



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:22 PM GMT

PDB ID : 3TOP
Title : Crystall Structure of the C-terminal Subunit of Human Maltase-Glucoamylase
in Complex with Acarbose
Authors : Shen, Y.; Qin, X.H.; Ren, L.M.
Deposited on : 2011-09-06
Resolution : 2.88 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

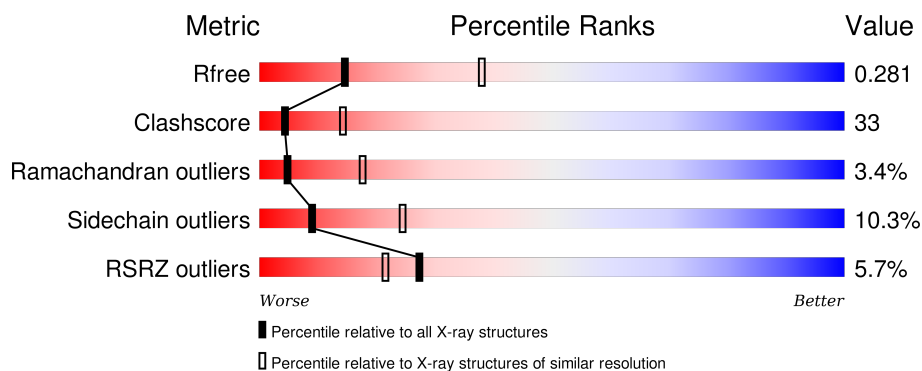
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	908	 4% 47% 42% 8% •
1	B	908	 7% 47% 43% 8% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14388 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 Maltase-glucoamylase, intestinal.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	890	Total	C	N	O	S	0	0	0
			7131	4572	1190	1338	31			
1	B	890	Total	C	N	O	S	0	0	0
			7131	4572	1190	1338	31			

There are 28 discrepancies between the modelled and reference sequences:

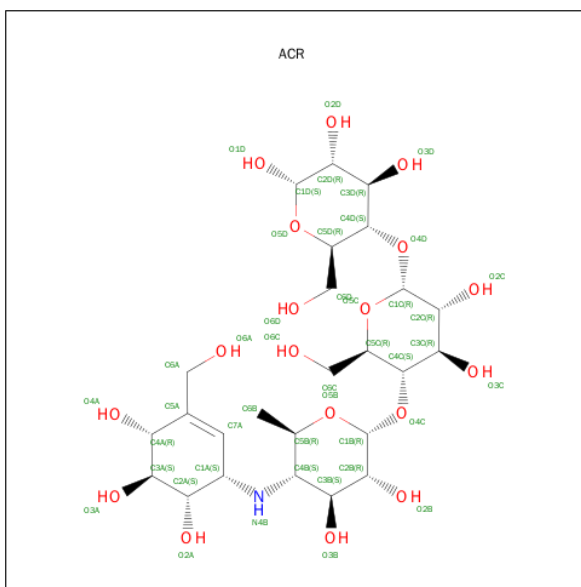
Chain	Residue	Modelled	Actual	Comment	Reference
A	952	TRP	-	EXPRESSION TAG	UNP O43451
A	953	SER	-	EXPRESSION TAG	UNP O43451
A	954	HIS	-	EXPRESSION TAG	UNP O43451
A	955	PRO	-	EXPRESSION TAG	UNP O43451
A	956	GLN	-	EXPRESSION TAG	UNP O43451
A	957	PHE	-	EXPRESSION TAG	UNP O43451
A	958	GLU	-	EXPRESSION TAG	UNP O43451
A	959	LYS	-	EXPRESSION TAG	UNP O43451
A	1854	HIS	-	EXPRESSION TAG	UNP O43451
A	1855	HIS	-	EXPRESSION TAG	UNP O43451
A	1856	HIS	-	EXPRESSION TAG	UNP O43451
A	1857	HIS	-	EXPRESSION TAG	UNP O43451
A	1858	HIS	-	EXPRESSION TAG	UNP O43451
A	1859	HIS	-	EXPRESSION TAG	UNP O43451
B	952	TRP	-	EXPRESSION TAG	UNP O43451
B	953	SER	-	EXPRESSION TAG	UNP O43451
B	954	HIS	-	EXPRESSION TAG	UNP O43451
B	955	PRO	-	EXPRESSION TAG	UNP O43451
B	956	GLN	-	EXPRESSION TAG	UNP O43451
B	957	PHE	-	EXPRESSION TAG	UNP O43451
B	958	GLU	-	EXPRESSION TAG	UNP O43451
B	959	LYS	-	EXPRESSION TAG	UNP O43451
B	1854	HIS	-	EXPRESSION TAG	UNP O43451
B	1855	HIS	-	EXPRESSION TAG	UNP O43451
B	1856	HIS	-	EXPRESSION TAG	UNP O43451

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1857	HIS	-	EXPRESSION TAG	UNP O43451
B	1858	HIS	-	EXPRESSION TAG	UNP O43451
B	1859	HIS	-	EXPRESSION TAG	UNP O43451

- Molecule 2 is SUGAR (ALPHA-ACARBOSE) (three-letter code: ACR) (formula: $C_{25}H_{43}NO_{18}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 44	C 25	N 1	O 18	0	0
2	B	1	Total 44	C 25	N 1	O 18	0	0

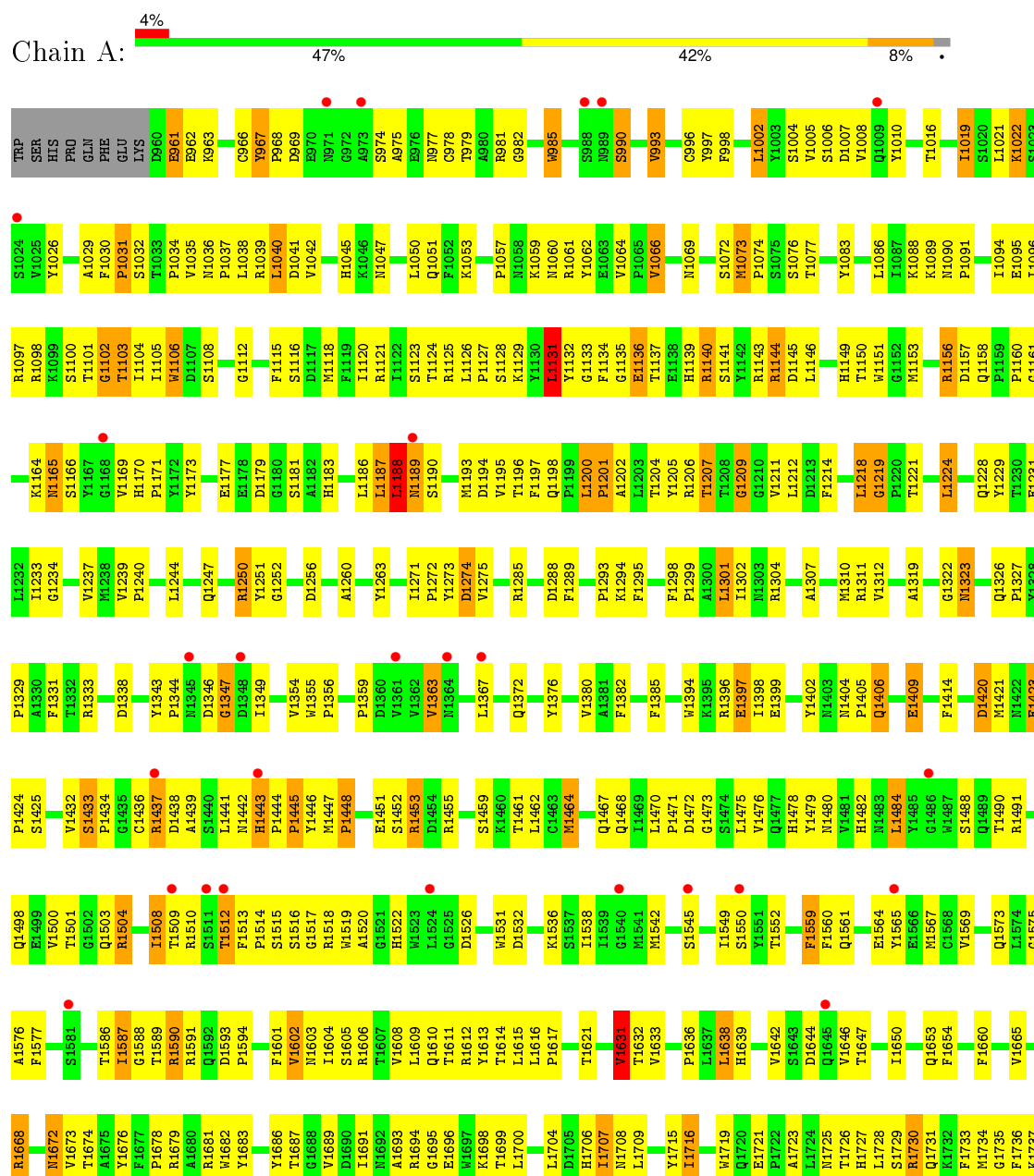
- Molecule 3 is water.

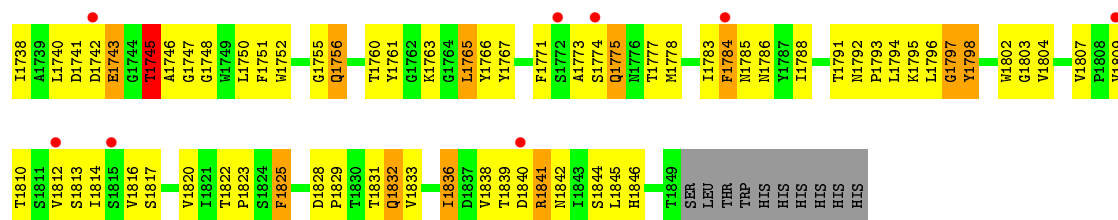
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	30	Total O 30 30	0	0
3	B	8	Total O 8 8	0	0

3 Residue-property plots

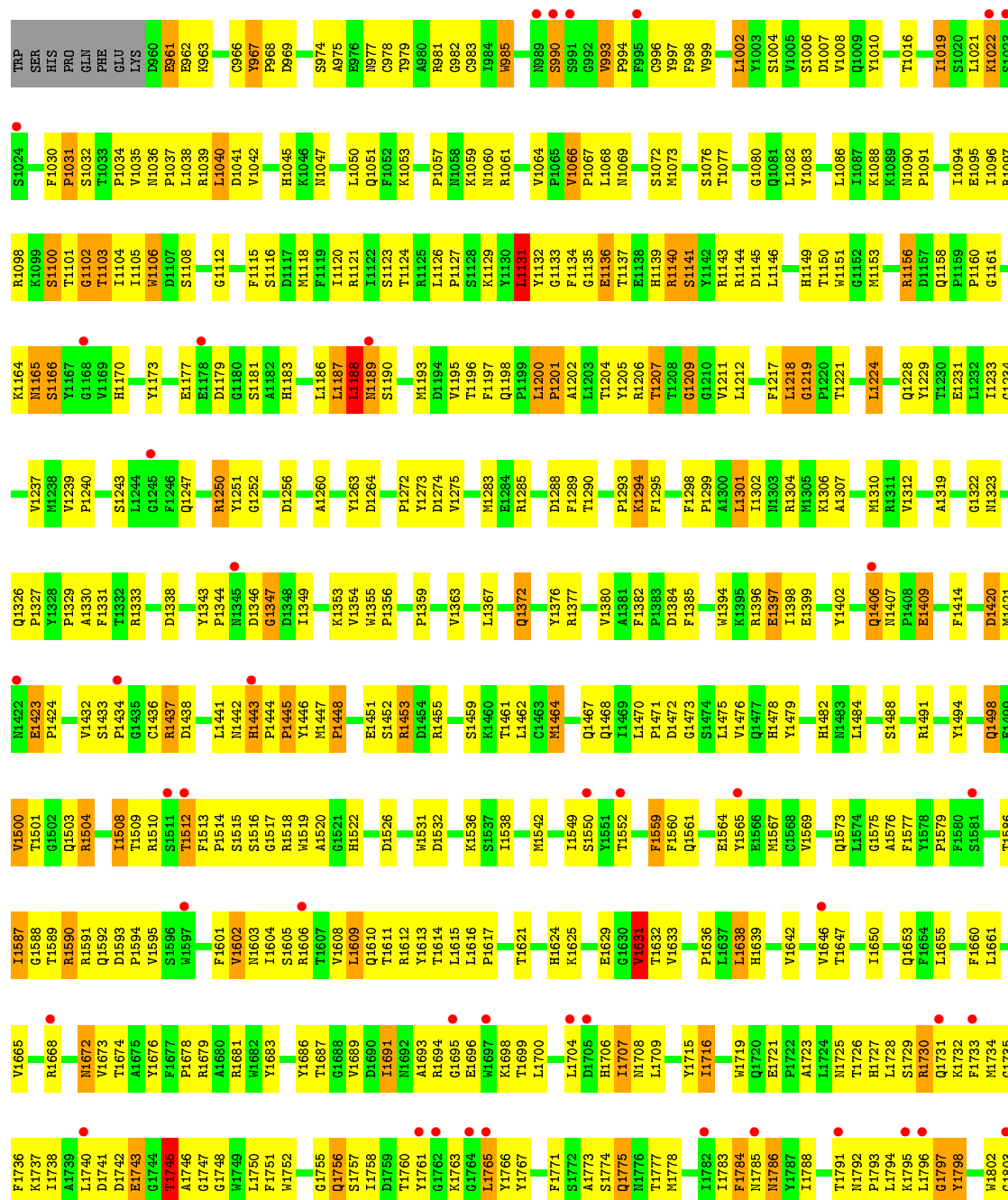
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

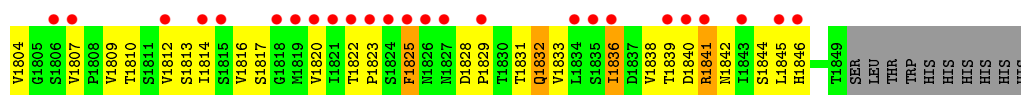
- Molecule 1: Maltase-glucoamylase, intestinal





• Molecule 1: Maltase-glucoamylase, intestinal





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.50 Å 105.50 Å 516.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.45 – 2.88 36.45 – 2.88	Depositor EDS
% Data completeness (in resolution range)	82.3 (36.45-2.88) 87.9 (36.45-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.90 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.218 , 0.284 0.222 , 0.281	Depositor DCC
R_{free} test set	3014 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 59342 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14388	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: ACR

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	0.44	2/7350 (0.0%)	0.63	2/10031 (0.0%)
1	B	0.44	0/7350	0.63	2/10031 (0.0%)
All	All	0.44	2/14700 (0.0%)	0.63	4/20062 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1144	ARG	CB-CG	6.16	1.69	1.52
1	A	1323	ASN	CB-CG	5.42	1.63	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1219	GLY	N-CA-C	-6.06	97.95	113.10
1	A	1131	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	1219	GLY	N-CA-C	-5.73	98.77	113.10
1	B	1131	LEU	CA-CB-CG	5.69	128.38	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	7131	0	6766	463	0
1	B	7131	0	6766	454	0
2	A	44	0	43	10	0
2	B	44	0	43	1	0
3	A	30	0	0	1	0
3	B	8	0	0	1	0
All	All	14388	0	13618	919	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 33.

All (919) 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:B:1734:MET:HE3	1:B:1794:LEU:HD21	1.29	1.10
1:A:1542:MET:HE1	1:A:1636:PRO:CB	1.81	1.10
1:B:967:TYR:CE2	1:B:1030:PHE:HZ	1.72	1.08
1:B:1542:MET:HE1	1:B:1636:PRO:HB3	1.09	1.06
1:B:1542:MET:HE1	1:B:1636:PRO:CB	1.85	1.06
1:A:1765:LEU:HD23	1:A:1765:LEU:H	1.16	1.05
1:A:1734:MET:HE3	1:A:1794:LEU:HD21	1.31	1.05
1:B:981:ARG:NH1	1:B:1030:PHE:HB2	1.71	1.04
1:B:1441:LEU:HD12	1:B:1464:MET:HB2	1.40	1.04
1:B:1765:LEU:HD23	1:B:1765:LEU:H	1.16	1.03
1:A:1542:MET:HE1	1:A:1636:PRO:HB3	1.04	1.02
1:A:967:TYR:CE2	1:A:1030:PHE:HZ	1.78	1.00
1:A:981:ARG:NH1	1:A:1030:PHE:HB2	1.77	1.00
1:A:1047:ASN:HD21	1:A:1077:THR:H	1.08	0.98
1:A:1681:ARG:HH11	1:A:1742:ASP:H	1.07	0.98
1:B:1047:ASN:HD21	1:B:1077:THR:H	1.12	0.96
1:A:1441:LEU:HD12	1:A:1464:MET:HB2	1.46	0.95
1:B:1681:ARG:HH11	1:B:1742:ASP:H	1.07	0.95
1:A:1538:ILE:O	1:A:1542:MET:HG3	1.68	0.92
1:B:1538:ILE:O	1:B:1542:MET:HG3	1.69	0.92
1:A:1030:PHE:CD2	1:A:1031:PRO:HD2	2.05	0.91
1:B:1030:PHE:CD2	1:B:1031:PRO:HD2	2.06	0.91
1:A:1542:MET:CE	1:A:1636:PRO:HB3	1.99	0.90
1:B:1030:PHE:HD2	1:B:1031:PRO:HD2	1.36	0.89
1:B:1441:LEU:CD1	1:B:1464:MET:H	1.87	0.88
1:A:1050:LEU:HD21	1:A:1083:TYR:CE1	2.07	0.88
1:B:1542:MET:CE	1:B:1636:PRO:HB3	2.02	0.88
1:A:1030:PHE:HD2	1:A:1031:PRO:HD2	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:LEU:CD1	1:A:1464:MET:H	1.86	0.87
1:A:1784:PHE:HE2	1:A:1786:ASN:HB2	1.41	0.86
1:A:1636:PRO:HG2	1:A:1639:HIS:CD2	2.10	0.86
1:A:1035:VAL:HG23	1:A:1038:LEU:HD21	1.57	0.86
1:A:1156:ARG:HH11	1:A:1158:GLN:HG2	1.40	0.86
1:B:967:TYR:CE2	1:B:1030:PHE:CZ	2.62	0.86
1:B:1120:ILE:HG21	1:B:1212:LEU:HD21	1.58	0.85
1:B:1035:VAL:HG23	1:B:1038:LEU:HD21	1.57	0.85
1:A:1021:LEU:HB2	1:A:1036:ASN:HD21	1.40	0.85
1:B:1816:VAL:HG22	1:B:1820:VAL:HG22	1.58	0.85
1:B:1256:ASP:HB2	1:B:1295:PHE:HA	1.58	0.85
1:B:1823:PRO:HB3	1:B:1841:ARG:HH21	1.41	0.85
1:A:961:GLU:HB3	1:A:1200:LEU:HB3	1.59	0.85
1:B:1021:LEU:HB2	1:B:1036:ASN:HD21	1.39	0.85
1:B:1526:ASP:HB3	1:B:1560:PHE:CE2	2.12	0.85
1:A:1716:ILE:HG12	1:A:1748:GLY:HA3	1.59	0.85
1:A:1716:ILE:HG22	1:A:1738:ILE:HA	1.59	0.85
1:B:1636:PRO:HG2	1:B:1639:HIS:CD2	2.11	0.84
1:B:1587:ILE:HG23	1:B:1588:GLY:H	1.41	0.84
1:B:1716:ILE:HG12	1:B:1748:GLY:HA3	1.55	0.84
1:B:1156:ARG:HH11	1:B:1158:GLN:HG2	1.42	0.84
1:A:1256:ASP:HB2	1:A:1295:PHE:HA	1.60	0.83
1:B:961:GLU:HB3	1:B:1200:LEU:HB3	1.61	0.83
1:B:1784:PHE:HE2	1:B:1786:ASN:HB2	1.43	0.83
1:B:1716:ILE:HG22	1:B:1738:ILE:HA	1.58	0.82
1:A:1526:ASP:HB3	1:A:1560:PHE:CE2	2.13	0.82
1:A:1681:ARG:HD3	1:A:1741:ASP:HA	1.59	0.82
1:B:1681:ARG:HD3	1:B:1741:ASP:HA	1.60	0.82
1:A:1587:ILE:HG23	1:A:1588:GLY:H	1.44	0.82
1:B:1468:GLN:NE2	1:B:1478:HIS:HD2	1.76	0.82
1:B:1726:THR:O	1:B:1730:ARG:HG2	1.81	0.81
1:A:1816:VAL:HG22	1:A:1820:VAL:HG22	1.63	0.81
1:A:1517:GLY:HA3	1:A:1549:ILE:HG12	1.62	0.81
1:A:1343:TYR:HB3	1:A:1344:PRO:HD2	1.63	0.80
1:A:967:TYR:CE2	1:A:1030:PHE:CZ	2.67	0.80
1:A:1165:ASN:HD21	1:A:1451:GLU:H	1.29	0.80
1:A:1823:PRO:HB3	1:A:1841:ARG:HH21	1.46	0.80
1:B:1517:GLY:HA3	1:B:1549:ILE:HG12	1.64	0.80
1:B:1050:LEU:HD21	1:B:1083:TYR:CE1	2.18	0.79
1:A:1120:ILE:HG21	1:A:1212:LEU:HD21	1.62	0.79
1:A:1468:GLN:NE2	1:A:1478:HIS:HD2	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1165:ASN:HD21	1:B:1451:GLU:H	1.31	0.78
1:B:1098:ARG:NH1	1:B:1181:SER:HB3	1.97	0.78
1:A:1726:THR:O	1:A:1730:ARG:HG2	1.84	0.78
1:B:1617:PRO:O	1:B:1621:THR:HG23	1.84	0.78
1:B:1765:LEU:HD23	1:B:1765:LEU:N	1.99	0.77
1:A:981:ARG:HH11	1:A:981:ARG:HG3	1.47	0.77
1:A:1088:LYS:HE2	1:A:1095:GLU:HB2	1.64	0.77
1:A:1617:PRO:O	1:A:1621:THR:HG23	1.85	0.77
1:B:1468:GLN:HE21	1:B:1478:HIS:HD2	1.31	0.77
1:B:1219:GLY:H	1:B:1228:GLN:HE22	1.30	0.77
1:B:981:ARG:HH12	1:B:1030:PHE:HB2	1.49	0.76
1:A:1665:VAL:HG22	1:A:1673:VAL:HG11	1.67	0.75
1:A:1219:GLY:H	1:A:1228:GLN:HE22	1.30	0.75
1:A:1039:ARG:HB3	1:A:1057:PRO:HG3	1.66	0.75
1:B:1088:LYS:HE2	1:B:1095:GLU:HB2	1.67	0.75
1:B:1765:LEU:H	1:B:1765:LEU:CD2	1.97	0.75
1:A:1165:ASN:ND2	1:A:1451:GLU:H	1.84	0.75
1:A:1765:LEU:HD23	1:A:1765:LEU:N	1.99	0.75
1:B:1343:TYR:HB3	1:B:1344:PRO:HD2	1.66	0.75
1:A:1559:PHE:CE2	1:A:1586:THR:HB	2.22	0.74
1:B:1039:ARG:HB3	1:B:1057:PRO:HG3	1.70	0.74
1:A:1653:GLN:HE22	1:A:1676:TYR:H	1.36	0.74
1:B:1723:ALA:HB1	1:B:1728:LEU:HB2	1.69	0.74
1:A:1665:VAL:HG22	1:A:1673:VAL:CG1	2.17	0.74
1:B:981:ARG:HG3	1:B:981:ARG:HH11	1.52	0.74
1:B:1165:ASN:ND2	1:B:1451:GLU:H	1.86	0.73
1:B:1665:VAL:HG22	1:B:1673:VAL:HG11	1.69	0.73
1:A:1468:GLN:HE21	1:A:1478:HIS:HD2	1.36	0.73
1:A:1030:PHE:CB	1:A:1031:PRO:HD2	2.18	0.73
1:B:1606:ARG:O	1:B:1610:GLN:HG3	1.88	0.73
1:A:1004:SER:OG	1:A:1022:LYS:HG2	1.87	0.73
1:B:1653:GLN:HE22	1:B:1676:TYR:H	1.37	0.72
1:A:1030:PHE:HD2	1:A:1031:PRO:CD	2.01	0.72
1:A:1123:SER:OG	1:A:1204:THR:HG23	1.89	0.72
1:B:1665:VAL:HG22	1:B:1673:VAL:CG1	2.19	0.72
1:A:962:GLU:HG3	1:A:1200:LEU:HD22	1.70	0.72
1:B:1030:PHE:HD2	1:B:1031:PRO:CD	2.02	0.72
1:B:1423:GLU:N	1:B:1424:PRO:HA	2.05	0.72
1:B:1559:PHE:CE2	1:B:1586:THR:HB	2.25	0.71
1:A:1120:ILE:HB	1:A:1207:THR:HG22	1.72	0.71
1:B:1146:LEU:HA	1:B:1197:PHE:HB3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1399:GLU:HA	1:B:1500:VAL:HG21	1.71	0.71
1:B:1614:THR:HG23	1:B:1719:TRP:HE3	1.55	0.71
1:A:1723:ALA:HB1	1:A:1728:LEU:HB2	1.72	0.71
1:A:1721:GLU:OE1	1:A:1733:PHE:HB2	1.90	0.71
1:A:1399:GLU:HA	1:A:1500:VAL:HG21	1.73	0.71
1:A:1647:THR:HA	1:A:1650:ILE:HG22	1.73	0.71
1:A:1437:ARG:HG2	1:A:1437:ARG:O	1.90	0.71
1:B:1467:GLN:NE2	1:B:1475:LEU:HD13	2.06	0.71
1:B:1681:ARG:HH11	1:B:1742:ASP:N	1.85	0.70
1:B:1251:TYR:CD1	1:B:1587:ILE:HB	2.27	0.70
1:B:1004:SER:OG	1:B:1022:LYS:HG2	1.91	0.70
1:A:1251:TYR:CD1	1:A:1587:ILE:HB	2.27	0.70
1:A:1681:ARG:HH11	1:A:1742:ASP:N	1.85	0.70
1:B:1437:ARG:O	1:B:1437:ARG:HG2	1.92	0.70
1:B:1129:LYS:HD2	1:B:1201:PRO:HG3	1.74	0.70
1:B:1120:ILE:HB	1:B:1207:THR:HG22	1.72	0.70
1:B:1035:VAL:CG2	1:B:1038:LEU:HD21	2.21	0.70
1:A:1606:ARG:O	1:A:1610:GLN:HG3	1.91	0.70
1:B:1444:PRO:O	1:B:1446:TYR:N	2.25	0.70
1:A:1098:ARG:NH1	1:A:1181:SER:HB3	2.07	0.69
1:A:1614:THR:HG23	1:A:1719:TRP:HE3	1.57	0.69
1:B:1083:TYR:HD2	1:B:1218:LEU:HD11	1.58	0.69
1:A:1047:ASN:HD21	1:A:1077:THR:N	1.87	0.69
1:B:1647:THR:HA	1:B:1650:ILE:HG22	1.72	0.69
1:A:1804:VAL:HG22	1:A:1832:GLN:O	1.93	0.69
1:A:1803:GLY:H	1:A:1832:GLN:HB2	1.56	0.69
1:B:1803:GLY:H	1:B:1832:GLN:HB2	1.59	0.68
1:A:981:ARG:HH12	1:A:1030:PHE:HB2	1.54	0.68
1:B:1804:VAL:HG22	1:B:1832:GLN:O	1.93	0.68
1:A:1765:LEU:CD2	1:A:1765:LEU:H	1.97	0.68
1:A:1030:PHE:HB3	1:A:1031:PRO:HD2	1.75	0.68
1:A:1035:VAL:CG2	1:A:1038:LEU:HD21	2.22	0.68
1:A:1807:VAL:O	1:A:1807:VAL:HG23	1.94	0.68
1:B:1021:LEU:HB2	1:B:1036:ASN:ND2	2.09	0.67
1:B:962:GLU:HG3	1:B:1200:LEU:HD22	1.76	0.67
1:A:1771:PHE:HB3	1:A:1778:MET:HE2	1.75	0.67
1:B:1030:PHE:CB	1:B:1031:PRO:HD2	2.24	0.67
1:A:1083:TYR:HD2	1:A:1218:LEU:HD11	1.59	0.67
1:B:1587:ILE:HG23	1:B:1588:GLY:N	2.10	0.67
1:A:1587:ILE:HG23	1:A:1588:GLY:N	2.09	0.67
1:A:1423:GLU:N	1:A:1424:PRO:HA	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:GLU:C	1:A:963:LYS:H	1.98	0.67
1:A:1503:GLN:HE22	1:A:1756:GLN:CD	1.97	0.67
1:B:1503:GLN:HE22	1:B:1756:GLN:CD	1.99	0.66
1:A:1129:LYS:HD2	1:A:1201:PRO:HG3	1.76	0.66
1:B:1251:TYR:O	1:B:1587:ILE:HA	1.94	0.66
1:B:1721:GLU:OE1	1:B:1733:PHE:HB2	1.95	0.66
1:B:1120:ILE:CG2	1:B:1212:LEU:HD21	2.25	0.66
1:B:1326:GLN:HB3	1:B:1327:PRO:HD2	1.77	0.66
1:A:1674:THR:HG22	1:A:1699:THR:OG1	1.95	0.66
1:A:1687:THR:OG1	1:A:1689:VAL:HG12	1.95	0.65
1:B:1733:PHE:CD1	1:B:1795:LYS:HB3	2.31	0.65
1:A:1139:HIS:CD2	1:A:1144:ARG:HD2	2.32	0.65
1:A:1131:LEU:HD22	1:A:1173:TYR:CD1	2.32	0.65
1:B:1139:HIS:CG	1:B:1144:ARG:HD2	2.31	0.65
1:A:1437:ARG:O	1:A:1438:ASP:HB2	1.96	0.65
1:B:1302:ILE:HD12	1:B:1312:VAL:HG21	1.77	0.65
1:B:1771:PHE:HB3	1:B:1778:MET:HE2	1.78	0.65
1:B:1437:ARG:O	1:B:1438:ASP:HB2	1.95	0.65
1:A:1146:LEU:HA	1:A:1197:PHE:HB3	1.76	0.65
1:A:1733:PHE:CD1	1:A:1795:LYS:HB3	2.31	0.65
1:A:1139:HIS:CG	1:A:1144:ARG:HD2	2.32	0.65
1:B:1200:LEU:O	1:B:1200:LEU:HG	1.97	0.64
1:A:1135:GLY:HA3	1:A:1170:HIS:H	1.61	0.64
1:B:1047:ASN:HD21	1:B:1077:THR:N	1.89	0.64
1:B:961:GLU:C	1:B:963:LYS:H	2.00	0.64
1:A:1021:LEU:HB2	1:A:1036:ASN:ND2	2.11	0.64
1:B:1687:THR:OG1	1:B:1689:VAL:HG12	1.98	0.64
1:B:1719:TRP:NE1	1:B:1735:GLY:HA3	2.12	0.64
1:A:1467:GLN:NE2	1:A:1475:LEU:HD13	2.13	0.64
1:A:1745:THR:HB	1:A:1773:ALA:O	1.98	0.64
1:B:963:LYS:HE2	1:B:997:TYR:CE2	2.33	0.64
1:A:1120:ILE:CG2	1:A:1212:LEU:HD21	2.28	0.63
1:A:1251:TYR:O	1:A:1587:ILE:HA	1.97	0.63
1:B:1098:ARG:CG	1:B:1100:SER:HB3	2.28	0.63
1:B:1135:GLY:HA3	1:B:1170:HIS:H	1.64	0.63
1:B:1467:GLN:HE22	1:B:1475:LEU:HD13	1.63	0.63
1:A:1289:PHE:CZ	1:A:1397:GLU:HB3	2.34	0.63
1:B:1745:THR:HB	1:B:1773:ALA:O	1.97	0.63
1:A:1433:SER:HB3	1:A:1434:PRO:HD3	1.81	0.62
1:B:1237:VAL:HG22	1:B:1518:ARG:C	2.19	0.62
1:B:1433:SER:HB3	1:B:1434:PRO:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:VAL:HG22	1:A:1518:ARG:C	2.19	0.62
1:A:1513:PHE:CD2	1:A:1514:PRO:HD2	2.34	0.62
1:A:1444:PRO:O	1:A:1446:TYR:N	2.31	0.62
1:B:1532:ASP:O	1:B:1536:LYS:HG2	1.99	0.62
1:B:1123:SER:OG	1:B:1204:THR:HG23	1.99	0.62
1:A:1200:LEU:HG	1:A:1200:LEU:O	1.99	0.62
1:B:1550:SER:HB2	1:B:1633:VAL:HG21	1.82	0.62
1:B:1030:PHE:HB3	1:B:1031:PRO:HD2	1.82	0.62
1:B:1726:THR:O	1:B:1730:ARG:CG	2.48	0.62
1:A:1730:ARG:HH12	1:A:1755:GLY:HA3	1.65	0.62
2:A:1:ACR:O2C	2:A:1:ACR:H6D2	2.00	0.62
1:A:981:ARG:HG3	1:A:981:ARG:NH1	2.15	0.61
1:A:1804:VAL:H	1:A:1832:GLN:HB3	1.63	0.61
1:B:1047:ASN:ND2	1:B:1077:THR:H	1.91	0.61
1:B:1531:TRP:CH2	1:B:1567:MET:HA	2.35	0.61
1:A:1513:PHE:H	1:A:1516:SER:HB2	1.65	0.61
1:B:1298:PHE:N	1:B:1299:PRO:CD	2.63	0.61
1:A:1135:GLY:HA2	1:A:1170:HIS:HB2	1.81	0.61
1:A:963:LYS:HE2	1:A:997:TYR:CE2	2.35	0.61
1:A:961:GLU:HG2	1:A:1200:LEU:N	2.15	0.61
1:B:1694:ARG:H	1:B:1696:GLU:HG3	1.66	0.61
1:B:1614:THR:HG23	1:B:1719:TRP:CE3	2.35	0.61
1:B:1135:GLY:HA2	1:B:1170:HIS:HB2	1.82	0.61
1:A:1326:GLN:HB3	1:A:1327:PRO:HD2	1.81	0.61
1:A:1726:THR:O	1:A:1730:ARG:CG	2.49	0.61
1:A:1298:PHE:N	1:A:1299:PRO:CD	2.64	0.61
1:A:966:CYS:SG	1:A:981:ARG:HD3	2.41	0.60
1:B:966:CYS:SG	1:B:981:ARG:HD3	2.41	0.60
1:A:1022:LYS:HD2	1:A:1022:LYS:O	2.01	0.60
1:B:1804:VAL:H	1:B:1832:GLN:HB3	1.65	0.60
1:B:1139:HIS:CD2	1:B:1144:ARG:HD2	2.37	0.60
1:A:1083:TYR:CD2	1:A:1218:LEU:HD11	2.37	0.60
1:A:1631:VAL:HG13	1:A:1632:THR:N	2.16	0.60
1:A:1105:ILE:HG23	1:A:1183:HIS:CD2	2.36	0.60
2:A:1:ACR:H5C	2:A:1:ACR:O3D	2.02	0.60
1:B:1611:THR:O	1:B:1614:THR:HB	2.02	0.60
1:B:1740:LEU:HA	1:B:1745:THR:O	2.02	0.60
1:B:1285:ARG:NH2	1:B:1359:PRO:HA	2.17	0.60
1:A:1461:THR:OG1	1:A:1462:LEU:N	2.33	0.60
1:B:1040:LEU:HD12	1:B:1041:ASP:N	2.17	0.60
1:A:1512:THR:HG22	1:A:1516:SER:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1719:TRP:NE1	1:A:1735:GLY:HA3	2.16	0.60
1:A:1550:SER:HB2	1:A:1633:VAL:HG21	1.84	0.60
1:B:1382:PHE:CD2	1:B:1462:LEU:HD21	2.37	0.60
1:A:1694:ARG:H	1:A:1696:GLU:HG3	1.67	0.59
1:B:1838:VAL:O	1:B:1838:VAL:HG12	2.00	0.59
1:B:1674:THR:HG22	1:B:1699:THR:OG1	2.00	0.59
1:B:1135:GLY:CA	1:B:1170:HIS:H	2.15	0.59
1:B:966:CYS:HB3	1:B:996:CYS:SG	2.42	0.59
1:B:1513:PHE:CD2	1:B:1514:PRO:HD2	2.37	0.59
1:A:1813:SER:HG	1:A:1825:PHE:HE2	1.50	0.59
1:B:1064:VAL:HG13	1:B:1066:VAL:HG13	1.84	0.59
1:B:961:GLU:HG2	1:B:1200:LEU:N	2.18	0.59
1:B:1101:THR:O	1:B:1103:THR:N	2.36	0.59
1:A:1803:GLY:HA2	1:A:1832:GLN:HG3	1.84	0.59
1:A:1136:GLU:OE1	1:A:1522:HIS:HE1	1.85	0.59
1:A:1740:LEU:HA	1:A:1745:THR:O	2.02	0.59
1:B:1807:VAL:O	1:B:1807:VAL:HG23	2.01	0.59
1:B:1396:ARG:O	1:B:1399:GLU:HB3	2.03	0.59
1:A:1098:ARG:CG	1:A:1100:SER:HB3	2.32	0.59
1:B:1120:ILE:HG21	1:B:1212:LEU:CD2	2.33	0.59
1:B:1512:THR:HG22	1:B:1516:SER:HB3	1.85	0.59
1:B:1136:GLU:OE1	1:B:1522:HIS:HE1	1.85	0.59
1:B:1289:PHE:CZ	1:B:1397:GLU:HB3	2.38	0.59
1:B:1823:PRO:HB3	1:B:1841:ARG:NH2	2.15	0.58
1:A:1207:THR:HG23	1:A:1209:GLY:H	1.68	0.58
1:A:1302:ILE:HD12	1:A:1312:VAL:HG21	1.84	0.58
1:A:1135:GLY:CA	1:A:1170:HIS:H	2.15	0.58
1:B:1686:TYR:CE2	1:B:1706:HIS:HE1	2.22	0.58
1:A:1040:LEU:HD12	1:A:1041:ASP:N	2.17	0.58
1:B:1621:THR:HG22	1:B:1751:PHE:H	1.67	0.58
1:A:1614:THR:HG23	1:A:1719:TRP:CE3	2.37	0.58
1:B:1576:ALA:O	1:B:1612:ARG:HD2	2.03	0.58
1:B:1186:LEU:HD12	1:B:1187:LEU:N	2.18	0.58
1:B:1745:THR:HG21	1:B:1774:SER:O	2.04	0.58
1:B:1083:TYR:CD2	1:B:1218:LEU:HD11	2.36	0.58
2:A:1:ACR:O2C	2:A:1:ACR:H4D	2.03	0.58
1:A:1382:PHE:CD2	1:A:1462:LEU:HD21	2.37	0.58
1:A:1621:THR:HG22	1:A:1751:PHE:H	1.67	0.58
1:B:1040:LEU:HD11	1:B:1042:VAL:HG23	1.86	0.58
1:A:1838:VAL:HG12	1:A:1838:VAL:O	2.03	0.58
1:B:1472:ASP:OD1	1:B:1473:GLY:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1615:LEU:HD11	1:B:1660:PHE:CZ	2.39	0.58
1:B:1104:ILE:O	1:B:1127:PRO:HB3	2.03	0.58
1:A:1260:ALA:HB2	1:A:1301:LEU:HD11	1.86	0.58
1:B:968:PRO:HB3	1:B:1206:ARG:NH1	2.19	0.58
1:A:1798:TYR:CD2	1:A:1798:TYR:N	2.71	0.58
1:A:966:CYS:HB3	1:A:996:CYS:SG	2.44	0.58
1:B:1461:THR:OG1	1:B:1462:LEU:N	2.33	0.58
1:A:1101:THR:O	1:A:1103:THR:N	2.36	0.57
1:B:1470:LEU:HD21	1:B:1476:VAL:HG21	1.86	0.57
1:B:1156:ARG:HD3	1:B:1158:GLN:CG	2.34	0.57
1:B:1784:PHE:CE2	1:B:1786:ASN:HB2	2.33	0.57
1:A:1823:PRO:HB3	1:A:1841:ARG:NH2	2.18	0.57
1:B:1803:GLY:HA2	1:B:1832:GLN:HG3	1.86	0.57
1:B:1813:SER:HG	1:B:1825:PHE:HE2	1.52	0.57
1:A:1784:PHE:C	1:A:1784:PHE:CD2	2.77	0.57
1:B:1367:LEU:HD12	1:B:1376:TYR:OH	2.05	0.57
1:A:1047:ASN:ND2	1:A:1077:THR:H	1.90	0.57
1:B:1098:ARG:HG2	1:B:1100:SER:HB3	1.85	0.57
1:B:1716:ILE:CG1	1:B:1748:GLY:HA3	2.30	0.57
1:B:961:GLU:N	1:B:961:GLU:OE1	2.37	0.57
1:B:1022:LYS:O	1:B:1022:LYS:HD2	2.05	0.57
1:A:1715:TYR:HA	1:A:1747:GLY:O	2.04	0.57
1:A:1784:PHE:CE2	1:A:1786:ASN:HB2	2.31	0.57
1:A:1156:ARG:HD3	1:A:1158:GLN:CG	2.35	0.57
1:A:1298:PHE:CZ	1:A:1302:ILE:HD11	2.40	0.57
1:A:1576:ALA:O	1:A:1612:ARG:HD2	2.05	0.57
1:A:1098:ARG:HG2	1:A:1100:SER:HB3	1.86	0.56
1:A:1532:ASP:O	1:A:1536:LYS:HG2	2.03	0.56
1:B:1715:TYR:HA	1:B:1747:GLY:O	2.04	0.56
1:B:1131:LEU:HD22	1:B:1173:TYR:CD1	2.40	0.56
1:A:1441:LEU:HD13	1:A:1464:MET:H	1.70	0.56
1:A:1531:TRP:CH2	1:A:1567:MET:HA	2.39	0.56
1:B:1035:VAL:CG2	1:B:1115:PHE:CD2	2.89	0.56
1:A:1086:LEU:HD22	1:B:1097:ARG:CZ	2.36	0.56
1:A:1745:THR:HG21	1:A:1774:SER:O	2.05	0.56
1:B:1750:LEU:HD21	1:B:1752:TRP:HD1	1.71	0.56
1:A:968:PRO:HB3	1:A:1206:ARG:NH1	2.21	0.56
1:B:1432:VAL:HG13	1:B:1433:SER:N	2.19	0.56
1:B:1794:LEU:HD22	1:B:1845:LEU:HD23	1.88	0.56
1:B:981:ARG:HG3	1:B:981:ARG:NH1	2.20	0.56
1:A:967:TYR:CD2	1:A:1030:PHE:HZ	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:LEU:HD11	1:A:1042:VAL:HG23	1.88	0.56
1:A:1219:GLY:N	1:A:1228:GLN:HE22	2.02	0.56
1:A:1250:ARG:NH2	1:A:1589:THR:HG23	2.21	0.56
1:A:1464:MET:HG3	1:A:1479:TYR:HA	1.88	0.56
1:A:1022:LYS:CD	1:A:1022:LYS:O	2.54	0.56
1:A:1686:TYR:CE2	1:A:1706:HIS:HE1	2.23	0.56
1:A:1784:PHE:C	1:A:1784:PHE:HD2	2.09	0.55
1:A:961:GLU:HB3	1:A:1200:LEU:CB	2.34	0.55
1:B:1513:PHE:H	1:B:1516:SER:HB2	1.70	0.55
1:B:1399:GLU:HA	1:B:1500:VAL:CG2	2.34	0.55
1:B:1522:HIS:O	1:B:1552:THR:HA	2.06	0.55
1:B:1153:MET:HE3	1:B:1193:MET:CG	2.35	0.55
1:B:1385:PHE:HB2	1:B:1488:SER:OG	2.05	0.55
1:A:1064:VAL:HG13	1:A:1066:VAL:HG13	1.87	0.55
1:B:1784:PHE:CD2	1:B:1784:PHE:C	2.78	0.55
1:A:1059:LYS:HD3	1:A:1060:ASN:H	1.72	0.55
1:B:1333:ARG:NH2	1:B:1396:ARG:HD3	2.21	0.55
1:A:1590:ARG:HD3	1:A:1591:ARG:O	2.07	0.55
1:A:1399:GLU:HA	1:A:1500:VAL:CG2	2.36	0.55
1:B:1406:GLN:HA	1:B:1406:GLN:HE21	1.72	0.55
1:B:961:GLU:HB3	1:B:1200:LEU:CB	2.34	0.55
1:A:981:ARG:HG2	1:A:982:GLY:H	1.72	0.55
1:A:1526:ASP:HB3	1:A:1560:PHE:HE2	1.71	0.55
1:A:1165:ASN:H	1:A:1165:ASN:HD22	1.54	0.55
1:A:1467:GLN:HE22	1:A:1475:LEU:HD13	1.71	0.55
1:B:1590:ARG:HD3	1:B:1591:ARG:O	2.07	0.55
1:A:1794:LEU:HD22	1:A:1845:LEU:HD23	1.89	0.55
1:B:1237:VAL:HG21	1:B:1520:ALA:N	2.22	0.55
1:A:1716:ILE:CG2	1:A:1738:ILE:HG23	2.37	0.55
1:A:1237:VAL:HG21	1:A:1520:ALA:N	2.22	0.55
1:B:1707:ILE:HD13	1:B:1709:LEU:HD21	1.87	0.55
1:A:1333:ARG:NH2	1:A:1396:ARG:HD3	2.22	0.54
1:A:1153:MET:HE3	1:A:1193:MET:CG	2.37	0.54
2:A:1:ACR:C5C	2:A:1:ACR:O3D	2.55	0.54
1:A:1406:GLN:HE21	1:A:1406:GLN:HA	1.71	0.54
1:A:1621:THR:HG21	1:A:1750:LEU:HA	1.89	0.54
1:A:961:GLU:O	1:A:963:LYS:N	2.40	0.54
1:B:1621:THR:HG21	1:B:1750:LEU:HA	1.89	0.54
1:B:1730:ARG:HH12	1:B:1755:GLY:HA3	1.73	0.54
1:A:1707:ILE:HG12	1:A:1708:ASN:N	2.22	0.54
1:B:1784:PHE:C	1:B:1784:PHE:HD2	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:961:GLU:O	1:B:963:LYS:N	2.40	0.54
1:A:1611:THR:O	1:A:1614:THR:HB	2.08	0.54
1:A:1145:ASP:O	1:A:1146:LEU:HB2	2.08	0.54
1:A:1045:HIS:CE1	1:A:1051:GLN:HG2	2.43	0.54
1:A:1030:PHE:CG	1:A:1031:PRO:HD2	2.42	0.54
1:B:1681:ARG:NH1	1:B:1742:ASP:HB2	2.23	0.54
1:A:1559:PHE:CZ	2:A:1:ACR:H6B3	2.43	0.54
1:A:1441:LEU:HD12	1:A:1464:MET:H	1.71	0.54
1:B:1036:ASN:OD1	1:B:1037:PRO:HA	2.07	0.54
1:B:1647:THR:HA	1:B:1650:ILE:CG2	2.38	0.54
1:A:1467:GLN:NE2	1:A:1475:LEU:HB3	2.23	0.54
1:B:1423:GLU:OE2	1:B:1510:ARG:NH2	2.38	0.54
1:B:1273:TYR:HA	1:B:1613:TYR:OH	2.08	0.54
1:A:981:ARG:HB2	1:A:1030:PHE:CE1	2.44	0.53
1:B:1560:PHE:O	1:B:1561:GLN:HB2	2.08	0.53
1:B:1250:ARG:NH2	1:B:1589:THR:HG23	2.23	0.53
1:A:961:GLU:HG2	1:A:1200:LEU:H	1.74	0.53
1:B:1526:ASP:HB3	1:B:1560:PHE:HE2	1.69	0.53
1:A:1120:ILE:HG21	1:A:1212:LEU:CD2	2.36	0.53
1:A:1319:ALA:HB1	1:A:1380:VAL:CG2	2.38	0.53
1:B:1141:SER:HB3	3:B:31:HOH:O	2.09	0.53
1:A:1396:ARG:O	1:A:1399:GLU:HB3	2.08	0.53
1:A:1750:LEU:HD21	1:A:1752:TRP:HD1	1.73	0.53
1:A:1432:VAL:HG13	1:A:1433:SER:N	2.24	0.53
1:B:1187:LEU:HD12	1:B:1205:TYR:CD2	2.43	0.53
1:A:1560:PHE:O	1:A:1561:GLN:HB2	2.07	0.53
1:B:1022:LYS:O	1:B:1022:LYS:CD	2.57	0.53
1:B:1260:ALA:HB2	1:B:1301:LEU:HD11	1.90	0.53
1:B:1741:ASP:C	1:B:1743:GLU:N	2.61	0.53
1:A:961:GLU:OE1	1:A:961:GLU:N	2.39	0.53
1:A:1237:VAL:HG21	1:A:1519:TRP:C	2.29	0.53
1:B:1263:TYR:CE1	1:B:1310:MET:HG3	2.44	0.53
1:B:1646:VAL:HG11	1:B:1676:TYR:CE1	2.43	0.53
1:A:1470:LEU:HD21	1:A:1476:VAL:HG21	1.91	0.53
1:B:1716:ILE:CG2	1:B:1738:ILE:HG23	2.39	0.53
1:B:1814:ILE:CB	1:B:1822:THR:HG22	2.39	0.53
1:A:1035:VAL:CG2	1:A:1115:PHE:CD2	2.92	0.52
1:A:1707:ILE:HD13	1:A:1709:LEU:HD21	1.91	0.52
1:B:967:TYR:CD2	1:B:1030:PHE:HZ	2.21	0.52
1:A:1247:GLN:HG2	1:A:1275:VAL:HB	1.90	0.52
1:B:981:ARG:HG2	1:B:982:GLY:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1423:GLU:N	1:B:1424:PRO:CA	2.72	0.52
1:B:1707:ILE:HG12	1:B:1708:ASN:N	2.23	0.52
1:B:1512:THR:HG21	1:B:1549:ILE:CD1	2.39	0.52
1:B:981:ARG:HB2	1:B:1030:PHE:CE1	2.44	0.52
1:A:1097:ARG:CZ	1:B:1086:LEU:HD22	2.40	0.52
1:B:1177:GLU:O	1:B:1179:ASP:O	2.27	0.52
1:A:1647:THR:HA	1:A:1650:ILE:CG2	2.39	0.52
1:B:1145:ASP:O	1:B:1146:LEU:HB2	2.08	0.52
1:B:1550:SER:HB2	1:B:1633:VAL:CG2	2.38	0.52
1:B:1032:SER:HB3	1:B:1116:SER:HB3	1.92	0.52
1:A:1298:PHE:N	1:A:1299:PRO:HD2	2.25	0.52
1:B:975:ALA:HA	1:B:985:TRP:CG	2.45	0.52
1:A:1472:ASP:OD1	1:A:1473:GLY:N	2.42	0.52
1:A:1322:GLY:HA3	1:A:1331:PHE:CE2	2.45	0.52
1:B:1322:GLY:HA3	1:B:1331:PHE:CE2	2.44	0.52
1:A:1542:MET:CE	1:A:1636:PRO:CB	2.73	0.52
1:B:1219:GLY:N	1:B:1228:GLN:HE22	2.03	0.52
1:A:1615:LEU:HD11	1:A:1660:PHE:CZ	2.46	0.52
1:A:1200:LEU:O	1:A:1201:PRO:C	2.49	0.51
1:B:1040:LEU:HD22	1:B:1094:ILE:HD11	1.92	0.51
1:A:1716:ILE:CG2	1:A:1738:ILE:HG12	2.40	0.51
1:B:1237:VAL:HG21	1:B:1519:TRP:C	2.30	0.51
1:A:981:ARG:HD2	1:A:1030:PHE:CD1	2.46	0.51
1:B:1420:ASP:CG	1:B:1421:MET:N	2.63	0.51
1:B:1441:LEU:HD13	1:B:1464:MET:H	1.69	0.51
1:B:1047:ASN:ND2	1:B:1076:SER:HA	2.25	0.51
1:B:1513:PHE:CG	1:B:1514:PRO:HD2	2.46	0.51
1:B:1298:PHE:CZ	1:B:1302:ILE:HD11	2.46	0.51
1:B:1247:GLN:HG2	1:B:1275:VAL:HB	1.92	0.51
1:B:1105:ILE:HG23	1:B:1183:HIS:CD2	2.45	0.51
1:B:1030:PHE:CG	1:B:1031:PRO:HD2	2.46	0.51
1:B:1464:MET:HG3	1:B:1479:TYR:HA	1.92	0.51
1:B:1165:ASN:HD22	1:B:1165:ASN:H	1.57	0.51
1:A:1423:GLU:OE2	1:A:1510:ARG:NH2	2.36	0.51
1:B:1045:HIS:CE1	1:B:1051:GLN:HG2	2.46	0.51
1:A:1186:LEU:HD12	1:A:1187:LEU:N	2.25	0.51
1:B:1156:ARG:HD3	1:B:1158:GLN:HG2	1.93	0.51
1:A:1420:ASP:CG	1:A:1421:MET:N	2.64	0.51
1:A:1059:LYS:HD3	1:A:1060:ASN:N	2.26	0.51
1:A:1638:LEU:HD12	1:A:1638:LEU:O	2.10	0.51
1:B:1035:VAL:HG21	1:B:1115:PHE:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:ACR:C4D	2:A:1:ACR:O2C	2.59	0.51
1:B:1433:SER:HB3	1:B:1434:PRO:CD	2.40	0.51
1:A:1187:LEU:HD12	1:A:1205:TYR:CD2	2.46	0.51
1:A:1613:TYR:HA	1:A:1616:LEU:HG	1.93	0.51
1:A:1668:ARG:HD2	3:A:12:HOH:O	2.11	0.51
1:A:1034:PRO:HA	1:A:1116:SER:HA	1.92	0.51
1:A:1737:LYS:HD3	1:A:1802:TRP:CH2	2.46	0.51
1:B:1765:LEU:N	1:B:1765:LEU:CD2	2.67	0.51
1:A:1050:LEU:HD21	1:A:1083:TYR:CZ	2.45	0.51
1:A:1513:PHE:CG	1:A:1514:PRO:HD2	2.45	0.51
1:B:1200:LEU:O	1:B:1201:PRO:C	2.49	0.51
1:B:1478:HIS:CE1	1:B:1482:HIS:ND1	2.79	0.51
1:A:1522:HIS:O	1:A:1552:THR:HA	2.11	0.51
1:A:1032:SER:HB3	1:A:1116:SER:HB3	1.92	0.51
1:A:1814:ILE:CB	1:A:1822:THR:HG22	2.40	0.51
1:B:961:GLU:HG2	1:B:1200:LEU:H	1.76	0.50
1:A:1731:GLN:O	1:A:1795:LYS:HE3	2.11	0.50
1:A:1302:ILE:HD12	1:A:1312:VAL:HG11	1.93	0.50
1:A:1150:THR:OG1	1:A:1196:THR:HG23	2.12	0.50
1:B:1613:TYR:HA	1:B:1616:LEU:HG	1.92	0.50
1:A:1177:GLU:O	1:A:1179:ASP:O	2.29	0.50
1:A:1601:PHE:O	1:A:1602:VAL:C	2.50	0.50
1:A:1367:LEU:HD12	1:A:1376:TYR:OH	2.11	0.50
1:B:1761:TYR:HA	1:B:1766:TYR:CD1	2.47	0.50
1:A:1421:MET:HE3	2:A:1:ACR:C7A	2.41	0.50
1:B:1491:ARG:HG3	1:B:1519:TRP:CE3	2.47	0.50
1:B:1441:LEU:CD1	1:B:1464:MET:HB2	2.26	0.50
1:B:1402:TYR:CD2	1:B:1500:VAL:HG13	2.46	0.50
1:B:1683:TYR:CE2	1:B:1740:LEU:O	2.64	0.50
1:A:1550:SER:HB2	1:A:1633:VAL:CG2	2.42	0.50
1:A:1681:ARG:NH1	1:A:1742:ASP:HB2	2.25	0.50
1:B:1272:PRO:HB2	1:B:1613:TYR:CE2	2.47	0.50
1:A:1700:LEU:HD12	1:A:1700:LEU:N	2.27	0.50
1:B:1638:LEU:O	1:B:1638:LEU:HD12	2.11	0.50
1:B:1775:GLN:O	1:B:1777:THR:HG23	2.10	0.50
1:A:1716:ILE:HG22	1:A:1738:ILE:CA	2.38	0.50
1:B:1731:GLN:O	1:B:1795:LYS:HE3	2.11	0.50
1:A:1097:ARG:NH1	1:B:1086:LEU:HD22	2.26	0.50
1:A:1273:TYR:HA	1:A:1613:TYR:OH	2.11	0.50
1:B:1798:TYR:CD2	1:B:1798:TYR:N	2.75	0.50
1:A:1285:ARG:NH2	1:A:1359:PRO:HA	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1229:TYR:CZ	1:B:1233:ILE:HD13	2.47	0.50
1:A:1137:THR:HG21	1:A:1151:TRP:CE3	2.47	0.50
1:A:1040:LEU:HD22	1:A:1094:ILE:HD11	1.94	0.50
1:A:975:ALA:HA	1:A:985:TRP:CG	2.47	0.50
1:B:1468:GLN:HE21	1:B:1478:HIS:CD2	2.21	0.50
1:B:1513:PHE:O	1:B:1516:SER:HB2	2.12	0.50
1:A:1559:PHE:CD2	1:A:1586:THR:HB	2.47	0.50
1:B:1783:ILE:HD12	1:B:1783:ILE:H	1.76	0.50
1:A:1765:LEU:CD2	1:A:1765:LEU:N	2.67	0.49
1:A:1478:HIS:CE1	1:A:1482:HIS:ND1	2.80	0.49
1:A:1433:SER:HB3	1:A:1434:PRO:CD	2.42	0.49
1:A:1189:ASN:HD22	1:A:1190:SER:N	2.10	0.49
1:B:1775:GLN:C	1:B:1777:THR:H	2.15	0.49
1:A:1402:TYR:CD2	1:A:1500:VAL:HG13	2.47	0.49
1:B:1467:GLN:NE2	1:B:1475:LEU:HB3	2.27	0.49
1:A:990:SER:O	1:A:993:VAL:HG22	2.12	0.49
1:A:1455:ARG:HB2	1:A:1459:SER:HB2	1.94	0.49
1:B:1376:TYR:CD2	1:B:1376:TYR:N	2.79	0.49
1:A:1106:TRP:CZ3	1:A:1108:SER:HB3	2.47	0.49
1:A:1621:THR:CG2	1:A:1751:PHE:H	2.25	0.49
1:A:1447:MET:O	1:A:1453:ARG:HD3	2.13	0.49
1:A:1831:THR:O	1:A:1833:VAL:N	2.45	0.49
1:A:1221:THR:OG1	1:A:1224:LEU:HD23	2.12	0.49
1:B:1207:THR:HG23	1:B:1209:GLY:H	1.76	0.49
1:A:1587:ILE:CG2	1:A:1588:GLY:H	2.22	0.49
1:B:1455:ARG:HB2	1:B:1459:SER:HB2	1.93	0.49
1:A:961:GLU:C	1:A:963:LYS:N	2.64	0.49
1:B:1621:THR:CG2	1:B:1751:PHE:H	2.26	0.49
1:A:1145:ASP:HB3	1:A:1149:HIS:HD2	1.77	0.49
1:B:1189:ASN:HD22	1:B:1190:SER:H	1.60	0.49
1:A:1104:ILE:O	1:A:1127:PRO:HB3	2.11	0.49
1:A:1250:ARG:HG3	1:A:1251:TYR:N	2.25	0.49
1:A:1161:GLY:HA3	1:A:1164:LYS:HD2	1.95	0.49
1:B:990:SER:O	1:B:993:VAL:HG22	2.13	0.49
1:B:1161:GLY:HA3	1:B:1164:LYS:HD2	1.95	0.49
1:A:1086:LEU:HD22	1:B:1097:ARG:NH1	2.27	0.49
1:B:1828:ASP:OD1	1:B:1829:PRO:HD2	2.13	0.49
1:A:1038:LEU:HD11	1:A:1115:PHE:HB3	1.95	0.49
1:A:1761:TYR:HA	1:A:1766:TYR:CD1	2.47	0.49
1:A:1035:VAL:HG21	1:A:1115:PHE:CD2	2.47	0.48
1:A:1036:ASN:OD1	1:A:1037:PRO:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1716:ILE:CG2	1:B:1738:ILE:HG12	2.44	0.48
1:B:1603:ASN:HA	1:B:1606:ARG:HD3	1.95	0.48
1:B:1237:VAL:HG22	1:B:1518:ARG:O	2.12	0.48
1:A:1716:ILE:CG1	1:A:1748:GLY:HA3	2.35	0.48
1:A:1603:ASN:HA	1:A:1606:ARG:HD3	1.95	0.48
1:A:1132:TYR:CE1	1:A:1143:ARG:HB2	2.47	0.48
1:B:961:GLU:C	1:B:963:LYS:N	2.66	0.48
1:B:1187:LEU:O	1:B:1189:ASN:N	2.42	0.48
1:A:1394:TRP:O	1:A:1398:ILE:HG12	2.12	0.48
1:A:1784:PHE:HD2	1:A:1785:ASN:N	2.11	0.48
1:A:1156:ARG:HD3	1:A:1158:GLN:HG2	1.95	0.48
1:B:1716:ILE:HG22	1:B:1738:ILE:CA	2.38	0.48
1:A:1513:PHE:O	1:A:1516:SER:HB2	2.14	0.48
1:B:1189:ASN:HD22	1:B:1190:SER:N	2.11	0.48
1:A:1260:ALA:HB2	1:A:1301:LEU:CD1	2.43	0.48
1:A:1691:ILE:O	1:A:1698:LYS:NZ	2.46	0.48
1:B:1319:ALA:HB1	1:B:1380:VAL:CG2	2.44	0.48
1:B:1038:LEU:HD11	1:B:1115:PHE:HB3	1.95	0.48
1:A:1512:THR:HG21	1:A:1549:ILE:CD1	2.44	0.48
1:A:1145:ASP:HB3	1:A:1149:HIS:CD2	2.48	0.48
1:A:1189:ASN:HD22	1:A:1190:SER:H	1.59	0.48
1:B:1059:LYS:HD3	1:B:1060:ASN:H	1.79	0.48
1:A:1775:GLN:C	1:A:1777:THR:H	2.17	0.48
1:B:981:ARG:HD2	1:B:1030:PHE:CD1	2.48	0.48
1:A:1784:PHE:CD2	1:A:1785:ASN:N	2.82	0.48
1:A:1274:ASP:OD1	1:A:1726:THR:HG23	2.14	0.48
1:A:1606:ARG:HH11	1:A:1606:ARG:CB	2.27	0.48
1:A:1237:VAL:HG22	1:A:1518:ARG:O	2.14	0.48
1:A:1061:ARG:HD3	1:A:1211:VAL:HG12	1.96	0.48
1:A:1683:TYR:CE2	1:A:1740:LEU:O	2.66	0.48
1:A:1229:TYR:CZ	1:A:1233:ILE:HD13	2.49	0.48
1:A:1019:ILE:HB	1:A:1038:LEU:HB2	1.96	0.48
1:B:1252:GLY:CA	1:B:1587:ILE:HD12	2.44	0.48
1:B:1509:THR:O	1:B:1522:HIS:HD2	1.96	0.48
1:B:1542:MET:HE1	1:B:1636:PRO:CA	2.43	0.48
1:B:1470:LEU:HB3	1:B:1471:PRO:CD	2.44	0.48
1:B:1831:THR:O	1:B:1833:VAL:N	2.47	0.48
1:A:1083:TYR:CD1	1:A:1083:TYR:C	2.87	0.47
1:B:1145:ASP:HB3	1:B:1149:HIS:HD2	1.79	0.47
1:A:1442:ASN:C	1:A:1444:PRO:CD	2.82	0.47
1:A:1446:TYR:O	1:A:1448:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1631:VAL:HG13	1:B:1632:THR:N	2.27	0.47
1:B:1137:THR:HG21	1:B:1151:TRP:CE3	2.49	0.47
1:A:1443:HIS:O	1:A:1444:PRO:C	2.52	0.47
1:B:1034:PRO:HA	1:B:1116:SER:HA	1.95	0.47
1:B:1737:LYS:HD3	1:B:1802:TRP:CH2	2.48	0.47
1:B:1053:LYS:HA	1:B:1212:LEU:O	2.15	0.47
1:B:1478:HIS:HE1	1:B:1482:HIS:ND1	2.13	0.47
1:A:1423:GLU:N	1:A:1424:PRO:CA	2.76	0.47
1:A:1565:TYR:O	1:A:1569:VAL:HG23	2.14	0.47
1:A:1542:MET:HE1	1:A:1636:PRO:CA	2.43	0.47
1:A:1047:ASN:ND2	1:A:1076:SER:HA	2.29	0.47
1:A:1134:PHE:CE1	1:A:1195:VAL:HG11	2.48	0.47
1:B:1798:TYR:HE2	1:B:1839:THR:CG2	2.27	0.47
1:B:1030:PHE:CD2	1:B:1031:PRO:CD	2.86	0.47
1:B:1446:TYR:O	1:B:1448:PRO:HD3	2.15	0.47
1:B:1504:ARG:HB3	1:B:1756:GLN:O	2.14	0.47
1:B:1302:ILE:HD12	1:B:1312:VAL:HG11	1.96	0.47
1:A:1683:TYR:HE2	1:A:1740:LEU:O	1.97	0.47
1:B:1683:TYR:HE2	1:B:1740:LEU:O	1.96	0.47
1:A:961:GLU:O	1:A:962:GLU:HB2	2.14	0.47
1:B:1129:LYS:CD	1:B:1201:PRO:HG3	2.44	0.47
1:A:1646:VAL:HG11	1:A:1676:TYR:CE1	2.49	0.47
1:B:1153:MET:HE3	1:B:1193:MET:HG3	1.96	0.47
1:B:1508:ILE:N	1:B:1508:ILE:CD1	2.78	0.47
1:A:1036:ASN:HA	1:A:1037:PRO:HA	1.59	0.47
1:A:1500:VAL:HG12	1:A:1501:THR:HG23	1.97	0.47
1:B:1498:GLN:OE1	1:B:1504:ARG:HA	2.15	0.47
1:B:1700:LEU:N	1:B:1700:LEU:HD12	2.29	0.47
1:B:1704:LEU:O	1:B:1704:LEU:HD12	2.15	0.47
1:A:1704:LEU:HD12	1:A:1704:LEU:O	2.15	0.47
1:B:1156:ARG:HG2	1:B:1158:GLN:HB2	1.96	0.47
1:A:1187:LEU:O	1:A:1189:ASN:N	2.44	0.47
1:B:1394:TRP:O	1:B:1398:ILE:HG12	2.15	0.47
1:B:1823:PRO:CB	1:B:1841:ARG:HH21	2.21	0.47
1:B:1298:PHE:N	1:B:1299:PRO:HD2	2.29	0.47
1:A:1263:TYR:CE1	1:A:1310:MET:HG3	2.49	0.47
1:B:1083:TYR:CD1	1:B:1083:TYR:C	2.88	0.47
1:A:1329:PRO:O	1:A:1333:ARG:HG3	2.15	0.47
1:B:1059:LYS:HD3	1:B:1060:ASN:N	2.29	0.47
1:B:1559:PHE:CD2	1:B:1586:THR:HB	2.50	0.46
1:B:1745:THR:O	1:B:1746:ALA:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1798:TYR:HE2	1:A:1839:THR:CG2	2.28	0.46
1:B:1260:ALA:HB2	1:B:1301:LEU:CD1	2.45	0.46
1:B:1134:PHE:CE1	1:B:1195:VAL:HG11	2.50	0.46
1:B:1788:ILE:HG22	1:B:1846:HIS:CD2	2.50	0.46
1:B:1784:PHE:HD2	1:B:1785:ASN:N	2.14	0.46
1:B:1136:GLU:HG2	1:B:1166:SER:HB3	1.97	0.46
1:B:1470:LEU:HB3	1:B:1471:PRO:HD2	1.97	0.46
1:A:1716:ILE:HG22	1:A:1738:ILE:HG12	1.96	0.46
1:B:1145:ASP:HB3	1:B:1149:HIS:CD2	2.50	0.46
1:A:1614:THR:CG2	1:A:1719:TRP:HB2	2.45	0.46
1:A:1442:ASN:C	1:A:1444:PRO:HD3	2.35	0.46
1:B:1798:TYR:HE2	1:B:1839:THR:HG23	1.81	0.46
1:B:1691:ILE:O	1:B:1698:LYS:NZ	2.49	0.46
1:A:1694:ARG:NH2	1:A:1743:GLU:HB2	2.30	0.46
1:B:1077:THR:HG23	1:B:1080:GLY:H	1.80	0.46
1:B:1681:ARG:NH1	1:B:1742:ASP:H	1.92	0.46
1:B:1784:PHE:CD2	1:B:1785:ASN:N	2.83	0.46
1:A:1104:ILE:O	1:A:1104:ILE:HG13	2.15	0.46
1:A:1741:ASP:C	1:A:1743:GLU:N	2.64	0.46
1:A:1694:ARG:HH22	1:A:1743:GLU:HB2	1.80	0.46
1:A:1053:LYS:HA	1:A:1212:LEU:O	2.14	0.46
1:B:1733:PHE:HB3	1:B:1797:GLY:HA3	1.98	0.46
1:A:1064:VAL:CG1	1:A:1066:VAL:HG13	2.45	0.46
1:A:1153:MET:HE3	1:A:1193:MET:HG3	1.98	0.46
1:A:1575:GLY:C	1:A:1577:PHE:H	2.19	0.46
1:B:1468:GLN:NE2	1:B:1478:HIS:CD2	2.68	0.46
1:A:1165:ASN:ND2	1:A:1165:ASN:H	2.14	0.46
1:B:1746:ALA:HB3	1:B:1773:ALA:HB3	1.97	0.46
1:B:1573:GLN:HA	1:B:1608:VAL:HG21	1.97	0.46
1:A:1733:PHE:HB3	1:A:1797:GLY:HA3	1.98	0.46
1:A:1746:ALA:HB3	1:A:1773:ALA:HB3	1.97	0.46
1:B:1136:GLU:OE1	1:B:1522:HIS:CE1	2.68	0.46
1:B:1791:THR:O	1:B:1793:PRO:HD3	2.15	0.46
1:A:1783:ILE:H	1:A:1783:ILE:HD12	1.81	0.46
1:B:1106:TRP:CZ3	1:B:1108:SER:HB3	2.50	0.46
1:A:1118:MET:HB2	1:A:1445:PRO:HG2	1.98	0.46
1:A:1346:ASP:O	1:A:1347:GLY:O	2.33	0.46
1:A:1156:ARG:HG2	1:A:1158:GLN:HB2	1.97	0.46
1:B:1443:HIS:O	1:B:1444:PRO:C	2.51	0.46
1:A:1090:ASN:HA	1:A:1091:PRO:HA	1.88	0.46
1:B:1283:MET:HA	1:B:1290:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1587:ILE:CG2	1:A:1588:GLY:N	2.79	0.45
1:B:1614:THR:CG2	1:B:1719:TRP:HB2	2.46	0.45
1:A:1272:PRO:HB2	1:A:1613:TYR:CE2	2.51	0.45
1:B:1638:LEU:C	1:B:1638:LEU:HD12	2.36	0.45
1:B:1229:TYR:CE1	1:B:1233:ILE:HD13	2.51	0.45
1:B:1609:LEU:HA	1:B:1609:LEU:HD13	1.81	0.45
1:A:1002:LEU:HD23	1:A:1002:LEU:N	2.31	0.45
1:B:1513:PHE:O	1:B:1514:PRO:C	2.54	0.45
1:B:1165:ASN:ND2	1:B:1165:ASN:H	2.15	0.45
1:B:1132:TYR:CE1	1:B:1143:ARG:HB2	2.50	0.45
1:B:1002:LEU:N	1:B:1002:LEU:HD23	2.31	0.45
1:A:1240:PRO:HA	1:A:1504:ARG:HH11	1.80	0.45
1:B:1512:THR:HG22	1:B:1516:SER:CB	2.47	0.45
1:B:1145:ASP:O	1:B:1146:LEU:CB	2.64	0.45
1:A:1229:TYR:CE1	1:A:1233:ILE:HD13	2.52	0.45
1:B:974:SER:OG	1:B:977:ASN:HB2	2.16	0.45
1:B:1221:THR:OG1	1:B:1224:LEU:HD23	2.17	0.45
1:A:979:THR:O	1:A:981:ARG:O	2.35	0.45
1:A:1129:LYS:CD	1:A:1201:PRO:HG3	2.45	0.45
1:B:961:GLU:O	1:B:962:GLU:HB2	2.16	0.45
1:A:1513:PHE:CE2	1:A:1514:PRO:HD2	2.51	0.45
1:B:1218:LEU:C	1:B:1219:GLY:O	2.49	0.45
1:B:1606:ARG:HH11	1:B:1606:ARG:CB	2.29	0.45
1:A:1333:ARG:NH2	1:A:1396:ARG:CD	2.80	0.45
1:B:1442:ASN:C	1:B:1444:PRO:CD	2.85	0.45
1:A:1508:ILE:CD1	1:A:1508:ILE:N	2.79	0.45
1:B:1624:HIS:CD2	1:B:1751:PHE:CE2	3.05	0.45
1:B:1333:ARG:NH2	1:B:1396:ARG:CD	2.79	0.45
1:A:1136:GLU:OE1	1:A:1522:HIS:CE1	2.69	0.45
1:B:1716:ILE:HG22	1:B:1738:ILE:HG12	1.99	0.45
1:A:1513:PHE:CG	1:A:1514:PRO:CD	3.00	0.45
1:B:1443:HIS:O	1:B:1445:PRO:N	2.50	0.45
1:A:1509:THR:O	1:A:1522:HIS:HD2	2.00	0.45
1:A:1157:ASP:HB2	1:A:1425:SER:HB2	1.99	0.45
1:A:1542:MET:HE2	1:A:1542:MET:HB3	1.36	0.45
1:B:1672:ASN:HD22	1:B:1673:VAL:N	2.15	0.45
1:A:1807:VAL:O	1:A:1807:VAL:CG2	2.64	0.45
1:A:1512:THR:HG22	1:A:1516:SER:CB	2.46	0.45
1:A:1145:ASP:O	1:A:1146:LEU:CB	2.65	0.45
1:A:1045:HIS:CE1	1:A:1051:GLN:HE21	2.35	0.45
1:A:1788:ILE:HG22	1:A:1846:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1414:PHE:C	1:A:1414:PHE:CD1	2.90	0.45
1:B:1264:ASP:OD2	1:B:1304:ARG:NH2	2.49	0.45
1:B:1118:MET:HB2	1:B:1445:PRO:HG2	1.99	0.45
1:A:1828:ASP:OD1	1:A:1829:PRO:HD2	2.17	0.45
1:B:1694:ARG:NH2	1:B:1743:GLU:HB2	2.32	0.44
1:B:1131:LEU:HD13	1:B:1132:TYR:N	2.32	0.44
1:B:1306:LYS:HA	1:B:1310:MET:O	2.18	0.44
1:A:1289:PHE:CE1	1:A:1397:GLU:HB3	2.53	0.44
1:B:1601:PHE:O	1:B:1602:VAL:C	2.55	0.44
1:B:1751:PHE:HA	1:B:1767:TYR:O	2.16	0.44
1:B:1022:LYS:O	1:B:1022:LYS:CG	2.66	0.44
1:B:1040:LEU:HD11	1:B:1042:VAL:CG2	2.47	0.44
1:B:1188:LEU:HA	1:B:1188:LEU:HD23	1.81	0.44
1:B:1693:ALA:HB1	1:B:1696:GLU:HB2	2.00	0.44
1:A:1745:THR:O	1:A:1746:ALA:HB2	2.17	0.44
1:B:1355:TRP:N	1:B:1356:PRO:CD	2.80	0.44
1:A:1593:ASP:HB2	1:A:1594:PRO:HD2	1.99	0.44
1:A:1459:SER:O	1:A:1461:THR:HG22	2.16	0.44
1:A:998:PHE:CZ	1:A:1112:GLY:HA2	2.52	0.44
1:B:1090:ASN:HA	1:B:1091:PRO:HA	1.91	0.44
1:A:1355:TRP:HE1	1:A:1421:MET:CE	2.30	0.44
1:A:1026:TYR:O	1:A:1029:ALA:HB3	2.18	0.44
1:B:1293:PRO:C	1:B:1295:PHE:H	2.21	0.44
1:B:1587:ILE:CG2	1:B:1588:GLY:H	2.21	0.44
1:B:1102:GLY:O	1:B:1103:THR:C	2.55	0.44
1:A:1751:PHE:HA	1:A:1767:TYR:O	2.17	0.44
1:A:1022:LYS:O	1:A:1022:LYS:CG	2.65	0.44
1:B:1240:PRO:HA	1:B:1504:ARG:HH11	1.81	0.44
1:A:1491:ARG:HG3	1:A:1519:TRP:CE3	2.52	0.44
1:B:1452:SER:HB3	1:B:1455:ARG:HG2	1.99	0.44
1:B:1686:TYR:CE2	1:B:1706:HIS:CE1	3.05	0.44
1:B:998:PHE:CZ	1:B:1112:GLY:HA2	2.53	0.44
1:B:962:GLU:CG	1:B:1200:LEU:HD22	2.47	0.44
1:B:1050:LEU:HD12	1:B:1096:ILE:HD13	1.99	0.44
1:A:1803:GLY:HA2	1:A:1832:GLN:CG	2.47	0.44
1:B:1353:LYS:HE2	1:B:1377:ARG:O	2.17	0.44
1:B:1565:TYR:O	1:B:1569:VAL:HG23	2.17	0.44
1:A:1200:LEU:O	1:A:1202:ALA:N	2.51	0.44
1:B:1250:ARG:HG3	1:B:1251:TYR:N	2.30	0.44
1:A:1319:ALA:HB1	1:A:1380:VAL:HG21	2.00	0.44
1:A:1169:VAL:HG12	1:A:1171:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1086:LEU:HD13	1:B:1097:ARG:NH2	2.33	0.43
1:A:1355:TRP:HB2	1:A:1356:PRO:HD3	1.99	0.43
1:B:1066:VAL:HA	1:B:1067:PRO:HD3	1.84	0.43
1:B:1355:TRP:HE1	1:B:1421:MET:CE	2.31	0.43
1:B:1069:ASN:OD1	1:B:1231:GLU:O	2.35	0.43
1:A:1604:ILE:HG22	1:A:1605:SER:N	2.33	0.43
1:A:1803:GLY:HA2	1:A:1832:GLN:CB	2.48	0.43
1:A:1798:TYR:HE2	1:A:1839:THR:HG23	1.83	0.43
1:A:1005:VAL:HG11	1:A:1089:LYS:HA	2.00	0.43
1:B:1272:PRO:O	1:B:1273:TYR:HB3	2.18	0.43
1:A:1484:LEU:HA	1:A:1484:LEU:HD12	1.77	0.43
1:B:1504:ARG:HH21	1:B:1760:THR:HG23	1.84	0.43
1:B:978:CYS:CB	1:B:985:TRP:HD1	2.32	0.43
1:B:1725:ASN:OD1	1:B:1727:HIS:HB3	2.19	0.43
1:A:1681:ARG:HD3	1:A:1741:ASP:CA	2.40	0.43
1:B:1200:LEU:O	1:B:1202:ALA:N	2.52	0.43
1:A:1252:GLY:CA	1:A:1587:ILE:HD12	2.48	0.43
1:A:1517:GLY:CA	1:A:1549:ILE:HG12	2.40	0.43
1:B:1050:LEU:HA	1:B:1050:LEU:HD23	1.70	0.43
1:B:1097:ARG:HG3	1:B:1102:GLY:O	2.18	0.43
1:B:1217:PHE:HB3	1:B:1228:GLN:HE21	1.84	0.43
1:B:1650:ILE:CD1	1:B:1653:GLN:HE21	2.31	0.43
1:B:1329:PRO:CB	1:B:1333:ARG:HD2	2.49	0.43
1:A:978:CYS:CB	1:A:985:TRP:HD1	2.30	0.43
1:B:1508:ILE:N	1:B:1508:ILE:HD12	2.33	0.43
1:A:1355:TRP:N	1:A:1356:PRO:CD	2.81	0.43
1:B:1288:ASP:HB3	1:B:1289:PHE:CD2	2.54	0.43
1:A:1293:PRO:C	1:A:1295:PHE:H	2.20	0.43
1:B:1500:VAL:HG12	1:B:1501:THR:HG23	2.00	0.43
1:B:1289:PHE:CE1	1:B:1397:GLU:HB3	2.52	0.43
1:B:1686:TYR:CD2	1:B:1706:HIS:HE1	2.36	0.43
1:B:1346:ASP:O	1:B:1347:GLY:O	2.37	0.43
1:B:1384:ASP:C	1:B:1384:ASP:OD1	2.56	0.43
1:B:1061:ARG:HG2	1:B:1061:ARG:NH1	2.33	0.43
1:A:1131:LEU:HD13	1:A:1132:TYR:N	2.34	0.43
1:B:1575:GLY:C	1:B:1577:PHE:H	2.21	0.43
1:B:1592:GLN:HB3	1:B:1592:GLN:HE21	1.68	0.43
1:B:1414:PHE:CD1	1:B:1414:PHE:C	2.92	0.43
1:A:1693:ALA:HB1	1:A:1696:GLU:HB2	2.01	0.43
1:B:1503:GLN:C	1:B:1758:ILE:HD11	2.40	0.43
1:B:1757:SER:HB2	1:B:1760:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1234:GLY:HA3	1:B:1518:ARG:HD3	2.00	0.43
1:A:1069:ASN:OD1	1:A:1231:GLU:O	2.36	0.43
1:A:1730:ARG:HE	1:A:1752:TRP:HZ3	1.67	0.43
1:B:1240:PRO:HG2	1:B:1243:SER:HB3	2.01	0.43
1:A:1838:VAL:C	1:A:1840:ASP:H	2.23	0.43
1:A:1251:TYR:CE1	1:A:1587:ILE:HB	2.53	0.42
1:B:1442:ASN:C	1:B:1444:PRO:HD3	2.39	0.42
1:A:1311:ARG:NH2	1:A:1756:GLN:OE1	2.52	0.42
1:B:1838:VAL:C	1:B:1840:ASP:H	2.21	0.42
1:B:1196:THR:OG1	1:B:1206:ARG:NH2	2.52	0.42
1:A:1836:ILE:HG22	1:A:1836:ILE:O	2.18	0.42
1:B:1407:ASN:HB3	1:B:1409:GLU:OE2	2.19	0.42
1:B:1679:ARG:HD3	1:B:1695:GLY:HA3	2.01	0.42
1:A:981:ARG:HG2	1:A:982:GLY:N	2.33	0.42
1:A:1218:LEU:C	1:A:1219:GLY:O	2.53	0.42
1:A:1650:ILE:CD1	1:A:1653:GLN:HE21	2.32	0.42
1:B:1045:HIS:CE1	1:B:1051:GLN:HE21	2.36	0.42
1:A:974:SER:OG	1:A:977:ASN:HB2	2.19	0.42
1:A:1791:THR:O	1:A:1793:PRO:HD3	2.19	0.42
1:A:1304:ARG:O	1:A:1307:ALA:HB3	2.18	0.42
1:A:1125:ARG:HA	1:A:1202:ALA:HB2	2.01	0.42
1:A:1478:HIS:HE1	1:A:1482:HIS:ND1	2.15	0.42
1:A:1329:PRO:CB	1:A:1333:ARG:HD2	2.49	0.42
1:A:1573:GLN:HA	1:A:1608:VAL:HG21	2.00	0.42
1:B:1083:TYR:HA	1:B:1097:ARG:O	2.19	0.42
1:A:1196:THR:OG1	1:A:1206:ARG:NH2	2.53	0.42
1:A:1221:THR:OG1	1:A:1224:LEU:HB2	2.20	0.42
1:B:1304:ARG:O	1:B:1307:ALA:HB3	2.20	0.42
1:A:1006:SER:OG	1:A:1007:ASP:N	2.52	0.42
1:A:1490:THR:HG22	1:A:1519:TRP:HB2	2.02	0.42
1:B:1531:TRP:CZ2	1:B:1567:MET:HA	2.54	0.42
1:A:1775:GLN:O	1:A:1777:THR:HG23	2.19	0.42
1:A:1404:ASN:OD1	1:A:1405:PRO:HD2	2.19	0.42
1:B:981:ARG:O	1:B:983:CYS:N	2.51	0.42
1:B:1036:ASN:HA	1:B:1037:PRO:HA	1.58	0.42
1:B:1803:GLY:HA2	1:B:1832:GLN:CG	2.49	0.42
1:A:1443:HIS:O	1:A:1445:PRO:N	2.52	0.42
1:A:1102:GLY:O	1:A:1103:THR:C	2.58	0.42
1:A:1272:PRO:O	1:A:1273:TYR:HB3	2.20	0.42
1:B:1050:LEU:HD21	1:B:1083:TYR:CZ	2.54	0.42
1:A:1234:GLY:HA3	1:A:1518:ARG:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1064:VAL:CG1	1:B:1066:VAL:HG13	2.49	0.42
1:B:1604:ILE:HG22	1:B:1605:SER:N	2.34	0.42
1:B:1694:ARG:HH22	1:B:1743:GLU:HB2	1.83	0.42
1:B:1019:ILE:HB	1:B:1038:LEU:HB2	2.01	0.42
1:A:1730:ARG:HH21	1:A:1752:TRP:HZ3	1.67	0.42
1:A:1672:ASN:HD22	1:A:1673:VAL:N	2.18	0.42
1:B:1436:CYS:O	1:B:1437:ARG:CD	2.67	0.42
1:A:1409:GLU:HG3	1:A:1409:GLU:H	1.48	0.42
1:B:1809:VAL:O	1:B:1809:VAL:HG13	2.20	0.42
1:B:1836:ILE:O	1:B:1836:ILE:HG22	2.20	0.42
1:B:981:ARG:HG2	1:B:982:GLY:N	2.35	0.42
1:B:1459:SER:O	1:B:1461:THR:HG22	2.20	0.42
1:A:1097:ARG:HG3	1:A:1102:GLY:O	2.19	0.42
1:A:1224:LEU:HD13	1:A:1224:LEU:HA	1.87	0.42
1:B:1542:MET:HB3	1:B:1542:MET:HE2	1.43	0.42
1:B:1513:PHE:CG	1:B:1514:PRO:CD	3.03	0.42
1:A:1730:ARG:NE	1:A:1752:TRP:CZ3	2.87	0.42
1:A:1421:MET:HE3	2:A:1:ACR:H7A	2.01	0.42
1:B:1139:HIS:HD2	1:B:1151:TRP:CH2	2.38	0.42
1:A:1188:LEU:HA	1:A:1188:LEU:HD23	1.88	0.42
1:A:981:ARG:HB2	1:A:1030:PHE:HE1	1.84	0.41
1:A:1513:PHE:O	1:A:1514:PRO:C	2.54	0.41
1:A:1298:PHE:HB3	1:A:1299:PRO:HD3	2.01	0.41
1:A:1686:TYR:CE2	1:A:1706:HIS:CE1	3.07	0.41
1:A:1679:ARG:HD3	1:A:1695:GLY:HA3	2.01	0.41
1:B:1251:TYR:CE1	1:B:1587:ILE:HB	2.54	0.41
1:B:1730:ARG:HH21	1:B:1752:TRP:HZ3	1.68	0.41
1:B:1750:LEU:HD21	1:B:1752:TRP:CD1	2.53	0.41
1:A:1244:LEU:HA	1:A:1244:LEU:HD23	1.79	0.41
2:B:1:ACR:H6B2	2:B:1:ACR:H7A	2.02	0.41
1:B:1593:ASP:HB2	1:B:1594:PRO:HD2	2.02	0.41
1:A:1030:PHE:CD2	1:A:1031:PRO:CD	2.84	0.41
1:A:1438:ASP:OD1	1:A:1439:ALA:N	2.52	0.41
1:B:1355:TRP:HB2	1:B:1356:PRO:HD3	2.01	0.41
1:A:1508:ILE:HD12	1:A:1508:ILE:N	2.34	0.41
1:A:1355:TRP:N	1:A:1356:PRO:HD2	2.36	0.41
1:B:1298:PHE:HB3	1:B:1299:PRO:HD3	2.02	0.41
1:A:1452:SER:HB3	1:A:1455:ARG:HG2	2.02	0.41
1:A:1825:PHE:CD1	1:A:1825:PHE:C	2.94	0.41
1:B:1355:TRP:N	1:B:1356:PRO:HD2	2.35	0.41
1:B:1061:ARG:HD3	1:B:1211:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:SER:O	1:A:1201:PRO:HB3	2.21	0.41
1:B:1730:ARG:NE	1:B:1752:TRP:CZ3	2.88	0.41
1:A:1088:LYS:HD3	1:A:1095:GLU:OE1	2.21	0.41
2:A:1:ACR:H4B	2:A:1:ACR:H7A	1.86	0.41
1:A:1498:GLN:OE1	1:A:1504:ARG:HA	2.20	0.41
1:A:1504:ARG:HH21	1:A:1760:THR:HG23	1.86	0.41
1:B:1372:GLN:HE22	1:B:1377:ARG:HH22	1.68	0.41
1:B:1008:VAL:HG12	1:B:1010:TYR:CE1	2.55	0.41
1:B:981:ARG:HB2	1:B:1030:PHE:HE1	1.84	0.41
1:B:979:THR:O	1:B:981:ARG:O	2.38	0.41
1:A:1421:MET:HE2	1:A:1421:MET:HB2	1.93	0.41
1:A:1131:LEU:CD2	1:A:1173:TYR:CD1	3.03	0.41
1:B:1736:PHE:CZ	1:B:1771:PHE:CE1	3.09	0.41
1:A:1288:ASP:HB3	1:A:1289:PHE:CD2	2.56	0.41
1:A:1288:ASP:O	1:A:1289:PHE:HB2	2.20	0.41
1:A:1682:TRP:HB2	1:A:1691:ILE:HG22	2.03	0.41
1:A:1239:VAL:HB	1:A:1240:PRO:HD2	2.02	0.41
1:B:1447:MET:O	1:B:1453:ARG:NH1	2.43	0.41
1:A:1385:PHE:HB2	1:A:1488:SER:OG	2.20	0.41
1:A:1062:TYR:CE2	1:A:1480:ASN:HB3	2.55	0.41
1:A:1468:GLN:NE2	1:A:1478:HIS:CD2	2.71	0.41
1:A:1644:ASP:OD2	1:A:1676:TYR:OH	2.36	0.41
1:A:1614:THR:HG23	1:A:1719:TRP:HB2	2.03	0.41
1:B:1140:ARG:HG3	1:B:1144:ARG:NH2	2.35	0.41
1:A:1660:PHE:HZ	1:A:1709:LEU:HD13	1.85	0.41
1:A:962:GLU:CG	1:A:1200:LEU:HD22	2.44	0.41
1:B:1513:PHE:CE2	1:B:1514:PRO:HD2	2.55	0.41
1:A:1559:PHE:HZ	2:A:1:ACR:H6B3	1.86	0.41
1:A:1153:MET:HE1	1:A:1195:VAL:HG13	2.03	0.41
1:A:1736:PHE:HD2	1:A:1736:PHE:HA	1.80	0.41
1:B:1098:ARG:HH12	1:B:1181:SER:HB3	1.79	0.41
1:A:1726:THR:HA	1:A:1729:SER:HB3	2.03	0.41
1:A:1436:CYS:O	1:A:1437:ARG:CD	2.69	0.41
1:B:1491:ARG:O	1:B:1494:TYR:HB3	2.21	0.41
1:B:1552:THR:O	1:B:1579:PRO:HD2	2.21	0.41
1:A:1470:LEU:HB3	1:A:1471:PRO:HD2	2.03	0.41
1:A:1187:LEU:HG	1:A:1214:PHE:CZ	2.56	0.41
1:A:1575:GLY:C	1:A:1577:PHE:N	2.74	0.41
1:B:1447:MET:O	1:B:1453:ARG:HD3	2.21	0.41
1:B:1006:SER:OG	1:B:1007:ASP:N	2.53	0.41
1:B:1726:THR:HA	1:B:1729:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1803:GLY:HA2	1:B:1832:GLN:CB	2.51	0.41
1:B:1150:THR:OG1	1:B:1196:THR:HG23	2.21	0.41
1:A:1050:LEU:CD2	1:A:1083:TYR:CZ	3.05	0.40
1:B:1813:SER:OG	1:B:1825:PHE:HE2	2.04	0.40
1:A:1725:ASN:OD1	1:A:1727:HIS:HB3	2.21	0.40
1:A:1140:ARG:HG3	1:A:1140:ARG:H	1.53	0.40
1:B:1655:LEU:HD23	1:B:1661:LEU:HA	2.03	0.40
1:A:998:PHE:CE1	1:A:1112:GLY:HA2	2.55	0.40
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.86	0.40
1:A:1538:ILE:HG23	1:A:1654:PHE:CD2	2.55	0.40
1:B:994:PRO:HB2	1:B:996:CYS:O	2.22	0.40
1:A:981:ARG:HB2	1:A:1030:PHE:CD1	2.57	0.40
1:A:1441:LEU:CD1	1:A:1464:MET:HB2	2.33	0.40
1:B:1443:HIS:N	1:B:1444:PRO:CD	2.85	0.40
1:B:1239:VAL:HB	1:B:1240:PRO:HD2	2.03	0.40
1:A:1040:LEU:HD12	1:A:1040:LEU:C	2.42	0.40
1:A:1073:MET:HB3	1:A:1074:PRO:HD2	2.03	0.40
1:A:1050:LEU:HD12	1:A:1096:ILE:HD13	2.03	0.40
1:B:1329:PRO:O	1:B:1330:ALA:C	2.60	0.40
1:B:1432:VAL:CG1	1:B:1433:SER:N	2.83	0.40
1:A:1363:VAL:HG23	1:A:1376:TYR:CE1	2.56	0.40
1:B:1625:LYS:O	1:B:1629:GLU:HB2	2.22	0.40
1:A:1008:VAL:HG12	1:A:1010:TYR:CE1	2.57	0.40
1:A:1228:GLN:HB2	1:A:1228:GLN:HE21	1.61	0.40
1:A:1139:HIS:HD2	1:A:1151:TRP:CH2	2.40	0.40
1:A:1194:ASP:OD1	1:A:1206:ARG:HB2	2.21	0.40
1:A:1271:ILE:HA	1:A:1272:PRO:HD3	1.92	0.40
1:B:1844:SER:OG	1:B:1846:HIS:HD2	2.04	0.40
1:A:1844:SER:OG	1:A:1846:HIS:HD2	2.05	0.40
1:A:1809:VAL:HG13	1:A:1809:VAL:O	2.22	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	888/908 (98%)	750 (84%)	109 (12%)	29 (3%)	5	18
1	B	888/908 (98%)	745 (84%)	111 (12%)	32 (4%)	4	16
All	All	1776/1816 (98%)	1495 (84%)	220 (12%)	61 (3%)	5	17

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	PRO
1	A	1136	GLU
1	A	1347	GLY
1	A	1443	HIS
1	A	1445	PRO
1	A	1631	VAL
1	A	1668	ARG
1	B	1031	PRO
1	B	1136	GLU
1	B	1347	GLY
1	B	1443	HIS
1	B	1445	PRO
1	B	1631	VAL
1	A	1102	GLY
1	A	1559	PHE
1	A	1832	GLN
1	B	1102	GLY
1	B	1188	LEU
1	B	1559	PHE
1	B	1668	ARG
1	B	1832	GLN
1	A	1188	LEU
1	A	1354	VAL
1	B	1338	ASP
1	B	1354	VAL
1	B	1587	ILE
1	B	1732	LYS
1	A	1338	ASP
1	A	1587	ILE
1	A	1745	THR
1	A	1756	GLN
1	B	1515	SER
1	B	1745	THR

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Mol	Chain	Res	Type
1	A	1515	SER
1	A	1678	PRO
1	B	961	GLU
1	B	1209	GLY
1	B	1294	LYS
1	B	1678	PRO
1	B	1786	ASN
1	B	1797	GLY
1	A	961	GLU
1	A	1160	PRO
1	A	1209	GLY
1	A	1797	GLY
1	B	1160	PRO
1	B	1756	GLN
1	A	1448	PRO
1	A	1602	VAL
1	B	1201	PRO
1	A	1201	PRO
1	B	1133	GLY
1	B	1448	PRO
1	A	1433	SER
1	A	1836	ILE
1	A	1133	GLY
1	A	1812	VAL
1	B	1812	VAL
1	B	1836	ILE
1	B	1595	VAL
1	B	1602	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	773/800 (97%)	696 (90%)	77 (10%)	9	26
1	B	773/800 (97%)	690 (89%)	83 (11%)	8	22
All	All	1546/1600 (97%)	1386 (90%)	160 (10%)	9	24

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	967	TYR
1	A	969	ASP
1	A	985	TRP
1	A	990	SER
1	A	993	VAL
1	A	1002	LEU
1	A	1016	THR
1	A	1019	ILE
1	A	1022	LYS
1	A	1040	LEU
1	A	1066	VAL
1	A	1072	SER
1	A	1073	MET
1	A	1103	THR
1	A	1106	TRP
1	A	1121	ARG
1	A	1124	THR
1	A	1126	LEU
1	A	1131	LEU
1	A	1140	ARG
1	A	1141	SER
1	A	1156	ARG
1	A	1165	ASN
1	A	1166	SER
1	A	1187	LEU
1	A	1188	LEU
1	A	1189	ASN
1	A	1198	GLN
1	A	1200	LEU
1	A	1207	THR
1	A	1218	LEU
1	A	1224	LEU
1	A	1250	ARG
1	A	1274	ASP
1	A	1294	LYS
1	A	1301	LEU
1	A	1323	ASN
1	A	1349	ILE
1	A	1363	VAL
1	A	1372	GLN
1	A	1397	GLU
1	A	1406	GLN

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Mol	Chain	Res	Type
1	A	1409	GLU
1	A	1420	ASP
1	A	1423	GLU
1	A	1437	ARG
1	A	1453	ARG
1	A	1464	MET
1	A	1484	LEU
1	A	1504	ARG
1	A	1508	ILE
1	A	1512	THR
1	A	1545	SER
1	A	1564	GLU
1	A	1590	ARG
1	A	1609	LEU
1	A	1631	VAL
1	A	1638	LEU
1	A	1642	VAL
1	A	1672	ASN
1	A	1707	ILE
1	A	1716	ILE
1	A	1730	ARG
1	A	1743	GLU
1	A	1745	THR
1	A	1763	LYS
1	A	1765	LEU
1	A	1775	GLN
1	A	1784	PHE
1	A	1792	ASN
1	A	1796	LEU
1	A	1798	TYR
1	A	1810	THR
1	A	1817	SER
1	A	1825	PHE
1	A	1841	ARG
1	A	1842	ASN
1	B	967	TYR
1	B	969	ASP
1	B	985	TRP
1	B	990	SER
1	B	993	VAL
1	B	999	VAL
1	B	1002	LEU

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Mol	Chain	Res	Type
1	B	1016	THR
1	B	1019	ILE
1	B	1022	LYS
1	B	1040	LEU
1	B	1066	VAL
1	B	1068	LEU
1	B	1072	SER
1	B	1073	MET
1	B	1082	LEU
1	B	1100	SER
1	B	1103	THR
1	B	1106	TRP
1	B	1121	ARG
1	B	1124	THR
1	B	1126	LEU
1	B	1131	LEU
1	B	1140	ARG
1	B	1141	SER
1	B	1156	ARG
1	B	1165	ASN
1	B	1166	SER
1	B	1187	LEU
1	B	1188	LEU
1	B	1189	ASN
1	B	1198	GLN
1	B	1200	LEU
1	B	1207	THR
1	B	1218	LEU
1	B	1224	LEU
1	B	1250	ARG
1	B	1274	ASP
1	B	1294	LYS
1	B	1301	LEU
1	B	1323	ASN
1	B	1349	ILE
1	B	1363	VAL
1	B	1372	GLN
1	B	1397	GLU
1	B	1406	GLN
1	B	1409	GLU
1	B	1420	ASP
1	B	1423	GLU

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Mol	Chain	Res	Type
1	B	1437	ARG
1	B	1453	ARG
1	B	1464	MET
1	B	1484	LEU
1	B	1498	GLN
1	B	1500	VAL
1	B	1504	ARG
1	B	1508	ILE
1	B	1512	THR
1	B	1564	GLU
1	B	1590	ARG
1	B	1609	LEU
1	B	1631	VAL
1	B	1638	LEU
1	B	1642	VAL
1	B	1672	ASN
1	B	1691	ILE
1	B	1707	ILE
1	B	1716	ILE
1	B	1730	ARG
1	B	1743	GLU
1	B	1745	THR
1	B	1763	LYS
1	B	1765	LEU
1	B	1775	GLN
1	B	1784	PHE
1	B	1792	ASN
1	B	1796	LEU
1	B	1798	TYR
1	B	1810	THR
1	B	1817	SER
1	B	1825	PHE
1	B	1841	ARG
1	B	1842	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1045	HIS
1	A	1047	ASN
1	A	1058	ASN
1	A	1165	ASN

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Mol	Chain	Res	Type
1	A	1183	HIS
1	A	1198	GLN
1	A	1228	GLN
1	A	1372	GLN
1	A	1406	GLN
1	A	1467	GLN
1	A	1468	GLN
1	A	1478	HIS
1	A	1503	GLN
1	A	1522	HIS
1	A	1592	GLN
1	A	1610	GLN
1	A	1653	GLN
1	A	1672	ASN
1	A	1706	HIS
1	A	1792	ASN
1	A	1846	HIS
1	B	1045	HIS
1	B	1047	ASN
1	B	1058	ASN
1	B	1165	ASN
1	B	1183	HIS
1	B	1198	GLN
1	B	1228	GLN
1	B	1372	GLN
1	B	1406	GLN
1	B	1467	GLN
1	B	1468	GLN
1	B	1478	HIS
1	B	1503	GLN
1	B	1522	HIS
1	B	1592	GLN
1	B	1610	GLN
1	B	1653	GLN
1	B	1672	ASN
1	B	1706	HIS
1	B	1792	ASN
1	B	1846	HIS

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	ACR	A	1	-	46,47,47	1.63	12 (26%)	58,70,70	2.06	11 (18%)
2	ACR	B	1	-	46,47,47	1.55	9 (19%)	58,70,70	1.72	5 (8%)

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	ACR	A	1	-	-	0/18/98/98	0/4/4/4
2	ACR	B	1	-	-	0/18/98/98	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ACR	C3A-C4A	-4.31	1.47	1.53
2	A	1	ACR	O5C-C5C	-2.63	1.37	1.44
2	A	1	ACR	O2B-C2B	-2.54	1.36	1.43
2	A	1	ACR	C3B-C4B	-2.51	1.48	1.53
2	A	1	ACR	O3C-C3C	-2.39	1.37	1.43
2	A	1	ACR	O4A-C4A	-2.36	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ACR	C3A-C4A	-2.36	1.50	1.53
2	B	1	ACR	O3C-C3C	-2.31	1.37	1.43
2	B	1	ACR	C3B-C4B	-2.30	1.48	1.53
2	B	1	ACR	O5C-C5C	-2.28	1.38	1.44
2	B	1	ACR	O2A-C2A	-2.23	1.37	1.43
2	A	1	ACR	O3A-C3A	-2.13	1.37	1.43
2	A	1	ACR	C3D-C4D	-2.10	1.46	1.52
2	B	1	ACR	O3B-C3B	2.04	1.47	1.43
2	B	1	ACR	C6D-C5D	2.08	1.59	1.51
2	A	1	ACR	O3B-C3B	2.09	1.48	1.43
2	A	1	ACR	C6D-C5D	2.18	1.59	1.51
2	A	1	ACR	O2D-C2D	2.94	1.50	1.43
2	A	1	ACR	C7A-C5A	3.18	1.37	1.32
2	B	1	ACR	O2D-C2D	3.48	1.51	1.43
2	B	1	ACR	C7A-C5A	3.78	1.38	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ACR	C1C-O4D-C4D	-4.49	106.26	118.01
2	B	1	ACR	C1B-O4C-C4C	-2.27	112.08	118.01
2	A	1	ACR	C3D-C4D-C5D	-2.21	105.85	110.84
2	A	1	ACR	C3B-C4B-C5B	-2.12	106.14	110.35
2	B	1	ACR	O6C-C6C-C5C	-2.12	104.34	111.33
2	A	1	ACR	O4A-C4A-C3A	-2.03	105.81	109.95
2	A	1	ACR	O4D-C1C-C2C	2.14	113.32	108.10
2	A	1	ACR	O3B-C3B-C4B	2.38	114.51	109.66
2	A	1	ACR	C2C-C3C-C4C	2.62	115.34	109.60
2	A	1	ACR	O5D-C1D-C2D	2.89	114.41	109.80
2	A	1	ACR	C1C-C2C-C3C	3.91	117.69	109.97
2	A	1	ACR	O5C-C1C-C2C	4.18	118.84	110.28
2	B	1	ACR	O5D-C5D-C4D	6.12	122.68	109.75
2	A	1	ACR	O5D-C5D-C4D	6.57	123.62	109.75
2	B	1	ACR	C1D-C2D-C3D	7.68	121.85	110.43
2	A	1	ACR	C1D-C2D-C3D	9.01	123.83	110.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	ACR	10	0
2	B	1	ACR	1	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	890/908 (98%)	0.21	34 (3%) 44 38	45, 81, 135, 207	0
1	B	890/908 (98%)	0.32	68 (7%) 17 11	50, 85, 141, 211	0
All	All	1780/1816 (98%)	0.26	102 (5%) 27 21	45, 83, 137, 211	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1443	HIS	7.4
1	B	1733	PHE	5.9
1	B	1821	ILE	5.8
1	B	991	SER	5.8
1	B	1815	SER	5.3
1	B	1823	PRO	5.3
1	B	1819	MET	5.0
1	B	1843	ILE	4.7
1	B	1840	ASP	4.6
1	B	1764	GLY	4.6
1	B	1806	SER	4.6
1	B	1820	VAL	4.5
1	B	1825	PHE	4.4
1	B	1836	ILE	4.4
1	A	989	ASN	4.1
1	B	1839	THR	4.1
1	B	1829	PRO	4.1
1	B	1765	LEU	3.8
1	B	1807	VAL	3.7
1	B	1434	PRO	3.7
1	A	1812	VAL	3.7
1	A	1809	VAL	3.6
1	A	1345	ASN	3.5
1	A	1645	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	1512	THR	3.3
1	B	1824	SER	3.1
1	A	1511	SER	3.0
1	B	1668	ARG	3.0
1	A	1009	GLN	2.9
1	A	1437	ARG	2.9
1	A	1565	TYR	2.9
1	A	1512	THR	2.9
1	A	1367	LEU	2.9
1	B	1697	TRP	2.9
1	B	1796	LEU	2.9
1	B	1822	THR	2.9
1	B	1826	ASN	2.8
1	B	1814	ILE	2.8
1	B	1845	LEU	2.8
1	A	1509	THR	2.7
1	B	1795	LYS	2.7
1	A	1364	ASN	2.7
1	B	1841	ARG	2.7
1	A	1550	SER	2.7
1	A	1545	SER	2.6
1	B	1406	GLN	2.6
1	A	1815	SER	2.6
1	A	1486	GLY	2.6
1	A	1774	SER	2.6
1	B	1695	GLY	2.6
1	B	1024	SER	2.6
1	B	1178	GLU	2.6
1	A	1840	ASP	2.5
1	B	989	ASN	2.5
1	B	1740	LEU	2.5
1	B	1834	LEU	2.5
1	A	988	SER	2.5
1	B	1168	GLY	2.5
1	A	1189	ASN	2.5
1	B	1761	TYR	2.5
1	A	971	ASN	2.4
1	B	1023	SER	2.4
1	A	1168	GLY	2.4
1	B	1704	LEU	2.4
1	B	1606	ARG	2.4
1	B	1791	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1812	VAL	2.4
1	B	1511	SER	2.4
1	B	1565	TYR	2.4
1	B	1827	ASN	2.4
1	B	1189	ASN	2.3
1	B	1245	GLY	2.3
1	B	1762	GLY	2.3
1	B	995	PHE	2.3
1	B	1550	SER	2.3
1	B	1835	SER	2.3
1	A	1524	LEU	2.3
1	A	973	ALA	2.3
1	B	1022	LYS	2.3
1	B	1581	SER	2.3
1	B	1597	TRP	2.3
1	A	1581	SER	2.2
1	B	1846	HIS	2.2
1	B	1785	ASN	2.2
1	A	1361	VAL	2.2
1	B	1782	ILE	2.2
1	B	990	SER	2.2
1	A	1742	ASP	2.2
1	A	1348	ASP	2.2
1	B	1705	ASP	2.1
1	A	1443	HIS	2.1
1	B	1646	VAL	2.1
1	A	1540	GLY	2.1
1	B	1731	GLN	2.1
1	B	1552	THR	2.1
1	A	1772	SER	2.1
1	B	1803	GLY	2.0
1	B	1422	ASN	2.0
1	A	1024	SER	2.0
1	A	1784	PHE	2.0
1	B	1345	ASN	2.0
1	B	1818	GLY	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	ACR	B	1	44/44	0.91	0.18	-0.42	54,88,110,121	0
2	ACR	A	1	44/44	0.92	0.18	-0.78	53,84,115,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.