



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:38 AM UTC

PDB ID : 5I6I / pdb_00005i6i
Title : Crystal structure of a dBCCP-variant of Chaetomium thermophilum acetyl-CoA carboxylase
Authors : Hunkeler, M.; Stuttfeld, E.; Hagmann, A.; Imseng, S.; Maier, T.
Deposited on : 2016-02-16
Resolution : 8.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

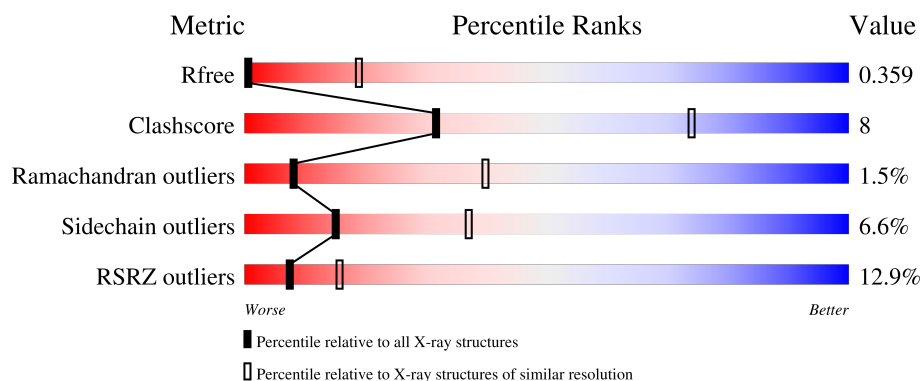
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.40 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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	2211	 9% 47% 14% • 37%
1	B	2211	 8% 48% 14% • 37%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 22445 atoms, of which 0 are hydrogens and 0 are deuteriums.

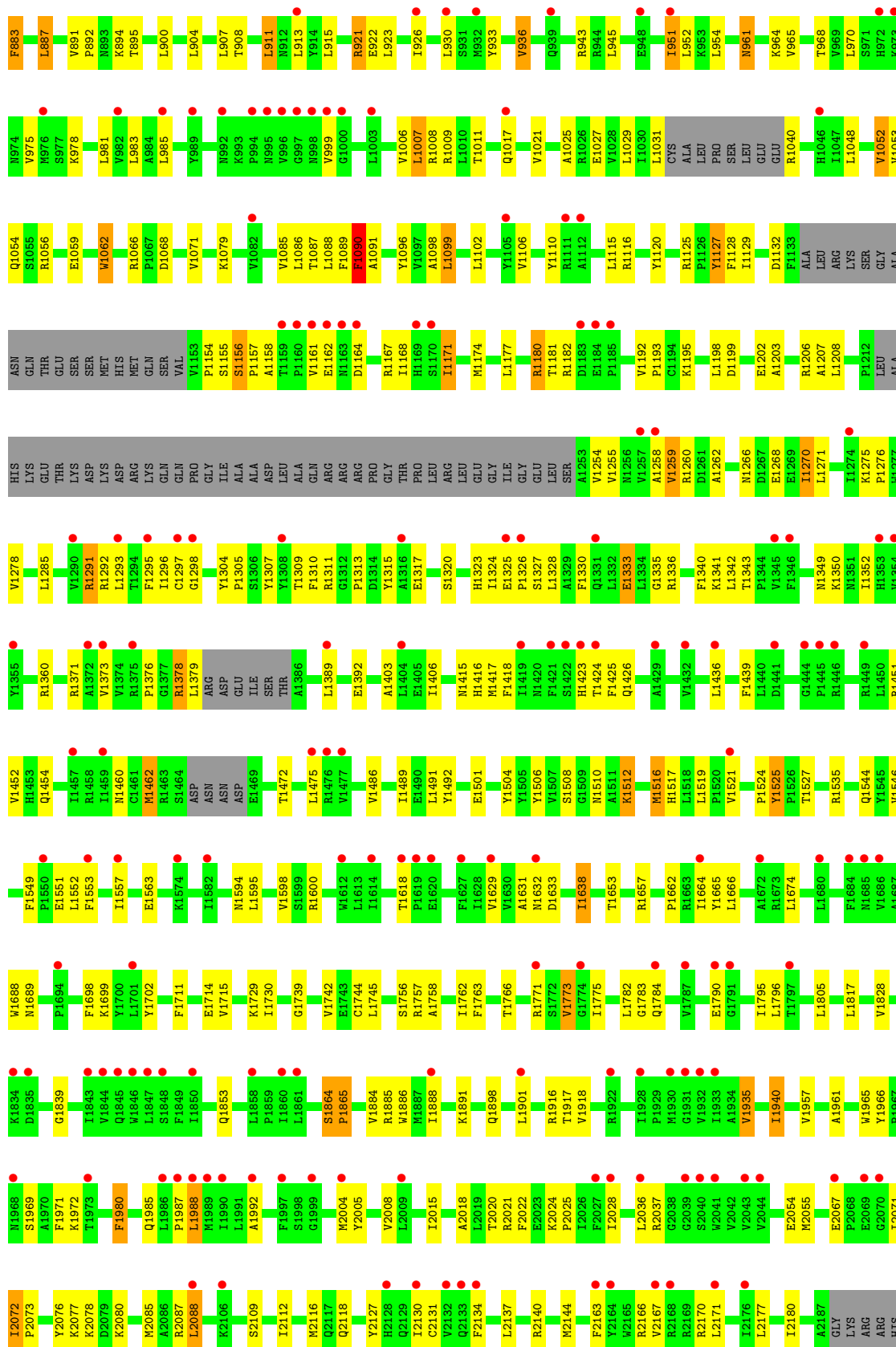
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein,Acetyl-CoA carboxylase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1399	Total	C	N	O	S	0	0	0
			11224	7122	1978	2086	38			
1	B	1394	Total	C	N	O	S	0	0	0
			11221	7120	1976	2086	39			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	GLY	-	expression tag	UNP G0S3L5
A	763	GLY	-	linker	UNP G0S3L5
A	764	SER	-	linker	UNP G0S3L5
A	765	GLY	-	linker	UNP G0S3L5
B	63	GLY	-	expression tag	UNP G0S3L5
B	763	GLY	-	linker	UNP G0S3L5
B	764	SER	-	linker	UNP G0S3L5
B	765	GLY	-	linker	UNP G0S3L5





4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	462.20Å 462.20Å 204.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.95 – 8.40 49.95 – 8.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.95-8.40) 99.0 (49.95-8.40)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 8.33Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.297 , 0.324 0.338 , 0.359	Depositor DCC
R_{free} test set	549 reflections (3.25%)	wwPDB-VP
Wilson B-factor (Å ²)	572.4	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 973.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	22445	wwPDB-VP
Average B, all atoms (Å ²)	250.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	2/11401 (0.0%)	1.32	39/15435 (0.3%)
1	B	0.75	1/11458 (0.0%)	1.31	35/15511 (0.2%)
All	All	0.75	3/22859 (0.0%)	1.32	74/30946 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2224	THR	CA-C	5.92	1.57	1.53
1	B	2072	ILE	CA-C	5.21	1.58	1.52
1	A	2072	ILE	CA-C	5.08	1.58	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1090	PHE	CA-CB-CG	6.40	120.20	113.80
1	B	1090	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	853	PRO	CA-C-N	6.37	129.45	120.28
1	B	853	PRO	C-N-CA	6.37	129.45	120.28
1	A	853	PRO	CA-C-N	6.34	129.41	120.28
1	A	853	PRO	C-N-CA	6.34	129.41	120.28
1	B	883	PHE	CA-CB-CG	6.12	119.92	113.80
1	A	883	PHE	CA-CB-CG	6.09	119.89	113.80
1	B	1971	PHE	CA-CB-CG	6.06	119.86	113.80
1	A	1090	PHE	CA-C-N	5.95	132.45	122.87
1	A	1090	PHE	C-N-CA	5.95	132.45	122.87
1	B	819	VAL	CA-C-N	5.82	128.87	120.38
1	B	819	VAL	C-N-CA	5.82	128.87	120.38
1	B	833	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	833	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	1971	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	1116	ARG	CA-C-N	5.66	128.88	120.90
1	A	1116	ARG	C-N-CA	5.66	128.88	120.90
1	B	1839	GLY	CA-C-N	5.65	127.89	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1839	GLY	C-N-CA	5.65	127.89	120.60
1	A	1839	GLY	CA-C-N	5.63	127.87	120.60
1	A	1839	GLY	C-N-CA	5.63	127.87	120.60
1	A	819	VAL	CA-C-N	5.60	128.56	120.38
1	A	819	VAL	C-N-CA	5.60	128.56	120.38
1	B	1091	ALA	CA-C-N	5.54	132.13	121.54
1	B	1091	ALA	C-N-CA	5.54	132.13	121.54
1	A	1535	ARG	CA-C-N	5.53	127.69	120.28
1	A	1535	ARG	C-N-CA	5.53	127.69	120.28
1	B	1961	ALA	CA-C-N	5.49	125.32	120.10
1	B	1961	ALA	C-N-CA	5.49	125.32	120.10
1	A	1961	ALA	CA-C-N	5.47	125.30	120.10
1	A	1961	ALA	C-N-CA	5.47	125.30	120.10
1	A	1510	ASN	CA-C-N	5.42	130.54	122.74
1	A	1510	ASN	C-N-CA	5.42	130.54	122.74
1	B	1594	ASN	CA-C-N	5.42	128.78	120.82
1	B	1594	ASN	C-N-CA	5.42	128.78	120.82
1	B	1828	VAL	N-CA-C	-5.41	105.57	110.82
1	B	1098	ALA	CA-C-N	5.38	127.43	120.44
1	B	1098	ALA	C-N-CA	5.38	127.43	120.44
1	B	1653	THR	CA-C-N	5.35	127.71	120.38
1	B	1653	THR	C-N-CA	5.35	127.71	120.38
1	A	1098	ALA	CA-C-N	5.34	127.39	120.44
1	A	1098	ALA	C-N-CA	5.34	127.39	120.44
1	A	1653	THR	CA-C-N	5.34	127.69	120.38
1	A	1653	THR	C-N-CA	5.34	127.69	120.38
1	A	1828	VAL	N-CA-C	-5.29	105.69	110.82
1	A	1594	ASN	CA-C-N	5.28	128.58	120.82
1	A	1594	ASN	C-N-CA	5.28	128.58	120.82
1	A	1439	PHE	CA-CB-CG	5.21	119.00	113.80
1	B	1110	TYR	CA-C-N	5.21	127.52	120.44
1	B	1110	TYR	C-N-CA	5.21	127.52	120.44
1	B	1439	PHE	CA-CB-CG	5.21	119.00	113.80
1	A	1783	GLY	CA-C-N	5.19	131.45	121.54
1	A	1783	GLY	C-N-CA	5.19	131.45	121.54
1	A	2015	ILE	CA-C-N	5.18	127.09	120.56
1	A	2015	ILE	C-N-CA	5.18	127.09	120.56
1	B	1261	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	2015	ILE	CA-C-N	5.13	127.03	120.56
1	B	2015	ILE	C-N-CA	5.13	127.03	120.56
1	A	1110	TYR	CA-C-N	5.12	127.41	120.44
1	A	1110	TYR	C-N-CA	5.12	127.41	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1980	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	1090	PHE	CA-C-N	5.10	132.02	122.74
1	B	1090	PHE	C-N-CA	5.10	132.02	122.74
1	B	807	MET	CA-C-N	5.09	127.10	120.28
1	B	807	MET	C-N-CA	5.09	127.10	120.28
1	B	1503	VAL	CA-C-N	5.04	129.51	122.41
1	B	1503	VAL	C-N-CA	5.04	129.51	122.41
1	A	1436	LEU	CA-C-N	5.03	127.28	120.38
1	A	1436	LEU	C-N-CA	5.03	127.28	120.38
1	B	1179	ARG	CA-C-N	5.03	131.15	121.54
1	B	1179	ARG	C-N-CA	5.03	131.15	121.54
1	A	807	MET	CA-C-N	5.01	127.00	120.28
1	A	807	MET	C-N-CA	5.01	127.00	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	11224	0	11148	187	0
1	B	11221	0	11191	181	0
All	All	22445	0	22339	363	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 8.

All (363) 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:1192:VAL:HG21	1:A:1203:ALA:HB1	1.48	0.94
1:B:1108:ARG:HH21	1:B:1375:ARG:HH22	1.21	0.85
1:B:1864:SER:HB2	1:B:1865:PRO:HD3	1.65	0.79
1:B:2054:GLU:HG3	1:B:2203:PRO:HG2	1.65	0.79
1:A:1864:SER:HB2	1:A:1865:PRO:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2054:GLU:HG3	1:A:2203:PRO:HG2	1.69	0.75
1:B:1091:ALA:HB2	1:B:1260:ARG:HG2	1.66	0.75
1:B:1131:TRP:O	1:B:1188:LYS:HA	1.87	0.74
1:B:1462:MET:HG2	1:B:1470:ASN:HB2	1.69	0.74
1:B:1415:ASN:HB2	1:B:1452:VAL:HA	1.71	0.73
1:A:1657:ARG:HD3	1:A:1758:ALA:HA	1.72	0.72
1:B:1516:MET:HG3	1:B:1519:LEU:HD12	1.71	0.71
1:A:1415:ASN:HB2	1:A:1452:VAL:HA	1.71	0.70
1:B:1657:ARG:HD3	1:B:1758:ALA:HA	1.71	0.70
1:A:961:ASN:HA	1:A:964:LYS:HB2	1.74	0.68
1:A:1546:VAL:HG21	1:A:1633:ASP:HA	1.75	0.68
1:B:961:ASN:HA	1:B:964:LYS:HB2	1.74	0.68
1:A:1007:LEU:HD12	1:A:1029:LEU:HG	1.76	0.67
1:B:1007:LEU:HD12	1:B:1029:LEU:HG	1.77	0.67
1:B:2037:ARG:HE	1:B:2067:GLU:HA	1.59	0.67
1:B:1546:VAL:HG21	1:B:1633:ASP:HA	1.75	0.67
1:B:926:ILE:HD12	1:B:985:LEU:HD11	1.78	0.66
1:B:1376:PRO:HB3	1:B:1423:HIS:HB2	1.77	0.66
1:B:1127:TYR:HB2	1:B:1193:PRO:HD2	1.78	0.65
1:B:1299:ARG:HD2	1:B:1303:SER:HB2	1.78	0.65
1:B:1180:ARG:HD2	1:B:1182:ARG:HD3	1.79	0.64
1:A:926:ILE:HD12	1:A:985:LEU:HD11	1.78	0.64
1:B:1662:PRO:HB3	1:B:1763:PHE:HB3	1.80	0.63
1:A:1171:ILE:HG23	1:A:1330:PHE:HB2	1.80	0.63
1:A:848:LEU:HD23	1:A:851:ARG:HG3	1.81	0.63
1:A:1180:ARG:HD2	1:A:1182:ARG:HD3	1.79	0.63
1:A:1195:LYS:HA	1:A:1260:ARG:HD2	1.81	0.63
1:B:1427:VAL:HG11	1:B:1459:ILE:HD12	1.80	0.63
1:A:1087:THR:HG21	1:A:1305:PRO:HG2	1.80	0.62
1:B:848:LEU:HD23	1:B:851:ARG:HG3	1.81	0.62
1:B:1007:LEU:HD11	1:B:1025:ALA:O	2.00	0.62
1:A:1007:LEU:HD11	1:A:1025:ALA:O	2.00	0.62
1:B:1711:PHE:HB3	1:B:1714:GLU:HB2	1.82	0.61
1:A:880:LEU:HD13	1:A:915:LEU:HD13	1.80	0.61
1:A:1711:PHE:HB3	1:A:1714:GLU:HB2	1.82	0.61
1:A:1161:VAL:HB	1:A:1330:PHE:HZ	1.66	0.60
1:B:1176:TYR:CE2	1:B:1291:ARG:HD3	2.36	0.60
1:A:1168:ILE:HB	1:A:1181:THR:HG21	1.83	0.60
1:B:1916:ARG:HB2	1:B:1940:ILE:HD13	1.83	0.60
1:A:1376:PRO:HG2	1:A:1423:HIS:HB2	1.82	0.60
1:B:1108:ARG:HH21	1:B:1375:ARG:NH2	1.96	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:MET:HB3	1:A:853:PRO:HD2	1.83	0.60
1:A:1517:HIS:HB3	1:A:1598:VAL:HG23	1.84	0.60
1:B:1341:LYS:HG3	1:B:1360:ARG:HG2	1.84	0.60
1:B:852:MET:HB3	1:B:853:PRO:HD2	1.83	0.60
1:B:1756:SER:HB2	1:B:1782:LEU:HD22	1.85	0.59
1:A:1091:ALA:CB	1:A:1260:ARG:HG2	2.33	0.59
1:B:1193:PRO:HB2	1:B:1260:ARG:HH21	1.66	0.59
1:B:1090:PHE:HB2	1:B:1193:PRO:HB3	1.85	0.59
1:A:2163:PHE:O	1:A:2167:VAL:HG23	2.03	0.59
1:B:1116:ARG:HE	1:B:1132:ASP:HB2	1.66	0.58
1:A:1756:SER:HB2	1:A:1782:LEU:HD22	1.85	0.58
1:B:2163:PHE:O	1:B:2167:VAL:HG23	2.04	0.58
1:A:1491:LEU:HB3	1:A:1508:SER:HA	1.86	0.58
1:B:1549:PHE:O	1:B:1553:PHE:HD1	1.87	0.58
1:A:1916:ARG:HB2	1:A:1940:ILE:HD13	1.85	0.58
1:A:1304:TYR:HB3	1:A:1350:LYS:HB2	1.86	0.58
1:B:1156:SER:HB2	1:B:1157:PRO:HD3	1.85	0.58
1:B:1254:VAL:HG12	1:B:1292:ARG:HB2	1.86	0.58
1:A:1068:ASP:HB3	1:A:1071:VAL:HG23	1.86	0.57
1:B:887:LEU:HD22	1:B:900:LEU:HB3	1.86	0.57
1:B:1307:TYR:H	1:B:1323:HIS:HA	1.70	0.57
1:A:1162:GLU:HG3	1:A:1501:GLU:HG2	1.86	0.57
1:B:1266:ASN:HB2	1:B:1270:ILE:HB	1.87	0.57
1:B:2025:PRO:HB3	1:B:2170:ARG:HD3	1.86	0.57
1:A:1087:THR:CB	1:A:1298:GLY:HA3	2.34	0.57
1:A:1549:PHE:O	1:A:1553:PHE:HD1	1.86	0.57
1:B:1884:VAL:HG21	1:B:1935:VAL:O	2.04	0.57
1:A:1918:VAL:HG13	1:A:1972:LYS:HD3	1.87	0.57
1:B:1081:THR:HG23	1:B:1375:ARG:HE	1.70	0.57
1:B:1517:HIS:HB3	1:B:1598:VAL:HG23	1.86	0.57
1:A:1884:VAL:HG21	1:A:1935:VAL:O	2.04	0.57
1:A:1492:TYR:HA	1:A:1506:TYR:HA	1.86	0.56
1:B:1310:PHE:HB3	1:B:1315:TYR:HB3	1.87	0.56
1:B:1059:GLU:HB3	1:B:1062:TRP:HZ3	1.70	0.56
1:A:2025:PRO:HB3	1:A:2170:ARG:HD3	1.86	0.56
1:A:1307:TYR:H	1:A:1323:HIS:HA	1.71	0.56
1:B:1918:VAL:HG13	1:B:1972:LYS:HD3	1.86	0.56
1:A:1087:THR:HG21	1:A:1305:PRO:CG	2.36	0.56
1:A:887:LEU:HD22	1:A:900:LEU:HB3	1.87	0.56
1:B:1068:ASP:HB3	1:B:1071:VAL:HG23	1.88	0.56
1:A:1059:GLU:HB3	1:A:1062:TRP:HZ3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:THR:OG1	1:A:1298:GLY:HA3	2.05	0.55
1:A:1156:SER:HB2	1:A:1157:PRO:HD3	1.87	0.55
1:A:2072:ILE:HD12	1:A:2131:CYS:HB2	1.89	0.55
1:B:1295:PHE:O	1:B:1307:TYR:HA	2.06	0.55
1:A:2072:ILE:HG23	1:A:2073:PRO:HD3	1.89	0.55
1:A:936:VAL:HG23	1:A:968:THR:HG23	1.89	0.55
1:B:1492:TYR:HA	1:B:1506:TYR:HA	1.87	0.55
1:B:2072:ILE:HG23	1:B:2073:PRO:HD3	1.88	0.55
1:B:936:VAL:HG23	1:B:968:THR:HG23	1.88	0.54
1:B:2072:ILE:HD12	1:B:2131:CYS:HB2	1.89	0.54
1:A:1333:GLU:HG2	1:A:1336:ARG:HG3	1.90	0.54
1:B:1516:MET:H	1:B:1600:ARG:HA	1.73	0.54
1:B:1176:TYR:HE2	1:B:1291:ARG:HD3	1.72	0.53
1:A:1371:ARG:HD3	1:A:1418:PHE:HB3	1.90	0.53
1:A:1295:PHE:O	1:A:1307:TYR:HA	2.07	0.53
1:A:1087:THR:HB	1:A:1298:GLY:HA3	1.91	0.53
1:B:1132:ASP:HA	1:B:1187:ARG:O	2.08	0.53
1:A:2037:ARG:HE	1:A:2067:GLU:HA	1.74	0.52
1:B:922:GLU:O	1:B:926:ILE:HG12	2.09	0.52
1:B:1116:ARG:HE	1:B:1132:ASP:CB	2.23	0.52
1:A:1688:TRP:HA	1:A:1698:PHE:HA	1.92	0.52
1:A:922:GLU:O	1:A:926:ILE:HG12	2.10	0.52
1:A:2256:MET:HA	1:A:2259:LEU:HD12	1.92	0.52
1:B:1059:GLU:HB3	1:B:1062:TRP:CZ3	2.45	0.52
1:B:1985:GLN:HB3	1:B:2024:LYS:HE3	1.92	0.52
1:B:1688:TRP:HA	1:B:1698:PHE:HA	1.92	0.51
1:A:1008:ARG:O	1:A:1011:THR:HG22	2.10	0.51
1:B:1133:PHE:HB2	1:B:1187:ARG:HB2	1.92	0.51
1:A:1349:ASN:HB3	1:A:1352:ILE:HG12	1.92	0.51
1:A:1702:TYR:HA	1:A:1729:LYS:HA	1.92	0.51
1:B:1702:TYR:HA	1:B:1729:LYS:HA	1.93	0.51
1:B:1096:TYR:CD1	1:B:1096:TYR:C	2.89	0.51
1:B:1026:ARG:HG2	1:B:1391:SER:OG	2.11	0.51
1:A:1333:GLU:CG	1:A:1336:ARG:HG3	2.41	0.51
1:A:1054:GLN:HB3	1:A:1062:TRP:CD1	2.46	0.51
1:A:1254:VAL:HG12	1:A:1292:ARG:HB2	1.92	0.51
1:A:1310:PHE:HB3	1:A:1315:TYR:HB3	1.92	0.51
1:A:1885:ARG:HA	1:A:1888:ILE:HD12	1.93	0.51
1:B:1006:VAL:O	1:B:1009:ARG:HG2	2.10	0.50
1:B:1008:ARG:O	1:B:1011:THR:HG22	2.10	0.50
1:B:1506:TYR:H	1:B:1517:HIS:CE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1340:PHE:CZ	1:A:1527:THR:HG22	2.47	0.50
1:B:1054:GLN:HB3	1:B:1062:TRP:CD1	2.47	0.50
1:B:1349:ASN:HB3	1:B:1352:ILE:HG12	1.93	0.50
1:A:1492:TYR:CD1	1:A:1506:TYR:HB3	2.46	0.50
1:B:1091:ALA:HB2	1:B:1260:ARG:CG	2.39	0.50
1:B:1885:ARG:HA	1:B:1888:ILE:HD12	1.93	0.50
1:A:907:LEU:O	1:A:911:LEU:HD13	2.12	0.50
1:A:1006:VAL:O	1:A:1009:ARG:HG2	2.11	0.50
1:A:1059:GLU:HB3	1:A:1062:TRP:CZ3	2.46	0.50
1:A:856:LEU:HB2	1:A:894:LYS:HE2	1.94	0.50
1:A:1091:ALA:HB1	1:A:1260:ARG:HG2	1.94	0.50
1:A:1096:TYR:C	1:A:1096:TYR:CD1	2.89	0.50
1:B:2210:LEU:O	1:B:2214:GLU:HB2	2.12	0.49
1:B:1535:ARG:HA	1:B:1545:TYR:HB2	1.94	0.49
1:A:1120:TYR:HD1	1:A:1129:ILE:HG22	1.78	0.49
1:A:1154:PRO:HB2	1:A:1158:ALA:HB2	1.93	0.49
1:B:907:LEU:O	1:B:911:LEU:HD13	2.12	0.49
1:A:1516:MET:H	1:A:1600:ARG:HA	1.77	0.49
1:A:1985:GLN:HB3	1:A:2024:LYS:HE3	1.93	0.49
1:B:1265:LYS:HE3	1:B:1299:ARG:HG3	1.93	0.49
1:B:1429:ALA:HB2	1:B:1475:LEU:HD13	1.94	0.49
1:A:827:PHE:O	1:A:831:LEU:HD23	2.13	0.49
1:B:1168:ILE:HB	1:B:1181:THR:HG21	1.95	0.49
1:A:1099:LEU:HA	1:A:1102:LEU:HD12	1.95	0.49
1:A:1506:TYR:HE2	1:A:1512:LYS:HA	1.77	0.49
1:A:1662:PRO:HB3	1:A:1763:PHE:HB3	1.94	0.49
1:A:1202:GLU:HB3	1:A:1206:ARG:HH12	1.78	0.49
1:B:827:PHE:O	1:B:831:LEU:HD23	2.13	0.49
1:B:1202:GLU:HB3	1:B:1206:ARG:HH12	1.78	0.48
1:A:1328:LEU:HD22	1:A:1373:VAL:HG21	1.94	0.48
1:A:1980:PHE:CB	1:A:1988:LEU:HD21	2.43	0.48
1:A:2028:ILE:HB	1:A:2055:MET:HG3	1.94	0.48
1:A:2210:LEU:O	1:A:2214:GLU:HB2	2.12	0.48
1:A:860:LEU:HG	1:A:879:LEU:HD22	1.95	0.48
1:B:860:LEU:HG	1:B:879:LEU:HD22	1.95	0.48
1:B:1053:VAL:HG23	1:B:1062:TRP:HB3	1.95	0.48
1:A:1091:ALA:HB2	1:A:1260:ARG:HG2	1.94	0.48
1:B:1192:VAL:HG11	1:B:1203:ALA:O	2.13	0.48
1:B:2028:ILE:HB	1:B:2055:MET:HG3	1.94	0.48
1:A:1415:ASN:HD22	1:A:1451:ARG:C	2.22	0.47
1:B:856:LEU:HB2	1:B:894:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:VAL:HG23	1:A:1062:TRP:HB3	1.96	0.47
1:A:1293:LEU:O	1:A:1309:THR:HA	2.15	0.47
1:B:895:THR:HG23	1:B:895:THR:O	2.15	0.47
1:B:895:THR:HB	1:B:900:LEU:HD12	1.95	0.47
1:A:895:THR:HB	1:A:900:LEU:HD12	1.95	0.47
1:A:1174:MET:SD	1:A:1335:GLY:HA3	2.55	0.47
1:A:1516:MET:HG3	1:A:1519:LEU:HD22	1.96	0.47
1:A:2085:MET:C	1:A:2087:ARG:H	2.23	0.47
1:A:1056:ARG:HD2	1:A:1062:TRP:CZ2	2.50	0.47
1:A:1090:PHE:HB2	1:A:1193:PRO:HB3	1.97	0.47
1:B:1403:ALA:O	1:B:1406:ILE:HG13	2.15	0.47
1:A:1426:GLN:HG3	1:A:1462:MET:HB3	1.97	0.47
1:B:1415:ASN:HD22	1:B:1451:ARG:C	2.22	0.47
1:B:1966:TYR:H	1:B:1969:SER:HB2	1.80	0.47
1:B:2085:MET:C	1:B:2087:ARG:H	2.23	0.47
1:A:895:THR:HG23	1:A:895:THR:O	2.15	0.47
1:A:1403:ALA:O	1:A:1406:ILE:HG13	2.14	0.46
1:A:1886:TRP:HB3	1:A:1891:LYS:HB2	1.98	0.46
1:A:2127:TYR:HA	1:A:2130:ILE:HD12	1.97	0.46
1:B:2127:TYR:HA	1:B:2130:ILE:HD12	1.97	0.46
1:A:1266:ASN:HB2	1:A:1270:ILE:HB	1.97	0.46
1:B:1056:ARG:HD2	1:B:1062:TRP:CZ2	2.50	0.46
1:B:1886:TRP:HB3	1:B:1891:LYS:HB2	1.98	0.46
1:A:1102:LEU:O	1:A:1106:VAL:HG23	2.15	0.46
1:B:1155:SER:HB2	1:B:1168:ILE:HG12	1.98	0.46
1:A:894:LYS:HG3	1:A:900:LEU:CD1	2.46	0.46
1:A:1492:TYR:CD1	1:A:1504:TYR:HB3	2.50	0.46
1:A:1966:TYR:H	1:A:1969:SER:HB2	1.81	0.46
1:B:1102:LEU:HD21	1:B:1193:PRO:HG3	1.97	0.46
1:B:1127:TYR:OH	1:B:1207:ALA:HB1	2.16	0.46
1:A:1416:HIS:HD2	1:A:1454:GLN:HG3	1.80	0.46
1:B:2203:PRO:HA	1:B:2206:ARG:HB3	1.97	0.46
1:B:2037:ARG:HH11	1:B:2068:PRO:HD3	1.81	0.46
1:B:945:LEU:HD13	1:B:951:ILE:HG13	1.98	0.46
1:B:1773:VAL:HG13	1:B:1795:ILE:HG23	1.98	0.46
1:A:1155:SER:HB2	1:A:1168:ILE:HG12	1.98	0.46
1:A:1992:ALA:HB1	1:A:2036:LEU:HD13	1.98	0.46
1:B:1531:LEU:HG	1:B:1535:ARG:HD2	1.98	0.46
1:B:933:TYR:HD1	1:B:978:LYS:HG2	1.81	0.45
1:B:1154:PRO:HB2	1:B:1158:ALA:HB2	1.97	0.45
1:B:1319:ASP:C	1:B:1344:PRO:HG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:GLU:HA	1:A:1271:LEU:HD12	1.98	0.45
1:B:1531:LEU:HD23	1:B:1535:ARG:NH1	2.31	0.45
1:A:1255:VAL:O	1:A:1293:LEU:HA	2.15	0.45
1:A:1519:LEU:HD11	1:A:1600:ARG:HD2	1.97	0.45
1:B:1007:LEU:HD11	1:B:1025:ALA:C	2.41	0.45
1:A:2004:MET:HA	1:A:2008:VAL:HG12	1.99	0.45
1:B:1253:ALA:O	1:B:1291:ARG:HG2	2.16	0.45
1:A:904:LEU:O	1:A:908:THR:HG23	2.17	0.45
1:B:1992:ALA:HB1	1:B:2036:LEU:HD13	1.98	0.45
1:A:1524:PRO:O	1:A:1525:TYR:C	2.60	0.45
1:B:2004:MET:HA	1:B:2008:VAL:HG12	1.99	0.45
1:A:1125:ARG:HH22	1:A:1199:ASP:CG	2.25	0.45
1:A:1773:VAL:HG13	1:A:1795:ILE:HG23	1.99	0.45
1:A:2020:THR:HG21	1:B:1757:ARG:HG2	1.98	0.45
1:B:1323:HIS:CE1	1:B:1350:LYS:HD2	2.51	0.45
1:A:852:MET:O	1:A:853:PRO:C	2.60	0.45
1:A:887:LEU:HD21	1:A:904:LEU:HD12	1.99	0.45
1:B:810:ILE:HD13	1:B:981:LEU:HD21	1.98	0.45
1:B:894:LYS:HG3	1:B:900:LEU:CD1	2.46	0.45
1:B:1268:GLU:HA	1:B:1271:LEU:HD12	1.97	0.45
1:B:1665:TYR:HB3	1:B:1766:THR:HG22	1.99	0.45
1:A:810:ILE:HD13	1:A:981:LEU:HD21	1.98	0.45
1:B:1291:ARG:HG3	1:B:1292:ARG:N	2.32	0.45
1:A:846:SER:HA	1:A:849:HIS:ND1	2.32	0.44
1:A:1007:LEU:HD11	1:A:1025:ALA:C	2.42	0.44
1:A:1333:GLU:C	1:A:1335:GLY:H	2.26	0.44
1:A:1665:TYR:HB3	1:A:1766:THR:HG22	2.00	0.44
1:A:2144:MET:HG2	1:B:1742:VAL:HG11	1.98	0.44
1:A:1087:THR:HG22	1:A:1296:ILE:HD11	1.99	0.44
1:B:1864:SER:HB2	1:B:1865:PRO:CD	2.43	0.44
1:A:923:LEU:HD21	1:A:999:VAL:HG12	2.00	0.44
1:A:1127:TYR:OH	1:A:1207:ALA:HB1	2.17	0.44
1:A:1325:GLU:CD	1:A:1326:PRO:HD2	2.42	0.44
1:A:1689:ASN:HA	1:A:1699:LYS:HE3	2.00	0.44
1:A:933:TYR:HD1	1:A:978:LYS:HG2	1.82	0.44
1:A:1629:VAL:HG22	1:A:1664:ILE:HB	1.99	0.44
1:B:846:SER:HA	1:B:849:HIS:ND1	2.33	0.44
1:A:1378:ARG:HD3	1:A:1392:GLU:HG2	1.99	0.44
1:A:1739:GLY:HA2	1:A:1744:CYS:SG	2.58	0.44
1:B:852:MET:O	1:B:853:PRO:C	2.60	0.44
1:B:1192:VAL:CG1	1:B:1203:ALA:HB1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:887:LEU:HD11	1:A:904:LEU:HB2	2.00	0.44
1:B:824:LEU:O	1:B:828:ILE:HG12	2.18	0.44
1:B:1153:VAL:N	1:B:1154:PRO:CD	2.81	0.44
1:A:824:LEU:O	1:A:828:ILE:HG12	2.18	0.44
1:A:1052:VAL:HG22	1:A:1096:TYR:CE1	2.53	0.44
1:B:2109:SER:HA	1:B:2112:ILE:HD12	2.00	0.44
1:B:1087:THR:OG1	1:B:1298:GLY:HA3	2.17	0.44
1:A:1757:ARG:HG2	1:B:2020:THR:HG21	2.00	0.43
1:A:2109:SER:HA	1:A:2112:ILE:HD12	1.99	0.43
1:B:904:LEU:O	1:B:908:THR:HG23	2.18	0.43
1:B:1544:GLN:HG3	1:B:1552:LEU:HD11	2.00	0.43
1:B:1742:VAL:HA	1:B:1745:LEU:HD12	1.99	0.43
1:A:945:LEU:HD13	1:A:951:ILE:HG13	2.00	0.43
1:A:1096:TYR:O	1:A:1099:LEU:HB3	2.18	0.43
1:A:1417:MET:HE3	1:A:1452:VAL:HG11	2.00	0.43
1:B:1473:MET:HE3	1:B:1475:LEU:HD21	2.00	0.43
1:B:891:VAL:HA	1:B:895:THR:HG22	2.01	0.43
1:A:891:VAL:HA	1:A:895:THR:HG22	2.00	0.43
1:A:1048:LEU:O	1:A:1052:VAL:HG23	2.18	0.43
1:B:887:LEU:HD21	1:B:904:LEU:HD12	1.99	0.43
1:B:1081:THR:OG1	1:B:1375:ARG:HB3	2.19	0.43
1:B:1116:ARG:NE	1:B:1132:ASP:HB2	2.31	0.43
1:B:1689:ASN:HA	1:B:1699:LYS:HE3	1.99	0.43
1:A:856:LEU:CB	1:A:894:LYS:HE2	2.48	0.43
1:A:1258:ALA:HA	1:A:1296:ILE:HG23	2.00	0.43
1:A:2177:LEU:HA	1:A:2180:ILE:HD12	2.00	0.43
1:B:975:VAL:HG11	1:B:1017:GLN:HG2	2.01	0.43
1:B:1052:VAL:HG22	1:B:1096:TYR:CE1	2.54	0.43
1:B:1739:GLY:HA2	1:B:1744:CYS:SG	2.58	0.43
1:A:1266:ASN:CB	1:A:1270:ILE:HB	2.49	0.43
1:A:1262:ALA:HB2	1:A:1298:GLY:O	2.19	0.43
1:B:831:LEU:HD12	1:B:922:GLU:HA	2.01	0.43
1:A:1066:ARG:HH12	1:A:1120:TYR:HB3	1.84	0.43
1:A:1742:VAL:HA	1:A:1745:LEU:HD12	1.99	0.43
1:B:1108:ARG:NH2	1:B:1375:ARG:HH22	2.03	0.43
1:B:1164:ASP:H	1:B:1167:ARG:NE	2.17	0.43
1:B:2137:LEU:HA	1:B:2140:ARG:HD3	2.01	0.43
1:A:1164:ASP:H	1:A:1167:ARG:NE	2.17	0.43
1:B:1099:LEU:HA	1:B:1102:LEU:HD12	2.00	0.43
1:A:831:LEU:HD12	1:A:922:GLU:HA	2.01	0.42
1:B:1096:TYR:O	1:B:1099:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1504:TYR:HE1	1:B:1521:VAL:HA	1.83	0.42
1:B:1629:VAL:HG22	1:B:1664:ILE:HB	2.00	0.42
1:A:2137:LEU:HA	1:A:2140:ARG:HD3	2.00	0.42
1:A:831:LEU:HD13	1:A:921:ARG:CZ	2.49	0.42
1:A:836:LEU:HG	1:A:921:ARG:HH12	1.84	0.42
1:A:1631:ALA:HB2	1:A:1666:LEU:HB2	2.01	0.42
1:B:1417:MET:HE3	1:B:1452:VAL:HG11	2.01	0.42
1:A:1127:TYR:CD2	1:A:1127:TYR:C	2.96	0.42
1:A:1040:ARG:HH21	1:A:1085:VAL:HB	1.84	0.42
1:A:1389:LEU:HD11	1:A:1425:PHE:CG	2.53	0.42
1:B:831:LEU:HD13	1:B:921:ARG:CZ	2.49	0.42
1:B:856:LEU:CB	1:B:894:LYS:HE2	2.50	0.42
1:B:1275:LYS:N	1:B:1276:PRO:HD2	2.34	0.42
1:A:1325:GLU:HG3	1:A:1327:SER:H	1.83	0.42
1:A:1275:LYS:N	1:A:1276:PRO:HD2	2.35	0.42
1:A:1291:ARG:HE	1:A:1291:ARG:HB2	1.73	0.42
1:A:975:VAL:HG11	1:A:1017:GLN:HG2	2.02	0.42
1:A:1099:LEU:C	1:A:1099:LEU:HD23	2.45	0.41
1:A:1259:VAL:HG23	1:A:1297:CYS:HA	2.02	0.41
1:B:1170:SER:HB2	1:B:1187:ARG:HH22	1.85	0.41
1:B:887:LEU:HD11	1:B:904:LEU:HB2	2.01	0.41
1:B:1170:SER:HB3	1:B:1173:ASP:HB3	2.02	0.41
1:B:1631:ALA:HB2	1:B:1666:LEU:HB2	2.02	0.41
1:A:2116:MET:C	1:A:2118:GLN:H	2.28	0.41
1:B:1048:LEU:O	1:B:1052:VAL:HG23	2.19	0.41
1:B:1096:TYR:C	1:B:1096:TYR:HD1	2.28	0.41
1:A:1027:GLU:O	1:A:1031:LEU:HG	2.20	0.41
1:A:2018:ALA:HA	1:A:2021:ARG:HD2	2.01	0.41
1:A:1052:VAL:HG22	1:A:1096:TYR:CD1	2.56	0.41
1:A:1504:TYR:HE1	1:A:1521:VAL:HA	1.86	0.41
1:A:2203:PRO:HA	1:A:2206:ARG:HB3	2.01	0.41
1:B:2169:ARG:O	1:B:2173:GLU:HB2	2.21	0.41
1:B:1052:VAL:HG22	1:B:1096:TYR:CD1	2.56	0.41
1:B:1504:TYR:CE1	1:B:1521:VAL:HA	2.56	0.41
1:A:961:ASN:O	1:A:965:VAL:HG23	2.21	0.41
1:A:1208:LEU:HD21	1:A:1285:LEU:HD23	2.03	0.41
1:A:1275:LYS:HA	1:A:1278:VAL:HG12	2.03	0.41
1:B:836:LEU:HG	1:B:921:ARG:HH12	1.84	0.41
1:B:1333:GLU:C	1:B:1335:GLY:H	2.29	0.41
1:A:1544:GLN:HG3	1:A:1552:LEU:HD11	2.02	0.41
1:B:820:MET:HA	1:B:823:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1098:ALA:O	1:B:1102:LEU:HG	2.21	0.41
1:B:1127:TYR:CG	1:B:1128:PHE:N	2.88	0.41
1:B:1265:LYS:HG3	1:B:1299:ARG:HE	1.86	0.41
1:B:2116:MET:C	1:B:2118:GLN:H	2.28	0.41
1:A:1460:ASN:HD22	1:A:1472:THR:HG21	1.86	0.41
1:A:2088:LEU:HG	1:B:1686:VAL:HG23	2.01	0.41
1:B:1027:GLU:O	1:B:1031:LEU:HG	2.20	0.41
1:B:1054:GLN:HB3	1:B:1062:TRP:NE1	2.36	0.41
1:B:1066:ARG:HH12	1:B:1120:TYR:HB3	1.86	0.41
1:A:1054:GLN:HB3	1:A:1062:TRP:NE1	2.36	0.41
1:A:1341:LYS:HG3	1:A:1360:ARG:HG2	2.02	0.41
1:A:2134:PHE:HA	1:A:2137:LEU:HD12	2.03	0.41
1:B:923:LEU:HD21	1:B:999:VAL:HG12	2.01	0.41
1:B:1076:VAL:HG11	1:B:1107:ARG:HB3	2.03	0.41
1:A:1096:TYR:C	1:A:1096:TYR:HD1	2.28	0.40
1:B:1530:TRP:O	1:B:1533:PRO:HD2	2.21	0.40
1:A:1089:PHE:C	1:A:1091:ALA:H	2.28	0.40
1:A:1864:SER:HB2	1:A:1865:PRO:CD	2.43	0.40
1:A:1987:PRO:HG3	1:A:2171:LEU:HD21	2.03	0.40
1:A:1988:LEU:HG	1:A:2022:PHE:CZ	2.57	0.40
1:B:1162:GLU:HG3	1:B:1522:SER:OG	2.20	0.40
1:B:993:LYS:HG2	1:B:1031:LEU:HD22	2.03	0.40
1:B:1794:ILE:HD12	1:B:1823:MET:HG3	2.04	0.40
1:A:2005:TYR:HA	1:B:1826:ASN:HD22	1.87	0.40
1:B:1340:PHE:CZ	1:B:1527:THR:HG22	2.56	0.40
1:A:820:MET:HA	1:A:823:LYS:HE3	2.02	0.40
1:A:2077:LYS:H	1:A:2080:LYS:HD2	1.87	0.40
1:B:1052:VAL:HA	1:B:1096:TYR:CZ	2.57	0.40
1:B:1099:LEU:HD23	1:B:1099:LEU:C	2.47	0.40
1:B:1527:THR:O	1:B:1530:TRP:CD1	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	1373/2211 (62%)	1229 (90%)	123 (9%)	21 (2%)	8	40
1	B	1380/2211 (62%)	1249 (90%)	110 (8%)	21 (2%)	8	40
All	All	2753/4422 (62%)	2478 (90%)	233 (8%)	42 (2%)	8	40

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	943	ARG
1	A	1156	SER
1	A	1516	MET
1	A	1784	GLN
1	A	1864	SER
1	B	943	ARG
1	B	1092	HIS
1	B	1156	SER
1	B	1864	SER
1	A	887	LEU
1	A	1128	PHE
1	A	1180	ARG
1	A	2225	ASN
1	B	887	LEU
1	B	1180	ARG
1	A	853	PRO
1	A	1486	VAL
1	A	1512	LYS
1	B	853	PRO
1	B	1160	PRO
1	B	1426	GLN
1	B	1516	MET
1	B	1638	ILE
1	B	1784	GLN
1	B	2225	ASN
1	A	892	PRO
1	A	1333	GLU
1	A	1638	ILE
1	A	1790	GLU
1	B	892	PRO
1	B	1128	PHE
1	B	1486	VAL
1	B	1790	GLU

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Mol	Chain	Res	Type
1	A	1313	PRO
1	A	1317	GLU
1	A	1865	PRO
1	B	1313	PRO
1	B	1865	PRO
1	B	1317	GLU
1	A	1052	VAL
1	B	1052	VAL
1	A	1525	TYR

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	1208/1879 (64%)	1127 (93%)	81 (7%)	15	36
1	B	1215/1879 (65%)	1137 (94%)	78 (6%)	16	37
All	All	2423/3758 (64%)	2264 (93%)	159 (7%)	15	37

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	819	VAL
1	A	824	LEU
1	A	836	LEU
1	A	848	LEU
1	A	852	MET
1	A	860	LEU
1	A	880	LEU
1	A	883	PHE
1	A	911	LEU
1	A	913	LEU
1	A	921	ARG
1	A	930	LEU
1	A	936	VAL
1	A	951	ILE

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Mol	Chain	Res	Type
1	A	952	LEU
1	A	954	LEU
1	A	961	ASN
1	A	970	LEU
1	A	983	LEU
1	A	1007	LEU
1	A	1021	VAL
1	A	1062	TRP
1	A	1079	LYS
1	A	1086	LEU
1	A	1088	LEU
1	A	1090	PHE
1	A	1099	LEU
1	A	1115	LEU
1	A	1127	TYR
1	A	1132	ASP
1	A	1171	ILE
1	A	1177	LEU
1	A	1198	LEU
1	A	1259	VAL
1	A	1270	ILE
1	A	1291	ARG
1	A	1311	ARG
1	A	1320	SER
1	A	1324	ILE
1	A	1342	LEU
1	A	1343	THR
1	A	1378	ARG
1	A	1379	LEU
1	A	1424	THR
1	A	1462	MET
1	A	1475	LEU
1	A	1489	ILE
1	A	1551	GLU
1	A	1557	ILE
1	A	1563	GLU
1	A	1595	LEU
1	A	1618	THR
1	A	1632	ASN
1	A	1638	ILE
1	A	1674	LEU
1	A	1715	VAL

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Mol	Chain	Res	Type
1	A	1730	ILE
1	A	1762	ILE
1	A	1771	ARG
1	A	1773	VAL
1	A	1775	ILE
1	A	1796	LEU
1	A	1805	LEU
1	A	1817	LEU
1	A	1853	GLN
1	A	1898	GLN
1	A	1901	LEU
1	A	1917	THR
1	A	1935	VAL
1	A	1940	ILE
1	A	1957	VAL
1	A	1965	TRP
1	A	1988	LEU
1	A	2071	ILE
1	A	2076	TYR
1	A	2078	LYS
1	A	2088	LEU
1	A	2166	ARG
1	A	2196	ASN
1	A	2234	GLU
1	A	2240	ILE
1	B	819	VAL
1	B	824	LEU
1	B	836	LEU
1	B	848	LEU
1	B	852	MET
1	B	860	LEU
1	B	880	LEU
1	B	883	PHE
1	B	911	LEU
1	B	913	LEU
1	B	915	LEU
1	B	921	ARG
1	B	930	LEU
1	B	936	VAL
1	B	951	ILE
1	B	952	LEU
1	B	954	LEU

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Mol	Chain	Res	Type
1	B	961	ASN
1	B	970	LEU
1	B	983	LEU
1	B	1007	LEU
1	B	1021	VAL
1	B	1032	CYS
1	B	1062	TRP
1	B	1086	LEU
1	B	1088	LEU
1	B	1090	PHE
1	B	1099	LEU
1	B	1115	LEU
1	B	1118	VAL
1	B	1127	TYR
1	B	1177	LEU
1	B	1186	ILE
1	B	1192	VAL
1	B	1198	LEU
1	B	1254	VAL
1	B	1296	ILE
1	B	1324	ILE
1	B	1327	SER
1	B	1331	GLN
1	B	1332	LEU
1	B	1378	ARG
1	B	1427	VAL
1	B	1430	ASP
1	B	1434	GLU
1	B	1489	ILE
1	B	1551	GLU
1	B	1557	ILE
1	B	1563	GLU
1	B	1595	LEU
1	B	1618	THR
1	B	1632	ASN
1	B	1638	ILE
1	B	1674	LEU
1	B	1715	VAL
1	B	1730	ILE
1	B	1762	ILE
1	B	1771	ARG
1	B	1773	VAL

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Mol	Chain	Res	Type
1	B	1775	ILE
1	B	1796	LEU
1	B	1805	LEU
1	B	1817	LEU
1	B	1853	GLN
1	B	1898	GLN
1	B	1901	LEU
1	B	1917	THR
1	B	1935	VAL
1	B	1940	ILE
1	B	1957	VAL
1	B	1965	TRP
1	B	2007	GLU
1	B	2071	ILE
1	B	2076	TYR
1	B	2078	LYS
1	B	2088	LEU
1	B	2166	ARG
1	B	2196	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	812	ASN
1	A	844	GLN
1	A	854	HIS
1	A	878	GLN
1	A	918	GLN
1	A	939	GLN
1	A	957	GLN
1	A	1017	GLN
1	A	1331	GLN
1	A	1415	ASN
1	A	1416	HIS
1	A	1453	HIS
1	A	1470	ASN
1	A	1481	ASN
1	A	1713	ASN
1	A	1856	ASN
1	A	1942	ASN
1	A	1985	GLN
1	A	2001	GLN

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Mol	Chain	Res	Type
1	A	2049	ASN
1	A	2129	GLN
1	A	2133	GLN
1	B	812	ASN
1	B	844	GLN
1	B	854	HIS
1	B	878	GLN
1	B	918	GLN
1	B	939	GLN
1	B	957	GLN
1	B	992	ASN
1	B	1017	GLN
1	B	1353	HIS
1	B	1415	ASN
1	B	1416	HIS
1	B	1453	HIS
1	B	1460	ASN
1	B	1470	ASN
1	B	1481	ASN
1	B	1488	GLN
1	B	1713	ASN
1	B	1856	ASN
1	B	1942	ASN
1	B	1985	GLN
1	B	2001	GLN
1	B	2129	GLN
1	B	2133	GLN
1	B	2236	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1387/2211 (62%)	0.53	189 (13%)	7 15	25, 211, 483, 500	0
1	B	1394/2211 (63%)	0.51	169 (12%)	8 17	5, 245, 486, 500	0
All	All	2781/4422 (62%)	0.52	358 (12%)	7 16	5, 230, 485, 500	0

All (358) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1862	SER	20.1
1	A	792	VAL	17.5
1	B	1796	LEU	16.4
1	B	1389	LEU	11.3
1	A	2069	GLU	11.2
1	A	2043	VAL	10.7
1	B	2130	ILE	10.3
1	A	1987	PRO	9.8
1	A	1684	PHE	9.4
1	B	1989	MET	8.9
1	B	1459	ILE	8.6
1	B	1701	LEU	8.5
1	B	1191	ILE	8.2
1	B	2168	ARG	8.1
1	B	1421	PHE	8.0
1	A	1928	ILE	7.9
1	B	1475	LEU	7.9
1	B	2134	PHE	7.7
1	A	790	VAL	7.6
1	B	1933	ILE	7.5
1	B	2131	CYS	7.5
1	B	1860	ILE	7.4
1	B	907	LEU	7.4
1	B	1730	ILE	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	791	VAL	7.2
1	A	1159	THR	7.2
1	A	1619	PRO	7.2
1	A	2044	VAL	7.1
1	B	1932	VAL	6.8
1	B	1795	ILE	6.8
1	B	879	LEU	6.8
1	B	851	ARG	6.7
1	A	2168	ARG	6.7
1	A	2199	LEU	6.7
1	B	1797	THR	6.7
1	B	1684	PHE	6.4
1	B	1285	LEU	6.4
1	A	1933	ILE	6.4
1	A	1999	GLY	6.4
1	B	1424	THR	6.4
1	B	2127	TYR	6.3
1	B	1372	ALA	6.2
1	B	1293	LEU	6.2
1	B	2213	LEU	6.2
1	A	1930	MET	6.2
1	B	1778	TYR	6.2
1	B	1373	VAL	6.1
1	A	1372	ALA	6.1
1	B	2176	ILE	6.1
1	B	903	THR	6.1
1	B	904	LEU	6.0
1	B	906	PRO	6.0
1	B	1105	TYR	6.0
1	B	1255	VAL	5.9
1	A	1989	MET	5.9
1	B	1419	ILE	5.8
1	A	846	SER	5.8
1	A	868	GLN	5.8
1	B	1374	VAL	5.7
1	B	2216	TRP	5.6
1	B	1106	VAL	5.6
1	A	2134	PHE	5.6
1	A	835	LYS	5.6
1	A	1160	PRO	5.6
1	A	1422	SER	5.5
1	A	1574	LYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	995	ASN	5.4
1	B	1934	ALA	5.4
1	A	2167	VAL	5.4
1	B	1930	MET	5.4
1	B	985	LEU	5.4
1	B	1794	ILE	5.3
1	B	2233	TYR	5.3
1	A	1701	LEU	5.2
1	B	848	LEU	5.2
1	A	1419	ILE	5.2
1	B	2163	PHE	5.2
1	A	2106	LYS	5.2
1	B	1861	LEU	4.9
1	A	1553	PHE	4.9
1	A	1686	VAL	4.9
1	A	1835	ASP	4.9
1	B	1388	TYR	4.8
1	B	2256	MET	4.8
1	A	1629	VAL	4.8
1	B	1457	ILE	4.7
1	A	1858	LEU	4.7
1	B	1256	ASN	4.6
1	B	1425	PHE	4.6
1	B	1208	LEU	4.6
1	B	2234	GLU	4.5
1	A	2009	LEU	4.5
1	B	2172	ILE	4.5
1	A	1000	GLY	4.5
1	B	2167	VAL	4.5
1	A	997	GLY	4.4
1	A	1846	TRP	4.4
1	A	1331	GLN	4.4
1	A	1986	LEU	4.4
1	B	800	PHE	4.4
1	A	994	PRO	4.4
1	A	2027	PHE	4.4
1	A	2040	SER	4.3
1	B	1204	LEU	4.3
1	A	793	GLY	4.3
1	A	992	ASN	4.3
1	A	1990	ILE	4.3
1	A	2039	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	1475	LEU	4.2
1	A	1432	VAL	4.1
1	B	948	GLU	4.1
1	B	844	GLN	4.1
1	B	1686	VAL	4.1
1	A	1988	LEU	4.0
1	A	2132	VAL	4.0
1	B	804	TYR	4.0
1	A	1843	ILE	4.0
1	B	2133	GLN	3.9
1	A	1112	ALA	3.9
1	A	1844	VAL	3.9
1	B	1680	LEU	3.9
1	A	1290	VAL	3.9
1	A	1521	VAL	3.8
1	B	1477	VAL	3.8
1	A	939	GLN	3.8
1	B	1290	VAL	3.8
1	B	2259	LEU	3.8
1	A	842	SER	3.8
1	A	1680	LEU	3.8
1	B	1863	PRO	3.7
1	A	1847	LEU	3.7
1	A	1295	PHE	3.7
1	B	1190	VAL	3.7
1	B	2129	GLN	3.7
1	A	2088	LEU	3.7
1	A	1184	GLU	3.7
1	B	878	GLN	3.7
1	B	1460	ASN	3.7
1	A	996	VAL	3.7
1	A	1860	ILE	3.7
1	A	2163	PHE	3.7
1	B	989	TYR	3.7
1	B	1845	GLN	3.7
1	A	1163	ASN	3.7
1	A	1185	PRO	3.7
1	A	982	VAL	3.6
1	B	1685	ASN	3.6
1	A	2133	GLN	3.6
1	A	1685	ASN	3.5
1	B	926	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	807	MET	3.5
1	A	2256	MET	3.5
1	A	1441	ASP	3.5
1	A	2164	TYR	3.5
1	A	1429	ALA	3.5
1	A	789	PRO	3.5
1	A	976	MET	3.5
1	A	1550	PRO	3.5
1	B	841	PHE	3.4
1	B	898	ASP	3.4
1	A	1672	ALA	3.4
1	A	2067	GLU	3.4
1	B	1103	GLU	3.4
1	A	1003	LEU	3.4
1	B	1473	MET	3.4
1	A	1459	ILE	3.4
1	B	1003	LEU	3.4
1	B	1295	PHE	3.3
1	B	1102	LEU	3.3
1	B	1030	ILE	3.3
1	A	1169	HIS	3.3
1	A	998	ASN	3.3
1	A	985	LEU	3.3
1	A	1845	GLN	3.3
1	A	1627	PHE	3.3
1	A	1389	LEU	3.3
1	B	852	MET	3.3
1	A	1557	ILE	3.3
1	B	892	PRO	3.3
1	A	1901	LEU	3.2
1	A	948	GLU	3.2
1	B	986	LEU	3.2
1	B	2240	ILE	3.2
1	A	930	LEU	3.2
1	B	827	PHE	3.2
1	A	1373	VAL	3.2
1	B	1075	VAL	3.2
1	A	865	GLU	3.2
1	B	970	LEU	3.2
1	B	1798	GLY	3.1
1	B	1257	VAL	3.1
1	A	973	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	815	ASP	3.0
1	A	1346	PHE	3.0
1	B	1129	ILE	3.0
1	A	840	GLU	3.0
1	A	1308	TYR	3.0
1	A	1618	THR	3.0
1	A	1771	ARG	3.0
1	B	1627	PHE	3.0
1	B	2132	VAL	3.0
1	B	1476	ARG	3.0
1	B	875	PRO	2.9
1	B	2035	GLU	2.9
1	A	1931	GLY	2.9
1	A	1612	TRP	2.9
1	A	1449	ARG	2.9
1	A	1183	ASP	2.9
1	A	2215	SER	2.9
1	A	999	VAL	2.9
1	B	929	LEU	2.9
1	A	951	ILE	2.8
1	A	1111	ARG	2.8
1	A	1375	ARG	2.8
1	A	1105	TYR	2.8
1	A	1423	HIS	2.8
1	B	1423	HIS	2.8
1	A	1424	THR	2.8
1	A	2171	LEU	2.8
1	B	1553	PHE	2.8
1	B	1026	ARG	2.8
1	B	1991	LEU	2.8
1	B	860	LEU	2.8
1	A	1973	THR	2.8
1	B	1284	ASP	2.8
1	B	1131	TRP	2.8
1	A	1476	ARG	2.7
1	A	1445	PRO	2.7
1	B	928	ASP	2.7
1	A	1888	ILE	2.7
1	B	2002	ARG	2.7
1	A	1477	VAL	2.7
1	B	874	PHE	2.7
1	A	1582	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1457	ILE	2.7
1	A	1932	VAL	2.7
1	A	1293	LEU	2.7
1	A	2028	ILE	2.6
1	A	2130	ILE	2.6
1	B	888	ASP	2.6
1	B	1987	PRO	2.6
1	A	1968	ASN	2.6
1	A	1354	VAL	2.6
1	B	818	VAL	2.6
1	A	1404	LEU	2.6
1	B	1990	ILE	2.6
1	A	2223	LYS	2.6
1	B	2027	PHE	2.6
1	A	1774	GLY	2.5
1	B	952	LEU	2.5
1	B	1606	SER	2.5
1	B	930	LEU	2.5
1	A	1784	GLN	2.5
1	A	1355	TYR	2.5
1	A	1997	PHE	2.5
1	B	1733	ILE	2.5
1	B	1840	VAL	2.5
1	B	2159	SER	2.5
1	B	1349	ASN	2.5
1	B	1458	ARG	2.5
1	B	801	ALA	2.5
1	A	1861	LEU	2.5
1	B	1420	ASN	2.5
1	A	1353	HIS	2.5
1	B	1867	PRO	2.4
1	B	1888	ILE	2.4
1	A	1170	SER	2.4
1	A	1297	CYS	2.4
1	A	2070	GLY	2.4
1	A	2233	TYR	2.4
1	A	2041	TRP	2.4
1	B	1068	ASP	2.4
1	A	1161	VAL	2.4
1	B	1995	ARG	2.4
1	A	1790	GLU	2.4
1	A	1258	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1421	PHE	2.4
1	B	1731	ILE	2.4
1	A	989	TYR	2.4
1	A	1017	GLN	2.3
1	A	1992	ALA	2.3
1	A	1046	HIS	2.3
1	B	1104	VAL	2.3
1	A	849	HIS	2.3
1	A	1325	GLU	2.3
1	B	2196	ASN	2.3
1	A	913	LEU	2.3
1	A	1436	LEU	2.3
1	B	1159	THR	2.3
1	A	1614	ILE	2.3
1	B	1844	VAL	2.3
1	A	807	MET	2.3
1	B	1905	ASP	2.3
1	A	2198	SER	2.3
1	B	1055	SER	2.3
1	A	2176	ILE	2.2
1	A	1298	GLY	2.2
1	A	2220	PRO	2.2
1	A	1787	VAL	2.2
1	B	876	ALA	2.2
1	B	2244	LEU	2.2
1	A	1446	ARG	2.2
1	A	844	GLN	2.2
1	B	1050	SER	2.2
1	B	1956	GLN	2.2
1	A	1694	PRO	2.2
1	A	869	ASN	2.2
1	A	1444	GLY	2.2
1	B	1919	VAL	2.2
1	A	1850	ILE	2.2
1	B	982	VAL	2.2
1	A	1326	PRO	2.2
1	A	1664	ILE	2.2
1	B	1155	SER	2.2
1	B	1817	LEU	2.2
1	B	1432	VAL	2.2
1	A	932	MET	2.2
1	B	1107	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1399	ASP	2.2
1	B	1444	GLY	2.2
1	B	1326	PRO	2.2
1	A	2036	LEU	2.2
1	B	1579	GLY	2.1
1	A	1345	VAL	2.1
1	A	2214	GLU	2.1
1	A	1164	ASP	2.1
1	B	1993	ASN	2.1
1	A	1848	SER	2.1
1	A	2128	HIS	2.1
1	B	2039	GLY	2.1
1	B	845	PHE	2.1
1	A	1797	THR	2.1
1	A	1791	GLY	2.1
1	B	925	LEU	2.1
1	B	1637	LYS	2.1
1	B	1677	ALA	2.1
1	B	1821	GLN	2.1
1	A	1274	ILE	2.1
1	A	1620	GLU	2.1
1	B	966	VAL	2.1
1	A	1632	ASN	2.1
1	A	926	ILE	2.1
1	B	1928	ILE	2.1
1	B	2038	GLY	2.1
1	B	968	THR	2.1
1	A	1257	VAL	2.1
1	A	1922	ARG	2.0
1	A	1834	LYS	2.0
1	A	861	THR	2.0
1	A	1162	GLU	2.0
1	B	2123	LEU	2.0
1	A	1316	ALA	2.0
1	A	972	HIS	2.0
1	B	1348	GLN	2.0
1	A	1082	VAL	2.0
1	B	1559	ASN	2.0
1	A	2004	MET	2.0
1	B	1644	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.