



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:20 AM UTC

PDB ID : 3BWE / pdb_00003bwe
Title : Crystal structure of aggregated form of DJ1
Authors : Cha, S.S.
Deposited on : 2008-01-09
Resolution : 2.40 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:

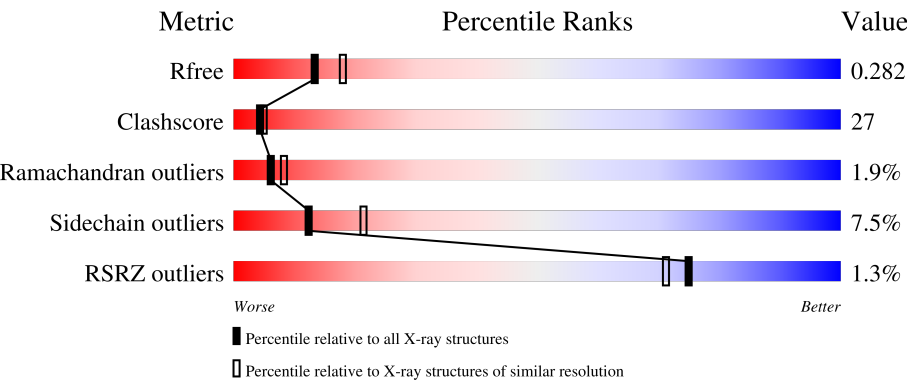
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	189	% 60%34%5% ..
1	B	189	% 59%35%5% ..
1	C	189	2% 52%40%7% ..
1	D	189	% 57%37% ..
1	E	189	2% 42%47%10% ..

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Mol	Chain	Length	Quality of chain
1	F	189	% 58% 37%
1	G	189	2% 44% 47% 7%

2 Entry composition [i](#)

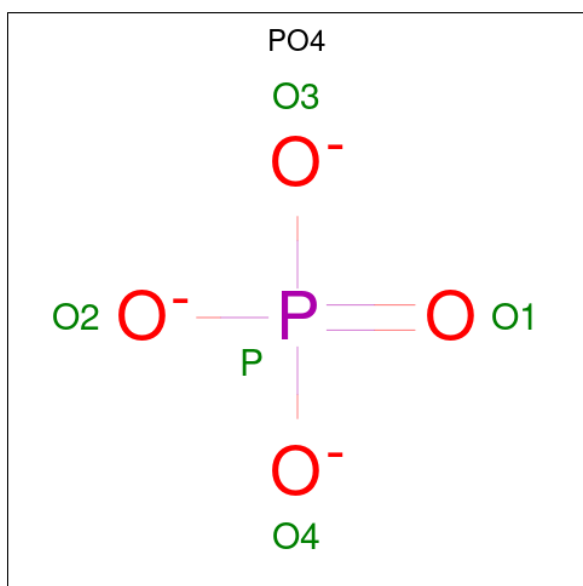
There are 3 unique types of molecules in this entry. The entry contains 9808 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein DJ-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	Se	0	0	0
			1368	859	238	264	3	4			
1	B	187	Total	C	N	O	S	Se	0	0	0
			1363	857	238	261	3	4			
1	C	188	Total	C	N	O	S	Se	0	0	0
			1368	859	238	264	3	4			
1	D	186	Total	C	N	O	S	Se	0	0	0
			1358	854	237	260	3	4			
1	E	188	Total	C	N	O	S	Se	0	0	0
			1351	849	238	257	3	4			
1	F	186	Total	C	N	O	S	Se	0	0	0
			1350	849	236	258	3	4			
1	G	186	Total	C	N	O	S	Se	0	0	0
			1332	838	231	256	3	4			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

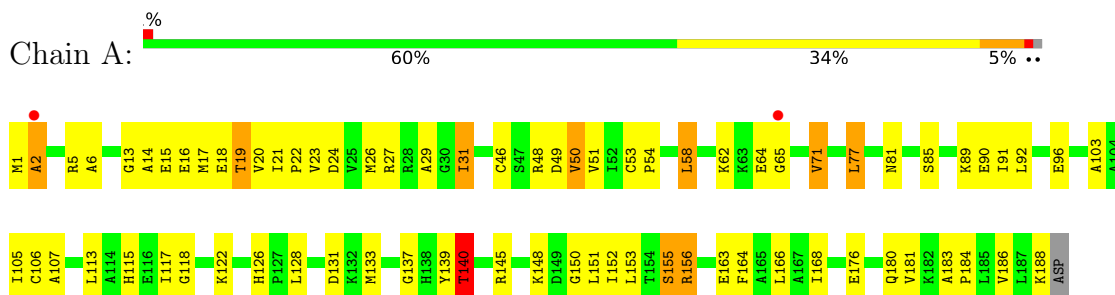
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	37	Total O 37 37	0	0
3	B	60	Total O 60 60	0	0
3	C	56	Total O 56 56	0	0
3	D	54	Total O 54 54	0	0
3	E	42	Total O 42 42	0	0
3	F	22	Total O 22 22	0	0
3	G	12	Total O 12 12	0	0

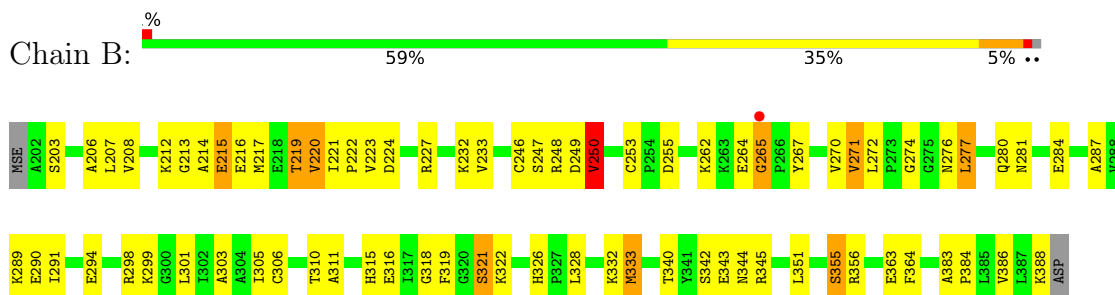
3 Residue-property plots

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

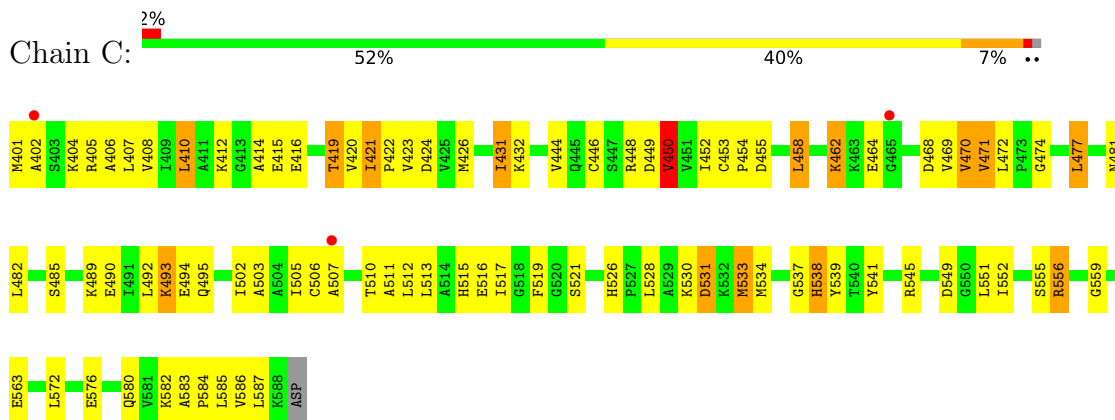
• Molecule 1: Protein DJ-1



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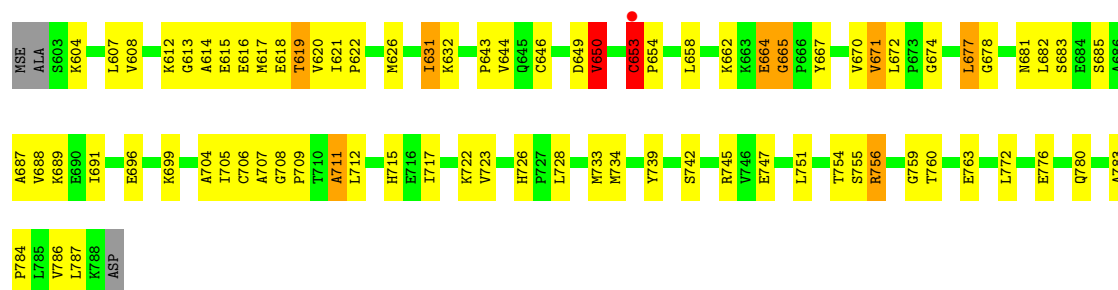


• Molecule 1: Protein DJ-1

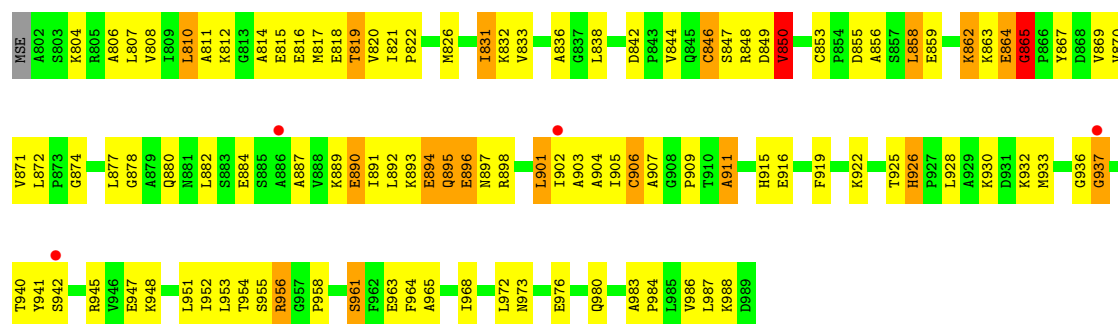
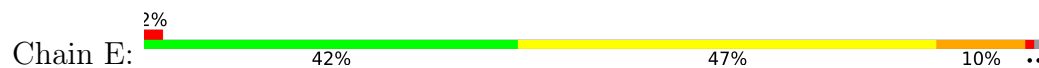


• Molecule 1: Protein DJ-1

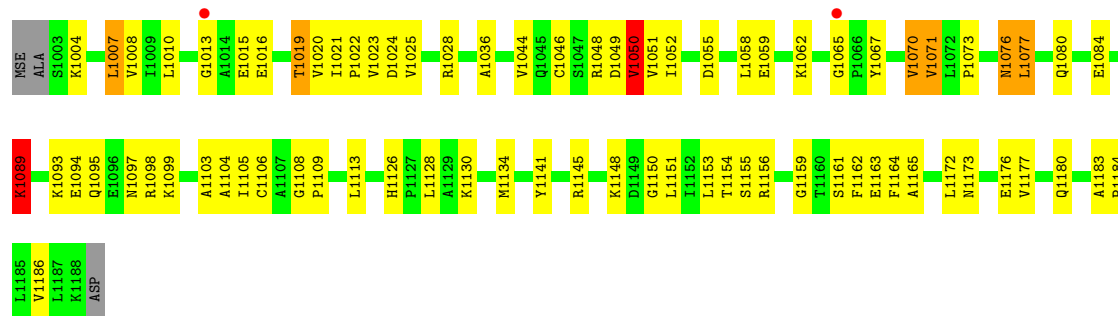




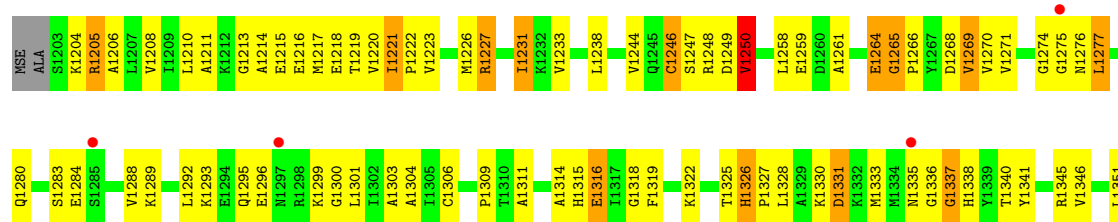
● Molecule 1: Protein DJ-1



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● Molecule 1: Protein DJ-1



I1352	I1353	T1354	S1355	R1356	G1357	P1358	G1359	T1360	S1361
F1364	A1365	L1366	A1367	I1368					
L1372	N1373	G1374	K1375	E1376					
Q1380	V1381	K1382	A1383	P1384					
L1387	K1388	ASP							

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.62Å 102.58Å 85.53Å 90.00° 113.69° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.99-2.40) 94.4 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.282 0.232 , 0.282	Depositor DCC
R_{free} test set	5761 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9808	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.51	0/1381	1.04	5/1863 (0.3%)
1	B	0.52	0/1376	1.04	7/1855 (0.4%)
1	C	0.55	1/1381 (0.1%)	1.07	9/1863 (0.5%)
1	D	0.53	0/1371	1.12	8/1848 (0.4%)
1	E	0.48	0/1364	1.09	13/1840 (0.7%)
1	F	0.48	0/1363	1.05	5/1839 (0.3%)
1	G	0.51	0/1345	1.05	10/1819 (0.5%)
All	All	0.51	1/9581 (0.0%)	1.06	57/12927 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	421	ILE	CA-CB	5.10	1.57	1.54

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	653	CYS	CA-C-N	12.16	135.04	119.84
1	D	653	CYS	C-N-CA	12.16	135.04	119.84
1	C	556	ARG	N-CA-C	8.98	124.66	112.90
1	C	453	CYS	CA-C-N	8.73	128.79	119.89
1	C	453	CYS	C-N-CA	8.73	128.79	119.89
1	E	894	GLU	N-CA-C	-8.46	101.75	110.97
1	F	1049	ASP	N-CA-C	8.04	122.67	112.86
1	A	156	ARG	N-CA-C	7.96	123.10	113.23
1	E	956	ARG	N-CA-C	7.92	121.45	111.24
1	B	356	ARG	N-CA-C	7.42	122.62	113.50
1	E	858	LEU	N-CA-C	-7.34	103.30	111.82
1	F	1156	ARG	N-CA-C	6.92	121.96	112.90
1	D	756	ARG	N-CA-C	6.70	119.58	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	VAL	N-CA-C	-6.36	100.56	109.21
1	D	650	VAL	N-CA-C	-6.32	101.39	109.80
1	D	707	ALA	N-CA-C	-6.29	105.61	113.28
1	C	511	ALA	N-CA-C	-6.06	104.23	111.69
1	C	453	CYS	CB-CA-C	6.01	116.12	110.17
1	G	1221	ILE	CB-CA-C	-6.00	108.00	113.70
1	G	1246	CYS	N-CA-C	5.99	118.62	110.35
1	B	249	ASP	N-CA-C	5.98	121.88	113.56
1	A	85	SER	N-CA-C	5.97	118.46	108.73
1	F	1055	ASP	N-CA-C	-5.85	105.64	112.89
1	E	911	ALA	N-CA-C	-5.83	105.43	112.54
1	G	1311	ALA	N-CA-C	-5.82	104.94	111.28
1	G	1326	HIS	N-CA-C	-5.80	101.77	110.24
1	F	1050	VAL	N-CA-C	-5.80	101.54	109.55
1	C	449	ASP	N-CA-C	5.74	121.54	113.56
1	E	907	ALA	N-CA-C	-5.66	106.37	113.28
1	E	895	GLN	N-CA-C	-5.64	101.50	109.96
1	A	107	ALA	N-CA-C	-5.61	106.60	113.50
1	B	311	ALA	N-CA-C	-5.55	105.31	111.36
1	D	649	ASP	N-CA-C	5.45	122.00	113.72
1	C	450	VAL	N-CA-C	-5.43	101.83	109.21
1	G	1374	GLY	N-CA-C	5.42	118.89	112.33
1	E	846	CYS	N-CA-C	5.40	118.32	110.17
1	A	140	THR	N-CA-C	-5.38	100.94	109.76
1	B	255	ASP	N-CA-C	-5.35	105.61	111.82
1	G	1357	GLY	CA-C-N	5.34	124.79	119.24
1	G	1357	GLY	C-N-CA	5.34	124.79	119.24
1	D	653	CYS	CB-CA-C	5.34	116.22	110.08
1	G	1220	VAL	N-CA-C	5.29	115.50	110.42
1	C	485	SER	N-CA-C	5.28	116.91	108.41
1	E	849	ASP	N-CA-C	5.25	121.70	113.72
1	A	49	ASP	N-CA-C	5.25	121.11	113.40
1	B	220	VAL	N-CA-C	5.25	115.46	110.53
1	G	1249	ASP	N-CA-C	5.25	121.97	110.80
1	F	1089	LYS	N-CA-C	-5.12	105.70	111.28
1	E	865	GLY	CA-C-N	5.07	125.51	120.14
1	E	865	GLY	C-N-CA	5.07	125.51	120.14
1	E	926	HIS	N-CA-C	-5.04	103.13	110.08
1	G	1250	VAL	N-CA-C	-5.04	103.08	109.58
1	E	855	ASP	N-CA-C	-5.02	105.90	112.23
1	E	850	VAL	N-CA-C	-5.02	103.10	109.58
1	D	711	ALA	N-CA-C	-5.01	105.94	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASN	N-CA-C	-5.00	103.88	110.43
1	C	455	ASP	N-CA-C	-5.00	106.69	112.89

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	1368	0	1403	71	0
1	B	1363	0	1405	67	0
1	C	1368	0	1399	85	0
1	D	1358	0	1399	69	0
1	E	1351	0	1377	89	0
1	F	1350	0	1385	54	0
1	G	1332	0	1348	107	0
2	A	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	0	0
3	A	37	0	0	1	0
3	B	60	0	0	4	0
3	C	56	0	0	2	0
3	D	54	0	0	1	0
3	E	42	0	0	2	0
3	F	22	0	0	1	0
3	G	12	0	0	1	0
All	All	9808	0	9716	514	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 27.

All (514) 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:113:LEU:HB2	1:A:133:MSE:HE1	1.23	1.15
1:B:203:SER:HB2	1:B:232:LYS:HE2	1.38	1.05
1:G:1205:ARG:HH11	1:G:1205:ARG:HB3	0.90	1.04
1:G:1205:ARG:HB3	1:G:1205:ARG:NH1	1.73	1.03
1:G:1205:ARG:HH11	1:G:1205:ARG:CB	1.75	0.98
1:A:16:GLU:HG2	1:A:50:VAL:HG22	1.45	0.95
1:A:6:ALA:HB2	1:A:31:ILE:HD11	1.47	0.94
1:D:705:ILE:HG13	1:D:755:SER:HB3	1.50	0.94
1:F:1070:VAL:HG12	1:F:1095:GLN:HE21	1.34	0.91
1:E:831:ILE:HD11	1:E:833:VAL:HG22	1.52	0.91
1:G:1221:ILE:HB	1:G:1222:PRO:HD3	1.51	0.91
1:E:948:LYS:HD3	1:E:953:LEU:HD12	1.53	0.90
1:F:1134:MSE:HE2	1:F:1141:TYR:HB2	1.55	0.89
1:B:383:ALA:HB3	1:B:384:PRO:HD3	1.54	0.88
1:B:310:THR:HA	1:B:333:MSE:HE1	1.56	0.88
1:A:113:LEU:HB2	1:A:133:MSE:CE	2.03	0.88
1:A:92:LEU:HB3	1:A:117:ILE:CD1	2.05	0.85
1:B:333:MSE:CE	1:B:333:MSE:HA	2.06	0.84
1:B:290:GLU:O	1:B:294:GLU:HG3	1.78	0.83
1:C:416:GLU:OE2	1:C:450:VAL:HG13	1.77	0.83
1:G:1383:ALA:HB3	1:G:1384:PRO:HD3	1.59	0.82
1:C:583:ALA:HB3	1:C:584:PRO:HD3	1.61	0.82
1:A:62:LYS:HE2	1:A:91:ILE:HG13	1.62	0.82
1:A:183:ALA:HB3	1:A:184:PRO:HD3	1.59	0.82
1:A:156:ARG:HH11	1:A:156:ARG:HG2	1.44	0.81
1:B:280:GLN:O	1:B:284:GLU:HG3	1.79	0.81
1:E:816:GLU:HG2	1:E:850:VAL:HG13	1.62	0.80
1:G:1210:LEU:HD12	1:G:1244:VAL:HG21	1.63	0.80
1:E:815:GLU:O	1:E:819:THR:HG22	1.82	0.80
1:B:305:ILE:HG13	1:B:355:SER:HB3	1.62	0.80
1:D:615:GLU:O	1:D:619:THR:HG22	1.82	0.80
1:A:16:GLU:HG2	1:A:50:VAL:CG2	2.13	0.79
1:C:526:HIS:HD2	1:C:528:LEU:H	1.30	0.78
1:G:1210:LEU:C	1:G:1210:LEU:HD13	2.10	0.76
1:C:410:LEU:HD22	1:C:444:VAL:HG11	1.66	0.76
1:B:318:GLY:O	1:B:321:SER:HB2	1.86	0.75
1:C:406:ALA:HB2	1:C:431:ILE:HD11	1.67	0.75
1:F:1148:LYS:HE2	1:F:1150:GLY:O	1.86	0.75
1:F:1016:GLU:HG2	1:F:1050:VAL:HG13	1.68	0.75
1:C:492:LEU:HB3	1:C:517:ILE:HD13	1.68	0.74
1:G:1295:GLN:NE2	1:G:1300:GLY:HA3	2.03	0.74
1:A:13:GLY:HA3	1:A:77:LEU:HB3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MSE:HE3	1:A:133:MSE:HA	1.68	0.74
1:B:333:MSE:HA	1:B:333:MSE:HE3	1.69	0.73
1:G:1213:GLY:HA2	1:G:1277:LEU:HD12	1.70	0.73
1:B:310:THR:HA	1:B:333:MSE:CE	2.17	0.73
1:D:621:ILE:HB	1:D:622:PRO:HD3	1.70	0.73
1:G:1264:GLU:O	1:G:1265:GLY:O	2.06	0.73
1:A:16:GLU:OE2	1:A:50:VAL:HG13	1.89	0.73
1:E:816:GLU:HG2	1:E:850:VAL:CG1	2.20	0.72
1:G:1210:LEU:CD1	1:G:1244:VAL:HG11	2.18	0.72
1:A:6:ALA:CB	1:A:31:ILE:HD11	2.19	0.72
1:F:1105:ILE:HG13	1:F:1155:SER:HB3	1.72	0.72
1:C:416:GLU:HG3	1:C:446:CYS:CB	2.20	0.72
1:A:16:GLU:HG3	1:A:46:CYS:CB	2.20	0.71
1:C:516:GLU:HA	1:C:519:PHE:CE1	2.26	0.71
1:E:863:LYS:O	1:E:865:GLY:N	2.23	0.70
1:G:1213:GLY:HA3	1:G:1277:LEU:HB2	1.71	0.70
1:E:905:ILE:HG13	1:E:955:SER:HB3	1.73	0.70
1:F:1013:GLY:HA3	1:F:1077:LEU:HB3	1.71	0.70
1:D:616:GLU:HG2	1:D:650:VAL:HG22	1.73	0.70
1:G:1214:ALA:O	1:G:1246:CYS:HB3	1.91	0.70
1:G:1213:GLY:CA	1:G:1277:LEU:HD12	2.23	0.69
1:G:1216:GLU:OE2	1:G:1216:GLU:N	2.23	0.69
1:B:232:LYS:HD2	1:C:401:MSE:O	1.91	0.69
1:A:16:GLU:HG3	1:A:46:CYS:HB2	1.73	0.69
1:B:208:VAL:HG22	1:B:271:VAL:HG22	1.73	0.69
1:D:722:LYS:HE2	1:D:742:SER:HB2	1.76	0.68
1:E:821:ILE:HB	1:E:822:PRO:HD3	1.75	0.68
1:C:551:LEU:C	1:C:552:ILE:HD12	2.19	0.68
1:B:216:GLU:HG2	1:B:250:VAL:HG22	1.76	0.67
1:D:674:GLY:HA3	1:D:706:CYS:HB3	1.76	0.67
1:F:1183:ALA:HB3	1:F:1184:PRO:HD3	1.76	0.67
1:G:1219:THR:O	1:G:1223:VAL:HG23	1.94	0.67
1:C:526:HIS:CD2	1:C:528:LEU:H	2.13	0.67
1:G:1210:LEU:HD11	1:G:1244:VAL:HG11	1.75	0.67
1:E:859:GLU:HA	1:E:862:LYS:NZ	2.10	0.66
1:G:1204:LYS:O	1:G:1231:ILE:HG13	1.95	0.66
1:G:1216:GLU:HG2	1:G:1250:VAL:HG22	1.77	0.66
1:G:1275:GLY:O	1:G:1277:LEU:HG	1.95	0.66
1:A:21:ILE:HB	1:A:22:PRO:HD3	1.76	0.66
1:G:1316:GLU:HB3	1:G:1319:PHE:CE2	2.31	0.66
1:C:416:GLU:HG3	1:C:446:CYS:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:810:LEU:HD22	1:E:844:VAL:HG11	1.78	0.66
1:F:1016:GLU:HG3	1:F:1050:VAL:HG22	1.78	0.66
1:G:1210:LEU:HD13	1:G:1211:ALA:N	2.10	0.65
1:A:122:LYS:HG3	1:A:140:THR:HG22	1.77	0.65
1:D:783:ALA:HB3	1:D:784:PRO:HD3	1.79	0.65
1:E:877:LEU:HB2	1:G:1376:GLU:HG3	1.79	0.65
1:B:213:GLY:HA3	1:B:277:LEU:HB3	1.79	0.65
1:E:906:CYS:HA	1:E:956:ARG:O	1.97	0.65
1:E:804:LYS:HG2	1:E:973:ASN:HD21	1.61	0.64
1:A:26:MSE:O	1:A:31:ILE:HG23	1.97	0.64
1:B:345:ARG:HD3	1:B:363:GLU:OE1	1.97	0.64
1:D:687:ALA:O	1:D:691:ILE:HG12	1.98	0.64
1:F:1108:GLY:N	1:F:1109:PRO:HD2	2.13	0.63
1:C:533:MSE:CE	1:C:533:MSE:HA	2.28	0.63
1:B:333:MSE:HA	1:B:333:MSE:HE2	1.80	0.63
1:B:345:ARG:NH2	1:B:363:GLU:OE2	2.31	0.63
1:F:1019:THR:HG22	1:F:1073:PRO:HB3	1.80	0.63
1:D:662:LYS:HD3	1:D:691:ILE:HD11	1.79	0.63
1:A:113:LEU:CB	1:A:133:MSE:HE1	2.15	0.63
1:D:631:ILE:HD12	1:D:632:LYS:N	2.13	0.63
1:A:156:ARG:HG2	1:A:156:ARG:NH1	2.09	0.63
1:D:745:ARG:HA	1:D:756:ARG:HG3	1.79	0.63
1:A:96:GLU:CD	1:A:117:ILE:HG23	2.25	0.62
1:E:831:ILE:HD12	1:E:831:ILE:C	2.24	0.62
1:G:1217:MSE:O	1:G:1221:ILE:HG12	1.99	0.62
1:C:510:THR:HA	1:C:533:MSE:HE1	1.80	0.62
1:C:582:LYS:HA	1:C:585:LEU:HD12	1.80	0.62
1:E:826:MSE:HE2	1:E:831:ILE:HG12	1.80	0.62
1:B:316:GLU:HA	1:B:319:PHE:CE1	2.34	0.62
1:G:1275:GLY:O	1:G:1276:ASN:HB3	1.98	0.62
1:E:814:ALA:O	1:E:846:CYS:HB3	1.99	0.62
1:E:880:GLN:O	1:E:884:GLU:HG3	1.99	0.62
1:E:808:VAL:HG22	1:E:871:VAL:CG1	2.29	0.62
1:E:902:ILE:C	1:E:902:ILE:HD12	2.25	0.61
1:F:1016:GLU:HG2	1:F:1050:VAL:CG1	2.29	0.61
1:E:986:VAL:HG12	1:E:986:VAL:O	2.00	0.61
1:A:58:LEU:O	1:A:62:LYS:HB2	2.01	0.61
1:E:816:GLU:OE1	1:E:850:VAL:HG13	2.01	0.61
1:F:1080:GLN:O	1:F:1084:GLU:HG3	2.01	0.61
1:G:1330:LYS:HE3	1:G:1341:TYR:CD2	2.36	0.61
1:A:1:MSE:O	1:A:2:ALA:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:ILE:CG1	1:D:755:SER:HB3	2.29	0.61
1:E:976:GLU:O	1:E:980:GLN:HG3	2.01	0.61
1:F:1089:LYS:O	1:F:1093:LYS:HG2	2.01	0.60
1:G:1216:GLU:HG3	1:G:1246:CYS:HB2	1.81	0.60
1:E:831:ILE:HD11	1:E:833:VAL:CG2	2.27	0.60
1:C:408:VAL:HG22	1:C:471:VAL:CG2	2.32	0.60
1:C:408:VAL:HG22	1:C:471:VAL:HG22	1.84	0.60
1:D:616:GLU:HG2	1:D:650:VAL:CG2	2.31	0.60
1:C:416:GLU:HG2	1:C:450:VAL:HG13	1.84	0.60
1:B:208:VAL:HG22	1:B:271:VAL:CG2	2.30	0.60
1:A:126:HIS:CD2	1:A:128:LEU:H	2.20	0.60
1:A:145:ARG:HD3	1:A:163:GLU:OE1	2.01	0.60
1:F:1059:GLU:HA	1:F:1062:LYS:HE3	1.82	0.60
1:D:786:VAL:HG12	1:D:786:VAL:O	2.00	0.59
1:E:901:LEU:HD12	1:E:972:LEU:HD11	1.84	0.59
1:G:1216:GLU:HG3	1:G:1246:CYS:CB	2.31	0.59
1:A:53:CYS:SG	1:B:253:CYS:SG	3.00	0.59
1:G:1216:GLU:HG2	1:G:1250:VAL:CG2	2.31	0.59
1:D:626:MSE:HB3	1:D:631:ILE:HG12	1.85	0.59
1:E:847:SER:OG	1:E:848:ARG:NH1	2.31	0.59
1:G:1325:THR:HG21	1:G:1333:MSE:HB2	1.83	0.59
1:A:105:ILE:HG13	1:A:155:SER:HB3	1.83	0.59
1:B:332:LYS:HE2	3:B:439:HOH:O	2.03	0.59
1:E:887:ALA:O	1:E:890:GLU:HB2	2.03	0.59
1:A:133:MSE:HE2	1:A:139:TYR:CE1	2.38	0.59
1:B:262:LYS:HD2	3:B:435:HOH:O	2.02	0.59
1:C:420:VAL:HG21	1:D:620:VAL:HG21	1.85	0.58
1:E:826:MSE:HE2	1:E:831:ILE:CD1	2.33	0.58
1:E:922:LYS:HG2	1:E:947:GLU:HG2	1.85	0.58
1:A:14:ALA:O	1:A:46:CYS:HB3	2.04	0.58
1:A:24:ASP:CG	1:B:217:MSE:HE2	2.28	0.58
1:E:838:LEU:HD12	1:E:858:LEU:HD22	1.86	0.58
1:G:1376:GLU:O	1:G:1380:GLN:HG3	2.03	0.58
1:C:415:GLU:O	1:C:419:THR:HG22	2.04	0.58
1:E:889:LYS:HB2	1:E:915:HIS:ND1	2.19	0.57
1:B:216:GLU:OE1	1:B:248:ARG:N	2.35	0.57
1:C:545:ARG:HD3	1:C:563:GLU:OE1	2.03	0.57
1:B:326:HIS:CD2	1:B:328:LEU:H	2.22	0.57
1:F:1104:ALA:O	1:F:1154:THR:HA	2.04	0.57
1:D:608:VAL:HG13	1:D:671:VAL:CG2	2.33	0.57
1:C:533:MSE:HA	1:C:533:MSE:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1024:ASP:O	1:F:1028:ARG:HG3	2.05	0.57
1:G:1216:GLU:CG	1:G:1250:VAL:HG22	2.34	0.57
1:A:151:LEU:C	1:A:152:ILE:HD12	2.30	0.57
1:G:1351:LEU:O	1:G:1352:ILE:HD12	2.05	0.57
1:F:1015:GLU:O	1:F:1019:THR:HG23	2.04	0.57
1:E:826:MSE:HB3	1:E:831:ILE:CG1	2.35	0.56
1:G:1218:GLU:OE1	1:G:1306:CYS:HB2	2.05	0.56
1:E:983:ALA:HB3	1:E:984:PRO:HD3	1.87	0.56
1:G:1216:GLU:HG2	1:G:1250:VAL:HG13	1.87	0.56
1:G:1303:ALA:HA	1:G:1353:LEU:O	2.06	0.56
1:A:145:ARG:NH2	1:A:163:GLU:OE2	2.39	0.56
1:F:1021:ILE:O	1:F:1025:VAL:HG23	2.06	0.56
1:B:384:PRO:O	1:B:386:VAL:HG23	2.06	0.56
1:E:859:GLU:HA	1:E:862:LYS:HZ2	1.70	0.56
1:G:1238:LEU:HD12	1:G:1258:LEU:HD12	1.86	0.56
1:A:16:GLU:CG	1:A:50:VAL:HG22	2.29	0.56
1:D:616:GLU:CG	1:D:650:VAL:HG22	2.35	0.55
1:C:521:SER:HA	1:C:549:ASP:OD2	2.06	0.55
1:G:1289:LYS:HG3	1:G:1315:HIS:CG	2.41	0.55
1:B:216:GLU:CG	1:B:250:VAL:HG22	2.35	0.55
1:F:1008:VAL:HG22	1:F:1071:VAL:HG22	1.89	0.55
1:A:126:HIS:HD2	1:A:128:LEU:H	1.53	0.55
1:C:474:GLY:HA3	1:C:506:CYS:HB3	1.87	0.55
1:B:287:ALA:O	1:B:291:ILE:HG12	2.07	0.54
1:C:421:ILE:HB	1:C:422:PRO:HD3	1.89	0.54
1:D:723:VAL:HB	1:D:754:THR:HG21	1.89	0.54
1:G:1210:LEU:HD11	1:G:1244:VAL:CG1	2.37	0.54
1:B:215:GLU:O	1:B:219:THR:HG22	2.07	0.54
1:C:416:GLU:HG2	1:C:450:VAL:HG22	1.90	0.54
1:E:821:ILE:HD12	1:E:961:SER:HB3	1.89	0.54
1:E:838:LEU:HD12	1:E:858:LEU:CD2	2.37	0.54
1:G:1210:LEU:C	1:G:1210:LEU:CD1	2.79	0.54
1:C:414:ALA:O	1:C:446:CYS:HB3	2.08	0.54
1:A:15:GLU:O	1:A:19:THR:HG22	2.07	0.54
1:A:20:VAL:HG21	1:B:220:VAL:HG21	1.90	0.53
1:B:322:LYS:HE2	1:B:342:SER:HB2	1.90	0.53
1:F:1008:VAL:HG22	1:F:1071:VAL:CG2	2.39	0.53
1:B:298:ARG:HG2	1:B:298:ARG:O	2.08	0.53
1:B:345:ARG:HH21	1:B:363:GLU:CD	2.17	0.53
1:E:872:LEU:HD23	1:E:911:ALA:HB3	1.90	0.53
1:G:1280:GLN:HG2	1:G:1284:GLU:OE2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:HD12	1:B:351:LEU:O	2.09	0.53
1:G:1216:GLU:HG2	1:G:1250:VAL:CG1	2.38	0.53
1:D:689:LYS:HB2	1:D:715:HIS:ND1	2.24	0.53
1:G:1345:ARG:HH11	1:G:1345:ARG:HG2	1.74	0.53
1:C:462:LYS:HD2	1:C:462:LYS:O	2.09	0.53
1:C:477:LEU:HD22	1:C:481:ASN:ND2	2.24	0.53
1:F:1021:ILE:HB	1:F:1022:PRO:HD3	1.90	0.53
1:A:92:LEU:HB3	1:A:117:ILE:HD12	1.89	0.53
1:A:155:SER:HB2	1:A:164:PHE:CD1	2.44	0.53
1:B:216:GLU:HG2	1:B:250:VAL:CG2	2.38	0.53
1:B:355:SER:HB2	1:B:364:PHE:CD1	2.43	0.53
1:D:608:VAL:HG13	1:D:671:VAL:HG22	1.91	0.53
1:E:816:GLU:CG	1:E:850:VAL:HG13	2.35	0.53
1:E:987:LEU:HD23	1:F:1159:GLY:CA	2.39	0.53
1:F:1022:PRO:HA	1:F:1165:ALA:HB2	1.91	0.52
1:F:1177:VAL:HG23	3:F:164:HOH:O	2.08	0.52
1:G:1335:ASN:O	1:G:1336:GLY:C	2.52	0.52
1:B:221:ILE:HB	1:B:222:PRO:HD3	1.92	0.52
1:D:672:LEU:N	1:D:672:LEU:HD12	2.24	0.52
1:E:901:LEU:HD12	1:E:972:LEU:CD1	2.38	0.52
1:A:16:GLU:O	1:A:20:VAL:HG23	2.10	0.52
1:E:818:GLU:OE2	1:E:874:GLY:HA3	2.10	0.52
1:D:745:ARG:HG3	3:D:123:HOH:O	2.08	0.52
1:D:622:PRO:O	1:D:626:MSE:HG3	2.09	0.52
1:D:677:LEU:HD22	1:D:681:ASN:ND2	2.24	0.52
1:A:5:ARG:HH22	1:A:64:GLU:HG2	1.74	0.52
1:B:227:ARG:HD3	3:B:395:HOH:O	2.09	0.52
1:C:545:ARG:NH1	1:D:786:VAL:O	2.43	0.52
1:G:1268:ASP:O	1:G:1269:VAL:HB	2.10	0.52
1:G:1299:LYS:C	1:G:1351:LEU:HD13	2.35	0.52
1:A:92:LEU:HB3	1:A:117:ILE:HD11	1.91	0.52
1:B:223:VAL:O	1:B:227:ARG:HG3	2.10	0.52
1:D:678:GLY:O	1:D:682:LEU:HD13	2.08	0.52
1:B:212:LYS:O	1:B:277:LEU:HD13	2.10	0.51
1:G:1322:LYS:HA	1:G:1340:THR:HB	1.90	0.51
1:E:987:LEU:HD23	1:F:1159:GLY:HA2	1.91	0.51
1:G:1316:GLU:HA	1:G:1319:PHE:CZ	2.45	0.51
1:A:188:LYS:N	1:B:345:ARG:NH1	2.58	0.51
1:C:510:THR:HA	1:C:533:MSE:CE	2.40	0.51
1:D:616:GLU:HG3	1:D:646:CYS:HB2	1.93	0.51
1:D:745:ARG:NH2	1:D:760:THR:HG22	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1213:GLY:O	1:G:1277:LEU:HD12	2.10	0.51
1:G:1330:LYS:O	1:G:1331:ASP:C	2.54	0.51
1:C:490:GLU:HG2	1:C:494:GLU:OE2	2.10	0.51
1:E:807:LEU:HB2	1:E:867:TYR:CG	2.45	0.51
1:F:1094:GLU:O	1:F:1098:ARG:HB2	2.10	0.51
1:B:214:ALA:O	1:B:246:CYS:HB3	2.10	0.51
1:C:586:VAL:HG12	1:C:586:VAL:O	2.10	0.51
1:G:1223:VAL:O	1:G:1227:ARG:HG3	2.11	0.51
1:G:1366:LEU:HD11	1:G:1382:LYS:HG3	1.93	0.51
1:C:426:MSE:O	1:C:431:ILE:HG23	2.10	0.51
1:G:1326:HIS:CD2	1:G:1328:LEU:H	2.29	0.51
1:D:604:LYS:HB3	1:D:772:LEU:HD23	1.93	0.51
1:G:1208:VAL:HG22	1:G:1271:VAL:CG2	2.40	0.51
1:C:408:VAL:HA	1:C:471:VAL:HG22	1.93	0.50
1:D:616:GLU:HG2	1:D:650:VAL:HG13	1.92	0.50
1:D:643:PRO:HG3	1:D:653:CYS:HB3	1.93	0.50
1:D:734:MSE:HE1	1:D:739:TYR:O	2.10	0.50
1:B:271:VAL:HA	1:B:303:ALA:O	2.10	0.50
1:F:1036:ALA:HB1	1:F:1058:LEU:HA	1.92	0.50
1:G:1315:HIS:O	1:G:1316:GLU:C	2.53	0.50
1:C:416:GLU:CG	1:C:446:CYS:HB2	2.41	0.50
1:C:471:VAL:HA	1:C:503:ALA:O	2.10	0.50
1:E:826:MSE:HE2	1:E:831:ILE:CG1	2.41	0.50
1:C:513:LEU:HB3	1:C:533:MSE:HE1	1.94	0.50
1:F:1176:GLU:O	1:F:1180:GLN:HG3	2.10	0.50
1:G:1216:GLU:CG	1:G:1246:CYS:HB2	2.42	0.50
1:A:126:HIS:HE1	1:B:384:PRO:O	1.94	0.50
1:B:326:HIS:HD2	1:B:328:LEU:H	1.58	0.49
1:C:416:GLU:HG2	1:C:450:VAL:CG1	2.42	0.49
1:D:723:VAL:HG21	1:D:733:MSE:CE	2.42	0.49
1:G:1215:GLU:HA	1:G:1247:SER:OG	2.12	0.49
1:G:1345:ARG:HG2	1:G:1345:ARG:NH1	2.27	0.49
1:A:89:LYS:HB2	1:A:115:HIS:CE1	2.47	0.49
1:C:494:GLU:HA	3:C:237:HOH:O	2.11	0.49
1:E:806:ALA:HB2	1:E:826:MSE:HE1	1.93	0.49
1:E:926:HIS:CD2	1:E:928:LEU:H	2.30	0.49
1:F:1019:THR:O	1:F:1023:VAL:HG23	2.11	0.49
1:E:902:ILE:CG1	1:E:952:ILE:HD13	2.42	0.49
1:A:77:LEU:HD22	1:A:81:ASN:ND2	2.26	0.49
1:E:902:ILE:HD12	1:E:902:ILE:O	2.13	0.49
1:E:964:PHE:O	1:E:968:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLU:CG	1:A:46:CYS:HB2	2.41	0.49
1:E:816:GLU:HG3	1:E:846:CYS:CB	2.42	0.49
1:A:103:ALA:HA	1:A:153:LEU:O	2.12	0.49
1:B:216:GLU:HG3	1:B:246:CYS:HB2	1.95	0.49
1:C:405:ARG:NH2	1:C:464:GLU:O	2.46	0.49
1:D:616:GLU:HG3	1:D:646:CYS:CB	2.43	0.49
1:E:836:ALA:HA	1:E:856:ALA:O	2.13	0.49
1:E:916:GLU:HA	1:E:919:PHE:CE2	2.47	0.49
1:B:274:GLY:HA3	1:B:306:CYS:HB3	1.95	0.48
1:E:811:ALA:O	1:E:812:LYS:C	2.54	0.48
1:C:472:LEU:HD11	1:C:492:LEU:HD11	1.95	0.48
1:E:878:GLY:O	1:E:882:LEU:HG	2.12	0.48
1:B:310:THR:HG22	1:B:333:MSE:HE3	1.94	0.48
1:C:431:ILE:HD12	1:C:572:LEU:HD23	1.95	0.48
1:C:492:LEU:HB3	1:C:517:ILE:CD1	2.40	0.48
1:D:607:LEU:HB2	1:D:667:TYR:CG	2.48	0.48
1:E:945:ARG:HD3	1:E:963:GLU:OE1	2.14	0.48
1:G:1303:ALA:HB1	1:G:1364:PHE:CZ	2.49	0.48
1:G:1277:LEU:HD23	1:G:1277:LEU:N	2.28	0.48
1:G:1216:GLU:OE1	1:G:1248:ARG:N	2.43	0.48
1:A:117:ILE:HG22	1:A:118:GLY:N	2.29	0.48
1:F:1058:LEU:C	1:F:1058:LEU:HD13	2.39	0.48
1:F:1099:LYS:C	1:F:1151:LEU:HD13	2.39	0.48
1:A:17:MSE:HE2	1:B:224:ASP:CG	2.39	0.47
1:D:671:VAL:C	1:D:672:LEU:HD12	2.39	0.47
1:E:951:LEU:N	1:E:951:LEU:HD22	2.29	0.47
1:C:489:LYS:HG2	1:C:493:LYS:CE	2.44	0.47
1:E:831:ILE:HD12	1:E:832:LYS:N	2.29	0.47
1:E:894:GLU:O	1:E:897:ASN:HB3	2.14	0.47
1:G:1204:LYS:HG2	1:G:1373:ASN:HD21	1.79	0.47
1:D:699:LYS:C	1:D:751:LEU:HD13	2.38	0.47
1:G:1330:LYS:HG3	1:G:1341:TYR:CE1	2.50	0.47
1:D:683:SER:OG	1:D:711:ALA:HA	2.14	0.47
1:D:616:GLU:HG2	1:D:650:VAL:CG1	2.44	0.47
1:B:305:ILE:CG1	1:B:355:SER:HB3	2.38	0.47
1:C:406:ALA:CB	1:C:431:ILE:HD11	2.40	0.47
1:C:505:ILE:HG13	1:C:555:SER:HB3	1.97	0.47
1:C:519:PHE:CD2	1:C:538:HIS:HB3	2.49	0.47
1:C:583:ALA:CB	1:C:584:PRO:HD3	2.40	0.47
1:D:696:GLU:CD	1:D:717:ILE:HG23	2.40	0.47
1:G:1326:HIS:HD2	1:G:1328:LEU:H	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LYS:HB3	1:B:262:LYS:HE2	1.68	0.47
1:B:289:LYS:HG3	1:B:315:HIS:HB3	1.96	0.47
1:C:587:LEU:HD23	1:D:759:GLY:HA2	1.97	0.47
1:E:872:LEU:HD21	1:E:892:LEU:HD11	1.97	0.47
1:F:1016:GLU:CD	1:F:1048:ARG:H	2.22	0.47
1:F:1145:ARG:NH2	1:F:1163:GLU:OE2	2.48	0.47
1:G:1206:ALA:HB2	1:G:1231:ILE:HD11	1.97	0.47
1:G:1206:ALA:HB3	1:G:1233:VAL:HG22	1.97	0.47
1:G:1296:GLU:OE2	1:G:1318:GLY:N	2.48	0.47
1:D:704:ALA:O	1:D:754:THR:HA	2.14	0.47
1:A:1:MSE:O	1:A:2:ALA:CB	2.63	0.46
1:C:469:VAL:HG22	1:C:470:VAL:N	2.29	0.46
1:F:1161:SER:O	1:F:1164:PHE:HB3	2.15	0.46
1:A:164:PHE:O	1:A:168:ILE:HG13	2.14	0.46
1:D:726:HIS:CD2	1:D:728:LEU:H	2.32	0.46
1:C:526:HIS:HA	1:C:556:ARG:O	2.15	0.46
1:D:608:VAL:HG22	1:D:671:VAL:HG22	1.98	0.46
1:D:708:GLY:N	1:D:709:PRO:HD2	2.29	0.46
1:A:51:VAL:HB	1:B:253:CYS:HB2	1.97	0.46
1:E:895:GLN:HG2	1:E:902:ILE:HG22	1.97	0.46
1:B:219:THR:O	1:B:223:VAL:HG23	2.16	0.46
1:B:299:LYS:C	1:B:351:LEU:HD13	2.40	0.46
1:D:685:SER:HB3	1:D:688:VAL:HB	1.98	0.46
1:E:871:VAL:HA	1:E:903:ALA:O	2.16	0.46
1:E:895:GLN:O	1:E:896:GLU:CB	2.64	0.46
1:E:945:ARG:HG3	3:E:141:HOH:O	2.15	0.46
1:D:612:LYS:HA	1:D:644:VAL:HG13	1.96	0.46
1:E:820:VAL:HG21	1:F:1020:VAL:HG21	1.97	0.46
1:G:1283:SER:HB3	1:G:1314:ALA:CB	2.45	0.46
1:A:186:VAL:HG12	1:A:186:VAL:O	2.15	0.46
1:G:1269:VAL:HA	1:G:1301:LEU:O	2.17	0.46
1:G:1274:GLY:HA3	1:G:1306:CYS:HB3	1.97	0.46
1:B:216:GLU:HG3	1:B:246:CYS:CB	2.46	0.45
1:D:664:GLU:O	1:D:665:GLY:O	2.34	0.45
1:D:613:GLY:HA3	1:D:677:LEU:HB3	1.97	0.45
1:E:930:LYS:HE3	1:E:941:TYR:CD2	2.52	0.45
1:G:1247:SER:C	1:G:1248:ARG:HD2	2.40	0.45
1:G:1275:GLY:O	1:G:1276:ASN:CB	2.65	0.45
1:C:526:HIS:HE1	1:D:784:PRO:O	1.99	0.45
1:E:893:LYS:O	1:E:897:ASN:HB3	2.16	0.45
1:F:1010:LEU:HG	1:F:1044:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1319:PHE:CD1	1:G:1338:HIS:HB3	2.51	0.45
1:E:816:GLU:HG3	1:E:846:CYS:HB2	1.97	0.45
1:F:1008:VAL:HA	1:F:1071:VAL:HG22	1.98	0.45
1:G:1276:ASN:HB3	1:G:1277:LEU:HD23	1.98	0.45
1:E:817:MSE:SE	1:F:1162:PHE:CZ	3.20	0.45
1:F:1076:ASN:C	1:F:1076:ASN:HD22	2.24	0.45
1:F:1172:LEU:C	1:F:1173:ASN:HD22	2.23	0.45
1:G:1204:LYS:C	1:G:1231:ILE:HG13	2.41	0.45
1:A:148:LYS:NZ	1:A:150:GLY:O	2.44	0.45
1:B:247:SER:C	1:B:248:ARG:HD2	2.42	0.45
1:G:1261:ALA:O	1:G:1264:GLU:HB2	2.17	0.45
1:G:1387:LEU:O	1:G:1388:LYS:C	2.59	0.45
1:E:858:LEU:HD11	1:E:891:ILE:CD1	2.47	0.45
1:E:901:LEU:HD23	1:E:951:LEU:O	2.16	0.45
1:E:904:ALA:O	1:E:954:THR:HA	2.17	0.45
1:G:1355:SER:HB2	1:G:1364:PHE:CD1	2.52	0.45
1:D:614:ALA:O	1:D:646:CYS:HB3	2.16	0.45
1:G:1352:ILE:O	1:G:1352:ILE:HG22	2.16	0.45
1:G:1304:ALA:O	1:G:1354:THR:HA	2.17	0.45
1:A:29:ALA:HA	1:A:181:VAL:HG21	1.99	0.45
1:C:587:LEU:HD23	1:D:759:GLY:CA	2.47	0.45
1:D:621:ILE:CB	1:D:622:PRO:HD3	2.45	0.45
1:F:1022:PRO:HA	1:F:1165:ALA:CB	2.47	0.45
1:A:176:GLU:O	1:A:180:GLN:HG3	2.17	0.44
1:C:489:LYS:HG3	1:C:515:HIS:HB3	1.99	0.44
1:E:889:LYS:O	1:E:893:LYS:HG2	2.17	0.44
1:F:1113:LEU:HD12	1:F:1113:LEU:O	2.17	0.44
1:G:1292:LEU:O	1:G:1293:LYS:C	2.60	0.44
1:C:552:ILE:HD12	1:C:552:ILE:N	2.31	0.44
1:G:1351:LEU:C	1:G:1352:ILE:HD12	2.43	0.44
1:G:1364:PHE:O	1:G:1368:ILE:HG13	2.17	0.44
1:A:71:VAL:HA	1:A:103:ALA:O	2.17	0.44
1:D:631:ILE:HD12	1:D:632:LYS:C	2.42	0.44
1:A:62:LYS:NZ	1:A:90:GLU:OE2	2.51	0.44
1:C:416:GLU:HG2	1:C:450:VAL:CG2	2.47	0.44
1:G:1221:ILE:HB	1:G:1222:PRO:CD	2.34	0.44
1:G:1247:SER:HA	1:G:1277:LEU:CD1	2.48	0.44
1:C:576:GLU:O	1:C:580:GLN:HG3	2.18	0.44
1:D:618:GLU:OE1	1:D:706:CYS:HB2	2.17	0.44
1:E:945:ARG:NH1	1:F:1186:VAL:O	2.51	0.44
1:G:1226:MSE:O	1:G:1231:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASP:HB2	3:A:207:HOH:O	2.17	0.44
1:A:113:LEU:HD22	1:A:133:MSE:HE3	1.99	0.44
1:A:145:ARG:NH1	1:B:388:LYS:N	2.65	0.44
1:C:416:GLU:CD	1:C:448:ARG:H	2.26	0.44
1:C:495:GLN:HA	1:C:495:GLN:OE1	2.18	0.44
1:E:853:CYS:HB2	1:F:1051:VAL:HB	1.99	0.44
1:D:726:HIS:HD2	1:D:728:LEU:H	1.66	0.44
1:C:587:LEU:C	1:D:745:ARG:NH1	2.76	0.43
1:G:1221:ILE:HG21	1:G:1361:SER:HB3	2.00	0.43
1:A:184:PRO:O	1:A:186:VAL:HG23	2.18	0.43
1:C:502:ILE:HG21	1:C:512:LEU:HD21	2.00	0.43
1:E:909:PRO:CG	1:E:925:THR:HG22	2.48	0.43
1:C:424:ASP:CG	1:D:617:MSE:HE2	2.43	0.43
1:D:723:VAL:HG21	1:D:733:MSE:HE2	2.00	0.43
1:F:1004:LYS:HB3	1:F:1172:LEU:HD23	1.99	0.43
1:G:1231:ILE:HD12	1:G:1372:LEU:HD12	2.01	0.43
1:G:1276:ASN:O	1:G:1280:GLN:HB2	2.18	0.43
1:A:153:LEU:HD23	1:A:168:ILE:HG12	2.01	0.43
1:C:530:LYS:HG3	1:C:541:TYR:CE1	2.53	0.43
1:G:1336:GLY:O	1:G:1337:GLY:C	2.61	0.43
1:A:145:ARG:NH1	1:B:386:VAL:O	2.51	0.43
1:A:152:ILE:HD12	1:A:152:ILE:N	2.32	0.43
1:D:709:PRO:O	1:D:712:LEU:HB2	2.19	0.43
1:E:932:LYS:O	1:E:933:MSE:C	2.61	0.43
1:E:958:PRO:O	1:E:961:SER:HB2	2.19	0.43
1:F:1097:ASN:N	1:F:1097:ASN:HD22	2.16	0.43
1:C:559:GLY:HA2	1:D:787:LEU:HD23	2.01	0.43
1:C:506:CYS:SG	1:C:507:ALA:N	2.91	0.43
1:E:909:PRO:HG2	1:E:925:THR:HG22	2.00	0.43
1:C:416:GLU:CD	1:C:450:VAL:HG13	2.42	0.43
1:B:264:GLU:O	1:B:265:GLY:O	2.36	0.43
1:F:1016:GLU:CD	1:F:1046:CYS:HB2	2.43	0.43
1:G:1277:LEU:CD2	1:G:1277:LEU:H	2.24	0.43
1:G:1325:THR:HG21	1:G:1333:MSE:CB	2.49	0.43
1:G:1333:MSE:C	1:G:1335:ASN:H	2.26	0.43
1:C:416:GLU:CG	1:C:450:VAL:HG13	2.47	0.42
1:C:492:LEU:CB	1:C:517:ILE:CD1	2.97	0.42
1:A:53:CYS:HA	1:A:54:PRO:HD3	1.81	0.42
1:E:926:HIS:HD2	1:E:928:LEU:H	1.65	0.42
1:E:936:GLY:O	1:E:937:GLY:C	2.61	0.42
1:G:1277:LEU:HD23	1:G:1277:LEU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD13	1:B:281:ASN:ND2	2.34	0.42
1:C:419:THR:O	1:C:423:VAL:HG23	2.19	0.42
1:D:604:LYS:N	1:D:604:LYS:HD2	2.34	0.42
1:D:616:GLU:O	1:D:619:THR:HG23	2.18	0.42
1:G:1304:ALA:HB1	1:G:1309:PRO:N	2.35	0.42
1:A:184:PRO:O	1:B:326:HIS:HE1	2.02	0.42
1:C:533:MSE:HA	1:C:533:MSE:HE2	2.01	0.42
1:D:776:GLU:O	1:D:780:GLN:HG3	2.20	0.42
1:E:869:VAL:HG23	1:E:901:LEU:HB3	2.01	0.42
1:E:945:ARG:HA	1:E:956:ARG:HG3	2.02	0.42
1:E:988:LYS:CB	1:F:1145:ARG:NH2	2.82	0.42
1:G:1358:PRO:C	1:G:1360:THR:H	2.28	0.42
1:C:462:LYS:HE3	3:C:83:HOH:O	2.20	0.42
1:D:664:GLU:O	1:D:665:GLY:C	2.63	0.42
1:A:18:GLU:O	1:A:22:PRO:HG2	2.20	0.42
1:D:653:CYS:HA	1:D:654:PRO:HD3	1.59	0.42
1:D:722:LYS:HD3	1:D:747:GLU:OE2	2.20	0.42
1:E:847:SER:C	1:E:848:ARG:HD2	2.45	0.42
1:E:850:VAL:HA	3:E:276:HOH:O	2.19	0.42
1:F:1007:LEU:HD12	1:F:1067:TYR:CD2	2.55	0.42
1:F:1010:LEU:HD21	1:F:1052:ILE:HB	2.01	0.42
1:B:318:GLY:HA2	3:B:407:HOH:O	2.19	0.41
1:C:404:LYS:HD2	1:C:468:ASP:CG	2.46	0.41
1:C:452:ILE:O	1:C:454:PRO:HD3	2.20	0.41
1:C:513:LEU:CB	1:C:533:MSE:HE1	2.50	0.41
1:B:216:GLU:CD	1:B:246:CYS:HB2	2.45	0.41
1:C:458:LEU:HD23	1:C:458:LEU:HA	1.94	0.41
1:G:1346:VAL:O	1:G:1346:VAL:HG23	2.20	0.41
1:B:207:LEU:HB2	1:B:267:TYR:CG	2.54	0.41
1:G:1208:VAL:HG22	1:G:1271:VAL:HG22	2.02	0.41
1:A:166:LEU:HA	1:A:166:LEU:HD23	1.84	0.41
1:C:412:LYS:O	1:C:481:ASN:ND2	2.53	0.41
1:C:416:GLU:HG3	1:C:446:CYS:HB3	2.01	0.41
1:E:822:PRO:HA	1:E:965:ALA:HB2	2.02	0.41
1:E:891:ILE:C	1:E:893:LYS:H	2.28	0.41
1:A:16:GLU:OE2	1:A:48:ARG:HB2	2.20	0.41
1:B:206:ALA:HB3	1:B:233:VAL:HG22	2.02	0.41
1:C:489:LYS:HG2	1:C:493:LYS:HE3	2.03	0.41
1:C:489:LYS:HE3	1:C:493:LYS:HE2	2.03	0.41
1:E:817:MSE:HE2	1:F:1024:ASP:CG	2.45	0.41
1:G:1283:SER:O	1:G:1315:HIS:CE1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1288:VAL:O	1:G:1292:LEU:HG	2.21	0.41
1:C:472:LEU:HD22	1:C:482:LEU:HD13	2.03	0.41
1:C:534:MSE:HE1	1:C:539:TYR:O	2.20	0.41
1:D:631:ILE:HD12	1:D:631:ILE:C	2.45	0.41
1:G:1213:GLY:C	1:G:1277:LEU:HD12	2.46	0.41
1:G:1382:LYS:HG3	1:G:1387:LEU:HD12	2.01	0.41
1:A:23:VAL:O	1:A:27:ARG:HG3	2.22	0.40
1:C:537:GLY:O	1:C:539:TYR:N	2.54	0.40
1:F:1126:HIS:CD2	1:F:1128:LEU:H	2.40	0.40
1:G:1216:GLU:CD	1:G:1246:CYS:HB2	2.47	0.40
1:G:1258:LEU:O	1:G:1259:GLU:C	2.63	0.40
1:C:422:PRO:O	1:C:426:MSE:HG3	2.20	0.40
1:E:817:MSE:O	1:E:821:ILE:HG13	2.21	0.40
1:G:1227:ARG:HD3	3:G:167:HOH:O	2.20	0.40
1:B:322:LYS:HA	1:B:340:THR:HB	2.04	0.40
1:G:1218:GLU:CD	1:G:1306:CYS:HB2	2.46	0.40
1:G:1283:SER:O	1:G:1315:HIS:HE1	2.04	0.40
1:C:408:VAL:HG22	1:C:471:VAL:HG21	2.02	0.40
1:E:897:ASN:O	1:E:897:ASN:CG	2.64	0.40
1:F:1016:GLU:OE1	1:F:1048:ARG:N	2.54	0.40
1:F:1103:ALA:HA	1:F:1153:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	186/189 (98%)	179 (96%)	3 (2%)	4 (2%)	5	6
1	B	185/189 (98%)	180 (97%)	3 (2%)	2 (1%)	11	18
1	C	186/189 (98%)	173 (93%)	10 (5%)	3 (2%)	7	11
1	D	184/189 (97%)	177 (96%)	6 (3%)	1 (0%)	24	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	186/189 (98%)	172 (92%)	9 (5%)	5 (3%)	4	4
1	F	184/189 (97%)	176 (96%)	6 (3%)	2 (1%)	11	18
1	G	184/189 (97%)	158 (86%)	19 (10%)	7 (4%)	2	2
All	All	1295/1323 (98%)	1215 (94%)	56 (4%)	24 (2%)	6	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	665	GLY
1	E	864	GLU
1	G	1265	GLY
1	A	2	ALA
1	B	265	GLY
1	C	538	HIS
1	E	865	GLY
1	G	1337	GLY
1	G	1356	ARG
1	A	65	GLY
1	A	137	GLY
1	B	276	ASN
1	C	402	ALA
1	C	531	ASP
1	E	896	GLU
1	F	1065	GLY
1	G	1264	GLU
1	E	906	CYS
1	F	1106	CYS
1	G	1269	VAL
1	G	1331	ASP
1	A	106	CYS
1	E	937	GLY
1	G	1266	PRO

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	142/142 (100%)	134 (94%)	8 (6%)	19	33
1	B	142/142 (100%)	131 (92%)	11 (8%)	12	20
1	C	142/142 (100%)	128 (90%)	14 (10%)	7	11
1	D	142/142 (100%)	132 (93%)	10 (7%)	14	24
1	E	137/142 (96%)	123 (90%)	14 (10%)	7	11
1	F	140/142 (99%)	131 (94%)	9 (6%)	16	28
1	G	136/142 (96%)	128 (94%)	8 (6%)	18	31
All	All	981/994 (99%)	907 (92%)	74 (8%)	12	21

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	31	ILE
1	A	50	VAL
1	A	58	LEU
1	A	71	VAL
1	A	77	LEU
1	A	140	THR
1	A	155	SER
1	B	215	GLU
1	B	219	THR
1	B	250	VAL
1	B	270	VAL
1	B	271	VAL
1	B	272	LEU
1	B	277	LEU
1	B	321	SER
1	B	333	MSE
1	B	343	GLU
1	B	355	SER
1	C	407	LEU
1	C	410	LEU
1	C	419	THR
1	C	431	ILE
1	C	432	LYS
1	C	450	VAL
1	C	458	LEU
1	C	462	LYS
1	C	470	VAL
1	C	471	VAL

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Mol	Chain	Res	Type
1	C	477	LEU
1	C	493	LYS
1	C	531	ASP
1	C	533	MSE
1	D	619	THR
1	D	631	ILE
1	D	650	VAL
1	D	653	CYS
1	D	658	LEU
1	D	664	GLU
1	D	670	VAL
1	D	671	VAL
1	D	677	LEU
1	D	763	GLU
1	E	810	LEU
1	E	819	THR
1	E	831	ILE
1	E	842	ASP
1	E	850	VAL
1	E	862	LYS
1	E	864	GLU
1	E	870	VAL
1	E	890	GLU
1	E	898	ARG
1	E	901	LEU
1	E	940	THR
1	E	942	SER
1	E	961	SER
1	F	1007	LEU
1	F	1019	THR
1	F	1050	VAL
1	F	1070	VAL
1	F	1071	VAL
1	F	1076	ASN
1	F	1077	LEU
1	F	1089	LYS
1	F	1130	LYS
1	G	1205	ARG
1	G	1227	ARG
1	G	1231	ILE
1	G	1250	VAL
1	G	1270	VAL

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Mol	Chain	Res	Type
1	G	1277	LEU
1	G	1316	GLU
1	G	1327	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	81	ASN
1	A	97	ASN
1	A	126	HIS
1	A	138	HIS
1	A	173	ASN
1	B	245	GLN
1	B	280	GLN
1	B	297	ASN
1	B	326	HIS
1	B	373	ASN
1	C	480	GLN
1	C	497	ASN
1	C	526	HIS
1	C	573	ASN
1	D	645	GLN
1	D	697	ASN
1	D	726	HIS
1	D	744	ASN
1	E	845	GLN
1	E	895	GLN
1	E	926	HIS
1	E	935	ASN
1	E	973	ASN
1	F	1076	ASN
1	F	1097	ASN
1	F	1126	HIS
1	F	1173	ASN
1	G	1245	GLN
1	G	1281	ASN
1	G	1295	GLN
1	G	1326	HIS
1	G	1344	ASN
1	G	1373	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 ⓘ

7 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	PO4	D	1	-	4,4,4	2.01	3 (75%)	6,6,6	0.41	0
2	PO4	F	5	-	4,4,4	1.93	3 (75%)	6,6,6	0.45	0
2	PO4	A	190	-	4,4,4	2.28	3 (75%)	6,6,6	0.42	0
2	PO4	A	191	-	4,4,4	2.32	3 (75%)	6,6,6	0.50	0
2	PO4	C	3	-	4,4,4	2.15	3 (75%)	6,6,6	0.45	0
2	PO4	F	4	-	4,4,4	1.96	2 (50%)	6,6,6	0.47	0
2	PO4	E	6	-	4,4,4	2.05	3 (75%)	6,6,6	0.42	0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	191	PO4	P-O3	-2.67	1.46	1.54
2	A	191	PO4	P-O4	-2.60	1.47	1.54
2	C	3	PO4	P-O2	-2.58	1.47	1.54
2	A	190	PO4	P-O3	-2.57	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	PO4	P-O4	-2.46	1.47	1.54
2	A	190	PO4	P-O4	-2.45	1.47	1.54
2	E	6	PO4	P-O2	-2.43	1.47	1.54
2	A	190	PO4	P-O2	-2.42	1.47	1.54
2	A	191	PO4	P-O2	-2.35	1.47	1.54
2	D	1	PO4	P-O4	-2.32	1.47	1.54
2	E	6	PO4	P-O3	-2.30	1.47	1.54
2	C	3	PO4	P-O4	-2.30	1.47	1.54
2	D	1	PO4	P-O3	-2.30	1.48	1.54
2	C	3	PO4	P-O3	-2.27	1.48	1.54
2	F	5	PO4	P-O2	-2.20	1.48	1.54
2	F	5	PO4	P-O3	-2.17	1.48	1.54
2	F	5	PO4	P-O4	-2.14	1.48	1.54
2	E	6	PO4	P-O4	-2.11	1.48	1.54
2	F	4	PO4	P-O3	-2.06	1.48	1.54
2	D	1	PO4	P-O2	-2.05	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	183/189 (96%)	-0.06	2 (1%) 78 74	13, 24, 37, 46	0
1	B	183/189 (96%)	-0.09	1 (0%) 87 85	13, 23, 34, 42	0
1	C	183/189 (96%)	-0.01	3 (1%) 70 66	13, 25, 34, 44	0
1	D	182/189 (96%)	-0.08	1 (0%) 87 85	14, 26, 36, 40	0
1	E	184/189 (97%)	0.33	4 (2%) 62 58	20, 34, 43, 47	0
1	F	182/189 (96%)	0.21	2 (1%) 78 74	19, 30, 38, 45	0
1	G	182/189 (96%)	0.49	4 (2%) 62 58	26, 36, 45, 50	0
All	All	1279/1323 (96%)	0.11	17 (1%) 75 71	13, 28, 41, 50	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	942	SER	3.8
1	C	465	GLY	3.6
1	F	1065	GLY	3.5
1	G	1275	GLY	3.0
1	C	402	ALA	3.0
1	D	653	CYS	2.8
1	A	65	GLY	2.7
1	B	265	GLY	2.4
1	G	1335	ASN	2.4
1	E	937	GLY	2.3
1	G	1297	ASN	2.3
1	G	1285	SER	2.3
1	A	2	ALA	2.3
1	F	1013	GLY	2.2
1	E	886	ALA	2.2
1	C	507	ALA	2.0
1	E	902	ILE	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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	A	191	5/5	0.94	0.12	33,33,34,35	0
2	PO4	F	5	5/5	0.96	0.09	43,44,44,45	0
2	PO4	C	3	5/5	0.97	0.08	32,33,35,35	0
2	PO4	D	1	5/5	0.97	0.07	39,40,41,43	0
2	PO4	A	190	5/5	0.97	0.09	29,30,32,33	0
2	PO4	F	4	5/5	0.98	0.05	37,37,38,38	0
2	PO4	E	6	5/5	0.98	0.05	35,35,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.