Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:59 AM GMT

PDB ID	:	3QMZ
Title	:	Crystal structure of the cytoplasmic dynein heavy chain motor domain
Authors	:	Cho, C.; Carter, A.P.; Jin, L.; Vale, R.D.
Deposited on	:	2011-02-07
Resolution	:	6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

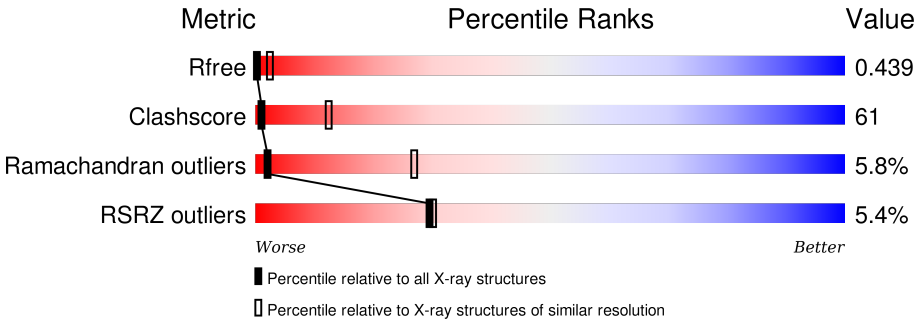
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
RSRZ outliers	91569	1001 (8.30-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2486	3% 53% 19% 10% • 14%
1	B	2486	4% 53% 19% 10% • 14%
2	S	219	20% 92% 5% ••
2	T	219	14% 91% 6% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytoplasmic dynein heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	2136	Total	C	N	O	0	0	0
			10585	6313	2136	2136			
1	B	2136	Total	C	N	O	0	0	0
			10586	6314	2136	2136			

- Molecule 2 is a protein called Glutathione-S-transferase.

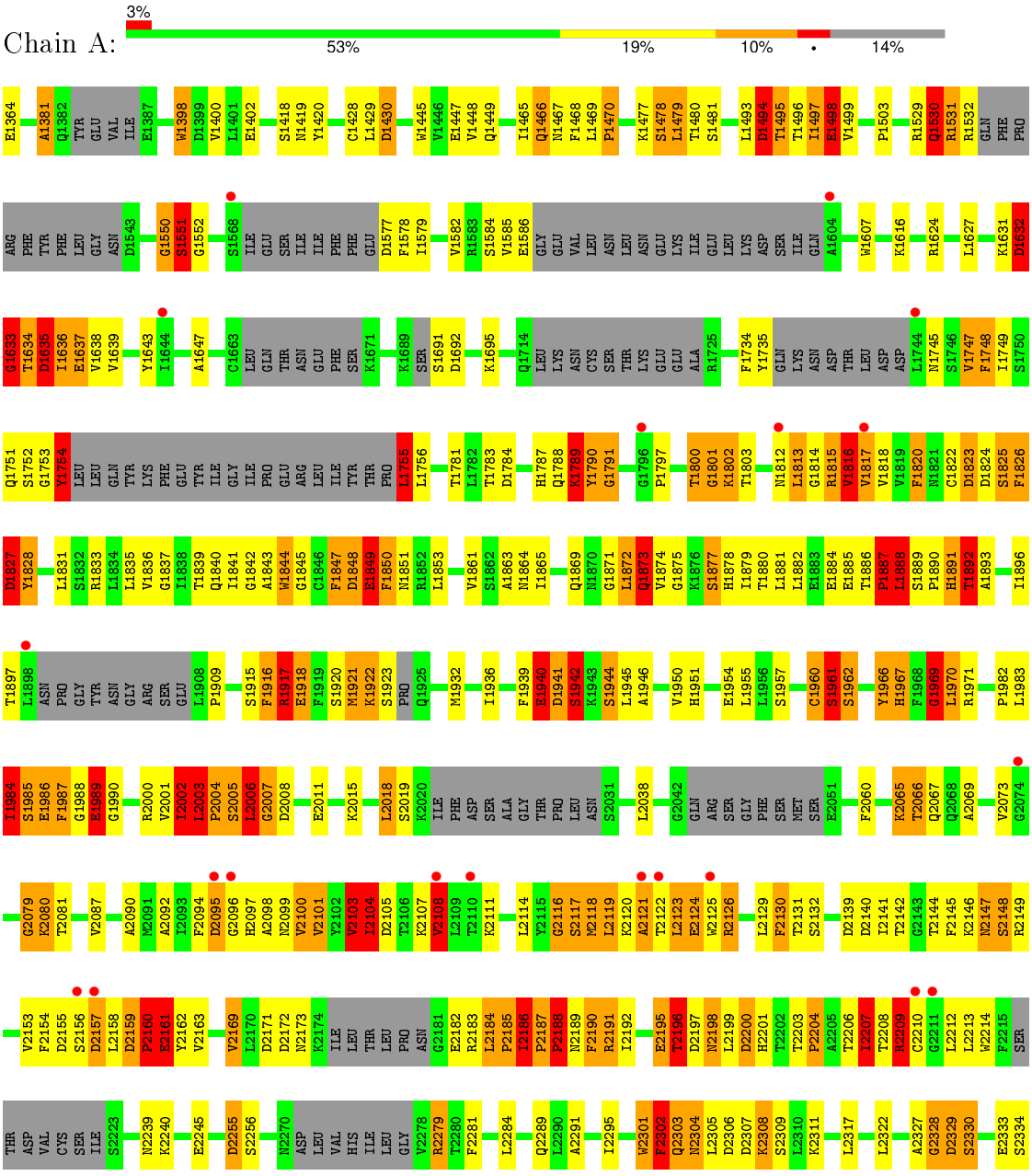
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	T	216	Total	C	N	O	0	0	0
			1066	634	216	216			
2	S	216	Total	C	N	O	0	0	0
			1065	633	216	216			

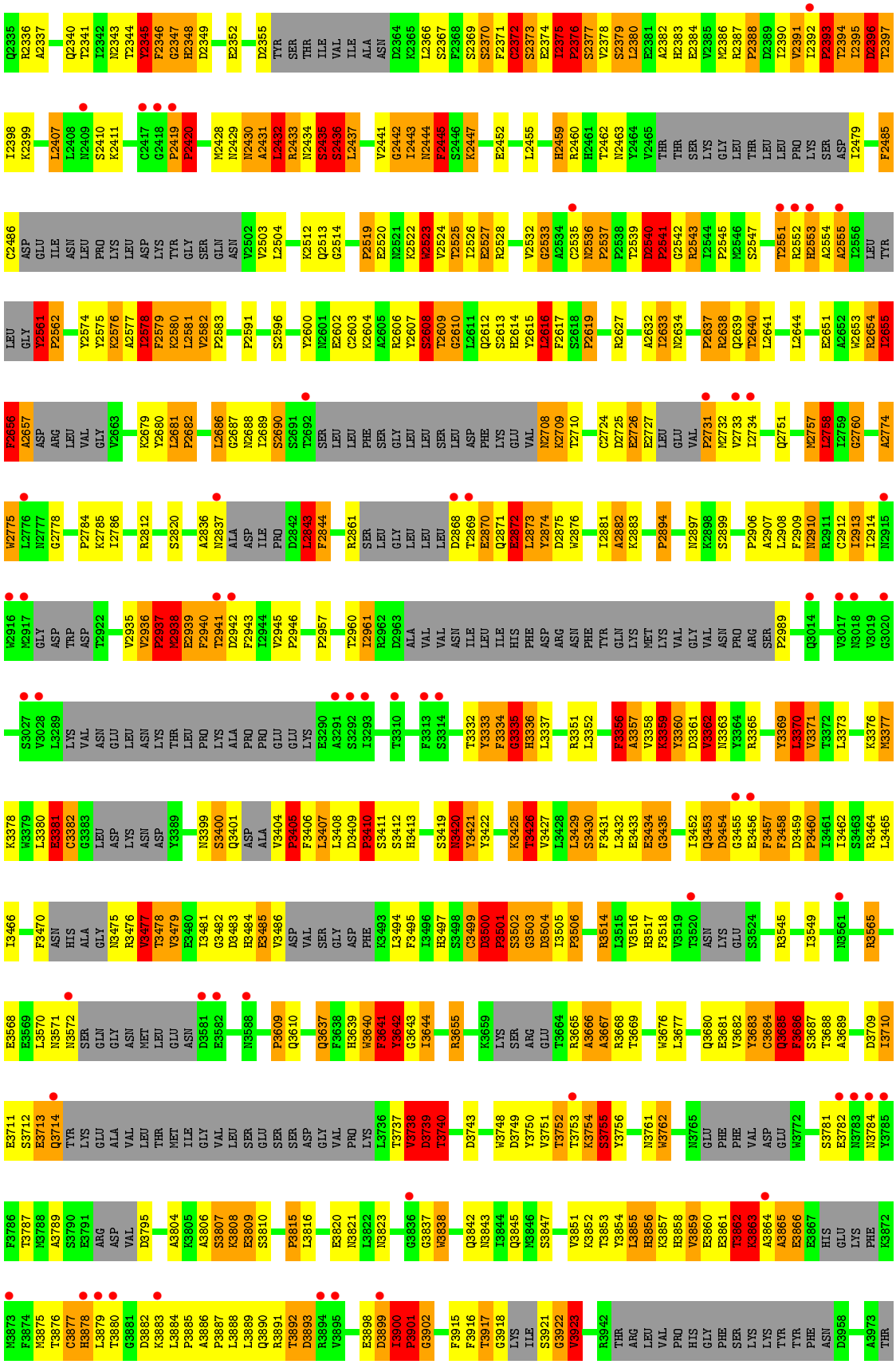
3 Residue-property plots (i)

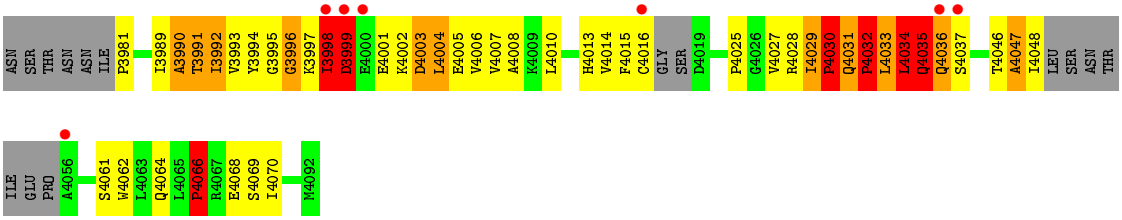
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytoplasmic dynein heavy chain

Chain A:

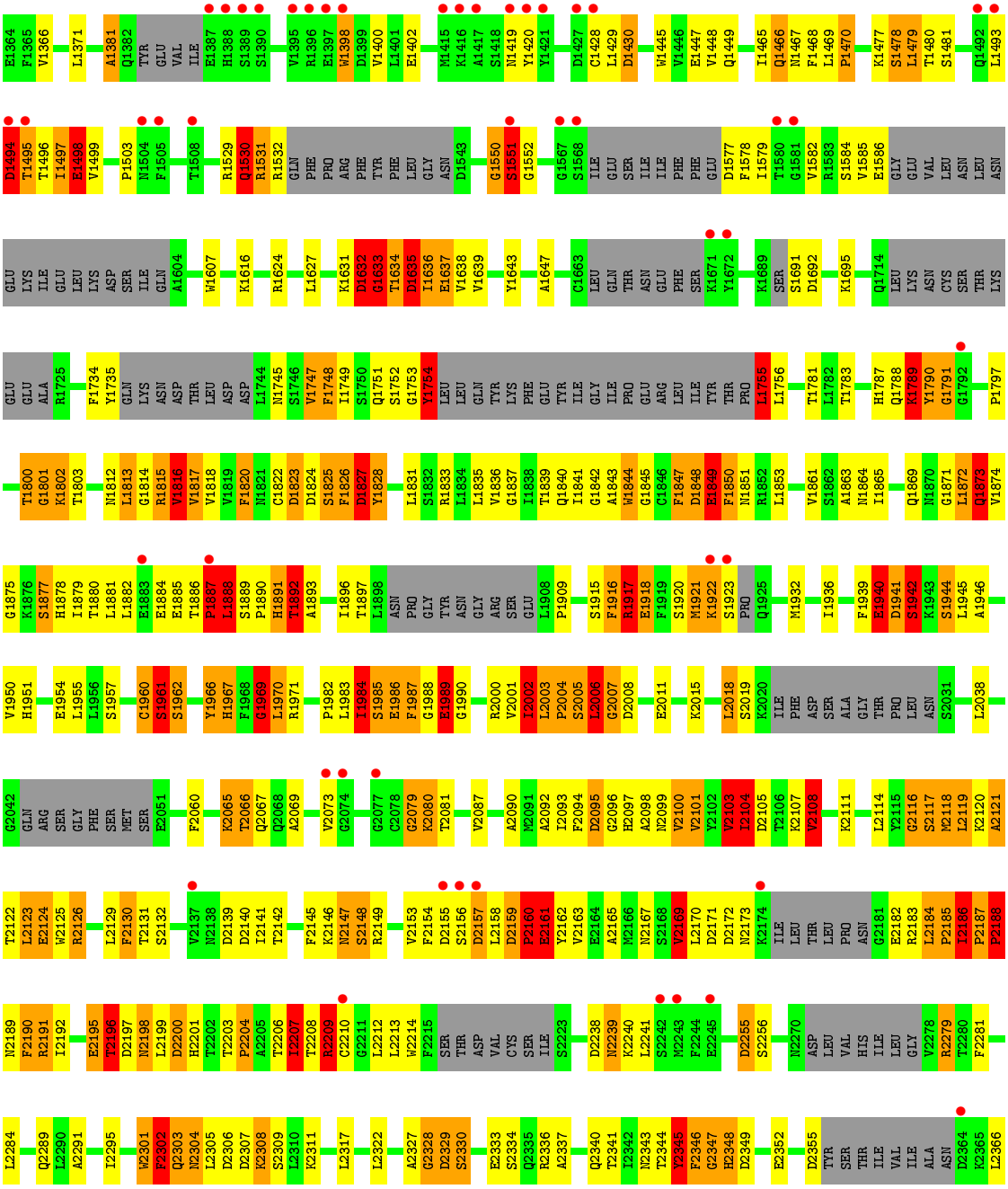


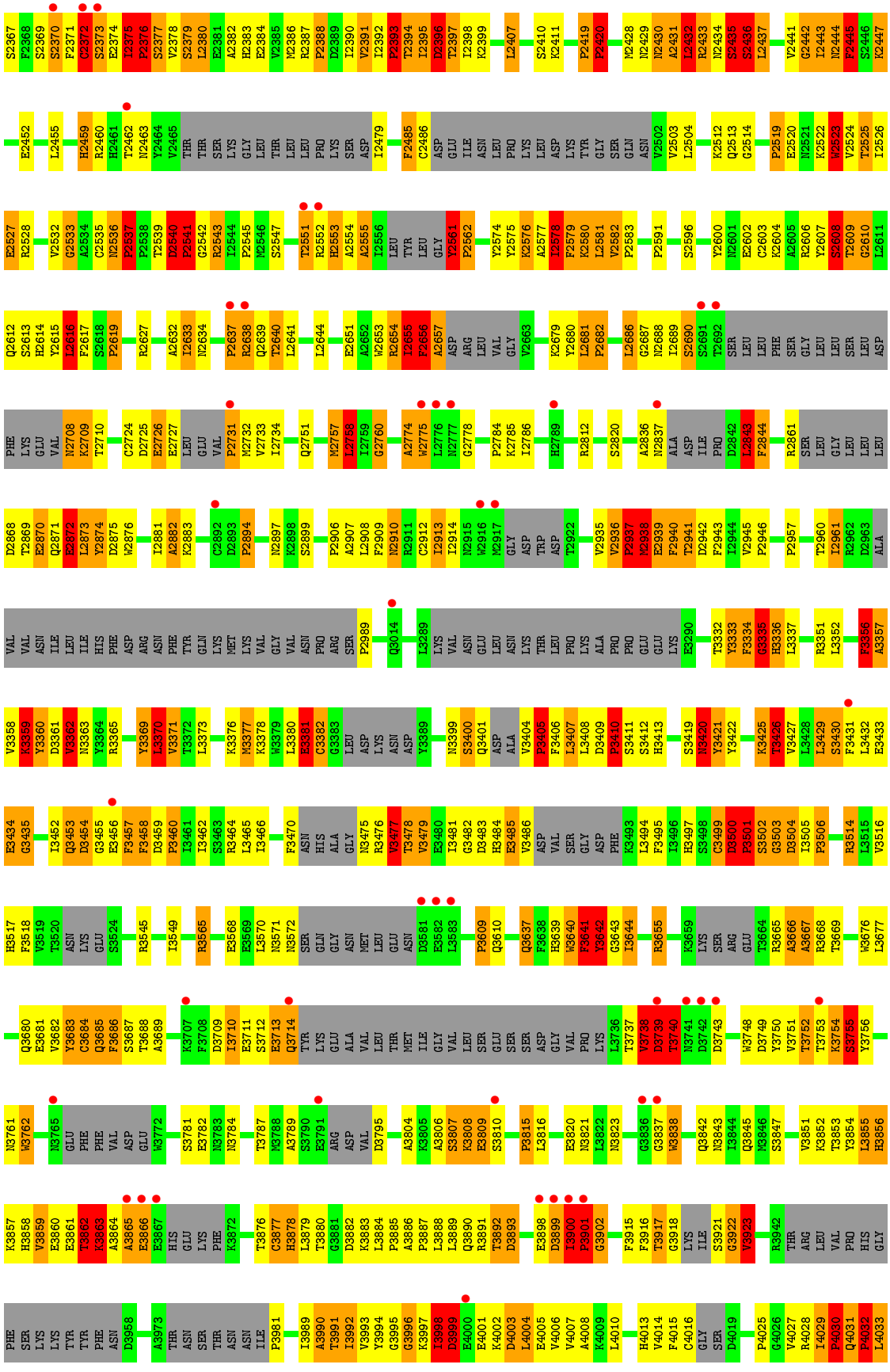


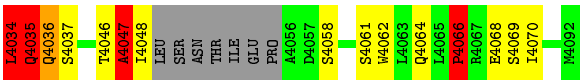


• Molecule 1: Cytoplasmic dynein heavy chain

Chain B:

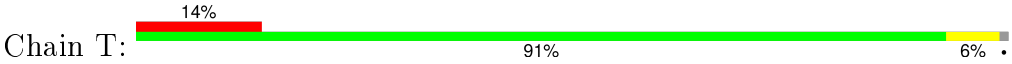


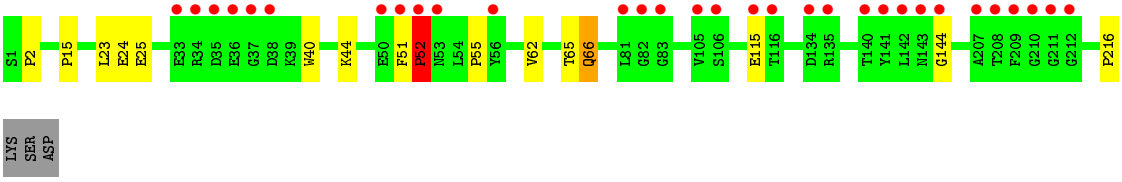

S2367 F2368 S2369 S2370 F2371 C2372 S2373 E2374 I2375 P2376 S2377 V2378 S2379 L2380 E2381 A2382 H2383 E2384 V2385 M2386 R2387 P2388 D2389 I2390 V2391 I2392 P2393 T2394 I2395 D2396 T2397 I2398 K2399 L2407 S2410 K2411 P2419 P2420 M2428 N2429 N2430 A2431 L2432 R2433 N2434 S2435 S2436 L2437 V2441 G2442 I2443 N2444 F2445 S2446 K2447
E2452 L2455 H2459 R2460 H2461 T2462 N2463 V2464 V2465 THR THR SER LYS GLY LEU THR LEU LEU PRO PRO LYS SER ASP I2479 F2485 C2486 ASP GLU ILE ASN LEU PRO LYS LEU ASP LYS TYR GLY SER GLN ASN V2502 V2503 L2504 K2512 Q2513 G2514 P2519 E2520 N2521 K2522 W2523 V2524 T2525 I2526
E2527 R2528 V2532 G2533 A2534 C2535 N2536 P2537 P2538 T2539 D2540 P2541 G2542 R2543 I2544 P2545 M2546 S2547 T2551 R2552 H2553 A2554 A2555 I2556 LEU TYR LEU GLY Y2561 P2562 Y2574 Y2575 K2576 A2577 I2578 F2579 K2580 L2581 V2582 P2583 P2591 S2596 Y2600 N2601 E2602 C2603 K2604 A2605 R2606 Y2607 S2608 T2609 G2610 L2611
Q2612 S2613 H2614 Y2615 L2616 F2617 S2618 P2619 R2627 A2632 I2633 N2634 P2637 R2638 Q2639 T2640 L2641 L2644 E2651 A2652 W2653 R2654 I2655 F2656 A2657 ASP ARG LEU VAL GLY V2663 K2679 Y2680 L2681 P2682 L2686 G2687 N2688 I2689 S2690 S2691 T2692 SER LEU LEU PHE SER GLY LEU LEU SER LEU ASP
PHE LYS GLU VAL N2708 K2709 T2710 C2724 D2725 E2726 E2727 LEU GLU VAL P2731 M2732 V2733 I2734 Q2751 M2757 L2758 I2759 G2760 A2774 W2775 L2776 N2777 G2778 P2784 K2785 I2786 H2789 R2812 S2820 A2836 N2837 ALA ASP ILE PRO D2842 L2843 F2844 R2861 SER LEU GLY LEU LEU LEU
D2868 T2869 E2870 Q2871 E2872 L2873 Y2874 D2875 W2876 I2881 A2882 K2883 C2892 D2893 P2894 N2897 K2898 S2899 P2906 A2907 L2908 F2909 N2910 R2911 C2912 I2913 I2914 N2915 W2916 M2917 GLY ASP TRP ASP T2922 V2935 V2936 P2937 M2938 E2939 P2940 T2941 D2942 F2943 I2944 V2945 P2946 P2957 T2960 I2961 R2962 D2963 ALA
VAL VAL ASN ILE LEU ILE HIS PHE ASP ARG ASN PHE TYR GLN LYS MET LYS VAL GLY VAL ASN PRO ARG SER P2989 Q3014 L3289 LYS VAL ASN GLU LEU ASN LYS THR LEU PRO LYS ALA PRO PRO GLU GLU LYS E3290 T3332 Y3333 F3334 G3335 H3336 L3337 R3351 L3352 F3356 A3357
V3358 K3359 Y3360 D3361 W3362 N3363 Y3364 R3365 Y3369 L3370 V3371 T3372 L3373 K3376 M3377 K3378 W3379 L3380 E3381 C3382 G3383 LEU ASP LYS ASN ASP Y3389 N3399 S3400 Q3401 ASP ALA V3404 P3405 F3406 L3407 L3408 D3409 P3410 S3411 S3412 H3413 S3419 N3420 Y3421 Y3422 K3425 T3426 V3427 L3428 L3429 S3430 F3431 L3432 E3433
E3434 G3435 I3452 Q3453 D3454 G3455 E3456 F3457 F3458 D3459 P3460 I3461 I3462 S3463 R3464 L3465 I3466 F3470 ASN HIS ALA GLY N3475 R3476 W3477 T3478 V3479 E3480 I3481 G3482 D3483 H3484 E3485 V3486 ASP VAL SER GLY ASP PHE H3493 L3494 F3495 I3496 H3497 S3498 C3499 D3500 P3501 S3502 G3503 D3504 I3505 P3506 R3514 L3515 V3516
H3517 F3518 Y3519 T3520 ASN LYS GLU S3524 R3545 I3549 R3565 E3568 E3569 L3570 N3571 N3572 SER GLN GLY ASN MET LEU LEU GLU ASN D3581 E3582 L3583 P3609 Q3610 Q3637 F3638 H3639 W3640 F3641 Y3642 G3643 I3644 R3655 K3659 LYS SER ARG GLU T3664 R3665 A3666 A3667 R3668 T3669 W3676 L3677
Q3680 E3681 V3682 Y3683 C3684 Q3685 F3686 S3687 T3688 A3689 K3707 F3708 D3709 I3710 E3711 S3712 E3713 Q3714 TYR LYS GLU ALA VAL LEU THR MET ILE GLY VAL LEU SER GLU SER SER ASP GLY VAL PRO LYS L3736 T3737 V3738 D3739 T3740 N3741 D3742 D3743 W3748 D3749 Y3750 V3751 T3752 T3753 K3754 S3755 Y3756
N3761 W3762 N3765 GLU PHE PHE VAL ASP GLU W3772 S3781 E3782 N3783 N3784 T3787 N3788 A3789 S3790 E3791 ARG ASP VAL D3795 A3804 K3805 A3806 S3807 K3808 E3809 S3810 P3815 I3816 E3820 N3821 L3822 N3823 G3836 G3837 W3838 Q3842 N3843 I3844 Q3845 K3846 S3847 V3851 K3852 T3853 Y3854 L3855 H3856
K3857 H3858 V3859 E3860 E3861 T3862 K3863 A3864 A3865 E3866 E3867 HIS GLU LYS PHE K3872 T3876 C3877 H3878 L3879 T3880 G3881 D3882 K3883 L3884 P3885 A3886 P3887 L3888 L3889 Q3890 R3891 T3892 D3893 E3898 D3899 I3900 P3901 G3902 F3915 F3916 T3917 G3918 LYS ILE S3921 G3922 V3923 R3942 THR ARG LEU VAL PRO HIS GLY
PHE SER LYS LYS TYR TYR PHE ASN D3958 A3973 THR ASN SER THR ASN ASN ILE P3981 I3989 A3990 T3991 I3992 V3993 Y3994 G3995 G3996 K3997 I3998 D3999 E4000 E4001 K4002 D4003 L4004 E4005 V4006 V4007 A4008 K4009 L4010 H4013 V4014 F4015 C4016 GLY SER D4019 P4025 G4026 V4027 R4028 I4029 P4030 Q4031 P4032 L4033



- Molecule 2: Glutathione-S-transferase

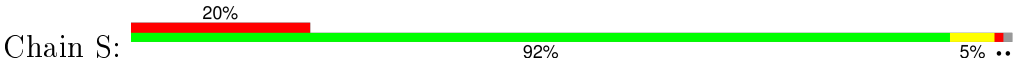
Chain T:

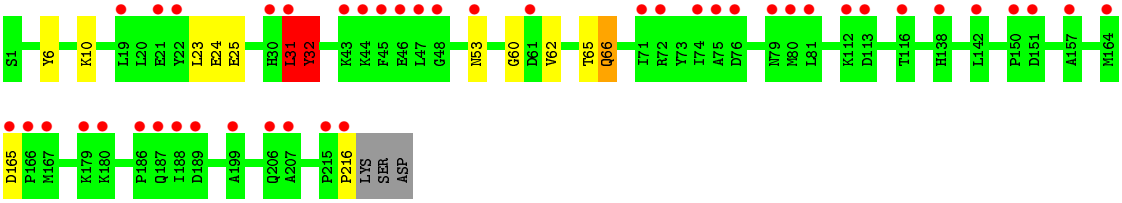




- Molecule 2: Glutathione-S-transferase

Chain S:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	174.08Å 118.92Å 200.51Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	50.00 – 6.00 50.13 – 6.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-6.00) 99.9 (50.13-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	9.38 (at 6.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.430 , 0.430 0.445 , 0.439	Depositor DCC
R_{free} test set	1079 reflections (5.47%)	DCC
Wilson B-factor (Å^2)	259.8	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 749.2	EDS
Estimated twinning fraction	0.014 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 20819 reflections	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	23302	wwPDB-VP
Average B, all atoms (Å^2)	222.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.63	201/10536 (1.9%)	2.24	571/14615 (3.9%)
1	B	1.63	201/10537 (1.9%)	2.24	572/14617 (3.9%)
2	S	1.94	2/1064 (0.2%)	0.86	3/1479 (0.2%)
2	T	0.39	0/1065	0.78	6/1481 (0.4%)
All	All	1.61	404/23202 (1.7%)	2.15	1152/32192 (3.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	3	136
1	B	3	136
2	S	0	3
All	All	6	275

All (404) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	32	TYR	N-CA	49.28	2.44	1.46
2	S	32	TYR	CA-C	37.84	2.51	1.52
1	B	4047	ALA	C-N	-30.16	0.64	1.34
1	A	4047	ALA	C-N	-30.14	0.64	1.34
1	A	3426	THR	C-N	-25.27	0.76	1.34
1	B	3426	THR	C-N	-25.26	0.76	1.34
1	A	3899	ASP	C-N	24.02	1.89	1.34
1	B	3899	ASP	C-N	24.01	1.89	1.34
1	A	3382	CYS	C-N	-22.36	0.92	1.33
1	B	3382	CYS	C-N	-22.33	0.92	1.33
1	A	3754	LYS	C-N	22.06	1.84	1.34
1	B	3754	LYS	C-N	22.05	1.84	1.34
1	A	2936	VAL	C-N	-21.28	0.93	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2936	VAL	C-N	-21.25	0.93	1.34
1	A	3360	TYR	C-N	21.00	1.82	1.34
1	B	3360	TYR	C-N	21.00	1.82	1.34
1	B	1844	TRP	C-N	20.24	1.69	1.33
1	A	1844	TRP	C-N	20.24	1.69	1.33
1	B	2709	LYS	C-N	19.80	1.79	1.34
1	A	2709	LYS	C-N	19.80	1.79	1.34
1	B	2103	VAL	C-N	-19.69	0.88	1.34
1	A	2103	VAL	C-N	-19.66	0.88	1.34
1	B	2147	ASN	C-N	-19.13	0.90	1.34
1	A	2147	ASN	C-N	-19.12	0.90	1.34
1	A	3334	PHE	C-N	18.31	1.66	1.33
1	B	3334	PHE	C-N	18.30	1.66	1.33
1	A	1815	ARG	C-N	18.10	1.75	1.34
1	B	1815	ARG	C-N	18.08	1.75	1.34
1	A	1801	GLY	C-N	-16.91	0.95	1.34
1	B	1801	GLY	C-N	-16.89	0.95	1.34
1	A	2346	PHE	C-N	16.75	1.63	1.33
1	B	2346	PHE	C-N	16.71	1.63	1.33
1	B	2301	TRP	C-N	16.65	1.72	1.34
1	A	2301	TRP	C-N	16.64	1.72	1.34
1	B	1986	GLU	C-N	16.51	1.72	1.34
1	A	1986	GLU	C-N	16.50	1.72	1.34
1	B	3642	TYR	C-N	16.38	1.62	1.33
1	A	3642	TYR	C-N	16.36	1.62	1.33
1	A	1632	ASP	C-N	16.04	1.61	1.33
1	B	1632	ASP	C-N	16.03	1.61	1.33
1	A	4015	PHE	C-N	-16.01	0.97	1.34
1	B	4015	PHE	C-N	-15.98	0.97	1.34
1	A	3901	PRO	C-N	15.92	1.61	1.33
1	B	3901	PRO	C-N	15.91	1.61	1.33
1	B	1466	GLN	C-N	15.86	1.70	1.34
1	A	1466	GLN	C-N	15.86	1.70	1.34
1	B	2002	ILE	C-N	-15.69	0.97	1.34
1	A	2002	ILE	C-N	-15.68	0.97	1.34
1	B	2774	ALA	C-N	15.17	1.69	1.34
1	A	2774	ALA	C-N	15.14	1.68	1.34
1	A	2279	ARG	C-N	-15.08	0.99	1.34
1	B	2279	ARG	C-N	-15.07	0.99	1.34
1	A	1877	SER	C-N	-14.88	0.99	1.34
1	B	1941	ASP	C-N	14.88	1.68	1.34
1	A	1941	ASP	C-N	14.87	1.68	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1877	SER	C-N	-14.86	0.99	1.34
1	B	3457	PHE	C-N	-14.43	1.00	1.34
1	A	3457	PHE	C-N	-14.42	1.00	1.34
1	B	1962	SER	C-N	-14.38	1.00	1.34
1	A	1962	SER	C-N	-14.36	1.01	1.34
1	B	2158	LEU	C-N	14.10	1.66	1.34
1	A	2158	LEU	C-N	14.09	1.66	1.34
1	A	1802	LYS	C-N	-14.01	1.01	1.34
1	B	1802	LYS	C-N	-14.00	1.01	1.34
1	B	2561	TYR	C-N	13.91	1.60	1.34
1	A	2561	TYR	C-N	13.90	1.60	1.34
1	B	3500	ASP	C-N	13.90	1.60	1.34
1	A	3500	ASP	C-N	13.89	1.60	1.34
1	A	3755	SER	C-N	13.88	1.66	1.34
1	B	3755	SER	C-N	13.88	1.66	1.34
1	A	1635	ASP	C-N	-13.84	1.02	1.34
1	B	1635	ASP	C-N	-13.83	1.02	1.34
1	B	2432	LEU	C-N	-13.78	1.02	1.34
1	A	2432	LEU	C-N	-13.77	1.02	1.34
1	B	3923	VAL	C-N	13.59	1.65	1.34
1	A	3923	VAL	C-N	13.59	1.65	1.34
1	B	2118	MET	C-N	13.25	1.64	1.34
1	A	2118	MET	C-N	13.22	1.64	1.34
1	A	2655	ILE	C-N	12.92	1.63	1.34
1	B	2655	ILE	C-N	12.91	1.63	1.34
1	B	2609	THR	C-N	12.84	1.56	1.33
1	A	2609	THR	C-N	12.83	1.56	1.33
1	A	3565	ARG	C-N	-12.68	1.04	1.34
1	B	3565	ARG	C-N	-12.67	1.04	1.34
1	A	2540	ASP	C-N	-12.61	1.10	1.34
1	B	2540	ASP	C-N	-12.59	1.10	1.34
1	A	2436	SER	C-N	12.53	1.62	1.34
1	B	1891	HIS	C-N	-12.53	1.05	1.34
1	B	2436	SER	C-N	12.52	1.62	1.34
1	A	1891	HIS	C-N	-12.50	1.05	1.34
1	A	3996	GLY	C-N	12.40	1.62	1.34
1	B	3996	GLY	C-N	12.39	1.62	1.34
1	A	3333	TYR	C-N	12.38	1.62	1.34
1	B	3333	TYR	C-N	12.37	1.62	1.34
1	A	1892	THR	C-N	12.27	1.62	1.34
1	B	1892	THR	C-N	12.23	1.62	1.34
1	B	1494	ASP	C-N	12.18	1.62	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1494	ASP	C-N	12.16	1.62	1.34
1	B	2579	PHE	C-N	12.16	1.62	1.34
1	A	2579	PHE	C-N	12.14	1.61	1.34
1	B	1985	SER	C-N	12.09	1.61	1.34
1	A	1985	SER	C-N	12.08	1.61	1.34
1	A	3499	CYS	C-N	12.02	1.61	1.34
1	B	3499	CYS	C-N	11.99	1.61	1.34
1	B	2574	TYR	C-N	11.90	1.61	1.34
1	A	2574	TYR	C-N	11.89	1.61	1.34
1	A	3892	THR	C-N	11.76	1.61	1.34
1	B	3892	THR	C-N	11.73	1.61	1.34
1	B	3684	CYS	C-N	-11.68	1.07	1.34
1	A	3684	CYS	C-N	-11.66	1.07	1.34
1	B	2758	LEU	C-N	11.58	1.60	1.34
1	A	2758	LEU	C-N	11.55	1.60	1.34
1	A	4035	GLN	C-N	11.52	1.60	1.34
1	B	4035	GLN	C-N	11.51	1.60	1.34
1	B	2101	VAL	C-N	-11.50	1.07	1.34
1	A	2101	VAL	C-N	-11.48	1.07	1.34
1	A	3893	ASP	C-N	11.46	1.60	1.34
1	B	3893	ASP	C-N	11.45	1.60	1.34
1	B	3637	GLN	C-N	11.43	1.60	1.34
1	A	3637	GLN	C-N	11.41	1.60	1.34
1	A	2186	ILE	C-N	11.39	1.55	1.34
1	B	2186	ILE	C-N	11.36	1.55	1.34
1	B	1800	THR	C-N	-11.19	1.12	1.33
1	A	1800	THR	C-N	-11.17	1.12	1.33
1	A	1850	PHE	C-N	11.14	1.59	1.34
1	B	1850	PHE	C-N	11.13	1.59	1.34
1	A	1967	HIS	C-N	11.09	1.59	1.34
1	A	2201	HIS	C-O	-11.07	1.02	1.23
1	B	2201	HIS	C-O	-11.06	1.02	1.23
1	A	3504	ASP	C-N	-11.06	1.08	1.34
1	B	1967	HIS	C-N	11.05	1.59	1.34
1	B	3504	ASP	C-N	-11.04	1.08	1.34
1	B	2195	GLU	C-N	11.03	1.59	1.34
1	A	2195	GLU	C-N	11.02	1.59	1.34
1	A	2460	ARG	C-N	-10.94	1.08	1.34
1	B	2460	ARG	C-N	-10.94	1.08	1.34
1	B	1849	GLU	C-N	-10.66	1.09	1.34
1	A	1849	GLU	C-N	-10.65	1.09	1.34
1	A	2124	GLU	C-O	10.61	1.43	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2935	VAL	C-N	10.60	1.58	1.34
1	B	2124	GLU	C-O	10.59	1.43	1.23
1	B	2935	VAL	C-N	10.58	1.58	1.34
1	A	2160	PRO	C-N	10.57	1.58	1.34
1	B	2160	PRO	C-N	10.57	1.58	1.34
1	A	4034	LEU	C-N	10.57	1.58	1.34
1	B	4034	LEU	C-N	10.56	1.58	1.34
1	B	3898	GLU	C-N	10.53	1.58	1.34
1	B	1430	ASP	C-N	-10.51	1.09	1.34
1	A	3898	GLU	C-N	10.50	1.58	1.34
1	A	1872	LEU	CA-C	-10.49	1.25	1.52
1	A	1430	ASP	C-N	-10.48	1.09	1.34
1	B	1872	LEU	CA-C	-10.48	1.25	1.52
1	A	1820	PHE	C-N	10.35	1.57	1.34
1	B	1820	PHE	C-N	10.34	1.57	1.34
1	B	1816	VAL	C-N	10.21	1.57	1.34
1	A	1816	VAL	C-N	10.21	1.57	1.34
1	A	2199	LEU	C-N	-10.19	1.10	1.34
1	B	2199	LEU	C-N	-10.18	1.10	1.34
1	A	2637	PRO	C-N	-10.17	1.10	1.34
1	B	2637	PRO	C-N	-10.17	1.10	1.34
1	B	3640	TRP	C-N	-9.90	1.11	1.34
1	A	3640	TRP	C-N	-9.90	1.11	1.34
1	A	3430	SER	C-N	9.83	1.56	1.34
1	A	2732	MET	C-N	9.81	1.56	1.34
1	B	3430	SER	C-N	9.81	1.56	1.34
1	B	2732	MET	C-N	9.80	1.56	1.34
1	A	2066	THR	C-N	9.71	1.56	1.34
1	B	2066	THR	C-N	9.68	1.56	1.34
1	B	2690	SER	C-N	9.67	1.56	1.34
1	A	1990	GLY	C-N	9.65	1.56	1.34
1	B	1990	GLY	C-N	9.65	1.56	1.34
1	A	2690	SER	C-N	9.64	1.56	1.34
1	A	2209	ARG	C-N	9.62	1.56	1.34
1	B	2209	ARG	C-N	9.61	1.56	1.34
1	B	2731	PRO	C-N	9.48	1.55	1.34
1	A	2731	PRO	C-N	9.47	1.55	1.34
1	A	2616	LEU	C-N	9.45	1.55	1.34
1	B	2616	LEU	C-N	9.44	1.55	1.34
1	A	1634	THR	C-N	9.29	1.55	1.34
1	B	1634	THR	C-N	9.28	1.55	1.34
1	A	2018	LEU	C-N	-9.27	1.12	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3420	ASN	C-N	9.24	1.55	1.34
1	B	2018	LEU	C-N	-9.24	1.12	1.34
1	B	3420	ASN	C-N	9.24	1.55	1.34
1	B	4033	LEU	C-N	-9.18	1.12	1.34
1	A	4033	LEU	C-N	-9.17	1.12	1.34
1	B	1984	ILE	C-N	9.09	1.54	1.34
1	A	1984	ILE	C-N	9.09	1.54	1.34
1	B	3666	ALA	C-N	-9.06	1.13	1.34
1	B	4005	GLU	N-CA	-9.05	1.28	1.46
1	A	4005	GLU	N-CA	-9.05	1.28	1.46
1	A	3666	ALA	C-N	-9.03	1.13	1.34
1	B	4036	GLN	C-N	-9.03	1.13	1.34
1	A	4036	GLN	C-N	-9.01	1.13	1.34
1	A	3667	ALA	C-N	8.96	1.54	1.34
1	B	3667	ALA	C-N	8.94	1.54	1.34
1	A	2005	SER	C-N	-8.94	1.13	1.34
1	B	2005	SER	C-N	-8.92	1.13	1.34
1	A	3644	ILE	C-N	8.85	1.54	1.34
1	B	3644	ILE	C-N	8.82	1.54	1.34
1	A	3685	GLN	C-N	8.79	1.54	1.34
1	B	3685	GLN	C-N	8.77	1.54	1.34
1	B	2309	SER	C-N	-8.72	1.14	1.34
1	A	2309	SER	C-N	-8.72	1.14	1.34
1	B	2372	CYS	C-N	8.65	1.53	1.34
1	A	2372	CYS	C-N	8.63	1.53	1.34
1	A	3856	HIS	CA-CB	-8.48	1.35	1.53
1	B	3856	HIS	CA-CB	-8.47	1.35	1.53
1	B	2200	ASP	C-N	-8.42	1.14	1.34
1	A	2200	ASP	C-N	-8.41	1.14	1.34
1	B	2689	ILE	C-N	-8.41	1.14	1.34
1	A	2725	ASP	C-N	8.40	1.53	1.34
1	A	2689	ILE	C-N	-8.39	1.14	1.34
1	B	2725	ASP	C-N	8.39	1.53	1.34
1	B	1983	LEU	C-N	-8.33	1.14	1.34
1	B	3795	ASP	C-N	-8.32	1.18	1.33
1	A	3405	PRO	C-N	-8.31	1.15	1.34
1	A	3795	ASP	C-N	-8.31	1.18	1.33
1	B	3405	PRO	C-N	-8.30	1.15	1.34
1	A	1983	LEU	C-N	-8.30	1.15	1.34
1	A	2117	SER	C-N	8.30	1.53	1.34
1	B	2117	SER	C-N	8.30	1.53	1.34
1	A	1825	SER	C-N	8.24	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2239	ASN	C-N	8.24	1.53	1.34
1	A	2240	LYS	C-O	-8.23	1.07	1.23
1	A	2239	ASN	C-N	8.22	1.52	1.34
1	B	1825	SER	C-N	8.22	1.52	1.34
1	A	2322	LEU	CA-CB	-8.20	1.34	1.53
1	B	2240	LYS	C-O	-8.19	1.07	1.23
1	B	2322	LEU	CA-CB	-8.19	1.34	1.53
1	B	2447	LYS	C-N	-8.18	1.15	1.34
1	A	2447	LYS	C-N	-8.16	1.15	1.34
1	A	3853	THR	CA-CB	-8.11	1.32	1.53
1	B	3853	THR	CA-CB	-8.11	1.32	1.53
1	B	2607	TYR	C-N	-8.04	1.15	1.34
1	A	2607	TYR	C-N	-8.04	1.15	1.34
1	A	2961	ILE	C-N	-8.03	1.15	1.34
1	B	2961	ILE	C-N	-8.02	1.15	1.34
1	A	1812	ASN	C-N	-8.01	1.15	1.34
1	B	1812	ASN	C-N	-8.01	1.15	1.34
1	A	2240	LYS	C-N	7.96	1.52	1.34
1	B	2240	LYS	C-N	7.96	1.52	1.34
1	A	3359	LYS	C-N	-7.95	1.15	1.34
1	B	1498	GLU	C-N	-7.95	1.15	1.34
1	B	3359	LYS	C-N	-7.95	1.15	1.34
1	A	1498	GLU	C-N	-7.94	1.15	1.34
1	A	1790	TYR	C-N	7.87	1.47	1.33
1	B	1790	TYR	C-N	7.85	1.47	1.33
1	B	2462	THR	C-N	-7.80	1.16	1.34
1	A	2462	THR	C-N	-7.78	1.16	1.34
1	B	2157	ASP	C-N	-7.76	1.16	1.34
1	A	2157	ASP	C-N	-7.75	1.16	1.34
1	B	1987	PHE	C-N	7.72	1.47	1.33
1	A	1987	PHE	C-N	7.71	1.47	1.33
1	B	1872	LEU	N-CA	-7.64	1.31	1.46
1	A	1828	TYR	C-N	7.62	1.51	1.34
1	A	1872	LEU	N-CA	-7.62	1.31	1.46
1	B	3503	GLY	C-N	-7.59	1.16	1.34
1	B	1828	TYR	C-N	7.58	1.51	1.34
1	A	2201	HIS	N-CA	7.57	1.61	1.46
1	A	2638	ARG	C-N	-7.56	1.16	1.34
1	A	3503	GLY	C-N	-7.55	1.16	1.34
1	B	2201	HIS	N-CA	7.54	1.61	1.46
1	B	2638	ARG	C-N	-7.53	1.16	1.34
1	A	4003	ASP	C-N	7.50	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4003	ASP	C-N	7.49	1.51	1.34
1	B	1969	GLY	C-N	-7.46	1.17	1.34
1	A	1969	GLY	C-N	-7.43	1.17	1.34
1	A	2843	LEU	C-N	7.43	1.51	1.34
1	B	2843	LEU	C-N	7.42	1.51	1.34
1	A	2187	PRO	C-N	7.40	1.48	1.34
1	A	1823	ASP	C-N	7.40	1.51	1.34
1	B	1823	ASP	C-N	7.40	1.51	1.34
1	B	2187	PRO	C-N	7.38	1.48	1.34
1	A	3362	VAL	C-N	7.32	1.50	1.34
1	B	3362	VAL	C-N	7.28	1.50	1.34
1	A	1848	ASP	C-N	-7.27	1.17	1.34
1	B	1848	ASP	C-N	-7.27	1.17	1.34
1	A	1871	GLY	C-N	-7.23	1.17	1.34
1	A	2941	THR	C-N	7.22	1.50	1.34
1	B	1871	GLY	C-N	-7.22	1.17	1.34
1	B	2941	THR	C-N	7.21	1.50	1.34
1	B	2196	THR	C-N	-7.19	1.17	1.34
1	B	3854	TYR	CA-C	-7.17	1.34	1.52
1	A	2196	THR	C-N	-7.17	1.17	1.34
1	A	3854	TYR	CA-C	-7.16	1.34	1.52
1	B	3399	ASN	C-N	7.06	1.50	1.34
1	A	2523	TRP	C-N	-7.03	1.17	1.34
1	A	1888	LEU	C-N	-7.02	1.17	1.34
1	A	3399	ASN	C-N	7.02	1.50	1.34
1	B	1888	LEU	C-N	-7.02	1.18	1.34
1	B	2523	TRP	C-N	-7.01	1.18	1.34
1	B	2396	ASP	C-N	7.01	1.50	1.34
1	A	2373	SER	C-N	-7.00	1.18	1.34
1	A	2396	ASP	C-N	7.00	1.50	1.34
1	B	2373	SER	C-N	-6.96	1.18	1.34
1	A	2240	LYS	N-CA	6.92	1.60	1.46
1	B	1942	SER	C-N	6.91	1.50	1.34
1	A	1942	SER	C-N	6.90	1.50	1.34
1	B	2240	LYS	N-CA	6.89	1.60	1.46
1	A	2444	ASN	C-N	-6.77	1.18	1.34
1	B	2444	ASN	C-N	-6.76	1.18	1.34
1	A	2939	GLU	C-O	6.75	1.36	1.23
1	B	2199	LEU	C-O	-6.74	1.10	1.23
1	A	2199	LEU	C-O	-6.71	1.10	1.23
1	B	2939	GLU	C-O	6.71	1.36	1.23
1	A	1478	SER	C-N	-6.67	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1478	SER	C-N	-6.64	1.18	1.34
1	A	2430	ASN	C-N	-6.64	1.18	1.34
1	B	2430	ASN	C-N	-6.64	1.18	1.34
1	A	2108	VAL	C-N	-6.63	1.18	1.34
1	B	2108	VAL	C-N	-6.62	1.18	1.34
1	A	2308	LYS	C-N	-6.58	1.19	1.34
1	B	2308	LYS	C-N	-6.58	1.19	1.34
1	A	3855	LEU	N-CA	-6.56	1.33	1.46
1	B	3855	LEU	N-CA	-6.55	1.33	1.46
1	B	2632	ALA	C-N	6.49	1.49	1.34
1	A	1497	ILE	C-N	-6.46	1.19	1.34
1	A	2726	GLU	C-N	-6.46	1.19	1.34
1	B	1497	ILE	C-N	-6.46	1.19	1.34
1	A	2632	ALA	C-N	6.46	1.48	1.34
1	B	2726	GLU	C-N	-6.45	1.19	1.34
1	A	3877	CYS	C-N	6.40	1.48	1.34
1	B	3877	CYS	C-N	6.39	1.48	1.34
1	A	2555	ALA	C-N	-6.38	1.19	1.34
1	B	2555	ALA	C-N	-6.36	1.19	1.34
1	A	1813	LEU	C-N	-6.32	1.21	1.33
1	B	1813	LEU	C-N	-6.32	1.21	1.33
1	A	2757	MET	C-N	-6.31	1.19	1.34
1	B	2757	MET	C-N	-6.27	1.19	1.34
1	A	1496	THR	C-N	6.21	1.48	1.34
1	B	4006	VAL	C-O	6.20	1.35	1.23
1	A	1754	TYR	C-N	6.20	1.48	1.34
1	B	1496	THR	C-N	6.19	1.48	1.34
1	B	1754	TYR	C-N	6.19	1.48	1.34
1	A	4006	VAL	C-O	6.19	1.35	1.23
1	A	1495	THR	C-N	-6.12	1.20	1.34
1	B	1495	THR	C-N	-6.11	1.20	1.34
1	A	3429	LEU	C-N	6.10	1.48	1.34
1	B	3683	TYR	C-N	6.09	1.48	1.34
1	A	3683	TYR	C-N	6.09	1.48	1.34
1	B	3429	LEU	C-N	6.08	1.48	1.34
1	B	2119	LEU	N-CA	6.01	1.58	1.46
1	A	2119	LEU	N-CA	6.00	1.58	1.46
1	A	3998	ILE	C-N	5.99	1.47	1.34
1	B	3998	ILE	C-N	5.98	1.47	1.34
1	A	3857	LYS	CA-C	-5.97	1.37	1.52
1	B	3857	LYS	CA-C	-5.95	1.37	1.52
1	A	3682	VAL	C-N	-5.94	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3682	VAL	C-N	-5.93	1.20	1.34
1	A	3854	TYR	N-CA	-5.86	1.34	1.46
1	B	3854	TYR	N-CA	-5.86	1.34	1.46
1	B	2139	ASP	C-N	-5.85	1.20	1.34
1	A	2139	ASP	C-N	-5.82	1.20	1.34
1	B	3655	ARG	C-N	5.82	1.47	1.34
1	A	3655	ARG	C-N	5.81	1.47	1.34
1	B	2760	GLY	C-N	-5.80	1.20	1.34
1	A	2760	GLY	C-N	-5.79	1.20	1.34
1	B	2208	THR	C-N	5.74	1.47	1.34
1	A	2208	THR	C-N	5.74	1.47	1.34
1	A	2541	PRO	C-N	5.71	1.43	1.33
1	B	2541	PRO	C-N	5.69	1.43	1.33
1	A	2527	GLU	C-N	-5.65	1.21	1.34
1	B	2527	GLU	C-N	-5.65	1.21	1.34
1	A	2006	LEU	C-N	-5.64	1.22	1.33
1	B	1966	TYR	C-N	5.63	1.47	1.34
1	A	1966	TYR	C-N	5.62	1.47	1.34
1	B	2006	LEU	C-N	-5.60	1.23	1.33
1	B	3858	HIS	N-CA	-5.60	1.35	1.46
1	A	1872	LEU	C-O	-5.57	1.12	1.23
1	B	1872	LEU	C-O	-5.56	1.12	1.23
1	A	3858	HIS	N-CA	-5.56	1.35	1.46
1	B	1398	TRP	C-N	5.55	1.46	1.34
1	A	1398	TRP	C-N	5.54	1.46	1.34
1	A	3853	THR	CA-C	-5.49	1.38	1.52
1	B	3853	THR	CA-C	-5.47	1.38	1.52
1	A	2633	ILE	C-N	-5.46	1.21	1.34
1	B	2445	PHE	C-N	5.46	1.46	1.34
1	A	2445	PHE	C-N	5.44	1.46	1.34
1	B	2633	ILE	C-N	-5.43	1.21	1.34
1	A	2118	MET	C-O	-5.42	1.13	1.23
1	B	2118	MET	C-O	-5.39	1.13	1.23
1	B	4004	LEU	CA-C	-5.32	1.39	1.52
1	A	4004	LEU	CA-C	-5.32	1.39	1.52
1	B	2207	ILE	N-CA	-5.18	1.35	1.46
1	A	2201	HIS	CA-C	-5.16	1.39	1.52
1	B	2201	HIS	CA-C	-5.16	1.39	1.52
1	B	1827	ASP	C-N	5.15	1.46	1.34
1	A	1827	ASP	C-N	5.14	1.45	1.34
1	A	2207	ILE	N-CA	-5.14	1.36	1.46
1	A	2940	PHE	C-N	-5.14	1.22	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1381	ALA	C-N	5.14	1.45	1.34
1	B	2940	PHE	C-N	-5.12	1.22	1.34
1	B	1381	ALA	C-N	5.11	1.45	1.34
1	B	3363	ASN	C-N	5.07	1.45	1.34
1	A	3363	ASN	C-N	5.06	1.45	1.34
1	A	1847	PHE	C-N	5.05	1.45	1.34
1	B	1847	PHE	C-N	5.04	1.45	1.34
1	A	1551	SER	C-N	5.02	1.42	1.33
1	B	1551	SER	C-N	5.02	1.42	1.33
1	A	3855	LEU	C-O	-5.01	1.13	1.23
1	B	3855	LEU	C-O	-5.01	1.13	1.23
1	B	2302	PHE	C-N	-5.01	1.22	1.34
1	A	2302	PHE	C-N	-5.00	1.22	1.34

All (1152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1466	GLN	O-C-N	-31.44	72.39	122.70
1	A	1466	GLN	O-C-N	-31.43	72.42	122.70
1	B	2436	SER	O-C-N	-28.51	77.09	122.70
1	A	2436	SER	O-C-N	-28.49	77.12	122.70
1	B	1466	GLN	CA-C-N	-28.26	55.02	117.20
1	A	1466	GLN	CA-C-N	-28.26	55.03	117.20
1	B	3501	PRO	N-CA-CB	25.79	134.25	103.30
1	A	3501	PRO	N-CA-CB	25.78	134.24	103.30
1	A	2655	ILE	O-C-N	-25.32	82.20	122.70
1	B	2655	ILE	O-C-N	-25.28	82.25	122.70
1	A	3435	GLY	O-C-N	-24.00	84.31	122.70
1	B	3435	GLY	O-C-N	-23.98	84.34	122.70
1	A	3434	GLU	O-C-N	-23.61	83.06	123.20
1	B	3434	GLU	O-C-N	-23.60	83.08	123.20
1	A	1815	ARG	CA-C-N	-23.39	65.75	117.20
1	B	1815	ARG	CA-C-N	-23.38	65.76	117.20
1	B	3917	THR	O-C-N	23.26	162.75	123.20
1	A	3917	THR	O-C-N	23.24	162.71	123.20
1	B	2555	ALA	O-C-N	-23.00	85.90	122.70
1	A	2555	ALA	O-C-N	-22.98	85.93	122.70
1	A	2656	PHE	O-C-N	-21.84	87.76	122.70
1	B	2656	PHE	O-C-N	-21.83	87.77	122.70
1	B	2121	ALA	CA-C-N	-21.78	69.28	117.20
1	A	2121	ALA	CA-C-N	-21.77	69.31	117.20
1	B	3381	GLU	O-C-N	-21.28	88.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1961	SER	CB-CA-C	-21.28	69.66	110.10
1	A	3381	GLU	O-C-N	-21.27	88.67	122.70
1	A	1961	SER	CB-CA-C	-21.26	69.71	110.10
1	B	3917	THR	CA-C-N	-20.76	74.67	116.20
1	A	3917	THR	CA-C-N	-20.74	74.71	116.20
1	A	2561	TYR	O-C-N	-20.11	82.90	121.10
1	B	2561	TYR	O-C-N	-20.09	82.92	121.10
1	B	2393	PRO	O-C-N	-20.05	90.62	122.70
1	A	1381	ALA	O-C-N	-20.04	90.63	122.70
1	A	2393	PRO	O-C-N	-20.04	90.64	122.70
1	B	1381	ALA	O-C-N	-20.03	90.65	122.70
1	A	3382	CYS	C-N-CA	20.01	164.33	122.30
1	B	3382	CYS	C-N-CA	20.00	164.31	122.30
1	A	2121	ALA	CA-C-O	19.59	161.24	120.10
1	B	2121	ALA	CA-C-O	19.58	161.21	120.10
1	B	1960	CYS	C-N-CA	19.40	170.21	121.70
1	A	2375	ILE	CB-CA-C	19.40	150.40	111.60
1	A	1960	CYS	C-N-CA	19.39	170.17	121.70
1	B	2375	ILE	CB-CA-C	19.38	150.36	111.60
1	A	2121	ALA	O-C-N	-19.24	91.92	122.70
1	B	2121	ALA	O-C-N	-19.23	91.92	122.70
1	A	3434	GLU	CA-C-N	19.11	154.43	116.20
1	B	1961	SER	O-C-N	-19.10	92.13	122.70
1	A	1961	SER	O-C-N	-19.09	92.15	122.70
1	B	3434	GLU	CA-C-N	19.09	154.39	116.20
2	S	32	TYR	N-CA-C	-19.08	59.48	111.00
1	A	1987	PHE	O-C-N	-19.02	90.87	123.20
1	B	1987	PHE	O-C-N	-19.00	90.89	123.20
1	A	2577	ALA	CB-CA-C	18.96	138.54	110.10
1	B	1466	GLN	C-N-CA	18.95	169.08	121.70
1	B	2577	ALA	CB-CA-C	18.95	138.52	110.10
1	A	1466	GLN	C-N-CA	18.95	169.07	121.70
1	A	2843	LEU	CB-CA-C	18.78	145.88	110.20
1	B	2843	LEU	CB-CA-C	18.78	145.88	110.20
1	B	2005	SER	O-C-N	-18.73	92.74	122.70
1	A	2005	SER	O-C-N	-18.72	92.75	122.70
1	B	2005	SER	C-N-CA	18.44	167.79	121.70
1	A	2005	SER	C-N-CA	18.44	167.79	121.70
1	A	3739	ASP	N-CA-C	18.41	160.72	111.00
1	B	3739	ASP	N-CA-C	18.41	160.69	111.00
1	A	1985	SER	O-C-N	18.08	151.63	122.70
1	B	1985	SER	O-C-N	18.08	151.62	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1962	SER	N-CA-CB	-18.07	83.39	110.50
1	A	1962	SER	N-CA-CB	-18.07	83.40	110.50
1	B	2101	VAL	O-C-N	-18.00	93.90	122.70
1	A	2101	VAL	O-C-N	-17.96	93.96	122.70
1	A	2432	LEU	O-C-N	-17.96	93.97	122.70
1	B	2432	LEU	O-C-N	-17.96	93.97	122.70
1	B	3335	GLY	O-C-N	-17.57	94.58	122.70
1	A	3335	GLY	O-C-N	-17.57	94.58	122.70
1	B	3685	GLN	C-N-CA	-17.49	77.98	121.70
1	A	3685	GLN	C-N-CA	-17.48	77.99	121.70
1	B	1635	ASP	CB-CA-C	17.42	145.23	110.40
1	A	1635	ASP	CB-CA-C	17.40	145.20	110.40
1	A	1635	ASP	O-C-N	-17.30	95.01	122.70
1	B	1635	ASP	O-C-N	-17.30	95.01	122.70
1	B	1813	LEU	O-C-N	-16.77	94.69	123.20
1	A	1813	LEU	O-C-N	-16.77	94.70	123.20
1	B	3999	ASP	N-CA-C	16.71	156.12	111.00
1	A	3999	ASP	N-CA-C	16.71	156.12	111.00
1	A	3685	GLN	N-CA-CB	-16.61	80.70	110.60
1	B	3685	GLN	N-CA-CB	-16.61	80.71	110.60
1	A	3900	ILE	O-C-N	16.60	152.65	121.10
1	B	3900	ILE	O-C-N	16.57	152.58	121.10
1	B	3382	CYS	N-CA-C	16.48	155.50	111.00
1	A	3382	CYS	N-CA-C	16.48	155.49	111.00
1	B	3405	PRO	N-CA-C	16.44	154.84	112.10
1	A	3405	PRO	N-CA-C	16.44	154.83	112.10
1	B	1960	CYS	O-C-N	16.34	148.85	122.70
1	A	1960	CYS	O-C-N	16.33	148.83	122.70
1	B	3892	THR	C-N-CA	16.29	162.43	121.70
1	A	3892	THR	C-N-CA	16.29	162.41	121.70
1	A	2018	LEU	C-N-CA	16.21	162.22	121.70
1	B	2018	LEU	C-N-CA	16.21	162.22	121.70
1	A	3401	GLN	CB-CA-C	-16.10	78.21	110.40
1	B	3401	GLN	CB-CA-C	-16.09	78.22	110.40
1	A	1987	PHE	CA-C-N	16.08	148.36	116.20
1	B	1987	PHE	CA-C-N	16.08	148.35	116.20
1	A	1816	VAL	CA-C-N	-16.02	81.96	117.20
1	B	1816	VAL	CA-C-N	-16.01	81.98	117.20
1	A	3382	CYS	CB-CA-C	-15.89	78.63	110.40
1	B	3382	CYS	CB-CA-C	-15.88	78.64	110.40
1	A	3866	GLU	N-CA-C	-15.84	68.23	111.00
1	B	3866	GLU	N-CA-C	-15.84	68.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3400	SER	O-C-N	-15.77	97.47	122.70
1	A	3400	SER	O-C-N	-15.77	97.47	122.70
1	B	3369	TYR	N-CA-C	15.74	153.50	111.00
1	A	3369	TYR	N-CA-C	15.74	153.50	111.00
1	A	3709	ASP	C-N-CA	15.69	160.93	121.70
1	B	3709	ASP	C-N-CA	15.67	160.88	121.70
1	A	1530	GLN	C-N-CA	-15.55	82.83	121.70
1	B	1530	GLN	C-N-CA	-15.54	82.86	121.70
1	A	1961	SER	C-N-CA	-15.53	82.87	121.70
1	B	1961	SER	C-N-CA	-15.52	82.89	121.70
1	B	3999	ASP	CB-CA-C	-15.50	79.39	110.40
1	A	3999	ASP	CB-CA-C	-15.50	79.40	110.40
1	B	2348	HIS	N-CA-CB	-15.45	82.80	110.60
1	A	2348	HIS	N-CA-CB	-15.44	82.80	110.60
1	B	2279	ARG	C-N-CA	-15.37	83.27	121.70
1	A	2005	SER	CB-CA-C	-15.37	80.89	110.10
1	B	2005	SER	CB-CA-C	-15.37	80.89	110.10
1	A	2279	ARG	C-N-CA	-15.37	83.29	121.70
1	A	2655	ILE	C-N-CA	15.29	159.94	121.70
1	B	2655	ILE	C-N-CA	15.29	159.92	121.70
1	A	2005	SER	N-CA-C	15.26	152.20	111.00
1	B	2005	SER	N-CA-C	15.24	152.15	111.00
1	A	3435	GLY	CA-C-N	15.17	150.58	117.20
1	B	3435	GLY	CA-C-N	15.16	150.56	117.20
1	B	1816	VAL	N-CA-C	15.15	151.90	111.00
1	A	1816	VAL	N-CA-C	15.13	151.86	111.00
1	B	2065	LYS	CB-CA-C	-15.02	80.37	110.40
1	A	2065	LYS	CB-CA-C	-15.00	80.41	110.40
1	B	2961	ILE	O-C-N	-14.91	98.84	122.70
1	A	2961	ILE	O-C-N	-14.91	98.85	122.70
1	B	2579	PHE	O-C-N	14.86	146.47	122.70
1	A	2579	PHE	O-C-N	14.86	146.47	122.70
1	B	3898	GLU	C-N-CA	14.80	158.71	121.70
1	A	3898	GLU	C-N-CA	14.80	158.69	121.70
1	B	2003	LEU	O-C-N	-14.75	93.07	121.10
1	A	2003	LEU	O-C-N	-14.75	93.08	121.10
1	A	1827	ASP	CB-CA-C	-14.70	81.00	110.40
1	B	1827	ASP	CB-CA-C	-14.70	81.01	110.40
1	B	1941	ASP	N-CA-CB	-14.69	84.16	110.60
1	A	1941	ASP	N-CA-CB	-14.68	84.17	110.60
1	B	1815	ARG	O-C-N	-14.68	99.20	122.70
1	A	1815	ARG	O-C-N	-14.67	99.23	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2437	LEU	N-CA-CB	-14.63	81.14	110.40
1	B	2437	LEU	N-CA-CB	-14.62	81.16	110.40
1	B	1813	LEU	C-N-CA	14.57	152.90	122.30
1	A	1813	LEU	C-N-CA	14.56	152.87	122.30
1	A	3682	VAL	O-C-N	-14.54	99.44	122.70
1	B	3682	VAL	O-C-N	-14.53	99.45	122.70
1	A	3709	ASP	O-C-N	-14.52	99.47	122.70
1	B	3709	ASP	O-C-N	-14.51	99.49	122.70
1	B	3644	ILE	O-C-N	14.46	145.84	122.70
1	A	3644	ILE	O-C-N	14.44	145.81	122.70
1	A	3899	ASP	CA-C-N	-14.42	85.48	117.20
1	B	3899	ASP	CA-C-N	-14.42	85.48	117.20
1	A	2066	THR	N-CA-CB	14.21	137.31	110.30
1	B	2066	THR	N-CA-CB	14.21	137.31	110.30
1	A	3682	VAL	C-N-CA	14.19	157.17	121.70
1	B	3682	VAL	C-N-CA	14.19	157.16	121.70
1	A	1801	GLY	O-C-N	-14.16	100.05	122.70
1	B	1801	GLY	O-C-N	-14.14	100.08	122.70
1	B	2345	TYR	C-N-CA	13.96	156.59	121.70
1	A	1820	PHE	O-C-N	-13.95	100.38	122.70
1	B	1820	PHE	O-C-N	-13.95	100.38	122.70
1	A	4015	PHE	C-N-CA	13.95	156.56	121.70
1	A	2345	TYR	C-N-CA	13.93	156.51	121.70
1	A	3684	CYS	CB-CA-C	-13.93	82.55	110.40
1	B	4015	PHE	C-N-CA	13.92	156.50	121.70
1	B	2066	THR	O-C-N	13.92	144.97	122.70
1	B	3684	CYS	CB-CA-C	-13.91	82.59	110.40
1	A	2066	THR	O-C-N	13.90	144.95	122.70
1	B	3333	TYR	C-N-CA	-13.73	87.38	121.70
1	A	3333	TYR	C-N-CA	-13.72	87.39	121.70
1	A	3405	PRO	C-N-CA	13.69	155.93	121.70
1	B	3405	PRO	C-N-CA	13.68	155.90	121.70
1	A	1985	SER	CA-C-N	-13.58	87.32	117.20
1	B	1985	SER	CA-C-N	-13.58	87.32	117.20
1	A	1940	GLU	N-CA-C	13.41	147.20	111.00
1	B	1940	GLU	N-CA-C	13.40	147.18	111.00
1	B	2199	LEU	O-C-N	13.38	144.11	122.70
1	A	2199	LEU	O-C-N	13.35	144.06	122.70
1	B	2005	SER	CA-C-N	13.29	146.43	117.20
1	A	1634	THR	N-CA-CB	-13.29	85.06	110.30
1	B	1634	THR	N-CA-CB	-13.29	85.06	110.30
1	A	2005	SER	CA-C-N	13.28	146.41	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1960	CYS	CA-C-N	-13.26	88.04	117.20
1	A	1960	CYS	CA-C-N	-13.24	88.07	117.20
1	A	3421	TYR	N-CA-CB	-13.24	86.78	110.60
1	B	3421	TYR	N-CA-CB	-13.23	86.79	110.60
1	B	1984	ILE	O-C-N	-13.15	101.66	122.70
1	A	1984	ILE	O-C-N	-13.13	101.70	122.70
1	B	2159	ASP	O-C-N	13.07	145.94	121.10
1	A	2159	ASP	O-C-N	13.06	145.92	121.10
1	A	2348	HIS	N-CA-C	13.04	146.22	111.00
1	B	2348	HIS	N-CA-C	13.04	146.21	111.00
1	A	3684	CYS	O-C-N	-13.00	101.90	122.70
1	B	1888	LEU	N-CA-C	12.99	146.08	111.00
1	B	3684	CYS	O-C-N	-12.99	101.92	122.70
1	A	1888	LEU	N-CA-C	12.99	146.06	111.00
1	A	3753	THR	N-CA-C	12.98	146.03	111.00
1	B	3753	THR	N-CA-C	12.97	146.01	111.00
1	B	2120	LYS	N-CA-CB	-12.91	87.36	110.60
1	A	2120	LYS	N-CA-CB	-12.89	87.39	110.60
1	A	2187	PRO	N-CA-CB	12.85	118.72	103.30
1	B	2555	ALA	CA-C-N	12.84	145.45	117.20
1	B	2187	PRO	N-CA-CB	12.84	118.70	103.30
1	A	2555	ALA	CA-C-N	12.82	145.42	117.20
1	B	1849	GLU	C-N-CA	12.82	153.75	121.70
1	A	1849	GLU	C-N-CA	12.81	153.73	121.70
1	B	1984	ILE	C-N-CA	-12.76	89.81	121.70
1	A	1984	ILE	C-N-CA	-12.76	89.81	121.70
1	A	2709	LYS	O-C-N	12.74	143.09	122.70
1	A	2688	ASN	N-CA-C	12.74	145.40	111.00
1	B	2709	LYS	O-C-N	12.74	143.08	122.70
1	B	2688	ASN	N-CA-C	12.73	145.36	111.00
1	A	3369	TYR	CB-CA-C	-12.70	85.00	110.40
1	A	1636	ILE	N-CA-CB	12.69	139.99	110.80
1	B	3369	TYR	CB-CA-C	-12.69	85.02	110.40
1	B	3681	GLU	CB-CA-C	-12.69	85.02	110.40
1	B	1636	ILE	N-CA-CB	12.69	139.98	110.80
1	A	3681	GLU	CB-CA-C	-12.67	85.06	110.40
1	A	2279	ARG	O-C-N	-12.61	102.52	122.70
1	A	3998	ILE	CA-C-N	-12.61	89.46	117.20
1	B	3998	ILE	CA-C-N	-12.60	89.47	117.20
1	B	2279	ARG	O-C-N	-12.60	102.54	122.70
1	B	2372	CYS	N-CA-C	12.57	144.93	111.00
1	B	2882	ALA	C-N-CA	-12.56	90.30	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2372	CYS	N-CA-C	12.55	144.89	111.00
1	A	2882	ALA	C-N-CA	-12.55	90.32	121.70
1	A	2126	ARG	N-CA-C	12.50	144.74	111.00
1	B	2126	ARG	N-CA-C	12.49	144.74	111.00
1	B	2555	ALA	C-N-CA	12.49	152.92	121.70
1	A	2555	ALA	C-N-CA	12.47	152.89	121.70
1	A	3998	ILE	C-N-CA	-12.46	90.54	121.70
1	B	3998	ILE	C-N-CA	-12.45	90.57	121.70
1	A	3863	LYS	O-C-N	-12.44	102.80	122.70
1	B	3863	LYS	O-C-N	-12.43	102.81	122.70
1	A	1479	LEU	O-C-N	-12.43	102.81	122.70
1	B	1479	LEU	O-C-N	-12.42	102.83	122.70
1	A	3370	LEU	N-CA-C	-12.39	77.55	111.00
1	B	3370	LEU	N-CA-C	-12.38	77.58	111.00
1	B	3644	ILE	CA-C-N	-12.37	89.98	117.20
1	A	3644	ILE	CA-C-N	-12.37	90.00	117.20
1	B	3684	CYS	C-N-CA	12.35	152.58	121.70
1	A	3684	CYS	C-N-CA	12.35	152.57	121.70
1	B	1755	LEU	N-CA-C	12.29	144.19	111.00
1	A	1635	ASP	CA-C-N	12.29	144.24	117.20
1	A	1755	LEU	N-CA-C	12.29	144.18	111.00
1	B	1635	ASP	CA-C-N	12.27	144.20	117.20
1	A	2432	LEU	CA-C-N	12.24	144.13	117.20
1	B	2432	LEU	CA-C-N	12.24	144.12	117.20
1	B	3333	TYR	O-C-N	12.19	142.20	122.70
1	B	3335	GLY	CA-C-N	12.17	143.98	117.20
1	A	3333	TYR	O-C-N	12.16	142.16	122.70
1	A	3335	GLY	CA-C-N	12.16	143.96	117.20
1	A	2379	SER	CB-CA-C	12.10	133.09	110.10
1	B	2379	SER	CB-CA-C	12.10	133.09	110.10
1	B	3865	ALA	CB-CA-C	12.03	128.14	110.10
1	A	3865	ALA	CB-CA-C	12.02	128.13	110.10
1	A	1813	LEU	CA-C-N	12.01	140.21	116.20
1	B	1813	LEU	CA-C-N	12.01	140.21	116.20
1	B	3360	TYR	O-C-N	11.93	141.79	122.70
1	A	3360	TYR	O-C-N	11.92	141.77	122.70
1	B	1802	LYS	O-C-N	-11.76	103.88	122.70
1	B	3426	THR	CA-C-N	-11.74	91.36	117.20
1	A	2002	ILE	O-C-N	11.74	141.48	122.70
1	A	3426	THR	CA-C-N	-11.74	91.37	117.20
1	A	1802	LYS	O-C-N	-11.74	103.92	122.70
1	B	2582	VAL	N-CA-CB	-11.71	85.73	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2688	ASN	CB-CA-C	-11.71	86.98	110.40
1	A	2582	VAL	N-CA-CB	-11.71	85.75	111.50
1	B	2688	ASN	CB-CA-C	-11.70	87.00	110.40
1	B	2002	ILE	O-C-N	11.70	141.42	122.70
1	A	2119	LEU	N-CA-C	11.70	142.58	111.00
1	B	2431	ALA	O-C-N	-11.70	103.98	122.70
1	B	1494	ASP	C-N-CA	-11.70	92.46	121.70
1	A	1494	ASP	C-N-CA	-11.69	92.47	121.70
1	A	2431	ALA	O-C-N	-11.69	104.00	122.70
1	B	2119	LEU	N-CA-C	11.68	142.54	111.00
1	A	3892	THR	N-CA-C	11.64	142.44	111.00
1	B	3892	THR	N-CA-C	11.64	142.43	111.00
1	A	1825	SER	N-CA-C	-11.63	79.59	111.00
1	B	1825	SER	N-CA-C	-11.63	79.58	111.00
1	A	1789	LYS	O-C-N	11.61	141.28	122.70
1	A	1828	TYR	N-CA-C	11.62	142.36	111.00
1	B	1828	TYR	N-CA-CB	-11.61	89.70	110.60
1	B	1789	LYS	O-C-N	11.61	141.27	122.70
1	B	1828	TYR	N-CA-C	11.60	142.31	111.00
1	A	1828	TYR	N-CA-CB	-11.60	89.73	110.60
1	B	3426	THR	C-N-CA	-11.59	92.72	121.70
1	A	3426	THR	C-N-CA	-11.59	92.73	121.70
1	B	3420	ASN	O-C-N	-11.56	104.20	122.70
1	A	3420	ASN	O-C-N	-11.56	104.20	122.70
1	A	2844	PHE	N-CA-CB	11.51	131.31	110.60
1	B	2844	PHE	N-CA-CB	11.51	131.31	110.60
1	B	3878	HIS	O-C-N	-11.49	104.32	122.70
1	A	3336	HIS	N-CA-CB	11.49	131.28	110.60
1	B	3336	HIS	N-CA-CB	11.49	131.28	110.60
1	A	3878	HIS	O-C-N	-11.46	104.36	122.70
1	A	3381	GLU	C-N-CA	11.43	150.28	121.70
1	B	3405	PRO	O-C-N	-11.43	104.42	122.70
1	A	3405	PRO	O-C-N	-11.42	104.43	122.70
1	B	3381	GLU	C-N-CA	11.40	150.21	121.70
1	A	3740	THR	CB-CA-C	-11.37	80.89	111.60
1	B	3740	THR	CB-CA-C	-11.37	80.89	111.60
1	A	3514	ARG	O-C-N	11.33	140.83	122.70
1	B	3514	ARG	O-C-N	11.32	140.81	122.70
1	B	2579	PHE	CA-C-N	-11.31	92.32	117.20
1	A	3421	TYR	N-CA-C	11.30	141.50	111.00
1	B	3421	TYR	N-CA-C	11.29	141.49	111.00
1	A	1477	LYS	N-CA-C	11.29	141.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2579	PHE	CA-C-N	-11.29	92.37	117.20
1	B	1477	LYS	N-CA-C	11.29	141.48	111.00
1	A	3400	SER	C-N-CA	11.27	149.87	121.70
1	B	3400	SER	C-N-CA	11.26	149.84	121.70
1	B	1636	ILE	N-CA-C	-11.25	80.62	111.00
1	B	3710	ILE	O-C-N	-11.25	104.69	122.70
1	A	1636	ILE	N-CA-C	-11.24	80.64	111.00
1	A	3710	ILE	O-C-N	-11.24	104.72	122.70
1	A	1817	VAL	CB-CA-C	-11.21	90.11	111.40
1	B	1817	VAL	CB-CA-C	-11.20	90.12	111.40
1	B	2937	PRO	O-C-N	-11.19	104.80	122.70
1	A	2002	ILE	CA-C-N	-11.19	92.59	117.20
1	B	2002	ILE	CA-C-N	-11.17	92.62	117.20
1	A	2937	PRO	O-C-N	-11.16	104.84	122.70
1	B	2108	VAL	O-C-N	-11.11	104.93	122.70
1	A	2108	VAL	O-C-N	-11.10	104.93	122.70
1	A	1633	GLY	O-C-N	-11.06	105.00	122.70
1	B	1633	GLY	O-C-N	-11.05	105.02	122.70
1	A	3900	ILE	C-N-CA	11.03	168.34	122.00
1	A	2578	ILE	O-C-N	-11.02	105.07	122.70
1	B	2578	ILE	O-C-N	-11.01	105.08	122.70
1	B	3900	ILE	C-N-CA	11.01	168.26	122.00
1	A	4036	GLN	O-C-N	-10.97	105.16	122.70
1	B	4036	GLN	O-C-N	-10.94	105.20	122.70
1	B	2709	LYS	CA-C-N	-10.72	93.62	117.20
1	A	2709	LYS	CA-C-N	-10.71	93.64	117.20
1	A	1989	GLU	C-N-CA	10.57	144.49	122.30
1	A	1969	GLY	O-C-N	-10.55	105.81	122.70
1	B	1969	GLY	O-C-N	-10.55	105.82	122.70
1	B	1989	GLU	C-N-CA	10.55	144.46	122.30
1	B	1940	GLU	CB-CA-C	-10.55	89.30	110.40
1	A	1940	GLU	CB-CA-C	-10.54	89.33	110.40
1	A	1817	VAL	N-CA-C	10.50	139.34	111.00
1	B	1817	VAL	N-CA-C	10.49	139.33	111.00
1	A	2640	THR	CB-CA-C	-10.46	83.37	111.60
1	B	2640	THR	CB-CA-C	-10.46	83.37	111.60
1	B	3333	TYR	CA-C-N	-10.42	94.28	117.20
1	A	2486	CYS	N-CA-CB	-10.40	91.87	110.60
1	B	2486	CYS	N-CA-CB	-10.40	91.88	110.60
1	A	3333	TYR	CA-C-N	-10.40	94.32	117.20
1	B	2018	LEU	O-C-N	-10.40	106.06	122.70
1	A	2018	LEU	O-C-N	-10.39	106.07	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4047	ALA	CA-C-N	-10.38	94.38	117.20
1	A	2003	LEU	CA-C-N	10.36	146.10	117.10
1	B	4047	ALA	CA-C-N	-10.35	94.42	117.20
1	B	2003	LEU	CA-C-N	10.34	146.06	117.10
1	A	2066	THR	CA-C-N	-10.33	94.47	117.20
1	B	2066	THR	CA-C-N	-10.33	94.47	117.20
1	A	2581	LEU	CB-CA-C	-10.32	90.60	110.20
1	B	2581	LEU	CB-CA-C	-10.30	90.62	110.20
1	A	3709	ASP	CA-C-N	10.28	139.82	117.20
1	B	3709	ASP	CA-C-N	10.26	139.77	117.20
1	A	2196	THR	O-C-N	-10.25	106.31	122.70
1	A	3360	TYR	CA-C-N	-10.25	94.66	117.20
1	A	2870	GLU	N-CA-C	-10.24	83.35	111.00
1	B	2870	GLU	N-CA-C	-10.24	83.34	111.00
1	B	3360	TYR	CA-C-N	-10.24	94.67	117.20
1	B	2196	THR	O-C-N	-10.24	106.32	122.70
1	A	2462	THR	O-C-N	10.23	139.06	122.70
1	B	2485	PHE	CB-CA-C	-10.20	89.99	110.40
1	B	2462	THR	O-C-N	10.20	139.01	122.70
1	A	2485	PHE	CB-CA-C	-10.19	90.02	110.40
1	B	3755	SER	O-C-N	-10.18	106.41	122.70
1	A	3755	SER	O-C-N	-10.17	106.42	122.70
1	A	1801	GLY	CA-C-N	10.09	139.40	117.20
1	B	1801	GLY	CA-C-N	10.09	139.39	117.20
1	A	2432	LEU	C-N-CA	10.05	146.83	121.70
1	B	2432	LEU	C-N-CA	10.05	146.83	121.70
1	B	3682	VAL	CA-C-N	10.04	139.28	117.20
1	A	3682	VAL	CA-C-N	10.03	139.26	117.20
1	A	1820	PHE	C-N-CA	10.01	146.72	121.70
1	B	1820	PHE	C-N-CA	10.01	146.72	121.70
1	A	3501	PRO	N-CA-C	-10.00	86.10	112.10
1	B	3501	PRO	N-CA-C	-10.00	86.10	112.10
1	A	4047	ALA	O-C-N	9.96	138.64	122.70
1	B	4047	ALA	O-C-N	9.96	138.64	122.70
1	B	2843	LEU	N-CA-C	-9.94	84.16	111.00
1	A	2843	LEU	N-CA-C	-9.94	84.17	111.00
1	A	3400	SER	CA-C-N	9.91	139.01	117.20
1	B	3400	SER	CA-C-N	9.91	139.01	117.20
1	B	1789	LYS	CA-C-N	-9.89	95.44	117.20
1	A	1789	LYS	CA-C-N	-9.88	95.47	117.20
1	A	3900	ILE	CA-C-N	-9.85	89.52	117.10
1	B	3739	ASP	CB-CA-C	-9.83	90.74	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3739	ASP	CB-CA-C	-9.82	90.75	110.40
1	B	2638	ARG	O-C-N	-9.82	106.98	122.70
1	B	3900	ILE	CA-C-N	-9.82	89.60	117.10
1	B	2309	SER	O-C-N	-9.79	107.03	122.70
1	A	2309	SER	O-C-N	-9.78	107.05	122.70
1	A	2638	ARG	O-C-N	-9.78	107.06	122.70
1	B	3866	GLU	CB-CA-C	-9.64	91.11	110.40
1	A	2345	TYR	N-CA-C	-9.63	84.99	111.00
1	A	3866	GLU	CB-CA-C	-9.63	91.14	110.40
1	B	2345	TYR	N-CA-C	-9.62	85.01	111.00
1	A	1633	GLY	C-N-CA	-9.61	97.67	121.70
1	B	1633	GLY	C-N-CA	-9.60	97.71	121.70
1	A	2198	ASN	C-N-CA	9.57	145.63	121.70
1	A	1983	LEU	C-N-CA	9.55	145.59	121.70
1	B	2198	ASN	C-N-CA	9.56	145.59	121.70
1	B	1983	LEU	C-N-CA	9.55	145.58	121.70
1	B	1815	ARG	C-N-CA	9.54	145.54	121.70
1	A	1815	ARG	C-N-CA	9.53	145.54	121.70
1	A	2485	PHE	N-CA-C	9.49	136.63	111.00
1	B	2485	PHE	N-CA-C	9.49	136.62	111.00
1	A	2006	LEU	C-N-CA	-9.47	102.41	122.30
1	B	2006	LEU	C-N-CA	-9.47	102.42	122.30
1	A	2640	THR	N-CA-C	9.46	136.55	111.00
1	B	2640	THR	N-CA-C	9.46	136.55	111.00
1	A	3917	THR	C-N-CA	-9.45	102.45	122.30
1	B	3917	THR	C-N-CA	-9.45	102.46	122.30
1	B	1888	LEU	C-N-CA	9.37	145.12	121.70
1	B	1962	SER	N-CA-C	9.36	136.28	111.00
1	A	1888	LEU	C-N-CA	9.36	145.09	121.70
1	A	1962	SER	N-CA-C	9.35	136.25	111.00
1	A	4047	ALA	C-N-CA	-9.35	98.33	121.70
1	B	4047	ALA	C-N-CA	-9.35	98.33	121.70
2	S	32	TYR	CA-C-O	-9.34	100.48	120.10
1	A	2633	ILE	O-C-N	-9.34	107.76	122.70
1	B	2303	GLN	N-CA-C	-9.34	85.80	111.00
1	B	2633	ILE	O-C-N	-9.33	107.77	122.70
1	A	2303	GLN	N-CA-C	-9.32	85.83	111.00
1	A	3514	ARG	CA-C-N	-9.30	96.73	117.20
1	B	3514	ARG	CA-C-N	-9.30	96.74	117.20
1	A	2373	SER	N-CA-CB	9.26	124.38	110.50
1	B	2373	SER	N-CA-CB	9.26	124.38	110.50
1	A	2527	GLU	O-C-N	-9.25	107.90	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2527	GLU	O-C-N	-9.24	107.91	122.70
1	B	3899	ASP	O-C-N	-9.20	107.97	122.70
1	A	3899	ASP	O-C-N	-9.19	107.99	122.70
1	B	1849	GLU	O-C-N	9.18	137.38	122.70
1	A	1849	GLU	O-C-N	9.17	137.37	122.70
1	A	1825	SER	CB-CA-C	-9.16	92.70	110.10
1	B	1825	SER	CB-CA-C	-9.15	92.71	110.10
1	B	3641	PHE	N-CA-C	9.10	135.57	111.00
1	A	3641	PHE	N-CA-C	9.10	135.56	111.00
1	A	2758	LEU	O-C-N	9.04	137.17	122.70
1	B	2758	LEU	O-C-N	9.00	137.10	122.70
1	B	2159	ASP	CA-C-N	-8.99	91.92	117.10
1	A	2159	ASP	CA-C-N	-8.99	91.94	117.10
1	B	2116	GLY	O-C-N	8.97	137.06	122.70
1	A	2116	GLY	O-C-N	8.96	137.04	122.70
1	B	1877	SER	O-C-N	-8.94	108.40	122.70
1	A	1877	SER	O-C-N	-8.93	108.41	122.70
1	B	2435	SER	O-C-N	-8.92	108.42	122.70
1	B	3425	LYS	O-C-N	-8.92	108.43	122.70
1	A	3425	LYS	O-C-N	-8.92	108.43	122.70
1	A	2435	SER	O-C-N	-8.90	108.46	122.70
1	A	3893	ASP	O-C-N	8.89	136.92	122.70
1	B	3893	ASP	O-C-N	8.88	136.91	122.70
1	B	3684	CYS	CA-C-N	8.87	136.71	117.20
1	A	3684	CYS	CA-C-N	8.86	136.70	117.20
1	A	3996	GLY	O-C-N	8.86	136.87	122.70
1	B	1892	THR	CA-C-N	-8.86	97.72	117.20
1	A	3667	ALA	O-C-N	8.85	136.87	122.70
1	B	3996	GLY	O-C-N	8.85	136.87	122.70
1	A	1892	THR	CA-C-N	-8.85	97.74	117.20
1	B	3667	ALA	O-C-N	8.83	136.82	122.70
1	A	3754	LYS	N-CA-C	-8.77	87.32	111.00
1	B	3754	LYS	N-CA-C	-8.76	87.34	111.00
1	B	3899	ASP	C-N-CA	-8.76	99.79	121.70
1	A	3899	ASP	C-N-CA	-8.76	99.81	121.70
1	B	1800	THR	O-C-N	-8.76	108.31	123.20
1	A	1800	THR	O-C-N	-8.75	108.32	123.20
1	A	2637	PRO	C-N-CA	8.74	143.56	121.70
1	B	2637	PRO	C-N-CA	8.73	143.53	121.70
1	B	2596	SER	C-N-CA	8.71	143.49	121.70
1	A	2596	SER	C-N-CA	8.71	143.46	121.70
1	A	3862	THR	O-C-N	-8.69	108.80	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3862	THR	O-C-N	-8.68	108.81	122.70
1	B	2158	LEU	CA-C-N	-8.68	98.11	117.20
1	A	2158	LEU	CA-C-N	-8.68	98.11	117.20
1	B	1633	GLY	N-CA-C	-8.67	91.43	113.10
1	A	1633	GLY	N-CA-C	-8.66	91.44	113.10
1	B	2775	TRP	O-C-N	8.66	136.56	122.70
1	B	1800	THR	C-N-CA	8.65	140.47	122.30
1	B	2186	ILE	O-C-N	8.64	137.52	121.10
1	A	2186	ILE	O-C-N	8.64	137.51	121.10
1	A	2775	TRP	O-C-N	8.63	136.51	122.70
1	A	1800	THR	C-N-CA	8.62	140.41	122.30
1	B	2602	GLU	C-N-CA	8.59	143.16	121.70
1	A	1635	ASP	N-CA-C	-8.58	87.83	111.00
1	A	2602	GLU	C-N-CA	8.58	143.15	121.70
1	B	1635	ASP	N-CA-C	-8.58	87.83	111.00
1	A	1823	ASP	O-C-N	8.48	136.27	122.70
1	B	1823	ASP	O-C-N	8.46	136.24	122.70
1	B	2161	GLU	CB-CA-C	-8.46	93.47	110.40
1	A	2161	GLU	CB-CA-C	-8.45	93.50	110.40
1	B	2634	ASN	O-C-N	8.43	136.19	122.70
1	A	2634	ASN	O-C-N	8.42	136.17	122.70
1	B	1962	SER	C-N-CA	8.42	142.75	121.70
1	A	1962	SER	C-N-CA	8.42	142.74	121.70
1	B	3405	PRO	CB-CA-C	-8.34	91.15	112.00
1	A	2066	THR	CB-CA-C	-8.33	89.11	111.60
1	A	3405	PRO	CB-CA-C	-8.33	91.18	112.00
1	B	2066	THR	CB-CA-C	-8.33	89.11	111.60
1	B	2303	GLN	CB-CA-C	8.33	127.05	110.40
1	A	2303	GLN	CB-CA-C	8.31	127.03	110.40
1	B	1986	GLU	C-N-CA	-8.26	101.06	121.70
1	A	1986	GLU	C-N-CA	-8.25	101.07	121.70
1	A	2158	LEU	O-C-N	8.25	135.90	122.70
1	B	2523	TRP	O-C-N	-8.25	109.50	122.70
1	A	2523	TRP	O-C-N	-8.24	109.51	122.70
1	B	2158	LEU	O-C-N	8.24	135.88	122.70
1	A	2656	PHE	N-CA-C	-8.22	88.81	111.00
1	B	2656	PHE	N-CA-C	-8.22	88.81	111.00
1	A	1789	LYS	C-N-CA	-8.21	101.18	121.70
1	B	1789	LYS	C-N-CA	-8.20	101.19	121.70
1	B	2431	ALA	CA-C-N	8.20	135.24	117.20
1	A	2431	ALA	CA-C-N	8.18	135.21	117.20
1	A	1961	SER	N-CA-C	8.14	132.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1961	SER	N-CA-C	8.13	132.95	111.00
1	A	1818	VAL	N-CA-C	8.10	132.88	111.00
1	B	1818	VAL	N-CA-C	8.10	132.86	111.00
1	B	1802	LYS	CA-C-N	8.05	134.91	117.20
1	A	1802	LYS	CA-C-N	8.04	134.90	117.20
1	A	2198	ASN	O-C-N	-8.04	109.83	122.70
1	A	1755	LEU	N-CA-CB	-8.04	94.32	110.40
1	A	4036	GLN	CA-C-N	8.04	134.88	117.20
1	B	1755	LEU	N-CA-CB	-8.04	94.33	110.40
1	B	4036	GLN	CA-C-N	8.04	134.88	117.20
1	B	2198	ASN	O-C-N	-8.03	109.85	122.70
1	B	3923	VAL	CA-C-N	-8.01	99.59	117.20
1	A	2616	LEU	O-C-N	-8.00	109.89	122.70
1	A	3923	VAL	CA-C-N	-8.00	99.60	117.20
1	B	2616	LEU	O-C-N	-8.00	109.91	122.70
1	B	1827	ASP	C-N-CA	-7.96	101.79	121.70
1	B	3901	PRO	O-C-N	7.96	136.73	123.20
1	A	1827	ASP	C-N-CA	-7.95	101.82	121.70
1	A	2345	TYR	CB-CA-C	-7.95	94.51	110.40
1	B	2345	TYR	CB-CA-C	-7.94	94.53	110.40
1	A	3901	PRO	O-C-N	7.93	136.69	123.20
1	A	2436	SER	C-N-CA	-7.93	101.87	121.70
1	B	3878	HIS	CA-C-N	7.93	134.65	117.20
1	B	2436	SER	C-N-CA	-7.93	101.87	121.70
1	A	3878	HIS	CA-C-N	7.93	134.64	117.20
1	A	2462	THR	CA-C-N	-7.90	99.82	117.20
1	A	1941	ASP	C-N-CA	-7.89	101.98	121.70
1	B	2462	THR	CA-C-N	-7.88	99.86	117.20
1	B	1941	ASP	C-N-CA	-7.88	102.00	121.70
1	B	1922	LYS	CB-CA-C	7.88	126.15	110.40
1	A	3641	PHE	C-N-CA	7.88	141.39	121.70
1	B	2201	HIS	O-C-N	7.87	135.30	122.70
1	A	1922	LYS	CB-CA-C	7.87	126.14	110.40
1	B	3641	PHE	C-N-CA	7.86	141.36	121.70
1	A	2201	HIS	O-C-N	7.85	135.27	122.70
1	B	2190	PHE	CB-CA-C	-7.85	94.69	110.40
1	A	2190	PHE	CB-CA-C	-7.84	94.71	110.40
1	A	2616	LEU	N-CA-CB	-7.77	94.85	110.40
1	B	2616	LEU	N-CA-CB	-7.76	94.88	110.40
1	B	2689	ILE	C-N-CA	7.73	141.03	121.70
1	A	2689	ILE	C-N-CA	7.73	141.03	121.70
1	B	2375	ILE	C-N-CA	7.73	154.47	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2375	ILE	C-N-CA	7.72	154.44	122.00
1	B	2938	MET	N-CA-C	-7.71	90.19	111.00
1	A	2938	MET	N-CA-C	-7.70	90.21	111.00
1	B	2582	VAL	N-CA-C	7.68	131.73	111.00
1	A	2582	VAL	N-CA-C	7.68	131.73	111.00
1	A	3898	GLU	O-C-N	7.67	134.98	122.70
1	B	3477	VAL	CB-CA-C	7.67	125.97	111.40
1	A	3477	VAL	CB-CA-C	7.66	125.95	111.40
1	B	3410	PRO	CB-CA-C	-7.65	92.86	112.00
1	B	3898	GLU	O-C-N	7.65	134.94	122.70
1	A	3410	PRO	CB-CA-C	-7.64	92.90	112.00
1	A	2942	ASP	N-CA-C	7.63	131.60	111.00
1	B	2942	ASP	N-CA-C	7.63	131.60	111.00
1	B	3866	GLU	C-N-CA	7.62	140.76	121.70
1	A	3866	GLU	C-N-CA	7.62	140.75	121.70
1	B	3738	VAL	CB-CA-C	7.55	125.75	111.40
1	A	1984	ILE	CA-C-N	7.55	133.81	117.20
1	B	1984	ILE	CA-C-N	7.54	133.80	117.20
1	A	3738	VAL	CB-CA-C	7.54	125.73	111.40
1	B	1827	ASP	CA-C-N	-7.48	100.75	117.20
1	A	1827	ASP	CA-C-N	-7.47	100.77	117.20
1	B	3755	SER	CB-CA-C	7.46	124.27	110.10
1	A	3878	HIS	C-N-CA	-7.43	103.13	121.70
1	A	2108	VAL	CA-C-N	7.43	133.54	117.20
1	B	3878	HIS	C-N-CA	-7.42	103.14	121.70
1	A	3755	SER	CB-CA-C	7.42	124.20	110.10
1	B	2108	VAL	CA-C-N	7.42	133.52	117.20
1	B	2302	PHE	O-C-N	-7.41	110.84	122.70
1	B	2120	LYS	N-CA-C	7.41	131.01	111.00
1	A	2120	LYS	N-CA-C	7.41	131.00	111.00
1	A	2302	PHE	O-C-N	-7.40	110.86	122.70
1	A	2119	LEU	CB-CA-C	-7.40	96.14	110.20
1	B	2116	GLY	CA-C-N	-7.39	100.94	117.20
1	B	2119	LEU	CB-CA-C	-7.39	96.16	110.20
1	A	2116	GLY	CA-C-N	-7.39	100.95	117.20
1	A	2186	ILE	CA-C-N	-7.36	96.49	117.10
1	A	4003	ASP	O-C-N	7.35	134.46	122.70
1	B	2186	ILE	CA-C-N	-7.34	96.54	117.10
1	B	4003	ASP	O-C-N	7.34	134.44	122.70
1	A	3681	GLU	N-CA-C	7.33	130.81	111.00
1	B	3681	GLU	N-CA-C	7.33	130.80	111.00
1	A	1918	GLU	O-C-N	7.31	134.40	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1632	ASP	CA-C-N	-7.31	101.59	116.20
1	B	1632	ASP	CA-C-N	-7.30	101.59	116.20
1	B	1918	GLU	O-C-N	7.30	134.38	122.70
1	A	1917	ARG	O-C-N	-7.30	111.03	122.70
1	B	1917	ARG	O-C-N	-7.29	111.03	122.70
1	A	1816	VAL	C-N-CA	7.25	139.82	121.70
1	B	1816	VAL	C-N-CA	7.25	139.81	121.70
1	B	2103	VAL	O-C-N	7.24	134.28	122.70
1	A	2169	VAL	CB-CA-C	-7.23	97.66	111.40
1	A	3407	LEU	CB-CA-C	-7.23	96.46	110.20
1	B	3407	LEU	CB-CA-C	-7.23	96.47	110.20
1	B	2169	VAL	CB-CA-C	-7.22	97.68	111.40
1	A	2373	SER	N-CA-C	-7.22	91.51	111.00
1	B	2373	SER	N-CA-C	-7.21	91.54	111.00
1	B	2561	TYR	CA-C-N	7.20	137.26	117.10
1	A	2561	TYR	CA-C-N	7.20	137.26	117.10
1	A	2657	ALA	N-CA-CB	7.20	120.18	110.10
1	A	2103	VAL	O-C-N	7.20	134.21	122.70
1	A	1818	VAL	N-CA-CB	-7.19	95.67	111.50
1	B	1818	VAL	N-CA-CB	-7.19	95.67	111.50
1	A	3893	ASP	CA-C-N	-7.19	101.38	117.20
1	B	3893	ASP	CA-C-N	-7.18	101.40	117.20
1	B	2657	ALA	N-CA-CB	7.18	120.15	110.10
1	A	1983	LEU	O-C-N	-7.15	111.25	122.70
1	B	1983	LEU	O-C-N	-7.14	111.27	122.70
1	A	2161	GLU	O-C-N	-7.11	111.32	122.70
1	A	2940	PHE	C-N-CA	7.11	139.47	121.70
1	B	2940	PHE	C-N-CA	7.11	139.47	121.70
1	B	2161	GLU	O-C-N	-7.10	111.33	122.70
1	B	2689	ILE	N-CA-C	7.10	130.18	111.00
1	A	2689	ILE	N-CA-C	7.09	130.15	111.00
1	B	2199	LEU	CA-C-N	-7.08	101.63	117.20
1	A	1823	ASP	C-N-CA	-7.07	104.02	121.70
1	A	2199	LEU	CA-C-N	-7.06	101.66	117.20
1	B	1823	ASP	C-N-CA	-7.06	104.05	121.70
1	B	1826	PHE	C-N-CA	7.05	139.33	121.70
1	A	2190	PHE	N-CA-C	7.05	130.04	111.00
1	A	1826	PHE	C-N-CA	7.05	139.31	121.70
1	A	3740	THR	C-N-CA	7.04	139.31	121.70
1	A	2938	MET	O-C-N	-7.04	111.43	122.70
1	B	2938	MET	O-C-N	-7.04	111.43	122.70
1	B	2190	PHE	N-CA-C	7.04	130.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3740	THR	C-N-CA	7.03	139.28	121.70
1	B	2758	LEU	CA-C-N	-7.02	101.76	117.20
1	A	1823	ASP	CA-C-N	-7.02	101.77	117.20
1	A	1477	LYS	CB-CA-C	-7.01	96.37	110.40
1	A	2758	LEU	CA-C-N	-7.01	101.77	117.20
1	B	1823	ASP	CA-C-N	-7.00	101.79	117.20
1	B	1477	LYS	CB-CA-C	-7.00	96.41	110.40
1	A	3504	ASP	O-C-N	6.99	133.89	122.70
1	A	3755	SER	CA-C-N	6.99	132.58	117.20
1	B	3755	SER	CA-C-N	6.98	132.56	117.20
1	B	2393	PRO	CA-C-N	6.98	132.55	117.20
1	A	2393	PRO	CA-C-N	6.97	132.54	117.20
1	A	3410	PRO	C-N-CA	-6.96	104.29	121.70
1	B	3410	PRO	C-N-CA	-6.96	104.30	121.70
1	B	3504	ASP	O-C-N	6.95	133.82	122.70
1	B	3420	ASN	CB-CA-C	-6.92	96.56	110.40
1	A	2937	PRO	CB-CA-C	-6.91	94.72	112.00
1	A	3420	ASN	CB-CA-C	-6.91	96.58	110.40
1	B	2937	PRO	CB-CA-C	-6.91	94.72	112.00
1	A	2445	PHE	N-CA-C	6.90	129.64	111.00
1	B	2732	MET	O-C-N	6.90	133.74	122.70
1	B	2445	PHE	N-CA-C	6.90	129.63	111.00
1	A	2732	MET	O-C-N	6.89	133.73	122.70
1	B	3820	GLU	N-CA-C	6.88	129.58	111.00
1	A	3820	GLU	N-CA-C	6.87	129.56	111.00
1	A	4034	LEU	C-N-CA	-6.87	104.54	121.70
1	B	4034	LEU	C-N-CA	-6.86	104.55	121.70
1	A	2882	ALA	CA-C-N	-6.85	102.12	117.20
1	B	2882	ALA	CA-C-N	-6.85	102.12	117.20
1	A	2774	ALA	O-C-N	-6.85	111.74	122.70
1	B	2774	ALA	O-C-N	-6.84	111.75	122.70
1	A	2256	SER	N-CA-CB	-6.84	100.24	110.50
1	B	2256	SER	N-CA-CB	-6.83	100.26	110.50
1	A	2118	MET	O-C-N	-6.81	111.81	122.70
1	B	2118	MET	O-C-N	-6.81	111.81	122.70
1	B	2634	ASN	CA-C-N	-6.80	102.23	117.20
1	A	2634	ASN	CA-C-N	-6.80	102.25	117.20
1	A	1877	SER	CA-C-N	6.77	132.09	117.20
1	B	3996	GLY	CA-C-N	-6.77	102.31	117.20
1	A	3996	GLY	CA-C-N	-6.76	102.32	117.20
1	A	3499	CYS	C-N-CA	-6.75	104.81	121.70
1	A	2372	CYS	O-C-N	6.75	133.50	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2372	CYS	O-C-N	6.75	133.51	122.70
1	B	1877	SER	CA-C-N	6.75	132.05	117.20
1	A	3667	ALA	CA-C-N	-6.75	102.36	117.20
1	B	3499	CYS	C-N-CA	-6.74	104.86	121.70
1	B	1850	PHE	O-C-N	6.73	133.47	122.70
1	B	2302	PHE	C-N-CA	6.73	138.53	121.70
1	A	2302	PHE	C-N-CA	6.73	138.53	121.70
1	A	3992	ILE	N-CA-C	-6.73	92.83	111.00
1	B	3992	ILE	N-CA-C	-6.73	92.83	111.00
1	B	3667	ALA	CA-C-N	-6.72	102.41	117.20
1	B	3357	ALA	N-CA-CB	-6.71	100.71	110.10
1	A	1850	PHE	O-C-N	6.71	133.43	122.70
1	A	3357	ALA	N-CA-CB	-6.70	100.72	110.10
1	B	1850	PHE	CA-C-N	-6.70	102.47	117.20
1	A	1850	PHE	CA-C-N	-6.70	102.47	117.20
1	A	3655	ARG	CA-C-N	-6.69	102.47	117.20
1	A	2616	LEU	C-N-CA	-6.69	104.97	121.70
1	B	2616	LEU	C-N-CA	-6.69	104.98	121.70
1	A	1816	VAL	CB-CA-C	-6.69	98.69	111.40
1	B	1816	VAL	CB-CA-C	-6.69	98.70	111.40
1	B	3655	ARG	CA-C-N	-6.68	102.50	117.20
1	A	1989	GLU	O-C-N	-6.67	111.85	123.20
1	A	2442	GLY	N-CA-C	6.66	129.76	113.10
1	B	2442	GLY	N-CA-C	6.66	129.76	113.10
1	A	2578	ILE	C-N-CA	6.66	138.34	121.70
1	B	2578	ILE	C-N-CA	6.65	138.33	121.70
1	B	1989	GLU	O-C-N	-6.65	111.89	123.20
1	B	2943	PHE	N-CA-C	-6.64	93.08	111.00
1	A	2943	PHE	N-CA-C	-6.63	93.09	111.00
1	A	3420	ASN	N-CA-C	-6.62	93.12	111.00
1	B	3420	ASN	N-CA-C	-6.62	93.12	111.00
1	A	3457	PHE	O-C-N	6.62	133.29	122.70
1	A	2936	VAL	O-C-N	-6.61	108.54	121.10
1	B	2936	VAL	O-C-N	-6.61	108.54	121.10
1	B	2346	PHE	C-N-CA	-6.60	108.44	122.30
1	B	3457	PHE	O-C-N	6.60	133.26	122.70
1	A	2346	PHE	C-N-CA	-6.59	108.46	122.30
1	B	3755	SER	N-CA-C	-6.58	93.24	111.00
1	B	2304	ASN	N-CA-C	6.58	128.75	111.00
1	A	2304	ASN	N-CA-C	6.57	128.75	111.00
1	A	3755	SER	N-CA-C	-6.57	93.26	111.00
1	B	1849	GLU	CA-C-N	-6.57	102.75	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2686	LEU	CB-CA-C	6.56	122.67	110.20
1	B	1812	ASN	O-C-N	-6.56	112.20	122.70
1	A	1849	GLU	CA-C-N	-6.55	102.78	117.20
1	A	2686	LEU	CB-CA-C	6.55	122.64	110.20
1	A	2462	THR	C-N-CA	-6.54	105.34	121.70
1	B	2373	SER	O-C-N	-6.54	112.23	122.70
1	A	2373	SER	O-C-N	-6.54	112.24	122.70
1	A	1812	ASN	O-C-N	-6.53	112.25	122.70
1	B	2462	THR	C-N-CA	-6.53	105.38	121.70
1	B	2775	TRP	CA-C-N	-6.53	102.84	117.20
1	A	2775	TRP	CA-C-N	-6.52	102.86	117.20
1	B	3682	VAL	N-CA-C	-6.51	93.42	111.00
1	A	3682	VAL	N-CA-C	-6.51	93.43	111.00
1	B	3382	CYS	O-C-N	-6.48	112.19	123.20
1	A	3382	CYS	O-C-N	-6.48	112.19	123.20
1	B	2159	ASP	C-N-CA	-6.48	94.80	122.00
1	A	2159	ASP	C-N-CA	-6.47	94.80	122.00
1	A	3901	PRO	N-CA-CB	6.44	111.03	103.30
2	T	144	GLY	N-CA-C	6.44	129.20	113.10
1	A	3641	PHE	O-C-N	-6.44	112.40	122.70
1	B	1826	PHE	O-C-N	-6.43	112.41	122.70
1	B	3901	PRO	N-CA-CB	6.43	111.02	103.30
1	A	2578	ILE	CA-C-N	6.43	131.34	117.20
1	A	1826	PHE	O-C-N	-6.43	112.42	122.70
1	B	3641	PHE	O-C-N	-6.42	112.42	122.70
1	B	2578	ILE	CA-C-N	6.42	131.33	117.20
1	A	2006	LEU	CB-CA-C	-6.42	98.00	110.20
1	B	2006	LEU	CB-CA-C	-6.42	98.01	110.20
1	A	3710	ILE	CB-CA-C	6.38	124.35	111.60
1	B	3710	ILE	CB-CA-C	6.37	124.34	111.60
1	B	2541	PRO	O-C-N	6.36	134.02	123.20
1	A	2541	PRO	O-C-N	6.36	134.01	123.20
1	A	2002	ILE	C-N-CA	6.35	137.56	121.70
1	B	2002	ILE	C-N-CA	6.32	137.51	121.70
1	A	3754	LYS	N-CA-CB	-6.32	99.22	110.60
1	B	2732	MET	CA-C-N	-6.31	103.31	117.20
1	B	3898	GLU	CA-C-N	-6.31	103.32	117.20
1	A	2732	MET	CA-C-N	-6.30	103.33	117.20
1	A	3898	GLU	CA-C-N	-6.30	103.33	117.20
1	B	3754	LYS	N-CA-CB	-6.30	99.25	110.60
1	A	3359	LYS	C-N-CA	6.29	137.42	121.70
1	A	2774	ALA	C-N-CA	-6.28	106.01	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2774	ALA	C-N-CA	-6.27	106.02	121.70
1	B	3359	LYS	C-N-CA	6.27	137.38	121.70
2	T	15	PRO	N-CA-CB	6.27	110.83	103.30
1	A	1634	THR	N-CA-C	6.27	127.92	111.00
1	B	2579	PHE	C-N-CA	-6.26	106.05	121.70
1	A	2309	SER	CA-C-N	6.26	130.97	117.20
1	B	1634	THR	N-CA-C	6.26	127.89	111.00
1	B	2309	SER	CA-C-N	6.26	130.97	117.20
1	A	2004	PRO	N-CA-CB	6.25	110.81	103.30
1	A	2376	PRO	N-CA-CB	6.25	110.80	103.30
1	A	2579	PHE	C-N-CA	-6.25	106.08	121.70
1	B	2004	PRO	N-CA-CB	6.25	110.80	103.30
1	A	2201	HIS	N-CA-CB	-6.24	99.37	110.60
1	B	2376	PRO	N-CA-CB	6.22	110.77	103.30
1	B	2201	HIS	N-CA-CB	-6.22	99.40	110.60
1	A	2126	ARG	CB-CA-C	-6.22	97.97	110.40
1	B	2126	ARG	CB-CA-C	-6.21	97.98	110.40
1	A	2682	PRO	N-CA-CB	6.21	110.75	103.30
1	B	2682	PRO	N-CA-CB	6.21	110.75	103.30
1	B	2255	ASP	CB-CA-C	-6.20	98.00	110.40
1	A	2255	ASP	CB-CA-C	-6.18	98.05	110.40
1	A	2637	PRO	O-C-N	-6.18	112.82	122.70
1	B	2637	PRO	O-C-N	-6.17	112.83	122.70
1	B	3860	GLU	N-CA-C	6.16	127.64	111.00
1	B	2160	PRO	N-CA-CB	6.16	110.69	103.30
1	B	2523	TRP	CB-CA-C	6.16	122.72	110.40
2	T	52	PRO	N-CA-CB	6.16	110.69	103.30
1	A	2523	TRP	CB-CA-C	6.16	122.71	110.40
1	B	2161	GLU	N-CA-C	-6.16	94.38	111.00
1	B	2873	LEU	N-CA-C	-6.16	94.38	111.00
1	B	1918	GLU	CA-C-N	-6.15	103.66	117.20
1	A	1918	GLU	CA-C-N	-6.15	103.67	117.20
1	A	2160	PRO	N-CA-CB	6.15	110.68	103.30
1	A	3860	GLU	N-CA-C	6.15	127.60	111.00
1	A	2873	LEU	N-CA-C	-6.15	94.41	111.00
1	B	2784	PRO	N-CA-CB	6.15	110.67	103.30
1	A	2161	GLU	N-CA-C	-6.14	94.41	111.00
1	A	3642	TYR	O-C-N	-6.14	112.75	123.20
1	B	3642	TYR	O-C-N	-6.14	112.76	123.20
1	B	1800	THR	CA-C-N	6.13	128.47	116.20
1	A	2784	PRO	N-CA-CB	6.12	110.65	103.30
1	A	1800	THR	CA-C-N	6.12	128.45	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3683	TYR	CA-C-N	-6.12	103.74	117.20
1	A	3683	TYR	CA-C-N	-6.12	103.74	117.20
1	A	2937	PRO	N-CA-CB	6.11	110.63	103.30
1	A	2946	PRO	N-CA-CB	6.09	110.61	103.30
1	B	2937	PRO	N-CA-CB	6.09	110.61	103.30
1	B	2946	PRO	N-CA-CB	6.08	110.60	103.30
1	B	2957	PRO	N-CA-CB	6.05	110.56	103.30
1	B	1969	GLY	CA-C-N	6.05	130.51	117.20
1	B	2591	PRO	N-CA-CB	6.05	110.56	103.30
1	A	1969	GLY	CA-C-N	6.04	130.50	117.20
1	A	2957	PRO	N-CA-CB	6.04	110.55	103.30
1	B	3991	THR	C-N-CA	-6.04	106.61	121.70
1	A	2591	PRO	N-CA-CB	6.04	110.54	103.30
1	A	3991	THR	C-N-CA	-6.04	106.61	121.70
1	A	3815	PRO	N-CA-CB	6.03	110.54	103.30
1	B	3815	PRO	N-CA-CB	6.03	110.54	103.30
1	B	2157	ASP	C-N-CA	6.03	136.76	121.70
1	A	2731	PRO	N-CA-CB	6.02	110.53	103.30
1	B	2731	PRO	N-CA-CB	6.02	110.53	103.30
1	B	1990	GLY	O-C-N	-6.02	113.07	122.70
1	A	2655	ILE	CA-C-N	-6.02	103.96	117.20
1	B	2655	ILE	CA-C-N	-6.02	103.96	117.20
1	B	3637	GLN	O-C-N	-6.02	113.07	122.70
1	B	2188	PRO	N-CA-CB	6.01	110.52	103.30
1	A	2185	PRO	N-CA-CB	6.01	110.52	103.30
1	B	2185	PRO	N-CA-CB	6.01	110.51	103.30
1	B	2394	THR	CB-CA-C	-6.01	95.37	111.60
1	A	2394	THR	CB-CA-C	-6.01	95.38	111.60
1	A	3637	GLN	O-C-N	-6.01	113.09	122.70
1	A	1470	PRO	N-CA-CB	6.00	110.50	103.30
1	A	3863	LYS	CA-C-N	6.00	130.41	117.20
1	B	1470	PRO	N-CA-CB	6.00	110.50	103.30
1	A	1990	GLY	O-C-N	-6.00	113.10	122.70
1	A	2157	ASP	C-N-CA	6.00	136.70	121.70
1	B	2393	PRO	N-CA-CB	6.00	110.50	103.30
1	B	3863	LYS	CA-C-N	6.00	130.40	117.20
1	A	2545	PRO	N-CA-CB	5.99	110.48	103.30
1	B	2103	VAL	C-N-CA	5.99	136.67	121.70
1	B	2545	PRO	N-CA-CB	5.99	110.49	103.30
1	A	2103	VAL	C-N-CA	5.99	136.66	121.70
1	B	2537	PRO	N-CA-CB	5.98	110.48	103.30
1	B	2906	PRO	N-CA-CB	5.98	110.48	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2393	PRO	N-CA-CB	5.98	110.47	103.30
1	A	4066	PRO	N-CA-CB	5.97	110.47	103.30
1	B	2583	PRO	N-CA-CB	5.97	110.47	103.30
1	A	2370	SER	CB-CA-C	5.97	121.45	110.10
1	A	2537	PRO	N-CA-CB	5.97	110.47	103.30
1	A	4035	GLN	O-C-N	-5.97	113.14	122.70
1	B	2370	SER	CB-CA-C	5.97	121.45	110.10
1	B	4035	GLN	O-C-N	-5.97	113.15	122.70
1	A	2906	PRO	N-CA-CB	5.97	110.46	103.30
1	A	2188	PRO	N-CA-CB	5.96	110.46	103.30
1	B	1503	PRO	N-CA-CB	5.96	110.45	103.30
1	B	4066	PRO	N-CA-CB	5.96	110.44	103.30
1	B	2541	PRO	N-CA-CB	5.95	110.44	103.30
1	B	2204	PRO	N-CA-CB	5.95	110.44	103.30
1	A	3435	GLY	C-N-CA	5.95	136.56	121.70
1	B	2894	PRO	N-CA-CB	5.94	110.43	103.30
1	A	1887	PRO	N-CA-CB	5.94	110.43	103.30
1	B	2346	PHE	N-CA-CB	-5.94	99.90	110.60
1	A	2541	PRO	N-CA-CB	5.94	110.43	103.30
1	B	2637	PRO	N-CA-CB	5.94	110.43	103.30
1	B	2690	SER	CA-C-N	-5.94	104.13	117.20
1	B	3435	GLY	C-N-CA	5.94	136.55	121.70
1	B	3460	PRO	N-CA-CB	5.94	110.43	103.30
1	B	4025	PRO	N-CA-CB	5.94	110.43	103.30
1	A	2961	ILE	CA-C-N	5.94	130.26	117.20
1	A	2690	SER	CA-C-N	-5.93	104.15	117.20
1	A	3609	PRO	N-CA-CB	5.93	110.42	103.30
1	A	2583	PRO	N-CA-CB	5.93	110.42	103.30
1	A	4025	PRO	N-CA-CB	5.93	110.41	103.30
1	B	2961	ILE	CA-C-N	5.93	130.25	117.20
1	B	3609	PRO	N-CA-CB	5.93	110.41	103.30
1	A	3460	PRO	N-CA-CB	5.93	110.41	103.30
1	A	3356	PHE	C-N-CA	-5.93	106.88	121.70
1	B	3356	PHE	C-N-CA	-5.93	106.88	121.70
1	A	2204	PRO	N-CA-CB	5.92	110.41	103.30
1	A	2637	PRO	N-CA-CB	5.92	110.41	103.30
1	A	2346	PHE	N-CA-CB	-5.92	99.94	110.60
1	A	1503	PRO	N-CA-CB	5.92	110.40	103.30
1	A	1909	PRO	N-CA-CB	5.92	110.40	103.30
1	A	4032	PRO	N-CA-CB	5.92	110.40	103.30
1	A	2894	PRO	N-CA-CB	5.91	110.39	103.30
1	A	4035	GLN	C-N-CA	-5.91	106.91	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4030	PRO	N-CA-CB	5.91	110.39	103.30
1	A	3981	PRO	N-CA-CB	5.91	110.39	103.30
1	B	4035	GLN	C-N-CA	-5.91	106.93	121.70
1	A	3999	ASP	C-N-CA	5.91	136.46	121.70
1	B	1887	PRO	N-CA-CB	5.90	110.39	103.30
1	B	4032	PRO	N-CA-CB	5.90	110.38	103.30
1	B	3999	ASP	C-N-CA	5.90	136.45	121.70
1	B	4030	PRO	N-CA-CB	5.90	110.38	103.30
1	A	2388	PRO	N-CA-CB	5.88	110.36	103.30
1	B	1909	PRO	N-CA-CB	5.88	110.36	103.30
1	B	3981	PRO	N-CA-CB	5.88	110.36	103.30
1	B	1816	VAL	N-CA-CB	-5.88	98.56	111.50
1	B	2606	ARG	N-CA-C	5.88	126.87	111.00
1	B	2388	PRO	N-CA-CB	5.88	110.35	103.30
1	A	1816	VAL	N-CA-CB	-5.87	98.59	111.50
1	A	2606	ARG	N-CA-C	5.86	126.83	111.00
1	A	2065	LYS	O-C-N	-5.85	113.33	122.70
1	A	1916	PHE	N-CA-C	5.85	126.80	111.00
1	B	1916	PHE	N-CA-C	5.85	126.79	111.00
1	B	2989	PRO	N-CA-CB	5.85	110.32	103.30
1	A	2989	PRO	N-CA-CB	5.84	110.31	103.30
1	B	2065	LYS	O-C-N	-5.84	113.35	122.70
1	A	2018	LEU	CA-C-N	5.84	130.05	117.20
1	B	3990	ALA	N-CA-C	-5.84	95.23	111.00
1	A	2562	PRO	N-CA-CB	5.83	110.30	103.30
1	B	2562	PRO	N-CA-CB	5.83	110.30	103.30
1	A	3990	ALA	N-CA-C	-5.83	95.25	111.00
1	B	2641	LEU	N-CA-CB	-5.83	98.74	110.40
1	B	2437	LEU	N-CA-C	5.83	126.74	111.00
1	A	2437	LEU	N-CA-C	5.83	126.73	111.00
1	A	2641	LEU	N-CA-CB	-5.83	98.75	110.40
1	B	2103	VAL	CA-C-N	-5.83	104.38	117.20
1	B	2018	LEU	CA-C-N	5.82	130.01	117.20
1	A	2103	VAL	CA-C-N	-5.81	104.42	117.20
1	B	2943	PHE	N-CA-CB	5.81	121.06	110.60
1	A	2943	PHE	N-CA-CB	5.79	121.03	110.60
1	A	3457	PHE	CA-C-N	-5.79	104.47	117.20
1	A	3754	LYS	O-C-N	5.78	131.95	122.70
1	A	2196	THR	CA-C-N	5.78	129.92	117.20
1	B	3457	PHE	CA-C-N	-5.77	104.50	117.20
1	A	2108	VAL	CB-CA-C	5.76	122.35	111.40
1	B	1754	TYR	CB-CA-C	5.76	121.93	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3754	LYS	O-C-N	5.76	131.92	122.70
1	A	1754	TYR	CB-CA-C	5.76	121.93	110.40
1	B	2196	THR	CA-C-N	5.76	129.88	117.20
1	B	2108	VAL	CB-CA-C	5.76	122.34	111.40
1	B	3405	PRO	N-CA-CB	5.76	110.21	103.30
1	B	1884	GLU	O-C-N	5.75	131.90	122.70
1	B	3887	PRO	N-CA-CB	5.75	110.20	103.30
1	B	1989	GLU	CB-CA-C	-5.75	98.91	110.40
1	A	2610	GLY	N-CA-C	-5.74	98.74	113.10
1	A	3405	PRO	N-CA-CB	5.74	110.19	103.30
1	B	1797	PRO	N-CA-CB	5.74	110.19	103.30
1	A	1884	GLU	O-C-N	5.74	131.89	122.70
1	A	3887	PRO	N-CA-CB	5.74	110.19	103.30
1	B	2610	GLY	N-CA-C	-5.74	98.76	113.10
1	A	1989	GLU	CB-CA-C	-5.72	98.95	110.40
1	A	1797	PRO	N-CA-CB	5.72	110.16	103.30
1	A	1892	THR	C-N-CA	-5.72	107.40	121.70
1	A	1430	ASP	C-N-CA	-5.72	107.41	121.70
1	B	1892	THR	C-N-CA	-5.72	107.41	121.70
1	B	1430	ASP	C-N-CA	-5.71	107.41	121.70
2	T	62	VAL	N-CA-C	-5.71	95.58	111.00
1	A	2519	PRO	N-CA-CB	5.70	110.14	103.30
1	A	2608	SER	O-C-N	-5.70	113.59	122.70
1	B	3410	PRO	N-CA-CB	5.69	110.13	103.30
1	A	1577	ASP	C-N-CA	5.68	135.91	121.70
1	A	3410	PRO	N-CA-CB	5.68	110.12	103.30
2	S	31	LEU	C-N-CA	5.68	135.90	121.70
1	B	2608	SER	O-C-N	-5.67	113.62	122.70
1	B	2519	PRO	N-CA-CB	5.67	110.11	103.30
1	B	2654	ARG	O-C-N	5.67	131.77	122.70
1	B	1577	ASP	C-N-CA	5.67	135.87	121.70
1	B	3506	PRO	N-CA-CB	5.66	110.09	103.30
1	A	2123	LEU	O-C-N	5.65	131.74	122.70
1	A	2654	ARG	O-C-N	5.65	131.74	122.70
1	B	2123	LEU	O-C-N	5.65	131.74	122.70
2	T	2	PRO	N-CA-CB	5.65	110.08	103.30
1	A	2104	ILE	O-C-N	5.64	131.72	122.70
1	A	3506	PRO	N-CA-CB	5.64	110.06	103.30
1	B	2104	ILE	O-C-N	5.64	131.72	122.70
1	A	2523	TRP	N-CA-C	-5.63	95.81	111.00
1	B	2523	TRP	N-CA-C	-5.62	95.82	111.00
1	A	3739	ASP	N-CA-CB	-5.62	100.48	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3739	ASP	N-CA-CB	-5.62	100.49	110.60
1	B	3838	TRP	N-CA-CB	-5.61	100.50	110.60
1	A	3838	TRP	N-CA-CB	-5.61	100.50	110.60
1	B	3359	LYS	O-C-N	5.60	131.65	122.70
1	B	3714	GLN	N-CA-C	5.59	126.10	111.00
1	A	3359	LYS	O-C-N	5.59	131.65	122.70
1	A	1478	SER	N-CA-CB	-5.58	102.13	110.50
1	B	1872	LEU	N-CA-CB	5.58	121.56	110.40
1	A	1872	LEU	N-CA-CB	5.58	121.56	110.40
1	A	3714	GLN	N-CA-C	5.58	126.06	111.00
1	B	1478	SER	N-CA-CB	-5.57	102.14	110.50
1	B	2541	PRO	CA-C-N	-5.56	105.07	116.20
1	A	2619	PRO	N-CA-CB	5.56	109.97	103.30
1	A	1982	PRO	N-CA-CB	5.56	109.97	103.30
1	A	2541	PRO	CA-C-N	-5.55	105.11	116.20
1	B	1982	PRO	N-CA-CB	5.54	109.95	103.30
1	B	2619	PRO	N-CA-CB	5.54	109.95	103.30
1	A	1944	SER	N-CA-C	-5.52	96.10	111.00
1	A	2447	LYS	C-N-CA	5.51	135.48	121.70
1	B	1944	SER	N-CA-C	-5.51	96.13	111.00
1	B	3478	THR	N-CA-CB	5.50	120.75	110.30
1	A	3478	THR	N-CA-CB	5.50	120.74	110.30
1	B	2447	LYS	C-N-CA	5.50	135.44	121.70
1	B	1825	SER	O-C-N	5.50	131.49	122.70
1	A	3504	ASP	CA-C-N	-5.49	105.13	117.20
1	A	1478	SER	N-CA-C	-5.48	96.21	111.00
1	A	1825	SER	O-C-N	5.47	131.46	122.70
1	B	3500	ASP	CA-C-N	-5.47	101.77	117.10
1	B	1478	SER	N-CA-C	-5.47	96.23	111.00
1	B	3504	ASP	CA-C-N	-5.47	105.16	117.20
1	A	2689	ILE	N-CA-CB	-5.47	98.22	110.80
1	B	2689	ILE	N-CA-CB	-5.47	98.22	110.80
1	A	3500	ASP	CA-C-N	-5.46	101.81	117.10
1	B	1892	THR	O-C-N	5.46	131.44	122.70
1	A	1985	SER	C-N-CA	-5.46	108.05	121.70
1	B	1985	SER	C-N-CA	-5.46	108.06	121.70
1	A	1634	THR	C-N-CA	-5.45	108.08	121.70
1	A	2447	LYS	N-CA-C	-5.44	96.31	111.00
1	A	1892	THR	O-C-N	5.44	131.40	122.70
1	A	1941	ASP	N-CA-C	5.44	125.68	111.00
1	B	1634	THR	C-N-CA	-5.43	108.11	121.70
1	B	2447	LYS	N-CA-C	-5.43	96.32	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1632	ASP	N-CA-C	5.43	125.67	111.00
1	A	1632	ASP	N-CA-C	5.43	125.65	111.00
1	A	2633	ILE	C-N-CA	5.43	135.27	121.70
1	B	1890	PRO	N-CA-CB	5.43	109.81	103.30
1	B	1941	ASP	N-CA-C	5.42	125.65	111.00
1	B	2007	GLY	N-CA-C	-5.42	99.54	113.10
2	T	55	PRO	N-CA-CB	5.42	109.80	103.30
1	A	2007	GLY	N-CA-C	-5.42	99.56	113.10
1	A	1890	PRO	N-CA-CB	5.42	109.80	103.30
1	B	2633	ILE	C-N-CA	5.41	135.23	121.70
1	A	1873	GLN	N-CA-CB	5.41	120.34	110.60
1	A	2407	LEU	O-C-N	-5.41	114.05	122.70
1	B	2938	MET	N-CA-CB	5.40	120.33	110.60
1	A	2938	MET	N-CA-CB	5.40	120.33	110.60
1	A	2117	SER	CA-C-N	-5.40	105.33	117.20
1	B	2117	SER	CA-C-N	-5.40	105.33	117.20
1	B	1873	GLN	N-CA-CB	5.39	120.31	110.60
1	B	2407	LEU	O-C-N	-5.39	114.08	122.70
1	A	1632	ASP	CB-CA-C	-5.39	99.62	110.40
1	B	1632	ASP	CB-CA-C	-5.39	99.62	110.40
1	B	2431	ALA	C-N-CA	-5.38	108.24	121.70
1	B	1873	GLN	CA-C-O	-5.38	108.80	120.10
1	A	2431	ALA	C-N-CA	-5.37	108.27	121.70
1	A	2640	THR	O-C-N	-5.37	114.11	122.70
1	B	2751	GLN	N-CA-C	5.37	125.48	111.00
1	A	1873	GLN	CA-C-O	-5.36	108.84	120.10
1	A	2897	ASN	N-CA-CB	-5.35	100.96	110.60
1	B	2459	HIS	O-C-N	-5.34	114.15	122.70
1	A	2751	GLN	N-CA-C	5.34	125.43	111.00
1	A	2459	HIS	O-C-N	-5.34	114.16	122.70
1	B	2640	THR	O-C-N	-5.34	114.16	122.70
1	B	3685	GLN	N-CA-C	5.33	125.38	111.00
1	B	3713	GLU	CB-CA-C	-5.33	99.75	110.40
1	B	2872	GLU	O-C-N	-5.32	114.19	122.70
1	A	4004	LEU	O-C-N	5.32	131.21	122.70
1	B	2897	ASN	N-CA-CB	-5.32	101.03	110.60
1	A	2420	PRO	N-CA-CB	5.32	109.68	103.30
1	A	3401	GLN	N-CA-C	5.32	125.35	111.00
1	A	3685	GLN	N-CA-C	5.32	125.35	111.00
1	A	2757	MET	C-N-CA	5.31	134.99	121.70
1	A	1791	GLY	O-C-N	5.31	132.23	123.20
1	A	3655	ARG	N-CA-C	5.31	125.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3713	GLU	CB-CA-C	-5.31	99.78	110.40
1	B	2420	PRO	N-CA-CB	5.31	109.67	103.30
1	A	2872	GLU	O-C-N	-5.31	114.21	122.70
1	B	4004	LEU	O-C-N	5.31	131.19	122.70
1	B	2607	TYR	O-C-N	-5.31	114.21	122.70
1	B	1791	GLY	O-C-N	5.31	132.22	123.20
1	B	3655	ARG	N-CA-C	5.30	125.32	111.00
1	B	3401	GLN	N-CA-C	5.30	125.32	111.00
1	A	3356	PHE	O-C-N	-5.30	114.22	122.70
1	B	2757	MET	C-N-CA	5.30	134.95	121.70
1	B	3356	PHE	O-C-N	-5.29	114.23	122.70
1	A	2607	TYR	O-C-N	-5.29	114.24	122.70
1	A	2527	GLU	CA-C-N	5.29	128.83	117.20
1	A	1802	LYS	C-N-CA	5.28	134.91	121.70
1	B	1802	LYS	C-N-CA	5.28	134.91	121.70
1	B	2527	GLU	CA-C-N	5.28	128.82	117.20
1	A	2347	GLY	N-CA-C	5.27	126.28	113.10
1	B	2347	GLY	N-CA-C	5.27	126.28	113.10
1	B	2372	CYS	CA-C-N	-5.27	105.61	117.20
1	A	4005	GLU	CA-C-N	-5.27	105.61	117.20
1	A	2372	CYS	CA-C-N	-5.26	105.64	117.20
1	B	4005	GLU	CA-C-N	-5.26	105.64	117.20
1	A	1816	VAL	O-C-N	-5.25	114.30	122.70
1	A	2191	ARG	N-CA-C	5.25	125.17	111.00
1	B	1917	ARG	CA-C-N	5.25	128.75	117.20
1	A	1791	GLY	C-N-CA	-5.25	111.28	122.30
1	A	1917	ARG	CA-C-N	5.25	128.74	117.20
1	B	1816	VAL	O-C-N	-5.25	114.31	122.70
1	B	2191	ARG	N-CA-C	5.25	125.17	111.00
1	B	3740	THR	N-CA-C	5.24	125.15	111.00
1	B	1791	GLY	C-N-CA	-5.24	111.30	122.30
1	A	3740	THR	N-CA-C	5.23	125.12	111.00
1	A	3754	LYS	C-N-CA	-5.22	108.65	121.70
1	A	4003	ASP	CA-C-N	-5.22	105.72	117.20
1	B	3754	LYS	C-N-CA	-5.21	108.68	121.70
1	B	4003	ASP	CA-C-N	-5.21	105.74	117.20
1	A	2195	GLU	C-N-CA	-5.21	108.68	121.70
1	B	2195	GLU	C-N-CA	-5.20	108.71	121.70
1	B	1957	SER	O-C-N	5.17	130.97	122.70
1	B	2638	ARG	CA-C-N	5.16	128.55	117.20
1	A	1989	GLU	CA-C-N	5.16	126.51	116.20
1	B	2607	TYR	C-N-CA	5.16	134.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1957	SER	O-C-N	5.15	130.95	122.70
1	B	1989	GLU	CA-C-N	5.15	126.50	116.20
1	A	2607	TYR	C-N-CA	5.15	134.57	121.70
1	A	2638	ARG	CA-C-N	5.14	128.50	117.20
1	B	1872	LEU	CB-CA-C	-5.13	100.46	110.20
1	A	3405	PRO	CA-C-N	5.12	128.48	117.20
1	B	2760	GLY	C-N-CA	5.12	134.51	121.70
1	A	1635	ASP	C-N-CA	-5.12	108.90	121.70
1	B	3755	SER	C-N-CA	5.12	134.49	121.70
1	A	2760	GLY	C-N-CA	5.12	134.49	121.70
1	B	3405	PRO	CA-C-N	5.12	128.46	117.20
1	A	1872	LEU	CB-CA-C	-5.11	100.49	110.20
1	B	1635	ASP	C-N-CA	-5.11	108.92	121.70
1	A	3755	SER	C-N-CA	5.11	134.47	121.70
1	B	1942	SER	CA-C-N	-5.10	105.97	117.20
1	A	1942	SER	CA-C-N	-5.10	105.98	117.20
1	B	2654	ARG	CA-C-N	-5.09	105.99	117.20
1	A	3359	LYS	CA-C-N	-5.08	106.01	117.20
1	A	2654	ARG	CA-C-N	-5.08	106.02	117.20
1	A	2551	THR	C-N-CA	5.08	134.40	121.70
1	B	2551	THR	C-N-CA	5.07	134.38	121.70
1	B	3359	LYS	CA-C-N	-5.07	106.04	117.20
1	A	2302	PHE	CA-C-N	5.07	128.35	117.20
1	A	3686	PHE	O-C-N	-5.07	114.59	122.70
1	B	2302	PHE	CA-C-N	5.07	128.35	117.20
1	A	2101	VAL	CA-C-N	5.07	128.34	117.20
1	B	3686	PHE	O-C-N	-5.06	114.60	122.70
1	B	2101	VAL	CA-C-N	5.06	128.33	117.20
1	A	3859	VAL	N-CA-C	5.04	124.61	111.00
1	A	2255	ASP	N-CA-C	5.03	124.58	111.00
1	B	2255	ASP	N-CA-C	5.03	124.58	111.00
1	B	3859	VAL	N-CA-C	5.03	124.57	111.00
1	A	3989	ILE	O-C-N	5.02	130.73	122.70
1	B	3989	ILE	O-C-N	5.01	130.72	122.70
1	B	1430	ASP	CA-C-N	-5.01	106.18	117.20

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1888	LEU	CA
1	A	2375	ILE	CA
1	A	3641	PHE	CA

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Mol	Chain	Res	Type	Atom
1	B	1888	LEU	CA
1	B	2375	ILE	CA
1	B	3641	PHE	CA

All (275) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1381	ALA	Mainchain
1	A	1430	ASP	Mainchain
1	A	1479	LEU	Mainchain
1	A	1494	ASP	Mainchain,Peptide
1	A	1530	GLN	Peptide
1	A	1531	ARG	Peptide
1	A	1632	ASP	Mainchain
1	A	1633	GLY	Mainchain,Peptide
1	A	1800	THR	Mainchain
1	A	1803	THR	Mainchain
1	A	1813	LEU	Mainchain
1	A	1816	VAL	Mainchain
1	A	1820	PHE	Mainchain
1	A	1825	SER	Peptide
1	A	1827	ASP	Mainchain,Peptide
1	A	1849	GLU	Peptide
1	A	1887	PRO	Mainchain
1	A	1888	LEU	Peptide
1	A	1892	THR	Mainchain
1	A	1917	ARG	Peptide
1	A	1921	MET	Mainchain
1	A	1942	SER	Mainchain
1	A	1961	SER	Mainchain,Peptide
1	A	1962	SER	Peptide
1	A	1969	GLY	Mainchain
1	A	1984	ILE	Mainchain
1	A	1989	GLU	Peptide
1	A	2002	ILE	Mainchain,Peptide
1	A	2005	SER	Peptide
1	A	2006	LEU	Peptide
1	A	2018	LEU	Mainchain,Peptide
1	A	2065	LYS	Mainchain
1	A	2101	VAL	Mainchain,Peptide
1	A	2103	VAL	Peptide
1	A	2126	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	2130	PHE	Mainchain
1	A	2148	SER	Mainchain
1	A	2160	PRO	Mainchain
1	A	2161	GLU	Mainchain,Peptide
1	A	2186	ILE	Mainchain
1	A	2196	THR	Mainchain
1	A	2198	ASN	Mainchain
1	A	2207	ILE	Mainchain,Peptide
1	A	2209	ARG	Mainchain
1	A	2279	ARG	Mainchain
1	A	2345	TYR	Peptide
1	A	2372	CYS	Peptide
1	A	2375	ILE	Peptide
1	A	2393	PRO	Mainchain,Peptide
1	A	2394	THR	Peptide
1	A	2432	LEU	Mainchain
1	A	2435	SER	Mainchain
1	A	2436	SER	Mainchain
1	A	2447	LYS	Mainchain,Peptide
1	A	2523	TRP	Mainchain
1	A	2527	GLU	Mainchain
1	A	2555	ALA	Mainchain
1	A	2561	TYR	Mainchain
1	A	2578	ILE	Mainchain
1	A	2608	SER	Mainchain
1	A	2616	LEU	Mainchain,Peptide
1	A	2617	PHE	Mainchain
1	A	2633	ILE	Mainchain
1	A	2638	ARG	Mainchain
1	A	2655	ILE	Mainchain,Peptide
1	A	2656	PHE	Mainchain,Peptide
1	A	2690	SER	Mainchain
1	A	2708	ASN	Peptide
1	A	2731	PRO	Mainchain
1	A	2843	LEU	Mainchain
1	A	2872	GLU	Mainchain
1	A	2882	ALA	Mainchain
1	A	2936	VAL	Mainchain
1	A	2937	PRO	Mainchain,Peptide
1	A	2938	MET	Mainchain
1	A	2960	THR	Mainchain
1	A	2961	ILE	Mainchain

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Mol	Chain	Res	Type	Group
1	A	3335	GLY	Mainchain
1	A	3356	PHE	Mainchain,Peptide
1	A	3359	LYS	Peptide
1	A	3381	GLU	Mainchain
1	A	3382	CYS	Mainchain
1	A	3400	SER	Mainchain
1	A	3405	PRO	Mainchain,Peptide
1	A	3410	PRO	Peptide
1	A	3420	ASN	Mainchain
1	A	3425	LYS	Mainchain
1	A	3426	THR	Mainchain
1	A	3434	GLU	Mainchain,Peptide
1	A	3435	GLY	Mainchain
1	A	3500	ASP	Mainchain,Peptide
1	A	3565	ARG	Mainchain
1	A	3641	PHE	Peptide
1	A	3642	TYR	Mainchain
1	A	3655	ARG	Mainchain
1	A	3683	TYR	Mainchain
1	A	3684	CYS	Peptide
1	A	3685	GLN	Mainchain,Peptide
1	A	3686	PHE	Mainchain
1	A	3710	ILE	Mainchain,Peptide
1	A	3739	ASP	Mainchain
1	A	3740	THR	Peptide
1	A	3862	THR	Mainchain
1	A	3863	LYS	Mainchain
1	A	3866	GLU	Peptide
1	A	3900	ILE	Peptide
1	A	3917	THR	Peptide
1	A	3923	VAL	Mainchain
1	A	3998	ILE	Mainchain,Peptide
1	A	3999	ASP	Peptide
1	A	4034	LEU	Mainchain
1	A	4035	GLN	Mainchain
1	A	4047	ALA	Mainchain,Peptide
1	B	1381	ALA	Mainchain
1	B	1430	ASP	Mainchain
1	B	1479	LEU	Mainchain
1	B	1494	ASP	Mainchain,Peptide
1	B	1530	GLN	Peptide
1	B	1531	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	1632	ASP	Mainchain
1	B	1633	GLY	Mainchain,Peptide
1	B	1800	THR	Mainchain
1	B	1803	THR	Mainchain
1	B	1813	LEU	Mainchain
1	B	1816	VAL	Mainchain
1	B	1820	PHE	Mainchain
1	B	1825	SER	Peptide
1	B	1827	ASP	Mainchain,Peptide
1	B	1849	GLU	Peptide
1	B	1887	PRO	Mainchain
1	B	1888	LEU	Peptide
1	B	1892	THR	Mainchain
1	B	1917	ARG	Peptide
1	B	1921	MET	Mainchain
1	B	1942	SER	Mainchain
1	B	1961	SER	Mainchain,Peptide
1	B	1962	SER	Peptide
1	B	1969	GLY	Mainchain
1	B	1984	ILE	Mainchain
1	B	1989	GLU	Peptide
1	B	2002	ILE	Mainchain,Peptide
1	B	2005	SER	Peptide
1	B	2006	LEU	Peptide
1	B	2018	LEU	Mainchain,Peptide
1	B	2065	LYS	Mainchain
1	B	2101	VAL	Mainchain,Peptide
1	B	2103	VAL	Peptide
1	B	2126	ARG	Peptide
1	B	2130	PHE	Mainchain
1	B	2148	SER	Mainchain
1	B	2160	PRO	Mainchain
1	B	2161	GLU	Mainchain,Peptide
1	B	2186	ILE	Mainchain
1	B	2196	THR	Mainchain
1	B	2198	ASN	Mainchain
1	B	2207	ILE	Mainchain,Peptide
1	B	2209	ARG	Mainchain
1	B	2279	ARG	Mainchain
1	B	2345	TYR	Peptide
1	B	2372	CYS	Peptide
1	B	2375	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	2393	PRO	Mainchain,Peptide
1	B	2394	THR	Peptide
1	B	2432	LEU	Mainchain
1	B	2435	SER	Mainchain
1	B	2436	SER	Mainchain
1	B	2447	LYS	Mainchain,Peptide
1	B	2523	TRP	Mainchain
1	B	2527	GLU	Mainchain
1	B	2555	ALA	Mainchain
1	B	2561	TYR	Mainchain
1	B	2578	ILE	Mainchain
1	B	2608	SER	Mainchain
1	B	2616	LEU	Mainchain,Peptide
1	B	2617	PHE	Mainchain
1	B	2633	ILE	Mainchain
1	B	2638	ARG	Mainchain
1	B	2655	ILE	Mainchain,Peptide
1	B	2656	PHE	Mainchain,Peptide
1	B	2690	SER	Mainchain
1	B	2708	ASN	Peptide
1	B	2731	PRO	Mainchain
1	B	2843	LEU	Mainchain
1	B	2872	GLU	Mainchain
1	B	2882	ALA	Mainchain
1	B	2936	VAL	Mainchain
1	B	2937	PRO	Mainchain,Peptide
1	B	2938	MET	Mainchain
1	B	2960	THR	Mainchain
1	B	2961	ILE	Mainchain
1	B	3335	GLY	Mainchain
1	B	3356	PHE	Mainchain,Peptide
1	B	3359	LYS	Peptide
1	B	3381	GLU	Mainchain
1	B	3382	CYS	Mainchain
1	B	3400	SER	Mainchain
1	B	3405	PRO	Mainchain,Peptide
1	B	3410	PRO	Peptide
1	B	3420	ASN	Mainchain
1	B	3425	LYS	Mainchain
1	B	3426	THR	Mainchain
1	B	3434	GLU	Mainchain,Peptide
1	B	3435	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	B	3500	ASP	Mainchain,Peptide
1	B	3565	ARG	Mainchain
1	B	3641	PHE	Peptide
1	B	3642	TYR	Mainchain
1	B	3655	ARG	Mainchain
1	B	3683	TYR	Mainchain
1	B	3684	CYS	Peptide
1	B	3685	GLN	Mainchain,Peptide
1	B	3686	PHE	Mainchain
1	B	3710	ILE	Mainchain,Peptide
1	B	3739	ASP	Mainchain
1	B	3740	THR	Peptide
1	B	3862	THR	Mainchain
1	B	3863	LYS	Mainchain
1	B	3866	GLU	Peptide
1	B	3900	ILE	Peptide
1	B	3917	THR	Peptide
1	B	3923	VAL	Mainchain
1	B	3998	ILE	Mainchain,Peptide
1	B	3999	ASP	Peptide
1	B	4034	LEU	Mainchain
1	B	4035	GLN	Mainchain
1	B	4047	ALA	Mainchain,Peptide
2	S	31	LEU	Peptide
2	S	32	TYR	Mainchain,Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10585	0	4454	1006	3
1	B	10586	0	4455	994	3
2	S	1065	0	464	9	0
2	T	1066	0	465	22	0
All	All	23302	0	9838	2013	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

All (2013) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:GLU:CA	2:T:216:PRO:HA	1.19	1.65
1:A:1932:MET:CB	1:A:1946:ALA:HB1	1.24	1.64
1:B:2060:PHE:CB	1:B:2087:VAL:CB	1.78	1.62
1:A:2060:PHE:CB	1:A:2087:VAL:CB	1.78	1.57
1:A:3666:ALA:HB2	1:A:3668:ARG:CB	1.32	1.57
1:B:3666:ALA:HB2	1:B:3668:ARG:CB	1.32	1.57
1:B:1932:MET:CB	1:B:1946:ALA:HB1	1.24	1.56
1:B:3666:ALA:CA	1:B:3668:ARG:H	1.08	1.55
1:A:3666:ALA:CA	1:A:3668:ARG:H	1.08	1.54
1:B:2002:ILE:HA	1:B:2003:LEU:CB	1.19	1.49
1:B:1634:THR:HA	1:B:1635:ASP:CB	1.22	1.46
1:B:1941:ASP:C	1:B:1942:SER:N	1.68	1.46
1:A:2774:ALA:C	1:A:2775:TRP:N	1.68	1.46
1:B:2441:VAL:CB	1:B:2442:GLY:N	1.80	1.44
1:B:3886:ALA:O	1:B:3890:GLN:CA	1.66	1.44
1:A:2512:LYS:CB	1:A:2523:TRP:CB	1.94	1.44
1:B:2774:ALA:C	1:B:2775:TRP:N	1.68	1.43
1:B:2512:LYS:CB	1:B:2523:TRP:CB	1.94	1.43
1:B:1986:GLU:C	1:B:1987:PHE:N	1.72	1.43
1:A:2301:TRP:C	1:A:2302:PHE:N	1.72	1.43
1:A:2441:VAL:CB	1:A:2442:GLY:N	1.80	1.43
1:B:3666:ALA:HA	1:B:3668:ARG:N	1.34	1.42
1:A:1844:TRP:C	1:A:1845:GLY:N	1.69	1.42
1:A:1941:ASP:C	1:A:1942:SER:N	1.68	1.42
1:A:3666:ALA:HA	1:A:3668:ARG:N	1.34	1.42
1:B:1844:TRP:C	1:B:1845:GLY:N	1.69	1.42
1:A:1634:THR:HA	1:A:1635:ASP:CB	1.22	1.41
1:B:1932:MET:CB	1:B:1946:ALA:CB	1.99	1.41
1:A:2118:MET:N	1:A:2129:LEU:CB	1.83	1.41
1:B:2118:MET:N	1:B:2129:LEU:CB	1.83	1.41
1:A:2002:ILE:HA	1:A:2003:LEU:CB	1.19	1.41
1:A:4028:ARG:HA	1:A:4029:ILE:CB	1.47	1.40
1:B:2301:TRP:C	1:B:2302:PHE:N	1.72	1.40
1:A:3886:ALA:O	1:A:3890:GLN:CA	1.66	1.40
1:A:1932:MET:CB	1:A:1946:ALA:CB	1.99	1.39
1:A:1986:GLU:C	1:A:1987:PHE:N	1.72	1.39
1:B:3739:ASP:HA	1:B:3740:THR:CB	1.31	1.38
1:A:2435:SER:CB	1:A:2479:ILE:CA	2.01	1.38
1:B:2785:LYS:O	1:B:3458:PHE:CA	1.69	1.38
1:A:1843:ALA:CB	1:A:1893:ALA:N	1.80	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2785:LYS:O	1:A:3458:PHE:CA	1.69	1.37
1:B:2435:SER:CB	1:B:2479:ILE:CA	2.01	1.37
1:B:3432:LEU:N	1:B:3455:GLY:O	1.57	1.37
1:B:1634:THR:CA	1:B:1635:ASP:CB	2.03	1.36
1:B:4028:ARG:HA	1:B:4029:ILE:CB	1.47	1.36
1:A:2435:SER:CB	1:A:2479:ILE:HA	1.56	1.36
1:A:3739:ASP:HA	1:A:3740:THR:CB	1.31	1.36
1:A:2709:LYS:C	1:A:2710:THR:N	1.79	1.36
1:A:1364:GLU:CA	2:T:216:PRO:CA	1.82	1.35
1:B:2435:SER:CB	1:B:2479:ILE:HA	1.56	1.35
1:B:3847:SER:CB	1:B:3851:VAL:CB	2.03	1.35
1:A:3432:LEU:N	1:A:3455:GLY:O	1.57	1.35
1:A:3847:SER:CB	1:A:3851:VAL:CB	2.03	1.35
1:B:1843:ALA:CB	1:B:1893:ALA:N	1.80	1.35
1:A:2369:SER:CB	1:A:2372:CYS:CB	2.03	1.34
1:B:2369:SER:CB	1:B:2372:CYS:CB	2.03	1.34
1:A:3666:ALA:CA	1:A:3668:ARG:N	1.89	1.34
1:B:2785:LYS:C	1:B:3458:PHE:HA	1.45	1.33
1:A:2785:LYS:C	1:A:3458:PHE:HA	1.45	1.33
1:B:3859:VAL:CB	1:B:3888:LEU:CB	2.07	1.33
1:A:4031:GLN:CB	1:A:4032:PRO:HA	1.50	1.33
1:A:1364:GLU:HA	2:T:216:PRO:CA	0.86	1.32
1:B:3360:TYR:C	1:B:3361:ASP:N	1.82	1.32
1:B:2105:ASP:HA	1:B:2154:PHE:O	1.23	1.32
1:B:2709:LYS:C	1:B:2710:THR:N	1.79	1.32
1:A:3356:PHE:CB	1:A:3357:ALA:HA	1.51	1.32
1:A:1843:ALA:CB	1:A:1844:TRP:HA	1.55	1.32
1:B:3356:PHE:CB	1:B:3357:ALA:HA	1.51	1.32
1:A:3859:VAL:CB	1:A:3888:LEU:CB	2.07	1.31
1:A:3360:TYR:C	1:A:3361:ASP:N	1.82	1.31
1:A:2600:TYR:CB	1:A:2613:SER:O	1.79	1.30
1:A:3754:LYS:C	1:A:3755:SER:N	1.84	1.30
1:A:3713:GLU:CB	1:A:3714:GLN:HA	1.58	1.30
1:B:1843:ALA:CB	1:B:1844:TRP:HA	1.55	1.30
1:B:3666:ALA:CA	1:B:3668:ARG:N	1.89	1.30
1:B:3713:GLU:CB	1:B:3714:GLN:HA	1.58	1.30
1:A:1634:THR:CA	1:A:1635:ASP:CB	2.03	1.30
1:A:4061:SER:O	1:A:4066:PRO:HA	1.17	1.30
1:A:1920:SER:CB	1:A:3998:ILE:C	2.01	1.29
1:B:4031:GLN:CB	1:B:4032:PRO:HA	1.51	1.29
1:B:3754:LYS:C	1:B:3755:SER:N	1.84	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1843:ALA:HB1	1:A:1844:TRP:CA	1.62	1.29
1:B:1920:SER:CB	1:B:3998:ILE:C	2.01	1.29
1:B:1843:ALA:HB1	1:B:1844:TRP:CA	1.62	1.29
1:A:1364:GLU:HA	2:T:216:PRO:C	1.48	1.28
1:B:2600:TYR:CB	1:B:2613:SER:O	1.80	1.28
1:A:1942:SER:O	1:A:1945:LEU:N	1.64	1.28
1:A:1364:GLU:CA	2:T:216:PRO:C	2.01	1.27
1:A:2786:ILE:HA	1:A:3458:PHE:C	1.36	1.27
1:A:2105:ASP:HA	1:A:2154:PHE:O	1.23	1.27
1:B:1942:SER:O	1:B:1945:LEU:N	1.64	1.27
1:B:3922:GLY:HA2	1:B:3923:VAL:CB	1.62	1.27
1:A:3500:ASP:CB	1:A:3501:PRO:HA	1.60	1.27
1:A:2006:LEU:CB	1:A:2007:GLY:HA2	1.64	1.26
1:B:4061:SER:O	1:B:4066:PRO:HA	1.17	1.26
1:A:3369:TYR:HA	1:A:3370:LEU:CB	1.49	1.26
1:B:2657:ALA:C	1:B:2914:ILE:O	1.73	1.26
1:B:3500:ASP:CB	1:B:3501:PRO:HA	1.60	1.26
1:A:1633:GLY:H	1:A:1634:THR:CA	1.43	1.25
1:A:2657:ALA:C	1:A:2914:ILE:O	1.73	1.25
1:A:3899:ASP:C	1:A:3900:ILE:N	1.89	1.25
1:B:3899:ASP:C	1:B:3900:ILE:N	1.89	1.25
1:B:1814:GLY:C	1:B:1815:ARG:CB	2.04	1.25
1:A:1466:GLN:CB	1:A:1469:LEU:H	1.49	1.25
1:A:1814:GLY:C	1:A:1815:ARG:CB	2.04	1.25
1:B:2873:LEU:O	1:B:2875:ASP:N	1.69	1.24
1:A:2873:LEU:O	1:A:2875:ASP:N	1.69	1.24
1:B:2006:LEU:CB	1:B:2007:GLY:HA2	1.64	1.24
1:A:1633:GLY:N	1:A:1635:ASP:CB	2.00	1.24
1:B:3369:TYR:HA	1:B:3370:LEU:CB	1.49	1.23
1:B:1869:GLN:O	1:B:1873:GLN:CB	1.87	1.23
1:B:2306:ASP:CB	1:B:2311:LYS:H	1.52	1.23
1:A:1869:GLN:O	1:A:1873:GLN:CB	1.87	1.23
1:B:1633:GLY:H	1:B:1634:THR:CA	1.43	1.23
1:B:1633:GLY:N	1:B:1635:ASP:CB	2.00	1.22
1:B:3886:ALA:O	1:B:3890:GLN:C	1.77	1.22
1:A:3406:PHE:CB	1:A:3514:ARG:O	1.88	1.22
1:B:1466:GLN:CB	1:B:1469:LEU:H	1.49	1.22
1:A:2306:ASP:CB	1:A:2311:LYS:H	1.52	1.22
1:B:3861:GLU:O	1:B:3863:LYS:N	1.73	1.22
1:B:3406:PHE:CB	1:B:3514:ARG:O	1.88	1.22
1:A:3666:ALA:CB	1:A:3668:ARG:CB	2.18	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2002:ILE:CA	1:A:2003:LEU:CB	2.16	1.21
1:A:3995:GLY:O	1:A:3997:LYS:N	1.74	1.21
1:A:3421:TYR:CB	1:A:3422:TYR:HA	1.70	1.21
1:A:4013:HIS:O	1:A:4016:CYS:HA	1.06	1.21
1:B:2002:ILE:CA	1:B:2003:LEU:CB	2.16	1.21
1:B:3886:ALA:O	1:B:3890:GLN:O	1.58	1.21
1:B:3666:ALA:CB	1:B:3668:ARG:N	2.04	1.21
1:A:2153:VAL:O	1:A:2195:GLU:CB	1.89	1.21
1:B:3421:TYR:CB	1:B:3422:TYR:HA	1.70	1.21
1:B:2206:THR:O	1:B:2209:ARG:O	1.54	1.21
1:B:1984:ILE:CB	1:B:1985:SER:HA	1.63	1.20
1:A:2206:THR:O	1:A:2209:ARG:O	1.54	1.20
1:A:3886:ALA:O	1:A:3890:GLN:C	1.77	1.20
1:B:4013:HIS:O	1:B:4016:CYS:HA	1.06	1.20
1:B:3666:ALA:CB	1:B:3668:ARG:CB	2.18	1.20
1:B:2153:VAL:O	1:B:2195:GLU:CB	1.89	1.20
1:B:3995:GLY:O	1:B:3997:LYS:N	1.74	1.20
1:A:3666:ALA:CB	1:A:3668:ARG:N	2.04	1.19
1:A:3861:GLU:O	1:A:3863:LYS:N	1.73	1.19
1:A:3886:ALA:O	1:A:3890:GLN:O	1.58	1.19
1:B:3807:SER:HA	1:B:3809:GLU:N	1.58	1.19
1:A:3922:GLY:HA2	1:A:3923:VAL:CB	1.62	1.18
1:B:2785:LYS:O	1:B:3458:PHE:N	1.76	1.18
1:A:2006:LEU:CA	1:A:2008:ASP:H	1.55	1.18
1:A:2411:LYS:CB	1:A:2554:ALA:HB3	1.72	1.18
1:A:1447:GLU:HA	1:A:1449:GLN:N	1.57	1.18
1:B:2153:VAL:O	1:B:2195:GLU:CA	1.91	1.18
1:B:2006:LEU:CA	1:B:2008:ASP:H	1.55	1.18
1:B:2411:LYS:CB	1:B:2554:ALA:HB3	1.72	1.18
1:B:1447:GLU:HA	1:B:1449:GLN:N	1.57	1.18
1:A:2785:LYS:O	1:A:3458:PHE:N	1.76	1.18
1:A:3336:HIS:N	1:A:3337:LEU:HA	1.44	1.18
1:A:2092:ALA:HB1	1:A:2097:HIS:CA	1.72	1.17
1:A:3807:SER:HA	1:A:3809:GLU:N	1.58	1.17
1:B:2092:ALA:HB1	1:B:2097:HIS:CA	1.72	1.17
1:A:2153:VAL:O	1:A:2195:GLU:CA	1.91	1.16
1:A:1842:GLY:HA2	1:A:1891:HIS:HA	1.23	1.16
1:B:2114:LEU:HA	1:B:2119:LEU:N	1.53	1.16
1:A:1941:ASP:CB	1:A:1942:SER:HA	1.76	1.16
1:A:1985:SER:C	1:A:1987:PHE:CB	2.14	1.16
1:B:4013:HIS:O	1:B:4016:CYS:CA	1.94	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2366:LEU:CB	1:B:2367:SER:HA	1.76	1.16
1:A:3666:ALA:CB	1:A:3668:ARG:H	1.57	1.15
1:B:3666:ALA:HB1	1:B:3669:THR:H	1.00	1.15
1:B:1985:SER:C	1:B:1987:PHE:CB	2.14	1.15
1:A:2114:LEU:HA	1:A:2119:LEU:N	1.53	1.15
1:A:4031:GLN:CB	1:A:4032:PRO:CA	2.24	1.15
1:A:2328:GLY:CA	1:A:2329:ASP:CB	2.25	1.15
1:B:3666:ALA:HB1	1:B:3669:THR:N	1.59	1.14
1:B:2328:GLY:HA2	1:B:2329:ASP:CB	1.76	1.14
1:B:1941:ASP:CB	1:B:1942:SER:HA	1.76	1.14
1:B:3500:ASP:CB	1:B:3501:PRO:CA	2.21	1.14
1:B:1493:LEU:O	1:B:1495:THR:N	1.79	1.14
1:A:3665:ARG:O	1:A:3667:ALA:HB3	1.48	1.14
1:B:3356:PHE:CB	1:B:3358:VAL:HA	1.78	1.14
1:A:4013:HIS:O	1:A:4016:CYS:CA	1.94	1.14
1:A:3666:ALA:HB1	1:A:3669:THR:N	1.59	1.14
1:A:3356:PHE:CB	1:A:3358:VAL:HA	1.78	1.14
1:B:4031:GLN:CB	1:B:4032:PRO:CA	2.24	1.14
1:B:3666:ALA:CB	1:B:3668:ARG:H	1.57	1.13
1:B:2006:LEU:CB	1:B:2007:GLY:CA	2.26	1.13
1:A:3890:GLN:H	1:A:3891:ARG:CA	1.62	1.13
1:B:3430:SER:CB	1:B:3454:ASP:CB	2.26	1.13
1:A:2786:ILE:HA	1:A:3458:PHE:O	1.45	1.13
1:A:3500:ASP:CB	1:A:3501:PRO:CA	2.21	1.13
1:A:2107:LYS:O	1:A:2504:LEU:N	1.81	1.13
1:A:1493:LEU:O	1:A:1495:THR:N	1.79	1.13
1:A:2092:ALA:CB	1:A:2098:ALA:H	1.62	1.13
1:A:3886:ALA:O	1:A:3890:GLN:HA	1.33	1.12
1:A:3430:SER:CB	1:A:3454:ASP:CB	2.26	1.12
1:A:3845:GLN:CB	1:A:3880:THR:CB	2.28	1.12
1:A:2006:LEU:CB	1:A:2007:GLY:CA	2.26	1.12
1:B:3665:ARG:O	1:B:3667:ALA:HB3	1.48	1.12
1:A:3739:ASP:CA	1:A:3740:THR:CB	2.27	1.12
1:A:1984:ILE:CB	1:A:1985:SER:HA	1.63	1.12
1:A:4035:GLN:HA	1:A:4036:GLN:CB	1.78	1.12
1:A:3807:SER:HA	1:A:3808:LYS:C	1.69	1.12
1:B:2092:ALA:CB	1:B:2098:ALA:H	1.62	1.12
1:B:1842:GLY:HA2	1:B:1891:HIS:HA	1.23	1.12
1:B:3739:ASP:CA	1:B:3740:THR:CB	2.27	1.11
1:B:4035:GLN:HA	1:B:4036:GLN:CB	1.78	1.11
1:A:2366:LEU:CB	1:A:2367:SER:HA	1.76	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2786:ILE:HA	1:B:3458:PHE:O	1.45	1.11
1:B:3430:SER:HA	1:B:3454:ASP:CB	1.80	1.11
1:A:3430:SER:HA	1:A:3454:ASP:CB	1.80	1.11
1:B:3886:ALA:O	1:B:3890:GLN:HA	1.33	1.11
1:A:2435:SER:CB	1:A:2479:ILE:N	2.13	1.11
1:B:2328:GLY:CA	1:B:2329:ASP:CB	2.25	1.11
1:B:1497:ILE:O	1:B:1499:VAL:N	1.83	1.11
1:B:2160:PRO:O	1:B:2162:TYR:N	1.83	1.11
1:A:4032:PRO:N	1:A:4033:LEU:HA	1.61	1.11
1:A:2600:TYR:CB	1:A:2613:SER:C	2.19	1.11
1:B:2600:TYR:CB	1:B:2613:SER:C	2.19	1.11
1:B:2107:LYS:O	1:B:2504:LEU:N	1.81	1.11
1:B:3890:GLN:H	1:B:3891:ARG:CA	1.62	1.10
1:A:2378:VAL:CB	1:A:2379:SER:CB	2.29	1.10
1:A:2371:PHE:H	1:A:2372:CYS:CB	1.63	1.10
1:B:2371:PHE:H	1:B:2372:CYS:CB	1.64	1.10
1:B:2092:ALA:CB	1:B:2097:HIS:HA	1.81	1.10
1:A:1497:ILE:O	1:A:1499:VAL:N	1.83	1.10
1:B:3336:HIS:N	1:B:3337:LEU:HA	1.44	1.10
1:A:2118:MET:H	1:A:2129:LEU:CB	1.54	1.10
1:A:2092:ALA:CB	1:A:2097:HIS:HA	1.82	1.10
1:A:2160:PRO:O	1:A:2162:TYR:N	1.83	1.10
1:B:2435:SER:CB	1:B:2479:ILE:N	2.13	1.10
1:B:3845:GLN:CB	1:B:3880:THR:CB	2.28	1.10
1:B:2378:VAL:CB	1:B:2379:SER:CB	2.30	1.10
1:A:4028:ARG:CA	1:A:4029:ILE:CB	2.30	1.10
1:B:4028:ARG:CA	1:B:4029:ILE:CB	2.30	1.10
1:B:3453:GLN:CB	1:B:3454:ASP:CB	2.30	1.10
1:A:3453:GLN:CB	1:A:3454:ASP:CB	2.30	1.10
1:B:1447:GLU:HA	1:B:1449:GLN:H	0.95	1.09
1:A:2328:GLY:HA2	1:A:2329:ASP:CB	1.76	1.09
1:B:3878:HIS:CB	1:B:3879:LEU:O	2.00	1.09
1:B:2785:LYS:O	1:B:3458:PHE:CB	2.00	1.09
1:A:2006:LEU:HA	1:A:2008:ASP:H	0.95	1.09
1:B:3421:TYR:CB	1:B:3422:TYR:CA	2.29	1.09
1:A:3878:HIS:CB	1:A:3879:LEU:O	2.00	1.09
1:A:3666:ALA:HB1	1:A:3669:THR:H	1.00	1.09
1:A:2785:LYS:O	1:A:3458:PHE:CB	2.00	1.09
1:A:3369:TYR:CA	1:A:3370:LEU:CB	2.30	1.09
1:A:3404:VAL:O	1:A:3495:PHE:HA	1.53	1.08
1:B:3890:GLN:H	1:B:3891:ARG:C	1.57	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2118:MET:H	1:B:2129:LEU:CB	1.54	1.08
1:A:1447:GLU:CA	1:A:1449:GLN:H	1.65	1.08
1:B:1447:GLU:CA	1:B:1449:GLN:H	1.65	1.08
1:A:1791:GLY:O	1:A:1915:SER:O	1.71	1.08
1:A:1550:GLY:HA2	1:A:1551:SER:C	1.71	1.08
1:B:1791:GLY:O	1:B:1915:SER:O	1.71	1.08
1:A:3998:ILE:O	1:A:3999:ASP:CB	1.94	1.08
1:B:2578:ILE:O	1:B:2580:LYS:N	1.85	1.08
1:A:3421:TYR:CB	1:A:3422:TYR:CA	2.29	1.08
1:A:2578:ILE:O	1:A:2580:LYS:N	1.85	1.08
1:B:2786:ILE:HA	1:B:3458:PHE:C	1.36	1.07
1:A:1447:GLU:HA	1:A:1449:GLN:H	0.95	1.07
1:B:4032:PRO:N	1:B:4033:LEU:HA	1.61	1.07
1:B:3431:PHE:C	1:B:3455:GLY:O	1.87	1.07
1:A:3713:GLU:CB	1:A:3714:GLN:CA	2.32	1.07
1:A:3878:HIS:CB	1:A:3879:LEU:C	2.23	1.07
1:B:3404:VAL:O	1:B:3495:PHE:HA	1.53	1.07
1:B:2435:SER:CA	1:B:2479:ILE:HA	1.85	1.07
1:B:2708:ASN:CB	1:B:2709:LYS:HA	1.84	1.07
1:B:1550:GLY:HA2	1:B:1551:SER:C	1.71	1.07
1:A:2435:SER:N	1:A:2479:ILE:HA	1.68	1.07
1:B:3878:HIS:CB	1:B:3879:LEU:C	2.23	1.07
1:A:1633:GLY:CA	1:A:1635:ASP:CB	2.31	1.06
1:A:1633:GLY:H	1:A:1634:THR:CB	1.67	1.06
1:A:2435:SER:CA	1:A:2479:ILE:HA	1.85	1.06
1:B:1633:GLY:H	1:B:1634:THR:CB	1.67	1.06
1:B:2435:SER:N	1:B:2479:ILE:HA	1.68	1.06
1:B:3369:TYR:CA	1:B:3370:LEU:CB	2.30	1.06
1:B:3807:SER:HA	1:B:3808:LYS:C	1.69	1.06
1:B:1633:GLY:CA	1:B:1635:ASP:CB	2.31	1.06
1:A:2708:ASN:CB	1:A:2709:LYS:HA	1.84	1.06
1:B:2006:LEU:HA	1:B:2008:ASP:H	0.95	1.06
1:A:3453:GLN:O	1:A:3497:HIS:O	1.71	1.06
1:B:1844:TRP:C	1:B:1893:ALA:O	1.94	1.06
1:A:1985:SER:O	1:A:1987:PHE:CB	2.03	1.06
1:B:3998:ILE:O	1:B:3999:ASP:CB	1.94	1.06
1:B:2441:VAL:CA	1:B:2442:GLY:N	2.18	1.06
1:B:3713:GLU:CB	1:B:3714:GLN:CA	2.32	1.06
1:A:2441:VAL:CA	1:A:2442:GLY:N	2.18	1.05
1:A:3890:GLN:H	1:A:3891:ARG:C	1.57	1.05
1:B:2443:ILE:N	1:B:2485:PHE:O	1.90	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1932:MET:CB	1:B:1946:ALA:CA	2.34	1.05
1:B:1985:SER:O	1:B:1987:PHE:CB	2.03	1.05
1:B:3453:GLN:O	1:B:3497:HIS:O	1.71	1.05
1:A:1932:MET:CB	1:A:1946:ALA:CA	2.34	1.05
1:B:3408:LEU:O	1:B:3518:PHE:CB	2.05	1.05
1:B:1878:HIS:CB	1:B:1888:LEU:O	2.05	1.05
1:B:2000:ARG:O	1:B:2212:LEU:N	1.89	1.04
1:A:1844:TRP:C	1:A:1893:ALA:O	1.94	1.04
1:A:3997:LYS:O	1:A:3999:ASP:CB	2.04	1.04
1:A:2000:ARG:O	1:A:2212:LEU:N	1.89	1.04
1:B:3997:LYS:O	1:B:3999:ASP:CB	2.04	1.04
1:A:3408:LEU:O	1:A:3518:PHE:CB	2.05	1.04
1:A:1880:THR:N	1:A:1887:PRO:O	1.90	1.04
1:B:1941:ASP:CB	1:B:1942:SER:CB	2.35	1.04
1:B:1633:GLY:N	1:B:1634:THR:CA	2.13	1.04
1:A:2434:ASN:CB	1:A:2435:SER:HA	1.87	1.04
1:B:3899:ASP:CB	1:B:3900:ILE:N	2.20	1.04
1:A:4013:HIS:C	1:A:4016:CYS:HA	1.77	1.04
1:B:1941:ASP:CB	1:B:1942:SER:CA	2.35	1.04
1:B:3356:PHE:CB	1:B:3357:ALA:CA	2.35	1.04
1:A:3899:ASP:CB	1:A:3900:ILE:N	2.20	1.04
1:A:1941:ASP:CB	1:A:1942:SER:CA	2.35	1.04
1:A:3431:PHE:C	1:A:3455:GLY:O	1.87	1.04
1:A:1878:HIS:CB	1:A:1888:LEU:O	2.05	1.04
1:A:1941:ASP:CB	1:A:1942:SER:CB	2.35	1.03
1:A:2443:ILE:N	1:A:2485:PHE:O	1.90	1.03
1:A:3409:ASP:CB	1:A:3518:PHE:CB	2.36	1.03
1:A:3430:SER:CA	1:A:3454:ASP:CB	2.37	1.03
1:B:1880:THR:N	1:B:1887:PRO:O	1.90	1.03
1:B:2653:TRP:O	1:B:2656:PHE:CB	2.07	1.03
1:A:3356:PHE:CB	1:A:3357:ALA:CA	2.35	1.03
1:B:4013:HIS:C	1:B:4016:CYS:HA	1.77	1.03
1:A:2653:TRP:O	1:A:2656:PHE:CB	2.07	1.03
1:A:3666:ALA:CB	1:A:3668:ARG:CA	2.37	1.03
1:A:1814:GLY:C	1:A:1816:VAL:N	2.11	1.03
1:A:4010:LEU:O	1:A:4014:VAL:N	1.92	1.03
1:B:3430:SER:CA	1:B:3454:ASP:CB	2.37	1.03
1:A:1633:GLY:N	1:A:1634:THR:CA	2.13	1.02
1:B:1814:GLY:C	1:B:1816:VAL:N	2.11	1.02
1:A:1364:GLU:N	2:T:216:PRO:HA	1.74	1.02
1:B:3666:ALA:CB	1:B:3668:ARG:CA	2.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2434:ASN:CB	1:B:2435:SER:HA	1.87	1.02
1:A:3922:GLY:CA	1:A:3923:VAL:CB	2.37	1.02
1:B:2105:ASP:CA	1:B:2154:PHE:O	2.07	1.02
1:B:3409:ASP:CB	1:B:3518:PHE:CB	2.36	1.02
1:A:1843:ALA:HB3	1:A:1893:ALA:N	1.56	1.02
1:A:2459:HIS:O	1:A:2463:ASN:CB	2.08	1.02
1:A:2105:ASP:CA	1:A:2154:PHE:O	2.07	1.01
1:B:2006:LEU:HA	1:B:2008:ASP:N	1.75	1.01
1:B:1843:ALA:HB3	1:B:1893:ALA:N	1.56	1.01
1:B:2786:ILE:N	1:B:3458:PHE:HA	1.50	1.01
1:A:3432:LEU:CB	1:A:3457:PHE:N	2.11	1.01
1:B:3922:GLY:CA	1:B:3923:VAL:CB	2.37	1.01
1:A:2871:GLN:O	1:A:2874:TYR:CB	2.09	1.01
1:B:4010:LEU:O	1:B:4014:VAL:N	1.92	1.01
1:B:2105:ASP:C	1:B:2157:ASP:CB	2.29	1.01
1:A:4003:ASP:O	1:A:4007:VAL:N	1.94	1.00
1:B:2092:ALA:HB1	1:B:2097:HIS:HA	1.01	1.00
1:B:1839:THR:O	1:B:1891:HIS:CB	2.09	1.00
1:A:2105:ASP:C	1:A:2157:ASP:CB	2.29	1.00
1:A:2006:LEU:HA	1:A:2008:ASP:N	1.75	1.00
1:B:2871:GLN:O	1:B:2874:TYR:CB	2.09	1.00
1:B:2459:HIS:O	1:B:2463:ASN:CB	2.08	1.00
1:A:2092:ALA:HB1	1:A:2097:HIS:HA	1.01	1.00
1:B:2346:PHE:C	1:B:2348:HIS:CB	2.30	1.00
1:A:4061:SER:O	1:A:4066:PRO:CA	2.10	1.00
1:A:1839:THR:O	1:A:1891:HIS:CB	2.09	0.99
1:A:2346:PHE:C	1:A:2348:HIS:CB	2.30	0.99
1:A:3877:CYS:CB	1:A:3878:HIS:C	2.30	0.99
1:B:2006:LEU:CA	1:B:2008:ASP:N	2.25	0.99
1:B:3807:SER:CA	1:B:3809:GLU:N	2.25	0.99
1:A:1364:GLU:CB	2:T:216:PRO:C	2.31	0.99
1:B:3432:LEU:N	1:B:3455:GLY:C	2.16	0.99
1:B:1844:TRP:CA	1:B:1893:ALA:O	2.10	0.99
1:B:3336:HIS:N	1:B:3337:LEU:CA	2.25	0.99
1:B:3878:HIS:CB	1:B:3879:LEU:HA	1.93	0.99
1:A:3807:SER:CA	1:A:3809:GLU:N	2.25	0.99
1:B:2337:ALA:O	1:B:2341:THR:CB	2.11	0.99
1:B:3877:CYS:CB	1:B:3878:HIS:C	2.30	0.98
1:A:3432:LEU:N	1:A:3455:GLY:C	2.16	0.98
1:A:2092:ALA:HB2	1:A:2098:ALA:H	1.28	0.98
1:A:3336:HIS:N	1:A:3337:LEU:CA	2.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3878:HIS:CB	1:A:3879:LEU:HA	1.93	0.98
1:B:3737:THR:CB	1:B:3738:VAL:CB	2.41	0.98
1:B:3545:ARG:O	1:B:3549:ILE:CB	2.12	0.98
1:B:4003:ASP:O	1:B:4007:VAL:N	1.94	0.98
1:B:4061:SER:O	1:B:4066:PRO:CA	2.10	0.98
1:A:2337:ALA:O	1:A:2341:THR:CB	2.11	0.98
1:B:1936:ILE:HA	1:B:1942:SER:CB	1.94	0.98
1:B:2092:ALA:HB2	1:B:2098:ALA:H	1.28	0.98
1:A:1844:TRP:CA	1:A:1893:ALA:O	2.10	0.98
1:A:2615:TYR:HA	1:A:2616:LEU:CB	1.92	0.97
1:A:1936:ILE:HA	1:A:1942:SER:CB	1.94	0.97
1:A:2155:ASP:CB	1:A:2156:SER:HA	1.94	0.97
1:A:2006:LEU:CA	1:A:2008:ASP:N	2.25	0.97
1:B:2435:SER:H	1:B:2479:ILE:HA	1.25	0.97
1:B:2615:TYR:HA	1:B:2616:LEU:CB	1.92	0.97
1:B:2155:ASP:CB	1:B:2156:SER:HA	1.94	0.97
1:A:3737:THR:CB	1:A:3738:VAL:CB	2.41	0.97
1:B:1691:SER:CB	1:B:1692:ASP:HA	1.94	0.96
1:B:3890:GLN:H	1:B:3891:ARG:HA	1.30	0.96
1:A:2435:SER:H	1:A:2479:ILE:HA	1.25	0.96
1:A:3545:ARG:O	1:A:3549:ILE:CB	2.12	0.96
1:A:1633:GLY:HA3	1:A:1635:ASP:CB	1.95	0.96
1:A:2396:ASP:O	1:A:2398:ILE:N	1.99	0.96
1:A:1633:GLY:N	1:A:1634:THR:HA	1.79	0.96
1:A:2117:SER:HA	1:A:2129:LEU:CB	1.95	0.96
1:A:3888:LEU:C	1:A:3890:GLN:CB	2.34	0.96
1:B:2434:ASN:HA	1:B:2435:SER:O	1.66	0.96
1:A:4035:GLN:CA	1:A:4036:GLN:CB	2.42	0.96
1:A:2786:ILE:N	1:A:3458:PHE:HA	1.50	0.96
1:A:3878:HIS:CB	1:A:3879:LEU:CA	2.43	0.96
1:B:2015:LYS:O	1:B:2019:SER:CB	2.14	0.96
1:A:2435:SER:CB	1:A:2479:ILE:CB	2.43	0.95
1:A:2015:LYS:O	1:A:2019:SER:CB	2.14	0.95
1:B:3429:LEU:O	1:B:3452:ILE:HA	1.65	0.95
1:B:2117:SER:HA	1:B:2129:LEU:CB	1.95	0.95
1:A:3429:LEU:O	1:A:3452:ILE:HA	1.65	0.95
1:B:2396:ASP:O	1:B:2398:ILE:N	1.99	0.95
1:B:3888:LEU:C	1:B:3890:GLN:CB	2.34	0.95
1:B:3878:HIS:CB	1:B:3879:LEU:CA	2.43	0.95
1:A:2002:ILE:O	1:A:2213:LEU:HA	1.67	0.95
1:A:2434:ASN:HA	1:A:2435:SER:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2435:SER:CB	1:B:2479:ILE:CB	2.43	0.95
1:A:3810:SER:CB	1:A:3837:GLY:HA3	1.97	0.95
1:A:2378:VAL:N	1:A:2379:SER:CB	2.30	0.95
1:A:1624:ARG:CB	1:A:1647:ALA:CB	2.45	0.95
1:A:1920:SER:CB	1:A:3998:ILE:O	2.15	0.95
1:B:2002:ILE:O	1:B:2213:LEU:HA	1.67	0.95
1:B:1631:LYS:C	1:B:1635:ASP:CB	2.35	0.95
1:B:1633:GLY:N	1:B:1634:THR:HA	1.79	0.95
1:B:1633:GLY:HA3	1:B:1635:ASP:CB	1.95	0.95
1:A:3751:VAL:N	1:A:3752:THR:CB	2.30	0.95
1:B:3751:VAL:N	1:B:3752:THR:CB	2.30	0.95
1:B:1843:ALA:HB1	1:B:1893:ALA:N	1.81	0.94
1:A:1734:PHE:O	1:A:1756:LEU:CB	2.15	0.94
1:B:3810:SER:CB	1:B:3837:GLY:HA3	1.97	0.94
1:B:1788:GLN:O	1:B:1790:TYR:N	2.00	0.94
1:A:1466:GLN:CB	1:A:1469:LEU:N	2.31	0.94
1:A:1631:LYS:C	1:A:1635:ASP:CB	2.35	0.94
1:A:3453:GLN:N	1:A:3454:ASP:CB	2.30	0.94
1:A:3749:ASP:C	1:A:3752:THR:CB	2.36	0.94
1:B:2378:VAL:N	1:B:2379:SER:CB	2.30	0.94
1:B:3749:ASP:C	1:B:3752:THR:CB	2.36	0.94
1:B:3859:VAL:CB	1:B:3888:LEU:CA	2.46	0.94
1:A:1843:ALA:HB1	1:A:1893:ALA:N	1.81	0.94
1:A:2708:ASN:CB	1:A:2709:LYS:CA	2.46	0.94
1:B:1814:GLY:CA	1:B:1815:ARG:CB	2.46	0.94
1:A:2092:ALA:HB1	1:A:2098:ALA:N	1.83	0.94
1:A:1691:SER:CB	1:A:1692:ASP:HA	1.94	0.94
1:B:1920:SER:CB	1:B:3998:ILE:O	2.15	0.94
1:B:3453:GLN:N	1:B:3454:ASP:CB	2.30	0.94
1:B:2581:LEU:CB	1:B:2582:VAL:CA	2.43	0.94
1:A:1788:GLN:C	1:A:1790:TYR:H	1.67	0.94
1:B:1984:ILE:CB	1:B:1985:SER:CA	2.46	0.93
1:B:1734:PHE:O	1:B:1756:LEU:CB	2.15	0.93
1:A:2378:VAL:H	1:A:2379:SER:CB	1.80	0.93
1:A:1788:GLN:O	1:A:1790:TYR:N	2.00	0.93
1:B:1624:ARG:CB	1:B:1647:ALA:CB	2.45	0.93
1:A:1814:GLY:CA	1:A:1815:ARG:CB	2.46	0.93
1:A:1848:ASP:CB	1:A:1849:GLU:C	2.37	0.93
1:A:2547:SER:O	1:A:2551:THR:CB	2.17	0.93
1:A:3358:VAL:C	1:A:3360:TYR:CB	2.37	0.93
1:B:2378:VAL:H	1:B:2379:SER:CB	1.80	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2581:LEU:CB	1:A:2582:VAL:CA	2.43	0.93
1:B:2708:ASN:CB	1:B:2709:LYS:CA	2.46	0.93
1:A:2107:LYS:O	1:A:2108:VAL:CB	2.15	0.93
1:A:2003:LEU:O	1:A:2004:PRO:C	2.02	0.93
1:A:3859:VAL:CB	1:A:3888:LEU:CA	2.46	0.93
1:B:2726:GLU:CB	1:B:2727:GLU:HA	1.99	0.93
1:B:2786:ILE:CA	1:B:3458:PHE:C	2.27	0.93
1:B:3754:LYS:O	1:B:3756:TYR:N	2.02	0.93
1:B:2160:PRO:C	1:B:2162:TYR:H	1.72	0.93
1:A:2172:ASP:O	1:A:2183:ARG:HA	1.69	0.92
1:B:2003:LEU:O	1:B:2004:PRO:C	2.02	0.92
1:B:1848:ASP:CB	1:B:1849:GLU:C	2.37	0.92
1:B:2306:ASP:CB	1:B:2311:LYS:N	2.31	0.92
1:B:1466:GLN:CB	1:B:1469:LEU:N	2.31	0.92
1:A:2306:ASP:CB	1:A:2311:LYS:N	2.31	0.92
1:A:2786:ILE:CA	1:A:3458:PHE:C	2.27	0.92
1:A:1848:ASP:N	1:A:1849:GLU:HA	1.84	0.92
1:A:3890:GLN:H	1:A:3891:ARG:HA	1.30	0.92
1:B:3358:VAL:C	1:B:3360:TYR:CB	2.38	0.92
1:B:2547:SER:O	1:B:2551:THR:CB	2.17	0.92
1:B:4035:GLN:CA	1:B:4036:GLN:CB	2.42	0.92
1:B:3808:LYS:O	1:B:3810:SER:N	2.03	0.92
1:B:2092:ALA:HB1	1:B:2098:ALA:N	1.83	0.92
1:B:1848:ASP:N	1:B:1849:GLU:HA	1.84	0.92
1:A:3754:LYS:O	1:A:3756:TYR:N	2.02	0.92
1:A:2614:HIS:O	1:A:2616:LEU:HA	1.70	0.92
1:A:3808:LYS:O	1:A:3810:SER:N	2.03	0.92
1:B:3478:THR:HA	1:B:3483:ASP:HA	1.51	0.91
1:B:3738:VAL:HA	1:B:3739:ASP:CB	2.01	0.91
1:B:2378:VAL:CB	1:B:2379:SER:CA	2.46	0.91
1:B:3899:ASP:CA	1:B:3900:ILE:N	2.33	0.91
1:A:2160:PRO:C	1:A:2162:TYR:H	1.72	0.91
1:B:2614:HIS:O	1:B:2616:LEU:HA	1.70	0.91
1:B:1814:GLY:HA3	1:B:1815:ARG:N	1.85	0.91
1:B:2105:ASP:O	1:B:2157:ASP:CB	2.18	0.91
1:B:3453:GLN:CA	1:B:3454:ASP:CB	2.49	0.91
1:B:3432:LEU:CB	1:B:3457:PHE:N	2.11	0.91
1:B:2172:ASP:O	1:B:2183:ARG:HA	1.69	0.91
1:B:2604:LYS:CB	1:B:2610:GLY:HA3	2.01	0.91
1:A:2604:LYS:CB	1:A:2610:GLY:HA3	2.01	0.91
1:A:3899:ASP:CA	1:A:3900:ILE:N	2.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2431:ALA:N	1:B:2432:LEU:HA	1.86	0.91
1:A:3478:THR:HA	1:A:3483:ASP:HA	1.52	0.91
1:A:1984:ILE:CB	1:A:1985:SER:CA	2.47	0.91
1:A:1842:GLY:HA2	1:A:1891:HIS:CA	2.01	0.91
1:B:2378:VAL:CA	1:B:2379:SER:CB	2.49	0.90
1:A:1827:ASP:CB	1:A:1828:TYR:HA	2.00	0.90
1:A:2105:ASP:O	1:A:2157:ASP:CB	2.18	0.90
1:A:1814:GLY:HA3	1:A:1815:ARG:N	1.85	0.90
1:A:1364:GLU:HA	2:T:216:PRO:CB	2.01	0.90
1:A:3453:GLN:CA	1:A:3454:ASP:CB	2.49	0.90
1:A:2726:GLU:CB	1:A:2727:GLU:HA	1.99	0.90
1:B:2188:PRO:CB	1:B:2189:ASN:C	2.40	0.90
1:B:1842:GLY:HA2	1:B:1891:HIS:CA	2.01	0.90
1:A:2938:MET:O	1:A:2939:GLU:C	2.01	0.90
1:B:2107:LYS:O	1:B:2108:VAL:CB	2.15	0.90
1:A:2188:PRO:CB	1:A:2189:ASN:C	2.40	0.89
1:A:1624:ARG:CB	1:A:1647:ALA:HB3	2.02	0.89
1:A:3737:THR:CA	1:A:3738:VAL:CB	2.50	0.89
1:A:2378:VAL:CA	1:A:2379:SER:CB	2.49	0.89
1:A:1843:ALA:HB3	1:A:1893:ALA:H	1.11	0.89
1:A:3738:VAL:HA	1:A:3739:ASP:CB	2.01	0.89
1:B:2107:LYS:N	1:B:2503:VAL:O	2.06	0.89
1:B:1827:ASP:CB	1:B:1828:TYR:HA	2.00	0.89
1:B:3737:THR:CA	1:B:3738:VAL:CB	2.50	0.89
1:A:3807:SER:N	1:A:3809:GLU:H	1.70	0.89
1:B:3430:SER:CB	1:B:3453:GLN:CB	2.51	0.89
1:A:2107:LYS:N	1:A:2503:VAL:O	2.06	0.89
1:B:1624:ARG:CB	1:B:1647:ALA:HB3	2.02	0.89
1:B:3666:ALA:HB1	1:B:3668:ARG:N	1.88	0.89
1:A:1578:PHE:CB	1:A:1616:LYS:CB	2.51	0.89
1:B:3995:GLY:C	1:B:3997:LYS:H	1.67	0.89
1:B:1920:SER:CB	1:B:3998:ILE:CA	2.51	0.89
1:A:2431:ALA:N	1:A:2432:LEU:HA	1.86	0.89
1:A:2434:ASN:CB	1:A:2435:SER:CA	2.50	0.89
1:A:3430:SER:CB	1:A:3453:GLN:CB	2.51	0.89
1:A:2378:VAL:CB	1:A:2379:SER:CA	2.46	0.89
1:B:1986:GLU:HA	1:B:1987:PHE:C	1.93	0.88
1:A:1632:ASP:CB	1:A:1633:GLY:HA2	2.03	0.88
1:A:3457:PHE:O	1:A:3460:PRO:N	2.06	0.88
1:B:2434:ASN:CB	1:B:2435:SER:CA	2.50	0.88
1:A:2107:LYS:O	1:A:2503:VAL:C	2.11	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4004:LEU:O	1:B:4008:ALA:N	2.06	0.88
1:A:1986:GLU:HA	1:A:1987:PHE:C	1.93	0.88
1:B:3807:SER:N	1:B:3809:GLU:H	1.70	0.88
1:A:1840:GLN:CB	1:A:1889:SER:CB	2.52	0.88
1:B:2600:TYR:HA	1:B:2613:SER:CB	2.04	0.88
1:B:1840:GLN:CB	1:B:1889:SER:CB	2.51	0.88
1:B:3666:ALA:HA	1:B:3668:ARG:H	0.73	0.88
1:B:3886:ALA:O	1:B:3890:GLN:CB	2.21	0.88
1:A:3457:PHE:O	1:A:3459:ASP:N	2.07	0.88
1:B:1788:GLN:C	1:B:1790:TYR:H	1.67	0.88
1:B:1578:PHE:CB	1:B:1616:LYS:CB	2.51	0.88
1:B:1843:ALA:HB3	1:B:1893:ALA:H	1.11	0.88
1:B:2098:ALA:HB1	1:B:2149:ARG:H	1.39	0.88
1:B:1787:HIS:CB	1:B:3992:ILE:CB	2.51	0.88
1:A:1787:HIS:CB	1:A:3992:ILE:CB	2.51	0.88
1:A:3666:ALA:HB1	1:A:3668:ARG:N	1.88	0.88
1:A:1920:SER:CB	1:A:3998:ILE:CA	2.51	0.88
1:A:3336:HIS:H	1:A:3337:LEU:HA	1.38	0.88
1:B:2092:ALA:HB1	1:B:2098:ALA:H	1.36	0.88
1:B:2107:LYS:O	1:B:2503:VAL:C	2.11	0.88
1:B:3457:PHE:O	1:B:3460:PRO:N	2.06	0.88
1:A:2600:TYR:HA	1:A:2613:SER:CB	2.04	0.88
1:B:3901:PRO:CB	1:B:3902:GLY:HA2	2.04	0.88
1:B:2938:MET:O	1:B:2939:GLU:C	2.01	0.88
1:A:2369:SER:C	1:A:2372:CYS:CB	2.42	0.88
1:A:3995:GLY:C	1:A:3997:LYS:H	1.67	0.88
1:A:2188:PRO:CB	1:A:2189:ASN:O	2.21	0.88
1:A:3666:ALA:HA	1:A:3668:ARG:H	0.73	0.88
1:A:3886:ALA:O	1:A:3890:GLN:CB	2.21	0.88
1:B:2369:SER:C	1:B:2372:CYS:CB	2.42	0.88
1:B:1632:ASP:CB	1:B:1633:GLY:HA2	2.03	0.87
1:B:2188:PRO:CB	1:B:2189:ASN:O	2.21	0.87
1:B:3336:HIS:O	1:B:3517:HIS:N	2.07	0.87
1:B:1530:GLN:O	1:B:1531:ARG:C	2.02	0.87
1:A:2098:ALA:HB1	1:A:2149:ARG:H	1.39	0.87
1:A:2155:ASP:CB	1:A:2156:SER:CA	2.52	0.87
1:B:2366:LEU:CB	1:B:2367:SER:CA	2.52	0.87
1:A:3815:PRO:O	1:A:3842:GLN:O	1.91	0.87
1:B:3457:PHE:O	1:B:3459:ASP:N	2.07	0.87
1:B:2371:PHE:N	1:B:2372:CYS:CB	2.36	0.87
1:A:2371:PHE:N	1:A:2372:CYS:CB	2.36	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2153:VAL:O	1:B:2195:GLU:N	2.07	0.87
1:A:2366:LEU:CB	1:A:2367:SER:CA	2.52	0.87
1:A:4004:LEU:O	1:A:4008:ALA:N	2.06	0.87
1:A:3336:HIS:O	1:A:3517:HIS:N	2.07	0.87
1:A:2092:ALA:HB1	1:A:2098:ALA:H	1.36	0.87
1:B:2539:THR:O	1:B:2541:PRO:N	2.08	0.87
1:A:3901:PRO:CB	1:A:3902:GLY:HA2	2.04	0.87
1:B:3815:PRO:O	1:B:3842:GLN:O	1.91	0.87
1:A:2578:ILE:C	1:A:2580:LYS:H	1.74	0.86
1:A:1941:ASP:C	1:A:1942:SER:CA	2.44	0.86
1:B:3666:ALA:HA	1:B:3667:ALA:HB3	1.55	0.86
1:B:3990:ALA:O	1:B:3993:VAL:N	2.06	0.86
1:B:2154:PHE:CA	1:B:2195:GLU:CB	2.54	0.86
1:B:2155:ASP:CB	1:B:2156:SER:CA	2.53	0.86
1:A:2153:VAL:O	1:A:2195:GLU:N	2.07	0.86
1:A:2539:THR:O	1:A:2541:PRO:N	2.08	0.85
1:A:1530:GLN:O	1:A:1531:ARG:C	2.02	0.85
1:A:3890:GLN:N	1:A:3891:ARG:C	2.28	0.85
1:A:3807:SER:CA	1:A:3808:LYS:C	2.45	0.85
1:B:1691:SER:CB	1:B:1692:ASP:CA	2.54	0.85
1:A:2778:GLY:O	1:A:2812:ARG:CB	2.24	0.85
1:B:2778:GLY:O	1:B:2812:ARG:CB	2.24	0.85
1:A:3666:ALA:HB2	1:A:3668:ARG:CA	2.03	0.85
1:B:2154:PHE:HA	1:B:2195:GLU:CB	2.06	0.85
1:B:3807:SER:CA	1:B:3808:LYS:C	2.45	0.85
1:A:2686:LEU:H	1:A:2687:GLY:HA2	1.41	0.85
1:B:2372:CYS:HA	1:B:2373:SER:CB	2.06	0.85
1:A:2154:PHE:CA	1:A:2195:GLU:CB	2.54	0.85
1:A:3499:CYS:O	1:A:3501:PRO:CB	2.24	0.85
1:B:2092:ALA:CB	1:B:2098:ALA:N	2.37	0.85
1:B:1941:ASP:C	1:B:1942:SER:CA	2.44	0.85
1:A:2154:PHE:HA	1:A:2195:GLU:CA	2.06	0.85
1:A:2369:SER:CB	1:A:2372:CYS:O	2.25	0.85
1:B:2154:PHE:HA	1:B:2195:GLU:CA	2.06	0.85
1:A:2154:PHE:HA	1:A:2195:GLU:CB	2.06	0.85
1:B:2107:LYS:O	1:B:2504:LEU:CA	2.25	0.85
1:B:3890:GLN:N	1:B:3891:ARG:C	2.28	0.85
1:A:3890:GLN:N	1:A:3891:ARG:CA	2.39	0.85
1:B:3457:PHE:O	1:B:3458:PHE:C	2.12	0.85
1:A:3851:VAL:O	1:A:3855:LEU:CB	2.25	0.85
1:B:2369:SER:CB	1:B:2372:CYS:O	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1788:GLN:C	1:A:1790:TYR:N	2.29	0.85
1:B:1986:GLU:C	1:B:1987:PHE:CA	2.46	0.84
1:B:2154:PHE:HA	1:B:2195:GLU:HA	1.59	0.84
1:A:3666:ALA:HA	1:A:3667:ALA:HB3	1.55	0.84
1:B:3851:VAL:O	1:B:3855:LEU:CB	2.25	0.84
1:A:2154:PHE:HA	1:A:2195:GLU:HA	1.59	0.84
1:A:3503:GLY:O	1:A:3506:PRO:N	2.10	0.84
1:A:2378:VAL:CB	1:A:2379:SER:HA	2.07	0.84
1:B:2686:LEU:H	1:B:2687:GLY:HA2	1.41	0.84
1:A:1691:SER:CB	1:A:1692:ASP:CA	2.55	0.84
1:A:1986:GLU:C	1:A:1987:PHE:CA	2.46	0.84
1:B:3807:SER:N	1:B:3809:GLU:N	2.25	0.84
1:B:2378:VAL:CB	1:B:2379:SER:HA	2.07	0.84
1:A:3739:ASP:N	1:A:3740:THR:CB	2.40	0.84
1:A:2107:LYS:O	1:A:2504:LEU:CA	2.25	0.84
1:A:2680:TYR:N	1:A:2681:LEU:HA	1.93	0.84
1:B:3739:ASP:N	1:B:3740:THR:CB	2.40	0.84
1:B:3499:CYS:O	1:B:3501:PRO:CB	2.24	0.84
1:B:2171:ASP:CB	1:B:2184:LEU:O	2.26	0.84
1:B:1942:SER:O	1:B:1945:LEU:CA	2.26	0.84
1:B:1497:ILE:O	1:B:1498:GLU:C	2.15	0.84
1:B:2785:LYS:C	1:B:3458:PHE:CA	2.19	0.83
1:A:2171:ASP:CB	1:A:2184:LEU:O	2.26	0.83
1:B:2117:SER:CA	1:B:2129:LEU:CB	2.57	0.83
1:A:2396:ASP:O	1:A:2399:LYS:N	2.11	0.83
1:A:1942:SER:O	1:A:1945:LEU:CA	2.26	0.83
1:B:3421:TYR:CB	1:B:3422:TYR:C	2.47	0.83
1:B:3476:ARG:HA	1:B:3485:GLU:CB	2.09	0.83
1:A:3476:ARG:HA	1:A:3485:GLU:CB	2.09	0.83
1:A:3990:ALA:O	1:A:3993:VAL:N	2.06	0.83
1:B:3890:GLN:N	1:B:3891:ARG:CA	2.39	0.83
1:A:3457:PHE:O	1:A:3458:PHE:C	2.12	0.83
1:A:2600:TYR:O	1:A:2610:GLY:HA2	1.79	0.83
1:A:3807:SER:N	1:A:3809:GLU:N	2.25	0.83
1:B:3503:GLY:O	1:B:3506:PRO:N	2.10	0.83
1:B:3336:HIS:H	1:B:3337:LEU:HA	1.38	0.83
1:B:1788:GLN:C	1:B:1790:TYR:N	2.29	0.83
1:A:1801:GLY:O	1:A:1802:LYS:C	2.16	0.83
1:B:1636:ILE:O	1:B:1639:VAL:N	2.12	0.82
1:A:2117:SER:CA	1:A:2129:LEU:CB	2.57	0.82
1:A:2372:CYS:HA	1:A:2373:SER:CB	2.06	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2396:ASP:O	1:B:2399:LYS:N	2.11	0.82
1:B:2430:ASN:C	1:B:2432:LEU:HA	2.00	0.82
1:B:2441:VAL:HA	1:B:2442:GLY:N	1.94	0.82
1:A:1636:ILE:O	1:A:1639:VAL:N	2.12	0.82
1:B:2600:TYR:O	1:B:2610:GLY:HA2	1.79	0.82
1:A:2092:ALA:CB	1:A:2098:ALA:N	2.37	0.82
1:A:3421:TYR:CB	1:A:3422:TYR:C	2.47	0.82
1:B:1530:GLN:O	1:B:1531:ARG:O	1.97	0.82
1:B:2680:TYR:N	1:B:2681:LEU:HA	1.93	0.82
1:A:2709:LYS:CA	1:A:2710:THR:N	2.43	0.82
1:A:2441:VAL:HA	1:A:2442:GLY:N	1.94	0.82
1:A:1633:GLY:H	1:A:1635:ASP:CB	1.92	0.82
1:A:3335:GLY:C	1:A:3337:LEU:HA	1.99	0.82
1:B:3335:GLY:C	1:B:3337:LEU:HA	1.99	0.82
1:B:1631:LYS:O	1:B:1635:ASP:CB	2.28	0.81
1:A:1530:GLN:O	1:A:1531:ARG:O	1.97	0.81
1:A:1631:LYS:O	1:A:1635:ASP:CB	2.28	0.81
1:B:2709:LYS:CA	1:B:2710:THR:N	2.43	0.81
1:A:2159:ASP:C	1:A:2161:GLU:N	2.30	0.81
1:A:1932:MET:C	1:A:1946:ALA:HB2	2.01	0.81
1:B:2159:ASP:C	1:B:2161:GLU:N	2.30	0.81
1:A:4034:LEU:O	1:A:4035:GLN:C	2.18	0.81
1:A:4046:THR:O	1:A:4048:ILE:CB	2.29	0.81
1:A:2430:ASN:C	1:A:2432:LEU:HA	2.00	0.81
1:B:3889:LEU:N	1:B:3890:GLN:CB	2.44	0.81
1:B:4034:LEU:O	1:B:4035:GLN:C	2.18	0.80
1:B:3789:ALA:O	1:B:3879:LEU:N	2.13	0.80
1:B:1550:GLY:HA2	1:B:1551:SER:O	1.81	0.80
1:B:1633:GLY:H	1:B:1635:ASP:CB	1.92	0.80
1:A:3889:LEU:N	1:A:3890:GLN:CB	2.44	0.80
1:A:3789:ALA:O	1:A:3879:LEU:N	2.13	0.80
1:B:2430:ASN:C	1:B:2432:LEU:CB	2.49	0.80
1:A:2206:THR:C	1:A:2209:ARG:O	2.19	0.80
1:B:3666:ALA:HB1	1:B:3668:ARG:CA	2.07	0.80
1:B:2160:PRO:O	1:B:2163:VAL:N	2.14	0.80
1:B:1932:MET:C	1:B:1946:ALA:HB2	2.01	0.80
1:B:3921:SER:CB	1:B:3922:GLY:O	2.30	0.80
1:B:2206:THR:C	1:B:2209:ARG:O	2.19	0.80
1:A:3749:ASP:O	1:A:3752:THR:CB	2.30	0.80
1:B:3640:TRP:O	1:B:3641:PHE:CB	2.28	0.80
1:A:4033:LEU:O	1:A:4036:GLN:CB	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:ILE:O	1:A:1498:GLU:C	2.15	0.80
1:B:3749:ASP:O	1:B:3752:THR:CB	2.30	0.80
1:B:3737:THR:HA	1:B:3738:VAL:CB	2.12	0.80
1:B:3739:ASP:O	1:B:3743:ASP:N	2.15	0.80
1:A:3360:TYR:CB	1:A:3361:ASP:N	2.45	0.80
1:B:3408:LEU:O	1:B:3518:PHE:N	2.15	0.80
1:B:1801:GLY:O	1:B:1802:LYS:C	2.16	0.80
1:A:3739:ASP:O	1:A:3743:ASP:N	2.15	0.80
1:B:2347:GLY:CA	1:B:2348:HIS:CB	2.56	0.80
1:A:3666:ALA:HB1	1:A:3668:ARG:CA	2.07	0.79
1:A:2434:ASN:CA	1:A:2435:SER:O	2.30	0.79
1:B:3360:TYR:CB	1:B:3361:ASP:N	2.45	0.79
1:B:3900:ILE:CB	1:B:3901:PRO:CA	2.60	0.79
1:A:2581:LEU:CB	1:A:2582:VAL:HA	2.11	0.79
1:B:1550:GLY:CA	1:B:1551:SER:C	2.50	0.79
1:A:2172:ASP:O	1:A:2183:ARG:CA	2.30	0.79
1:A:3640:TRP:O	1:A:3641:PHE:CB	2.28	0.79
1:B:2117:SER:C	1:B:2129:LEU:CB	2.51	0.79
1:A:3737:THR:HA	1:A:3738:VAL:CB	2.12	0.79
1:A:2430:ASN:C	1:A:2432:LEU:CB	2.49	0.79
1:B:4033:LEU:O	1:B:4036:GLN:CB	2.30	0.79
1:B:3452:ILE:C	1:B:3454:ASP:CB	2.51	0.79
1:A:3478:THR:CB	1:A:3483:ASP:CB	2.61	0.79
1:B:2434:ASN:CA	1:B:2435:SER:O	2.30	0.79
1:A:3900:ILE:CB	1:A:3901:PRO:CA	2.60	0.79
1:B:3475:ASN:O	1:B:3485:GLU:CB	2.30	0.79
1:B:4046:THR:O	1:B:4048:ILE:CB	2.29	0.79
2:S:32:TYR:N	2:S:32:TYR:CA	2.44	0.79
1:B:2155:ASP:CB	1:B:2157:ASP:N	2.46	0.79
1:B:2172:ASP:O	1:B:2183:ARG:CA	2.30	0.79
2:S:32:TYR:C	2:S:32:TYR:CA	2.51	0.79
1:A:2103:VAL:CB	1:A:2104:ILE:CB	2.61	0.79
1:B:3878:HIS:CA	1:B:3879:LEU:C	2.49	0.79
1:A:2347:GLY:CA	1:A:2348:HIS:CB	2.56	0.79
1:B:1848:ASP:N	1:B:1849:GLU:CA	2.46	0.79
1:A:2160:PRO:O	1:A:2163:VAL:N	2.14	0.79
1:A:2392:ILE:O	1:A:2393:PRO:CB	2.31	0.79
1:A:1747:VAL:CB	1:A:1752:SER:CB	2.60	0.79
1:A:2603:CYS:CB	1:A:2609:THR:CB	2.61	0.79
1:A:3921:SER:CB	1:A:3922:GLY:O	2.30	0.79
1:A:2155:ASP:CB	1:A:2157:ASP:N	2.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3452:ILE:C	1:A:3454:ASP:CB	2.51	0.79
1:B:1747:VAL:CB	1:B:1752:SER:CB	2.60	0.79
1:A:2653:TRP:O	1:A:2656:PHE:CA	2.31	0.78
1:B:1872:LEU:O	1:B:1875:GLY:N	2.17	0.78
1:B:2653:TRP:O	1:B:2656:PHE:CA	2.31	0.78
1:B:2392:ILE:O	1:B:2393:PRO:CB	2.31	0.78
1:A:2436:SER:O	1:A:2437:LEU:CB	2.29	0.78
1:A:3878:HIS:CA	1:A:3879:LEU:C	2.50	0.78
1:A:3815:PRO:O	1:A:3843:ASN:CB	2.32	0.78
1:B:2382:ALA:HB1	1:B:2386:MET:CB	2.12	0.78
1:A:3475:ASN:O	1:A:3485:GLU:CB	2.30	0.78
1:A:3485:GLU:O	1:A:3486:VAL:CB	2.32	0.78
1:A:1881:LEU:HA	1:A:1885:GLU:O	1.83	0.78
1:A:2785:LYS:C	1:A:3458:PHE:CA	2.19	0.78
1:A:3408:LEU:O	1:A:3518:PHE:N	2.15	0.78
1:A:1872:LEU:O	1:A:1875:GLY:N	2.17	0.78
1:B:3478:THR:CB	1:B:3483:ASP:CB	2.61	0.78
1:A:2514:GLY:HA3	1:A:2520:GLU:O	1.83	0.78
1:A:2105:ASP:CA	1:A:2157:ASP:CB	2.61	0.78
1:B:2581:LEU:CB	1:B:2582:VAL:HA	2.11	0.78
1:A:2117:SER:C	1:A:2129:LEU:CB	2.51	0.78
1:A:1848:ASP:N	1:A:1849:GLU:CA	2.46	0.78
1:B:3485:GLU:O	1:B:3486:VAL:CB	2.32	0.78
1:A:2444:ASN:O	1:A:2445:PHE:CB	2.31	0.78
1:A:2774:ALA:C	1:A:2775:TRP:CA	2.52	0.78
1:A:2442:GLY:HA2	1:A:2485:PHE:CB	2.13	0.78
1:B:2103:VAL:CB	1:B:2104:ILE:CB	2.61	0.78
1:B:2603:CYS:CB	1:B:2609:THR:CB	2.61	0.78
1:A:3409:ASP:C	1:A:3411:SER:HA	2.04	0.78
1:B:2006:LEU:CB	1:B:2007:GLY:C	2.53	0.78
1:B:2514:GLY:HA3	1:B:2520:GLU:O	1.83	0.78
1:B:1941:ASP:H	1:B:1942:SER:CB	1.96	0.78
1:A:1550:GLY:HA2	1:A:1551:SER:O	1.81	0.78
1:A:1941:ASP:H	1:A:1942:SER:CB	1.96	0.77
1:B:2774:ALA:C	1:B:2775:TRP:CA	2.52	0.77
1:A:3806:ALA:O	1:A:3807:SER:CB	2.31	0.77
1:B:3666:ALA:CB	1:B:3669:THR:H	1.91	0.77
1:B:2140:ASP:O	1:B:2142:THR:N	2.18	0.77
1:B:2442:GLY:HA2	1:B:2485:PHE:CB	2.13	0.77
1:B:3409:ASP:C	1:B:3411:SER:HA	2.04	0.77
1:B:2386:MET:O	1:B:2390:ILE:CB	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2140:ASP:O	1:A:2142:THR:N	2.18	0.77
1:B:2396:ASP:O	1:B:2397:THR:C	2.21	0.77
1:B:2432:LEU:O	1:B:2433:ARG:CB	2.29	0.77
1:B:2542:GLY:O	1:B:2543:ARG:CB	2.33	0.77
1:B:2153:VAL:O	1:B:2195:GLU:HA	1.82	0.77
1:A:3360:TYR:CA	1:A:3361:ASP:N	2.47	0.77
1:A:2604:LYS:N	1:A:2610:GLY:N	2.32	0.77
1:A:2092:ALA:HB1	1:A:2097:HIS:C	2.05	0.77
1:A:2542:GLY:O	1:A:2543:ARG:CB	2.33	0.77
1:B:1881:LEU:HA	1:B:1885:GLU:O	1.83	0.77
1:A:4027:VAL:O	1:A:4029:ILE:CB	2.33	0.77
1:B:3360:TYR:CA	1:B:3361:ASP:N	2.47	0.77
1:B:2604:LYS:N	1:B:2610:GLY:N	2.32	0.77
1:A:2105:ASP:O	1:A:2156:SER:O	2.03	0.77
1:A:2153:VAL:O	1:A:2195:GLU:HA	1.82	0.77
1:B:3861:GLU:C	1:B:3863:LYS:H	1.88	0.77
1:B:3806:ALA:O	1:B:3807:SER:CB	2.32	0.77
1:B:2444:ASN:O	1:B:2445:PHE:CB	2.30	0.77
1:A:2382:ALA:HB1	1:A:2386:MET:CB	2.12	0.77
1:A:2386:MET:O	1:A:2390:ILE:CB	2.33	0.77
1:B:4027:VAL:O	1:B:4029:ILE:CB	2.33	0.77
1:A:2188:PRO:CB	1:A:2189:ASN:CA	2.63	0.77
1:B:3815:PRO:O	1:B:3843:ASN:CB	2.32	0.77
1:B:2105:ASP:CA	1:B:2157:ASP:CB	2.61	0.77
1:B:3901:PRO:CB	1:B:3902:GLY:CA	2.63	0.77
1:B:2092:ALA:HB1	1:B:2097:HIS:C	2.05	0.77
1:A:1627:LEU:O	1:A:1631:LYS:CB	2.33	0.77
1:A:2172:ASP:O	1:A:2183:ARG:CB	2.33	0.77
1:B:2524:VAL:O	1:B:2525:THR:CB	2.33	0.76
1:A:2006:LEU:CB	1:A:2007:GLY:C	2.53	0.76
1:B:1814:GLY:C	1:B:1815:ARG:O	2.24	0.76
1:A:1532:ARG:O	1:A:1607:TRP:HA	1.85	0.76
1:B:2105:ASP:O	1:B:2156:SER:O	2.03	0.76
1:B:2188:PRO:CB	1:B:2189:ASN:CA	2.63	0.76
1:B:1532:ARG:O	1:B:1607:TRP:HA	1.85	0.76
1:A:3877:CYS:HA	1:A:3878:HIS:CB	2.16	0.76
1:B:1987:PHE:O	1:B:1988:GLY:C	2.22	0.76
1:A:1987:PHE:O	1:A:1988:GLY:C	2.22	0.76
1:B:2369:SER:O	1:B:2372:CYS:CB	2.32	0.76
1:B:1627:LEU:O	1:B:1631:LYS:CB	2.33	0.76
1:B:2172:ASP:O	1:B:2183:ARG:CB	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2843:LEU:HA	1:A:2844:PHE:CB	2.15	0.76
1:B:3754:LYS:C	1:B:3755:SER:C	2.45	0.76
1:B:3404:VAL:O	1:B:3495:PHE:CA	2.34	0.76
1:A:2396:ASP:O	1:A:2397:THR:C	2.21	0.76
1:A:1364:GLU:O	2:T:216:PRO:CB	2.34	0.76
1:B:3890:GLN:N	1:B:3891:ARG:HA	1.98	0.76
1:A:2369:SER:O	1:A:2372:CYS:CB	2.32	0.76
1:B:3713:GLU:CB	1:B:3714:GLN:C	2.54	0.76
1:A:2154:PHE:C	1:A:2195:GLU:CB	2.55	0.76
1:A:1814:GLY:C	1:A:1815:ARG:O	2.24	0.76
1:A:1747:VAL:HA	1:A:1752:SER:HA	1.67	0.76
1:B:2436:SER:O	1:B:2437:LEU:CB	2.29	0.76
1:A:1466:GLN:CB	1:A:1469:LEU:CB	2.63	0.75
1:B:1466:GLN:CB	1:B:1469:LEU:CB	2.63	0.75
1:A:2006:LEU:CB	1:A:2008:ASP:N	2.49	0.75
1:B:2578:ILE:C	1:B:2580:LYS:H	1.74	0.75
1:A:3754:LYS:C	1:A:3755:SER:C	2.45	0.75
1:A:3901:PRO:CB	1:A:3902:GLY:CA	2.63	0.75
1:B:2006:LEU:CB	1:B:2008:ASP:N	2.49	0.75
1:A:2328:GLY:HA3	1:A:2329:ASP:CB	2.16	0.75
1:B:2108:VAL:CB	1:B:2504:LEU:CB	2.64	0.75
1:A:2432:LEU:O	1:A:2433:ARG:CB	2.29	0.75
1:A:3665:ARG:O	1:A:3667:ALA:CB	2.32	0.75
1:B:2154:PHE:C	1:B:2195:GLU:CB	2.55	0.75
1:B:3501:PRO:O	1:B:3502:SER:CB	2.35	0.75
1:A:3861:GLU:C	1:A:3863:LYS:H	1.88	0.75
1:A:2108:VAL:CB	1:A:2504:LEU:CB	2.64	0.75
1:A:3478:THR:O	1:A:3479:VAL:CB	2.34	0.75
1:A:3404:VAL:O	1:A:3495:PHE:CA	2.34	0.75
1:A:3713:GLU:CB	1:A:3714:GLN:C	2.54	0.75
1:B:2640:THR:O	1:B:2644:LEU:CB	2.35	0.75
1:A:2524:VAL:O	1:A:2525:THR:CB	2.33	0.75
1:B:2328:GLY:HA3	1:B:2329:ASP:CB	2.16	0.75
1:B:3877:CYS:HA	1:B:3878:HIS:CB	2.16	0.75
1:A:1932:MET:CA	1:A:1946:ALA:CB	2.64	0.75
1:A:2640:THR:O	1:A:2644:LEU:CB	2.35	0.75
1:B:3886:ALA:C	1:B:3890:GLN:O	2.24	0.74
1:B:1932:MET:CA	1:B:1946:ALA:CB	2.64	0.74
1:A:1814:GLY:HA3	1:A:1815:ARG:CA	2.17	0.74
1:B:2411:LYS:HA	1:B:2554:ALA:O	1.86	0.74
1:B:2430:ASN:C	1:B:2432:LEU:CA	2.56	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3890:GLN:N	1:A:3891:ARG:HA	1.98	0.74
1:B:3478:THR:O	1:B:3479:VAL:CB	2.34	0.74
1:A:2430:ASN:C	1:A:2432:LEU:CA	2.56	0.74
1:A:2411:LYS:HA	1:A:2554:ALA:O	1.86	0.74
1:B:1747:VAL:HA	1:B:1752:SER:HA	1.68	0.74
1:A:3886:ALA:C	1:A:3890:GLN:O	2.24	0.74
1:A:3501:PRO:O	1:A:3502:SER:CB	2.35	0.74
1:B:3419:SER:O	1:B:3421:TYR:N	2.21	0.74
1:B:2173:ASN:HA	1:B:2182:GLU:O	1.88	0.74
1:A:1843:ALA:CB	1:A:1893:ALA:H	1.69	0.74
1:B:1932:MET:CB	1:B:1946:ALA:HA	2.18	0.73
1:B:1627:LEU:CB	1:B:1643:TYR:CB	2.66	0.73
1:A:3419:SER:O	1:A:3421:TYR:N	2.21	0.73
1:A:1364:GLU:C	2:T:216:PRO:C	2.46	0.73
1:A:3370:LEU:O	1:A:3373:LEU:N	2.22	0.73
1:A:4010:LEU:O	1:A:4013:HIS:C	2.27	0.73
1:B:2843:LEU:HA	1:B:2844:PHE:CB	2.15	0.73
1:A:1627:LEU:CB	1:A:1643:TYR:CB	2.66	0.73
1:B:3370:LEU:O	1:B:3373:LEU:N	2.22	0.73
1:B:2209:ARG:CB	1:B:2210:CYS:CB	2.67	0.73
1:B:4010:LEU:O	1:B:4013:HIS:C	2.27	0.73
1:A:3452:ILE:O	1:A:3453:GLN:C	2.27	0.73
1:A:2173:ASN:HA	1:A:2182:GLU:O	1.88	0.73
1:B:2657:ALA:O	1:B:2914:ILE:CB	2.37	0.73
1:A:2657:ALA:O	1:A:2914:ILE:CB	2.37	0.73
1:A:2209:ARG:CB	1:A:2210:CYS:CB	2.66	0.73
1:B:2329:ASP:O	1:B:2330:SER:O	2.05	0.73
1:B:1843:ALA:CB	1:B:1893:ALA:H	1.69	0.72
1:B:1734:PHE:O	1:B:1755:LEU:O	2.07	0.72
1:A:2430:ASN:O	1:A:2432:LEU:CB	2.38	0.72
1:A:1932:MET:C	1:A:1946:ALA:CB	2.57	0.72
1:B:3666:ALA:HB1	1:B:3668:ARG:C	2.10	0.72
1:A:3877:CYS:CB	1:A:3879:LEU:N	2.52	0.72
1:A:1747:VAL:O	1:A:1748:PHE:CB	2.38	0.72
1:A:3991:THR:O	1:A:3992:ILE:C	2.21	0.72
1:A:3666:ALA:HB1	1:A:3668:ARG:C	2.10	0.72
1:B:2301:TRP:O	1:B:2302:PHE:O	2.07	0.72
1:A:2329:ASP:O	1:A:2330:SER:O	2.05	0.72
1:A:3877:CYS:CA	1:A:3878:HIS:CB	2.67	0.72
1:B:2430:ASN:O	1:B:2432:LEU:CB	2.38	0.72
1:B:3915:PHE:O	1:B:3916:PHE:C	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1932:MET:C	1:B:1946:ALA:CB	2.57	0.72
1:A:3503:GLY:O	1:A:3505:ILE:N	2.23	0.72
1:B:1814:GLY:HA3	1:B:1815:ARG:CA	2.17	0.72
1:B:1747:VAL:O	1:B:1748:PHE:CB	2.38	0.72
1:B:2038:LEU:CB	1:B:2090:ALA:HB2	2.19	0.72
1:B:3877:CYS:CA	1:B:3878:HIS:CB	2.67	0.72
1:B:3877:CYS:CB	1:B:3879:LEU:N	2.52	0.72
1:A:2038:LEU:CB	1:A:2090:ALA:HB2	2.19	0.72
1:B:3899:ASP:C	1:B:3900:ILE:CA	2.58	0.71
1:A:3864:ALA:O	1:A:3865:ALA:HB2	1.90	0.71
1:A:3915:PHE:O	1:A:3916:PHE:C	2.25	0.71
1:A:2372:CYS:C	1:A:2374:GLU:N	2.40	0.71
1:A:3899:ASP:C	1:A:3900:ILE:CA	2.58	0.71
1:B:4001:GLU:O	1:B:4002:LYS:CB	2.38	0.71
1:A:3666:ALA:CB	1:A:3669:THR:H	1.91	0.71
1:A:1734:PHE:O	1:A:1755:LEU:O	2.07	0.71
1:A:1932:MET:CB	1:A:1946:ALA:HA	2.18	0.71
1:A:2301:TRP:O	1:A:2302:PHE:O	2.07	0.71
1:B:1814:GLY:HA3	1:B:1815:ARG:CB	2.19	0.71
1:B:2374:GLU:O	1:B:2375:ILE:C	2.27	0.71
1:A:2374:GLU:O	1:A:2375:ILE:C	2.27	0.71
1:B:3452:ILE:O	1:B:3453:GLN:C	2.27	0.71
1:A:1848:ASP:CB	1:A:1850:PHE:N	2.54	0.71
1:B:3665:ARG:O	1:B:3667:ALA:CB	2.32	0.71
1:A:3687:SER:O	1:A:3689:ALA:N	2.24	0.71
1:B:1478:SER:O	1:B:1481:SER:N	2.24	0.71
1:B:3864:ALA:O	1:B:3865:ALA:HB2	1.90	0.71
1:B:3687:SER:O	1:B:3689:ALA:N	2.24	0.71
1:A:4001:GLU:O	1:A:4002:LYS:CB	2.38	0.71
1:B:2434:ASN:CB	1:B:2435:SER:O	2.39	0.70
1:B:3503:GLY:O	1:B:3505:ILE:N	2.23	0.70
1:A:1814:GLY:HA3	1:A:1815:ARG:CB	2.19	0.70
1:A:2616:LEU:H	1:A:2619:PRO:CB	2.04	0.70
1:A:1881:LEU:HA	1:A:1886:THR:HA	1.73	0.70
1:A:3359:LYS:N	1:A:3360:TYR:CB	2.55	0.70
1:A:2346:PHE:O	1:A:2348:HIS:CB	2.39	0.70
1:B:1848:ASP:CB	1:B:1850:PHE:N	2.54	0.70
1:B:3991:THR:O	1:B:3992:ILE:C	2.21	0.70
1:B:1747:VAL:CB	1:B:1752:SER:HA	2.21	0.70
1:A:3666:ALA:HA	1:A:3667:ALA:CB	2.15	0.70
1:B:2785:LYS:C	1:B:3458:PHE:CB	2.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1747:VAL:CB	1:A:1752:SER:HA	2.21	0.70
1:B:1881:LEU:HA	1:B:1886:THR:HA	1.73	0.70
1:A:1939:PHE:O	1:A:1940:GLU:CB	2.40	0.70
1:A:2153:VAL:C	1:A:2195:GLU:CB	2.60	0.70
1:A:2411:LYS:CB	1:A:2554:ALA:CB	2.62	0.70
1:B:2346:PHE:O	1:B:2348:HIS:CB	2.39	0.70
1:B:2616:LEU:H	1:B:2619:PRO:CB	2.04	0.70
1:B:3478:THR:CB	1:B:3483:ASP:HA	2.21	0.70
1:A:1986:GLU:CA	1:A:1987:PHE:CB	2.70	0.69
1:A:1916:PHE:O	1:A:1917:ARG:CB	2.39	0.69
1:A:3478:THR:CB	1:A:3483:ASP:HA	2.21	0.69
1:A:3677:LEU:HA	1:A:3680:GLN:CB	2.22	0.69
1:A:1843:ALA:HA	1:A:1844:TRP:O	1.92	0.69
1:A:2434:ASN:CB	1:A:2435:SER:O	2.39	0.69
2:S:32:TYR:N	2:S:32:TYR:C	2.46	0.69
1:B:2002:ILE:O	1:B:2212:LEU:O	2.11	0.69
1:B:1843:ALA:HA	1:B:1844:TRP:O	1.92	0.69
1:A:2002:ILE:C	1:A:2212:LEU:O	2.31	0.69
1:B:3359:LYS:N	1:B:3360:TYR:CB	2.55	0.69
1:B:3677:LEU:HA	1:B:3680:GLN:CB	2.22	0.69
1:B:1823:ASP:HA	1:B:1853:LEU:CB	2.22	0.69
1:B:2002:ILE:C	1:B:2212:LEU:O	2.31	0.69
1:B:1986:GLU:CA	1:B:1987:PHE:CB	2.70	0.69
1:B:1960:CYS:HA	1:B:1961:SER:CB	2.23	0.69
1:A:1478:SER:O	1:A:1481:SER:N	2.24	0.69
1:A:1823:ASP:HA	1:A:1853:LEU:CB	2.22	0.69
1:B:1986:GLU:HA	1:B:1987:PHE:O	1.92	0.69
1:B:1843:ALA:HB1	1:B:1893:ALA:O	1.93	0.69
1:A:1986:GLU:HA	1:A:1987:PHE:O	1.92	0.69
1:B:1872:LEU:C	1:B:1874:VAL:N	2.45	0.69
1:A:1843:ALA:HB1	1:A:1844:TRP:HA	0.74	0.69
1:B:2153:VAL:C	1:B:2195:GLU:CB	2.60	0.69
1:B:3370:LEU:O	1:B:3371:VAL:C	2.32	0.69
1:A:1960:CYS:HA	1:A:1961:SER:CB	2.23	0.69
1:A:2369:SER:CA	1:A:2372:CYS:CB	2.71	0.68
1:A:2873:LEU:C	1:A:2875:ASP:N	2.47	0.68
1:B:1916:PHE:O	1:B:1917:ARG:CB	2.39	0.68
1:B:4004:LEU:O	1:B:4008:ALA:CB	2.41	0.68
1:A:1843:ALA:HB1	1:A:1893:ALA:O	1.93	0.68
1:B:2372:CYS:C	1:B:2374:GLU:N	2.40	0.68
1:B:1466:GLN:HA	1:B:1468:PHE:N	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2346:PHE:CB	1:A:2349:ASP:HA	2.23	0.68
1:B:1939:PHE:O	1:B:1940:GLU:CB	2.40	0.68
1:B:2004:PRO:N	1:B:2214:TRP:CB	2.56	0.68
1:A:4004:LEU:O	1:A:4008:ALA:CB	2.41	0.68
1:B:2419:PRO:O	1:B:2420:PRO:CB	2.41	0.68
1:B:1932:MET:CA	1:B:1946:ALA:HB1	2.19	0.68
1:B:1633:GLY:N	1:B:1634:THR:CB	2.51	0.68
1:A:2004:PRO:N	1:A:2214:TRP:CB	2.56	0.68
1:A:2419:PRO:O	1:A:2420:PRO:CB	2.42	0.68
1:B:2147:ASN:O	1:B:2148:SER:C	2.29	0.68
1:B:2369:SER:CA	1:B:2372:CYS:CB	2.71	0.68
1:B:2411:LYS:CB	1:B:2554:ALA:CB	2.62	0.68
1:B:2912:CYS:O	1:B:2913:ILE:CB	2.42	0.68
1:A:1844:TRP:CB	1:A:1893:ALA:O	2.41	0.68
1:A:2002:ILE:O	1:A:2212:LEU:O	2.11	0.68
1:A:3370:LEU:O	1:A:3371:VAL:C	2.32	0.68
1:B:3484:HIS:O	1:B:3485:GLU:CB	2.42	0.68
1:B:1843:ALA:HB1	1:B:1844:TRP:HA	0.74	0.68
1:A:1497:ILE:C	1:A:1499:VAL:N	2.45	0.68
1:B:1735:TYR:C	1:B:1756:LEU:N	2.47	0.68
1:A:3484:HIS:O	1:A:3485:GLU:CB	2.42	0.68
1:A:1585:VAL:O	1:A:1586:GLU:CB	2.42	0.68
1:A:1735:TYR:C	1:A:1756:LEU:N	2.47	0.67
1:B:1844:TRP:CB	1:B:1893:ALA:O	2.41	0.67
1:A:3750:TYR:C	1:A:3752:THR:CB	2.62	0.67
1:A:2912:CYS:O	1:A:2913:ILE:CB	2.42	0.67
1:A:1633:GLY:N	1:A:1634:THR:CB	2.51	0.67
1:A:2785:LYS:C	1:A:3458:PHE:CB	2.56	0.67
1:B:1872:LEU:O	1:B:1874:VAL:N	2.27	0.67
1:B:2346:PHE:CB	1:B:2349:ASP:HA	2.23	0.67
1:B:1932:MET:O	1:B:1946:ALA:HB2	1.93	0.67
1:A:2907:ALA:O	1:A:2909:PHE:N	2.28	0.67
1:B:2329:ASP:H	1:B:2333:GLU:CB	2.08	0.67
1:A:2539:THR:O	1:A:2540:ASP:C	2.33	0.67
1:A:1932:MET:O	1:A:1946:ALA:HB2	1.93	0.67
1:B:1941:ASP:N	1:B:1942:SER:CB	2.58	0.67
1:A:4030:PRO:O	1:A:4031:GLN:C	2.33	0.67
1:A:2329:ASP:H	1:A:2333:GLU:CB	2.08	0.67
1:B:3890:GLN:CB	1:B:3891:ARG:O	2.43	0.67
1:B:3410:PRO:O	1:B:3413:HIS:N	2.27	0.67
1:A:1872:LEU:O	1:A:1874:VAL:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:TRP:O	1:A:1448:VAL:CB	2.42	0.67
1:B:3750:TYR:C	1:B:3752:THR:CB	2.62	0.67
1:A:1631:LYS:O	1:A:1635:ASP:HA	1.95	0.67
1:A:3890:GLN:CB	1:A:3891:ARG:O	2.43	0.67
1:B:1445:TRP:O	1:B:1448:VAL:CB	2.42	0.67
1:B:2907:ALA:O	1:B:2909:PHE:N	2.28	0.67
1:A:1941:ASP:N	1:A:1942:SER:CB	2.58	0.67
1:B:2686:LEU:N	1:B:2687:GLY:HA2	2.09	0.67
1:B:1631:LYS:O	1:B:1635:ASP:HA	1.95	0.66
1:A:2371:PHE:CB	1:A:2372:CYS:CA	2.72	0.66
1:A:3410:PRO:O	1:A:3413:HIS:N	2.27	0.66
1:B:2371:PHE:CB	1:B:2372:CYS:CA	2.72	0.66
1:B:4030:PRO:O	1:B:4031:GLN:C	2.33	0.66
1:A:2147:ASN:O	1:A:2148:SER:C	2.29	0.66
1:A:3807:SER:H	1:A:3808:LYS:CB	2.08	0.66
1:A:3407:LEU:CB	1:A:3497:HIS:HA	2.26	0.66
1:A:2347:GLY:N	1:A:2348:HIS:CB	2.59	0.66
1:A:2616:LEU:O	1:A:2619:PRO:N	2.29	0.66
1:B:2616:LEU:O	1:B:2619:PRO:N	2.29	0.66
1:B:2343:ASN:O	1:B:2345:TYR:O	2.14	0.66
1:B:1844:TRP:HA	1:B:1893:ALA:O	1.94	0.66
1:B:2007:GLY:O	1:B:2011:GLU:CB	2.44	0.66
1:B:3807:SER:H	1:B:3808:LYS:CB	2.08	0.66
1:B:1493:LEU:O	1:B:1494:ASP:C	2.34	0.66
1:A:3748:TRP:O	1:A:3752:THR:CB	2.43	0.66
1:B:2724:CYS:HA	1:B:2726:GLU:H	1.59	0.66
1:B:1747:VAL:CB	1:B:1751:GLN:O	2.44	0.66
1:A:3332:THR:C	1:A:3334:PHE:H	1.99	0.66
1:B:1842:GLY:CA	1:B:1891:HIS:HA	2.14	0.66
1:B:2873:LEU:C	1:B:2875:ASP:N	2.47	0.66
1:A:2724:CYS:HA	1:A:2726:GLU:H	1.59	0.66
1:A:2726:GLU:CB	1:A:2727:GLU:CA	2.73	0.66
1:A:1747:VAL:CB	1:A:1751:GLN:O	2.44	0.66
1:B:2099:ASN:CB	1:B:2100:VAL:CB	2.74	0.66
1:A:3478:THR:CB	1:A:3482:GLY:O	2.44	0.66
1:A:2786:ILE:CA	1:A:3458:PHE:O	2.35	0.65
1:B:2155:ASP:CB	1:B:2157:ASP:H	2.09	0.65
1:A:2435:SER:N	1:A:2479:ILE:CA	2.55	0.65
1:B:3407:LEU:CB	1:B:3497:HIS:HA	2.26	0.65
1:A:3877:CYS:CB	1:A:3878:HIS:CB	2.75	0.65
1:B:3748:TRP:O	1:B:3752:THR:CB	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1585:VAL:O	1:B:1586:GLU:CB	2.42	0.65
1:B:2604:LYS:N	1:B:2610:GLY:H	1.95	0.65
1:B:2111:LYS:CB	1:B:2116:GLY:N	2.60	0.65
1:A:2343:ASN:O	1:A:2345:TYR:O	2.14	0.65
1:B:2435:SER:H	1:B:2479:ILE:CA	2.07	0.65
1:B:2539:THR:O	1:B:2540:ASP:C	2.33	0.65
1:A:2007:GLY:O	1:A:2011:GLU:CB	2.44	0.65
1:A:1872:LEU:C	1:A:1874:VAL:N	2.45	0.65
1:A:3861:GLU:O	1:A:3862:THR:C	2.34	0.65
1:B:2615:TYR:CA	1:B:2616:LEU:CB	2.74	0.65
1:B:1848:ASP:CB	1:B:1849:GLU:O	2.44	0.65
1:A:2301:TRP:C	1:A:2302:PHE:CA	2.64	0.65
1:A:2604:LYS:N	1:A:2610:GLY:H	1.95	0.65
1:A:2103:VAL:C	1:A:2105:ASP:H	1.94	0.65
1:B:2347:GLY:N	1:B:2348:HIS:CB	2.59	0.65
1:B:3478:THR:CB	1:B:3482:GLY:O	2.44	0.65
1:A:2382:ALA:CB	1:A:2386:MET:CB	2.75	0.65
1:A:2111:LYS:CB	1:A:2116:GLY:N	2.60	0.65
1:B:3889:LEU:N	1:B:3890:GLN:CA	2.59	0.65
1:A:3889:LEU:N	1:A:3890:GLN:CA	2.59	0.65
1:B:3432:LEU:CB	1:B:3456:GLU:CB	2.74	0.65
1:A:3739:ASP:H	1:A:3740:THR:CB	2.10	0.65
1:A:2099:ASN:CB	1:A:2100:VAL:CB	2.74	0.65
1:B:2604:LYS:O	1:B:2608:SER:CB	2.44	0.65
1:B:2098:ALA:HB1	1:B:2149:ARG:N	2.12	0.65
1:B:3877:CYS:CB	1:B:3878:HIS:CB	2.75	0.65
1:B:1691:SER:CB	1:B:1692:ASP:O	2.45	0.65
1:B:2726:GLU:CB	1:B:2727:GLU:CA	2.73	0.65
1:A:1691:SER:CB	1:A:1692:ASP:O	2.45	0.65
1:A:1848:ASP:CB	1:A:1849:GLU:O	2.44	0.65
1:A:2686:LEU:N	1:A:2687:GLY:HA2	2.09	0.65
1:A:1918:GLU:O	1:A:3996:GLY:HA2	1.97	0.65
1:A:3997:LYS:C	1:A:3999:ASP:CB	2.65	0.65
1:B:1848:ASP:CA	1:B:1849:GLU:C	2.66	0.65
1:B:1986:GLU:HA	1:B:1987:PHE:CA	2.27	0.64
1:A:1844:TRP:HA	1:A:1893:ALA:O	1.94	0.64
1:A:1631:LYS:HA	1:A:1635:ASP:HA	1.78	0.64
1:B:2786:ILE:CA	1:B:3458:PHE:O	2.35	0.64
1:A:3432:LEU:CB	1:A:3456:GLU:CB	2.74	0.64
1:B:2103:VAL:C	1:B:2105:ASP:H	1.94	0.64
1:A:1822:CYS:O	1:A:1824:ASP:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2382:ALA:CB	1:B:2386:MET:CB	2.74	0.64
1:A:1986:GLU:HA	1:A:1987:PHE:CA	2.27	0.64
1:A:2155:ASP:CB	1:A:2157:ASP:H	2.09	0.64
1:A:4034:LEU:C	1:A:4036:GLN:CB	2.66	0.64
1:A:2604:LYS:O	1:A:2608:SER:CB	2.44	0.64
1:B:3861:GLU:O	1:B:3862:THR:C	2.34	0.64
1:B:1827:ASP:CB	1:B:1828:TYR:CA	2.76	0.64
1:B:1636:ILE:O	1:B:1638:VAL:N	2.31	0.64
1:B:2372:CYS:N	1:B:2373:SER:CB	2.61	0.64
1:B:3332:THR:C	1:B:3334:PHE:H	1.99	0.64
1:B:1631:LYS:HA	1:B:1635:ASP:HA	1.78	0.64
1:B:3997:LYS:C	1:B:3999:ASP:CB	2.65	0.64
1:B:2435:SER:N	1:B:2479:ILE:CA	2.55	0.64
1:A:1493:LEU:O	1:A:1494:ASP:C	2.34	0.64
1:A:1824:ASP:O	1:A:1826:PHE:O	2.16	0.64
1:B:1918:GLU:O	1:B:3996:GLY:HA2	1.97	0.64
1:B:1822:CYS:O	1:B:1824:ASP:N	2.29	0.64
1:B:1747:VAL:CA	1:B:1752:SER:HA	2.27	0.64
1:A:1636:ILE:O	1:A:1638:VAL:N	2.31	0.63
1:B:2301:TRP:C	1:B:2302:PHE:CA	2.64	0.63
1:A:2372:CYS:N	1:A:2373:SER:CB	2.61	0.63
1:B:3335:GLY:O	1:B:3337:LEU:HA	1.99	0.63
1:A:1747:VAL:CA	1:A:1752:SER:HA	2.27	0.63
1:A:3335:GLY:O	1:A:3337:LEU:HA	1.99	0.63
1:A:3859:VAL:CB	1:A:3888:LEU:HA	2.28	0.63
1:B:4034:LEU:C	1:B:4036:GLN:CB	2.66	0.63
1:B:1824:ASP:O	1:B:1826:PHE:O	2.16	0.63
1:A:2188:PRO:CB	1:A:2189:ASN:HA	2.28	0.63
1:A:3666:ALA:CA	1:A:3667:ALA:HB3	2.27	0.63
1:B:1632:ASP:CB	1:B:1633:GLY:CA	2.75	0.63
1:A:2159:ASP:O	1:A:2160:PRO:C	2.35	0.63
1:A:4064:GLN:CB	1:A:4070:ILE:CB	2.77	0.63
1:A:2708:ASN:CB	1:A:2709:LYS:CB	2.77	0.63
1:B:3336:HIS:H	1:B:3337:LEU:CA	2.03	0.63
1:B:2390:ILE:O	1:B:2391:VAL:C	2.37	0.63
1:A:2603:CYS:CB	1:A:2610:GLY:H	2.12	0.63
1:A:3750:TYR:N	1:A:3752:THR:CB	2.62	0.63
1:A:3478:THR:CB	1:A:3483:ASP:CA	2.77	0.63
1:A:1969:GLY:O	1:A:1970:LEU:C	2.37	0.63
1:B:3750:TYR:N	1:B:3752:THR:CB	2.62	0.63
1:A:1848:ASP:CA	1:A:1849:GLU:C	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2873:LEU:O	1:A:2874:TYR:C	2.35	0.62
1:B:2188:PRO:CB	1:B:2189:ASN:HA	2.28	0.62
1:A:1842:GLY:C	1:A:1892:THR:N	2.53	0.62
1:A:1364:GLU:C	2:T:216:PRO:CA	2.64	0.62
1:B:3478:THR:CB	1:B:3483:ASP:CA	2.77	0.62
1:A:2000:ARG:O	1:A:2212:LEU:C	2.38	0.62
1:B:1747:VAL:CB	1:B:1752:SER:CA	2.77	0.62
1:B:1986:GLU:CA	1:B:1987:PHE:CA	2.77	0.62
1:B:2603:CYS:CB	1:B:2610:GLY:H	2.12	0.62
1:B:2861:ARG:HA	1:B:2868:ASP:CB	2.29	0.62
1:A:1632:ASP:CB	1:A:1633:GLY:CA	2.75	0.62
1:A:1986:GLU:CA	1:A:1987:PHE:CA	2.77	0.62
1:B:2873:LEU:O	1:B:2874:TYR:C	2.35	0.62
1:A:1747:VAL:CB	1:A:1752:SER:CA	2.77	0.62
1:B:2000:ARG:O	1:B:2212:LEU:C	2.38	0.62
1:B:1631:LYS:O	1:B:1636:ILE:HA	2.00	0.62
1:B:1631:LYS:C	1:B:1635:ASP:HA	2.20	0.62
1:B:2155:ASP:CB	1:B:2156:SER:C	2.68	0.62
1:B:2708:ASN:CB	1:B:2709:LYS:CB	2.77	0.62
1:A:2390:ILE:O	1:A:2391:VAL:C	2.37	0.62
1:B:1950:VAL:O	1:B:1954:GLU:CB	2.48	0.62
1:A:2155:ASP:CB	1:A:2156:SER:C	2.67	0.62
1:A:2195:GLU:O	1:A:2196:THR:C	2.37	0.62
1:A:2098:ALA:HB1	1:A:2149:ARG:N	2.12	0.62
1:A:2123:LEU:O	1:A:2124:GLU:CB	2.47	0.62
1:B:1842:GLY:C	1:B:1892:THR:N	2.53	0.62
1:A:2561:TYR:CB	1:A:2562:PRO:HA	2.30	0.62
1:A:2861:ARG:HA	1:A:2868:ASP:CB	2.29	0.62
1:A:1950:VAL:O	1:A:1954:GLU:CB	2.48	0.62
1:A:1753:GLY:O	1:A:1754:TYR:CB	2.48	0.62
1:B:2123:LEU:O	1:B:2124:GLU:CB	2.47	0.62
1:A:1631:LYS:C	1:A:1635:ASP:HA	2.20	0.62
1:B:3739:ASP:H	1:B:3740:THR:CB	2.10	0.62
1:A:3751:VAL:CB	1:A:3752:THR:HA	2.29	0.62
1:B:4064:GLN:CB	1:B:4070:ILE:CB	2.77	0.62
1:B:2195:GLU:O	1:B:2196:THR:C	2.37	0.61
1:B:2540:ASP:O	1:B:2542:GLY:N	2.33	0.61
1:B:1753:GLY:O	1:B:1754:TYR:CB	2.48	0.61
1:A:1364:GLU:CA	2:T:216:PRO:CB	2.67	0.61
1:B:1844:TRP:CA	1:B:1845:GLY:N	2.62	0.61
1:A:1550:GLY:CA	1:A:1551:SER:C	2.50	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3877:CYS:CB	1:A:3878:HIS:CA	2.78	0.61
1:A:3410:PRO:N	1:A:3411:SER:HA	2.16	0.61
1:A:2540:ASP:O	1:A:2542:GLY:N	2.33	0.61
1:A:2203:THR:O	1:A:2207:ILE:CB	2.48	0.61
1:A:3426:THR:CB	1:A:3427:VAL:N	2.27	0.61
1:A:1877:SER:O	1:A:1878:HIS:C	2.39	0.61
1:B:3478:THR:CA	1:B:3483:ASP:HA	2.27	0.61
1:B:3751:VAL:CB	1:B:3752:THR:HA	2.29	0.61
1:B:1840:GLN:HA	1:B:1889:SER:O	2.01	0.61
1:B:2561:TYR:CB	1:B:2562:PRO:HA	2.29	0.61
1:B:3666:ALA:CA	1:B:3667:ALA:HB3	2.27	0.61
1:A:3478:THR:CA	1:A:3483:ASP:HA	2.27	0.61
1:A:1840:GLN:HA	1:A:1889:SER:O	2.01	0.61
1:B:2203:THR:O	1:B:2207:ILE:CB	2.48	0.60
1:B:1932:MET:CB	1:B:1946:ALA:C	2.70	0.60
1:B:3859:VAL:CB	1:B:3888:LEU:HA	2.28	0.60
1:B:3410:PRO:N	1:B:3411:SER:HA	2.16	0.60
1:B:1466:GLN:N	1:B:1468:PHE:H	1.98	0.60
1:B:3877:CYS:CB	1:B:3878:HIS:CA	2.78	0.60
1:A:2907:ALA:C	1:A:2909:PHE:H	2.04	0.60
1:A:2130:PHE:C	1:A:2132:SER:N	2.54	0.60
1:B:3821:ASN:O	1:B:3823:ASN:N	2.30	0.60
1:B:1966:TYR:O	1:B:1967:HIS:CB	2.49	0.60
1:B:2159:ASP:O	1:B:2160:PRO:C	2.35	0.60
1:A:1631:LYS:O	1:A:1636:ILE:HA	2.00	0.60
1:B:2369:SER:O	1:B:2371:PHE:N	2.35	0.60
1:B:3807:SER:H	1:B:3809:GLU:H	1.48	0.60
1:B:1941:ASP:CA	1:B:1942:SER:CA	2.79	0.60
1:B:2107:LYS:O	1:B:2504:LEU:HA	2.02	0.60
1:B:1827:ASP:CB	1:B:1831:LEU:CB	2.79	0.60
1:A:1966:TYR:O	1:A:1967:HIS:CB	2.49	0.60
1:A:1466:GLN:N	1:A:1468:PHE:H	1.98	0.60
1:B:1466:GLN:CA	1:B:1468:PHE:N	2.64	0.60
1:A:2459:HIS:CB	1:A:2463:ASN:CB	2.80	0.60
1:A:1827:ASP:CB	1:A:1831:LEU:CB	2.80	0.60
1:A:2428:MET:O	1:A:2433:ARG:CB	2.49	0.60
1:B:4031:GLN:CB	1:B:4032:PRO:C	2.70	0.60
1:A:1872:LEU:O	1:A:1873:GLN:C	2.40	0.60
1:A:2411:LYS:CA	1:A:2554:ALA:O	2.49	0.60
1:A:3332:THR:C	1:A:3334:PHE:N	2.55	0.60
1:B:2130:PHE:C	1:B:2132:SER:N	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2369:SER:O	1:A:2371:PHE:N	2.34	0.60
1:A:4031:GLN:CB	1:A:4032:PRO:C	2.70	0.60
1:B:1872:LEU:O	1:B:1873:GLN:C	2.40	0.60
1:B:2459:HIS:CB	1:B:2463:ASN:CB	2.80	0.60
1:A:1851:ASN:CB	1:A:1897:THR:O	2.50	0.60
1:B:1848:ASP:O	1:B:1851:ASN:CB	2.50	0.60
1:A:2679:LYS:C	1:A:2681:LEU:HA	2.23	0.60
1:A:1529:ARG:HA	1:A:1532:ARG:CB	2.31	0.60
1:B:1969:GLY:O	1:B:1970:LEU:C	2.37	0.60
1:B:1942:SER:O	1:B:1945:LEU:CB	2.50	0.60
1:A:2785:LYS:O	1:A:3458:PHE:HA	1.53	0.60
1:A:2188:PRO:N	1:A:2189:ASN:HA	2.16	0.60
1:B:1529:ARG:HA	1:B:1532:ARG:CB	2.31	0.60
1:B:2639:GLN:O	1:B:2640:THR:CB	2.50	0.60
1:A:3376:LYS:O	1:A:3380:LEU:N	2.31	0.60
1:B:2371:PHE:CA	1:B:2372:CYS:CB	2.80	0.60
1:A:3754:LYS:C	1:A:3755:SER:CA	2.69	0.60
1:A:2307:ASP:O	1:A:2308:LYS:CB	2.50	0.60
1:B:1636:ILE:O	1:B:1637:GLU:C	2.40	0.59
1:A:1848:ASP:O	1:A:1851:ASN:CB	2.50	0.59
1:B:2428:MET:O	1:B:2433:ARG:CB	2.49	0.59
1:A:1827:ASP:CB	1:A:1828:TYR:CA	2.76	0.59
1:B:2307:ASP:O	1:B:2308:LYS:CB	2.50	0.59
1:A:1941:ASP:CA	1:A:1942:SER:CA	2.79	0.59
1:A:1942:SER:O	1:A:1945:LEU:CB	2.50	0.59
1:A:2579:PHE:O	1:A:2580:LYS:CB	2.49	0.59
1:A:2079:GLY:O	1:A:2080:LYS:C	2.40	0.59
1:A:1466:GLN:CA	1:A:1468:PHE:N	2.64	0.59
1:B:2411:LYS:CA	1:B:2554:ALA:O	2.49	0.59
1:A:3821:ASN:O	1:A:3823:ASN:N	2.30	0.59
1:B:1984:ILE:CB	1:B:1985:SER:CB	2.81	0.59
1:A:1984:ILE:CB	1:A:1985:SER:CB	2.81	0.59
1:B:1851:ASN:CB	1:B:1897:THR:O	2.50	0.59
1:A:2429:ASN:HA	1:A:2433:ARG:CB	2.32	0.59
1:A:1932:MET:CB	1:A:1946:ALA:C	2.70	0.59
1:A:3808:LYS:O	1:A:3809:GLU:C	2.41	0.59
1:B:2429:ASN:HA	1:B:2433:ARG:CB	2.32	0.59
1:A:2103:VAL:C	1:A:2105:ASP:N	2.56	0.59
1:B:1447:GLU:CA	1:B:1448:VAL:CB	2.71	0.59
1:A:1842:GLY:CA	1:A:1891:HIS:HA	2.14	0.59
1:B:2907:ALA:C	1:B:2909:PHE:H	2.04	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2371:PHE:CA	1:A:2372:CYS:CB	2.80	0.59
1:B:1942:SER:C	1:B:1945:LEU:H	2.05	0.59
1:A:3409:ASP:CA	1:A:3518:PHE:CB	2.81	0.59
1:A:3336:HIS:H	1:A:3337:LEU:CA	2.04	0.59
1:B:1986:GLU:HA	1:B:1987:PHE:CB	2.33	0.59
1:B:3754:LYS:C	1:B:3755:SER:CA	2.69	0.59
1:A:4013:HIS:O	1:A:4016:CYS:CB	2.51	0.59
1:A:2724:CYS:HA	1:A:2726:GLU:N	2.18	0.59
1:B:2679:LYS:C	1:B:2681:LEU:HA	2.22	0.59
1:B:4013:HIS:O	1:B:4016:CYS:CB	2.50	0.59
1:B:3808:LYS:O	1:B:3809:GLU:C	2.41	0.59
1:B:3845:GLN:CB	1:B:3878:HIS:HA	2.33	0.59
1:A:1398:TRP:HA	1:A:1402:GLU:CB	2.33	0.59
1:B:2000:ARG:C	1:B:2212:LEU:H	2.06	0.58
1:B:2513:GLN:O	1:B:2522:LYS:N	2.36	0.58
1:B:2379:SER:O	1:B:2380:LEU:O	2.20	0.58
1:B:2579:PHE:O	1:B:2580:LYS:CB	2.49	0.58
1:B:2724:CYS:HA	1:B:2726:GLU:N	2.18	0.58
1:B:3332:THR:C	1:B:3334:PHE:N	2.55	0.58
1:B:2376:PRO:O	1:B:2377:SER:C	2.41	0.58
1:B:1398:TRP:HA	1:B:1402:GLU:CB	2.33	0.58
1:A:1986:GLU:HA	1:A:1987:PHE:CB	2.33	0.58
1:A:2657:ALA:O	1:A:2914:ILE:O	2.21	0.58
1:A:3845:GLN:CB	1:A:3878:HIS:HA	2.33	0.58
1:B:2581:LEU:CB	1:B:2582:VAL:CB	2.80	0.58
1:B:2459:HIS:C	1:B:2463:ASN:CB	2.71	0.58
1:A:1942:SER:C	1:A:1945:LEU:H	2.05	0.58
1:A:2513:GLN:O	1:A:2522:LYS:N	2.36	0.58
1:B:2881:ILE:C	1:B:2883:LYS:N	2.56	0.58
1:A:2000:ARG:C	1:A:2212:LEU:H	2.06	0.58
1:B:3499:CYS:O	1:B:3501:PRO:CA	2.52	0.58
1:B:2188:PRO:N	1:B:2189:ASN:HA	2.16	0.58
1:A:2639:GLN:O	1:A:2640:THR:CB	2.50	0.58
1:A:1631:LYS:CA	1:A:1635:ASP:HA	2.33	0.58
1:B:1631:LYS:CA	1:B:1635:ASP:HA	2.33	0.58
1:B:3409:ASP:CA	1:B:3518:PHE:CB	2.81	0.58
1:A:2107:LYS:O	1:A:2504:LEU:HA	2.02	0.58
1:B:2079:GLY:O	1:B:2080:LYS:C	2.40	0.58
1:A:1364:GLU:HA	2:T:216:PRO:HA	0.58	0.58
1:A:2369:SER:C	1:A:2371:PHE:H	2.07	0.58
1:A:2376:PRO:O	1:A:2377:SER:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1465:ILE:O	1:A:1467:ASN:N	2.37	0.58
1:A:1636:ILE:O	1:A:1637:GLU:C	2.40	0.58
1:A:2873:LEU:O	1:A:2876:TRP:N	2.36	0.58
1:A:2581:LEU:CB	1:A:2582:VAL:CB	2.80	0.58
1:A:1478:SER:O	1:A:1480:THR:N	2.37	0.58
1:B:1465:ILE:O	1:B:1467:ASN:N	2.37	0.58
1:B:2103:VAL:C	1:B:2105:ASP:N	2.56	0.58
1:A:3900:ILE:CB	1:A:3901:PRO:HA	2.34	0.58
1:A:2379:SER:O	1:A:2380:LEU:O	2.20	0.58
1:A:2459:HIS:C	1:A:2463:ASN:CB	2.71	0.58
1:A:2347:GLY:N	1:A:2348:HIS:C	2.58	0.58
1:B:2909:PHE:O	1:B:2910:ASN:CB	2.52	0.58
1:A:2552:ARG:O	1:A:2553:HIS:C	2.42	0.58
1:B:2103:VAL:O	1:B:2105:ASP:N	2.35	0.57
1:A:3998:ILE:CA	1:A:3999:ASP:CB	2.79	0.57
1:B:2347:GLY:N	1:B:2348:HIS:C	2.58	0.57
1:B:1755:LEU:O	1:B:1756:LEU:CB	2.50	0.57
1:A:3499:CYS:O	1:A:3501:PRO:CA	2.52	0.57
1:B:2346:PHE:CB	1:B:2348:HIS:O	2.52	0.57
1:A:1849:GLU:CB	1:A:1850:PHE:C	2.73	0.57
1:A:2881:ILE:C	1:A:2883:LYS:N	2.56	0.57
1:A:3408:LEU:CB	1:A:3516:VAL:CB	2.83	0.57
1:B:2873:LEU:O	1:B:2875:ASP:CA	2.52	0.57
1:A:2346:PHE:CB	1:A:2348:HIS:O	2.52	0.57
1:B:3426:THR:CB	1:B:3427:VAL:N	2.27	0.57
1:A:1932:MET:CA	1:A:1946:ALA:HB1	2.18	0.57
1:B:3408:LEU:CB	1:B:3516:VAL:CB	2.83	0.57
1:A:1755:LEU:O	1:A:1756:LEU:CB	2.50	0.57
1:B:3376:LYS:O	1:B:3380:LEU:N	2.31	0.57
1:B:2000:ARG:O	1:B:2212:LEU:O	2.23	0.57
1:A:1844:TRP:CA	1:A:1845:GLY:N	2.62	0.57
1:B:3453:GLN:CB	1:B:3454:ASP:CA	2.82	0.57
1:B:2578:ILE:CB	1:B:2581:LEU:O	2.53	0.57
1:B:2301:TRP:CA	1:B:2302:PHE:N	2.66	0.57
1:A:3921:SER:CA	1:A:3922:GLY:O	2.53	0.57
1:B:1478:SER:O	1:B:1480:THR:N	2.37	0.57
1:B:2881:ILE:C	1:B:2883:LYS:H	2.07	0.57
1:A:2881:ILE:C	1:A:2883:LYS:H	2.07	0.57
1:B:1631:LYS:O	1:B:1635:ASP:CA	2.53	0.57
1:B:3899:ASP:CB	1:B:3900:ILE:CB	2.82	0.57
1:A:3453:GLN:CB	1:A:3454:ASP:CA	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1849:GLU:CB	1:B:1850:PHE:C	2.73	0.57
1:B:3864:ALA:O	1:B:3865:ALA:CB	2.53	0.57
1:B:1847:PHE:O	1:B:1896:ILE:HA	2.05	0.57
1:B:3900:ILE:CB	1:B:3901:PRO:HA	2.34	0.56
1:A:3751:VAL:N	1:A:3752:THR:CA	2.68	0.56
1:B:2709:LYS:CB	1:B:2710:THR:N	2.69	0.56
1:A:3899:ASP:CB	1:A:3900:ILE:CB	2.82	0.56
1:A:3807:SER:HA	1:A:3809:GLU:CA	2.34	0.56
1:B:2121:ALA:O	1:B:2122:THR:C	2.41	0.56
1:B:2512:LYS:CB	1:B:2522:LYS:O	2.53	0.56
1:A:3738:VAL:CA	1:A:3739:ASP:CB	2.77	0.56
1:B:2369:SER:C	1:B:2371:PHE:H	2.07	0.56
1:B:3921:SER:CA	1:B:3922:GLY:O	2.53	0.56
1:A:3807:SER:H	1:A:3809:GLU:H	1.49	0.56
1:B:2149:ARG:CB	1:B:2190:PHE:CB	2.83	0.56
1:B:1877:SER:O	1:B:1878:HIS:C	2.39	0.56
1:A:2909:PHE:O	1:A:2910:ASN:CB	2.52	0.56
1:B:2907:ALA:C	1:B:2909:PHE:N	2.58	0.56
1:B:2552:ARG:O	1:B:2553:HIS:C	2.42	0.56
1:A:2121:ALA:O	1:A:2122:THR:C	2.41	0.56
1:A:2317:LEU:CB	1:A:2355:ASP:CB	2.84	0.56
1:A:2512:LYS:CB	1:A:2522:LYS:O	2.54	0.56
1:B:2873:LEU:O	1:B:2876:TRP:N	2.36	0.56
1:B:2873:LEU:C	1:B:2875:ASP:H	2.06	0.56
1:A:1847:PHE:O	1:A:1896:ILE:HA	2.05	0.56
1:A:2149:ARG:CB	1:A:2190:PHE:CB	2.83	0.56
1:A:2873:LEU:O	1:A:2875:ASP:CA	2.52	0.56
1:B:2306:ASP:CB	1:B:2311:LYS:CB	2.84	0.56
1:A:2329:ASP:O	1:A:2330:SER:C	2.43	0.56
1:A:2907:ALA:C	1:A:2909:PHE:N	2.58	0.56
1:A:2343:ASN:C	1:A:2345:TYR:H	2.09	0.56
1:A:2301:TRP:O	1:A:2302:PHE:C	2.44	0.56
1:B:3358:VAL:O	1:B:3360:TYR:CB	2.54	0.56
1:B:2067:GLN:HA	1:B:2191:ARG:CB	2.35	0.56
1:B:1371:LEU:CB	2:S:165:ASP:HA	2.36	0.56
1:A:1631:LYS:O	1:A:1635:ASP:CA	2.53	0.56
1:A:1631:LYS:HA	1:A:1639:VAL:CB	2.36	0.56
1:A:3503:GLY:O	1:A:3504:ASP:C	2.42	0.56
1:A:3751:VAL:H	1:A:3752:THR:CB	2.18	0.56
1:A:2067:GLN:HA	1:A:2191:ARG:CB	2.35	0.56
1:A:2000:ARG:O	1:A:2212:LEU:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1466:GLN:HA	1:A:1468:PHE:N	2.06	0.56
1:B:3751:VAL:N	1:B:3752:THR:CA	2.68	0.56
1:A:3891:ARG:CB	1:A:3892:THR:CB	2.84	0.56
1:A:2578:ILE:CB	1:A:2581:LEU:O	2.53	0.56
1:A:2709:LYS:CB	1:A:2710:THR:N	2.69	0.55
1:A:2604:LYS:N	1:A:2610:GLY:CA	2.69	0.55
1:B:2329:ASP:O	1:B:2330:SER:C	2.43	0.55
1:A:2429:ASN:CA	1:A:2432:LEU:O	2.54	0.55
1:A:3358:VAL:O	1:A:3360:TYR:CB	2.54	0.55
1:B:2600:TYR:O	1:B:2610:GLY:CA	2.53	0.55
1:B:2343:ASN:C	1:B:2345:TYR:H	2.09	0.55
1:B:2317:LEU:CB	1:B:2355:ASP:CB	2.84	0.55
1:B:2774:ALA:C	1:B:2775:TRP:HA	2.26	0.55
1:B:2657:ALA:O	1:B:2914:ILE:O	2.21	0.55
1:B:3891:ARG:CB	1:B:3892:THR:CB	2.84	0.55
1:B:1844:TRP:O	1:B:1893:ALA:O	2.25	0.55
1:B:2604:LYS:N	1:B:2610:GLY:CA	2.69	0.55
1:A:3408:LEU:O	1:A:3518:PHE:CA	2.54	0.55
1:B:3751:VAL:H	1:B:3752:THR:CB	2.18	0.55
1:B:2429:ASN:CA	1:B:2432:LEU:O	2.54	0.55
1:A:1942:SER:O	1:A:1946:ALA:N	2.38	0.55
1:A:2600:TYR:O	1:A:2610:GLY:CA	2.53	0.55
1:A:2155:ASP:CA	1:A:2156:SER:C	2.75	0.55
1:B:3408:LEU:O	1:B:3518:PHE:CA	2.54	0.55
1:A:2615:TYR:CA	1:A:2616:LEU:CB	2.74	0.55
1:B:1951:HIS:O	1:B:1955:LEU:CB	2.54	0.55
1:B:1942:SER:O	1:B:1946:ALA:N	2.38	0.55
1:B:1631:LYS:HA	1:B:1639:VAL:CB	2.36	0.55
1:B:2600:TYR:CA	1:B:2613:SER:CB	2.83	0.55
1:A:1814:GLY:CA	1:A:1815:ARG:O	2.55	0.55
1:A:2306:ASP:CB	1:A:2311:LYS:CB	2.84	0.55
1:A:2774:ALA:C	1:A:2775:TRP:HA	2.26	0.55
1:B:2301:TRP:O	1:B:2302:PHE:C	2.44	0.55
1:B:2609:THR:HA	1:B:2612:GLN:CB	2.37	0.55
1:A:2105:ASP:HA	1:A:2154:PHE:C	2.16	0.55
1:B:3807:SER:HA	1:B:3809:GLU:CA	2.33	0.55
1:A:2435:SER:H	1:A:2479:ILE:CA	2.07	0.55
1:B:3356:PHE:H	1:B:3357:ALA:HB2	1.71	0.55
1:B:3336:HIS:O	1:B:3517:HIS:CB	2.56	0.54
1:B:2396:ASP:C	1:B:2398:ILE:N	2.61	0.54
1:B:3852:LYS:O	1:B:3856:HIS:N	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:HIS:O	1:A:1955:LEU:CB	2.54	0.54
1:A:3356:PHE:H	1:A:3357:ALA:HB2	1.71	0.54
1:B:2653:TRP:O	1:B:2656:PHE:HA	2.06	0.54
1:A:1364:GLU:O	2:T:216:PRO:C	2.45	0.54
1:A:2200:ASP:O	1:A:2204:PRO:N	2.40	0.54
1:A:1920:SER:CB	1:A:3998:ILE:HA	2.37	0.54
1:B:3998:ILE:CA	1:B:3999:ASP:CB	2.79	0.54
1:B:2155:ASP:CA	1:B:2156:SER:C	2.75	0.54
1:B:2200:ASP:O	1:B:2204:PRO:N	2.40	0.54
1:A:2627:ARG:CB	1:A:2651:GLU:CB	2.86	0.54
1:A:2653:TRP:O	1:A:2656:PHE:HA	2.06	0.54
1:A:2614:HIS:O	1:A:2616:LEU:CA	2.50	0.54
1:B:2614:HIS:O	1:B:2616:LEU:CA	2.50	0.54
1:B:2094:PHE:O	1:B:2095:ASP:CB	2.56	0.54
1:A:2869:THR:C	1:A:2870:GLU:O	2.41	0.54
1:B:2105:ASP:HA	1:B:2154:PHE:C	2.16	0.54
1:B:3503:GLY:O	1:B:3504:ASP:C	2.42	0.54
1:B:1814:GLY:CA	1:B:1815:ARG:O	2.55	0.54
1:A:1932:MET:CA	1:A:1946:ALA:HA	2.38	0.54
1:A:2609:THR:HA	1:A:2612:GLN:CB	2.37	0.54
1:A:3336:HIS:O	1:A:3517:HIS:CB	2.56	0.54
1:A:2396:ASP:C	1:A:2398:ILE:N	2.61	0.54
1:A:2118:MET:CA	1:A:2129:LEU:CB	2.81	0.54
1:A:2873:LEU:C	1:A:2875:ASP:H	2.06	0.54
1:B:1932:MET:CA	1:B:1946:ALA:HA	2.38	0.54
1:A:2937:PRO:O	1:A:2938:MET:C	2.47	0.54
1:B:2627:ARG:CB	1:B:2651:GLU:CB	2.86	0.54
1:A:3609:PRO:O	1:A:3610:GLN:CB	2.56	0.54
1:A:3452:ILE:O	1:A:3454:ASP:N	2.40	0.53
1:B:2937:PRO:O	1:B:2938:MET:C	2.47	0.53
1:B:2159:ASP:CB	1:B:2161:GLU:H	2.22	0.53
1:B:2869:THR:C	1:B:2870:GLU:O	2.41	0.53
1:B:3609:PRO:O	1:B:3610:GLN:CB	2.56	0.53
1:A:2000:ARG:O	1:A:2212:LEU:CA	2.55	0.53
1:B:1920:SER:CB	1:B:3998:ILE:HA	2.37	0.53
1:A:2347:GLY:N	1:A:2348:HIS:CA	2.71	0.53
1:B:2000:ARG:O	1:B:2212:LEU:CA	2.55	0.53
1:A:2604:LYS:CB	1:A:2610:GLY:CA	2.83	0.53
1:A:2094:PHE:O	1:A:2095:ASP:CB	2.56	0.53
1:B:3452:ILE:O	1:B:3454:ASP:N	2.40	0.53
1:A:2304:ASN:O	1:A:2305:LEU:CB	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:GLU:C	2:T:216:PRO:CB	2.77	0.53
1:B:2733:VAL:CB	1:B:2734:ILE:HA	2.39	0.53
1:B:2209:ARG:CB	1:B:2210:CYS:CA	2.87	0.53
1:A:3864:ALA:O	1:A:3865:ALA:CB	2.53	0.53
1:A:1844:TRP:O	1:A:1893:ALA:O	2.25	0.53
1:A:3499:CYS:O	1:A:3501:PRO:HA	2.09	0.53
1:A:2209:ARG:CB	1:A:2210:CYS:CA	2.87	0.53
1:B:3499:CYS:O	1:B:3501:PRO:HA	2.09	0.53
1:A:2733:VAL:CB	1:A:2734:ILE:HA	2.39	0.53
2:T:65:THR:O	2:T:66:GLN:CB	2.57	0.53
1:A:2604:LYS:H	1:A:2610:GLY:CA	2.21	0.53
2:T:23:LEU:O	2:T:25:GLU:N	2.42	0.53
1:B:3807:SER:CB	1:B:3809:GLU:CB	2.87	0.52
1:A:2159:ASP:CB	1:A:2161:GLU:H	2.22	0.52
1:A:2346:PHE:CA	1:A:2348:HIS:O	2.57	0.52
1:A:3852:LYS:O	1:A:3856:HIS:N	2.32	0.52
1:A:2301:TRP:CA	1:A:2302:PHE:N	2.66	0.52
1:B:3738:VAL:CA	1:B:3739:ASP:CB	2.77	0.52
1:A:3807:SER:CB	1:A:3809:GLU:CB	2.87	0.52
1:A:2757:MET:O	1:A:2758:LEU:CB	2.58	0.52
1:A:2774:ALA:CA	1:A:2775:TRP:HA	2.39	0.52
1:A:1447:GLU:CA	1:A:1448:VAL:CB	2.71	0.52
1:A:3809:GLU:O	1:A:3838:TRP:N	2.40	0.52
1:B:1497:ILE:C	1:B:1499:VAL:N	2.45	0.52
1:A:3333:TYR:O	1:A:3335:GLY:N	2.42	0.52
1:B:3333:TYR:O	1:B:3335:GLY:N	2.42	0.52
1:A:3748:TRP:O	1:A:3752:THR:HA	2.10	0.52
1:B:2430:ASN:CA	1:B:2432:LEU:CB	2.87	0.52
1:B:2304:ASN:O	1:B:2305:LEU:CB	2.57	0.52
1:A:2600:TYR:CA	1:A:2613:SER:CB	2.83	0.52
1:B:2604:LYS:H	1:B:2610:GLY:CA	2.21	0.52
1:A:1493:LEU:C	1:A:1495:THR:N	2.59	0.52
1:B:2346:PHE:CA	1:B:2348:HIS:O	2.57	0.52
1:B:1691:SER:O	1:B:1695:LYS:CB	2.58	0.52
1:A:2430:ASN:CA	1:A:2432:LEU:CB	2.87	0.52
1:B:1493:LEU:C	1:B:1495:THR:N	2.59	0.52
1:A:1691:SER:O	1:A:1695:LYS:CB	2.58	0.52
1:B:2774:ALA:CA	1:B:2775:TRP:HA	2.39	0.52
1:A:3878:HIS:HA	1:A:3880:THR:CB	2.40	0.52
1:B:2347:GLY:N	1:B:2348:HIS:CA	2.71	0.52
1:A:2336:ARG:O	1:A:2340:GLN:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1843:ALA:HB1	1:A:1844:TRP:C	2.27	0.52
1:B:3809:GLU:O	1:B:3838:TRP:N	2.40	0.52
1:B:2118:MET:CA	1:B:2129:LEU:CB	2.81	0.51
1:B:3336:HIS:O	1:B:3517:HIS:CA	2.58	0.51
1:B:2114:LEU:CB	1:B:2119:LEU:O	2.51	0.51
1:A:4033:LEU:O	1:A:4034:LEU:C	2.48	0.51
1:B:2429:ASN:HA	1:B:2432:LEU:O	2.11	0.51
1:A:1844:TRP:C	1:A:1845:GLY:CA	2.73	0.51
1:B:2434:ASN:CB	1:B:2435:SER:C	2.79	0.51
1:B:3995:GLY:C	1:B:3997:LYS:N	2.37	0.51
1:A:2103:VAL:O	1:A:2105:ASP:N	2.35	0.51
1:A:2429:ASN:HA	1:A:2432:LEU:O	2.11	0.51
1:B:2336:ARG:O	1:B:2340:GLN:CB	2.58	0.51
1:B:2291:ALA:O	1:B:2295:ILE:N	2.43	0.51
1:A:2114:LEU:O	1:A:2118:MET:O	2.29	0.51
1:B:2604:LYS:CA	1:B:2610:GLY:HA3	2.41	0.51
1:A:3336:HIS:O	1:A:3517:HIS:CA	2.58	0.51
1:B:2346:PHE:CB	1:B:2352:GLU:CB	2.89	0.51
1:B:3787:THR:O	1:B:3876:THR:HA	2.11	0.51
1:A:2371:PHE:CB	1:A:2372:CYS:CB	2.89	0.51
1:A:3502:SER:O	1:A:3503:GLY:C	2.49	0.51
1:B:4033:LEU:O	1:B:4034:LEU:C	2.48	0.51
1:B:3878:HIS:HA	1:B:3880:THR:CB	2.40	0.51
1:A:1428:CYS:CB	1:A:1429:LEU:HA	2.40	0.51
1:B:2757:MET:O	1:B:2758:LEU:CB	2.58	0.51
1:A:2434:ASN:CB	1:A:2435:SER:C	2.79	0.51
1:B:3748:TRP:O	1:B:3752:THR:HA	2.10	0.51
1:A:1734:PHE:O	1:A:1755:LEU:C	2.48	0.51
1:B:1428:CYS:CB	1:B:1429:LEU:HA	2.40	0.51
1:B:2114:LEU:O	1:B:2118:MET:O	2.29	0.51
1:A:2096:GLY:HA3	1:A:2146:LYS:CB	2.41	0.51
1:A:1624:ARG:CB	1:A:1647:ALA:HB2	2.38	0.51
1:A:2369:SER:C	1:A:2371:PHE:N	2.64	0.50
1:A:2346:PHE:CB	1:A:2352:GLU:CB	2.89	0.50
1:B:4061:SER:O	1:B:4062:TRP:C	2.47	0.50
1:A:1814:GLY:C	1:A:1815:ARG:CA	2.78	0.50
1:B:3404:VAL:HA	1:B:3494:LEU:CB	2.41	0.50
1:B:1734:PHE:O	1:B:1755:LEU:C	2.48	0.50
1:A:3637:GLN:C	1:A:3639:HIS:H	2.15	0.50
1:B:2371:PHE:CB	1:B:2372:CYS:CB	2.89	0.50
1:A:3750:TYR:CA	1:A:3752:THR:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3750:TYR:CA	1:B:3752:THR:CB	2.89	0.50
1:B:1843:ALA:HB1	1:B:1844:TRP:C	2.27	0.50
1:B:1844:TRP:HA	1:B:1893:ALA:N	2.27	0.50
1:A:4061:SER:O	1:A:4062:TRP:C	2.47	0.50
1:B:3502:SER:O	1:B:3503:GLY:C	2.49	0.50
1:A:1822:CYS:C	1:A:1824:ASP:N	2.65	0.50
1:A:3787:THR:O	1:A:3876:THR:HA	2.11	0.50
1:B:3420:ASN:O	1:B:3421:TYR:CB	2.60	0.50
1:B:2395:ILE:O	1:B:2397:THR:N	2.45	0.50
1:B:3637:GLN:C	1:B:3639:HIS:H	2.15	0.50
1:A:2604:LYS:CA	1:A:2610:GLY:HA3	2.41	0.50
1:B:1814:GLY:C	1:B:1815:ARG:CA	2.78	0.50
1:B:2096:GLY:HA3	1:B:2146:LYS:CB	2.41	0.50
1:A:2654:ARG:HA	1:A:2656:PHE:CB	2.42	0.50
1:B:4047:ALA:N	1:B:4048:ILE:N	2.24	0.50
1:A:2327:ALA:O	1:A:2328:GLY:O	2.30	0.50
1:A:3916:PHE:O	1:A:3918:GLY:HA3	2.12	0.50
2:T:40:TRP:O	2:T:44:LYS:N	2.44	0.50
1:B:1822:CYS:C	1:B:1824:ASP:N	2.65	0.49
1:A:3754:LYS:CA	1:A:3755:SER:N	2.71	0.49
1:B:2654:ARG:HA	1:B:2656:PHE:CB	2.42	0.49
1:A:2390:ILE:O	1:A:2391:VAL:O	2.30	0.49
1:B:2836:ALA:O	1:B:2837:ASN:CB	2.60	0.49
1:A:1941:ASP:CA	1:A:1942:SER:N	2.70	0.49
1:B:2195:GLU:O	1:B:2197:ASP:N	2.45	0.49
1:A:2395:ILE:O	1:A:2397:THR:N	2.45	0.49
1:B:1465:ILE:O	1:B:1467:ASN:CB	2.60	0.49
1:A:2069:ALA:HA	1:A:2192:ILE:O	2.11	0.49
1:B:1814:GLY:C	1:B:1815:ARG:C	2.71	0.49
1:A:4004:LEU:O	1:A:4008:ALA:HB2	2.12	0.49
1:B:3916:PHE:O	1:B:3918:GLY:HA3	2.12	0.49
1:B:1969:GLY:O	1:B:1971:ARG:N	2.45	0.49
1:A:1921:MET:O	1:A:1922:LYS:CB	2.58	0.49
1:A:1814:GLY:CA	1:A:1815:ARG:CA	2.86	0.49
1:A:1842:GLY:HA2	1:A:1892:THR:N	2.28	0.49
1:B:3781:SER:O	1:B:3782:GLU:CB	2.60	0.49
1:B:1921:MET:O	1:B:1922:LYS:CB	2.58	0.49
1:B:1922:LYS:O	1:B:1923:SER:CB	2.61	0.49
1:A:2532:VAL:O	1:A:2533:GLY:O	2.30	0.49
1:B:2369:SER:C	1:B:2371:PHE:N	2.64	0.49
1:A:3404:VAL:HA	1:A:3494:LEU:CB	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1624:ARG:CB	1:B:1647:ALA:HB2	2.38	0.49
1:A:2291:ALA:O	1:A:2295:ILE:N	2.43	0.49
1:A:1932:MET:HA	1:A:1946:ALA:HA	1.94	0.49
1:B:1942:SER:O	1:B:1944:SER:N	2.46	0.49
1:A:1844:TRP:HA	1:A:1893:ALA:N	2.27	0.49
1:B:2604:LYS:CB	1:B:2610:GLY:CA	2.83	0.49
1:A:2155:ASP:HA	1:A:2156:SER:C	2.33	0.49
1:B:2092:ALA:CA	1:B:2097:HIS:HA	2.39	0.49
1:B:3336:HIS:CB	1:B:3517:HIS:CB	2.91	0.49
1:A:1447:GLU:CA	1:A:1449:GLN:N	2.41	0.49
1:B:2069:ALA:HA	1:B:2192:ILE:O	2.11	0.49
1:B:3882:ASP:O	1:B:3883:LYS:CB	2.60	0.49
1:B:2327:ALA:O	1:B:2328:GLY:O	2.30	0.49
1:A:3676:TRP:O	1:A:3680:GLN:CB	2.61	0.49
1:A:1465:ILE:O	1:A:1467:ASN:CB	2.61	0.49
1:A:1922:LYS:O	1:A:1923:SER:CB	2.61	0.49
1:B:2532:VAL:O	1:B:2533:GLY:O	2.30	0.49
1:A:3781:SER:O	1:A:3782:GLU:CB	2.60	0.49
1:B:1366:VAL:CB	2:S:216:PRO:C	2.81	0.49
1:B:1986:GLU:C	1:B:1987:PHE:CB	2.81	0.49
1:A:1843:ALA:CA	1:A:1844:TRP:O	2.61	0.49
1:B:2155:ASP:HA	1:B:2156:SER:C	2.33	0.49
1:B:3921:SER:HA	1:B:3922:GLY:O	2.13	0.49
1:B:3479:VAL:N	1:B:3482:GLY:O	2.46	0.49
1:A:1942:SER:O	1:A:1944:SER:N	2.45	0.48
1:A:2301:TRP:C	1:A:2302:PHE:C	2.71	0.48
1:B:3807:SER:CA	1:B:3809:GLU:CB	2.91	0.48
1:A:2160:PRO:C	1:A:2162:TYR:N	2.43	0.48
1:A:1790:TYR:O	1:A:1916:PHE:CB	2.61	0.48
1:A:1969:GLY:O	1:A:1971:ARG:N	2.45	0.48
1:A:2289:GLN:CB	1:A:2407:LEU:CB	2.91	0.48
1:B:2289:GLN:CB	1:B:2407:LEU:CB	2.91	0.48
1:B:3665:ARG:C	1:B:3667:ALA:HB3	2.28	0.48
1:B:3360:TYR:C	1:B:3361:ASP:CA	2.76	0.48
1:A:2872:GLU:O	1:A:2873:LEU:C	2.51	0.48
1:A:2329:ASP:N	1:A:2333:GLU:CB	2.77	0.48
1:A:2836:ALA:O	1:A:2837:ASN:CB	2.60	0.48
1:B:1843:ALA:CA	1:B:1844:TRP:O	2.61	0.48
1:B:2301:TRP:C	1:B:2302:PHE:C	2.71	0.48
1:A:3336:HIS:CB	1:A:3517:HIS:CB	2.91	0.48
1:A:2107:LYS:CA	1:A:2503:VAL:C	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2107:LYS:CA	1:B:2503:VAL:C	2.81	0.48
1:B:1790:TYR:O	1:B:1916:PHE:CB	2.60	0.48
1:B:1918:GLU:O	1:B:3996:GLY:CA	2.61	0.48
1:A:1986:GLU:N	1:A:1987:PHE:CB	2.76	0.48
2:S:6:TYR:O	2:S:31:LEU:HA	2.12	0.48
1:B:3351:ARG:CB	1:B:3352:LEU:HA	2.43	0.48
1:A:3665:ARG:C	1:A:3667:ALA:HB3	2.28	0.48
1:B:3997:LYS:CB	1:B:4003:ASP:CB	2.92	0.48
1:A:2195:GLU:O	1:A:2197:ASP:N	2.45	0.48
1:A:2092:ALA:CA	1:A:2097:HIS:HA	2.39	0.48
1:B:1497:ILE:O	1:B:1499:VAL:CA	2.61	0.48
1:A:3991:THR:HA	1:A:3994:TYR:CB	2.44	0.48
1:A:1918:GLU:O	1:A:3996:GLY:CA	2.61	0.48
1:B:2001:VAL:O	1:B:2212:LEU:O	2.32	0.48
1:A:1814:GLY:C	1:A:1815:ARG:C	2.71	0.48
1:A:3420:ASN:O	1:A:3421:TYR:CB	2.60	0.48
1:B:2390:ILE:O	1:B:2391:VAL:O	2.30	0.48
1:A:3882:ASP:O	1:A:3883:LYS:CB	2.60	0.48
1:B:1986:GLU:N	1:B:1987:PHE:CB	2.76	0.48
1:B:2189:ASN:O	1:B:2190:PHE:CB	2.61	0.48
1:B:1842:GLY:HA2	1:B:1892:THR:N	2.28	0.48
1:A:1879:ILE:C	1:A:1887:PRO:O	2.50	0.48
1:B:3676:TRP:O	1:B:3680:GLN:CB	2.61	0.48
1:A:2343:ASN:C	1:A:2345:TYR:N	2.65	0.48
1:A:3754:LYS:CB	1:A:3755:SER:N	2.77	0.48
1:B:2329:ASP:N	1:B:2333:GLU:CB	2.77	0.48
1:B:3377:MET:O	1:B:3381:GLU:N	2.37	0.48
1:A:3351:ARG:CB	1:A:3352:LEU:HA	2.43	0.48
1:A:1986:GLU:C	1:A:1987:PHE:CB	2.81	0.48
1:B:2872:GLU:O	1:B:2873:LEU:C	2.51	0.48
1:A:3921:SER:HA	1:A:3922:GLY:O	2.13	0.48
1:A:3807:SER:CA	1:A:3809:GLU:CB	2.91	0.48
1:A:3479:VAL:N	1:A:3482:GLY:O	2.46	0.48
1:B:2343:ASN:C	1:B:2345:TYR:N	2.65	0.48
1:A:2122:THR:CB	1:A:2125:TRP:CB	2.91	0.48
1:A:1364:GLU:CB	2:T:216:PRO:CA	2.81	0.48
1:A:1691:SER:CB	1:A:1692:ASP:C	2.82	0.48
1:B:3991:THR:HA	1:B:3994:TYR:CB	2.44	0.48
1:B:1932:MET:HA	1:B:1946:ALA:HA	1.95	0.47
1:B:1844:TRP:C	1:B:1845:GLY:CA	2.73	0.47
1:A:2096:GLY:O	1:A:2097:HIS:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2522:LYS:O	1:B:2523:TRP:CB	2.62	0.47
1:B:3419:SER:O	1:B:3420:ASN:C	2.52	0.47
1:A:2189:ASN:O	1:A:2190:PHE:CB	2.61	0.47
1:B:1745:ASN:HA	1:B:1754:TYR:CB	2.44	0.47
1:A:2513:GLN:O	1:A:2522:LYS:CB	2.62	0.47
1:B:2155:ASP:N	1:B:2195:GLU:CB	2.76	0.47
1:A:3997:LYS:CB	1:A:4003:ASP:CB	2.92	0.47
1:A:2155:ASP:N	1:A:2195:GLU:CB	2.76	0.47
1:A:3411:SER:CB	1:A:3499:CYS:CB	2.93	0.47
1:B:2317:LEU:CB	1:B:2355:ASP:O	2.62	0.47
1:A:1987:PHE:O	1:A:1989:GLU:N	2.47	0.47
1:B:3754:LYS:CB	1:B:3755:SER:N	2.77	0.47
1:B:2159:ASP:O	1:B:2162:TYR:N	2.48	0.47
1:A:1941:ASP:CA	1:A:1942:SER:CB	2.93	0.47
1:B:3891:ARG:CB	1:B:3892:THR:CA	2.93	0.47
1:A:2604:LYS:HA	1:A:2608:SER:HA	1.96	0.47
1:B:2096:GLY:O	1:B:2097:HIS:C	2.53	0.47
1:A:1745:ASN:HA	1:A:1754:TYR:CB	2.44	0.47
1:B:2122:THR:CB	1:B:2125:TRP:CB	2.91	0.47
1:B:2513:GLN:O	1:B:2522:LYS:CB	2.62	0.47
1:A:3456:GLU:C	1:A:3460:PRO:CB	2.83	0.47
1:B:2434:ASN:CA	1:B:2435:SER:C	2.82	0.47
1:B:2459:HIS:CA	1:B:2463:ASN:CB	2.93	0.47
1:B:1691:SER:CB	1:B:1692:ASP:C	2.82	0.47
1:A:2317:LEU:CB	1:A:2355:ASP:O	2.62	0.47
1:A:3891:ARG:CB	1:A:3892:THR:CA	2.93	0.47
1:B:3889:LEU:N	1:B:3890:GLN:HA	2.30	0.47
1:B:3411:SER:CB	1:B:3499:CYS:CB	2.93	0.47
1:B:1843:ALA:HB1	1:B:1893:ALA:CA	2.45	0.47
1:A:1632:ASP:N	1:A:1633:GLY:CA	2.78	0.47
1:A:3360:TYR:C	1:A:3361:ASP:CA	2.76	0.47
1:B:2604:LYS:CA	1:B:2610:GLY:CA	2.93	0.47
1:A:2092:ALA:O	1:A:2097:HIS:N	2.48	0.47
1:B:4004:LEU:O	1:B:4008:ALA:HB2	2.12	0.47
1:A:2386:MET:HA	1:A:2390:ILE:CB	2.45	0.47
2:T:23:LEU:C	2:T:25:GLU:N	2.68	0.47
1:B:1632:ASP:N	1:B:1633:GLY:CA	2.78	0.46
1:B:1987:PHE:O	1:B:1989:GLU:N	2.47	0.46
1:A:3859:VAL:CB	1:A:3888:LEU:N	2.78	0.46
1:B:2786:ILE:O	1:B:3459:ASP:N	2.46	0.46
1:B:1814:GLY:CA	1:B:1815:ARG:CA	2.86	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1497:ILE:O	1:A:1499:VAL:CA	2.61	0.46
1:A:2459:HIS:CA	1:A:2463:ASN:CB	2.93	0.46
1:A:3761:ASN:O	1:A:3762:TRP:O	2.33	0.46
1:A:2001:VAL:O	1:A:2212:LEU:O	2.32	0.46
1:B:3456:GLU:C	1:B:3460:PRO:CB	2.83	0.46
1:B:2604:LYS:HA	1:B:2608:SER:HA	1.96	0.46
1:A:3419:SER:O	1:A:3420:ASN:C	2.52	0.46
2:S:65:THR:O	2:S:66:GLN:CB	2.64	0.46
1:A:2604:LYS:CA	1:A:2610:GLY:CA	2.93	0.46
1:A:2159:ASP:O	1:A:2162:TYR:N	2.48	0.46
1:B:2386:MET:HA	1:B:2390:ILE:CB	2.45	0.46
1:B:2410:SER:O	1:B:2553:HIS:CB	2.64	0.46
1:B:2514:GLY:CA	1:B:2520:GLU:O	2.58	0.46
1:B:3761:ASN:O	1:B:3762:TRP:O	2.33	0.46
1:B:3754:LYS:CA	1:B:3755:SER:N	2.71	0.46
1:B:1869:GLN:O	1:B:1873:GLN:CA	2.61	0.46
1:B:1879:ILE:C	1:B:1887:PRO:O	2.50	0.46
1:A:2786:ILE:O	1:A:3459:ASP:N	2.46	0.46
1:B:2105:ASP:HA	1:B:2157:ASP:CB	2.43	0.46
1:B:2429:ASN:C	1:B:2432:LEU:C	2.73	0.46
1:B:3821:ASN:C	1:B:3823:ASN:H	2.17	0.46
1:A:1495:THR:O	1:A:1497:ILE:N	2.49	0.46
1:A:2383:HIS:O	1:A:2386:MET:N	2.47	0.46
1:A:2079:GLY:O	1:A:2081:THR:N	2.49	0.46
1:A:2532:VAL:O	1:A:2533:GLY:C	2.54	0.46
1:A:1843:ALA:HB1	1:A:1893:ALA:CA	2.45	0.46
1:A:4061:SER:C	1:A:4066:PRO:HA	2.18	0.46
1:B:1466:GLN:CB	1:B:1469:LEU:CA	2.94	0.46
1:B:2092:ALA:O	1:B:2097:HIS:N	2.48	0.46
1:B:2149:ARG:O	1:B:2190:PHE:HA	2.16	0.46
1:A:2116:GLY:O	1:A:2130:PHE:CB	2.64	0.46
1:A:2861:ARG:CB	1:A:2868:ASP:CB	2.94	0.46
1:A:2105:ASP:HA	1:A:2157:ASP:CB	2.43	0.46
1:B:3877:CYS:CB	1:B:3878:HIS:O	2.64	0.46
1:B:2861:ARG:CB	1:B:2868:ASP:CB	2.94	0.46
1:B:3711:GLU:HA	1:B:3712:SER:HA	1.53	0.46
1:B:3859:VAL:CB	1:B:3888:LEU:N	2.78	0.46
1:A:2522:LYS:O	1:A:2523:TRP:CB	2.62	0.46
1:A:3889:LEU:N	1:A:3890:GLN:HA	2.30	0.46
1:B:3410:PRO:C	1:B:3412:SER:N	2.68	0.46
1:A:2149:ARG:O	1:A:2190:PHE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3430:SER:O	1:A:3433:GLU:CB	2.64	0.46
1:B:3570:LEU:C	1:B:3572:ASN:N	2.68	0.46
1:A:2434:ASN:CA	1:A:2435:SER:C	2.82	0.45
1:B:1495:THR:O	1:B:1497:ILE:N	2.49	0.45
1:A:2680:TYR:N	1:A:2681:LEU:CA	2.74	0.45
1:A:3711:GLU:HA	1:A:3712:SER:HA	1.53	0.45
1:B:3409:ASP:O	1:B:3410:PRO:CB	2.63	0.45
1:A:3845:GLN:CB	1:A:3878:HIS:CA	2.95	0.45
1:B:2384:GLU:O	1:B:2387:ARG:N	2.48	0.45
1:A:2410:SER:O	1:A:2553:HIS:CB	2.64	0.45
1:B:2532:VAL:O	1:B:2533:GLY:C	2.54	0.45
1:A:2609:THR:O	1:A:2610:GLY:C	2.54	0.45
1:B:2092:ALA:C	1:B:2097:HIS:HA	2.37	0.45
1:A:1789:LYS:O	1:A:1790:TYR:CB	2.59	0.45
1:B:2073:VAL:O	1:B:2214:TRP:HA	2.17	0.45
1:B:2609:THR:O	1:B:2610:GLY:C	2.54	0.45
1:A:1872:LEU:C	1:A:1875:GLY:H	2.19	0.45
1:B:3845:GLN:CB	1:B:3878:HIS:CA	2.95	0.45
1:B:3666:ALA:CB	1:B:3669:THR:N	2.54	0.45
1:B:3456:GLU:O	1:B:3460:PRO:CB	2.65	0.45
1:B:3899:ASP:CB	1:B:3900:ILE:CA	2.95	0.45
1:A:2092:ALA:C	1:A:2097:HIS:HA	2.37	0.45
1:A:2333:GLU:O	1:A:2334:SER:C	2.51	0.45
1:A:3570:LEU:C	1:A:3572:ASN:N	2.68	0.45
1:A:1942:SER:C	1:A:1944:SER:N	2.70	0.45
1:A:3409:ASP:O	1:A:3410:PRO:CB	2.63	0.45
1:A:3821:ASN:C	1:A:3823:ASN:H	2.17	0.45
1:B:2535:CYS:O	1:B:2536:ASN:C	2.54	0.45
1:B:1941:ASP:CA	1:B:1942:SER:CB	2.93	0.45
1:B:3359:LYS:CA	1:B:3360:TYR:CB	2.95	0.45
1:A:1466:GLN:CB	1:A:1469:LEU:CA	2.94	0.45
1:B:1789:LYS:O	1:B:1790:TYR:CB	2.59	0.45
1:B:2774:ALA:HA	1:B:2775:TRP:HA	1.99	0.45
1:A:1466:GLN:CA	1:A:1468:PHE:H	2.27	0.45
1:B:3430:SER:O	1:B:3433:GLU:CB	2.64	0.45
2:S:60:GLY:C	2:S:62:VAL:H	2.20	0.45
1:A:2073:VAL:O	1:A:2214:TRP:HA	2.17	0.45
1:A:3456:GLU:O	1:A:3460:PRO:CB	2.65	0.45
1:A:2514:GLY:CA	1:A:2520:GLU:O	2.58	0.45
1:A:2114:LEU:CB	1:A:2119:LEU:O	2.51	0.45
1:A:2001:VAL:C	1:A:2212:LEU:O	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3361:ASP:O	1:A:3362:VAL:CB	2.65	0.45
1:B:1466:GLN:CA	1:B:1468:PHE:H	2.27	0.45
1:B:2116:GLY:O	1:B:2130:PHE:CB	2.64	0.45
1:B:1579:ILE:HA	1:B:1584:SER:HA	1.98	0.45
1:B:2079:GLY:O	1:B:2081:THR:N	2.49	0.44
1:A:2940:PHE:HA	1:A:2941:THR:CB	2.48	0.44
1:B:2001:VAL:C	1:B:2212:LEU:O	2.55	0.44
1:A:2774:ALA:HA	1:A:2775:TRP:HA	1.99	0.44
1:B:2686:LEU:H	1:B:2687:GLY:CA	2.22	0.44
1:A:2140:ASP:C	1:A:2142:THR:N	2.71	0.44
1:A:2535:CYS:O	1:A:2536:ASN:C	2.54	0.44
1:B:2003:LEU:N	1:B:2212:LEU:O	2.51	0.44
1:A:3359:LYS:CA	1:A:3360:TYR:CB	2.95	0.44
1:B:3921:SER:HA	1:B:3922:GLY:HA3	1.87	0.44
1:A:2206:THR:HA	1:A:2209:ARG:O	2.17	0.44
1:B:2206:THR:HA	1:B:2209:ARG:O	2.17	0.44
1:B:1986:GLU:CA	1:B:1987:PHE:C	2.77	0.44
1:A:2442:GLY:CA	1:A:2485:PHE:CB	2.92	0.44
1:A:3754:LYS:O	1:A:3755:SER:C	2.55	0.44
1:A:1550:GLY:C	1:A:1552:GLY:N	2.71	0.44
1:B:2654:ARG:C	1:B:2656:PHE:N	2.71	0.44
1:B:3748:TRP:O	1:B:3752:THR:CA	2.66	0.44
1:A:1579:ILE:HA	1:A:1584:SER:HA	1.98	0.44
1:B:1941:ASP:CA	1:B:1942:SER:N	2.70	0.44
1:A:2003:LEU:N	1:A:2212:LEU:O	2.51	0.44
1:B:2302:PHE:O	1:B:2303:GLN:C	2.55	0.44
1:A:4035:GLN:HA	1:A:4037:SER:N	2.33	0.44
1:A:3410:PRO:C	1:A:3412:SER:N	2.68	0.44
1:B:2333:GLU:O	1:B:2334:SER:C	2.51	0.44
1:B:1848:ASP:N	1:B:1849:GLU:C	2.71	0.44
1:A:1882:LEU:N	1:A:1885:GLU:O	2.51	0.44
1:B:1942:SER:C	1:B:1944:SER:N	2.70	0.44
1:A:3787:THR:N	1:A:3875:MET:O	2.50	0.44
1:A:3378:LYS:O	1:A:3381:GLU:O	2.35	0.44
1:A:3666:ALA:CB	1:A:3669:THR:N	2.54	0.43
1:A:1635:ASP:HA	1:A:1636:ILE:HA	1.69	0.43
1:A:2107:LYS:CA	1:A:2503:VAL:O	2.66	0.43
1:A:3748:TRP:O	1:A:3752:THR:CA	2.66	0.43
1:A:1848:ASP:N	1:A:1849:GLU:C	2.70	0.43
1:B:3476:ARG:O	1:B:3477:VAL:CB	2.66	0.43
1:B:3378:LYS:O	1:B:3381:GLU:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:ASN:HA	1:A:1420:TYR:C	2.39	0.43
1:A:3687:SER:C	1:A:3689:ALA:H	2.21	0.43
1:A:3642:TYR:O	1:A:3643:GLY:C	2.56	0.43
1:A:3890:GLN:CA	1:A:3891:ARG:O	2.67	0.43
1:B:1872:LEU:C	1:B:1875:GLY:H	2.19	0.43
1:A:1842:GLY:CA	1:A:1892:THR:N	2.82	0.43
1:A:2107:LYS:C	1:A:2503:VAL:C	2.77	0.43
1:B:1842:GLY:CA	1:B:1892:THR:N	2.82	0.43
1:A:2429:ASN:C	1:A:2432:LEU:C	2.73	0.43
1:B:2820:SER:CB	1:B:2899:SER:CB	2.96	0.43
2:T:51:PHE:O	2:T:52:PRO:C	2.57	0.43
1:A:3995:GLY:C	1:A:3997:LYS:N	2.37	0.43
1:B:4035:GLN:HA	1:B:4037:SER:N	2.33	0.43
1:B:1882:LEU:N	1:B:1885:GLU:O	2.51	0.43
1:B:3754:LYS:O	1:B:3755:SER:C	2.55	0.43
1:A:3877:CYS:CB	1:A:3879:LEU:HA	2.48	0.43
1:B:4046:THR:C	1:B:4048:ILE:N	2.72	0.43
1:B:3890:GLN:CA	1:B:3891:ARG:O	2.67	0.43
1:B:2603:CYS:O	1:B:2608:SER:N	2.52	0.43
1:A:3877:CYS:CB	1:A:3878:HIS:O	2.64	0.43
1:B:2107:LYS:CA	1:B:2503:VAL:O	2.66	0.43
1:B:3877:CYS:CB	1:B:3879:LEU:HA	2.48	0.43
1:B:2140:ASP:C	1:B:2142:THR:N	2.71	0.43
1:A:2281:PHE:O	1:A:2284:LEU:N	2.51	0.43
1:B:3361:ASP:O	1:B:3362:VAL:CB	2.65	0.43
1:B:3713:GLU:CA	1:B:3714:GLN:C	2.87	0.43
1:B:1951:HIS:O	1:B:1955:LEU:N	2.52	0.43
1:A:2820:SER:CB	1:A:2899:SER:CB	2.96	0.43
1:A:3784:ASN:O	1:A:3893:ASP:HA	2.19	0.43
1:A:1869:GLN:O	1:A:1873:GLN:CA	2.61	0.43
1:B:1550:GLY:C	1:B:1552:GLY:N	2.71	0.43
1:A:2654:ARG:C	1:A:2656:PHE:N	2.71	0.43
1:B:2410:SER:CB	1:B:2528:ARG:O	2.67	0.43
1:B:3642:TYR:O	1:B:3643:GLY:C	2.56	0.43
1:B:1419:ASN:HA	1:B:1420:TYR:C	2.39	0.43
1:A:2302:PHE:O	1:A:2303:GLN:C	2.55	0.43
1:A:3713:GLU:CA	1:A:3714:GLN:C	2.87	0.43
1:A:2384:GLU:O	1:A:2387:ARG:N	2.48	0.43
1:B:1823:ASP:O	1:B:1853:LEU:O	2.36	0.43
1:B:2940:PHE:HA	1:B:2941:THR:CB	2.47	0.43
1:A:2608:SER:N	1:A:2609:THR:CB	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1823:ASP:O	1:A:1853:LEU:O	2.36	0.43
1:A:2603:CYS:O	1:A:2608:SER:N	2.52	0.42
1:B:2608:SER:N	1:B:2609:THR:CB	2.82	0.42
1:A:3687:SER:O	1:A:3688:THR:C	2.58	0.42
1:A:2410:SER:CB	1:A:2528:ARG:O	2.67	0.42
1:A:1932:MET:CB	1:A:1946:ALA:O	2.68	0.42
1:A:2708:ASN:N	1:A:2709:LYS:CB	2.83	0.42
1:A:3998:ILE:CB	1:A:3999:ASP:CB	2.98	0.42
1:A:1447:GLU:HA	1:A:1448:VAL:CB	2.49	0.42
1:A:3685:GLN:O	1:A:3686:PHE:CB	2.64	0.42
1:A:2144:THR:HA	1:A:2145:PHE:C	2.40	0.42
1:B:2654:ARG:C	1:B:2656:PHE:H	2.22	0.42
1:A:3568:GLU:O	1:A:3571:ASN:CB	2.67	0.42
1:B:2281:PHE:O	1:B:2284:LEU:N	2.51	0.42
1:A:3410:PRO:O	1:A:3412:SER:N	2.53	0.42
1:B:3821:ASN:C	1:B:3823:ASN:N	2.73	0.42
1:B:3784:ASN:O	1:B:3893:ASP:HA	2.19	0.42
1:A:2654:ARG:C	1:A:2656:PHE:H	2.22	0.42
1:B:2383:HIS:O	1:B:2386:MET:N	2.47	0.42
1:A:3377:MET:O	1:A:3381:GLU:N	2.37	0.42
1:B:4068:GLU:O	1:B:4069:SER:CB	2.67	0.42
1:B:1447:GLU:HA	1:B:1448:VAL:CB	2.49	0.42
1:B:3462:ILE:C	1:B:3464:ARG:N	2.73	0.42
1:B:1833:ARG:C	1:B:1835:LEU:N	2.73	0.42
1:B:2708:ASN:N	1:B:2709:LYS:CB	2.83	0.42
1:A:3899:ASP:CB	1:A:3900:ILE:CA	2.95	0.42
1:B:2145:PHE:HA	1:B:2146:LYS:HA	1.68	0.42
1:B:3475:ASN:O	1:B:3485:GLU:CA	2.68	0.42
1:A:3475:ASN:O	1:A:3485:GLU:CA	2.68	0.42
1:A:2383:HIS:O	1:A:2384:GLU:C	2.57	0.42
1:B:2709:LYS:C	1:B:2710:THR:CA	2.81	0.42
1:B:4035:GLN:HA	1:B:4036:GLN:C	2.38	0.42
1:B:3998:ILE:CB	1:B:3999:ASP:CB	2.98	0.42
1:B:3410:PRO:O	1:B:3412:SER:N	2.53	0.42
1:A:1842:GLY:HA2	1:A:1891:HIS:C	2.40	0.42
1:B:1842:GLY:HA2	1:B:1891:HIS:C	2.41	0.42
1:B:2383:HIS:O	1:B:2384:GLU:C	2.57	0.42
1:A:2343:ASN:O	1:A:2345:TYR:N	2.53	0.42
1:B:2093:ILE:O	1:B:2094:PHE:C	2.59	0.42
1:B:3568:GLU:O	1:B:3571:ASN:CB	2.67	0.42
1:A:2575:TYR:O	1:A:2576:LYS:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2575:TYR:O	1:B:2576:LYS:O	2.38	0.42
1:B:1932:MET:CB	1:B:1946:ALA:O	2.68	0.42
1:A:3842:GLN:O	1:A:3843:ASN:CB	2.67	0.42
2:T:23:LEU:C	2:T:25:GLU:H	2.24	0.42
1:B:2442:GLY:CA	1:B:2485:PHE:CB	2.92	0.41
1:A:2709:LYS:C	1:A:2710:THR:CA	2.81	0.41
1:B:2540:ASP:O	1:B:2542:GLY:O	2.38	0.41
1:B:3842:GLN:O	1:B:3843:ASN:CB	2.67	0.41
1:B:2343:ASN:O	1:B:2345:TYR:N	2.53	0.41
1:B:1861:VAL:O	1:B:1864:ASN:N	2.53	0.41
1:B:2165:ALA:C	1:B:2167:ASN:N	2.73	0.41
1:B:2452:GLU:O	1:B:2455:LEU:N	2.53	0.41
1:A:1861:VAL:O	1:A:1864:ASN:N	2.53	0.41
1:B:3687:SER:C	1:B:3689:ALA:H	2.21	0.41
1:B:1833:ARG:O	1:B:1836:VAL:N	2.53	0.41
1:A:1833:ARG:C	1:A:1835:LEU:N	2.73	0.41
1:A:1781:THR:O	1:A:1784:ASP:N	2.53	0.41
1:B:3410:PRO:N	1:B:3411:SER:CA	2.83	0.41
1:B:2096:GLY:CA	1:B:2146:LYS:CB	2.98	0.41
1:B:1837:GLY:O	1:B:1841:ILE:CB	2.68	0.41
1:B:3409:ASP:O	1:B:3411:SER:HA	2.19	0.41
1:A:1865:ILE:O	1:A:1869:GLN:CB	2.69	0.41
1:A:1843:ALA:CB	1:A:1844:TRP:CA	2.37	0.41
1:A:3815:PRO:O	1:A:3816:LEU:CB	2.69	0.41
1:B:1781:THR:C	1:B:1783:THR:N	2.73	0.41
1:B:2149:ARG:O	1:B:2190:PHE:CA	2.69	0.41
1:B:2107:LYS:C	1:B:2503:VAL:C	2.77	0.41
1:B:3990:ALA:O	1:B:3993:VAL:CB	2.60	0.41
1:A:1418:SER:HA	1:A:1419:ASN:HA	1.91	0.41
1:B:3462:ILE:O	1:B:3465:LEU:N	2.53	0.41
1:A:1781:THR:C	1:A:1783:THR:N	2.73	0.41
1:B:3466:ILE:O	1:B:3470:PHE:CB	2.69	0.41
1:B:2238:ASP:O	1:B:2239:ASN:C	2.59	0.41
1:A:3807:SER:HA	1:A:3809:GLU:CB	2.50	0.41
1:A:3476:ARG:O	1:A:3477:VAL:CB	2.66	0.41
1:A:4068:GLU:O	1:A:4069:SER:CB	2.67	0.41
1:A:2301:TRP:N	1:A:2302:PHE:N	2.69	0.41
1:B:1826:PHE:O	1:B:1827:ASP:O	2.38	0.41
1:B:3784:ASN:O	1:B:3893:ASP:CB	2.69	0.41
1:A:1861:VAL:C	1:A:1863:ALA:N	2.73	0.41
1:A:3462:ILE:C	1:A:3464:ARG:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1932:MET:C	1:A:1946:ALA:HB1	2.37	0.41
1:B:4058:SER:O	1:B:4061:SER:N	2.52	0.41
1:A:1826:PHE:O	1:A:1827:ASP:O	2.38	0.41
1:B:2099:ASN:HA	1:B:2100:VAL:HA	1.87	0.41
1:A:3821:ASN:C	1:A:3823:ASN:N	2.73	0.41
1:A:3784:ASN:O	1:A:3893:ASP:CB	2.69	0.41
1:A:1833:ARG:O	1:A:1836:VAL:N	2.53	0.41
1:A:3462:ILE:O	1:A:3465:LEU:N	2.53	0.41
2:S:23:LEU:O	2:S:25:GLU:N	2.54	0.41
1:A:2452:GLU:O	1:A:2455:LEU:N	2.53	0.41
1:A:1837:GLY:O	1:A:1841:ILE:CB	2.68	0.41
1:A:2600:TYR:CB	1:A:2613:SER:CB	2.98	0.41
1:B:2600:TYR:CB	1:B:2613:SER:CB	2.98	0.41
1:A:4010:LEU:O	1:A:4013:HIS:N	2.54	0.41
1:B:4010:LEU:O	1:B:4013:HIS:N	2.54	0.41
1:B:3804:ALA:C	1:B:3806:ALA:H	2.24	0.41
1:A:2096:GLY:CA	1:A:2146:LYS:CB	2.98	0.41
1:B:1865:ILE:O	1:B:1869:GLN:CB	2.69	0.40
1:B:2535:CYS:O	1:B:2537:PRO:N	2.54	0.40
1:A:3466:ILE:O	1:A:3470:PHE:CB	2.69	0.40
1:B:2114:LEU:HA	1:B:2118:MET:C	2.40	0.40
1:B:2114:LEU:O	1:B:2119:LEU:CB	2.62	0.40
1:A:2149:ARG:O	1:A:2190:PHE:CA	2.69	0.40
1:A:2540:ASP:O	1:A:2542:GLY:O	2.38	0.40
1:A:2733:VAL:CB	1:A:2734:ILE:CA	3.00	0.40
1:A:3462:ILE:O	1:A:3464:ARG:N	2.55	0.40
1:B:2169:VAL:HA	1:B:2170:LEU:HA	1.73	0.40
1:B:1635:ASP:HA	1:B:1636:ILE:HA	1.69	0.40
1:A:2114:LEU:HA	1:A:2118:MET:C	2.40	0.40
1:B:2301:TRP:N	1:B:2302:PHE:N	2.69	0.40
1:B:2539:THR:C	1:B:2541:PRO:N	2.74	0.40
1:B:3815:PRO:O	1:B:3816:LEU:CB	2.69	0.40
1:B:2733:VAL:CB	1:B:2734:ILE:CA	3.00	0.40
1:A:1632:ASP:N	1:A:1635:ASP:CB	2.84	0.40
1:A:3503:GLY:C	1:A:3505:ILE:N	2.68	0.40
1:B:3807:SER:HA	1:B:3809:GLU:CB	2.50	0.40
1:B:2861:ARG:CA	1:B:2868:ASP:CB	2.98	0.40
1:B:2165:ALA:O	1:B:2167:ASN:N	2.55	0.40
1:A:3804:ALA:C	1:A:3806:ALA:H	2.24	0.40
1:A:2686:LEU:H	1:A:2687:GLY:CA	2.22	0.40
1:B:3687:SER:O	1:B:3688:THR:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1951:HIS:O	1:A:1955:LEU:N	2.52	0.40
1:B:1833:ARG:O	1:B:1835:LEU:N	2.55	0.40
1:B:1861:VAL:O	1:B:1863:ALA:N	2.55	0.40
1:A:1861:VAL:O	1:A:1863:ALA:N	2.55	0.40
1:A:1781:THR:O	1:A:1783:THR:N	2.55	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2245:GLU:N	1:B:2241:LEU:CB[1_554]	1.43	0.77
1:A:2245:GLU:CA	1:B:2241:LEU:CB[1_554]	1.81	0.39
1:A:2245:GLU:CB	1:B:2241:LEU:CB[1_554]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2039/2486 (82%)	1605 (79%)	307 (15%)	127 (6%)	2 25
1	B	2039/2486 (82%)	1605 (79%)	308 (15%)	126 (6%)	2 25
2	S	214/219 (98%)	194 (91%)	16 (8%)	4 (2%)	10 52
2	T	214/219 (98%)	190 (89%)	20 (9%)	4 (2%)	10 52
All	All	4506/5410 (83%)	3594 (80%)	651 (14%)	261 (6%)	2 27

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1470	PRO
1	A	1494	ASP
1	A	1498	GLU

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Mol	Chain	Res	Type
1	A	1635	ASP
1	A	1637	GLU
1	A	1748	PHE
1	A	1887	PRO
1	A	1917	ARG
1	A	1940	GLU
1	A	2108	VAL
1	A	2185	PRO
1	A	2187	PRO
1	A	2188	PRO
1	A	2302	PHE
1	A	2330	SER
1	A	2375	ILE
1	A	2376	PRO
1	A	2380	LEU
1	A	2388	PRO
1	A	2391	VAL
1	A	2393	PRO
1	A	2395	ILE
1	A	2419	PRO
1	A	2420	PRO
1	A	2433	ARG
1	A	2525	THR
1	A	2536	ASN
1	A	2540	ASP
1	A	2543	ARG
1	A	2553	HIS
1	A	2576	LYS
1	A	2578	ILE
1	A	2682	PRO
1	A	2758	LEU
1	A	2874	TYR
1	A	2894	PRO
1	A	2910	ASN
1	A	2913	ILE
1	A	3362	VAL
1	A	3370	LEU
1	A	3371	VAL
1	A	3405	PRO
1	A	3410	PRO
1	A	3453	GLN
1	A	3454	ASP

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Mol	Chain	Res	Type
1	A	3458	PHE
1	A	3479	VAL
1	A	3485	GLU
1	A	3500	ASP
1	A	3501	PRO
1	A	3502	SER
1	A	3762	TRP
1	A	3807	SER
1	A	3809	GLU
1	A	3862	THR
1	A	4029	ILE
1	A	4031	GLN
1	A	4066	PRO
1	B	1470	PRO
1	B	1494	ASP
1	B	1498	GLU
1	B	1635	ASP
1	B	1637	GLU
1	B	1748	PHE
1	B	1887	PRO
1	B	1917	ARG
1	B	1940	GLU
1	B	2108	VAL
1	B	2185	PRO
1	B	2187	PRO
1	B	2188	PRO
1	B	2302	PHE
1	B	2330	SER
1	B	2375	ILE
1	B	2376	PRO
1	B	2380	LEU
1	B	2388	PRO
1	B	2391	VAL
1	B	2393	PRO
1	B	2395	ILE
1	B	2419	PRO
1	B	2420	PRO
1	B	2433	ARG
1	B	2525	THR
1	B	2536	ASN
1	B	2540	ASP
1	B	2543	ARG

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Mol	Chain	Res	Type
1	B	2553	HIS
1	B	2576	LYS
1	B	2578	ILE
1	B	2682	PRO
1	B	2758	LEU
1	B	2874	TYR
1	B	2894	PRO
1	B	2910	ASN
1	B	2913	ILE
1	B	3362	VAL
1	B	3370	LEU
1	B	3371	VAL
1	B	3405	PRO
1	B	3410	PRO
1	B	3453	GLN
1	B	3454	ASP
1	B	3458	PHE
1	B	3479	VAL
1	B	3485	GLU
1	B	3500	ASP
1	B	3501	PRO
1	B	3502	SER
1	B	3762	TRP
1	B	3807	SER
1	B	3809	GLU
1	B	3862	THR
1	B	4029	ILE
1	B	4031	GLN
1	B	4066	PRO
1	A	1970	LEU
1	A	2095	ASP
1	A	2104	ILE
1	A	2131	THR
1	A	2186	ILE
1	A	2328	GLY
1	A	2329	ASP
1	A	2370	SER
1	A	2377	SER
1	A	2396	ASP
1	A	2445	PHE
1	A	2519	PRO
1	A	2533	GLY

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Mol	Chain	Res	Type
1	A	2580	LYS
1	A	3641	PHE
1	A	3740	THR
1	A	3923	VAL
1	B	1970	LEU
1	B	2095	ASP
1	B	2104	ILE
1	B	2131	THR
1	B	2186	ILE
1	B	2328	GLY
1	B	2329	ASP
1	B	2370	SER
1	B	2377	SER
1	B	2396	ASP
1	B	2445	PHE
1	B	2519	PRO
1	B	2533	GLY
1	B	2580	LYS
1	B	3641	PHE
1	B	3740	THR
1	B	3923	VAL
2	T	24	GLU
1	A	1400	VAL
1	A	1550	GLY
1	A	1582	VAL
1	A	1873	GLN
1	A	2066	THR
1	A	2079	GLY
1	A	2080	LYS
1	A	2209	ARG
1	A	2255	ASP
1	A	2344	THR
1	A	2637	PRO
1	A	2843	LEU
1	A	2908	LEU
1	A	2945	VAL
1	A	3755	SER
1	A	3808	LYS
1	A	3884	LEU
1	A	3900	ILE
1	A	3901	PRO
1	A	3998	ILE

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Mol	Chain	Res	Type
1	B	1400	VAL
1	B	1550	GLY
1	B	1582	VAL
1	B	1873	GLN
1	B	2066	THR
1	B	2079	GLY
1	B	2080	LYS
1	B	2209	ARG
1	B	2255	ASP
1	B	2344	THR
1	B	2397	THR
1	B	2637	PRO
1	B	2843	LEU
1	B	2908	LEU
1	B	2945	VAL
1	B	3755	SER
1	B	3808	LYS
1	B	3884	LEU
1	B	3900	ILE
1	B	3901	PRO
1	B	3998	ILE
2	T	66	GLN
2	T	115	GLU
2	S	10	LYS
2	S	24	GLU
2	S	66	GLN
1	A	1754	TYR
1	A	1755	LEU
1	A	2141	ILE
1	A	2397	THR
1	A	2443	ILE
1	A	2526	ILE
1	A	3481	ILE
1	A	3752	THR
1	A	3885	PRO
1	A	3922	GLY
1	B	1754	TYR
1	B	1755	LEU
1	B	2141	ILE
1	B	2443	ILE
1	B	2526	ILE
1	B	3481	ILE

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Mol	Chain	Res	Type
1	B	3752	THR
1	B	3885	PRO
1	B	3922	GLY
1	A	1551	SER
1	A	1749	ILE
1	A	1789	LYS
1	A	2541	PRO
1	A	2681	LEU
1	A	3365	ARG
1	A	4030	PRO
1	B	1551	SER
1	B	1749	ILE
1	B	1789	LYS
1	B	2541	PRO
1	B	2681	LEU
1	B	3365	ARG
1	B	4030	PRO
2	S	53	ASN
1	A	2184	LEU
1	A	3377	MET
1	A	4032	PRO
1	B	2184	LEU
1	B	3377	MET
1	B	4032	PRO
2	T	52	PRO
1	A	3738	VAL
1	B	3644	ILE
1	B	3738	VAL
1	A	2100	VAL
1	A	2169	VAL
1	A	3477	VAL
1	A	3644	ILE
1	B	2100	VAL
1	B	2169	VAL
1	B	3477	VAL
1	A	1747	VAL
1	A	2760	GLY
1	B	1747	VAL
1	B	2760	GLY
1	A	2655	ILE
1	A	3902	GLY
1	B	2655	ILE

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Mol	Chain	Res	Type
1	B	3902	GLY
1	A	1817	VAL
1	A	2003	LEU
1	A	2537	PRO
1	B	1817	VAL
1	B	2537	PRO

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	2136/2486 (85%)	0.02	86 (4%)	42	40	183, 210, 384, 480	0
1	B	2136/2486 (85%)	0.13	93 (4%)	38	36	183, 210, 384, 480	0
2	S	216/219 (98%)	1.06	44 (20%)	1	6	209, 233, 253, 268	0
2	T	216/219 (98%)	0.74	31 (14%)	3	9	201, 219, 248, 273	0
All	All	4704/5410 (86%)	0.15	254 (5%)	29	30	183, 210, 376, 480	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	80	MET	7.5
1	B	2156	SER	6.1
1	B	1397	GLU	5.9
1	B	3899	ASP	5.7
2	T	52	PRO	5.4
1	B	3867	GLU	5.3
1	A	4056	ALA	5.1
2	T	143	ASN	4.9
2	S	81	LEU	4.9
2	T	211	GLY	4.8
1	B	3742	ASP	4.5
1	A	3894	ARG	4.4
1	A	2916	TRP	4.4
1	A	3292	SER	4.3
2	S	206	GLN	4.3
1	B	1416	LYS	4.3
2	T	51	PHE	4.3
1	B	3866	GLU	4.3
2	S	75	ALA	4.3
1	B	3743	ASP	4.2
1	B	1568	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	S	215	PRO	4.1
1	B	3582	GLU	4.1
1	B	1671	LYS	4.0
2	S	79	ASN	4.0
1	A	2734	ILE	4.0
1	B	3900	ILE	3.9
2	S	189	ASP	3.9
2	T	82	GLY	3.9
1	A	3291	ALA	3.9
1	B	2776	LEU	3.9
2	S	179	LYS	3.9
2	T	142	LEU	3.9
2	S	46	GLU	3.9
1	B	2074	GLY	3.8
2	S	165	ASP	3.8
1	A	2211	GLY	3.8
1	A	2156	SER	3.8
2	T	141	TYR	3.7
1	B	1427	ASP	3.7
2	T	210	GLY	3.7
1	B	1396	ARG	3.7
1	A	4016	CYS	3.7
1	A	2157	ASP	3.7
1	A	3520	THR	3.7
1	B	1389	SER	3.7
1	B	1504	ASN	3.7
1	A	1796	GLY	3.6
1	B	2789	HIS	3.6
1	B	3898	GLU	3.6
1	A	2121	ALA	3.6
2	S	44	LYS	3.6
1	A	3581	ASP	3.5
1	A	2942	ASP	3.5
1	B	1420	TYR	3.4
1	A	2917	MET	3.4
2	S	76	ASP	3.4
2	T	208	THR	3.4
1	B	1672	TYR	3.3
1	A	3895	VAL	3.3
1	A	2210	CYS	3.3
2	S	47	LEU	3.3
1	B	2373	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	S	113	ASP	3.3
2	T	53	ASN	3.3
1	B	1388	HIS	3.3
1	A	2868	ASP	3.3
1	A	3880	THR	3.2
1	B	1580	THR	3.2
1	B	3581	ASP	3.2
1	A	2419	PRO	3.2
1	B	3753	THR	3.2
1	B	2837	ASN	3.2
1	B	1505	PHE	3.2
1	B	2916	TRP	3.2
1	A	3873	MET	3.2
1	A	2915	ASN	3.2
1	A	2074	GLY	3.2
2	S	216	PRO	3.2
1	A	3018	ASN	3.2
2	S	43	LYS	3.1
1	B	2243	MET	3.1
2	T	33	GLU	3.1
1	B	1387	GLU	3.1
2	S	22	TYR	3.0
1	B	3901	PRO	3.0
1	A	2122	THR	3.0
1	A	2776	LEU	3.0
2	S	199	ALA	3.0
1	B	3837	GLY	3.0
2	T	37	GLY	3.0
1	B	1421	TYR	3.0
1	B	1398	TRP	3.0
2	S	45	PHE	3.0
1	B	1567	GLY	3.0
1	B	2692	THR	3.0
1	B	2364	ASP	2.9
2	S	138	HIS	2.9
1	A	2417	CYS	2.9
1	B	3714	GLN	2.9
1	A	2418	GLY	2.9
2	S	74	ILE	2.9
2	T	115	GLU	2.9
1	B	3583	LEU	2.9
1	A	2837	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	S	48	GLY	2.8
2	S	157	ALA	2.8
2	T	134	ASP	2.8
2	S	142	LEU	2.8
2	T	81	LEU	2.8
1	B	1792	GLY	2.8
2	S	188	ILE	2.8
1	B	1494	ASP	2.8
2	T	50	GLU	2.8
1	A	2731	PRO	2.8
1	B	2155	ASP	2.8
2	T	212	GLY	2.7
2	S	180	LYS	2.7
1	B	3836	GLY	2.7
2	T	38	ASP	2.7
1	B	1508	THR	2.7
1	A	3878	HIS	2.7
1	B	3741	ASN	2.7
1	A	1817	VAL	2.7
1	A	1898	LEU	2.7
1	A	3999	ASP	2.6
2	T	35	ASP	2.6
1	B	1419	ASN	2.6
2	S	61	ASP	2.6
1	B	1922	LYS	2.6
1	B	2637	PRO	2.6
2	T	106	SER	2.6
2	S	186	PRO	2.6
1	A	3899	ASP	2.6
1	B	1417	ALA	2.6
1	B	2077	GLY	2.6
1	B	2073	VAL	2.6
1	B	2245	GLU	2.6
1	A	3782	GLU	2.6
1	B	3865	ALA	2.6
1	B	3014	GLN	2.6
2	S	53	ASN	2.6
2	S	166	PRO	2.5
1	A	1604	ALA	2.5
1	A	2108	VAL	2.5
1	A	3582	GLU	2.5
1	A	4000	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	3883	LYS	2.5
2	T	209	PHE	2.5
1	B	2372	CYS	2.5
1	A	3783	ASN	2.5
1	B	2775	TRP	2.5
1	A	2692	THR	2.5
1	A	2096	GLY	2.5
1	A	3998	ILE	2.4
2	S	21	GLU	2.4
1	A	2392	ILE	2.4
2	S	19	LEU	2.4
1	B	2777	ASN	2.4
2	S	151	ASP	2.4
2	S	112	LYS	2.4
1	A	2409	ASN	2.4
1	A	3784	ASN	2.4
1	B	1551	SER	2.4
2	T	135	ARG	2.4
1	A	3313	PHE	2.4
1	A	4036	GLN	2.4
2	S	116	THR	2.4
1	A	2095	ASP	2.4
1	B	2462	THR	2.4
1	A	3455	GLY	2.4
1	A	3014	GLN	2.4
1	B	1923	SER	2.4
1	B	3739	ASP	2.4
2	S	72	ARG	2.4
1	B	2552	ARG	2.3
2	T	34	ARG	2.3
2	S	187	GLN	2.3
1	B	1493	LEU	2.3
1	B	1495	THR	2.3
1	B	3765	ASN	2.3
1	A	2552	ARG	2.3
1	A	2553	HIS	2.3
2	S	71	ILE	2.3
1	A	3714	GLN	2.3
1	A	3753	THR	2.3
1	A	3836	GLY	2.3
2	T	36	GLU	2.3
1	A	3020	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	4000	GLU	2.3
1	A	3572	ASN	2.3
1	B	3456	GLU	2.3
1	A	2941	THR	2.2
1	B	2137	VAL	2.2
2	T	116	THR	2.2
1	B	3810	SER	2.2
1	A	3310	THR	2.2
1	B	1581	GLY	2.2
1	B	2157	ASP	2.2
1	B	1415	MET	2.2
1	B	2242	SER	2.2
1	B	2210	CYS	2.2
1	B	2370	SER	2.2
1	B	2917	MET	2.2
1	A	4037	SER	2.2
1	A	3561	ASN	2.2
2	T	83	GLY	2.2
1	A	3456	GLU	2.2
2	S	167	MET	2.2
1	A	3314	SER	2.2
1	B	1492	GLN	2.2
1	A	3785	TYR	2.2
2	S	207	ALA	2.2
1	B	2174	LYS	2.2
1	B	2638	ARG	2.2
1	A	2125	TRP	2.2
1	A	2869	THR	2.2
1	B	2731	PRO	2.1
1	A	1644	ILE	2.1
1	A	3588	ASN	2.1
1	A	3017	VAL	2.1
1	B	1887	PRO	2.1
1	B	1390	SER	2.1
1	B	2551	THR	2.1
2	T	140	THR	2.1
2	S	31	LEU	2.1
1	A	1812	ASN	2.1
1	A	2733	VAL	2.1
2	T	144	GLY	2.1
1	B	1883	GLU	2.1
1	A	2551	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2691	SER	2.1
1	A	2110	THR	2.1
1	A	3293	ILE	2.1
1	B	3791	GLU	2.1
1	A	3028	VAL	2.1
2	T	207	ALA	2.1
2	S	30	HIS	2.1
1	B	2892	CYS	2.1
2	S	150	PRO	2.1
1	A	2555	ALA	2.1
2	T	105	VAL	2.1
1	A	1568	SER	2.1
1	B	3707	LYS	2.1
1	A	3879	LEU	2.0
1	A	2535	CYS	2.0
1	B	1428	CYS	2.0
2	T	56	TYR	2.0
1	B	1395	VAL	2.0
2	S	164	MET	2.0
1	A	3864	ALA	2.0
1	A	1744	LEU	2.0
1	A	3027	SER	2.0
1	B	3431	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.