



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AOD
Title : Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors : Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on : 2010-09-23
Resolution : 3.30 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

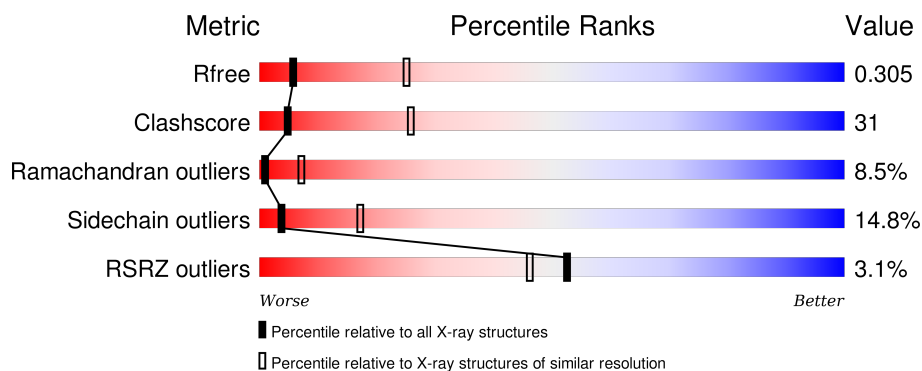
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

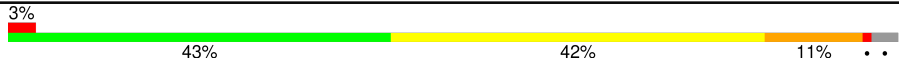


The reported resolution of this entry is 3.30 Å.

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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 $\leq 5\%$. 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	1053	 3% 43% 42% 11% ..
1	B	1053	 3% 40% 45% 11% ..
1	C	1053	 3% 44% 43% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23419 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.

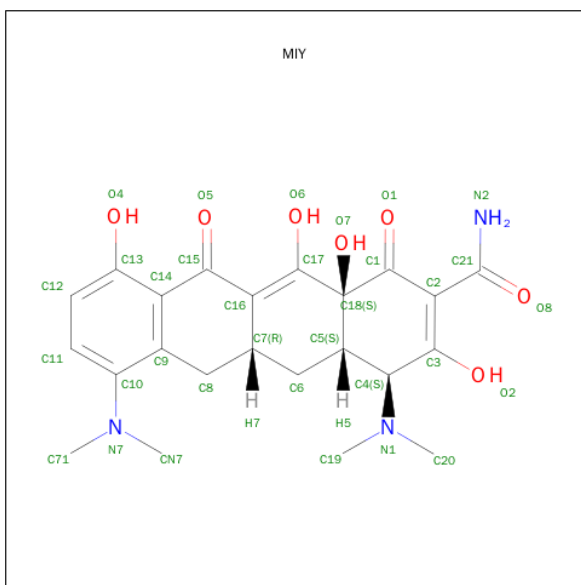
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

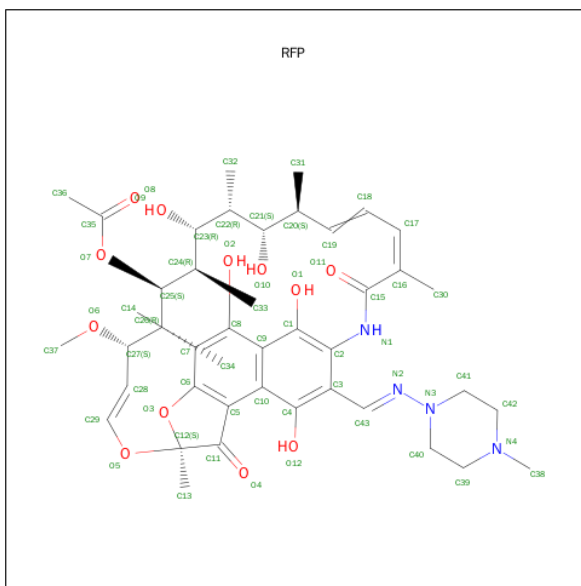
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	HIS	-	EXPRESSION TAG	UNP P31224
C	1051	HIS	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 3 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			59	43	4	12		

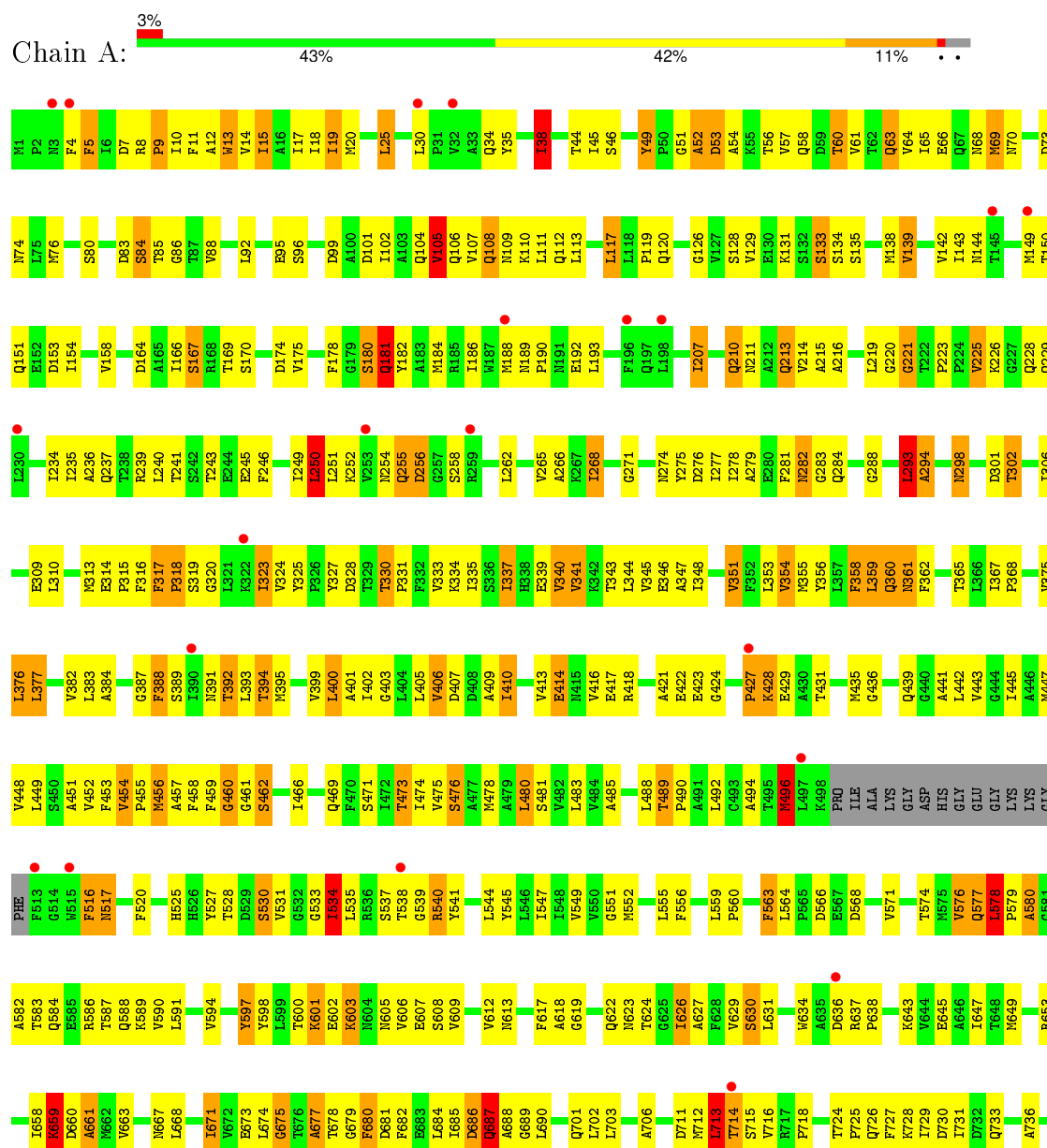
- Molecule 4 is water.

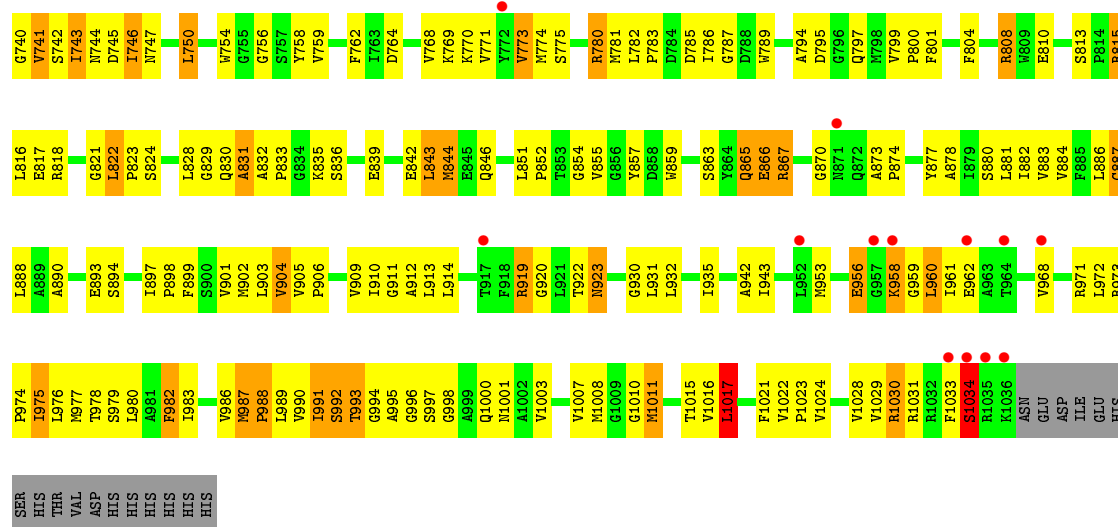
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	2	Total 2	O 2	0	0
4	C	1	Total 1	O 1	0	0

3 Residue-property plots

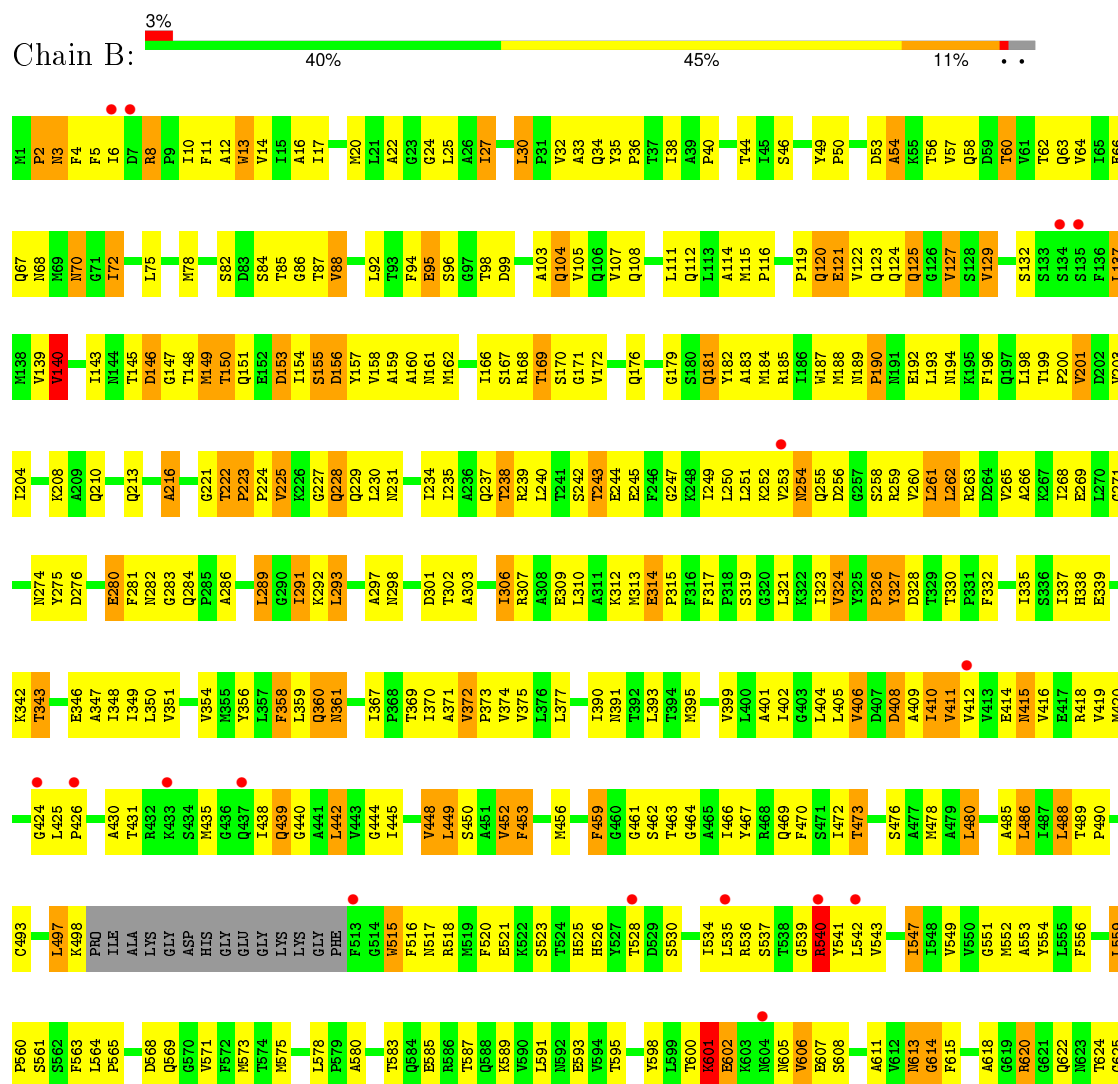
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

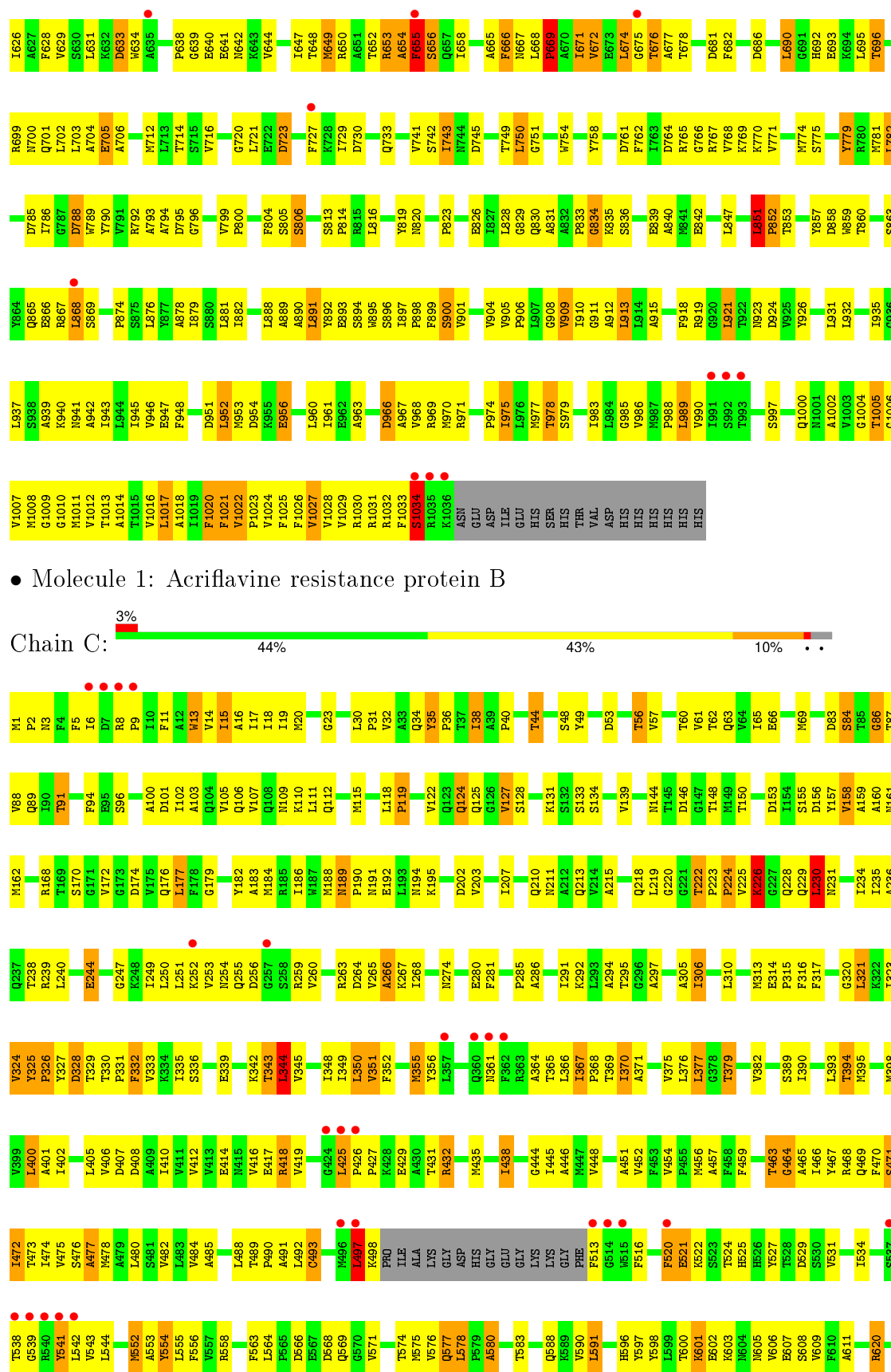
• Molecule 1: Acriflavine resistance protein B





• Molecule 1: Acriflavine resistance protein B





Q1000	G1004	T1005	G1006	V1007	M1008	M1011	V1012	T1013	A1014	T1015	V1016	L1017	A1018	I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ILE	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS	HIS	HIS								
L931	L932	T933	T934	I935	K940	N941	A942	T943	L944	T945	V946	E947	F948	A949	K950	D951	L952	K953	D954	K955	E956	G957	K958	G959	L960	T961	E962	A963	T964	L965	D966	A967	V968	R969	N970	R971	L972	R973	P974	T975	L976	N977	F982	T983	L984	G985	V986	L989	V990	T993	G994	S997	G998	A999
G854	V855	G856	V857	N859	S863	L868	S869	G870	N871	Q872	A873	P874	S875	S879	V883	V884	T885	L888	A889	A890	E893	S896	F899	S900	V901	V904	V905	P906	L907	G908	V909	T910	G911	L914	A915	R919	G920	L921	T922	V925	V926	F927	Q928	V929	G930									
V771	M774	S775	K778	T779	R780	M781	L782	P783	D784	D785	I786	W789	R792	D795	G796	Q797	M798	V799	P800	F801	S802	A803	F804	S805	S806	S807	R808	P814	R815	G821	L822	M825	Q830	A831	A832	P833	G834	K835	S836	E839	L843	M844	L847	A848	S849	K850	L851							
N623	T624	F628	V629	S630	L631	K632	D633	W634	A635	D636	R637	N642	K643	V644	I647	T648	M649	F655	S656	Q657	I658	K659	M662	V663	F664	A665	I671	V672	L674	G675	T676	A677	T678	G679	F680	D681	L684	I685	D686	Q687	L690	G691	H692	E693	K694	L695	T696	Q697	A698	R699				
L702	A707	P710	D711	M712	L713	T714	S715	V716	R717	G720	L721	E722	D723	T724	F727	K728	I729	D730	I731	D732	Q733	E734	K735	A736	Q737	A738	L739	G740	V741	S742	D745	I746	L750	Q751	A752	A753	W754	G755	G756	S757	Y758	V759	M760	D761	F762	I763	D764	R767	V768	K769	K770			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.60 Å 134.50 Å 162.83 Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	47.50 – 3.30 47.50 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.50-3.30) 97.3 (47.50-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.67 (at 3.33 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.258 , 0.318 0.251 , 0.305	Depositor DCC
R_{free} test set	3532 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	95.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 70728 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23419	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.65	0/7920	0.77	4/10756 (0.0%)
1	B	0.60	0/7920	0.76	2/10756 (0.0%)
1	C	0.65	0/7920	0.79	5/10756 (0.0%)
All	All	0.64	0/23760	0.77	11/32268 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	LEU	CA-CB-CG	7.38	132.26	115.30
1	B	868	LEU	CA-CB-CG	6.60	130.48	115.30
1	C	721	LEU	CA-CB-CG	6.58	130.42	115.30
1	A	400	LEU	CA-CB-CG	6.09	129.30	115.30
1	C	344	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	250	LEU	CA-CB-CG	5.68	128.35	115.30
1	A	578	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	989	LEU	CA-CB-CG	5.50	127.94	115.30
1	C	230	LEU	CA-CB-CG	5.30	127.49	115.30
1	C	720	GLY	N-CA-C	5.20	126.11	113.10
1	A	25	LEU	CA-CB-CG	5.18	127.21	115.30

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	7774	0	7931	510	0
1	B	7774	0	7931	537	0
1	C	7774	0	7931	503	0
2	A	33	0	24	0	0
3	C	59	0	56	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
All	All	23419	0	23873	1489	0

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 31.

All (1489) 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:713:LEU:CB	1:A:832:ALA:HA	1.80	1.11
1:C:44:THR:HG23	1:C:91:THR:HB	1.33	1.10
1:C:909:VAL:HG12	1:C:931:LEU:HD21	1.11	1.09
1:B:95:GLU:O	1:B:98:THR:HG22	1.50	1.09
1:C:115:MET:HE3	1:C:127:VAL:HG11	1.33	1.08
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.09	1.03
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.23	1.02
1:A:901:VAL:O	1:A:904:VAL:HG23	1.60	1.02
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.42	1.01
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.02	1.01
1:A:225:VAL:H	1:B:781:MET:HE2	1.25	1.01
1:B:222:THR:HB	1:B:223:PRO:HD3	1.38	1.01
1:A:713:LEU:HB3	1:A:832:ALA:CA	1.89	1.01
1:C:760:ASN:O	1:C:771:VAL:HG23	1.61	1.01
1:B:919:ARG:HD2	1:B:1005:THR:HG21	1.42	1.00
1:A:671:ILE:H	1:A:671:ILE:CD1	1.74	1.00
1:C:713:LEU:CD1	1:C:834:GLY:HA3	1.92	0.98
1:C:974:PRO:HA	1:C:977:MET:HE2	1.44	0.98
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.44	0.98
1:C:190:PRO:HD2	1:C:779:TYR:CD1	1.99	0.97
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.46	0.96
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.47	0.96
1:A:731:ILE:HG12	1:A:746:ILE:HG21	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LYS:HD2	1:A:660:ASP:H	1.33	0.93
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.50	0.93
1:A:356:TYR:HD1	1:A:361:ASN:H	1.17	0.93
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.50	0.92
1:A:911:GLY:H	1:A:914:LEU:HD13	1.34	0.92
1:C:184:MET:HA	1:C:184:MET:HE3	1.52	0.91
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.70	0.91
1:A:73:ASP:H	1:A:106:GLN:HE22	1.10	0.91
1:C:1025:PHE:O	1:C:1029:VAL:HB	1.70	0.91
1:C:115:MET:CE	1:C:127:VAL:HG11	2.00	0.91
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.52	0.90
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.50	0.89
1:C:758:TYR:HE2	1:C:770:LYS:HB3	1.34	0.89
1:C:564:LEU:HD13	1:C:671:ILE:HD12	1.54	0.89
1:A:713:LEU:HB2	1:A:833:PRO:HD3	1.54	0.89
1:C:211:ASN:HD22	1:C:240:LEU:HG	1.38	0.89
1:C:758:TYR:CE2	1:C:770:LYS:HB3	2.08	0.88
1:A:302:THR:O	1:A:306:ILE:HG12	1.73	0.88
1:A:462:SER:HB2	1:A:865:GLN:HG2	1.56	0.88
1:B:222:THR:HB	1:B:223:PRO:CD	2.03	0.88
1:C:848:ALA:HA	1:C:851:LEU:HD22	1.56	0.88
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.56	0.88
1:B:463:THR:HG21	1:B:869:SER:HB2	1.54	0.88
1:B:729:ILE:HG13	1:B:730:ASP:H	1.37	0.88
1:A:886:LEU:HD21	1:C:17:ILE:HG22	1.54	0.87
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.56	0.87
1:B:897:ILE:HB	1:B:1026:PHE:HE1	1.40	0.87
1:C:1:MET:HB2	1:C:2:PRO:CD	2.04	0.86
1:C:758:TYR:CE2	1:C:770:LYS:HD3	2.09	0.86
1:C:418:ARG:HH12	1:C:970:MET:HG2	1.39	0.86
1:A:447:MET:HB3	1:A:887:CYS:SG	2.16	0.86
1:C:281:PHE:CZ	1:C:324:VAL:HG21	2.11	0.86
1:A:14:VAL:HG21	1:B:890:ALA:HB2	1.55	0.86
1:A:15:ILE:O	1:A:19:ILE:HD13	1.73	0.86
1:B:150:THR:H	1:B:153:ASP:HB2	1.41	0.85
1:A:310:LEU:HD12	1:A:325:TYR:OH	1.76	0.85
1:C:848:ALA:HA	1:C:851:LEU:CD2	2.07	0.85
1:A:886:LEU:HG	1:C:14:VAL:HG23	1.57	0.85
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.06	0.84
1:A:454:VAL:HG12	1:A:455:PRO:HD3	1.57	0.84
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ALA:O	1:C:490:PRO:HD3	1.77	0.84
1:B:459:PHE:HZ	1:B:876:LEU:HG	1.40	0.83
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.59	0.83
1:C:713:LEU:HD11	1:C:834:GLY:CA	1.98	0.83
1:B:84:SER:HB3	1:B:814:PRO:HA	1.59	0.83
1:B:70:ASN:H	1:B:70:ASN:HD22	1.27	0.83
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.13	0.83
1:B:1020:PHE:O	1:B:1021:PHE:HB2	1.76	0.83
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.09	0.82
1:C:901:VAL:O	1:C:904:VAL:HG23	1.81	0.80
1:A:852:PRO:O	1:A:855:VAL:HG22	1.81	0.80
1:C:38:ILE:HD13	1:C:38:ILE:H	1.45	0.80
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.63	0.80
1:B:743:ILE:H	1:B:743:ILE:HD13	1.44	0.80
1:B:906:PRO:HA	1:B:909:VAL:HG22	1.63	0.80
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.63	0.79
1:C:34:GLN:HB3	1:C:333:VAL:CG2	2.12	0.79
1:C:696:THR:O	1:C:699:ARG:HG3	1.82	0.79
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.47	0.79
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.64	0.79
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.13	0.79
1:C:909:VAL:HG12	1:C:931:LEU:CD2	2.05	0.78
1:C:418:ARG:HH22	1:C:970:MET:CE	1.96	0.78
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.65	0.78
1:A:713:LEU:CB	1:A:833:PRO:HD3	2.14	0.78
1:A:4:PHE:O	1:A:8:ARG:NH2	2.16	0.78
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.65	0.78
1:A:671:ILE:H	1:A:671:ILE:HD13	1.47	0.78
1:A:756:GLY:HA2	1:A:774:MET:HB3	1.65	0.78
1:B:104:GLN:C	1:B:104:GLN:HE21	1.87	0.78
1:A:886:LEU:O	1:C:14:VAL:HG21	1.84	0.77
1:A:601:LYS:O	1:A:601:LYS:HG3	1.83	0.77
1:A:878:ALA:O	1:A:882:ILE:HD13	1.85	0.77
1:A:987:MET:H	1:A:988:PRO:HD3	1.47	0.77
1:A:104:GLN:HE21	1:A:131:LYS:HD3	1.50	0.77
1:A:832:ALA:CB	1:A:835:LYS:HB2	2.14	0.77
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.65	0.77
1:B:743:ILE:N	1:B:743:ILE:HD13	2.00	0.77
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.66	0.77
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.66	0.77
1:B:139:VAL:HG12	1:B:139:VAL:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:LEU:O	1:B:595:THR:HG22	1.85	0.76
1:C:343:THR:HG21	1:C:989:LEU:HD13	1.65	0.76
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.15	0.76
1:B:1020:PHE:N	1:B:1020:PHE:HD2	1.84	0.76
1:B:54:ALA:HB1	1:B:816:LEU:HD12	1.67	0.76
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.01	0.76
1:A:219:LEU:HD22	1:B:781:MET:O	1.86	0.76
1:A:987:MET:N	1:A:988:PRO:HD3	2.01	0.76
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.68	0.76
1:A:713:LEU:HD22	1:A:714:THR:H	1.51	0.75
1:A:729:ILE:HG22	1:A:730:ASP:N	2.01	0.75
1:A:466:ILE:O	1:A:469:GLN:HB2	1.86	0.75
1:A:775:SER:O	1:A:780:ARG:HD3	1.86	0.75
1:A:538:THR:H	1:A:540:ARG:NH2	1.84	0.75
1:C:444:GLY:O	1:C:448:VAL:HG23	1.87	0.75
1:A:457:ALA:O	1:A:458:PHE:HD1	1.68	0.75
1:A:13:TRP:O	1:A:17:ILE:HG12	1.86	0.75
1:C:184:MET:HA	1:C:184:MET:CE	2.17	0.74
1:C:189:ASN:C	1:C:189:ASN:HD22	1.90	0.74
1:A:367:ILE:HD11	1:A:413:VAL:HB	1.68	0.74
1:A:987:MET:O	1:A:987:MET:HG2	1.86	0.74
1:B:699:ARG:O	1:B:701:GLN:N	2.20	0.74
1:A:268:ILE:O	1:A:268:ILE:HG22	1.86	0.74
1:B:6:ILE:HD11	1:B:490:PRO:HB2	1.68	0.74
1:C:643:LYS:O	1:C:647:ILE:HG13	1.87	0.74
1:C:909:VAL:CG1	1:C:931:LEU:HD21	2.06	0.74
1:A:11:PHE:HD1	1:B:890:ALA:HB1	1.51	0.73
1:B:171:GLY:HA3	1:B:302:THR:CB	2.19	0.73
1:B:652:THR:O	1:B:656:SER:HB3	1.88	0.73
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.71	0.73
1:A:574:THR:HG1	1:A:598:TYR:HE1	1.37	0.73
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.70	0.73
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.54	0.73
1:C:252:LYS:HG2	1:C:260:VAL:CG1	2.18	0.73
1:A:52:ALA:HB1	1:A:57:VAL:HG23	1.71	0.72
1:C:758:TYR:HE2	1:C:770:LYS:HD3	1.54	0.72
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.54	0.72
1:B:280:GLU:HB2	1:B:284:GLN:O	1.88	0.72
1:B:171:GLY:HA3	1:B:302:THR:HB	1.71	0.72
1:C:554:TYR:O	1:C:556:PHE:N	2.22	0.72
1:C:950:LYS:HA	1:C:953:MET:CE	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:PHE:N	1:B:1020:PHE:CD2	2.55	0.72
1:B:671:ILE:HG22	1:B:672:VAL:N	2.03	0.72
1:C:950:LYS:HA	1:C:953:MET:HE2	1.70	0.72
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.70	0.72
1:A:808:ARG:HD2	1:A:808:ARG:H	1.53	0.72
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.88	0.72
1:A:80:SER:OG	1:A:818:ARG:HG3	1.90	0.72
1:A:990:VAL:O	1:A:991:ILE:HG12	1.90	0.71
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.71	0.71
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.25	0.71
1:A:1029:VAL:O	1:A:1030:ARG:HB2	1.89	0.71
1:A:216:ALA:HB2	1:B:750:LEU:HD13	1.72	0.71
1:B:986:VAL:O	1:B:990:VAL:HG23	1.90	0.71
1:B:158:VAL:HA	1:B:162:MET:CG	2.20	0.71
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.73	0.71
1:A:671:ILE:H	1:A:671:ILE:HD12	1.53	0.71
1:A:142:VAL:O	1:A:154:ILE:HG21	1.90	0.71
1:B:979:SER:O	1:B:983:ILE:HG13	1.90	0.71
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.91	0.71
1:C:115:MET:CE	1:C:118:LEU:HD23	2.20	0.71
1:C:524:THR:HG22	1:C:972:LEU:HD12	1.73	0.71
1:A:73:ASP:H	1:A:106:GLN:NE2	1.87	0.71
1:A:53:ASP:HA	1:A:84:SER:HA	1.73	0.71
1:A:178:PHE:HB2	1:A:288:GLY:H	1.55	0.70
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.73	0.70
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.25	0.70
1:C:552:MET:SD	1:C:909:VAL:HG23	2.30	0.70
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.72	0.70
1:A:713:LEU:CG	1:A:833:PRO:HD3	2.20	0.70
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.25	0.70
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.91	0.70
1:A:533:GLY:C	1:A:535:LEU:H	1.95	0.70
1:A:1033:PHE:O	1:A:1034:SER:HB2	1.91	0.70
1:C:695:LEU:HB3	1:C:825:MET:HE1	1.74	0.70
1:B:5:PHE:HE2	1:B:11:PHE:HD2	1.40	0.70
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.74	0.70
1:A:400:LEU:HD11	1:A:930:GLY:HA2	1.72	0.70
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.27	0.70
1:A:818:ARG:HA	1:A:824:SER:H	1.57	0.70
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.72	0.70
1:A:389:SER:O	1:A:394:THR:HG21	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ALA:O	1:C:469:GLN:HG2	1.91	0.69
1:B:727:PHE:HE1	1:B:786:ILE:HD11	1.57	0.69
1:C:538:THR:HG22	1:C:539:GLY:H	1.56	0.69
1:A:407:ASP:OD2	1:A:978:THR:HG21	1.91	0.69
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.07	0.69
1:B:332:PHE:CD1	1:B:569:GLN:HA	2.26	0.69
1:C:417:GLU:HA	1:C:417:GLU:OE2	1.90	0.69
1:B:459:PHE:O	1:B:464:GLY:HA3	1.92	0.69
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.73	0.69
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.28	0.69
1:B:898:PRO:C	1:B:900:SER:H	1.96	0.69
1:A:781:MET:HE2	1:C:225:VAL:H	1.58	0.69
1:B:729:ILE:HG13	1:B:730:ASP:N	2.07	0.69
1:A:603:LYS:HD3	1:A:603:LYS:H	1.58	0.69
1:C:600:THR:O	1:C:603:LYS:HB2	1.92	0.69
1:A:69:MET:O	1:C:168:ARG:HG2	1.93	0.69
1:A:901:VAL:O	1:A:904:VAL:CG2	2.40	0.68
1:C:454:VAL:HG23	1:C:475:VAL:HG21	1.75	0.68
1:A:7:ASP:O	1:A:9:PRO:HD3	1.93	0.68
1:B:704:ALA:O	1:B:705:GLU:HB2	1.94	0.68
1:B:523:SER:HA	1:B:526:HIS:CD2	2.28	0.68
1:C:727:PHE:CE2	1:C:807:SER:HB2	2.27	0.68
1:C:190:PRO:HD2	1:C:779:TYR:HD1	1.54	0.68
1:C:418:ARG:HD2	1:C:419:VAL:HG22	1.74	0.68
1:C:445:ILE:HG13	1:C:446:ALA:H	1.57	0.68
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.74	0.68
1:C:476:SER:O	1:C:478:MET:N	2.25	0.68
1:C:34:GLN:HB3	1:C:333:VAL:HG22	1.76	0.68
1:A:818:ARG:HB3	1:A:823:PRO:HA	1.74	0.68
1:A:10:ILE:HG12	1:B:895:TRP:HB2	1.74	0.68
1:C:265:VAL:O	1:C:266:ALA:HB2	1.93	0.68
1:C:101:ASP:O	1:C:105:VAL:HG23	1.93	0.68
1:B:190:PRO:HD3	1:B:779:TYR:CE2	2.28	0.68
1:C:554:TYR:HB3	1:C:558:ARG:HH21	1.57	0.68
1:B:648:THR:HG23	1:B:665:ALA:HB3	1.76	0.68
1:A:387:GLY:O	1:A:388:PHE:O	2.12	0.68
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.76	0.67
1:C:552:MET:SD	1:C:909:VAL:CG2	2.82	0.67
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.75	0.67
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.76	0.67
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.76	0.67
1:B:851:LEU:N	1:B:852:PRO:HD3	2.09	0.67
1:A:104:GLN:NE2	1:A:131:LYS:HD3	2.10	0.67
1:B:20:MET:HG2	1:B:377:LEU:HD12	1.77	0.67
1:B:229:GLN:HA	1:C:583:THR:HG21	1.77	0.67
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.77	0.67
1:B:696:THR:HG22	1:B:699:ARG:HH12	1.60	0.67
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.76	0.67
1:B:897:ILE:HB	1:B:1026:PHE:CE1	2.27	0.66
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.77	0.66
1:A:188:MET:HA	1:A:266:ALA:HB2	1.76	0.66
1:A:643:LYS:O	1:A:647:ILE:HG12	1.95	0.66
1:B:699:ARG:HG2	1:B:700:ASN:H	1.58	0.66
1:B:898:PRO:HA	1:B:901:VAL:HG23	1.77	0.66
1:A:746:ILE:HD12	1:A:804:PHE:CE1	2.30	0.66
1:B:1028:VAL:O	1:B:1032:ARG:HB2	1.96	0.66
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.77	0.66
1:B:692:HIS:HE1	1:B:723:ASP:OD1	1.78	0.66
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.25	0.66
1:C:189:ASN:ND2	1:C:191:ASN:H	1.93	0.66
1:A:842:GLU:O	1:A:846:GLN:HG3	1.95	0.66
1:A:298:ASN:HD22	1:A:301:ASP:H	1.43	0.66
1:B:727:PHE:CE1	1:B:786:ILE:HD11	2.31	0.66
1:C:712:MET:O	1:C:713:LEU:HD22	1.96	0.65
1:A:403:GLY:HA3	1:A:982:PHE:CZ	2.32	0.65
1:A:525:HIS:HA	1:A:528:THR:HG22	1.76	0.65
1:A:685:ILE:HG22	1:A:686:ASP:H	1.62	0.65
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.76	0.65
1:C:445:ILE:HG13	1:C:446:ALA:N	2.11	0.65
1:B:714:THR:CG2	1:B:830:GLN:HG3	2.26	0.65
1:C:945:ILE:HG13	1:C:946:VAL:H	1.62	0.65
1:C:489:THR:O	1:C:493:CYS:HB2	1.96	0.65
1:B:404:LEU:HD13	1:B:449:LEU:HD21	1.78	0.65
1:C:491:ALA:C	1:C:493:CYS:H	2.00	0.65
1:C:174:ASP:HB3	1:C:292:LYS:HB2	1.78	0.65
1:C:252:LYS:HG2	1:C:260:VAL:HG12	1.79	0.65
1:A:178:PHE:HB2	1:A:288:GLY:N	2.11	0.65
1:B:255:GLN:HG3	1:B:256:ASP:H	1.61	0.65
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.32	0.65
1:C:34:GLN:HB3	1:C:333:VAL:HG21	1.79	0.64
1:C:1018:ALA:O	1:C:1022:VAL:HG12	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:LYS:O	1:A:602:GLU:HG2	1.98	0.64
1:A:391:ASN:O	1:A:392:THR:C	2.36	0.64
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.79	0.64
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.28	0.64
1:A:441:ALA:O	1:A:445:ILE:HG23	1.97	0.64
1:B:1027:VAL:O	1:B:1031:ARG:HB3	1.97	0.64
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.79	0.64
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.78	0.64
1:B:425:LEU:HB3	1:B:498:LYS:C	2.18	0.64
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.79	0.64
1:A:729:ILE:CG2	1:A:730:ASP:N	2.60	0.64
1:B:459:PHE:CZ	1:B:876:LEU:HG	2.28	0.64
1:C:815:ARG:HH11	1:C:815:ARG:HG2	1.62	0.64
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.27	0.64
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.80	0.64
1:C:213:GLN:NE2	1:C:238:THR:HA	2.13	0.64
1:A:677:ALA:C	1:A:679:GLY:H	2.01	0.64
1:A:14:VAL:O	1:A:17:ILE:N	2.31	0.64
1:B:36:PRO:O	1:B:38:ILE:HG12	1.98	0.64
1:C:418:ARG:NH2	1:C:970:MET:CE	2.60	0.64
1:C:158:VAL:CG1	1:C:177:LEU:HD21	2.28	0.64
1:A:117:LEU:HD11	1:C:124:GLN:O	1.97	0.63
1:A:836:SER:OG	1:A:839:GLU:HG2	1.98	0.63
1:B:792:ARG:HG2	1:B:793:ALA:H	1.63	0.63
1:C:102:ILE:HA	1:C:105:VAL:HG23	1.79	0.63
1:A:328:ASP:OD1	1:A:330:THR:HB	1.98	0.63
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.29	0.63
1:A:9:PRO:HD2	1:B:893:GLU:OE2	1.98	0.63
1:B:298:ASN:HB2	1:B:301:ASP:HB2	1.79	0.63
1:A:886:LEU:HG	1:C:14:VAL:CG2	2.26	0.63
1:A:166:ILE:HD11	1:A:310:LEU:HD21	1.78	0.63
1:A:351:VAL:O	1:A:351:VAL:HG12	1.98	0.63
1:A:367:ILE:HG22	1:A:496:MET:CE	2.29	0.63
1:C:53:ASP:OD1	1:C:56:THR:HB	1.99	0.63
1:B:706:ALA:HB1	1:B:716:VAL:HG21	1.80	0.63
1:B:72:ILE:HD13	1:B:72:ILE:N	2.14	0.63
1:B:2:PRO:HB3	1:B:486:LEU:O	1.99	0.62
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.81	0.62
1:A:351:VAL:HG21	1:A:406:VAL:HG21	1.81	0.62
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.80	0.62
1:A:713:LEU:O	1:A:714:THR:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLY:HA2	1:B:891:LEU:HD11	1.81	0.62
1:B:281:PHE:HE1	1:B:608:SER:HB2	1.62	0.62
1:B:667:ASN:O	1:B:678:THR:HB	1.99	0.62
1:A:354:VAL:HG11	1:A:980:LEU:HB3	1.81	0.62
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.34	0.62
1:B:966:ASP:O	1:B:970:MET:HG3	1.98	0.62
1:B:228:GLN:NE2	1:C:781:MET:HB3	2.14	0.62
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.81	0.62
1:B:94:PHE:CB	1:B:98:THR:HG21	2.30	0.62
1:A:894:SER:OG	1:A:897:ILE:HB	1.99	0.62
1:B:671:ILE:CG2	1:B:672:VAL:H	2.12	0.62
1:B:274:ASN:HD22	1:B:276:ASP:HB2	1.64	0.62
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.81	0.62
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.27	0.62
1:C:15:ILE:O	1:C:19:ILE:HG12	1.99	0.62
1:C:222:THR:HG22	1:C:223:PRO:HD3	1.81	0.62
1:B:198:LEU:HD23	1:B:792:ARG:NH2	2.15	0.62
1:A:773:VAL:O	1:A:773:VAL:CG1	2.47	0.62
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.82	0.62
1:C:836:SER:HB3	1:C:839:GLU:HG2	1.82	0.62
1:B:158:VAL:HA	1:B:162:MET:HG3	1.81	0.62
1:B:255:GLN:CG	1:B:256:ASP:H	2.12	0.62
1:B:255:GLN:HG3	1:B:256:ASP:N	2.14	0.62
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.30	0.62
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.82	0.61
1:C:23:GLY:HA3	1:C:377:LEU:O	1.99	0.61
1:A:228:GLN:HG3	1:A:229:GLN:N	2.15	0.61
1:C:343:THR:O	1:C:343:THR:HG22	1.99	0.61
1:B:671:ILE:HG22	1:B:672:VAL:H	1.65	0.61
1:C:990:VAL:HG13	1:C:1005:THR:HG22	1.82	0.61
1:C:418:ARG:HH22	1:C:970:MET:HE2	1.63	0.61
1:B:5:PHE:HE2	1:B:11:PHE:CD2	2.18	0.61
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.35	0.61
1:C:945:ILE:HG13	1:C:946:VAL:N	2.16	0.61
1:B:671:ILE:CG2	1:B:672:VAL:N	2.63	0.61
1:A:367:ILE:HG22	1:A:496:MET:HE1	1.83	0.61
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.00	0.61
1:A:246:PHE:O	1:A:249:ILE:HG12	2.01	0.61
1:A:883:VAL:O	1:A:887:CYS:HB2	2.00	0.61
1:B:743:ILE:H	1:B:743:ILE:CD1	2.09	0.61
1:A:339:GLU:O	1:A:341:VAL:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HG21	1:A:481:SER:HA	1.81	0.61
1:C:974:PRO:HA	1:C:977:MET:CE	2.28	0.61
1:A:354:VAL:O	1:A:354:VAL:HG12	2.00	0.61
1:A:73:ASP:N	1:A:106:GLN:HE22	1.92	0.61
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.36	0.61
1:C:228:GLN:HG3	1:C:229:GLN:O	2.01	0.61
1:A:108:GLN:CD	1:B:112:GLN:HG3	2.21	0.61
1:C:1:MET:HB2	1:C:2:PRO:HD3	1.82	0.61
1:C:38:ILE:N	1:C:38:ILE:CD1	2.64	0.60
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.31	0.60
1:A:485:ALA:HA	1:A:489:THR:OG1	2.02	0.60
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.66	0.60
1:A:344:LEU:HD23	1:A:402:ILE:HD12	1.82	0.60
1:A:660:ASP:O	1:A:661:ALA:HB2	2.00	0.60
1:A:597:TYR:O	1:A:601:LYS:HB3	2.02	0.60
1:B:274:ASN:ND2	1:B:276:ASP:HB2	2.16	0.60
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.84	0.60
1:B:204:ILE:CG2	1:B:208:LYS:HE2	2.30	0.60
1:C:38:ILE:N	1:C:38:ILE:HD13	2.15	0.60
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.83	0.60
1:B:539:GLY:C	1:B:541:TYR:H	2.05	0.60
1:A:661:ALA:O	1:A:663:VAL:HG23	2.02	0.60
1:A:597:TYR:C	1:A:597:TYR:CD1	2.74	0.60
1:C:836:SER:HB3	1:C:839:GLU:CG	2.31	0.60
1:C:379:THR:HB	1:C:398:MET:CE	2.31	0.60
1:A:293:LEU:O	1:A:294:ALA:CB	2.49	0.60
1:B:665:ALA:O	1:B:666:PHE:HB2	2.01	0.60
1:A:993:THR:HB	1:A:997:SER:CB	2.32	0.60
1:C:162:MET:HA	1:C:313:MET:CE	2.32	0.60
1:C:973:ARG:N	1:C:974:PRO:HD2	2.17	0.60
1:B:282:ASN:O	1:B:284:GLN:N	2.34	0.60
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.81	0.60
1:B:146:ASP:O	1:B:148:THR:N	2.32	0.60
1:C:310:LEU:HD13	1:C:323:ILE:HD13	1.83	0.60
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.82	0.60
1:C:762:PHE:CE1	1:C:769:LYS:HB2	2.37	0.59
1:C:40:PRO:HB2	1:C:94:PHE:O	2.02	0.59
1:B:10:ILE:HG13	1:C:893:GLU:O	2.02	0.59
1:B:30:LEU:HD13	1:B:390:ILE:HD11	1.83	0.59
1:B:476:SER:O	1:B:480:LEU:HB2	2.03	0.59
1:C:945:ILE:HD11	1:C:1022:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.84	0.59
1:B:151:GLN:O	1:B:155:SER:HB2	2.02	0.59
1:C:948:PHE:HE1	1:C:971:ARG:HE	1.48	0.59
1:B:193:LEU:HD22	1:B:198:LEU:HB2	1.83	0.59
1:C:795:ASP:OD2	1:C:797:GLN:HB3	2.02	0.59
1:A:919:ARG:HG3	1:A:920:GLY:N	2.16	0.59
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.83	0.59
1:C:958:LYS:HG2	1:C:962:GLU:HB3	1.85	0.59
1:B:552:MET:SD	1:B:909:VAL:HG23	2.43	0.59
1:A:685:ILE:HG22	1:A:686:ASP:N	2.18	0.59
1:B:276:ASP:O	1:B:614:GLY:HA3	2.02	0.59
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.68	0.59
1:C:1:MET:CB	1:C:2:PRO:CD	2.80	0.59
1:C:418:ARG:NH2	1:C:970:MET:HE3	2.17	0.59
1:C:466:ILE:HG13	1:C:563:PHE:HZ	1.65	0.59
1:A:254:ASN:ND2	1:A:258:SER:OG	2.36	0.59
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.02	0.59
1:C:1017:LEU:O	1:C:1021:PHE:HB2	2.03	0.59
1:A:612:VAL:HG22	1:A:626:ILE:HG22	1.83	0.59
1:C:759:VAL:HB	1:C:760:ASN:ND2	2.17	0.59
1:B:876:LEU:CD2	1:B:932:LEU:HD11	2.32	0.59
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.84	0.59
1:A:293:LEU:O	1:A:294:ALA:HB2	2.03	0.59
1:A:649:MET:O	1:A:653:ARG:HD3	2.02	0.59
1:A:680:PHE:CE1	1:A:829:GLY:HA3	2.38	0.59
1:B:418:ARG:HH11	1:B:418:ARG:HB3	1.66	0.59
1:C:44:THR:CG2	1:C:91:THR:HB	2.22	0.59
1:A:671:ILE:HD13	1:A:671:ILE:N	2.15	0.59
1:B:876:LEU:HD22	1:B:932:LEU:HD11	1.85	0.59
1:C:38:ILE:H	1:C:38:ILE:CD1	2.16	0.59
1:B:375:VAL:HG13	1:B:480:LEU:HB3	1.85	0.59
1:B:910:ILE:HG23	1:B:911:GLY:H	1.67	0.59
1:A:169:THR:HG22	1:A:309:GLU:HG3	1.85	0.59
1:B:104:GLN:C	1:B:104:GLN:NE2	2.56	0.58
1:A:448:VAL:HG22	1:A:884:VAL:HG13	1.85	0.58
1:B:169:THR:O	1:B:172:VAL:HG23	2.02	0.58
1:A:987:MET:N	1:A:988:PRO:CD	2.66	0.58
1:A:919:ARG:HG3	1:A:920:GLY:H	1.69	0.58
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.85	0.58
1:A:239:ARG:HD3	1:A:762:PHE:HA	1.85	0.58
1:B:240:LEU:O	1:B:762:PHE:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:ILE:HG12	1:A:674:LEU:HB3	1.85	0.58
1:B:449:LEU:HB3	1:B:478:MET:HG3	1.85	0.58
1:C:474:ILE:O	1:C:478:MET:HB2	2.03	0.58
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.85	0.58
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.34	0.58
1:C:997:SER:O	1:C:999:ALA:N	2.36	0.58
1:B:782:LEU:N	1:B:785:ASP:OD1	2.36	0.58
1:B:70:ASN:N	1:B:70:ASN:HD22	1.99	0.58
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.39	0.58
1:A:216:ALA:CB	1:B:750:LEU:HD13	2.33	0.58
1:B:213:GLN:CG	1:C:56:THR:OG1	2.51	0.58
1:B:525:HIS:HA	1:B:528:THR:HG22	1.86	0.58
1:B:183:ALA:N	1:B:271:GLY:O	2.36	0.58
1:A:401:ALA:HB2	1:A:474:ILE:HG13	1.85	0.58
1:B:70:ASN:H	1:B:70:ASN:ND2	2.01	0.58
1:C:412:VAL:O	1:C:412:VAL:HG12	2.04	0.58
1:C:16:ALA:O	1:C:20:MET:HG3	2.04	0.58
1:C:355:MET:HB3	1:C:365:THR:HG23	1.86	0.58
1:A:713:LEU:HB3	1:A:832:ALA:CB	2.34	0.58
1:A:688:ALA:O	1:A:690:LEU:N	2.37	0.58
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.18	0.58
1:B:911:GLY:HA3	1:B:1013:THR:HB	1.86	0.58
1:C:577:GLN:HA	1:C:577:GLN:HE21	1.68	0.58
1:C:158:VAL:HG11	1:C:177:LEU:HD21	1.86	0.58
1:B:537:SER:HB2	1:B:540:ARG:HE	1.68	0.58
1:B:593:GLU:OE2	1:B:658:ILE:HD13	2.04	0.58
1:A:154:ILE:O	1:A:158:VAL:HG23	2.04	0.57
1:B:948:PHE:HB2	1:B:971:ARG:NH2	2.19	0.57
1:B:201:VAL:HG21	1:B:745:ASP:OD1	2.03	0.57
1:C:84:SER:HB2	1:C:814:PRO:HA	1.86	0.57
1:A:671:ILE:HG12	1:A:674:LEU:HD12	1.85	0.57
1:A:746:ILE:HG22	1:A:747:ASN:N	2.19	0.57
1:C:945:ILE:HG22	1:C:971:ARG:HB2	1.86	0.57
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.85	0.57
1:A:742:SER:OG	1:A:745:ASP:HB2	2.05	0.57
1:C:972:LEU:H	1:C:974:PRO:HD2	1.69	0.57
1:A:731:ILE:CG1	1:A:746:ILE:HG21	2.30	0.57
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.85	0.57
1:A:773:VAL:O	1:A:773:VAL:HG12	2.04	0.57
1:C:746:ILE:HD12	1:C:804:PHE:CE1	2.39	0.57
1:C:531:VAL:O	1:C:534:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASN:HD21	1:B:642:ASN:ND2	2.01	0.57
1:C:327:TYR:HB2	1:C:628:PHE:HB3	1.85	0.57
1:B:742:SER:OG	1:B:745:ASP:HB2	2.05	0.57
1:A:979:SER:OG	1:A:1015:THR:HG21	2.05	0.57
1:C:935:ILE:O	1:C:935:ILE:HG22	2.05	0.57
1:A:108:GLN:HG2	1:A:129:VAL:HB	1.86	0.57
1:B:49:TYR:CE1	1:B:60:THR:HG21	2.40	0.57
1:B:633:ASP:OD1	1:B:634:TRP:N	2.36	0.57
1:C:580:ALA:HA	1:C:623:ASN:ND2	2.20	0.57
1:A:712:MET:SD	1:A:835:LYS:HG2	2.45	0.56
1:A:365:THR:O	1:A:368:PRO:HD2	2.05	0.56
1:A:713:LEU:CG	1:A:832:ALA:HA	2.34	0.56
1:B:204:ILE:HG22	1:B:208:LYS:HE2	1.86	0.56
1:C:331:PRO:O	1:C:335:ILE:HG12	2.05	0.56
1:B:356:TYR:O	1:B:360:GLN:N	2.37	0.56
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.40	0.56
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.88	0.56
1:B:911:GLY:HA3	1:B:1013:THR:CB	2.35	0.56
1:A:395:MET:HA	1:A:395:MET:CE	2.35	0.56
1:B:187:TRP:O	1:B:266:ALA:HB1	2.04	0.56
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.88	0.56
1:A:324:VAL:HG12	1:A:325:TYR:H	1.71	0.56
1:A:780:ARG:HH22	1:C:223:PRO:HD2	1.69	0.56
1:A:563:PHE:O	1:A:564:LEU:HD12	2.05	0.56
1:A:30:LEU:HD21	1:A:384:ALA:CB	2.27	0.56
1:B:225:VAL:HG23	1:C:781:MET:SD	2.46	0.56
1:A:180:SER:O	1:A:181:GLN:HB2	2.05	0.56
1:B:192:GLU:O	1:B:196:PHE:HD2	1.89	0.56
1:B:898:PRO:C	1:B:900:SER:N	2.59	0.56
1:A:756:GLY:HA2	1:A:774:MET:CB	2.36	0.56
1:A:780:ARG:NH2	1:C:223:PRO:HD2	2.19	0.56
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.88	0.56
1:B:238:THR:HG23	1:B:239:ARG:N	2.20	0.56
1:A:1015:THR:O	1:A:1017:LEU:N	2.34	0.56
1:A:298:ASN:O	1:A:302:THR:HG23	2.05	0.56
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.36	0.56
1:A:740:GLY:HA3	1:A:794:ALA:H	1.71	0.56
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.41	0.56
1:C:686:ASP:C	1:C:686:ASP:OD1	2.44	0.56
1:A:449:LEU:O	1:A:453:PHE:HD1	1.89	0.56
1:B:159:ALA:HB1	1:B:181:GLN:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:909:VAL:CG1	1:C:935:ILE:HD11	2.36	0.56
1:C:247:GLY:HA3	1:C:263:ARG:CZ	2.36	0.56
1:B:188:MET:HA	1:B:266:ALA:HB2	1.88	0.56
1:A:740:GLY:HA3	1:A:794:ALA:CB	2.36	0.56
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.88	0.56
1:B:947:GLU:O	1:B:951:ASP:HB2	2.06	0.56
1:C:418:ARG:HH22	1:C:970:MET:HE3	1.71	0.56
1:B:1020:PHE:O	1:B:1021:PHE:CB	2.48	0.56
1:A:534:ILE:HG13	1:A:534:ILE:O	2.06	0.56
1:B:979:SER:HA	1:B:1011:MET:HE3	1.88	0.56
1:B:314:GLU:N	1:B:315:PRO:CD	2.69	0.56
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.88	0.56
1:C:962:GLU:HA	1:C:965:LEU:HD13	1.87	0.55
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.20	0.55
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.21	0.55
1:B:57:VAL:HG23	1:B:82:SER:HB2	1.87	0.55
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.86	0.55
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.54	0.55
1:A:729:ILE:CG2	1:A:730:ASP:H	2.20	0.55
1:B:237:GLN:HG2	1:B:238:THR:N	2.21	0.55
1:C:183:ALA:HB1	1:C:770:LYS:O	2.07	0.55
1:A:353:LEU:C	1:A:355:MET:H	2.09	0.55
1:B:4:PHE:O	1:B:5:PHE:HB2	2.07	0.55
1:B:682:PHE:CE1	1:B:857:TYR:CD1	2.95	0.55
1:A:986:VAL:HG13	1:A:986:VAL:O	2.06	0.55
1:C:190:PRO:CD	1:C:779:TYR:HD1	2.17	0.55
1:A:108:GLN:NE2	1:B:112:GLN:HG3	2.21	0.55
1:B:119:PRO:C	1:B:121:GLU:H	2.09	0.55
1:A:184:MET:HG3	1:A:186:ILE:HD11	1.88	0.55
1:A:150:THR:N	1:A:153:ASP:OD2	2.35	0.55
1:A:167:SER:OG	1:A:175:VAL:CG2	2.55	0.55
1:B:900:SER:OG	1:B:1029:VAL:HG11	2.07	0.55
1:A:583:THR:CG2	1:A:584:GLN:N	2.70	0.55
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.89	0.55
1:A:713:LEU:HG	1:A:833:PRO:CD	2.29	0.55
1:B:730:ASP:HB3	1:B:806:SER:HB3	1.89	0.55
1:C:601:LYS:C	1:C:603:LYS:H	2.10	0.55
1:A:606:VAL:HA	1:A:631:LEU:HD23	1.89	0.55
1:A:588:GLN:HG2	1:A:613:ASN:OD1	2.07	0.55
1:A:52:ALA:CB	1:A:57:VAL:HG23	2.36	0.55
1:B:375:VAL:HB	1:B:405:LEU:HD22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:CE2	1:B:11:PHE:HD2	2.23	0.55
1:C:577:GLN:HB2	3:C:2002:RFP:H402	1.89	0.55
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.22	0.55
1:A:733:GLN:OE1	1:A:743:ILE:CD1	2.56	0.54
1:A:207:ILE:HB	1:A:759:VAL:HG11	1.89	0.54
1:B:452:VAL:O	1:B:453:PHE:HB2	2.07	0.54
1:B:139:VAL:CG1	1:B:139:VAL:O	2.54	0.54
1:B:123:GLN:O	1:B:125:GLN:N	2.40	0.54
1:A:782:LEU:O	1:A:785:ASP:HB2	2.07	0.54
1:A:102:ILE:O	1:A:106:GLN:HG3	2.08	0.54
1:A:531:VAL:HG12	1:A:535:LEU:HD11	1.89	0.54
1:B:686:ASP:HB2	1:B:695:LEU:HD23	1.89	0.54
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.21	0.54
1:B:1033:PHE:O	1:B:1034:SER:HB2	2.07	0.54
1:C:401:ALA:O	1:C:405:LEU:HG	2.08	0.54
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.42	0.54
1:C:729:ILE:HD11	1:C:786:ILE:HD11	1.88	0.54
1:B:978:THR:HG22	1:B:979:SER:N	2.22	0.54
1:B:541:TYR:C	1:B:543:VAL:H	2.11	0.54
1:A:880:SER:O	1:A:884:VAL:HG23	2.08	0.54
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.08	0.54
1:B:898:PRO:O	1:B:900:SER:N	2.40	0.54
1:C:974:PRO:O	1:C:977:MET:HB2	2.08	0.54
1:B:888:LEU:C	1:B:890:ALA:H	2.11	0.54
1:B:551:GLY:HA2	1:B:554:TYR:HB3	1.90	0.54
1:A:991:ILE:O	1:A:992:SER:CB	2.56	0.54
1:C:265:VAL:HG23	1:C:265:VAL:O	2.06	0.54
1:C:365:THR:O	1:C:368:PRO:HD2	2.07	0.54
1:B:411:VAL:O	1:B:415:ASN:HB2	2.06	0.54
1:A:315:PRO:O	1:A:316:PHE:HB2	2.08	0.54
1:B:255:GLN:CG	1:B:256:ASP:N	2.70	0.54
1:B:948:PHE:HB2	1:B:971:ARG:CZ	2.37	0.54
1:A:750:LEU:O	1:A:754:TRP:HD1	1.90	0.54
1:B:99:ASP:OD2	1:B:99:ASP:C	2.46	0.54
1:B:552:MET:C	1:B:554:TYR:H	2.11	0.54
1:C:662:MET:HG3	1:C:664:PHE:CE1	2.43	0.54
1:C:144:ASN:HD21	1:C:148:THR:H	1.54	0.54
1:B:84:SER:HB3	1:B:814:PRO:CA	2.33	0.54
1:C:325:TYR:N	1:C:325:TYR:CD1	2.76	0.54
1:B:258:SER:C	1:B:259:ARG:HG2	2.28	0.54
1:C:552:MET:O	1:C:554:TYR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:VAL:O	1:C:266:ALA:CB	2.55	0.53
1:B:792:ARG:HG2	1:B:793:ALA:N	2.22	0.53
1:B:952:LEU:HG	1:B:956:GLU:OE2	2.08	0.53
1:C:210:GLN:HE22	1:C:249:ILE:HA	1.73	0.53
1:C:211:ASN:ND2	1:C:240:LEU:HG	2.16	0.53
1:C:815:ARG:NH1	1:C:815:ARG:HG2	2.23	0.53
1:B:335:ILE:HG13	1:B:634:TRP:CD1	2.43	0.53
1:B:518:ARG:HA	1:B:521:GLU:CD	2.28	0.53
1:A:360:GLN:HE22	1:A:517:ASN:HD21	1.56	0.53
1:C:906:PRO:HA	1:C:909:VAL:HG22	1.91	0.53
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.72	0.53
1:A:214:VAL:HG23	1:A:237:GLN:HB3	1.89	0.53
1:A:38:ILE:HG12	1:A:674:LEU:HD23	1.89	0.53
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.90	0.53
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.91	0.53
1:A:617:PHE:O	1:A:619:GLY:N	2.42	0.53
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.90	0.53
1:B:351:VAL:HG12	1:B:351:VAL:O	2.08	0.53
1:C:153:ASP:OD2	1:C:182:TYR:OH	2.27	0.53
1:C:379:THR:HB	1:C:398:MET:HE1	1.90	0.53
1:B:360:GLN:O	1:B:361:ASN:HB3	2.09	0.53
1:A:456:MET:O	1:A:458:PHE:N	2.42	0.53
1:A:688:ALA:C	1:A:690:LEU:H	2.12	0.53
1:B:188:MET:CE	1:B:203:VAL:HG21	2.37	0.53
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.90	0.53
1:C:907:LEU:HG	1:C:1017:LEU:HB3	1.91	0.53
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.43	0.53
1:B:419:VAL:HG12	1:B:419:VAL:O	2.09	0.53
1:B:699:ARG:HG2	1:B:700:ASN:N	2.24	0.53
1:B:282:ASN:C	1:B:284:GLN:H	2.12	0.53
1:B:878:ALA:O	1:B:882:ILE:HG12	2.09	0.53
1:C:139:VAL:HG12	1:C:326:PRO:HG2	1.90	0.53
1:C:176:GLN:HE22	1:C:620:ARG:NH1	2.07	0.53
1:A:8:ARG:HB3	1:B:893:GLU:OE1	2.08	0.53
1:A:600:THR:O	1:A:601:LYS:CB	2.57	0.53
1:B:420:MET:SD	1:B:424:GLY:HA2	2.49	0.53
1:C:552:MET:SD	1:C:909:VAL:HG21	2.49	0.52
1:C:418:ARG:NH2	1:C:970:MET:HE2	2.23	0.52
1:A:818:ARG:HA	1:A:824:SER:N	2.23	0.52
1:B:238:THR:CG2	1:B:239:ARG:N	2.71	0.52
1:B:967:ALA:C	1:B:969:ARG:N	2.61	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:O	1:A:904:VAL:N	2.41	0.52
1:C:847:LEU:HA	1:C:850:LYS:HG2	1.90	0.52
1:B:351:VAL:HA	1:B:354:VAL:HG22	1.91	0.52
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.91	0.52
1:B:154:ILE:HG23	1:B:321:LEU:HD11	1.92	0.52
1:B:63:GLN:O	1:B:66:GLU:N	2.42	0.52
1:B:20:MET:HG3	1:B:374:VAL:HA	1.90	0.52
1:A:442:LEU:HA	1:A:445:ILE:HG13	1.92	0.52
1:C:66:GLU:O	1:C:69:MET:N	2.38	0.52
1:C:714:THR:HG23	1:C:830:GLN:O	2.08	0.52
1:B:967:ALA:C	1:B:969:ARG:H	2.12	0.52
1:B:185:ARG:HB2	1:B:269:GLU:O	2.10	0.52
1:C:2:PRO:O	1:C:6:ILE:N	2.42	0.52
1:C:329:THR:C	1:C:331:PRO:HD2	2.30	0.52
1:C:963:ALA:C	1:C:965:LEU:H	2.11	0.52
1:A:451:ALA:O	1:A:453:PHE:N	2.42	0.52
1:C:351:VAL:HG13	1:C:369:THR:HG22	1.91	0.52
1:B:788:ASP:N	1:B:788:ASP:OD1	2.43	0.52
1:C:953:MET:SD	1:C:963:ALA:HB2	2.50	0.52
1:C:110:LYS:O	1:C:111:LEU:C	2.47	0.52
1:C:280:GLU:HA	1:C:286:ALA:HB3	1.92	0.52
1:A:909:VAL:CG1	1:A:913:LEU:HD22	2.40	0.52
1:B:251:LEU:HB2	1:B:261:LEU:HA	1.92	0.52
1:A:255:GLN:O	1:A:256:ASP:HB2	2.09	0.52
1:B:565:PRO:HD3	1:B:924:ASP:OD1	2.09	0.52
1:C:680:PHE:HE1	1:C:844:MET:HE3	1.74	0.52
1:C:1028:VAL:HA	1:C:1031:ARG:HB3	1.90	0.52
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.92	0.52
1:A:459:PHE:O	1:A:460:GLY:O	2.27	0.52
1:B:405:LEU:HD12	1:B:406:VAL:HG13	1.92	0.52
1:B:412:VAL:HG21	1:B:485:ALA:HB1	1.91	0.52
1:A:1011:MET:CE	1:A:1011:MET:HA	2.40	0.52
1:A:682:PHE:HE2	1:A:684:LEU:HD12	1.74	0.52
1:C:448:VAL:O	1:C:452:VAL:HG23	2.10	0.51
1:B:894:SER:CB	1:B:897:ILE:HG12	2.38	0.51
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.27	0.51
1:B:919:ARG:HD3	1:B:921:LEU:HD13	1.91	0.51
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.11	0.51
1:B:785:ASP:O	1:B:786:ILE:C	2.49	0.51
1:B:251:LEU:HD22	1:B:262:LEU:H	1.75	0.51
1:A:993:THR:HB	1:A:997:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:ILE:O	1:B:900:SER:OG	2.18	0.51
1:C:3:ASN:OD1	1:C:432:ARG:HG3	2.10	0.51
1:C:727:PHE:CE2	1:C:807:SER:CB	2.93	0.51
1:B:213:GLN:HG2	1:C:56:THR:OG1	2.10	0.51
1:B:692:HIS:CE1	1:B:723:ASP:OD1	2.60	0.51
1:C:580:ALA:HA	1:C:623:ASN:HD22	1.74	0.51
1:C:342:LYS:C	1:C:344:LEU:H	2.13	0.51
1:A:902:MET:O	1:A:905:VAL:HG23	2.11	0.51
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.92	0.51
1:A:169:THR:CG2	1:A:309:GLU:HG3	2.40	0.51
1:B:568:ASP:OD2	1:B:634:TRP:HH2	1.93	0.51
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.93	0.51
1:C:3:ASN:C	1:C:5:PHE:H	2.14	0.51
1:A:281:PHE:O	1:A:282:ASN:C	2.47	0.51
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.93	0.51
1:B:530:SER:O	1:B:534:ILE:HG12	2.10	0.51
1:C:472:ILE:HG22	1:C:473:THR:N	2.25	0.51
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.93	0.51
1:B:360:GLN:O	1:B:361:ASN:CB	2.59	0.51
1:A:151:GLN:NE2	1:A:279:ALA:H	2.07	0.51
1:A:151:GLN:NE2	1:A:279:ALA:N	2.59	0.51
1:A:189:ASN:CG	1:A:192:GLU:HB2	2.31	0.51
1:B:701:GLN:HB3	1:B:851:LEU:CD1	2.39	0.51
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.92	0.51
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.45	0.51
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.93	0.51
1:A:265:VAL:CG1	1:A:265:VAL:O	2.58	0.51
1:B:456:MET:HG3	1:B:467:TYR:CB	2.35	0.51
1:C:762:PHE:CZ	1:C:764:ASP:HB2	2.46	0.51
1:A:605:ASN:OD1	1:A:637:ARG:HG2	2.11	0.51
1:C:281:PHE:HE1	1:C:608:SER:HG	1.59	0.51
1:B:445:ILE:HG13	1:B:940:LYS:HG3	1.93	0.51
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.11	0.51
1:A:391:ASN:O	1:A:393:LEU:N	2.43	0.51
1:C:225:VAL:O	1:C:226:LYS:C	2.48	0.51
1:A:993:THR:HB	1:A:997:SER:HB3	1.92	0.51
1:A:1015:THR:C	1:A:1017:LEU:H	2.13	0.51
1:C:1028:VAL:HG12	1:C:1032:ARG:HB2	1.92	0.51
1:A:298:ASN:ND2	1:A:301:ASP:H	2.09	0.50
1:A:886:LEU:HD21	1:C:17:ILE:HG21	1.91	0.50
1:B:139:VAL:O	1:B:140:VAL:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.46	0.50
1:C:314:GLU:N	1:C:315:PRO:HD2	2.26	0.50
1:B:1027:VAL:O	1:B:1031:ARG:CB	2.59	0.50
1:C:144:ASN:ND2	1:C:148:THR:N	2.58	0.50
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.94	0.50
1:B:291:ILE:HD12	1:B:291:ILE:N	2.27	0.50
1:B:939:ALA:O	1:B:943:ILE:HG12	2.11	0.50
1:C:115:MET:HE2	1:C:118:LEU:HD23	1.93	0.50
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.46	0.50
1:C:956:GLU:HA	1:C:956:GLU:OE2	2.11	0.50
1:A:281:PHE:CZ	1:A:324:VAL:HG11	2.47	0.50
1:B:373:PRO:O	1:B:377:LEU:HG	2.11	0.50
1:C:218:GLN:HE21	1:C:231:ASN:HD21	1.60	0.50
1:B:600:THR:C	1:B:602:GLU:H	2.15	0.50
1:A:456:MET:HB2	1:A:471:SER:HB2	1.94	0.50
1:B:1010:GLY:HA2	1:B:1013:THR:HG22	1.93	0.50
1:C:158:VAL:HG12	1:C:177:LEU:HD21	1.93	0.50
1:A:909:VAL:HG12	1:A:913:LEU:HD22	1.93	0.50
1:C:983:ILE:HD11	1:C:1011:MET:HB3	1.92	0.50
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.94	0.50
1:C:948:PHE:O	1:C:952:LEU:HB3	2.11	0.50
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.92	0.50
1:A:591:LEU:HD12	1:A:613:ASN:HB2	1.94	0.50
1:A:728:LYS:NZ	1:C:236:ALA:O	2.45	0.50
1:C:513:PHE:CG	1:C:516:PHE:HB3	2.47	0.50
1:A:671:ILE:CG1	1:A:674:LEU:HD12	2.41	0.50
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.41	0.50
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.47	0.50
1:A:686:ASP:OD1	1:A:686:ASP:C	2.50	0.50
1:A:780:ARG:HH21	1:C:222:THR:H	1.58	0.50
1:B:681:ASP:OD2	1:B:826:GLU:OE1	2.29	0.50
1:C:752:ALA:O	1:C:774:MET:HA	2.11	0.50
1:C:350:LEU:HD22	1:C:984:LEU:HB3	1.92	0.50
1:B:631:LEU:HD11	1:B:644:VAL:HG12	1.93	0.50
1:B:493:CYS:O	1:B:497:LEU:CB	2.59	0.50
1:B:150:THR:HG23	1:B:153:ASP:OD1	2.11	0.50
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.42	0.50
1:C:220:GLY:HA2	1:C:228:GLN:HE21	1.77	0.50
1:B:338:HIS:HE1	1:B:342:LYS:HE3	1.76	0.50
1:B:166:ILE:C	1:B:168:ARG:H	2.14	0.50
1:C:189:ASN:C	1:C:189:ASN:ND2	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HG2	1:B:153:ASP:HB3	1.94	0.50
1:A:181:GLN:O	1:A:181:GLN:HG2	2.11	0.50
1:A:207:ILE:O	1:A:211:ASN:HB3	2.12	0.50
1:B:103:ALA:O	1:B:107:VAL:HG23	2.12	0.50
1:A:607:GLU:HB3	1:A:630:SER:O	2.12	0.50
1:A:221:GLY:H	1:B:622:GLN:HE22	1.60	0.50
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.93	0.49
1:C:56:THR:O	1:C:60:THR:HB	2.12	0.49
1:C:914:LEU:O	1:C:915:ALA:HB3	2.11	0.49
1:A:931:LEU:O	1:A:935:ILE:HG12	2.12	0.49
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.42	0.49
1:A:317:PHE:HE2	1:A:323:ILE:HG23	1.77	0.49
1:B:104:GLN:HE21	1:B:105:VAL:N	2.10	0.49
1:C:911:GLY:HA3	1:C:1013:THR:CB	2.42	0.49
1:C:908:GLY:CA	1:C:1014:ALA:HB2	2.39	0.49
1:B:213:GLN:HG3	1:C:56:THR:OG1	2.11	0.49
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.74	0.49
1:B:967:ALA:O	1:B:969:ARG:N	2.44	0.49
1:C:451:ALA:CB	1:C:883:VAL:HG12	2.42	0.49
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.28	0.49
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.95	0.49
1:B:420:MET:SD	1:B:425:LEU:N	2.77	0.49
1:C:986:VAL:O	1:C:990:VAL:HG23	2.12	0.49
1:B:462:SER:H	1:B:865:GLN:NE2	2.10	0.49
1:A:271:GLY:HA3	1:A:275:TYR:OH	2.12	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.95	0.49
1:B:1018:ALA:O	1:B:1022:VAL:HG22	2.12	0.49
1:C:161:ASN:O	1:C:313:MET:HE2	2.13	0.49
1:B:985:GLY:O	1:B:988:PRO:HD2	2.13	0.49
1:C:805:SER:O	1:C:806:SER:HB3	2.13	0.49
1:A:228:GLN:HG3	1:A:229:GLN:H	1.77	0.49
1:C:11:PHE:O	1:C:14:VAL:HG12	2.12	0.49
1:A:890:ALA:HB2	1:C:14:VAL:HG11	1.94	0.49
1:B:906:PRO:HA	1:B:909:VAL:CG2	2.39	0.49
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.94	0.49
1:C:859:TRP:HB3	1:C:863:SER:O	2.12	0.49
1:A:214:VAL:HG12	1:A:215:ALA:N	2.28	0.49
1:B:649:MET:O	1:B:653:ARG:HB2	2.11	0.49
1:A:235:ILE:O	1:A:235:ILE:HG22	2.13	0.49
1:C:655:PHE:O	1:C:657:GLN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:ILE:CD1	1:B:291:ILE:N	2.76	0.49
1:A:435:MET:SD	1:A:490:PRO:HB3	2.52	0.49
1:C:636:ASP:N	1:C:636:ASP:OD2	2.44	0.49
1:B:182:TYR:O	1:B:769:LYS:HD2	2.13	0.49
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.95	0.49
1:A:38:ILE:N	1:A:38:ILE:HD13	2.28	0.49
1:A:746:ILE:CD1	1:A:804:PHE:CE1	2.96	0.49
1:B:332:PHE:HB2	1:B:569:GLN:O	2.12	0.49
1:B:119:PRO:HG2	1:B:122:VAL:HG23	1.95	0.49
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.42	0.49
1:B:573:MET:HB2	1:B:575:MET:HE1	1.94	0.49
1:B:894:SER:C	1:B:896:SER:H	2.16	0.49
1:B:539:GLY:H	1:B:540:ARG:NH2	2.10	0.49
1:A:167:SER:OG	1:A:175:VAL:HG22	2.13	0.49
1:B:561:SER:HA	1:B:923:ASN:HB3	1.95	0.49
1:C:186:ILE:HG13	1:C:268:ILE:CD1	2.42	0.49
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.95	0.49
1:C:106:GLN:O	1:C:107:VAL:C	2.50	0.49
1:A:447:MET:CB	1:A:887:CYS:SG	2.97	0.49
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.78	0.49
1:A:990:VAL:C	1:A:991:ILE:HG12	2.33	0.48
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.94	0.48
1:A:578:LEU:HB3	1:A:579:PRO:CD	2.43	0.48
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.13	0.48
1:A:571:VAL:HG12	1:A:630:SER:HB3	1.94	0.48
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.96	0.48
1:B:401:ALA:O	1:B:405:LEU:HG	2.13	0.48
1:A:343:THR:HG21	1:A:399:VAL:HG13	1.94	0.48
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.95	0.48
1:C:162:MET:HA	1:C:313:MET:HE1	1.95	0.48
1:C:844:MET:O	1:C:847:LEU:HD22	2.13	0.48
1:B:931:LEU:O	1:B:935:ILE:HG12	2.13	0.48
1:C:962:GLU:HA	1:C:965:LEU:HB2	1.95	0.48
1:C:466:ILE:HG13	1:C:563:PHE:CZ	2.47	0.48
1:B:404:LEU:HD22	1:B:449:LEU:HD11	1.93	0.48
1:C:727:PHE:HE2	1:C:807:SER:CB	2.26	0.48
1:B:665:ALA:O	1:B:666:PHE:CB	2.61	0.48
1:C:431:THR:O	1:C:435:MET:HG2	2.13	0.48
1:C:935:ILE:O	1:C:935:ILE:CG2	2.61	0.48
1:C:712:MET:CB	1:C:835:LYS:HG3	2.44	0.48
1:B:404:LEU:HD21	1:B:937:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:963:ALA:HA	1:B:966:ASP:HB2	1.94	0.48
1:B:34:GLN:O	1:B:391:ASN:HB2	2.13	0.48
1:C:244:GLU:O	1:C:263:ARG:NH2	2.46	0.48
1:C:192:GLU:HB3	1:C:265:VAL:HG12	1.96	0.48
1:B:1022:VAL:HA	1:B:1025:PHE:CD1	2.48	0.48
1:B:193:LEU:CD2	1:B:198:LEU:HB2	2.44	0.48
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.48
1:C:732:ASP:O	1:C:733:GLN:C	2.51	0.48
1:B:945:ILE:HG23	1:B:975:ILE:HD11	1.94	0.48
1:C:211:ASN:ND2	1:C:240:LEU:H	2.12	0.48
1:C:491:ALA:O	1:C:493:CYS:N	2.46	0.48
1:A:178:PHE:HB2	1:A:288:GLY:CA	2.44	0.48
1:C:463:THR:O	1:C:465:ALA:N	2.47	0.48
1:B:754:TRP:HH2	1:B:785:ASP:HB2	1.76	0.48
1:C:229:GLN:O	1:C:230:LEU:HB3	2.13	0.48
1:B:314:GLU:OE2	1:B:323:ILE:HD12	2.14	0.48
1:C:144:ASN:HD21	1:C:148:THR:N	2.12	0.48
1:C:931:LEU:O	1:C:931:LEU:HD22	2.14	0.48
1:A:780:ARG:NH2	1:C:223:PRO:O	2.47	0.48
1:B:158:VAL:HA	1:B:162:MET:HG2	1.93	0.48
1:B:314:GLU:HA	1:B:317:PHE:CE2	2.47	0.48
1:A:912:ALA:HB2	1:A:1010:GLY:HA3	1.95	0.48
1:B:44:THR:OG1	1:B:132:SER:HB3	2.13	0.48
1:C:190:PRO:HB3	1:C:789:TRP:CE3	2.49	0.48
1:B:720:GLY:O	1:B:721:LEU:HD12	2.14	0.48
1:B:200:PRO:HD2	1:B:749:THR:HG23	1.94	0.48
1:B:372:VAL:HB	1:B:405:LEU:HD11	1.96	0.48
1:B:324:VAL:CG2	1:B:326:PRO:HD3	2.43	0.48
1:C:158:VAL:HG12	1:C:159:ALA:N	2.27	0.48
1:C:858:ASP:OD1	1:C:859:TRP:N	2.47	0.48
1:B:408:ASP:OD1	1:B:442:LEU:HA	2.13	0.48
1:A:729:ILE:HG22	1:A:730:ASP:H	1.76	0.48
1:B:200:PRO:HG2	1:B:749:THR:HG23	1.96	0.48
1:A:211:ASN:CG	1:A:211:ASN:O	2.52	0.48
1:C:119:PRO:HG2	1:C:122:VAL:HG23	1.96	0.48
1:C:948:PHE:HE1	1:C:971:ARG:NE	2.12	0.48
1:A:574:THR:HB	1:A:627:ALA:HB3	1.95	0.48
1:B:990:VAL:HG21	1:B:1008:MET:SD	2.54	0.48
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.44	0.48
1:B:655:PHE:O	1:B:658:ILE:HG13	2.13	0.48
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:LEU:O	1:C:370:ILE:N	2.42	0.48
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.48	0.47
1:B:940:LYS:NZ	1:B:978:THR:CG2	2.77	0.47
1:A:533:GLY:C	1:A:535:LEU:N	2.65	0.47
1:A:1033:PHE:O	1:A:1034:SER:CB	2.60	0.47
1:C:909:VAL:HG11	1:C:935:ILE:HD11	1.96	0.47
1:A:897:ILE:N	1:A:898:PRO:HD2	2.29	0.47
1:C:973:ARG:O	1:C:977:MET:HG3	2.14	0.47
1:B:1024:VAL:O	1:B:1028:VAL:HG23	2.14	0.47
1:A:987:MET:HA	1:A:990:VAL:O	2.14	0.47
1:B:940:LYS:HZ2	1:B:978:THR:CG2	2.28	0.47
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.49	0.47
1:A:649:MET:HG2	1:A:653:ARG:NH1	2.29	0.47
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.78	0.47
1:B:157:TYR:HA	1:B:161:ASN:ND2	2.29	0.47
1:A:144:ASN:HB2	1:A:149:MET:HE3	1.96	0.47
1:C:294:ALA:HB3	1:C:297:ALA:HB2	1.96	0.47
1:A:324:VAL:HG12	1:A:325:TYR:N	2.29	0.47
1:B:314:GLU:N	1:B:315:PRO:HD3	2.29	0.47
1:B:921:LEU:HD22	1:B:1005:THR:HB	1.97	0.47
1:B:221:GLY:HA3	1:C:780:ARG:HH12	1.79	0.47
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.95	0.47
1:B:342:LYS:O	1:B:346:GLU:HG3	2.13	0.47
1:A:51:GLY:O	1:C:215:ALA:HB1	2.13	0.47
1:A:674:LEU:HD13	1:A:675:GLY:N	2.29	0.47
1:C:778:LYS:HG3	1:C:779:TYR:CE2	2.50	0.47
1:A:991:ILE:O	1:A:992:SER:OG	2.26	0.47
1:A:818:ARG:NH1	1:A:821:GLY:O	2.47	0.47
1:B:692:HIS:ND1	1:B:692:HIS:O	2.48	0.47
1:B:881:LEU:O	1:B:882:ILE:C	2.53	0.47
1:B:210:GLN:NE2	1:B:249:ILE:HA	2.28	0.47
1:C:736:ALA:C	1:C:738:ALA:H	2.18	0.47
1:C:713:LEU:HD23	1:C:832:ALA:N	2.29	0.47
1:B:222:THR:CB	1:B:223:PRO:HD3	2.26	0.47
1:B:456:MET:CG	1:B:467:TYR:HB3	2.36	0.47
1:A:597:TYR:HD1	1:A:598:TYR:N	2.12	0.47
1:B:681:ASP:O	1:B:859:TRP:HE3	1.98	0.47
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.96	0.47
1:B:518:ARG:HA	1:B:521:GLU:CG	2.45	0.47
1:B:13:TRP:O	1:B:17:ILE:HG12	2.14	0.47
1:A:552:MET:HA	1:A:555:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.29	0.47
1:A:228:GLN:HB2	1:B:781:MET:HE1	1.96	0.47
1:C:2:PRO:O	1:C:6:ILE:HG13	2.14	0.47
1:A:314:GLU:O	1:A:317:PHE:HB2	2.15	0.47
1:A:688:ALA:C	1:A:690:LEU:N	2.68	0.47
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.96	0.47
1:B:910:ILE:HG23	1:B:911:GLY:N	2.28	0.47
1:B:666:PHE:HB3	1:B:678:THR:CG2	2.45	0.47
1:A:337:ILE:HG12	1:A:395:MET:SD	2.54	0.47
1:C:186:ILE:O	1:C:186:ILE:HG22	2.13	0.47
1:B:860:THR:O	1:B:863:SER:HB2	2.14	0.47
1:B:549:VAL:O	1:B:552:MET:HB3	2.14	0.47
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.30	0.47
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.78	0.47
1:C:376:LEU:O	1:C:379:THR:N	2.44	0.47
1:C:926:TYR:CE2	1:C:999:ALA:HB1	2.50	0.47
1:B:123:GLN:C	1:B:125:GLN:H	2.17	0.47
1:C:949:ALA:HB1	1:C:1026:PHE:CE2	2.50	0.47
1:A:608:SER:O	1:A:629:VAL:HG23	2.15	0.47
1:C:328:ASP:OD1	1:C:330:THR:HB	2.15	0.47
1:C:457:ALA:HB2	1:C:471:SER:CB	2.45	0.47
1:B:452:VAL:O	1:B:453:PHE:CB	2.63	0.47
1:B:78:MET:HG3	1:B:92:LEU:HG	1.97	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.49	0.47
1:A:974:PRO:O	1:A:975:ILE:C	2.53	0.47
1:C:497:LEU:HD12	1:C:498:LYS:HG3	1.96	0.47
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.96	0.47
1:C:713:LEU:HD13	1:C:713:LEU:N	2.29	0.47
1:A:808:ARG:N	1:A:808:ARG:HH11	2.12	0.47
1:A:351:VAL:HG21	1:A:406:VAL:CG2	2.45	0.47
1:A:150:THR:OG1	1:A:153:ASP:OD2	2.31	0.47
1:B:997:SER:HA	1:B:1000:GLN:HB2	1.97	0.47
1:C:350:LEU:CD2	1:C:984:LEU:HB3	2.45	0.47
1:A:431:THR:HB	1:A:494:ALA:HB2	1.95	0.47
1:A:673:GLU:O	1:A:673:GLU:HG3	2.15	0.47
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.96	0.46
1:C:463:THR:HG22	1:C:464:GLY:N	2.29	0.46
1:A:309:GLU:O	1:A:313:MET:HG2	2.15	0.46
1:C:305:ALA:O	1:C:306:ILE:C	2.53	0.46
1:A:681:ASP:H	1:A:863:SER:CB	2.28	0.46
1:A:66:GLU:C	1:A:68:ASN:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:H	1:B:72:ILE:HD13	1.79	0.46
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.97	0.46
1:B:62:THR:O	1:B:66:GLU:HB2	2.14	0.46
1:B:472:ILE:HG23	1:B:473:THR:N	2.30	0.46
1:B:469:GLN:O	1:B:473:THR:OG1	2.33	0.46
1:C:778:LYS:HG3	1:C:779:TYR:HE2	1.81	0.46
1:C:966:ASP:O	1:C:970:MET:N	2.29	0.46
1:C:484:VAL:HG13	1:C:488:LEU:HB3	1.98	0.46
1:C:821:GLY:O	1:C:822:LEU:HD23	2.15	0.46
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.97	0.46
1:B:2:PRO:O	1:B:4:PHE:N	2.48	0.46
1:A:680:PHE:CZ	1:A:844:MET:HE1	2.50	0.46
1:A:255:GLN:O	1:A:256:ASP:CB	2.63	0.46
1:C:655:PHE:C	1:C:657:GLN:N	2.68	0.46
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.79	0.46
1:C:899:PHE:H	1:C:899:PHE:HD1	1.62	0.46
1:A:711:ASP:C	1:A:713:LEU:H	2.17	0.46
1:A:281:PHE:O	1:A:283:GLY:N	2.48	0.46
1:C:1032:ARG:HG3	1:C:1036:LYS:HE2	1.97	0.46
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.97	0.46
1:C:734:GLU:HA	1:C:737:GLN:HG2	1.97	0.46
1:B:654:ALA:C	1:B:656:SER:H	2.18	0.46
1:B:1009:GLY:O	1:B:1012:VAL:HG22	2.16	0.46
1:C:601:LYS:O	1:C:603:LYS:N	2.48	0.46
1:C:160:ALA:HA	1:C:767:ARG:NE	2.31	0.46
1:B:50:PRO:HG2	1:B:125:GLN:HE22	1.80	0.46
1:C:680:PHE:CE1	1:C:844:MET:HE3	2.50	0.46
1:C:435:MET:HA	1:C:438:ILE:HG22	1.98	0.46
1:A:973:ARG:O	1:A:977:MET:HG3	2.16	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.15	0.46
1:B:828:LEU:HB3	1:B:829:GLY:H	1.59	0.46
1:B:111:LEU:HD21	1:B:127:VAL:HG13	1.97	0.46
1:B:445:ILE:O	1:B:449:LEU:HB2	2.16	0.46
1:A:702:LEU:HG	1:A:702:LEU:O	2.16	0.46
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.51	0.46
1:A:221:GLY:HA2	1:B:622:GLN:OE1	2.16	0.46
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.98	0.46
1:C:658:ILE:HD12	1:C:658:ILE:H	1.81	0.46
1:A:395:MET:HA	1:A:395:MET:HE2	1.97	0.46
1:A:274:ASN:OD1	1:A:275:TYR:N	2.49	0.46
1:C:317:PHE:CG	1:C:321:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:VAL:CG1	1:A:883:VAL:O	2.64	0.46
1:B:587:THR:HG22	1:B:591:LEU:HD23	1.98	0.46
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.44	0.46
1:C:379:THR:O	1:C:382:VAL:N	2.49	0.46
1:C:767:ARG:HH11	1:C:767:ARG:HG3	1.81	0.46
1:A:427:PRO:O	1:A:429:GLU:N	2.48	0.46
1:C:759:VAL:HG23	1:C:771:VAL:HB	1.98	0.46
1:A:391:ASN:H	1:A:394:THR:HG22	1.80	0.46
1:B:671:ILE:HD13	1:B:676:THR:HG22	1.98	0.46
1:A:677:ALA:C	1:A:679:GLY:N	2.69	0.46
1:C:997:SER:O	1:C:1000:GLN:N	2.41	0.46
1:A:167:SER:OG	1:A:175:VAL:HG21	2.16	0.46
1:A:427:PRO:C	1:A:429:GLU:H	2.18	0.46
1:B:328:ASP:OD2	1:B:328:ASP:C	2.54	0.46
1:A:729:ILE:HD13	1:C:234:ILE:CG2	2.44	0.45
1:C:731:ILE:HG12	1:C:746:ILE:HG21	1.98	0.45
1:C:531:VAL:HA	1:C:534:ILE:HG23	1.97	0.45
1:C:144:ASN:ND2	1:C:148:THR:H	2.14	0.45
1:A:799:VAL:CG1	1:A:800:PRO:HD2	2.46	0.45
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.98	0.45
1:B:764:ASP:O	1:B:766:GLY:N	2.49	0.45
1:C:14:VAL:HG13	1:C:15:ILE:N	2.31	0.45
1:A:389:SER:OG	1:A:391:ASN:ND2	2.48	0.45
1:B:1022:VAL:HA	1:B:1025:PHE:HD1	1.80	0.45
1:C:457:ALA:HB2	1:C:471:SER:OG	2.17	0.45
1:A:428:LYS:HG3	1:A:429:GLU:HG3	1.98	0.45
1:A:317:PHE:HE2	1:A:323:ILE:CG2	2.29	0.45
1:A:56:THR:O	1:A:60:THR:HB	2.16	0.45
1:C:156:ASP:O	1:C:157:TYR:C	2.55	0.45
1:C:758:TYR:HE2	1:C:770:LYS:CB	2.18	0.45
1:C:332:PHE:O	1:C:333:VAL:C	2.54	0.45
1:C:9:PRO:O	1:C:11:PHE:N	2.46	0.45
1:B:104:GLN:HE22	1:B:108:GLN:HE21	1.64	0.45
1:A:530:SER:O	1:A:534:ILE:HG23	2.15	0.45
1:B:399:VAL:O	1:B:402:ILE:HB	2.16	0.45
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.79	0.45
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.31	0.45
1:B:58:GLN:O	1:B:63:GLN:HG2	2.17	0.45
1:B:66:GLU:HG3	1:B:78:MET:SD	2.56	0.45
1:C:65:ILE:HD13	1:C:111:LEU:HD21	1.97	0.45
1:A:431:THR:CB	1:A:494:ALA:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:VAL:O	1:C:348:ILE:N	2.48	0.45
1:A:911:GLY:N	1:A:914:LEU:HD13	2.16	0.45
1:A:60:THR:HG23	1:A:119:PRO:HG3	1.97	0.45
1:B:314:GLU:HG3	1:B:317:PHE:CE2	2.51	0.45
1:C:352:PHE:HA	1:C:369:THR:HG21	1.98	0.45
1:A:909:VAL:O	1:A:912:ALA:HB3	2.16	0.45
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.99	0.45
1:A:727:PHE:CZ	1:A:783:PRO:HB3	2.51	0.45
1:C:901:VAL:HG11	1:C:943:ILE:HA	1.98	0.45
1:C:414:GLU:HG2	1:C:974:PRO:HB3	1.98	0.45
1:B:805:SER:O	1:B:806:SER:HB2	2.16	0.45
1:C:418:ARG:HD2	1:C:419:VAL:CG2	2.42	0.45
1:A:456:MET:C	1:A:458:PHE:N	2.69	0.45
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.47	0.45
1:B:348:ILE:HG12	1:B:372:VAL:HG21	1.98	0.45
1:B:154:ILE:C	1:B:156:ASP:N	2.70	0.45
1:C:872:GLN:HE21	1:C:875:SER:HB2	1.81	0.45
1:B:669:PRO:HG3	1:B:678:THR:HA	1.99	0.45
1:B:34:GLN:HG2	1:B:35:TYR:CD2	2.51	0.45
1:C:491:ALA:C	1:C:493:CYS:N	2.68	0.45
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.98	0.45
1:C:155:SER:OG	1:C:179:GLY:HA3	2.17	0.45
1:B:639:GLY:O	1:B:641:GLU:N	2.50	0.45
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.98	0.45
1:B:5:PHE:HA	1:B:8:ARG:HB2	1.99	0.45
1:C:188:MET:HA	1:C:266:ALA:HB2	1.98	0.45
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.99	0.45
1:B:493:CYS:O	1:B:497:LEU:HB2	2.17	0.45
1:B:44:THR:OG1	1:B:132:SER:CB	2.64	0.45
1:B:891:LEU:HD13	1:B:892:TYR:CE2	2.52	0.44
1:C:712:MET:C	1:C:713:LEU:HD22	2.37	0.44
1:C:925:VAL:HG23	1:C:926:TYR:N	2.32	0.44
1:A:750:LEU:O	1:A:754:TRP:CD1	2.70	0.44
1:B:410:ILE:HD13	1:B:977:MET:HG3	1.99	0.44
1:A:623:ASN:O	1:A:623:ASN:CG	2.54	0.44
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.36	0.44
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.46	0.44
1:A:69:MET:CG	1:A:92:LEU:HD21	2.48	0.44
1:C:102:ILE:O	1:C:103:ALA:C	2.54	0.44
1:A:83:ASP:O	1:A:85:THR:N	2.49	0.44
1:C:577:GLN:CA	1:C:577:GLN:HE21	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LEU:O	1:B:263:ARG:N	2.50	0.44
1:C:314:GLU:N	1:C:315:PRO:CD	2.80	0.44
1:B:291:ILE:CD1	1:B:291:ILE:H	2.30	0.44
1:C:1004:GLY:C	1:C:1006:GLY:H	2.20	0.44
1:B:601:LYS:HE2	1:B:601:LYS:HB2	1.90	0.44
1:B:280:GLU:HA	1:B:286:ALA:HB3	1.99	0.44
1:B:238:THR:HG23	1:B:239:ARG:H	1.82	0.44
1:C:859:TRP:CE3	1:C:863:SER:HB3	2.53	0.44
1:B:339:GLU:O	1:B:342:LYS:HB2	2.16	0.44
1:A:971:ARG:O	1:A:974:PRO:HD2	2.17	0.44
1:A:241:THR:N	1:A:245:GLU:OE1	2.40	0.44
1:A:250:LEU:HD22	1:A:250:LEU:H	1.81	0.44
1:B:891:LEU:HD13	1:B:892:TYR:CZ	2.52	0.44
1:B:892:TYR:CD1	1:B:897:ILE:HD11	2.51	0.44
1:B:863:SER:O	1:B:866:GLU:N	2.50	0.44
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.99	0.44
1:C:219:LEU:CD2	1:C:234:ILE:HD11	2.47	0.44
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.99	0.44
1:C:952:LEU:O	1:C:952:LEU:HG	2.18	0.44
1:A:574:THR:HG21	1:A:594:VAL:CG1	2.48	0.44
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.52	0.44
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.99	0.44
1:B:539:GLY:C	1:B:541:TYR:N	2.71	0.44
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.48	0.44
1:B:57:VAL:CG2	1:B:82:SER:HB2	2.47	0.44
1:A:359:LEU:O	1:A:360:GLN:HB2	2.17	0.44
1:B:942:ALA:O	1:B:945:ILE:HG13	2.17	0.44
1:A:367:ILE:HG22	1:A:496:MET:HE3	1.99	0.44
1:A:540:ARG:HD2	1:A:541:TYR:HE2	1.81	0.44
1:C:576:VAL:HG13	1:C:590:VAL:HG11	2.00	0.44
1:C:203:VAL:O	1:C:207:ILE:HG13	2.18	0.44
1:B:309:GLU:O	1:B:312:LYS:HB2	2.17	0.44
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.98	0.44
1:A:190:PRO:HB3	1:A:789:TRP:CD2	2.52	0.44
1:C:254:ASN:O	1:C:256:ASP:N	2.51	0.44
1:B:563:PHE:HB2	1:B:866:GLU:HG3	1.98	0.44
1:A:355:MET:CG	1:A:365:THR:HG22	2.48	0.44
1:B:298:ASN:CB	1:B:301:ASP:HB2	2.47	0.44
1:C:390:ILE:HA	1:C:394:THR:HG21	1.99	0.44
1:C:657:GLN:O	1:C:659:LYS:N	2.51	0.44
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ASN:ND2	1:B:231:ASN:C	2.68	0.44
1:C:928:GLN:HA	1:C:931:LEU:HB3	1.98	0.44
1:B:901:VAL:O	1:B:904:VAL:HG23	2.17	0.44
1:A:591:LEU:CD1	1:A:613:ASN:HB2	2.48	0.44
1:B:448:VAL:O	1:B:452:VAL:HG22	2.17	0.44
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.44
1:A:346:GLU:C	1:A:348:ILE:N	2.71	0.44
1:A:724:THR:HG22	1:A:725:PRO:N	2.33	0.44
1:A:956:GLU:HB3	1:A:958:LYS:HG3	2.00	0.44
1:B:624:THR:O	1:B:624:THR:HG23	2.17	0.44
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.87	0.44
1:C:931:LEU:O	1:C:935:ILE:HG13	2.18	0.44
1:B:560:PRO:HB2	1:B:836:SER:CB	2.41	0.44
1:A:46:SER:HA	1:A:88:VAL:O	2.17	0.44
1:A:252:LYS:HE3	1:A:254:ASN:HB3	2.00	0.44
1:B:450:SER:O	1:B:452:VAL:O	2.36	0.44
1:C:574:THR:HG23	1:C:665:ALA:HB2	1.98	0.44
1:C:520:PHE:C	1:C:522:LYS:H	2.22	0.44
1:A:959:GLY:HA3	1:A:962:GLU:HB3	2.00	0.44
1:C:963:ALA:O	1:C:965:LEU:N	2.51	0.43
1:A:780:ARG:NH2	1:C:222:THR:H	2.15	0.43
1:C:222:THR:CG2	1:C:223:PRO:HD3	2.47	0.43
1:B:749:THR:O	1:B:750:LEU:C	2.56	0.43
1:B:162:MET:HB3	1:B:313:MET:SD	2.58	0.43
1:A:733:GLN:HE22	1:A:743:ILE:HD12	1.83	0.43
1:A:579:PRO:O	1:A:580:ALA:C	2.55	0.43
1:B:367:ILE:HG22	1:B:489:THR:HG23	1.98	0.43
1:A:63:GLN:HG2	1:C:768:VAL:HG12	2.00	0.43
1:A:866:GLU:HG3	1:A:867:ARG:N	2.33	0.43
1:A:74:ASN:H	1:C:170:SER:HB2	1.83	0.43
1:C:541:TYR:C	1:C:543:VAL:H	2.21	0.43
1:C:901:VAL:O	1:C:904:VAL:CG2	2.60	0.43
1:B:894:SER:OG	1:B:897:ILE:HG23	2.18	0.43
1:C:779:TYR:CD2	1:C:779:TYR:N	2.85	0.43
1:C:3:ASN:C	1:C:5:PHE:N	2.71	0.43
1:C:963:ALA:C	1:C:965:LEU:N	2.71	0.43
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.47	0.43
1:B:358:PHE:CD1	1:B:977:MET:HB3	2.54	0.43
1:C:418:ARG:NH1	1:C:970:MET:HG2	2.20	0.43
1:C:36:PRO:HG3	1:C:469:GLN:HG3	2.01	0.43
1:C:230:LEU:HD13	1:C:230:LEU:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:H	1:B:622:GLN:NE2	2.16	0.43
1:B:129:VAL:HG23	1:C:109:ASN:HD21	1.83	0.43
1:C:194:ASN:O	1:C:195:LYS:C	2.57	0.43
1:B:25:LEU:HD11	1:C:879:ILE:HG12	1.99	0.43
1:C:707:ALA:O	1:C:710:PRO:HD3	2.18	0.43
1:A:138:MET:HB2	1:A:327:TYR:O	2.19	0.43
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.48	0.43
1:A:216:ALA:HA	1:B:751:GLY:HA2	2.00	0.43
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.83	0.43
1:C:687:GLN:HB3	1:C:687:GLN:HE21	1.52	0.43
1:C:591:LEU:HD12	1:C:611:ALA:HB1	2.00	0.43
1:C:609:VAL:HG22	1:C:629:VAL:HG22	2.01	0.43
1:C:456:MET:O	1:C:459:PHE:HD2	2.00	0.43
1:A:547:ILE:HA	1:A:547:ILE:HD13	1.95	0.43
1:A:80:SER:HG	1:A:818:ARG:HG3	1.81	0.43
1:B:190:PRO:HD3	1:B:779:TYR:CD2	2.53	0.43
1:B:119:PRO:HG2	1:B:122:VAL:HG21	2.00	0.43
1:A:451:ALA:C	1:A:453:PHE:H	2.20	0.43
1:A:431:THR:O	1:A:435:MET:HB2	2.18	0.43
1:C:672:VAL:HG13	1:C:675:GLY:N	2.33	0.43
1:A:1024:VAL:O	1:A:1028:VAL:HG23	2.19	0.43
1:B:307:ARG:HB2	1:B:307:ARG:HH11	1.83	0.43
1:C:742:SER:OG	1:C:745:ASP:HB2	2.18	0.43
1:C:115:MET:HA	1:C:118:LEU:CD2	2.49	0.43
1:B:921:LEU:HD21	1:B:1002:ALA:HA	2.00	0.43
1:A:685:ILE:HB	1:A:687:GLN:HE22	1.83	0.43
1:A:584:GLN:N	1:A:622:GLN:HB3	2.33	0.43
1:A:254:ASN:CG	1:A:258:SER:OG	2.57	0.43
1:A:979:SER:O	1:A:983:ILE:HG12	2.17	0.43
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.52	0.43
1:B:166:ILE:HD11	1:B:310:LEU:CD2	2.48	0.43
1:B:463:THR:OG1	1:B:464:GLY:N	2.52	0.43
1:B:705:GLU:HG3	1:B:847:LEU:HD13	2.01	0.43
1:B:674:LEU:O	1:B:676:THR:N	2.51	0.43
1:B:200:PRO:CD	1:B:749:THR:HG23	2.49	0.43
1:A:293:LEU:HB3	1:A:294:ALA:H	1.68	0.43
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.53	0.43
1:A:449:LEU:O	1:A:453:PHE:CD1	2.70	0.43
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.54	0.43
1:A:566:ASP:HB3	1:A:667:ASN:HD22	1.82	0.43
1:B:564:LEU:HD22	1:B:926:TYR:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LEU:HD13	1:C:901:VAL:HG23	2.00	0.43
1:C:741:VAL:HG11	1:C:746:ILE:HD11	2.01	0.43
1:B:338:HIS:CE1	1:B:342:LYS:HE3	2.54	0.43
1:A:346:GLU:C	1:A:348:ILE:H	2.22	0.43
1:C:520:PHE:O	1:C:522:LYS:N	2.52	0.43
1:A:45:ILE:HA	1:A:128:SER:O	2.19	0.43
1:B:235:ILE:O	1:C:728:LYS:HD2	2.19	0.43
1:C:940:LYS:HA	1:C:943:ILE:HD12	2.01	0.43
1:B:404:LEU:HD21	1:B:937:LEU:CD2	2.49	0.43
1:B:692:HIS:HE1	1:B:723:ASP:CG	2.22	0.43
1:B:49:TYR:HE1	1:B:60:THR:HG21	1.84	0.43
1:B:327:TYR:HB2	1:B:628:PHE:HB3	2.01	0.43
1:B:470:PHE:O	1:B:473:THR:N	2.52	0.43
1:C:83:ASP:HB2	1:C:87:THR:HB	2.01	0.43
1:B:32:VAL:O	1:B:33:ALA:HB2	2.18	0.43
1:C:400:LEU:HD12	1:C:933:THR:HG21	1.99	0.43
1:C:61:VAL:HA	1:C:118:LEU:HD12	2.00	0.43
1:C:1022:VAL:HA	1:C:1025:PHE:CE2	2.54	0.43
1:C:953:MET:SD	1:C:963:ALA:CB	3.07	0.43
1:B:852:PRO:O	1:B:853:THR:OG1	2.24	0.43
1:B:1013:THR:O	1:B:1017:LEU:HB3	2.18	0.43
1:B:947:GLU:HA	1:B:947:GLU:OE2	2.18	0.43
1:C:983:ILE:HD13	1:C:1008:MET:HA	2.00	0.43
1:C:658:ILE:O	1:C:659:LYS:HD2	2.18	0.43
1:C:672:VAL:HG12	1:C:672:VAL:O	2.18	0.43
1:C:18:ILE:O	1:C:19:ILE:C	2.58	0.42
1:C:192:GLU:HG2	1:C:264:ASP:O	2.19	0.42
1:C:355:MET:SD	1:C:410:ILE:HD11	2.59	0.42
1:B:192:GLU:O	1:B:196:PHE:CD2	2.71	0.42
1:C:690:LEU:HD11	1:C:854:GLY:HA3	2.00	0.42
1:B:154:ILE:O	1:B:157:TYR:N	2.52	0.42
1:C:983:ILE:HG23	1:C:1008:MET:HG3	2.01	0.42
1:C:189:ASN:HD21	1:C:191:ASN:HB2	1.84	0.42
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.50	0.42
1:A:736:ALA:HA	1:A:741:VAL:HG12	2.02	0.42
1:C:139:VAL:CG1	1:C:326:PRO:HG2	2.49	0.42
1:C:655:PHE:O	1:C:656:SER:C	2.56	0.42
1:C:687:GLN:OE1	1:C:856:GLY:HA3	2.18	0.42
1:B:349:ILE:HG22	1:B:350:LEU:HD23	2.01	0.42
1:A:476:SER:O	1:A:480:LEU:HB2	2.19	0.42
1:B:547:ILE:HD13	1:B:547:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:LEU:HA	1:C:956:GLU:HG2	1.99	0.42
1:A:317:PHE:HA	1:A:318:PRO:HD2	1.73	0.42
1:B:721:LEU:HB3	1:B:814:PRO:HG2	2.01	0.42
1:B:140:VAL:O	1:B:140:VAL:HG22	2.18	0.42
1:A:733:GLN:O	1:A:736:ALA:HB3	2.20	0.42
1:B:87:THR:HG21	1:B:620:ARG:HH12	1.79	0.42
1:C:597:TYR:CD1	1:C:601:LYS:HG3	2.54	0.42
1:A:69:MET:HG3	1:A:92:LEU:HD21	2.00	0.42
1:C:395:MET:O	1:C:398:MET:N	2.43	0.42
1:B:155:SER:OG	1:B:179:GLY:HA3	2.20	0.42
1:A:680:PHE:CZ	1:A:844:MET:CE	3.03	0.42
1:B:303:ALA:HA	1:B:306:ILE:HD13	2.00	0.42
1:B:391:ASN:O	1:B:395:MET:HG2	2.20	0.42
1:A:566:ASP:HB3	1:A:667:ASN:ND2	2.34	0.42
1:B:16:ALA:HB2	1:B:488:LEU:HG	2.01	0.42
1:C:554:TYR:HD1	1:C:558:ARG:NE	2.17	0.42
1:B:830:GLN:HB2	1:B:831:ALA:H	1.62	0.42
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.32	0.42
1:B:190:PRO:CD	1:B:779:TYR:CE2	3.01	0.42
1:B:335:ILE:HG13	1:B:634:TRP:HD1	1.82	0.42
1:A:180:SER:O	1:A:181:GLN:CB	2.67	0.42
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.49	0.42
1:B:327:TYR:O	1:B:327:TYR:HD1	2.03	0.42
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.22	0.42
1:B:216:ALA:O	1:B:234:ILE:HB	2.20	0.42
1:C:406:VAL:CG1	1:C:407:ASP:N	2.82	0.42
1:B:96:SER:HB3	1:B:461:GLY:HA2	2.00	0.42
1:C:489:THR:N	1:C:490:PRO:HD2	2.34	0.42
1:A:988:PRO:HB2	1:A:989:LEU:H	1.66	0.42
1:C:251:LEU:HB2	1:C:260:VAL:O	2.19	0.42
1:B:190:PRO:HG3	1:B:789:TRP:CZ2	2.55	0.42
1:A:240:LEU:N	1:A:240:LEU:HD12	2.35	0.42
1:B:327:TYR:C	1:B:327:TYR:CD1	2.92	0.42
1:A:959:GLY:O	1:A:961:ILE:N	2.53	0.42
1:C:343:THR:CG2	1:C:989:LEU:HD13	2.42	0.42
1:B:858:ASP:OD1	1:B:859:TRP:N	2.48	0.42
1:A:993:THR:HB	1:A:994:GLY:H	1.74	0.42
1:C:325:TYR:N	1:C:325:TYR:HD1	2.14	0.42
1:A:211:ASN:HA	1:A:240:LEU:HD13	2.02	0.42
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.82	0.42
1:A:34:GLN:HG2	1:A:35:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:VAL:HG21	1:B:1026:PHE:CE2	2.55	0.42
1:B:819:TYR:OH	1:B:860:THR:HB	2.20	0.42
1:B:401:ALA:HA	1:B:404:LEU:HB2	2.02	0.42
1:B:682:PHE:HB2	1:B:859:TRP:CZ3	2.55	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.89	0.42
1:C:395:MET:HA	1:C:395:MET:CE	2.50	0.42
1:A:590:VAL:O	1:A:591:LEU:C	2.56	0.42
1:C:295:THR:HG23	1:C:295:THR:O	2.20	0.42
1:C:186:ILE:HG13	1:C:268:ILE:HD13	2.00	0.42
1:B:833:PRO:O	1:B:834:GLY:O	2.37	0.42
1:A:577:GLN:HB2	1:A:577:GLN:HE21	1.62	0.42
1:A:713:LEU:CD2	1:A:714:THR:H	2.27	0.42
1:C:445:ILE:O	1:C:448:VAL:N	2.53	0.42
1:C:446:ALA:HB2	1:C:482:VAL:HG21	2.02	0.42
1:C:905:VAL:CB	1:C:906:PRO:HD3	2.47	0.42
1:C:942:ALA:HB1	1:C:1022:VAL:HG21	2.01	0.42
1:B:699:ARG:CG	1:B:700:ASN:H	2.28	0.42
1:B:911:GLY:HA3	1:B:1013:THR:HG21	2.02	0.42
1:A:330:THR:O	1:A:331:PRO:C	2.58	0.42
1:B:154:ILE:C	1:B:156:ASP:H	2.23	0.42
1:A:99:ASP:OD1	1:A:101:ASP:N	2.52	0.42
1:B:210:GLN:HE22	1:B:249:ILE:HA	1.85	0.42
1:A:830:GLN:HE21	1:A:831:ALA:H	1.68	0.42
1:C:575:MET:SD	1:C:575:MET:N	2.92	0.42
1:A:780:ARG:HH22	1:C:223:PRO:CD	2.32	0.42
1:B:700:ASN:O	1:B:704:ALA:CB	2.68	0.42
1:C:538:THR:HG22	1:C:539:GLY:N	2.30	0.42
1:A:1015:THR:C	1:A:1017:LEU:N	2.73	0.42
1:B:941:ASN:ND2	1:B:1014:ALA:O	2.50	0.42
1:C:425:LEU:H	1:C:426:PRO:CD	2.33	0.42
1:B:293:LEU:CD1	1:B:297:ALA:HB3	2.50	0.42
1:A:828:LEU:HD23	1:A:828:LEU:HA	1.83	0.42
1:B:556:PHE:HB2	1:B:913:LEU:HD21	2.01	0.42
1:A:52:ALA:HB3	1:A:86:GLY:CA	2.44	0.42
1:A:445:ILE:HD12	1:A:445:ILE:C	2.40	0.42
1:A:341:VAL:O	1:A:345:VAL:HG23	2.20	0.42
1:B:762:PHE:CD2	1:B:771:VAL:HG22	2.55	0.42
1:B:686:ASP:HB3	1:B:823:PRO:HG2	2.01	0.42
1:B:409:ALA:HB2	1:B:485:ALA:HB2	2.01	0.42
1:A:552:MET:HB3	1:A:910:ILE:HG23	2.01	0.42
1:B:137:LEU:HD13	1:B:293:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:923:ASN:HD22	1:A:923:ASN:C	2.22	0.42
1:B:866:GLU:O	1:B:869:SER:HB3	2.20	0.41
1:A:882:ILE:O	1:A:886:LEU:HB2	2.19	0.41
1:B:908:GLY:C	1:B:910:ILE:H	2.23	0.41
1:B:11:PHE:CD1	1:C:890:ALA:HB1	2.55	0.41
1:B:251:LEU:HA	1:B:251:LEU:HD12	1.82	0.41
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.48	0.41
1:C:210:GLN:NE2	1:C:249:ILE:HG23	2.35	0.41
1:B:166:ILE:O	1:B:168:ARG:N	2.53	0.41
1:C:451:ALA:HB1	1:C:883:VAL:HG12	2.02	0.41
1:B:799:VAL:CG2	1:B:804:PHE:CE2	3.03	0.41
1:A:822:LEU:HA	1:A:822:LEU:HD12	1.81	0.41
1:A:282:ASN:ND2	1:A:609:VAL:H	2.18	0.41
1:A:454:VAL:O	1:A:456:MET:O	2.38	0.41
1:B:552:MET:SD	1:B:909:VAL:CG2	3.08	0.41
1:A:686:ASP:OD2	1:A:690:LEU:HB2	2.20	0.41
1:B:53:ASP:O	1:B:54:ALA:C	2.59	0.41
1:C:577:GLN:HG3	1:C:577:GLN:O	2.20	0.41
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.32	0.41
1:B:68:ASN:ND2	1:B:114:ALA:HB2	2.34	0.41
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.55	0.41
1:B:568:ASP:OD2	1:B:634:TRP:CH2	2.72	0.41
1:C:100:ALA:HB1	1:C:295:THR:HG21	2.01	0.41
1:B:306:ILE:O	1:B:310:LEU:HG	2.20	0.41
1:A:582:ALA:HB3	1:A:623:ASN:HB2	2.02	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CE2	2.55	0.41
1:C:930:GLY:HA3	1:C:1007:VAL:CG2	2.50	0.41
1:C:904:VAL:O	1:C:906:PRO:N	2.54	0.41
1:C:393:LEU:HD11	1:C:466:ILE:HG23	2.02	0.41
1:B:743:ILE:CD1	1:B:743:ILE:N	2.69	0.41
1:A:527:TYR:OH	1:A:968:VAL:CG1	2.68	0.41
1:A:478:MET:O	1:A:481:SER:HB3	2.19	0.41
1:A:754:TRP:HZ2	1:A:786:ILE:HA	1.85	0.41
1:C:896:SER:OG	1:C:1033:PHE:HD1	2.03	0.41
1:A:368:PRO:HB3	1:A:409:ALA:HB1	2.02	0.41
1:A:574:THR:HG21	1:A:594:VAL:HG11	2.01	0.41
1:A:598:TYR:O	1:A:602:GLU:HB2	2.20	0.41
1:B:650:ARG:O	1:B:654:ALA:N	2.44	0.41
1:C:601:LYS:C	1:C:603:LYS:N	2.74	0.41
1:A:994:GLY:H	1:A:997:SER:HB3	1.85	0.41
1:B:314:GLU:H	1:B:315:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:THR:O	1:B:602:GLU:N	2.50	0.41
1:B:493:CYS:O	1:B:497:LEU:HB3	2.18	0.41
1:A:995:ALA:O	1:A:996:GLY:C	2.59	0.41
1:C:189:ASN:HD22	1:C:190:PRO:N	2.18	0.41
1:B:445:ILE:HG13	1:B:940:LYS:CG	2.50	0.41
1:A:781:MET:HE2	1:C:225:VAL:N	2.32	0.41
1:B:46:SER:HA	1:B:88:VAL:O	2.21	0.41
1:A:111:LEU:O	1:A:113:LEU:N	2.53	0.41
1:B:20:MET:CG	1:B:374:VAL:HA	2.51	0.41
1:B:72:ILE:HD11	1:B:75:LEU:HD22	2.01	0.41
1:B:485:ALA:HA	1:B:489:THR:HB	2.02	0.41
1:A:551:GLY:O	1:A:555:LEU:HD23	2.21	0.41
1:C:425:LEU:H	1:C:426:PRO:HD3	1.85	0.41
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.82	0.41
1:C:569:GLN:C	1:C:634:TRP:HZ2	2.24	0.41
1:C:13:TRP:O	1:C:17:ILE:HG13	2.20	0.41
1:A:534:ILE:HB	1:A:541:TYR:CE2	2.56	0.41
1:A:53:ASP:O	1:A:54:ALA:C	2.58	0.41
1:A:69:MET:CE	1:A:107:VAL:HG13	2.51	0.41
1:A:617:PHE:CE1	1:A:626:ILE:HD11	2.55	0.41
1:A:568:ASP:OD1	1:A:634:TRP:CZ3	2.74	0.41
1:C:350:LEU:HD21	1:C:984:LEU:HD22	2.03	0.41
1:C:119:PRO:HG2	1:C:122:VAL:CG2	2.51	0.41
1:A:681:ASP:H	1:A:863:SER:HB3	1.86	0.41
1:B:254:ASN:HA	1:B:254:ASN:HD22	1.58	0.41
1:B:704:ALA:O	1:B:705:GLU:CB	2.64	0.41
1:B:535:LEU:HD11	1:B:1023:PRO:O	2.20	0.41
1:A:706:ALA:HB1	1:A:716:VAL:HG11	2.02	0.41
1:C:735:LYS:O	1:C:739:LEU:HD13	2.20	0.41
1:C:712:MET:SD	1:C:843:LEU:HD22	2.61	0.41
1:C:189:ASN:ND2	1:C:191:ASN:N	2.66	0.41
1:C:950:LYS:HA	1:C:953:MET:HE1	1.99	0.41
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.56	0.41
1:A:316:PHE:O	1:A:317:PHE:C	2.60	0.41
1:B:280:GLU:CB	1:B:284:GLN:O	2.63	0.41
1:B:1012:VAL:HG23	1:B:1013:THR:H	1.83	0.41
1:B:369:THR:O	1:B:372:VAL:HG13	2.21	0.41
1:C:158:VAL:HG11	1:C:177:LEU:CD2	2.49	0.41
1:C:836:SER:HB3	1:C:839:GLU:HG3	2.03	0.41
1:B:541:TYR:O	1:B:543:VAL:N	2.54	0.41
1:C:997:SER:OG	1:C:998:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:C	1:A:453:PHE:N	2.74	0.41
1:B:181:GLN:HB3	1:B:181:GLN:HE21	1.52	0.41
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.86	0.41
1:B:439:GLN:HA	1:B:442:LEU:HD12	2.03	0.41
1:B:764:ASP:C	1:B:766:GLY:H	2.24	0.41
1:A:724:THR:HG22	1:A:725:PRO:O	2.21	0.41
1:C:648:THR:OG1	1:C:649:MET:N	2.53	0.41
1:A:414:GLU:C	1:A:416:VAL:H	2.23	0.41
1:A:516:PHE:CE2	1:A:520:PHE:HB2	2.56	0.41
1:B:578:LEU:HD23	1:B:578:LEU:N	2.36	0.41
1:C:648:THR:O	1:C:649:MET:C	2.59	0.41
1:C:919:ARG:HB3	1:C:921:LEU:HD23	2.03	0.41
1:B:1004:GLY:O	1:B:1006:GLY:N	2.54	0.41
1:A:133:SER:C	1:A:135:SER:H	2.23	0.41
1:A:38:ILE:H	1:A:38:ILE:HD13	1.86	0.41
1:A:886:LEU:HA	1:A:886:LEU:HD12	1.94	0.41
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.48	0.41
1:A:1029:VAL:O	1:A:1030:ARG:CB	2.66	0.41
1:B:415:ASN:HD21	1:B:971:ARG:HG2	1.86	0.41
1:B:1033:PHE:O	1:B:1034:SER:CB	2.68	0.41
1:B:370:ILE:HA	1:B:370:ILE:HD13	1.93	0.41
1:B:40:PRO:HB2	1:B:94:PHE:O	2.21	0.40
1:A:113:LEU:HD23	1:C:127:VAL:O	2.21	0.40
1:A:409:ALA:O	1:A:410:ILE:C	2.59	0.40
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.92	0.40
1:B:986:VAL:HG12	1:B:990:VAL:HG22	2.01	0.40
1:B:761:ASP:HB3	1:B:768:VAL:HG13	2.04	0.40
1:B:265:VAL:O	1:B:265:VAL:HG22	2.20	0.40
1:C:323:ILE:HG22	1:C:325:TYR:CE1	2.56	0.40
1:C:930:GLY:HA3	1:C:1007:VAL:HG22	2.03	0.40
1:A:20:MET:HG2	1:A:377:LEU:HD22	2.01	0.40
1:A:213:GLN:HB2	1:A:213:GLN:HE21	1.74	0.40
1:A:911:GLY:CA	1:A:914:LEU:HB2	2.49	0.40
1:C:965:LEU:HB3	1:C:966:ASP:H	1.61	0.40
1:B:909:VAL:O	1:B:913:LEU:HD22	2.21	0.40
1:B:115:MET:SD	1:B:127:VAL:HG11	2.61	0.40
1:C:815:ARG:CZ	3:C:2002:RFP:H302	2.50	0.40
1:A:742:SER:O	1:A:744:ASN:N	2.55	0.40
1:C:693:GLU:O	1:C:694:LYS:C	2.60	0.40
1:A:758:TYR:CE1	1:A:770:LYS:HB3	2.56	0.40
1:A:701:GLN:O	1:A:702:LEU:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.57	0.40
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.52	0.40
1:C:631:LEU:HB2	1:C:637:ARG:NH2	2.36	0.40
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.56	0.40
1:A:333:VAL:O	1:A:337:ILE:HB	2.22	0.40
1:C:210:GLN:HE22	1:C:250:LEU:H	1.69	0.40
1:B:63:GLN:O	1:B:64:VAL:C	2.60	0.40
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.57	0.40
1:A:961:ILE:HD12	1:A:1031:ARG:HH22	1.86	0.40
1:C:1015:THR:O	1:C:1019:ILE:HB	2.22	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.83	0.40
1:A:126:GLY:CA	1:B:116:PRO:HB3	2.43	0.40
1:B:5:PHE:HB3	1:B:12:ALA:HB2	2.03	0.40
1:B:754:TRP:CH2	1:B:785:ASP:HB2	2.54	0.40
3:C:2002:RFP:H323	3:C:2002:RFP:H311	2.03	0.40
1:C:717:ARG:NH2	3:C:2002:RFP:O8	2.53	0.40
1:C:686:ASP:OD2	1:C:690:LEU:N	2.54	0.40
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.96	0.40
1:B:613:ASN:O	1:B:615:PHE:N	2.49	0.40
1:A:959:GLY:C	1:A:961:ILE:N	2.74	0.40
1:B:289:LEU:CD1	1:B:289:LEU:N	2.84	0.40
1:C:832:ALA:CB	1:C:833:PRO:CD	2.99	0.40
1:C:34:GLN:HB2	1:C:35:TYR:CZ	2.56	0.40
1:A:883:VAL:HG12	1:A:883:VAL:O	2.20	0.40
1:A:12:ALA:O	1:A:488:LEU:HD13	2.21	0.40
1:B:910:ILE:C	1:B:912:ALA:H	2.25	0.40
1:B:4:PHE:O	1:B:5:PHE:CB	2.69	0.40
1:B:262:LEU:HA	1:B:265:VAL:HG12	2.04	0.40
1:B:541:TYR:C	1:B:543:VAL:N	2.75	0.40
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.56	0.40
1:A:923:ASN:ND2	1:A:923:ASN:C	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1018/1053 (97%)	752 (74%)	173 (17%)	93 (9%)	1	6
1	B	1018/1053 (97%)	730 (72%)	201 (20%)	87 (8%)	1	7
1	C	1018/1053 (97%)	760 (75%)	178 (18%)	80 (8%)	1	8
All	All	3054/3159 (97%)	2242 (73%)	552 (18%)	260 (8%)	1	7

All (260) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	181	GLN
1	A	182	TYR
1	A	282	ASN
1	A	293	LEU
1	A	294	ALA
1	A	319	SER
1	A	388	PHE
1	A	392	THR
1	A	439	GLN
1	A	580	ALA
1	A	601	LYS
1	A	659	LYS
1	A	661	ALA
1	A	677	ALA
1	A	678	THR
1	A	713	LEU
1	A	715	SER
1	A	746	ILE
1	A	831	ALA
1	A	893	GLU
1	A	960	LEU
1	A	992	SER
1	A	1016	VAL
1	B	2	PRO
1	B	22	ALA
1	B	54	ALA
1	B	124	GLN
1	B	147	GLY
1	B	228	GLN
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	326	PRO
1	B	358	PHE
1	B	583	THR
1	B	601	LYS
1	B	633	ASP
1	B	638	PRO
1	B	640	GLU
1	B	656	SER
1	B	669	PRO
1	B	671	ILE
1	B	675	GLY
1	B	676	THR
1	B	733	GLN
1	B	775	SER
1	B	806	SER
1	B	918	PHE
1	B	1016	VAL
1	B	1021	PHE
1	B	1034	SER
1	C	226	LYS
1	C	266	ALA
1	C	326	PRO
1	C	463	THR
1	C	464	GLY
1	C	520	PHE
1	C	553	ALA
1	C	580	ALA
1	C	602	GLU
1	C	678	THR
1	C	720	GLY
1	C	806	SER
1	C	832	ALA
1	C	869	SER
1	C	872	GLN
1	C	905	VAL
1	C	921	LEU
1	C	960	LEU
1	C	965	LEU
1	C	993	THR
1	C	998	GLY
1	A	19	ILE
1	A	52	ALA

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Mol	Chain	Res	Type
1	A	64	VAL
1	A	95	GLU
1	A	134	SER
1	A	170	SER
1	A	221	GLY
1	A	256	ASP
1	A	354	VAL
1	A	358	PHE
1	A	362	PHE
1	A	424	GLY
1	A	428	LYS
1	A	460	GLY
1	A	534	ILE
1	A	638	PRO
1	A	675	GLY
1	A	743	ILE
1	A	870	GLY
1	A	903	LEU
1	A	958	LYS
1	A	975	ILE
1	A	988	PRO
1	A	998	GLY
1	A	1017	LEU
1	A	1034	SER
1	B	140	VAL
1	B	216	ALA
1	B	227	GLY
1	B	243	THR
1	B	361	ASN
1	B	486	LEU
1	B	542	LEU
1	B	580	ALA
1	B	613	ASN
1	B	654	ALA
1	B	666	PHE
1	B	672	VAL
1	B	690	LEU
1	B	705	GLU
1	B	834	GLY
1	B	852	PRO
1	B	899	PHE
1	B	953	MET

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Mol	Chain	Res	Type
1	B	1005	THR
1	C	86	GLY
1	C	255	GLN
1	C	438	ILE
1	C	521	GLU
1	C	601	LYS
1	C	656	SER
1	C	674	LEU
1	C	711	ASP
1	C	713	LEU
1	C	952	LEU
1	C	953	MET
1	C	997	SER
1	C	1027	VAL
1	A	53	ASP
1	A	112	GLN
1	A	167	SER
1	A	174	ASP
1	A	236	ALA
1	A	436	GLY
1	A	452	VAL
1	A	618	ALA
1	B	167	SER
1	B	222	THR
1	B	319	SER
1	B	360	GLN
1	B	439	GLN
1	B	517	ASN
1	B	540	ARG
1	B	553	ALA
1	B	585	GLU
1	B	618	ALA
1	B	655	PHE
1	B	677	ALA
1	B	723	ASP
1	B	765	ARG
1	B	794	ALA
1	B	889	ALA
1	B	968	VAL
1	C	285	PRO
1	C	328	ASP
1	C	336	SER

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Mol	Chain	Res	Type
1	C	427	PRO
1	C	468	ARG
1	C	554	TYR
1	C	555	LEU
1	C	620	ARG
1	C	636	ASP
1	C	658	ILE
1	C	712	MET
1	C	721	LEU
1	C	722	GLU
1	C	756	GLY
1	C	873	ALA
1	C	994	GLY
1	A	317	PHE
1	A	376	LEU
1	A	427	PRO
1	A	517	ASN
1	A	539	GLY
1	A	953	MET
1	A	987	MET
1	B	120	GLN
1	B	127	VAL
1	B	453	PHE
1	B	796	GLY
1	B	820	ASN
1	B	909	VAL
1	C	377	LEU
1	C	425	LEU
1	C	497	LEU
1	C	541	TYR
1	C	675	GLY
1	C	802	SER
1	C	885	PHE
1	C	974	PRO
1	C	983	ILE
1	A	133	SER
1	A	180	SER
1	A	334	LYS
1	A	347	ALA
1	A	421	ALA
1	A	456	MET
1	A	689	GLY

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Mol	Chain	Res	Type
1	A	1030	ARG
1	B	440	GLY
1	B	442	LEU
1	B	515	TRP
1	B	614	GLY
1	B	851	LEU
1	B	974	PRO
1	B	1017	LEU
1	C	62	THR
1	C	477	ALA
1	C	552	MET
1	C	825	MET
1	C	964	THR
1	C	967	ALA
1	A	9	PRO
1	A	18	ILE
1	A	220	GLY
1	A	268	ILE
1	A	318	PRO
1	A	330	THR
1	A	360	GLN
1	A	496	MET
1	A	687	GLN
1	B	125	GLN
1	B	283	GLY
1	B	602	GLU
1	B	921	LEU
1	C	332	PHE
1	C	343	THR
1	C	751	GLY
1	C	784	ASP
1	C	1005	THR
1	C	1035	ARG
1	A	105	VAL
1	A	351	VAL
1	B	86	GLY
1	C	1028	VAL
1	A	38	ILE
1	A	335	ILE
1	B	975	ILE
1	C	935	ILE
1	C	1006	GLY

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Mol	Chain	Res	Type
1	A	15	ILE
1	A	139	VAL
1	A	320	GLY
1	A	410	ILE
1	A	787	GLY
1	B	201	VAL
1	B	306	ILE
1	C	15	ILE
1	A	461	GLY
1	B	223	PRO
1	B	647	ILE
1	B	874	PRO
1	B	961	ILE
1	C	222	THR
1	C	224	PRO
1	C	671	ILE
1	C	975	ILE
1	C	1016	VAL
1	A	340	VAL

5.3.2 Protein sidechains ⓘ

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	833/859 (97%)	707 (85%)	126 (15%)	3	16
1	B	833/859 (97%)	708 (85%)	125 (15%)	3	17
1	C	833/859 (97%)	715 (86%)	118 (14%)	4	19
All	All	2499/2577 (97%)	2130 (85%)	369 (15%)	4	17

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	13	TRP
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	44	THR
1	A	49	TYR
1	A	58	GLN
1	A	60	THR
1	A	63	GLN
1	A	65	ILE
1	A	69	MET
1	A	70	ASN
1	A	76	MET
1	A	96	SER
1	A	105	VAL
1	A	108	GLN
1	A	109	ASN
1	A	110	LYS
1	A	117	LEU
1	A	120	GLN
1	A	164	ASP
1	A	181	GLN
1	A	193	LEU
1	A	207	ILE
1	A	210	GLN
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	234	ILE
1	A	243	THR
1	A	250	LEU
1	A	255	GLN
1	A	277	ILE
1	A	284	GLN
1	A	293	LEU
1	A	298	ASN
1	A	302	THR
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	358	PHE
1	A	359	LEU
1	A	361	ASN
1	A	376	LEU
1	A	377	LEU

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Mol	Chain	Res	Type
1	A	382	VAL
1	A	394	THR
1	A	405	LEU
1	A	406	VAL
1	A	414	GLU
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	423	GLU
1	A	454	VAL
1	A	462	SER
1	A	473	THR
1	A	475	VAL
1	A	476	SER
1	A	480	LEU
1	A	483	LEU
1	A	489	THR
1	A	496	MET
1	A	516	PHE
1	A	530	SER
1	A	534	ILE
1	A	537	SER
1	A	540	ARG
1	A	544	LEU
1	A	549	VAL
1	A	556	PHE
1	A	563	PHE
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	586	ARG
1	A	589	LYS
1	A	597	TYR
1	A	603	LYS
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	636	ASP
1	A	645	GLU
1	A	658	ILE
1	A	659	LYS
1	A	668	LEU

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Mol	Chain	Res	Type
1	A	671	ILE
1	A	680	PHE
1	A	686	ASP
1	A	687	GLN
1	A	713	LEU
1	A	714	THR
1	A	741	VAL
1	A	750	LEU
1	A	768	VAL
1	A	773	VAL
1	A	780	ARG
1	A	801	PHE
1	A	808	ARG
1	A	810	GLU
1	A	815	ARG
1	A	817	GLU
1	A	822	LEU
1	A	843	LEU
1	A	844	MET
1	A	865	GLN
1	A	866	GLU
1	A	867	ARG
1	A	881	LEU
1	A	887	CYS
1	A	899	PHE
1	A	904	VAL
1	A	919	ARG
1	A	923	ASN
1	A	956	GLU
1	A	960	LEU
1	A	976	LEU
1	A	982	PHE
1	A	991	ILE
1	A	993	THR
1	A	1001	ASN
1	A	1008	MET
1	A	1011	MET
1	A	1017	LEU
1	A	1034	SER
1	B	3	ASN
1	B	8	ARG
1	B	13	TRP

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Mol	Chain	Res	Type
1	B	27	ILE
1	B	30	LEU
1	B	56	THR
1	B	60	THR
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	85	THR
1	B	88	VAL
1	B	95	GLU
1	B	104	GLN
1	B	120	GLN
1	B	121	GLU
1	B	129	VAL
1	B	137	LEU
1	B	140	VAL
1	B	145	THR
1	B	146	ASP
1	B	149	MET
1	B	150	THR
1	B	153	ASP
1	B	155	SER
1	B	156	ASP
1	B	169	THR
1	B	170	SER
1	B	176	GLN
1	B	181	GLN
1	B	189	ASN
1	B	190	PRO
1	B	194	ASN
1	B	199	THR
1	B	225	VAL
1	B	230	LEU
1	B	238	THR
1	B	243	THR
1	B	244	GLU
1	B	253	VAL
1	B	254	ASN
1	B	261	LEU
1	B	280	GLU
1	B	289	LEU
1	B	291	ILE

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Mol	Chain	Res	Type
1	B	292	LYS
1	B	293	LEU
1	B	314	GLU
1	B	324	VAL
1	B	327	TYR
1	B	330	THR
1	B	337	ILE
1	B	343	THR
1	B	359	LEU
1	B	372	VAL
1	B	406	VAL
1	B	408	ASP
1	B	410	ILE
1	B	411	VAL
1	B	414	GLU
1	B	415	ASN
1	B	435	MET
1	B	438	ILE
1	B	448	VAL
1	B	449	LEU
1	B	452	VAL
1	B	459	PHE
1	B	473	THR
1	B	480	LEU
1	B	488	LEU
1	B	497	LEU
1	B	515	TRP
1	B	516	PHE
1	B	520	PHE
1	B	536	ARG
1	B	540	ARG
1	B	547	ILE
1	B	559	LEU
1	B	571	VAL
1	B	589	LYS
1	B	601	LYS
1	B	606	VAL
1	B	607	GLU
1	B	620	ARG
1	B	629	VAL
1	B	649	MET
1	B	653	ARG

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Mol	Chain	Res	Type
1	B	655	PHE
1	B	668	LEU
1	B	669	PRO
1	B	674	LEU
1	B	690	LEU
1	B	693	GLU
1	B	696	THR
1	B	702	LEU
1	B	712	MET
1	B	741	VAL
1	B	743	ILE
1	B	750	LEU
1	B	758	TYR
1	B	770	LYS
1	B	774	MET
1	B	779	TYR
1	B	782	LEU
1	B	788	ASP
1	B	795	ASP
1	B	813	SER
1	B	842	GLU
1	B	851	LEU
1	B	879	ILE
1	B	891	LEU
1	B	900	SER
1	B	913	LEU
1	B	952	LEU
1	B	954	ASP
1	B	956	GLU
1	B	960	LEU
1	B	966	ASP
1	B	978	THR
1	B	989	LEU
1	B	1007	VAL
1	B	1020	PHE
1	B	1022	VAL
1	B	1027	VAL
1	B	1034	SER
1	C	8	ARG
1	C	13	TRP
1	C	32	VAL
1	C	35	TYR

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Mol	Chain	Res	Type
1	C	38	ILE
1	C	44	THR
1	C	48	SER
1	C	49	TYR
1	C	56	THR
1	C	63	GLN
1	C	84	SER
1	C	89	GLN
1	C	91	THR
1	C	96	SER
1	C	112	GLN
1	C	119	PRO
1	C	124	GLN
1	C	125	GLN
1	C	127	VAL
1	C	128	SER
1	C	133	SER
1	C	134	SER
1	C	150	THR
1	C	158	VAL
1	C	177	LEU
1	C	189	ASN
1	C	226	LYS
1	C	230	LEU
1	C	239	ARG
1	C	244	GLU
1	C	253	VAL
1	C	259	ARG
1	C	274	ASN
1	C	306	ILE
1	C	316	PHE
1	C	324	VAL
1	C	325	TYR
1	C	339	GLU
1	C	344	LEU
1	C	349	ILE
1	C	350	LEU
1	C	351	VAL
1	C	355	MET
1	C	356	TYR
1	C	367	ILE
1	C	370	ILE

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Mol	Chain	Res	Type
1	C	379	THR
1	C	394	THR
1	C	400	LEU
1	C	402	ILE
1	C	408	ASP
1	C	416	VAL
1	C	418	ARG
1	C	429	GLU
1	C	432	ARG
1	C	471	SER
1	C	472	ILE
1	C	480	LEU
1	C	492	LEU
1	C	493	CYS
1	C	497	LEU
1	C	521	GLU
1	C	525	HIS
1	C	529	ASP
1	C	542	LEU
1	C	544	LEU
1	C	566	ASP
1	C	571	VAL
1	C	577	GLN
1	C	578	LEU
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	605	ASN
1	C	624	THR
1	C	636	ASP
1	C	644	VAL
1	C	659	LYS
1	C	681	ASP
1	C	684	LEU
1	C	685	ILE
1	C	686	ASP
1	C	687	GLN
1	C	695	LEU
1	C	697	GLN
1	C	699	ARG
1	C	713	LEU
1	C	714	THR

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Mol	Chain	Res	Type
1	C	715	SER
1	C	722	GLU
1	C	724	THR
1	C	731	ILE
1	C	745	ASP
1	C	750	LEU
1	C	759	VAL
1	C	760	ASN
1	C	779	TYR
1	C	799	VAL
1	C	808	ARG
1	C	847	LEU
1	C	849	SER
1	C	851	LEU
1	C	868	LEU
1	C	869	SER
1	C	871	ASN
1	C	879	ILE
1	C	900	SER
1	C	901	VAL
1	C	907	LEU
1	C	922	THR
1	C	931	LEU
1	C	941	ASN
1	C	954	ASP
1	C	982	PHE
1	C	1017	LEU
1	C	1029	VAL
1	C	1033	PHE
1	C	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	67	GLN
1	A	89	GLN
1	A	104	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	191	ASN
1	A	210	GLN
1	A	213	GLN
1	A	254	ASN
1	A	282	ASN
1	A	298	ASN
1	A	360	GLN
1	A	361	ASN
1	A	577	GLN
1	A	584	GLN
1	A	687	GLN
1	A	709	HIS
1	A	719	ASN
1	A	726	GLN
1	A	830	GLN
1	A	846	GLN
1	A	923	ASN
1	A	928	GLN
1	A	1001	ASN
1	B	34	GLN
1	B	68	ASN
1	B	70	ASN
1	B	74	ASN
1	B	104	GLN
1	B	106	GLN
1	B	108	GLN
1	B	112	GLN
1	B	120	GLN
1	B	124	GLN
1	B	125	GLN
1	B	144	ASN
1	B	161	ASN
1	B	189	ASN
1	B	210	GLN
1	B	213	GLN
1	B	228	GLN
1	B	231	ASN
1	B	254	ASN
1	B	274	ASN
1	B	338	HIS
1	B	415	ASN

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Mol	Chain	Res	Type
1	B	517	ASN
1	B	526	HIS
1	B	569	GLN
1	B	605	ASN
1	B	642	ASN
1	B	692	HIS
1	B	744	ASN
1	B	846	GLN
1	B	865	GLN
1	C	63	GLN
1	C	68	ASN
1	C	89	GLN
1	C	104	GLN
1	C	109	ASN
1	C	123	GLN
1	C	124	GLN
1	C	125	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	210	GLN
1	C	211	ASN
1	C	213	GLN
1	C	231	ASN
1	C	274	ASN
1	C	577	GLN
1	C	588	GLN
1	C	657	GLN
1	C	726	GLN
1	C	737	GLN
1	C	760	ASN
1	C	871	ASN
1	C	872	GLN
1	C	928	GLN
1	C	941	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	MIY	A	2001	-	35,36,36	1.83	4 (11%)	40,58,58	1.91	11 (27%)
3	RFP	C	2002	-	63,63,63	1.73	3 (4%)	82,94,94	1.96	15 (18%)

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
2	MIY	A	2001	-	-	0/12/70/70	0/4/4/4
3	RFP	C	2002	-	-	0/60/85/85	0/1/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	MIY	C18-C1	-2.08	1.51	1.55
2	A	2001	MIY	C4-N1	2.04	1.51	1.47
2	A	2001	MIY	C16-C15	2.05	1.52	1.47
3	C	2002	RFP	O5-C29	2.85	1.48	1.39
3	C	2002	RFP	O7-C35	5.38	1.47	1.35
2	A	2001	MIY	O5-C15	9.72	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2002	RFP	O4-C11	11.34	1.43	1.21

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2002	RFP	O4-C11-C5	-7.99	115.37	132.02
2	A	2001	MIY	O5-C15-C14	-5.87	110.99	122.01
2	A	2001	MIY	O5-C15-C16	-5.43	112.64	120.73
2	A	2001	MIY	O6-C17-C16	-4.09	119.93	123.84
3	C	2002	RFP	C30-C16-C17	-3.41	115.14	123.22
3	C	2002	RFP	O4-C11-C12	-3.30	111.82	119.93
2	A	2001	MIY	C14-C15-C16	-2.55	114.64	118.68
3	C	2002	RFP	C12-C11-C5	-2.47	101.75	107.53
2	A	2001	MIY	C71-N7-CN7	-2.39	108.08	115.96
3	C	2002	RFP	C2-C3-C43	-2.13	121.12	123.56
2	A	2001	MIY	C11-C10-N7	-2.12	118.62	121.59
2	A	2001	MIY	C18-C5-C4	2.03	114.45	111.73
2	A	2001	MIY	O6-C17-C18	2.06	116.79	113.50
2	A	2001	MIY	C18-C1-C2	2.13	119.54	116.13
3	C	2002	RFP	O5-C12-O3	2.16	113.27	109.33
3	C	2002	RFP	C40-C39-N4	2.52	113.45	110.79
3	C	2002	RFP	C42-C41-N3	2.56	113.74	110.39
2	A	2001	MIY	C15-C16-C17	2.58	121.12	118.93
2	A	2001	MIY	C9-C10-N7	2.65	121.19	118.94
3	C	2002	RFP	C39-C40-N3	2.79	114.05	110.39
3	C	2002	RFP	O3-C6-C7	2.89	127.26	121.29
3	C	2002	RFP	C3-C43-N2	3.46	126.62	120.77
3	C	2002	RFP	C12-O5-C29	3.90	126.67	116.58
3	C	2002	RFP	C42-N4-C39	4.49	115.42	109.53
3	C	2002	RFP	O7-C35-C36	4.50	119.60	111.10
3	C	2002	RFP	C41-C42-N4	6.63	117.78	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2002	RFP	4	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, 95th 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	1022/1053 (97%)	0.05	34 (3%) 50 43	52, 102, 136, 167	0
1	B	1022/1053 (97%)	0.13	27 (2%) 59 53	65, 106, 140, 169	0
1	C	1022/1053 (97%)	0.01	34 (3%) 50 43	49, 100, 148, 183	0
All	All	3066/3159 (97%)	0.06	95 (3%) 52 46	49, 103, 142, 183	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	872	GLN	5.9
1	C	514	GLY	5.5
1	C	515	TRP	5.3
1	A	32	VAL	5.0
1	C	425	LEU	5.0
1	C	538	THR	4.5
1	A	145	THR	4.2
1	B	993	THR	4.1
1	B	675	GLY	4.0
1	C	424	GLY	3.9
1	C	540	ARG	3.9
1	A	198	LEU	3.7
1	A	1036	LYS	3.6
1	C	676	THR	3.5
1	A	1034	SER	3.4
1	A	515	TRP	3.3
1	C	871	ASN	3.3
1	C	833	PRO	3.3
1	C	7	ASP	3.3
1	C	539	GLY	3.2
1	C	362	PHE	3.1
1	A	871	ASN	3.1
1	A	513	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	538	THR	3.0
1	C	513	PHE	3.0
1	A	957	GLY	3.0
1	A	230	LEU	2.9
1	C	497	LEU	2.9
1	A	1033	PHE	2.9
1	C	8	ARG	2.9
1	B	6	ILE	2.9
1	A	188	MET	2.8
1	B	1034	SER	2.8
1	A	1035	ARG	2.8
1	C	537	SER	2.7
1	A	4	PHE	2.7
1	C	870	GLY	2.7
1	C	357	LEU	2.7
1	C	671	ILE	2.7
1	A	196	PHE	2.7
1	B	424	GLY	2.7
1	B	1036	LYS	2.7
1	B	604	ASN	2.7
1	C	962	GLU	2.7
1	B	134	SER	2.6
1	A	3	ASN	2.6
1	B	1035	ARG	2.6
1	C	361	ASN	2.6
1	A	917	THR	2.6
1	A	390	ILE	2.6
1	B	727	PHE	2.5
1	A	259	ARG	2.5
1	C	1033	PHE	2.5
1	B	655	PHE	2.5
1	C	520	PHE	2.5
1	B	437	GLN	2.5
1	C	496	MET	2.4
1	A	958	LYS	2.4
1	B	535	LEU	2.4
1	B	253	VAL	2.4
1	B	513	PHE	2.4
1	A	714	THR	2.4
1	B	7	ASP	2.3
1	B	635	ALA	2.3
1	C	9	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	869	SER	2.3
1	A	30	LEU	2.3
1	A	427	PRO	2.3
1	A	149	MET	2.3
1	C	257	GLY	2.3
1	B	426	PRO	2.3
1	A	962	GLU	2.3
1	C	541	TYR	2.3
1	B	412	VAL	2.2
1	A	497	LEU	2.2
1	C	426	PRO	2.2
1	B	542	LEU	2.2
1	B	540	ARG	2.2
1	C	360	GLN	2.2
1	A	952	LEU	2.1
1	B	135	SER	2.1
1	A	964	THR	2.1
1	B	992	SER	2.1
1	A	636	ASP	2.1
1	A	322	LYS	2.1
1	B	868	LEU	2.1
1	B	433	LYS	2.1
1	C	6	ILE	2.1
1	B	528	THR	2.1
1	C	252	LYS	2.1
1	C	542	LEU	2.0
1	A	772	TYR	2.0
1	A	968	VAL	2.0
1	B	991	ILE	2.0
1	A	253	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

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, 95th 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(\AA^2)	Q<0.9
2	MIY	A	2001	33/33	0.87	0.25	0.35	134,138,142,142	0
3	RFP	C	2002	59/59	0.91	0.26	0.17	131,136,139,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.