Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:12 PM GMT

PDB ID	:	1SJA
Title	:	X-ray structure of o-Succinylbenzoate Synthase complexed with N-acetylmethionine
Authors	:	Thoden, J.B.; Taylor-Ringia, E.A.; Garrett, J.B.; Gerlt, J.A.; Holden, H.M.; Rayment, I.
Deposited on	:	2004-03-03
Resolution	:	2.30 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:

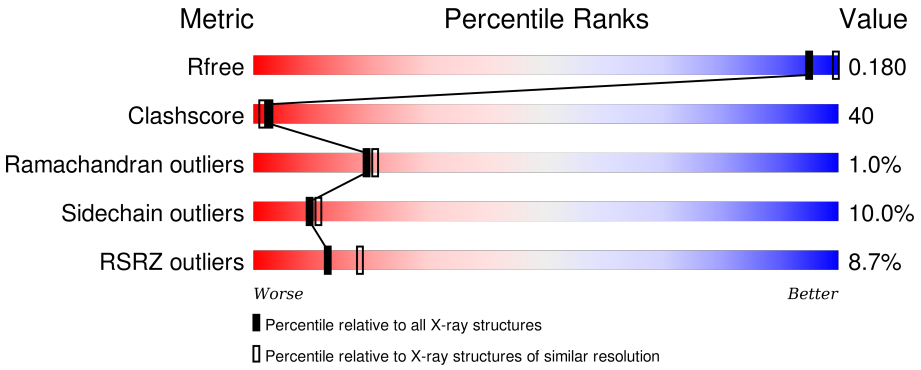
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	368	12% 37% 52% 10% •
1	B	368	2% 48% 42% 10% •
1	C	368	7% 43% 45% 11% •
1	D	368	14% 39% 48% 11% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AME	A	600	-	-	X	X
3	AME	B	700	-	-	X	X
3	AME	C	800	-	-	X	X
3	AME	D	900	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11704 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.

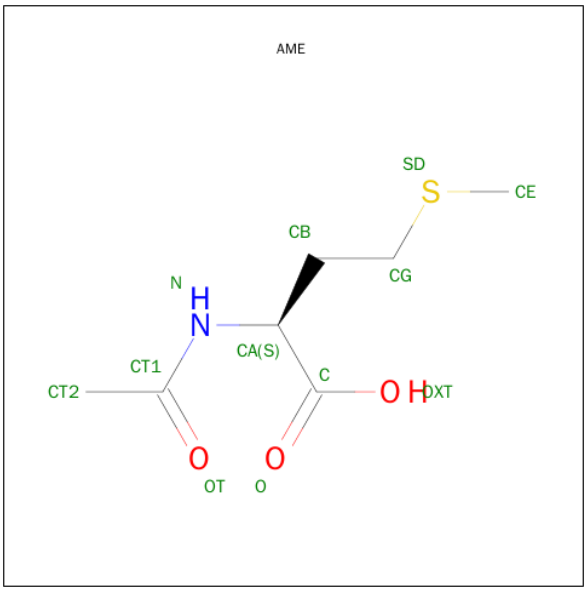
- Molecule 1 is a protein called N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	2	0
			2785	1769	487	517	12			
1	B	368	Total	C	N	O	S	0	3	0
			2796	1775	487	522	12			
1	C	368	Total	C	N	O	S	0	0	0
			2771	1761	481	517	12			
1	D	368	Total	C	N	O	S	0	1	0
			2778	1765	484	517	12			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is N-ACETYLMETHIONINE (three-letter code: AME) (formula: $C_7H_{13}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 7 1 3 1	0	0
3	B	1	Total C N O S 12 7 1 3 1	0	0
3	C	1	Total C N O S 12 7 1 3 1	0	0
3	D	1	Total C N O S 12 7 1 3 1	0	0

- Molecule 4 is water.

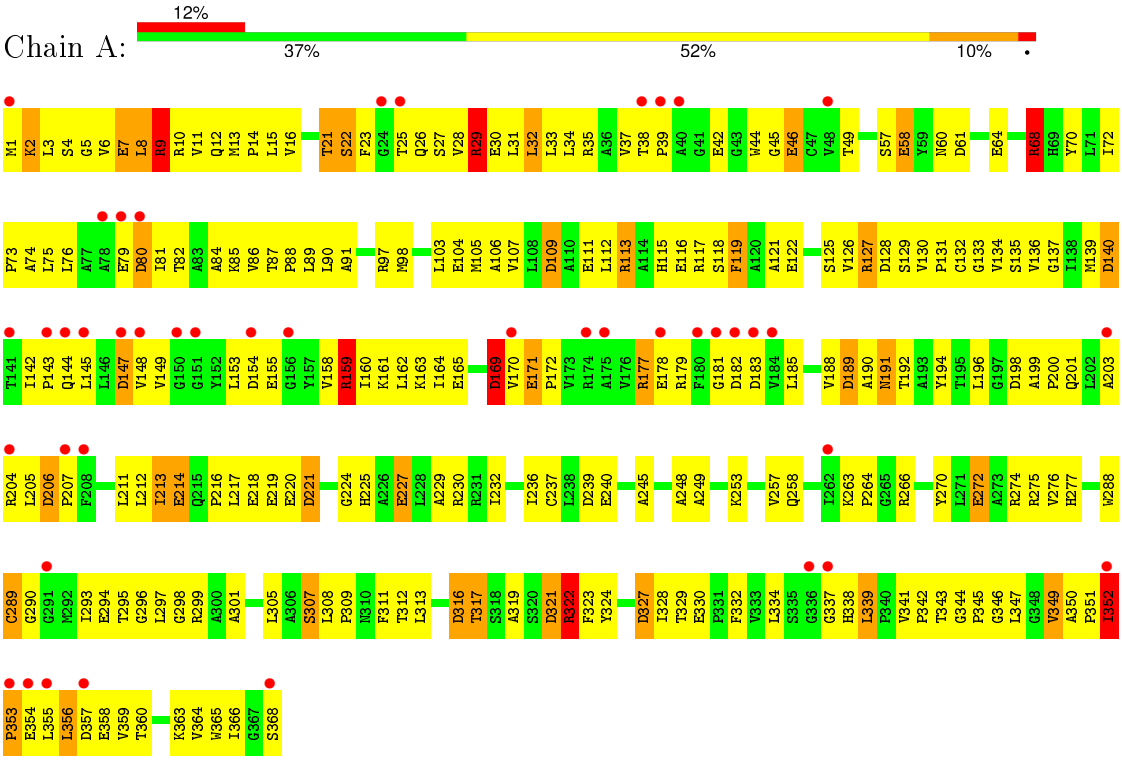
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	0	0
4	B	153	Total O 153 153	0	0
4	C	117	Total O 117 117	0	0
4	D	117	Total O 117 117	0	0

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.

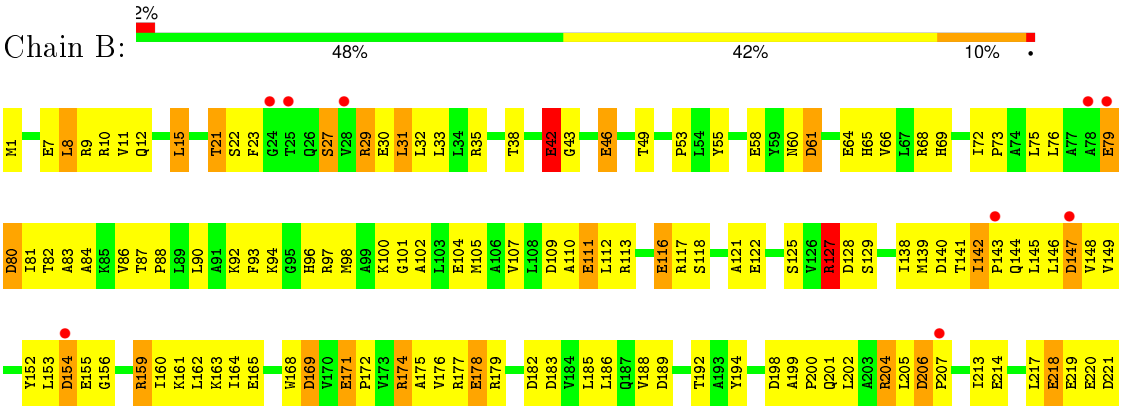
- Molecule 1: N-acylamino acid racemase

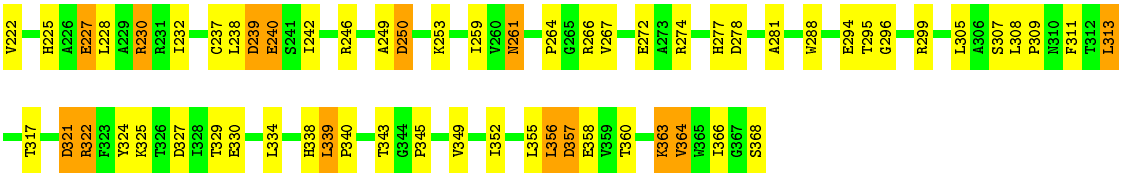
Chain A:



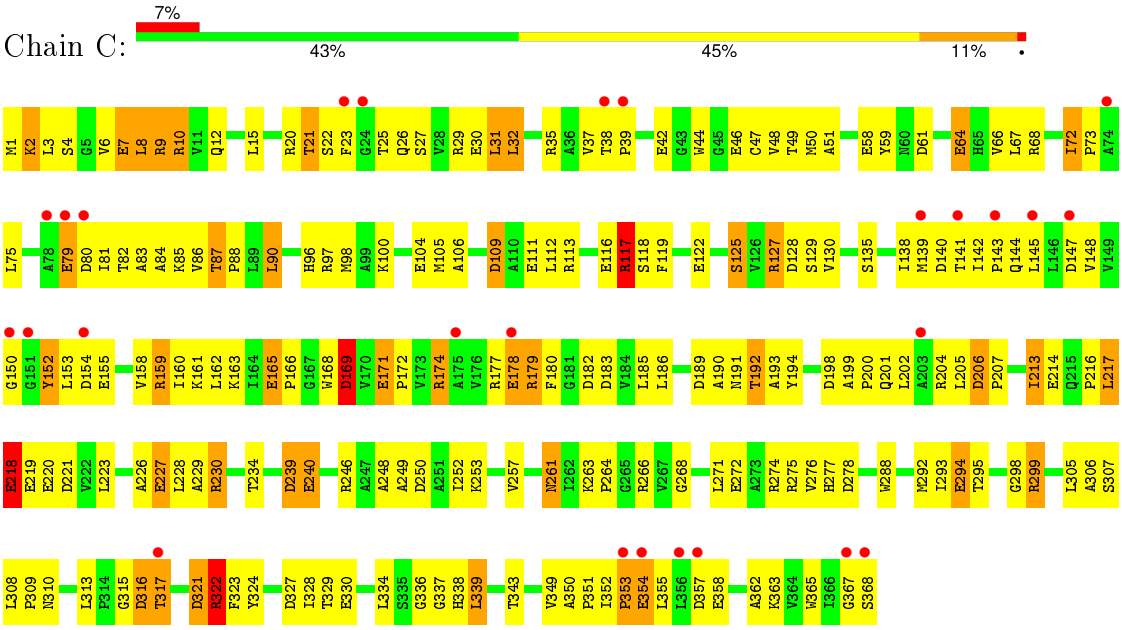
- Molecule 1: N-acylamino acid racemase

Chain B:

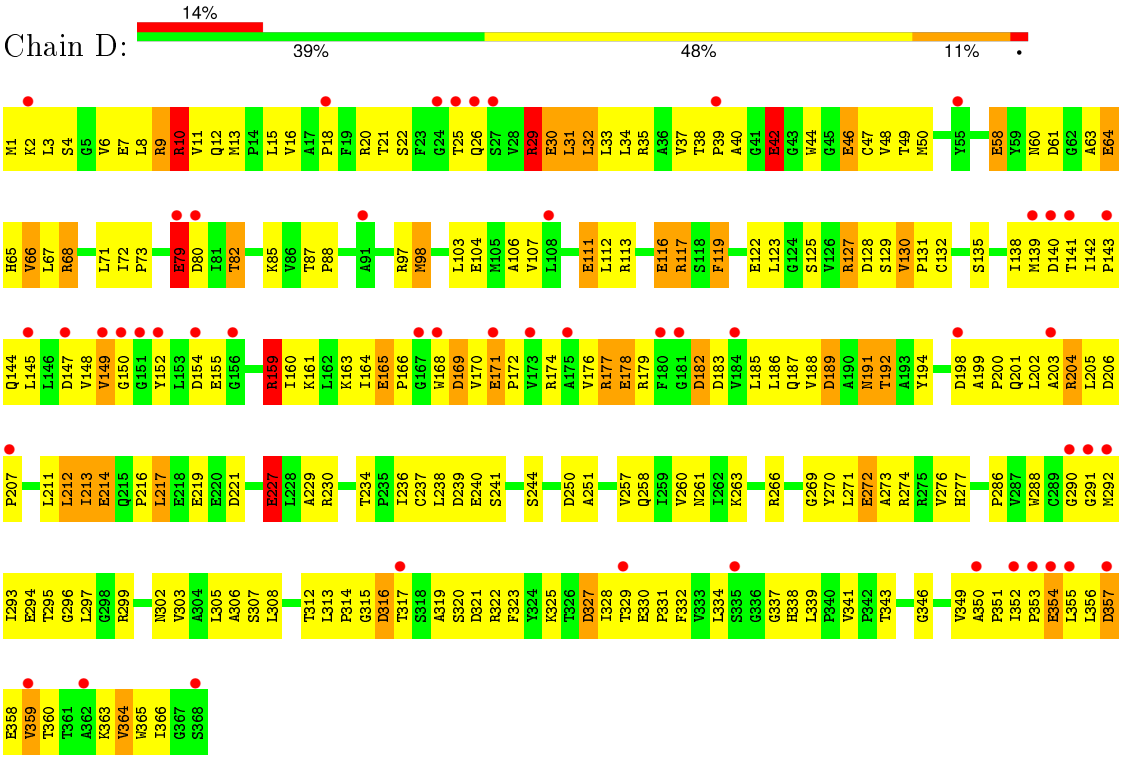




- Molecule 1: N-acylamino acid racemase



- Molecule 1: N-acylamino acid racemase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	215.30Å 215.30Å 259.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 29.86 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.30) 97.7 (29.86-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.24Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.211 , 0.280 0.178 , 0.180	Depositor DCC
R_{free} test set	10015 reflections (11.14%)	DCC
Wilson B-factor (Å^2)	13.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 395.2	EDS
Estimated twinning fraction	0.217 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.216 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.207 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Outliers	0 of 106040 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11704	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AME

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	1.00	25/2849 (0.9%)	1.35	41/3878 (1.1%)
1	B	1.04	26/2868 (0.9%)	1.40	41/3902 (1.1%)
1	C	1.03	23/2827 (0.8%)	1.44	41/3850 (1.1%)
1	D	1.00	23/2838 (0.8%)	1.43	44/3864 (1.1%)
All	All	1.02	97/11382 (0.9%)	1.40	167/15494 (1.1%)

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	165	GLU	CD-OE2	8.79	1.35	1.25
1	D	178	GLU	CD-OE2	7.80	1.34	1.25
1	D	79	GLU	CD-OE2	7.77	1.34	1.25
1	A	116	GLU	CD-OE2	7.66	1.34	1.25
1	C	171	GLU	CD-OE2	7.62	1.34	1.25
1	C	30	GLU	CD-OE2	7.54	1.33	1.25
1	B	46	GLU	CD-OE2	7.45	1.33	1.25
1	A	79	GLU	CD-OE2	7.36	1.33	1.25
1	B	294	GLU	CD-OE2	7.22	1.33	1.25
1	D	42	GLU	CD-OE2	7.19	1.33	1.25
1	A	171	GLU	CD-OE2	7.18	1.33	1.25
1	C	358	GLU	CD-OE2	7.16	1.33	1.25
1	D	116	GLU	CD-OE2	7.09	1.33	1.25
1	D	294	GLU	CD-OE2	7.04	1.33	1.25
1	B	358	GLU	CD-OE2	7.03	1.33	1.25
1	B	30	GLU	CD-OE2	7.03	1.33	1.25
1	A	30	GLU	CD-OE2	7.01	1.33	1.25
1	A	46	GLU	CD-OE2	6.92	1.33	1.25
1	D	30	GLU	CD-OE2	6.90	1.33	1.25
1	D	354	GLU	CD-OE2	6.86	1.33	1.25
1	B	111	GLU	CD-OE2	6.85	1.33	1.25
1	A	354	GLU	CD-OE2	6.74	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	GLU	CD-OE2	6.72	1.33	1.25
1	D	219	GLU	CD-OE2	6.62	1.32	1.25
1	A	240	GLU	CD-OE2	6.58	1.32	1.25
1	C	165	GLU	CD-OE2	6.58	1.32	1.25
1	D	272	GLU	CD-OE2	6.56	1.32	1.25
1	B	218	GLU	CD-OE2	6.47	1.32	1.25
1	B	155	GLU	CD-OE2	6.47	1.32	1.25
1	C	79	GLU	CD-OE2	6.44	1.32	1.25
1	B	58	GLU	CD-OE2	6.43	1.32	1.25
1	C	214	GLU	CD-OE2	6.41	1.32	1.25
1	C	218	GLU	CD-OE2	6.40	1.32	1.25
1	A	165	GLU	CD-OE2	6.40	1.32	1.25
1	C	155	GLU	CD-OE2	6.36	1.32	1.25
1	B	122	GLU	CD-OE2	6.34	1.32	1.25
1	A	272	GLU	CD-OE2	6.31	1.32	1.25
1	D	330	GLU	CD-OE2	6.30	1.32	1.25
1	C	330	GLU	CD-OE2	6.28	1.32	1.25
1	D	227	GLU	CD-OE2	6.23	1.32	1.25
1	D	240	GLU	CD-OE2	6.23	1.32	1.25
1	B	220	GLU	CD-OE2	6.19	1.32	1.25
1	A	214	GLU	CD-OE2	6.17	1.32	1.25
1	B	178	GLU	CD-OE2	6.17	1.32	1.25
1	B	42	GLU	CD-OE2	6.16	1.32	1.25
1	A	122	GLU	CD-OE2	6.14	1.32	1.25
1	C	7	GLU	CD-OE2	6.13	1.32	1.25
1	C	116	GLU	CD-OE2	6.13	1.32	1.25
1	A	111	GLU	CD-OE2	6.09	1.32	1.25
1	C	219	GLU	CD-OE2	6.08	1.32	1.25
1	A	42	GLU	CD-OE2	6.07	1.32	1.25
1	D	171	GLU	CD-OE2	6.06	1.32	1.25
1	B	330	GLU	CD-OE2	6.06	1.32	1.25
1	D	358	GLU	CD-OE2	6.04	1.32	1.25
1	D	104	GLU	CD-OE2	6.04	1.32	1.25
1	B	227	GLU	CD-OE2	6.01	1.32	1.25
1	A	178	GLU	CD-OE2	6.01	1.32	1.25
1	B	171	GLU	CD-OE2	5.99	1.32	1.25
1	A	155	GLU	CD-OE2	5.95	1.32	1.25
1	C	178	GLU	CD-OE2	5.88	1.32	1.25
1	A	227	GLU	CD-OE2	5.81	1.32	1.25
1	B	214	GLU	CD-OE2	5.76	1.31	1.25
1	B	79[A]	GLU	CD-OE2	5.73	1.31	1.25
1	B	79[B]	GLU	CD-OE2	5.73	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	79[C]	GLU	CD-OE2	5.73	1.31	1.25
1	C	354	GLU	CD-OE2	5.70	1.31	1.25
1	A	64	GLU	CD-OE2	5.69	1.31	1.25
1	C	220	GLU	CD-OE2	5.68	1.31	1.25
1	C	227	GLU	CD-OE2	5.67	1.31	1.25
1	B	219	GLU	CD-OE2	5.67	1.31	1.25
1	D	46	GLU	CD-OE2	5.67	1.31	1.25
1	B	64	GLU	CD-OE2	5.63	1.31	1.25
1	A	104	GLU	CD-OE2	5.62	1.31	1.25
1	C	111	GLU	CD-OE2	5.62	1.31	1.25
1	D	122	GLU	CD-OE2	5.60	1.31	1.25
1	C	294	GLU	CD-OE2	5.55	1.31	1.25
1	D	64	GLU	CD-OE2	5.51	1.31	1.25
1	A	58	GLU	CD-OE2	5.47	1.31	1.25
1	D	214	GLU	CD-OE2	5.46	1.31	1.25
1	B	165	GLU	CD-OE2	5.44	1.31	1.25
1	B	104	GLU	CD-OE2	5.42	1.31	1.25
1	C	104	GLU	CD-OE2	5.41	1.31	1.25
1	D	111	GLU	CD-OE2	5.39	1.31	1.25
1	C	46	GLU	CD-OE2	5.39	1.31	1.25
1	C	272	GLU	CD-OE2	5.37	1.31	1.25
1	A	330	GLU	CD-OE2	5.35	1.31	1.25
1	C	64	GLU	CD-OE2	5.34	1.31	1.25
1	D	58	GLU	CD-OE2	5.31	1.31	1.25
1	A	7	GLU	CD-OE2	5.27	1.31	1.25
1	A	219	GLU	CD-OE2	5.24	1.31	1.25
1	B	116	GLU	CD-OE2	5.19	1.31	1.25
1	B	7	GLU	CD-OE2	5.17	1.31	1.25
1	B	240	GLU	CD-OE2	5.17	1.31	1.25
1	D	155	GLU	CD-OE2	5.13	1.31	1.25
1	A	218	GLU	CD-OE2	5.10	1.31	1.25
1	A	358	GLU	CD-OE2	5.10	1.31	1.25
1	C	240	GLU	CD-OE2	5.02	1.31	1.25

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	299	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	D	80	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	C	147	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	B	206	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	C	321	ASP	CB-CG-OD2	-8.20	110.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	230	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	D	250	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	C	109	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	B	80	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	C	109	ASP	CB-CG-OD1	7.95	125.45	118.30
1	C	182	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	B	189	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	D	117	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	C	189	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	147	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	D	250	ASP	CB-CG-OD1	7.64	125.18	118.30
1	D	221	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	C	198	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	C	316	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	61	ASP	CB-CG-OD1	7.40	124.96	118.30
1	B	189	ASP	CB-CG-OD1	7.37	124.94	118.30
1	C	327	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	C	322	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	D	29	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	C	127	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	C	239	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	D	239	ASP	CB-CG-OD1	7.25	124.82	118.30
1	D	154	ASP	CB-CG-OD1	7.22	124.79	118.30
1	A	80	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	C	327	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	61	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	128	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	239	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	250	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	182	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	A	97	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	322	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	221	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	D	198	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	D	239	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	C	169	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	316	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	183	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	C	147	ASP	CB-CG-OD1	6.82	124.44	118.30
1	C	274	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	239	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	357	ASP	CB-CG-OD2	-6.79	112.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	239	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	D	159	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	B	321	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	A	183	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	140	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	D	204	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	127[A]	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	127[B]	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	182	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	154	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	109	ASP	CB-CG-OD1	6.65	124.29	118.30
1	C	183	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	D	80	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	169	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	183	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	140	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	239	ASP	CB-CG-OD1	6.54	124.19	118.30
1	C	80	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	C	230	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	206	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	C	321	ASP	CB-CG-OD1	6.48	124.14	118.30
1	A	182	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	221	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	250	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	327	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	183	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	198	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	D	357	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	C	154	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	B	154	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	117	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	140	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	80	ASP	CB-CG-OD1	6.29	123.96	118.30
1	C	357	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	127	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	154	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	357	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	204	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	321	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	221	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	97	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	154	ASP	CB-CG-OD1	6.07	123.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	322	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	198	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	68[A]	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	68[B]	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	128	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	D	183	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	61	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	152	TYR	CB-CG-CD2	5.98	124.59	121.00
1	B	198	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	154	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	299	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	D	183	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	204	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	C	140	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	182	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	C	61	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	270	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	D	189	ASP	CB-CG-OD1	5.82	123.53	118.30
1	D	182	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	10	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	321	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	189	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	C	189	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	183	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	109	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	C	250	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	189	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	B	299	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	182	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	B	128	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	147	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	68	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	C	316	ASP	CB-CG-OD1	5.66	123.40	118.30
1	D	331	PRO	N-CA-CB	5.66	110.09	103.30
1	A	9	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	128	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	61	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	61	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	239	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	312	THR	CA-CB-CG2	5.58	120.21	112.40
1	A	221	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	109	ASP	CB-CG-OD2	-5.53	113.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	221	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	327	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	321	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	343	THR	CA-CB-CG2	-5.44	104.79	112.40
1	C	117	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	352	ILE	C-N-CD	-5.41	108.70	120.60
1	C	128	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	A	169	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	206	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	D	140	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	321	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	C	182	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	250	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	189	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	29	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	72	ILE	CA-CB-CG2	-5.29	100.33	110.90
1	D	147	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	128	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	147	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	80	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	327	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	159	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	61	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	127	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	179	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	10	ARG	N-CA-CB	5.10	119.79	110.60
1	A	357	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	349	VAL	CB-CA-C	-5.10	101.72	111.40
1	D	327	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	128	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	246	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	152	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	B	278	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	97	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	D	316	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	159	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2785	0	2828	268	0
1	B	2796	0	2834	197	0
1	C	2771	0	2810	220	0
1	D	2778	0	2819	226	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	12	10	0
3	B	12	0	12	8	0
3	C	12	0	12	17	0
3	D	12	0	12	13	0
4	A	135	0	0	17	0
4	B	153	0	0	12	0
4	C	117	0	0	12	0
4	D	117	0	0	16	0
All	All	11704	0	11339	910	2

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 40.

All (910) 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:117:ARG:NH1	1:A:121:ALA:HB1	1.41	1.34
1:A:58:GLU:HB2	1:A:98:MET:CE	1.67	1.23
1:C:38:THR:HB	1:C:39:PRO:HD2	1.17	1.15
1:C:35:ARG:NH1	1:C:42:GLU:OE2	1.80	1.14
1:C:141:THR:CG2	1:C:143:PRO:HD2	1.76	1.13
1:B:10:ARG:NH2	1:B:61:ASP:OD1	1.80	1.13
1:A:58:GLU:HB2	1:A:98:MET:HE2	1.24	1.13
1:B:127[A]:ARG:HG2	1:B:127[A]:ARG:HH11	1.17	1.08
1:C:141:THR:HG22	1:C:143:PRO:CD	1.83	1.07
1:B:1:MET:HE2	1:B:38:THR:HG21	1.36	1.07
1:A:117:ARG:HH11	1:A:121:ALA:CB	1.69	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ILE:HD13	1:B:188:VAL:HG11	1.35	1.06
1:D:127[B]:ARG:NH2	1:D:308:LEU:O	1.87	1.06
1:D:29:ARG:HD3	1:D:31:LEU:HD23	1.35	1.05
1:C:67:LEU:O	1:C:72:ILE:HG13	1.54	1.05
1:C:49:THR:HG22	1:C:98:MET:HE3	1.06	1.03
1:D:33:LEU:O	1:D:34:LEU:HD23	1.59	1.02
1:A:21:THR:HG22	1:A:23:PHE:H	1.23	1.02
1:C:49:THR:HG22	1:C:98:MET:CE	1.89	1.02
1:D:163:LYS:NZ	3:D:900:AME:HN1	1.58	1.01
1:A:12:GLN:O	1:A:359:VAL:HG22	1.61	1.01
1:A:135:SER:CB	3:A:600:AME:HT23	1.91	1.01
1:C:135:SER:CB	3:C:800:AME:CT2	2.39	1.00
1:D:272:GLU:N	4:D:940:HOH:O	1.95	1.00
1:C:38:THR:HB	1:C:39:PRO:CD	1.92	1.00
1:D:60:ASN:HB2	4:D:920:HOH:O	1.64	0.97
1:A:82:THR:HG22	1:A:84:ALA:H	1.26	0.97
1:C:135:SER:CB	3:C:800:AME:HT23	1.93	0.96
1:C:58:GLU:HB2	1:C:98:MET:HE2	1.48	0.96
1:A:352:ILE:HG22	1:A:355:LEU:HG	1.48	0.95
1:A:117:ARG:NH1	1:A:121:ALA:CB	2.28	0.95
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.27	0.94
1:C:159:ARG:NH2	1:C:316:ASP:OD1	2.01	0.93
1:D:58:GLU:OE1	1:D:98:MET:HG3	1.68	0.93
1:A:87:THR:HB	1:A:88:PRO:HD3	1.49	0.93
1:A:21:THR:HG21	1:A:23:PHE:CE1	2.04	0.93
1:A:117:ARG:HH11	1:A:121:ALA:HB1	1.01	0.93
1:C:49:THR:CG2	1:C:98:MET:HE3	1.96	0.92
1:C:35:ARG:HD3	1:C:44:TRP:CZ2	2.03	0.92
1:D:206:ASP:HB2	1:D:207:PRO:HD3	1.48	0.92
1:B:82:THR:HG22	1:B:84:ALA:H	1.34	0.92
1:C:10:ARG:HG3	1:C:362:ALA:HB3	1.52	0.92
1:B:1:MET:CE	1:B:38:THR:HG21	2.01	0.91
1:C:21:THR:HG21	1:C:23:PHE:CE1	2.06	0.91
1:B:49:THR:HG22	1:B:98:MET:CE	2.01	0.90
1:A:58:GLU:CB	1:A:98:MET:CE	2.49	0.90
1:D:29:ARG:HD3	1:D:31:LEU:CD2	2.02	0.89
1:A:21:THR:HG21	1:A:23:PHE:CD1	2.08	0.89
1:C:58:GLU:HB2	1:C:98:MET:CE	2.02	0.89
1:C:248:ALA:O	1:C:252:ILE:HG13	1.73	0.89
1:C:125:SER:HB2	1:C:307:SER:OG	1.73	0.89
1:A:329:THR:HG22	1:A:350:ALA:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:SER:HB3	3:C:800:AME:CT2	2.01	0.88
1:C:139:MET:HB2	1:C:168:TRP:CZ2	2.08	0.88
1:D:21:THR:HG22	1:D:22:SER:N	1.86	0.88
1:D:211:LEU:O	1:D:212:LEU:HB3	1.69	0.88
1:C:141:THR:HG22	1:C:143:PRO:HD2	0.91	0.88
1:C:352:ILE:HB	1:C:355:LEU:HD12	1.55	0.88
1:B:82:THR:HG22	1:B:84:ALA:N	1.89	0.88
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.53	0.87
1:A:204[A]:ARG:HH11	1:A:204[A]:ARG:HG2	1.37	0.87
1:C:135:SER:OG	3:C:800:AME:HT23	1.75	0.87
1:B:15:LEU:HB2	1:B:27:SER:O	1.75	0.87
1:B:49:THR:CG2	1:B:98:MET:CE	2.52	0.87
1:B:21:THR:HG22	1:B:23:PHE:H	1.39	0.86
1:D:159:ARG:HD2	4:D:963:HOH:O	1.74	0.86
1:D:206:ASP:N	1:D:207:PRO:HD2	1.89	0.86
1:C:205:LEU:C	1:C:207:PRO:HD2	1.97	0.85
1:A:68[A]:ARG:HG2	1:A:68[A]:ARG:HH11	1.39	0.85
1:C:213:ILE:HG22	1:C:234:THR:HG22	1.57	0.85
1:A:159:ARG:HD2	4:A:666:HOH:O	1.76	0.85
1:C:206:ASP:N	1:C:207:PRO:CD	2.40	0.84
1:A:135:SER:CB	3:A:600:AME:CT2	2.56	0.84
1:D:216:PRO:C	1:D:217:LEU:HD23	1.98	0.84
1:D:44:TRP:O	1:D:106:ALA:HA	1.77	0.84
1:D:21:THR:HG22	1:D:22:SER:H	1.43	0.83
1:A:206:ASP:HB2	1:A:207:PRO:HD3	1.58	0.83
1:B:21:THR:HG21	1:B:23:PHE:CE1	2.13	0.83
1:A:139:MET:HG3	1:A:145:LEU:HA	1.59	0.83
1:D:29:ARG:CD	1:D:31:LEU:HD23	2.09	0.83
1:D:352:ILE:HG22	1:D:352:ILE:O	1.77	0.82
1:A:4:SER:HB2	1:A:37:VAL:HG12	1.57	0.82
1:B:127[A]:ARG:NH1	1:B:127[A]:ARG:HG2	1.82	0.82
1:A:10:ARG:NH2	1:A:60:ASN:HB3	1.94	0.82
1:C:87:THR:HG22	1:C:88:PRO:HD3	1.59	0.82
1:C:201:GLN:O	1:C:204:ARG:HB2	1.80	0.82
1:C:58:GLU:CB	1:C:98:MET:HE2	2.09	0.82
1:A:135:SER:HB2	3:A:600:AME:HT23	1.60	0.82
1:C:38:THR:CB	1:C:39:PRO:HD2	2.04	0.81
1:D:135:SER:OG	3:D:900:AME:HT23	1.79	0.81
1:D:135:SER:CB	3:D:900:AME:HT23	2.08	0.81
1:A:73:PRO:HA	1:A:76:LEU:HD12	1.60	0.81
1:D:29:ARG:NH2	1:D:50:MET:HG2	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASP:OD1	1:A:194:TYR:OH	1.97	0.81
1:B:164:ILE:HD13	1:B:188:VAL:CG1	2.10	0.81
1:D:47:CYS:SG	1:D:49:THR:HG23	2.21	0.81
1:B:281:ALA:O	1:C:246:ARG:NH2	2.14	0.80
1:B:29:ARG:HD2	1:B:31:LEU:CD2	2.12	0.80
1:A:293:ILE:O	1:A:293:ILE:HG22	1.81	0.80
1:D:29:ARG:HH21	1:D:50:MET:HG2	1.47	0.79
1:C:185:LEU:HA	4:C:870:HOH:O	1.81	0.79
1:B:49:THR:HG22	1:B:98:MET:HE2	1.64	0.79
1:A:10:ARG:NH2	1:A:60:ASN:CB	2.46	0.79
1:C:118:SER:HB2	4:C:852:HOH:O	1.80	0.79
1:A:296:GLY:HA3	1:A:329:THR:OG1	1.82	0.79
1:D:164:ILE:HB	1:D:168:TRP:O	1.83	0.78
1:A:135:SER:HB2	3:A:600:AME:CT2	2.14	0.78
1:D:206:ASP:N	1:D:207:PRO:CD	2.45	0.78
1:B:169:ASP:OD1	1:B:194:TYR:OH	2.01	0.78
1:A:87:THR:CB	1:A:88:PRO:HD3	2.11	0.78
1:B:175:ALA:O	1:B:178:GLU:HB3	1.84	0.78
1:B:164:ILE:HG23	1:B:188:VAL:HG13	1.66	0.78
1:A:109:ASP:O	1:A:113:ARG:HG3	1.83	0.78
1:B:72:ILE:HB	1:B:73:PRO:HD3	1.66	0.78
1:B:139:MET:HG3	1:B:145:LEU:HA	1.67	0.77
1:D:163:LYS:HZ2	3:D:900:AME:HN1	1.32	0.77
1:D:16:VAL:HG23	1:D:323:PHE:O	1.83	0.77
1:B:87:THR:HB	1:B:88:PRO:HD3	1.65	0.77
1:D:159:ARG:NH2	1:D:316:ASP:OD1	2.15	0.77
1:A:206:ASP:N	1:A:207:PRO:HD2	2.00	0.77
1:C:158:VAL:O	1:C:158:VAL:HG12	1.83	0.77
1:A:75:LEU:O	1:A:81:ILE:HD11	1.84	0.77
1:D:188:VAL:O	4:D:964:HOH:O	2.02	0.77
1:C:3:LEU:HB2	1:C:81:ILE:HD12	1.67	0.77
1:C:87:THR:CG2	1:C:88:PRO:HD3	2.14	0.76
1:B:111:GLU:OE2	1:C:117:ARG:NH2	2.19	0.76
1:C:206:ASP:N	1:C:207:PRO:HD2	2.01	0.76
1:B:10:ARG:NH1	1:B:60:ASN:HB3	2.00	0.76
1:D:13:MET:HE1	1:D:295:THR:HG22	1.68	0.76
1:D:328:ILE:HG13	1:D:329:THR:HG23	1.68	0.76
1:D:125:SER:HB2	1:D:307:SER:OG	1.87	0.75
1:C:87:THR:CB	1:C:88:PRO:HD3	2.16	0.75
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.69	0.75
1:A:334:LEU:HD12	1:A:339:LEU:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:HH12	1:A:121:ALA:HB1	1.46	0.75
1:D:327:ASP:O	1:D:355:LEU:HD13	1.87	0.75
1:B:49:THR:HA	1:B:98:MET:HE1	1.69	0.75
1:D:263:LYS:HB2	1:D:266:ARG:NH1	2.01	0.75
1:B:127[A]:ARG:CG	1:B:127[A]:ARG:HH11	1.99	0.74
1:D:212:LEU:HD12	1:D:212:LEU:O	1.87	0.74
1:D:142:ILE:HB	1:D:143:PRO:HD3	1.68	0.74
1:D:10:ARG:HD3	4:D:929:HOH:O	1.87	0.74
1:C:39:PRO:HG2	4:C:817:HOH:O	1.87	0.74
1:B:11:VAL:HG21	1:B:33:LEU:CD1	2.18	0.74
1:A:352:ILE:CG2	1:A:355:LEU:HG	2.17	0.73
1:D:352:ILE:O	1:D:355:LEU:HB2	1.87	0.73
1:D:213:ILE:HG22	1:D:234:THR:HG22	1.70	0.73
1:C:58:GLU:CB	1:C:98:MET:CE	2.65	0.73
1:A:263:LYS:HB2	1:A:266:ARG:NH1	2.04	0.73
1:B:141:THR:HB	1:B:143:PRO:HD2	1.71	0.73
1:A:82:THR:HG22	1:A:84:ALA:N	2.03	0.73
1:D:48:VAL:HG22	4:D:916:HOH:O	1.87	0.73
3:C:800:AME:OXT	4:C:895:HOH:O	2.06	0.73
1:A:301:ALA:HB2	1:A:347:LEU:HD23	1.71	0.73
1:C:135:SER:HB3	3:C:800:AME:HT21	1.72	0.72
1:B:11:VAL:HG21	1:B:33:LEU:HD12	1.71	0.72
1:D:363:LYS:O	1:D:364:VAL:HB	1.88	0.72
1:A:200:PRO:O	4:A:677:HOH:O	2.08	0.72
1:A:113:ARG:HA	1:A:345:PRO:HB2	1.71	0.72
1:D:127[A]:ARG:HB3	1:D:127[A]:ARG:HH11	1.55	0.72
1:B:206:ASP:HB2	1:B:207:PRO:HD3	1.71	0.72
1:A:21:THR:CG2	1:A:23:PHE:CD1	2.73	0.71
1:C:82:THR:HG22	1:C:84:ALA:H	1.53	0.71
1:D:199:ALA:N	1:D:200:PRO:HD2	2.05	0.71
1:D:163:LYS:NZ	3:D:900:AME:N	2.35	0.71
1:D:58:GLU:CD	1:D:98:MET:HG3	2.11	0.71
1:C:263:LYS:HE2	4:C:895:HOH:O	1.91	0.71
1:B:113:ARG:HA	1:B:345:PRO:HB2	1.72	0.70
1:A:149:VAL:HG13	1:A:160:ILE:HD13	1.73	0.70
1:C:139:MET:HG3	1:C:145:LEU:HA	1.72	0.70
1:A:139:MET:HG3	1:A:145:LEU:CA	2.20	0.70
1:D:201:GLN:O	1:D:204:ARG:HB2	1.91	0.70
1:C:10:ARG:HD2	1:C:64:GLU:OE1	1.91	0.70
1:C:29:ARG:HG2	1:C:31:LEU:HD21	1.73	0.70
1:D:206:ASP:CB	1:D:207:PRO:HD3	2.18	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:VAL:HB	1:D:131:PRO:HD2	1.73	0.69
1:D:135:SER:CB	3:D:900:AME:CT2	2.69	0.69
1:C:21:THR:HG22	1:C:23:PHE:H	1.57	0.69
1:B:29:ARG:HD2	1:B:31:LEU:HD21	1.75	0.69
1:D:213:ILE:HG22	1:D:234:THR:CG2	2.22	0.69
1:C:217:LEU:HD21	1:C:228:LEU:HD22	1.72	0.69
1:A:12:GLN:O	1:A:359:VAL:CG2	2.37	0.69
1:D:13:MET:CE	1:D:295:THR:HG22	2.23	0.69
1:D:350:ALA:HB1	1:D:351:PRO:HD2	1.74	0.69
1:B:147:ASP:HA	4:B:765:HOH:O	1.92	0.69
1:B:142:ILE:N	1:B:143:PRO:HD2	2.08	0.69
1:D:72:ILE:HB	1:D:73:PRO:HD3	1.75	0.69
1:D:217:LEU:N	1:D:217:LEU:HD23	2.07	0.68
1:B:206:ASP:N	1:B:207:PRO:CD	2.56	0.68
1:B:49:THR:CG2	1:B:98:MET:HE2	2.22	0.68
1:C:7:GLU:OE2	1:C:9:ARG:NH1	2.26	0.68
1:B:206:ASP:N	1:B:207:PRO:HD2	2.09	0.68
1:D:291:GLY:O	3:D:900:AME:OT	2.12	0.68
1:B:146:LEU:C	4:B:765:HOH:O	2.32	0.68
1:A:28:VAL:HG12	1:A:29:ARG:N	2.07	0.68
1:A:206:ASP:N	1:A:207:PRO:CD	2.57	0.68
1:A:308:LEU:CB	1:A:309:PRO:HD2	2.23	0.68
1:B:139:MET:HG3	1:B:145:LEU:CA	2.25	0.67
1:B:250:ASP:OD2	4:B:796:HOH:O	2.12	0.67
1:B:171:GLU:N	1:B:172:PRO:HD2	2.10	0.67
1:C:139:MET:HG3	1:C:145:LEU:CA	2.25	0.67
1:A:35:ARG:HG3	1:A:44:TRP:CE2	2.29	0.67
1:A:201:GLN:O	1:A:204[B]:ARG:HB2	1.95	0.67
1:A:352:ILE:O	1:A:355:LEU:HB2	1.94	0.67
1:D:212:LEU:HD12	1:D:212:LEU:C	2.14	0.67
1:D:21:THR:CG2	1:D:22:SER:N	2.57	0.67
1:A:21:THR:CG2	1:A:23:PHE:H	2.04	0.67
1:D:9:ARG:HH21	1:D:363:LYS:HE2	1.59	0.67
1:C:10:ARG:CD	1:C:64:GLU:OE1	2.44	0.66
1:D:21:THR:CG2	1:D:22:SER:H	2.08	0.66
1:D:350:ALA:HB1	1:D:351:PRO:CD	2.25	0.66
1:D:244:SER:HB2	4:D:988:HOH:O	1.95	0.66
1:D:10:ARG:NH1	1:D:10:ARG:HG3	1.98	0.66
1:B:101:GLY:O	4:B:753:HOH:O	2.12	0.66
1:A:29:ARG:HD2	1:A:31:LEU:HD23	1.77	0.66
1:D:16:VAL:HG22	1:D:325:LYS:HG3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ILE:O	1:A:355:LEU:N	2.24	0.66
1:B:194:TYR:CE2	1:B:202:LEU:HD21	2.31	0.66
1:B:171:GLU:HB2	1:B:172:PRO:HD3	1.78	0.66
1:D:13:MET:CE	1:D:31:LEU:HD11	2.26	0.65
1:A:9:ARG:NE	1:A:360:THR:HG21	2.12	0.65
1:C:87:THR:HG22	1:C:88:PRO:CD	2.25	0.65
1:A:199:ALA:HB3	1:A:200:PRO:CD	2.25	0.65
1:C:87:THR:HB	1:C:88:PRO:HD3	1.77	0.65
1:A:288:TRP:HA	4:A:662:HOH:O	1.94	0.65
1:D:38:THR:HB	1:D:39:PRO:HD2	1.79	0.65
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.79	0.65
1:D:29:ARG:NH2	1:D:50:MET:CG	2.60	0.65
1:B:147:ASP:N	4:B:765:HOH:O	2.30	0.65
1:B:288:TRP:HB3	1:B:313:LEU:HB2	1.78	0.65
1:C:191:ASN:C	1:C:192:THR:HG23	2.17	0.65
1:A:8:LEU:HD12	1:A:366:ILE:HD13	1.80	0.64
1:A:144:GLN:O	1:A:148:VAL:HG23	1.97	0.64
1:D:113:ARG:HG3	1:D:346:GLY:HA3	1.79	0.64
1:D:85:LYS:O	1:D:88:PRO:HD2	1.98	0.64
1:D:13:MET:HE3	1:D:31:LEU:HD11	1.78	0.64
1:C:329:THR:HG21	1:C:349:VAL:HG11	1.79	0.64
1:A:352:ILE:O	1:A:352:ILE:HG22	1.97	0.64
1:A:290:GLY:HA2	4:A:695:HOH:O	1.96	0.64
1:A:352:ILE:HG22	1:A:355:LEU:CG	2.26	0.64
1:C:86:VAL:HG13	1:C:90:LEU:HD11	1.79	0.64
1:A:319:ALA:HB1	1:A:332:PHE:O	1.97	0.64
1:C:349:VAL:HG12	1:C:350:ALA:N	2.13	0.64
1:B:21:THR:CG2	1:B:22:SER:N	2.60	0.64
1:D:328:ILE:O	1:D:351:PRO:HA	1.97	0.64
1:B:142:ILE:N	1:B:143:PRO:CD	2.61	0.64
1:B:29:ARG:CD	1:B:31:LEU:CD2	2.76	0.63
1:B:29:ARG:CD	1:B:31:LEU:HD23	2.28	0.63
1:D:141:THR:OG1	1:D:144:GLN:HB2	1.98	0.63
1:A:38:THR:HB	1:A:39:PRO:HD2	1.79	0.63
1:A:277:HIS:HD2	1:A:311:PHE:CE1	2.17	0.63
1:A:33:LEU:HD23	1:A:45:GLY:O	1.98	0.63
1:B:277:HIS:HD2	1:B:311:PHE:CE1	2.16	0.63
1:B:21:THR:HG23	1:B:22:SER:H	1.61	0.63
1:C:352:ILE:CB	1:C:355:LEU:HD12	2.29	0.63
1:B:163:LYS:NZ	3:B:700:AME:HB2	2.13	0.63
1:C:135:SER:HB2	3:C:800:AME:CT2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:O	1:A:204[A]:ARG:HB2	1.99	0.62
1:B:82:THR:O	1:B:86:VAL:HG23	1.99	0.62
1:C:186:LEU:N	4:C:870:HOH:O	2.07	0.62
1:D:205:LEU:C	1:D:207:PRO:HD2	2.18	0.62
1:D:352:ILE:HG22	1:D:355:LEU:H	1.64	0.62
1:B:261:ASN:C	1:B:261:ASN:OD1	2.37	0.62
1:B:8:LEU:HD23	1:B:32:LEU:HD11	1.82	0.62
1:A:8:LEU:HD23	1:A:32:LEU:CD2	2.29	0.62
1:D:169:ASP:OD1	1:D:194:TYR:OH	2.17	0.62
1:D:199:ALA:N	1:D:200:PRO:CD	2.62	0.62
1:D:82:THR:HG22	1:D:85:LYS:H	1.64	0.62
1:A:161:LYS:NZ	3:A:600:AME:OXT	2.28	0.62
1:A:87:THR:CB	1:A:88:PRO:CD	2.76	0.62
1:C:87:THR:CB	1:C:88:PRO:CD	2.77	0.62
1:C:171:GLU:N	1:C:172:PRO:HD2	2.14	0.62
1:A:6:VAL:HB	1:A:72:ILE:HD13	1.82	0.62
1:C:334:LEU:HD21	1:C:337:GLY:HA2	1.80	0.62
1:A:119:PHE:CD2	1:A:301:ALA:HB1	2.35	0.61
1:A:159:ARG:NH2	1:A:316:ASP:OD1	2.20	0.61
1:D:142:ILE:HB	1:D:143:PRO:CD	2.30	0.61
1:D:85:LYS:C	1:D:88:PRO:HD2	2.21	0.61
1:C:59:TYR:OH	1:D:65:HIS:HD2	1.83	0.61
1:A:10:ARG:NH2	1:A:60:ASN:HB2	2.14	0.61
1:A:232:ILE:O	4:A:688:HOH:O	2.16	0.61
1:B:205:LEU:C	1:B:207:PRO:HD2	2.20	0.61
1:C:51:ALA:O	1:C:59:TYR:HB2	2.01	0.61
1:A:203:ALA:HA	1:A:232:ILE:HG22	1.83	0.61
1:B:163:LYS:HZ1	3:B:700:AME:CB	2.14	0.61
1:C:191:ASN:O	1:C:192:THR:HG23	2.00	0.61
1:C:169:ASP:OD2	1:C:201:GLN:NE2	2.33	0.61
1:A:21:THR:HG22	1:A:23:PHE:N	2.06	0.61
1:D:9:ARG:HH11	1:D:356:LEU:CD2	2.13	0.61
1:A:351:PRO:O	1:A:353:PRO:HD3	2.01	0.61
1:D:144:GLN:O	1:D:148:VAL:HG23	2.00	0.61
1:A:7:GLU:OE2	1:A:35:ARG:NH1	2.34	0.61
1:B:159:ARG:HB2	1:B:185:LEU:CB	2.31	0.61
1:B:75:LEU:O	1:B:81:ILE:HD11	2.00	0.60
1:C:139:MET:HB2	1:C:168:TRP:CH2	2.34	0.60
1:A:171:GLU:HB2	1:A:172:PRO:HD3	1.83	0.60
1:B:159:ARG:HD2	1:B:159:ARG:C	2.21	0.60
1:A:46:GLU:OE1	1:A:297:LEU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ARG:HD3	1:B:32:LEU:HD13	1.82	0.60
1:A:201:GLN:O	1:A:201:GLN:HG3	2.02	0.60
1:D:295:THR:OG1	1:D:297:LEU:HB2	2.00	0.60
1:C:21:THR:HG21	1:C:23:PHE:CD1	2.37	0.60
1:B:147:ASP:CA	4:B:765:HOH:O	2.49	0.60
1:D:269:GLY:C	4:D:940:HOH:O	2.40	0.60
1:B:228:LEU:O	1:B:228:LEU:HD12	2.02	0.60
1:B:11:VAL:CG2	1:B:33:LEU:HD12	2.32	0.60
1:C:261:ASN:C	1:C:261:ASN:OD1	2.40	0.60
1:D:159:ARG:HB2	1:D:185:LEU:HB2	1.84	0.60
1:B:159:ARG:HA	1:B:185:LEU:HB2	1.82	0.60
1:B:164:ILE:CD1	1:B:188:VAL:CG1	2.79	0.60
1:A:274:ARG:O	1:A:277:HIS:HB3	2.02	0.60
1:C:223:LEU:O	1:C:226:ALA:HB3	2.01	0.59
1:D:60:ASN:O	1:D:63:ALA:HB3	2.02	0.59
1:A:9:ARG:HE	1:A:360:THR:HG21	1.67	0.59
1:A:72:ILE:HG22	1:A:76:LEU:HD11	1.83	0.59
1:A:35:ARG:HG3	1:A:44:TRP:CZ2	2.36	0.59
1:C:96:HIS:O	1:C:100:LYS:HG3	2.03	0.59
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.84	0.59
1:C:82:THR:HG22	1:C:84:ALA:N	2.16	0.59
1:A:171:GLU:N	1:A:172:PRO:HD2	2.17	0.59
1:B:87:THR:HB	1:B:88:PRO:CD	2.32	0.59
1:B:49:THR:HG23	1:B:98:MET:CE	2.31	0.59
1:C:29:ARG:CG	1:C:31:LEU:HD21	2.33	0.59
1:D:272:GLU:O	1:D:276:VAL:HG23	2.03	0.58
1:A:136:VAL:HB	1:A:162:LEU:HD23	1.84	0.58
1:B:227:GLU:HA	1:B:230:ARG:HH11	1.68	0.58
1:A:58:GLU:CB	1:A:98:MET:HE3	2.30	0.58
1:A:127:ARG:NH2	1:A:311:PHE:O	2.36	0.58
1:B:9:ARG:O	1:B:32:LEU:HD12	2.04	0.58
1:D:159:ARG:HG2	1:D:160:ILE:N	2.19	0.58
1:B:87:THR:CB	1:B:88:PRO:HD3	2.33	0.58
1:C:150:GLY:HA2	1:C:180:PHE:CE2	2.37	0.58
1:C:322:ARG:NH1	1:C:323:PHE:CE2	2.72	0.58
1:C:227:GLU:O	1:C:230:ARG:HB2	2.04	0.58
1:D:206:ASP:CB	1:D:207:PRO:CD	2.82	0.58
1:A:23:PHE:HZ	3:A:600:AME:SD	2.26	0.58
1:C:161:LYS:NZ	3:C:800:AME:OXT	2.36	0.58
1:D:169:ASP:OD2	1:D:201:GLN:NE2	2.37	0.58
1:B:49:THR:HA	1:B:98:MET:CE	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:VAL:O	1:C:158:VAL:CG1	2.51	0.58
1:A:169:ASP:OD2	1:A:201:GLN:NE2	2.32	0.57
1:B:29:ARG:HD2	1:B:31:LEU:HD23	1.84	0.57
1:B:21:THR:HG23	1:B:22:SER:N	2.18	0.57
1:A:301:ALA:HB2	1:A:347:LEU:CD2	2.34	0.57
1:C:20:ARG:HG2	1:C:138:ILE:HB	1.86	0.57
1:B:80:ASP:O	1:B:81:ILE:HG13	2.04	0.57
1:D:29:ARG:CD	1:D:31:LEU:CD2	2.75	0.57
1:C:171:GLU:N	1:C:172:PRO:CD	2.67	0.57
1:D:26:GLN:NE2	1:D:50:MET:SD	2.78	0.57
1:D:48:VAL:HG23	1:D:98:MET:SD	2.44	0.57
1:A:350:ALA:HB1	1:A:351:PRO:HD2	1.87	0.57
1:B:143:PRO:O	1:B:146:LEU:N	2.38	0.57
1:B:142:ILE:O	1:B:146:LEU:HG	2.05	0.57
1:B:141:THR:CB	1:B:143:PRO:HD2	2.35	0.57
1:A:1:MET:HE2	1:A:38:THR:HG21	1.87	0.56
1:A:28:VAL:HG12	1:A:29:ARG:H	1.70	0.56
1:A:356:LEU:CD2	1:A:360:THR:OG1	2.52	0.56
1:A:135:SER:HB3	3:A:600:AME:CT2	2.33	0.56
1:A:327:ASP:OD1	1:A:328:ILE:N	2.39	0.56
1:C:159:ARG:HD2	4:C:864:HOH:O	2.03	0.56
1:D:35:ARG:NE	1:D:42:GLU:OE2	2.38	0.56
1:D:191:ASN:C	1:D:192:THR:HG23	2.26	0.56
1:C:205:LEU:C	1:C:207:PRO:CD	2.71	0.56
1:D:352:ILE:HG22	1:D:355:LEU:HB2	1.86	0.56
1:C:349:VAL:HG13	4:C:893:HOH:O	2.05	0.56
1:B:35:ARG:HD2	1:B:42:GLU:OE2	2.06	0.56
1:A:5:GLY:HA2	1:A:76:LEU:HD21	1.88	0.56
1:D:103:LEU:O	1:D:107:VAL:HG23	2.05	0.56
1:B:159:ARG:HB2	1:B:185:LEU:HB2	1.87	0.56
1:A:49:THR:HG22	1:A:98:MET:HE3	1.87	0.56
1:D:365:TRP:O	1:D:366:ILE:HG13	2.06	0.56
1:D:159:ARG:HB2	1:D:185:LEU:CB	2.36	0.56
1:D:189:ASP:OD2	3:D:900:AME:OXT	2.24	0.56
1:A:212:LEU:HD12	1:A:212:LEU:O	2.06	0.55
1:A:21:THR:CG2	1:A:22:SER:N	2.69	0.55
1:B:21:THR:HG21	1:B:23:PHE:CZ	2.40	0.55
1:B:29:ARG:NE	1:B:31:LEU:CD2	2.69	0.55
1:B:334:LEU:HD12	1:B:338:HIS:O	2.07	0.55
1:B:201:GLN:O	1:B:204:ARG:HB2	2.06	0.55
1:C:50:MET:HE2	4:C:830:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HG3	4:B:751:HOH:O	2.06	0.55
1:A:169:ASP:O	1:A:172:PRO:HD2	2.07	0.55
1:A:68[A]:ARG:HH11	1:A:68[A]:ARG:CG	2.16	0.55
1:A:290:GLY:CA	4:A:695:HOH:O	2.52	0.55
1:D:171:GLU:N	1:D:172:PRO:HD2	2.20	0.55
1:C:8:LEU:CD2	1:C:32:LEU:HD22	2.35	0.55
1:C:21:THR:CG2	1:C:23:PHE:CD1	2.90	0.55
1:B:49:THR:HG22	1:B:98:MET:HE1	1.85	0.55
1:C:329:THR:HG21	1:C:349:VAL:CG1	2.36	0.55
1:D:274:ARG:O	1:D:277:HIS:HB3	2.07	0.55
1:A:204[A]:ARG:NH1	1:A:204[A]:ARG:HG2	2.16	0.55
1:A:11:VAL:HB	1:A:31:LEU:CD1	2.37	0.55
1:A:277:HIS:CD2	1:A:311:PHE:CE1	2.95	0.55
1:B:162:LEU:CD1	1:B:186:LEU:HD11	2.37	0.55
1:B:127[B]:ARG:NH2	1:B:308:LEU:O	2.39	0.55
1:C:58:GLU:HB2	1:C:98:MET:HE1	1.88	0.55
1:A:72:ILE:N	1:A:73:PRO:CD	2.69	0.55
1:D:142:ILE:O	1:D:145:LEU:HB3	2.07	0.55
1:C:127:ARG:HB2	1:C:307:SER:HB2	1.89	0.55
1:B:148:VAL:HG13	1:B:152:TYR:CE1	2.42	0.55
1:C:169:ASP:O	1:C:172:PRO:HD2	2.07	0.54
1:C:25:THR:CG2	1:C:26:GLN:N	2.69	0.54
1:D:11:VAL:HG22	1:D:360:THR:HA	1.89	0.54
1:B:96:HIS:O	1:B:100:LYS:HG3	2.07	0.54
1:B:81:ILE:CG2	1:B:82:THR:N	2.70	0.54
1:A:338:HIS:O	1:A:339:LEU:HD12	2.08	0.54
1:D:9:ARG:NH1	1:D:356:LEU:CD2	2.71	0.54
1:B:35:ARG:NH1	1:B:42:GLU:OE2	2.39	0.54
1:C:350:ALA:HB1	1:C:351:PRO:HD2	1.88	0.54
1:C:293:ILE:HD11	3:C:800:AME:CE	2.37	0.54
1:D:10:ARG:CG	1:D:10:ARG:HH11	2.13	0.54
1:C:112:LEU:HB3	1:C:117:ARG:O	2.08	0.54
1:D:46:GLU:OE2	1:D:295:THR:HG23	2.07	0.54
1:D:33:LEU:C	1:D:34:LEU:HD23	2.28	0.54
1:D:206:ASP:HB2	1:D:207:PRO:CD	2.31	0.54
1:A:204[A]:ARG:HH11	1:A:204[A]:ARG:CG	2.10	0.54
1:B:163:LYS:HZ1	3:B:700:AME:HB2	1.72	0.54
1:A:8:LEU:HD12	1:A:366:ILE:CD1	2.38	0.54
1:A:33:LEU:HD21	1:A:297:LEU:HD12	1.90	0.54
1:B:239:ASP:OD1	1:B:266:ARG:NH1	2.39	0.54
1:C:109:ASP:O	1:C:113:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:TYR:CG	1:D:202:LEU:HD11	2.43	0.54
1:A:229:ALA:HB2	1:A:236:ILE:HG13	1.90	0.54
1:D:160:ILE:O	1:D:186:LEU:HD12	2.08	0.54
1:C:169:ASP:C	1:C:172:PRO:HD2	2.27	0.54
1:B:145:LEU:O	1:B:145:LEU:HG	2.01	0.54
1:B:149:VAL:HG12	1:B:153:LEU:HD12	1.89	0.54
1:A:8:LEU:CD2	1:A:32:LEU:HD21	2.37	0.54
1:D:214:GLU:HA	1:D:237:CYS:HB3	1.89	0.54
1:B:199:ALA:N	1:B:200:PRO:HD2	2.22	0.54
1:B:81:ILE:HG22	1:B:82:THR:N	2.22	0.53
1:B:227:GLU:HA	1:B:230:ARG:NH1	2.22	0.53
1:A:125:SER:CB	1:A:307:SER:HG	2.21	0.53
1:A:272:GLU:O	1:A:276:VAL:HG23	2.08	0.53
1:C:1:MET:HE3	1:C:38:THR:HG21	1.89	0.53
1:C:194:TYR:CE2	1:C:202:LEU:HD21	2.44	0.53
1:D:58:GLU:OE1	1:D:98:MET:CG	2.49	0.53
1:A:135:SER:OG	3:A:600:AME:HT23	2.09	0.53
1:C:321:ASP:HA	1:C:324:TYR:O	2.08	0.53
1:C:329:THR:CG2	1:C:349:VAL:CG1	2.86	0.53
1:B:43:GLY:HA3	1:B:110:ALA:HB2	1.91	0.53
1:D:2:LYS:HD2	1:D:3:LEU:N	2.24	0.53
1:B:21:THR:HG21	1:B:23:PHE:CD1	2.44	0.53
1:A:2:LYS:HD2	1:A:39:PRO:HG3	1.90	0.53
1:A:177:ARG:HD2	1:A:181:GLY:O	2.09	0.53
1:C:352:ILE:HG22	1:C:352:ILE:O	2.08	0.53
1:B:81:ILE:CD1	4:B:716:HOH:O	2.56	0.53
1:A:199:ALA:CB	1:A:200:PRO:HD3	2.34	0.53
1:A:164:ILE:HG12	1:A:188:VAL:HB	1.89	0.53
1:B:138:ILE:HG23	1:B:168:TRP:CD1	2.43	0.53
1:A:159:ARG:HG2	1:A:160:ILE:N	2.23	0.53
1:A:199:ALA:N	1:A:200:PRO:HD2	2.23	0.53
1:D:258:GLN:O	1:D:286:PRO:HD2	2.09	0.53
1:C:292:MET:O	1:C:293:ILE:HB	2.09	0.53
1:A:1:MET:CE	1:A:38:THR:HG21	2.38	0.53
1:A:33:LEU:CD2	1:A:297:LEU:HD12	2.40	0.53
1:A:200:PRO:O	1:A:203:ALA:HB3	2.09	0.52
1:C:293:ILE:CD1	3:C:800:AME:CE	2.88	0.52
1:B:11:VAL:HG21	1:B:33:LEU:HD11	1.90	0.52
1:D:191:ASN:O	1:D:192:THR:HG23	2.08	0.52
1:B:72:ILE:N	1:B:73:PRO:HD2	2.25	0.52
1:D:64:GLU:O	1:D:67:LEU:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ASN:ND2	1:D:288:TRP:CH2	2.78	0.52
1:A:13:MET:HG2	1:A:359:VAL:HG21	1.91	0.52
1:A:33:LEU:CD2	1:A:45:GLY:O	2.56	0.52
1:A:135:SER:OG	1:A:161:LYS:HE2	2.10	0.52
1:A:9:ARG:NE	1:A:356:LEU:HD22	2.25	0.52
1:A:149:VAL:HG13	1:A:160:ILE:CD1	2.39	0.52
1:D:163:LYS:HE3	1:D:191:ASN:OD1	2.10	0.52
1:C:293:ILE:HG22	1:C:293:ILE:O	2.09	0.52
1:B:33:LEU:HD23	1:B:46:GLU:HG3	1.91	0.52
1:A:28:VAL:CG1	1:A:29:ARG:N	2.72	0.52
1:D:11:VAL:HG13	1:D:359:VAL:HB	1.91	0.52
1:D:271:LEU:N	4:D:940:HOH:O	2.42	0.52
1:A:293:ILE:CG2	1:A:293:ILE:O	2.52	0.52
1:D:365:TRP:C	1:D:366:ILE:HG13	2.29	0.52
1:D:18:PRO:HA	1:D:26:GLN:O	2.09	0.52
1:B:87:THR:CB	1:B:88:PRO:CD	2.88	0.52
1:C:29:ARG:CG	1:C:31:LEU:CD2	2.89	0.52
1:D:1:MET:SD	1:D:38:THR:HG21	2.50	0.52
1:C:329:THR:HB	1:C:349:VAL:CG1	2.40	0.52
1:A:212:LEU:HD11	4:A:667:HOH:O	2.10	0.51
1:D:174:ARG:O	1:D:178:GLU:HB2	2.11	0.51
1:C:352:ILE:O	1:C:355:LEU:N	2.44	0.51
1:B:29:ARG:NE	1:B:31:LEU:HD23	2.25	0.51
1:D:139:MET:HG3	1:D:145:LEU:HA	1.93	0.51
1:C:349:VAL:CG1	1:C:350:ALA:N	2.72	0.51
1:B:125:SER:HB2	1:B:307:SER:OG	2.10	0.51
1:D:60:ASN:CB	4:D:920:HOH:O	2.38	0.51
1:A:9:ARG:HE	1:A:356:LEU:HD22	1.74	0.51
1:A:356:LEU:O	1:A:359:VAL:HG12	2.11	0.51
1:C:159:ARG:HG2	1:C:160:ILE:N	2.23	0.51
1:B:72:ILE:N	1:B:73:PRO:CD	2.73	0.51
1:A:308:LEU:HB3	1:A:309:PRO:HD2	1.90	0.51
1:C:129:SER:C	1:C:130:VAL:CG1	2.77	0.51
1:A:356:LEU:HD23	1:A:360:THR:OG1	2.10	0.51
1:A:125:SER:CB	1:A:307:SER:OG	2.58	0.51
1:C:308:LEU:CB	1:C:309:PRO:CD	2.89	0.51
1:A:70:TYR:C	1:A:73:PRO:HD2	2.31	0.51
1:A:212:LEU:HD12	1:A:212:LEU:C	2.31	0.51
1:C:171:GLU:OE1	1:C:171:GLU:HA	2.11	0.51
1:C:367:GLY:O	1:C:368:SER:O	2.29	0.51
1:D:270:TYR:O	1:D:273:ALA:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:THR:HG23	1:A:22:SER:N	2.24	0.51
1:B:164:ILE:CG2	1:B:188:VAL:HG13	2.38	0.51
1:A:308:LEU:CB	1:A:309:PRO:CD	2.88	0.51
1:D:30:GLU:O	1:D:60:ASN:ND2	2.37	0.50
1:B:277:HIS:CD2	1:B:311:PHE:CE1	2.98	0.50
1:A:112:LEU:HB3	1:A:117:ARG:O	2.11	0.50
1:B:274:ARG:O	1:B:277:HIS:HB3	2.10	0.50
1:C:148:VAL:CG1	1:C:152:TYR:CE1	2.95	0.50
1:A:8:LEU:CD2	1:A:32:LEU:CD2	2.89	0.50
1:C:334:LEU:HD12	1:C:339:LEU:HD13	1.94	0.50
1:C:277:HIS:CD2	1:C:310:ASN:HB3	2.47	0.50
1:A:171:GLU:N	1:A:172:PRO:CD	2.75	0.50
1:C:83:ALA:O	1:C:86:VAL:HB	2.11	0.50
1:C:293:ILE:HD11	3:C:800:AME:HE3	1.93	0.50
1:C:329:THR:CG2	1:C:349:VAL:HG11	2.42	0.50
1:C:59:TYR:OH	1:D:65:HIS:CD2	2.64	0.50
1:D:60:ASN:CA	4:D:920:HOH:O	2.60	0.50
1:B:163:LYS:NZ	3:B:700:AME:CB	2.73	0.50
1:A:334:LEU:HD21	1:A:337:GLY:HA2	1.92	0.50
1:A:11:VAL:HB	1:A:31:LEU:HD12	1.93	0.50
1:B:171:GLU:N	1:B:172:PRO:CD	2.75	0.50
1:B:308:LEU:HB3	1:B:309:PRO:HD2	1.94	0.50
1:C:352:ILE:O	1:C:355:LEU:HB2	2.11	0.50
1:C:21:THR:HG21	1:C:23:PHE:CZ	2.46	0.50
1:C:213:ILE:HG22	1:C:234:THR:CG2	2.34	0.50
1:C:119:PHE:HB2	4:C:853:HOH:O	2.12	0.50
1:D:79:GLU:OE1	1:D:79:GLU:HA	2.10	0.50
1:C:35:ARG:HD3	1:C:44:TRP:CH2	2.45	0.50
1:D:25:THR:HG22	1:D:26:GLN:N	2.26	0.50
1:A:118:SER:HB2	4:A:654:HOH:O	2.11	0.50
1:A:125:SER:HB2	1:A:307:SER:OG	2.11	0.49
1:C:161:LYS:HE2	1:C:163:LYS:HE2	1.95	0.49
1:A:113:ARG:HG2	1:A:346:GLY:HA3	1.93	0.49
1:C:328:ILE:O	1:C:351:PRO:HA	2.12	0.49
1:C:148:VAL:HG13	1:C:152:TYR:CE1	2.46	0.49
1:A:58:GLU:CB	1:A:98:MET:HE2	2.18	0.49
1:B:10:ARG:HH12	1:B:60:ASN:HB3	1.74	0.49
1:A:87:THR:N	1:A:88:PRO:HD2	2.26	0.49
1:A:288:TRP:CE3	1:A:289:CYS:O	2.65	0.49
1:D:135:SER:HB3	3:D:900:AME:CT2	2.41	0.49
1:A:10:ARG:CZ	1:A:60:ASN:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:CG1	1:A:29:ARG:H	2.26	0.49
1:C:72:ILE:N	1:C:73:PRO:HD2	2.27	0.49
1:D:169:ASP:HB2	1:D:170:VAL:HG23	1.95	0.49
1:D:194:TYR:CD1	1:D:194:TYR:N	2.79	0.49
1:D:227:GLU:O	1:D:230:ARG:HB2	2.13	0.49
1:B:92:LYS:HD2	1:B:93:PHE:CZ	2.47	0.49
1:B:164:ILE:CG2	1:B:188:VAL:CG1	2.91	0.49
1:B:23:PHE:HZ	3:B:700:AME:HE1	1.76	0.49
1:B:249:ALA:O	1:B:253:LYS:HG3	2.12	0.49
1:C:293:ILE:CD1	3:C:800:AME:HE2	2.43	0.49
1:A:199:ALA:CB	1:A:200:PRO:CD	2.88	0.49
1:D:9:ARG:NH1	1:D:356:LEU:HG	2.27	0.49
1:A:91:ALA:O	4:A:646:HOH:O	2.19	0.49
1:C:293:ILE:HD12	3:C:800:AME:HE2	1.94	0.49
1:A:328:ILE:O	1:A:351:PRO:HA	2.12	0.49
1:B:86:VAL:O	1:B:90:LEU:HG	2.12	0.49
1:B:49:THR:HG23	1:B:98:MET:HE3	1.95	0.49
1:A:145:LEU:O	1:A:148:VAL:HB	2.12	0.49
1:C:153:LEU:HD12	1:C:180:PHE:CD2	2.47	0.49
1:A:134:VAL:O	1:A:134:VAL:HG13	2.13	0.49
1:A:221:ASP:O	1:A:225:HIS:ND1	2.39	0.49
1:A:46:GLU:OE2	1:A:294:GLU:HB3	2.13	0.49
1:B:55:TYR:CZ	1:B:240:GLU:HG3	2.48	0.49
1:D:4:SER:HB2	1:D:37:VAL:HG12	1.94	0.49
1:B:11:VAL:HG12	1:B:12:GLN:N	2.28	0.49
3:D:900:AME:SD	3:D:900:AME:CT1	3.01	0.48
1:D:169:ASP:HB2	1:D:170:VAL:H	1.37	0.48
1:A:329:THR:HG22	1:A:350:ALA:C	2.31	0.48
1:C:87:THR:HB	1:C:88:PRO:CD	2.41	0.48
1:B:171:GLU:HB2	1:B:172:PRO:CD	2.43	0.48
1:B:321:ASP:HA	1:B:324:TYR:O	2.13	0.48
1:C:139:MET:HG3	1:C:145:LEU:HB2	1.95	0.48
1:C:47:CYS:SG	1:C:49:THR:HG23	2.53	0.48
1:A:308:LEU:HG	1:A:309:PRO:HD2	1.95	0.48
1:D:171:GLU:HA	1:D:171:GLU:OE1	2.12	0.48
1:C:25:THR:HG22	1:C:26:GLN:N	2.28	0.48
1:D:4:SER:HB2	1:D:37:VAL:O	2.13	0.48
1:A:142:ILE:N	1:A:143:PRO:HD2	2.28	0.48
1:B:8:LEU:O	1:B:363:LYS:HA	2.13	0.48
1:C:21:THR:CG2	1:C:22:SER:N	2.76	0.48
1:B:21:THR:CG2	1:B:23:PHE:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LEU:HD21	1:D:29:ARG:HB2	1.95	0.48
1:A:352:ILE:O	1:A:355:LEU:CB	2.61	0.48
1:B:75:LEU:CD2	1:B:90:LEU:HD21	2.44	0.48
1:A:364:VAL:HG22	1:A:365:TRP:N	2.29	0.48
1:D:67:LEU:HD23	1:D:71:LEU:HB2	1.95	0.48
1:C:315:GLY:C	1:C:317:THR:H	2.16	0.48
1:D:211:LEU:O	1:D:212:LEU:CB	2.44	0.48
1:D:11:VAL:HG12	1:D:12:GLN:N	2.29	0.48
1:A:161:LYS:NZ	1:A:316:ASP:OD2	2.47	0.48
1:A:321:ASP:HA	1:A:324:TYR:O	2.13	0.48
1:D:199:ALA:HB3	1:D:200:PRO:CD	2.43	0.48
1:A:112:LEU:HD23	1:A:112:LEU:HA	1.72	0.47
1:D:130:VAL:O	1:D:338:HIS:HA	2.13	0.47
1:A:8:LEU:HB2	1:A:364:VAL:CG1	2.44	0.47
1:D:303:VAL:HG23	1:D:317:THR:HG21	1.96	0.47
1:D:20:ARG:HD3	1:D:138:ILE:HB	1.96	0.47
1:A:16:VAL:N	1:A:323:PHE:O	2.45	0.47
1:D:127[A]:ARG:NH1	1:D:129:SER:O	2.47	0.47
1:B:81:ILE:HD12	4:B:716:HOH:O	2.12	0.47
1:B:29:ARG:CD	1:B:31:LEU:HD21	2.41	0.47
1:D:170:VAL:HG22	1:D:205:LEU:HD23	1.96	0.47
1:B:225:HIS:CD2	1:B:238:LEU:HD21	2.50	0.47
1:B:217:LEU:HB2	1:B:225:HIS:CE1	2.50	0.47
1:D:48:VAL:HG12	1:D:292:MET:HB2	1.96	0.47
1:A:87:THR:N	1:A:88:PRO:CD	2.77	0.47
1:B:194:TYR:CD2	1:B:202:LEU:HD21	2.50	0.47
1:A:334:LEU:HD12	1:A:339:LEU:CD1	2.41	0.47
1:C:150:GLY:CA	1:C:180:PHE:CZ	2.98	0.47
1:B:237:CYS:HA	1:B:259:ILE:O	2.15	0.47
1:B:267:VAL:O	1:B:272:GLU:HG2	2.14	0.47
1:A:21:THR:CG2	1:A:23:PHE:CG	2.97	0.47
1:A:170:VAL:HA	1:A:205:LEU:HD21	1.96	0.47
1:C:162:LEU:HG	1:C:186:LEU:HD11	1.96	0.47
1:C:48:VAL:HG22	4:C:827:HOH:O	2.15	0.47
1:B:116:GLU:HA	1:B:345:PRO:HB3	1.97	0.47
1:B:296:GLY:HA3	1:B:329:THR:OG1	2.15	0.47
1:C:271:LEU:HA	1:C:271:LEU:HD23	1.55	0.47
1:D:6:VAL:HA	1:D:35:ARG:O	2.15	0.47
1:D:40:ALA:CB	4:D:906:HOH:O	2.63	0.47
1:C:6:VAL:HG12	1:C:7:GLU:N	2.30	0.46
1:B:127[B]:ARG:HB2	1:B:307:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:HB	1:B:73:PRO:CD	2.43	0.46
1:A:236:ILE:HG22	1:A:237:CYS:N	2.30	0.46
1:D:251:ALA:HB2	4:D:987:HOH:O	2.15	0.46
1:C:308:LEU:HB3	1:C:309:PRO:HD2	1.97	0.46
1:C:129:SER:C	1:C:130:VAL:HG13	2.34	0.46
1:A:213:ILE:HG12	1:A:216:PRO:HG3	1.97	0.46
1:C:143:PRO:O	1:C:144:GLN:C	2.53	0.46
1:A:190:ALA:O	1:A:191:ASN:C	2.53	0.46
1:A:322:ARG:NH1	1:A:323:PHE:CE2	2.82	0.46
1:D:319:ALA:HB1	1:D:332:PHE:O	2.15	0.46
1:A:112:LEU:HD22	1:A:117:ARG:HB3	1.96	0.46
1:B:75:LEU:HD21	1:B:90:LEU:HD21	1.97	0.46
1:C:3:LEU:HB2	1:C:81:ILE:CD1	2.42	0.46
1:D:132:CYS:HB2	1:D:334:LEU:HD11	1.96	0.46
1:D:238:LEU:HD13	1:D:241:SER:HB2	1.96	0.46
1:B:72:ILE:CB	1:B:73:PRO:HD3	2.43	0.46
1:C:135:SER:HG	3:C:800:AME:HT23	1.73	0.46
1:D:352:ILE:O	1:D:355:LEU:N	2.49	0.46
1:A:113:ARG:HA	1:A:345:PRO:CB	2.41	0.46
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.71	0.46
1:D:60:ASN:N	4:D:920:HOH:O	2.48	0.46
1:D:185:LEU:HA	1:D:185:LEU:HD23	1.68	0.46
1:B:161:LYS:NZ	3:B:700:AME:C	2.79	0.46
1:C:199:ALA:O	1:C:200:PRO:C	2.54	0.46
1:C:352:ILE:HA	1:C:353:PRO:HD3	1.75	0.46
1:C:109:ASP:HA	1:C:119:PHE:HE1	1.81	0.46
1:B:340:PRO:HG2	4:B:852:HOH:O	2.14	0.46
1:C:68:ARG:O	1:C:73:PRO:CD	2.64	0.46
1:C:249:ALA:O	1:C:253:LYS:HG3	2.16	0.46
1:A:316:ASP:OD2	4:A:695:HOH:O	2.20	0.46
1:D:142:ILE:N	1:D:143:PRO:HD2	2.30	0.46
1:B:264:PRO:HG3	1:B:305:LEU:HD22	1.98	0.46
1:B:146:LEU:HD23	1:B:176:VAL:HG22	1.98	0.45
1:D:290:GLY:HA2	4:D:1000:HOH:O	2.15	0.45
1:A:87:THR:HG22	1:A:88:PRO:N	2.31	0.45
1:A:206:ASP:HB2	1:A:207:PRO:CD	2.39	0.45
1:A:288:TRP:CA	4:A:662:HOH:O	2.57	0.45
1:B:159:ARG:HB2	1:B:185:LEU:HB3	1.98	0.45
1:C:32:LEU:HD23	1:C:32:LEU:HA	1.67	0.45
1:A:329:THR:HG21	1:A:349:VAL:HG23	1.98	0.45
1:C:135:SER:HB2	3:C:800:AME:HT22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:SER:HA	1:C:308:LEU:HD12	1.98	0.45
1:C:139:MET:HG3	1:C:145:LEU:CB	2.47	0.45
1:A:199:ALA:N	1:A:200:PRO:CD	2.79	0.45
1:C:171:GLU:HB2	1:C:172:PRO:HD3	1.98	0.45
1:C:141:THR:HG22	1:C:142:ILE:N	2.31	0.45
1:B:10:ARG:HH12	1:B:60:ASN:CB	2.30	0.45
1:A:356:LEU:HD22	1:A:360:THR:OG1	2.17	0.45
1:C:75:LEU:O	1:C:81:ILE:HD11	2.17	0.45
1:A:185:LEU:HD22	1:A:211:LEU:HD11	1.98	0.45
1:A:15:LEU:HD12	1:A:26:GLN:O	2.16	0.45
1:B:192:THR:HB	1:B:218:GLU:HA	1.97	0.45
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.72	0.45
1:C:275:ARG:O	1:C:276:VAL:C	2.53	0.45
1:A:163:LYS:HZ1	3:A:600:AME:HB2	1.81	0.45
1:D:159:ARG:HB3	1:D:314:PRO:HG2	1.98	0.45
1:B:222:VAL:O	1:B:225:HIS:N	2.50	0.45
1:A:103:LEU:O	1:A:107:VAL:HG23	2.16	0.45
1:A:49:THR:HG22	1:A:98:MET:CE	2.47	0.45
1:C:38:THR:CB	1:C:39:PRO:CD	2.65	0.45
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.66	0.45
1:C:264:PRO:HG3	1:C:305:LEU:HD22	1.98	0.45
1:D:72:ILE:HB	1:D:73:PRO:CD	2.44	0.45
1:B:55:TYR:OH	1:B:239:ASP:OD1	2.33	0.45
1:B:267:VAL:HG23	1:B:272:GLU:HB3	1.98	0.45
1:A:112:LEU:O	1:A:115:HIS:N	2.43	0.45
1:B:87:THR:N	1:B:88:PRO:HD2	2.32	0.45
1:C:135:SER:CB	3:C:800:AME:HT22	2.43	0.45
1:C:308:LEU:HD12	1:C:308:LEU:HA	1.62	0.45
1:C:352:ILE:HG22	1:C:355:LEU:HG	1.97	0.45
1:A:68[A]:ARG:HG2	1:A:68[A]:ARG:NH1	2.17	0.45
1:A:1:MET:HE2	1:A:38:THR:CG2	2.47	0.45
1:C:29:ARG:HG3	1:C:31:LEU:CD2	2.46	0.45
1:C:31:LEU:HD13	1:C:295:THR:HG23	1.98	0.45
1:B:68:ARG:HG3	1:B:366:ILE:CD1	2.47	0.45
1:B:8:LEU:HB2	1:B:364:VAL:HG12	1.98	0.44
1:A:205:LEU:C	1:A:207:PRO:HD2	2.36	0.44
1:C:298:GLY:O	1:C:299:ARG:C	2.53	0.44
1:D:212:LEU:C	1:D:212:LEU:CD1	2.85	0.44
1:A:203:ALA:CA	1:A:232:ILE:HG22	2.48	0.44
1:C:87:THR:N	1:C:88:PRO:HD2	2.32	0.44
1:A:44:TRP:O	1:A:106:ALA:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HB2	1:A:81:ILE:O	2.17	0.44
1:C:365:TRP:HE1	1:C:367:GLY:HA3	1.81	0.44
1:D:29:ARG:NH1	1:D:292:MET:O	2.51	0.44
1:B:80:ASP:C	1:B:81:ILE:HG13	2.37	0.44
1:A:5:GLY:HA2	1:A:76:LEU:CD2	2.47	0.44
1:A:257:VAL:HG22	1:A:258:GLN:N	2.31	0.44
1:A:328:ILE:O	1:A:352:ILE:N	2.38	0.44
1:B:102:ALA:O	1:B:105:MET:HB3	2.17	0.44
1:D:149:VAL:HG12	1:D:150:GLY:N	2.32	0.44
1:C:148:VAL:CG1	1:C:152:TYR:HE1	2.31	0.44
1:A:57:SER:HA	1:B:94:LYS:O	2.18	0.44
1:D:339:LEU:HD23	1:D:339:LEU:HA	1.53	0.44
1:A:249:ALA:O	1:A:253:LYS:HB2	2.17	0.44
1:B:23:PHE:HZ	3:B:700:AME:CE	2.31	0.44
1:A:288:TRP:HE3	1:A:289:CYS:O	2.00	0.44
1:D:11:VAL:CG1	1:D:12:GLN:N	2.80	0.44
1:C:288:TRP:HB3	1:C:313:LEU:HB2	1.99	0.44
1:B:339:LEU:HA	1:B:339:LEU:HD12	1.49	0.44
1:C:68:ARG:O	1:C:73:PRO:CG	2.66	0.44
1:C:72:ILE:N	1:C:73:PRO:CD	2.81	0.44
1:A:85:LYS:C	1:A:88:PRO:HD2	2.38	0.44
1:D:130:VAL:CB	1:D:131:PRO:HD2	2.39	0.44
1:C:129:SER:HA	1:C:339:LEU:O	2.17	0.44
1:C:293:ILE:CD1	3:C:800:AME:HE3	2.48	0.44
1:A:70:TYR:O	1:A:73:PRO:HD2	2.18	0.44
1:A:126:VAL:HG22	1:A:309:PRO:HD3	2.00	0.44
1:B:164:ILE:HG23	1:B:188:VAL:CG1	2.42	0.43
1:A:350:ALA:HB1	1:A:351:PRO:CD	2.48	0.43
1:B:159:ARG:CB	1:B:185:LEU:HB2	2.48	0.43
1:D:229:ALA:HB2	1:D:236:ILE:HG13	1.99	0.43
3:D:900:AME:N	3:D:900:AME:SD	2.91	0.43
1:D:9:ARG:HH11	1:D:356:LEU:HD21	1.82	0.43
1:B:272:GLU:HB2	4:B:747:HOH:O	2.16	0.43
1:C:97:ARG:O	1:C:268:GLY:HA2	2.18	0.43
1:A:9:ARG:HD3	1:A:360:THR:HG23	2.00	0.43
1:A:169:ASP:HB2	1:A:170:VAL:H	1.46	0.43
1:B:153:LEU:HG	1:B:160:ILE:HD11	1.99	0.43
1:D:329:THR:HG22	1:D:351:PRO:HA	2.01	0.43
1:C:336:GLY:O	1:C:338:HIS:HD2	2.01	0.43
1:D:302:ASN:O	1:D:305:LEU:HB3	2.18	0.43
1:C:166:PRO:HD3	1:C:193:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLU:O	1:D:166:PRO:C	2.56	0.43
1:A:147:ASP:HA	4:A:663:HOH:O	2.18	0.43
1:B:308:LEU:CB	1:B:309:PRO:HD2	2.48	0.43
1:A:129:SER:HA	1:A:339:LEU:O	2.18	0.43
1:C:20:ARG:HD3	1:C:138:ILE:HG22	1.99	0.43
1:A:16:VAL:HG23	1:A:323:PHE:O	2.19	0.43
1:A:86:VAL:O	1:A:90:LEU:HG	2.19	0.43
1:C:206:ASP:N	1:C:207:PRO:HD3	2.30	0.43
1:D:142:ILE:CB	1:D:143:PRO:CD	2.95	0.43
1:D:9:ARG:NH2	1:D:357:ASP:OD1	2.51	0.43
1:A:118:SER:HB3	1:A:344:GLY:O	2.18	0.43
1:D:295:THR:H	1:D:295:THR:HG23	1.48	0.43
1:C:294:GLU:O	1:C:299:ARG:NH2	2.46	0.43
1:C:21:THR:HG23	1:C:22:SER:N	2.33	0.43
1:A:169:ASP:O	1:A:172:PRO:HG2	2.19	0.43
1:B:171:GLU:O	1:B:174:ARG:N	2.52	0.43
1:D:66:VAL:CG1	1:D:67:LEU:N	2.81	0.43
1:C:174:ARG:O	1:C:178:GLU:HB2	2.18	0.43
1:D:177:ARG:HD2	1:D:182:ASP:HA	2.00	0.43
1:C:7:GLU:HB3	1:C:35:ARG:HB3	2.00	0.43
1:D:49:THR:OG1	1:D:60:ASN:OD1	2.37	0.43
1:A:23:PHE:CZ	3:A:600:AME:SD	3.09	0.43
1:B:83:ALA:O	1:B:86:VAL:HB	2.18	0.43
1:B:49:THR:CA	1:B:98:MET:CE	2.97	0.43
1:C:305:LEU:O	1:C:307:SER:N	2.52	0.43
1:D:119:PHE:HB2	4:D:951:HOH:O	2.19	0.43
1:C:122:GLU:HA	1:C:122:GLU:OE1	2.18	0.43
1:B:31:LEU:HD13	1:B:295:THR:HG23	2.00	0.43
1:D:139:MET:HB2	1:D:168:TRP:CH2	2.53	0.43
1:D:199:ALA:O	1:D:203:ALA:N	2.49	0.43
1:D:72:ILE:N	1:D:73:PRO:HD2	2.33	0.43
1:B:159:ARG:CD	1:B:159:ARG:C	2.86	0.43
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.67	0.43
1:C:190:ALA:HB3	1:C:216:PRO:HA	2.01	0.43
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.69	0.43
1:C:257:VAL:O	1:C:257:VAL:HG13	2.18	0.43
1:B:145:LEU:O	1:B:149:VAL:HG23	2.19	0.42
1:A:163:LYS:HE3	1:A:191:ASN:OD1	2.19	0.42
1:A:140:ASP:HB2	1:A:144:GLN:OE1	2.19	0.42
1:B:33:LEU:CD2	1:B:46:GLU:HG3	2.48	0.42
1:C:15:LEU:HD12	1:C:26:GLN:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.75	0.42
1:D:10:ARG:HG2	1:D:32:LEU:HD21	2.01	0.42
1:A:171:GLU:HB2	1:A:172:PRO:CD	2.48	0.42
1:C:3:LEU:HD12	1:C:3:LEU:HA	1.59	0.42
1:C:82:THR:HB	1:C:85:LYS:HG3	2.00	0.42
1:C:226:ALA:O	1:C:229:ALA:HB3	2.18	0.42
1:D:9:ARG:NH1	1:D:356:LEU:HD23	2.34	0.42
1:A:211:LEU:O	1:A:212:LEU:HB3	2.19	0.42
1:A:216:PRO:C	1:A:217:LEU:HD23	2.40	0.42
1:D:320:SER:HB2	1:D:332:PHE:H	1.85	0.42
1:A:133:GLY:HA2	1:A:159:ARG:H	1.85	0.42
1:B:49:THR:CG2	1:B:98:MET:HE3	2.44	0.42
1:D:143:PRO:O	1:D:144:GLN:C	2.58	0.42
1:A:177:ARG:O	1:A:181:GLY:O	2.37	0.42
1:A:245:ALA:O	1:A:248:ALA:HB3	2.20	0.42
1:A:119:PHE:CD2	1:A:301:ALA:CB	3.03	0.42
1:A:227:GLU:O	1:A:230:ARG:HB2	2.20	0.42
1:C:86:VAL:HG13	1:C:90:LEU:CD1	2.47	0.42
1:A:264:PRO:HG3	1:A:305:LEU:CD2	2.49	0.42
1:D:7:GLU:HB3	1:D:35:ARG:HB3	2.01	0.42
1:D:176:VAL:HG12	1:D:176:VAL:O	2.20	0.42
1:B:32:LEU:HA	1:B:32:LEU:HD12	1.79	0.42
1:D:127[A]:ARG:CB	1:D:127[A]:ARG:HH11	2.29	0.42
1:A:21:THR:HG21	1:A:23:PHE:CG	2.53	0.42
1:D:161:LYS:NZ	3:D:900:AME:C	2.82	0.42
1:C:165:GLU:O	1:C:166:PRO:C	2.57	0.42
1:D:257:VAL:HG21	1:D:260:VAL:HG23	2.02	0.42
1:A:312:THR:O	1:A:313:LEU:HG	2.20	0.42
1:D:297:LEU:HA	1:D:297:LEU:HD23	1.83	0.42
1:D:149:VAL:O	1:D:152:TYR:N	2.53	0.42
1:C:352:ILE:CG2	1:C:355:LEU:HG	2.50	0.42
1:D:296:GLY:O	1:D:349:VAL:HG21	2.20	0.42
1:C:350:ALA:HB1	1:C:351:PRO:CD	2.50	0.42
1:D:303:VAL:CG1	1:D:341:VAL:HA	2.50	0.42
1:A:341:VAL:HA	1:A:342:PRO:HD2	1.88	0.42
1:B:356:LEU:CD2	1:B:356:LEU:C	2.88	0.42
1:B:112:LEU:HD22	1:B:117:ARG:HB3	2.02	0.42
1:C:4:SER:HB2	1:C:37:VAL:O	2.19	0.42
1:A:295:THR:OG1	1:A:328:ILE:HD11	2.20	0.41
1:D:288:TRP:HB3	1:D:313:LEU:HB2	2.02	0.41
1:A:275:ARG:NH2	4:A:727:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127[A]:ARG:NH1	1:B:129:SER:O	2.54	0.41
1:D:145:LEU:O	1:D:148:VAL:HB	2.20	0.41
1:B:356:LEU:HD22	1:B:360:THR:OG1	2.20	0.41
1:A:132:CYS:O	1:A:158:VAL:HG23	2.20	0.41
1:A:74:ALA:HB2	4:A:640:HOH:O	2.19	0.41
1:D:9:ARG:HH21	1:D:363:LYS:CE	2.31	0.41
1:D:315:GLY:C	1:D:317:THR:H	2.23	0.41
1:C:239:ASP:HB3	1:C:240:GLU:OE1	2.20	0.41
1:C:105:MET:O	1:C:106:ALA:C	2.58	0.41
1:A:204[A]:ARG:NH1	1:A:204[A]:ARG:CG	2.72	0.41
1:B:143:PRO:O	1:B:144:GLN:C	2.59	0.41
1:A:214:GLU:HB2	4:A:667:HOH:O	2.20	0.41
1:A:25:THR:HG22	1:A:26:GLN:N	2.35	0.41
1:A:8:LEU:HG	1:A:34:LEU:HD23	2.03	0.41
1:D:353:PRO:O	1:D:354:GLU:C	2.59	0.41
1:A:191:ASN:C	1:A:192:THR:HG23	2.41	0.41
1:A:13:MET:HE2	1:A:324:TYR:CZ	2.55	0.41
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.88	0.41
1:B:242:ILE:HG23	1:B:242:ILE:HD12	1.83	0.41
1:D:295:THR:C	1:D:297:LEU:H	2.22	0.41
1:C:58:GLU:HB3	1:C:98:MET:CE	2.47	0.41
1:A:159:ARG:CD	4:A:666:HOH:O	2.50	0.41
1:B:161:LYS:HZ1	3:B:700:AME:C	2.34	0.41
1:A:68[A]:ARG:NH1	1:A:68[A]:ARG:CG	2.77	0.41
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.79	0.41
1:C:217:LEU:O	1:C:218:GLU:C	2.59	0.41
1:D:87:THR:N	1:D:88:PRO:HD2	2.35	0.41
1:B:199:ALA:N	1:B:200:PRO:CD	2.84	0.41
1:A:196:LEU:HD12	1:A:196:LEU:O	2.21	0.41
1:A:130:VAL:HA	1:A:131:PRO:HD3	1.67	0.41
1:B:9:ARG:NH2	1:B:357:ASP:OD1	2.53	0.41
1:A:163:LYS:HD2	1:A:189:ASP:HB3	2.03	0.41
1:D:149:VAL:HG13	1:D:160:ILE:HD13	2.03	0.41
1:D:161:LYS:HA	1:D:187:GLN:O	2.21	0.41
1:B:153:LEU:CG	1:B:160:ILE:HD11	2.51	0.41
1:D:296:GLY:HA3	1:D:329:THR:OG1	2.21	0.41
1:D:171:GLU:N	1:D:172:PRO:CD	2.82	0.41
1:B:118:SER:O	1:B:121:ALA:N	2.53	0.41
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.78	0.41
1:D:29:ARG:NH2	1:D:49:THR:O	2.54	0.41
1:D:141:THR:HB	1:D:143:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:HD3	1:C:138:ILE:CG2	2.51	0.41
1:C:239:ASP:OD1	1:C:266:ARG:NH1	2.51	0.41
1:C:72:ILE:HB	1:C:73:PRO:CD	2.49	0.40
1:D:163:LYS:HD2	1:D:189:ASP:HB3	2.03	0.40
1:B:82:THR:CG2	1:B:83:ALA:N	2.84	0.40
1:C:87:THR:N	1:C:88:PRO:CD	2.83	0.40
1:D:334:LEU:HD21	1:D:337:GLY:HA2	2.03	0.40
1:D:163:LYS:HA	1:D:163:LYS:HD2	1.89	0.40
1:D:216:PRO:O	1:D:217:LEU:HD23	2.20	0.40
1:A:308:LEU:CG	1:A:309:PRO:HD2	2.50	0.40
1:B:148:VAL:CG1	1:B:152:TYR:CE1	3.04	0.40
1:A:221:ASP:OD2	1:A:224:GLY:HA3	2.20	0.40
1:B:65:HIS:CD2	1:B:69:HIS:HD2	2.39	0.40
1:D:123:LEU:HA	1:D:123:LEU:HD23	1.91	0.40
1:D:58:GLU:HB2	1:D:98:MET:HE2	2.04	0.40
1:C:67:LEU:C	1:C:72:ILE:HG13	2.35	0.40
1:A:21:THR:HG22	1:A:23:PHE:CG	2.57	0.40
1:C:217:LEU:O	1:C:218:GLU:O	2.39	0.40
1:C:338:HIS:O	1:C:339:LEU:HD12	2.21	0.40
1:A:142:ILE:H	1:A:143:PRO:HD2	1.86	0.40
1:A:298:GLY:O	1:A:299:ARG:C	2.59	0.40
1:A:3:LEU:HA	1:A:3:LEU:HD12	1.38	0.40
1:C:2:LYS:HD3	4:C:818:HOH:O	2.20	0.40
1:D:159:ARG:HH21	1:D:161:LYS:CB	2.34	0.40
1:D:161:LYS:HZ3	3:D:900:AME:C	2.34	0.40
1:B:83:ALA:HA	1:B:107:VAL:HG11	2.03	0.40
1:A:339:LEU:HD12	1:A:339:LEU:HA	1.78	0.40
1:B:240:GLU:OE2	4:B:732:HOH:O	2.22	0.40
1:C:275:ARG:O	1:C:278:ASP:N	2.54	0.40
1:B:352:ILE:O	1:B:355:LEU:N	2.55	0.40
1:D:25:THR:CG2	1:D:26:GLN:N	2.84	0.40
1:A:2:LYS:HD3	1:A:2:LYS:C	2.42	0.40
1:A:105:MET:CE	1:A:347:LEU:HD21	2.51	0.40
1:A:8:LEU:HD23	1:A:32:LEU:HD21	1.99	0.40
1:D:85:LYS:O	1:D:88:PRO:CD	2.69	0.40
1:C:20:ARG:CG	1:C:138:ILE:HB	2.52	0.40
1:B:154:ASP:C	1:B:156:GLY:N	2.75	0.40

All (2) 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:D:325:LYS:CD	1:D:325:LYS:CD[6_556]	1.08	1.12
1:D:325:LYS:CD	1:D:325:LYS:CE[6_556]	1.84	0.36

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	368/368 (100%)	334 (91%)	29 (8%)	5 (1%)	14	13
1	B	370/368 (100%)	343 (93%)	26 (7%)	1 (0%)	46	57
1	C	366/368 (100%)	337 (92%)	25 (7%)	4 (1%)	17	18
1	D	367/368 (100%)	315 (86%)	47 (13%)	5 (1%)	14	13
All	All	1471/1472 (100%)	1329 (90%)	127 (9%)	15 (1%)	19	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	THR
1	C	218	GLU
1	A	191	ASN
1	C	306	ALA
1	D	212	LEU
1	A	113	ARG
1	B	53	PRO
1	C	192	THR
1	D	306	ALA
1	A	353	PRO
1	D	364	VAL
1	D	191	ASN
1	D	149	VAL
1	A	137	GLY
1	C	353	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	293/291 (101%)	264 (90%)	29 (10%)	10 11
1	B	295/291 (101%)	264 (90%)	31 (10%)	8 9
1	C	291/291 (100%)	261 (90%)	30 (10%)	9 10
1	D	292/291 (100%)	261 (89%)	31 (11%)	8 9
All	All	1171/1164 (101%)	1050 (90%)	121 (10%)	9 10

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	8	LEU
1	A	9	ARG
1	A	14	PRO
1	A	21	THR
1	A	22	SER
1	A	27	SER
1	A	29	ARG
1	A	32	LEU
1	A	68[A]	ARG
1	A	68[B]	ARG
1	A	80	ASP
1	A	119	PHE
1	A	159	ARG
1	A	169	ASP
1	A	177	ARG
1	A	179	ARG
1	A	213	ILE
1	A	289	CYS
1	A	307	SER
1	A	317	THR
1	A	322	ARG
1	A	339	LEU
1	A	343	THR

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Mol	Chain	Res	Type
1	A	349	VAL
1	A	352	ILE
1	A	356	LEU
1	A	363	LYS
1	A	368	SER
1	B	8	LEU
1	B	15	LEU
1	B	21	THR
1	B	27	SER
1	B	29	ARG
1	B	31	LEU
1	B	42	GLU
1	B	66	VAL
1	B	79[A]	GLU
1	B	79[B]	GLU
1	B	79[C]	GLU
1	B	127[A]	ARG
1	B	127[B]	ARG
1	B	142	ILE
1	B	159	ARG
1	B	169	ASP
1	B	174	ARG
1	B	177	ARG
1	B	179	ARG
1	B	213	ILE
1	B	232	ILE
1	B	261	ASN
1	B	313	LEU
1	B	317	THR
1	B	322	ARG
1	B	325	LYS
1	B	339	LEU
1	B	356	LEU
1	B	363	LYS
1	B	364	VAL
1	B	368	SER
1	C	2	LYS
1	C	8	LEU
1	C	9	ARG
1	C	10	ARG
1	C	12	GLN
1	C	21	THR

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Mol	Chain	Res	Type
1	C	27	SER
1	C	31	LEU
1	C	32	LEU
1	C	66	VAL
1	C	79	GLU
1	C	87	THR
1	C	90	LEU
1	C	117	ARG
1	C	125	SER
1	C	159	ARG
1	C	169	ASP
1	C	174	ARG
1	C	177	ARG
1	C	179	ARG
1	C	213	ILE
1	C	217	LEU
1	C	261	ASN
1	C	299	ARG
1	C	317	THR
1	C	322	ARG
1	C	339	LEU
1	C	343	THR
1	C	354	GLU
1	C	363	LYS
1	D	8	LEU
1	D	9	ARG
1	D	10	ARG
1	D	29	ARG
1	D	31	LEU
1	D	32	LEU
1	D	42	GLU
1	D	66	VAL
1	D	68	ARG
1	D	79	GLU
1	D	82	THR
1	D	98	MET
1	D	111	GLU
1	D	116	GLU
1	D	117	ARG
1	D	119	PHE
1	D	127[A]	ARG
1	D	127[B]	ARG

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Mol	Chain	Res	Type
1	D	130	VAL
1	D	159	ARG
1	D	169	ASP
1	D	177	ARG
1	D	179	ARG
1	D	192	THR
1	D	213	ILE
1	D	217	LEU
1	D	227	GLU
1	D	293	ILE
1	D	322	ARG
1	D	343	THR
1	D	359	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	258	GLN
1	B	65	HIS
1	B	69	HIS
1	C	12	GLN
1	C	65	HIS
1	C	69	HIS
1	C	338	HIS
1	D	65	HIS
1	D	69	HIS
1	D	258	GLN

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 (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AME	A	600	2	8,11,11	1.63	2 (25%)	6,13,13	1.28	1 (16%)
3	AME	B	700	2	8,11,11	1.65	2 (25%)	6,13,13	1.74	2 (33%)
3	AME	C	800	2	8,11,11	1.66	2 (25%)	6,13,13	1.34	1 (16%)
3	AME	D	900	2	8,11,11	1.63	2 (25%)	6,13,13	1.45	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AME	A	600	2	-	0/8/12/12	0/0/0/0
3	AME	B	700	2	-	0/8/12/12	0/0/0/0
3	AME	C	800	2	-	0/8/12/12	0/0/0/0
3	AME	D	900	2	-	0/8/12/12	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	900	AME	CT1-N	3.13	1.46	1.34
3	D	900	AME	OT-CT1	3.15	1.30	1.23
3	B	700	AME	CT1-N	3.15	1.46	1.34
3	A	600	AME	CT1-N	3.15	1.46	1.34
3	A	600	AME	OT-CT1	3.17	1.30	1.23
3	C	800	AME	CT1-N	3.22	1.46	1.34
3	B	700	AME	OT-CT1	3.24	1.30	1.23
3	C	800	AME	OT-CT1	3.26	1.30	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	900	AME	OT-CT1-CT2	-2.28	117.88	122.06
3	A	600	AME	OT-CT1-CT2	-2.25	117.94	122.06
3	B	700	AME	OT-CT1-CT2	-2.08	118.24	122.06
3	C	800	AME	CG-CB-CA	-2.06	107.02	113.06
3	D	900	AME	CT2-CT1-N	2.17	120.26	116.11
3	B	700	AME	CT2-CT1-N	3.44	122.70	116.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	AME	10	0
3	B	700	AME	8	0
3	C	800	AME	17	0
3	D	900	AME	13	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	368/368 (100%)	0.67	43 (11%) 6 10	23, 55, 88, 100	0
1	B	368/368 (100%)	0.23	9 (2%) 62 71	20, 40, 77, 100	0
1	C	368/368 (100%)	0.48	26 (7%) 19 26	24, 48, 84, 100	0
1	D	368/368 (100%)	0.79	50 (13%) 4 6	24, 58, 93, 100	0
All	All	1472/1472 (100%)	0.54	128 (8%) 13 18	20, 50, 87, 100	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	80	ASP	5.5
1	A	141	THR	5.3
1	D	24	GLY	5.2
1	C	143	PRO	5.0
1	D	359	VAL	5.0
1	A	39	PRO	4.5
1	C	151	GLY	4.3
1	D	175	ALA	4.3
1	B	24	GLY	4.3
1	B	143	PRO	4.2
1	C	39	PRO	4.1
1	D	353	PRO	4.0
1	A	25	THR	3.9
1	A	203	ALA	3.9
1	D	141	THR	3.9
1	A	156	GLY	3.8
1	D	151	GLY	3.8
1	A	151	GLY	3.8
1	D	355	LEU	3.8
1	C	141	THR	3.7
1	D	154	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	335	SER	3.6
1	A	38	THR	3.5
1	A	354	GLU	3.5
1	C	354	GLU	3.5
1	D	140	ASP	3.5
1	C	357	ASP	3.4
1	A	181	GLY	3.4
1	A	175	ALA	3.3
1	C	150	GLY	3.3
1	D	354	GLU	3.3
1	A	207	PRO	3.3
1	C	80	ASP	3.3
1	C	24	GLY	3.2
1	D	173	VAL	3.2
1	A	368	SER	3.0
1	A	40	ALA	3.0
1	A	208	PHE	3.0
1	D	150	GLY	3.0
1	A	357	ASP	3.0
1	A	150	GLY	3.0
1	D	145	LEU	3.0
1	D	198	ASP	2.9
1	D	27	SER	2.9
1	C	79	GLU	2.9
1	A	143	PRO	2.9
1	C	353	PRO	2.9
1	D	55	TYR	2.9
1	D	143	PRO	2.9
1	A	204[A]	ARG	2.9
1	C	145	LEU	2.9
1	D	357	ASP	2.9
1	B	79[A]	GLU	2.8
1	D	352	ILE	2.8
1	D	368	SER	2.8
1	A	80	ASP	2.8
1	A	147	ASP	2.8
1	D	181	GLY	2.7
1	D	207	PRO	2.7
1	D	329	THR	2.7
1	B	154	ASP	2.7
1	A	178	GLU	2.7
1	A	352	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	79	GLU	2.7
1	A	183	ASP	2.7
1	D	203	ALA	2.7
1	A	291	GLY	2.7
1	A	48	VAL	2.6
1	C	178	GLU	2.6
1	B	147	ASP	2.6
1	D	290	GLY	2.6
1	B	78	ALA	2.6
1	C	38	THR	2.6
1	A	24	GLY	2.5
1	C	74	ALA	2.5
1	D	292	MET	2.5
1	C	147	ASP	2.5
1	C	356	LEU	2.5
1	C	368	SER	2.5
1	D	184	VAL	2.5
1	C	367	GLY	2.5
1	D	25	THR	2.5
1	D	18	PRO	2.4
1	D	2	LYS	2.4
1	A	170	VAL	2.4
1	A	337	GLY	2.4
1	D	317	THR	2.4
1	D	362	ALA	2.4
1	C	139	MET	2.3
1	D	156	GLY	2.3
1	A	184	VAL	2.3
1	D	152	TYR	2.3
1	D	139	MET	2.3
1	C	203	ALA	2.3
1	D	39	PRO	2.3
1	A	180	PHE	2.3
1	D	149	VAL	2.3
1	A	78	ALA	2.3
1	A	353	PRO	2.3
1	A	174	ARG	2.3
1	D	171	GLU	2.3
1	A	148	VAL	2.3
1	C	154	ASP	2.3
1	B	207	PRO	2.2
1	D	167	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	262	ILE	2.2
1	D	291	GLY	2.2
1	A	182	ASP	2.2
1	C	175	ALA	2.2
1	D	168	TRP	2.2
1	C	23	PHE	2.2
1	D	79	GLU	2.2
1	D	26	GLN	2.2
1	D	180	PHE	2.2
1	A	336	GLY	2.1
1	A	355	LEU	2.1
1	D	91	ALA	2.1
1	A	145	LEU	2.1
1	D	147	ASP	2.1
1	C	78	ALA	2.1
1	A	154	ASP	2.1
1	C	317	THR	2.1
1	D	108	LEU	2.1
1	A	144	GLN	2.1
1	B	28	VAL	2.1
1	B	25	THR	2.0
1	A	1	MET	2.0
1	D	350	ALA	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	AME	A	600	12/12	0.88	0.33	3.44	62,88,100,100	0
3	AME	B	700	12/12	0.86	0.23	3.39	36,63,80,97	0
3	AME	C	800	12/12	0.93	0.22	2.34	26,97,100,100	0
3	AME	D	900	12/12	0.84	0.26	1.23	40,83,100,100	0
2	MG	A	601	1/1	0.98	0.13	-1.15	41,41,41,41	0
2	MG	D	901	1/1	0.99	0.12	-1.23	54,54,54,54	0
2	MG	B	701	1/1	0.97	0.13	-1.50	35,35,35,35	0
2	MG	C	801	1/1	0.94	0.10	-1.77	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.