



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:50 PM UTC

PDB ID : 3V0A / pdb_00003v0a
Title : 2.7 angstrom crystal structure of BoNT/Ai in complex with NTNHA
Authors : Gu, S.; Rumpel, S.; Zhou, J.; Strotmeier, J.; Bigalke, H.; Perry, K.; Shoemaker, C.B.; Rummel, A.; Jin, R.
Deposited on : 2011-12-07
Resolution : 2.70 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

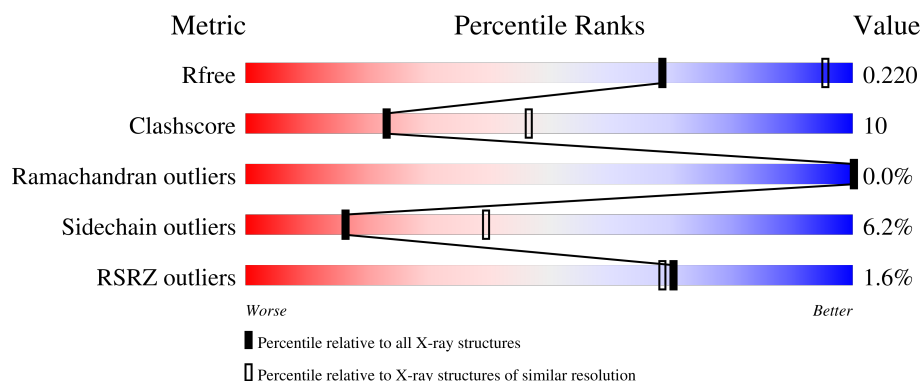
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	1296	78% 19% ..
2	B	1196	2% 72% 21% ..
3	C	152	3% 42% 34% 22%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21163 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 BoNT/A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1280	Total	C	N	O	S	36	0	0
			10418	6681	1721	1983	33			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLN	GLU	engineered mutation	UNP Q7B8V4
A	363	ALA	ARG	engineered mutation	UNP Q7B8V4
A	366	PHE	TYR	engineered mutation	UNP Q7B8V4
A	1158	ALA	THR	conflict	UNP Q7B8V4

- Molecule 2 is a protein called NTN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1150	Total	C	N	O	S	46	0	0
			9409	6022	1515	1840	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q45914
B	0	SER	-	expression tag	UNP Q45914
B	1194	PRO	-	expression tag	UNP Q45914

- Molecule 3 is a protein called Llama antibody F12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	119	Total	C	N	O	S	4	0	0
			892	551	156	181	4			

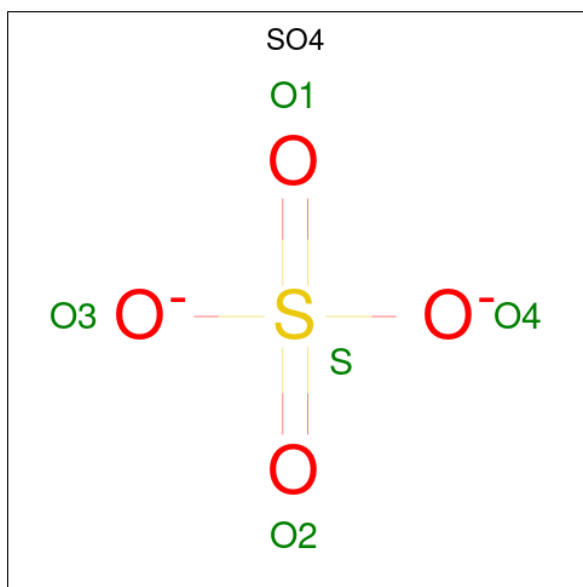
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



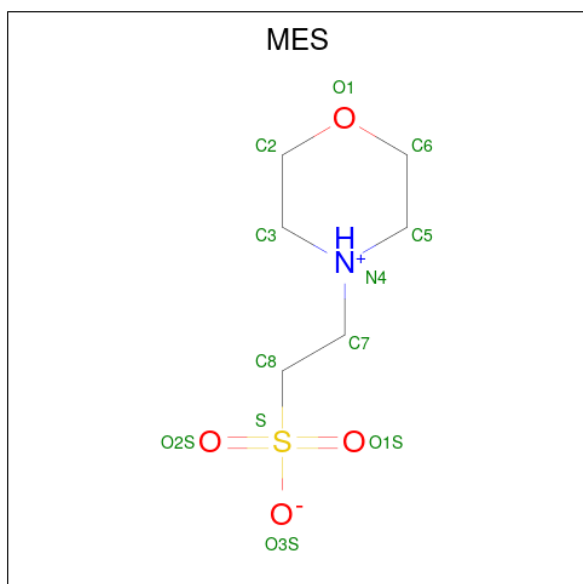
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

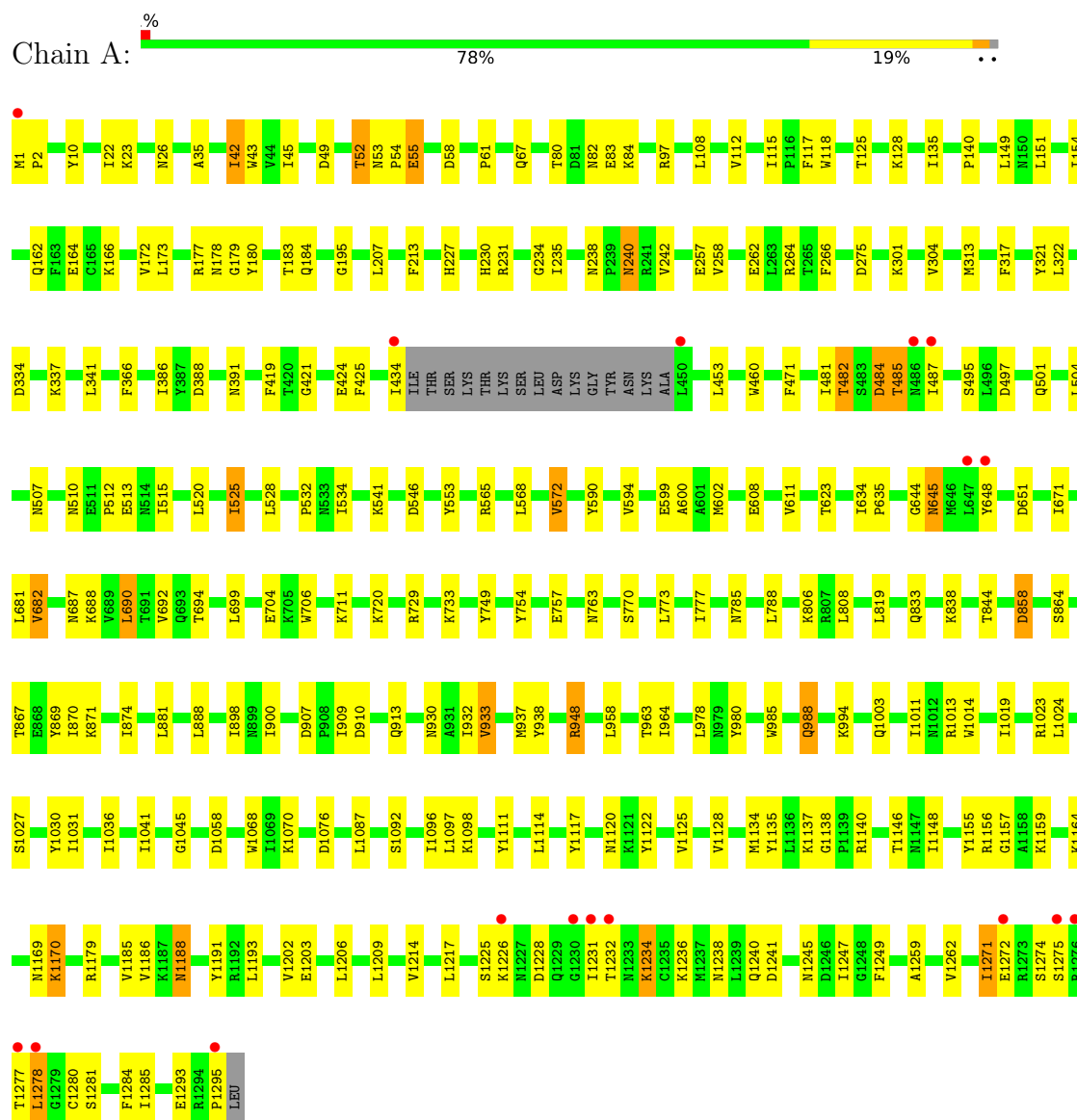
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	181	Total	O	0	0
			181	181		
8	B	112	Total	O	0	0
			112	112		
8	C	1	Total	O	0	0
			1	1		

3 Residue-property plots

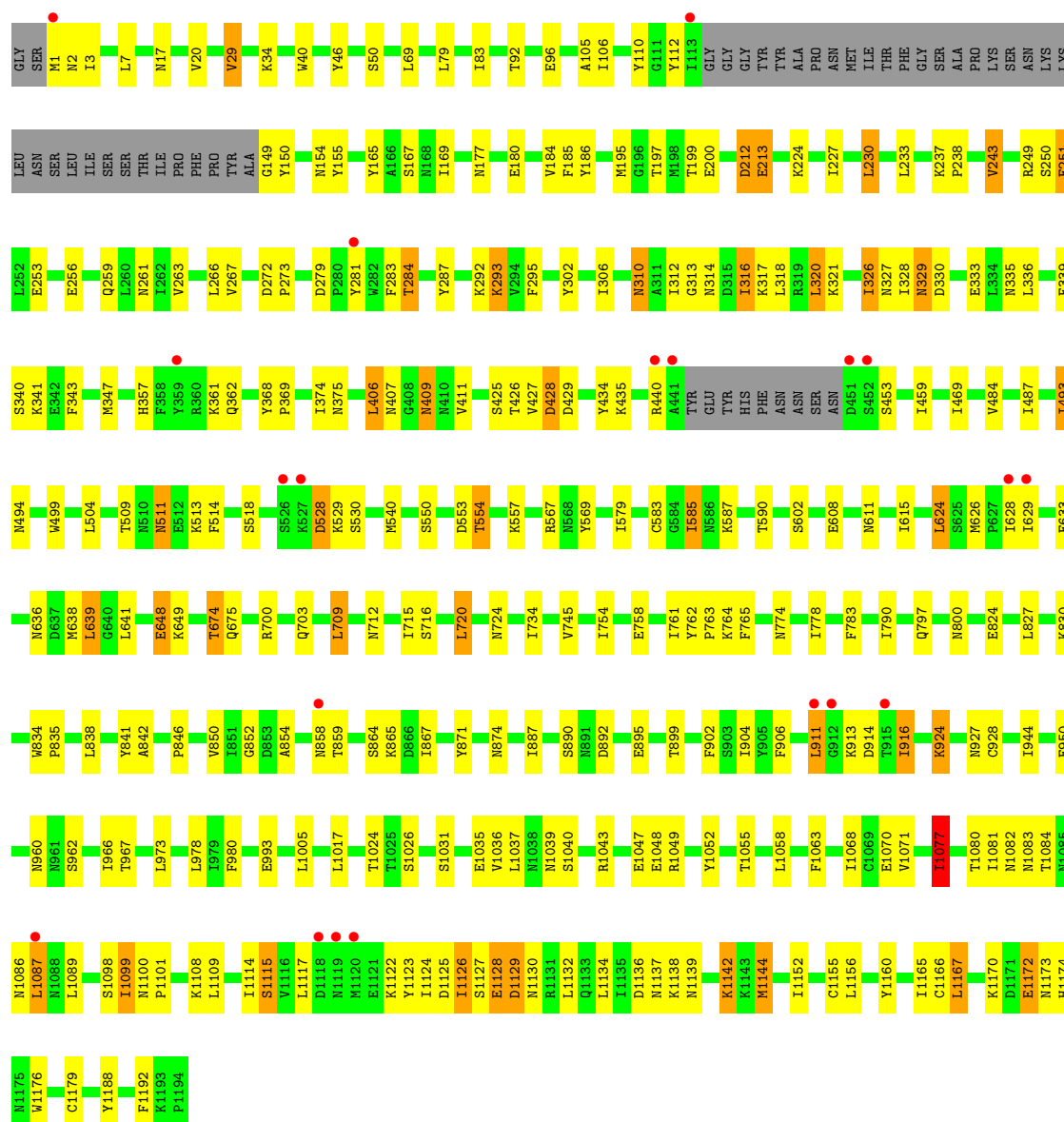
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: BoNT/A

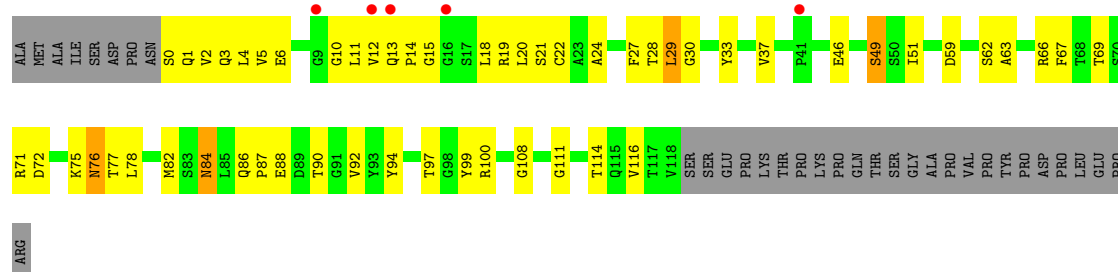


• Molecule 2: NTNH





• Molecule 3: Llama antibody F12



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.08Å 156.08Å 324.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.70 49.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.36-2.70) 99.6 (49.36-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.176 , 0.224 0.173 , 0.220	Depositor DCC
R_{free} test set	5477 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21163	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: SO4, ZN, MES, CA

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	0.39	0/10639	0.77	5/14405 (0.0%)
2	B	0.39	0/9604	0.80	12/13015 (0.1%)
3	C	0.31	0/912	0.75	0/1238
All	All	0.38	0/21155	0.78	17/28658 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1172	GLU	N-CA-C	7.72	120.82	111.40
2	B	425	SER	N-CA-C	6.57	120.23	109.85
2	B	899	THR	N-CA-C	6.14	120.93	113.38
1	A	932	ILE	N-CA-C	5.89	118.66	112.83
1	A	235	ILE	N-CA-C	5.80	117.74	112.29
1	A	1041	ILE	N-CA-C	5.70	118.37	112.90
1	A	938	TYR	N-CA-C	5.57	120.19	113.17
2	B	212	ASP	CB-CA-C	-5.57	109.66	117.23
2	B	1037	LEU	CA-C-N	-5.50	114.63	122.77
2	B	1037	LEU	C-N-CA	-5.50	114.63	122.77
1	A	1285	ILE	N-CA-C	5.32	112.82	107.55
2	B	284	THR	N-CA-C	5.22	115.18	108.34
2	B	1087	LEU	N-CA-C	-5.20	106.92	113.20
2	B	237	LYS	CA-C-N	5.17	125.15	120.03
2	B	237	LYS	C-N-CA	5.17	125.15	120.03
2	B	428	ASP	N-CA-CB	5.12	119.20	110.50
2	B	1077	ILE	N-CA-C	5.09	115.23	108.11

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	10418	0	10297	194	0
2	B	9409	0	9202	199	0
3	C	892	0	840	41	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	60	0	0	2	0
6	B	35	0	0	1	0
6	C	5	0	0	0	0
7	B	48	0	52	1	0
8	A	181	0	0	2	0
8	B	112	0	0	2	0
8	C	1	0	0	1	0
All	All	21163	0	20391	423	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 10.

All (423) 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:1275:SER:HA	2:B:827:LEU:HD21	1.22	1.21
2:B:528:ASP:HB2	2:B:530:SER:H	1.07	1.13
2:B:340:SER:HB2	2:B:347:MET:HE3	1.30	1.08
2:B:336:LEU:HB3	2:B:347:MET:HE1	1.31	1.07
2:B:528:ASP:HB2	2:B:530:SER:N	1.76	1.00
2:B:426:THR:HB	2:B:427:VAL:CA	1.91	0.99
2:B:426:THR:HB	2:B:427:VAL:HA	1.02	0.98
2:B:426:THR:CB	2:B:427:VAL:HA	1.93	0.98
1:A:421:GLY:H	1:A:424:GLU:HG3	1.33	0.93
1:A:1275:SER:CA	2:B:827:LEU:HD21	2.04	0.87
2:B:528:ASP:CB	2:B:530:SER:H	1.88	0.84
2:B:314:ASN:HB3	2:B:318:LEU:HD12	1.60	0.82
1:A:10:TYR:CZ	1:A:84:LYS:HD3	2.16	0.81
1:A:482:THR:HG22	1:A:484:ASP:H	1.47	0.80
2:B:1099:ILE:HD12	2:B:1099:ILE:H	1.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:GLN:HG3	1:A:994:LYS:HB3	1.64	0.80
2:B:426:THR:OG1	2:B:427:VAL:CG2	2.30	0.80
1:A:525:ILE:HD12	1:A:525:ILE:H	1.48	0.79
1:A:149:LEU:HD12	1:A:183:THR:CG2	2.11	0.79
3:C:18:LEU:HD22	3:C:20:LEU:HD12	1.64	0.79
1:A:80:THR:HG22	1:A:82:ASN:H	1.46	0.79
1:A:487:ILE:HG23	1:A:704:GLU:OE2	1.85	0.77
3:C:86:GLN:HB3	3:C:87:PRO:HD2	1.68	0.76
1:A:52:THR:HG23	1:A:528:LEU:HD11	1.66	0.75
2:B:602:SER:HB2	2:B:608:GLU:OE1	1.85	0.75
2:B:426:THR:HG21	2:B:428:ASP:OD2	1.86	0.75
1:A:1137:LYS:HG2	1:A:1138:GLY:H	1.53	0.74
1:A:421:GLY:N	1:A:424:GLU:HG3	2.02	0.74
2:B:1170:LYS:HE3	2:B:1173:ASN:HB3	1.69	0.73
2:B:1031:SER:O	2:B:1035:GLU:HG2	1.89	0.73
2:B:426:THR:OG1	2:B:427:VAL:HG22	1.89	0.72
2:B:251:GLU:HG2	2:B:357:HIS:HE1	1.54	0.72
3:C:18:LEU:HD23	3:C:19:ARG:N	2.05	0.72
1:A:149:LEU:HD12	1:A:183:THR:HG23	1.71	0.72
2:B:243:VAL:HG13	2:B:259:GLN:HB2	1.72	0.70
1:A:1278:LEU:HD23	1:A:1281:SER:OG	1.92	0.70
1:A:870:ILE:O	1:A:874:ILE:HG13	1.93	0.69
1:A:1275:SER:HA	2:B:827:LEU:CD2	2.13	0.69
2:B:336:LEU:HB3	2:B:347:MET:CE	2.18	0.69
1:A:482:THR:HG22	1:A:484:ASP:N	2.07	0.69
3:C:49:SER:HG	3:C:69:THR:HG1	1.34	0.69
2:B:715:ILE:HG22	2:B:720:LEU:HD22	1.76	0.68
2:B:243:VAL:CG1	2:B:259:GLN:HB2	2.22	0.68
2:B:1123:TYR:CE1	2:B:1138:LYS:HB2	2.28	0.68
2:B:834:TRP:HB2	2:B:835:PRO:HD2	1.74	0.68
2:B:96:GLU:HG2	2:B:459:ILE:HD13	1.75	0.67
2:B:426:THR:OG1	2:B:427:VAL:HG23	1.94	0.67
2:B:528:ASP:HB2	2:B:529:LYS:CA	2.25	0.66
2:B:528:ASP:HB2	2:B:529:LYS:HA	1.76	0.66
2:B:310:ASN:OD1	2:B:310:ASN:N	2.29	0.65
1:A:1228:ASP:HB3	1:A:1232:THR:H	1.60	0.65
2:B:295:PHE:CD1	2:B:328:ILE:HD11	2.32	0.65
1:A:1236:LYS:NZ	1:A:1280:CYS:SG	2.70	0.64
2:B:302:TYR:OH	2:B:321:LYS:HB2	1.98	0.64
2:B:493:ILE:HD11	2:B:499:TRP:CZ2	2.33	0.64
3:C:1:GLN:HG3	3:C:2:VAL:H	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:CD1	1:A:183:THR:HG21	2.27	0.64
1:A:1170:LYS:H	1:A:1170:LYS:HD3	1.60	0.64
1:A:1170:LYS:HD3	1:A:1170:LYS:N	2.13	0.64
1:A:453:LEU:HD23	1:A:453:LEU:H	1.62	0.64
2:B:1132:LEU:HD21	2:B:1165:ILE:HD13	1.80	0.64
1:A:149:LEU:HD12	1:A:183:THR:HG21	1.79	0.63
1:A:681:LEU:HD23	1:A:694:THR:HG22	1.81	0.63
1:A:1:MET:N	1:A:2:PRO:HD3	2.14	0.63
2:B:409:ASN:OD1	2:B:409:ASN:N	2.30	0.63
1:A:611:VAL:HG12	1:A:1024:LEU:HD11	1.81	0.63
1:A:117:PHE:HA	1:A:317:PHE:CE1	2.34	0.62
1:A:80:THR:HG22	1:A:82:ASN:N	2.12	0.62
1:A:1271:ILE:HG13	2:B:854:ALA:HB1	1.81	0.62
2:B:251:GLU:HG2	2:B:357:HIS:CE1	2.34	0.62
1:A:1170:LYS:O	1:A:1170:LYS:HG2	1.99	0.62
3:C:24:ALA:HB3	3:C:76:ASN:ND2	2.15	0.61
2:B:960:ASN:OD1	2:B:962:SER:HB3	2.00	0.61
1:A:948:ARG:NH1	8:A:1473:HOH:O	2.32	0.61
1:A:10:TYR:CZ	1:A:84:LYS:CD	2.84	0.61
1:A:52:THR:CG2	1:A:528:LEU:HD11	2.31	0.61
1:A:135:ILE:HD13	1:A:149:LEU:CD2	2.30	0.61
1:A:482:THR:CG2	1:A:484:ASP:H	2.14	0.60
1:A:53:ASN:OD1	1:A:55:GLU:HB2	2.01	0.60
1:A:67:GLN:O	1:A:460:TRP:HZ2	1.85	0.60
2:B:567:ARG:NH2	8:B:1301:HOH:O	2.33	0.60
2:B:1142:LYS:HD3	2:B:1160:TYR:CE1	2.36	0.60
1:A:184:GLN:OE1	1:A:231:ARG:HD3	2.01	0.60
1:A:1092:SER:O	1:A:1098:LYS:NZ	2.34	0.60
3:C:97:THR:HG21	3:C:108:GLY:CA	2.31	0.60
1:A:963:THR:HB	1:A:1058:ASP:HB3	1.84	0.59
2:B:638:MET:HE3	2:B:649:LYS:HD3	1.84	0.59
2:B:639:LEU:HD12	2:B:783:PHE:CE1	2.37	0.59
1:A:706:TRP:CD2	1:A:808:LEU:HD13	2.37	0.59
1:A:149:LEU:CD1	1:A:183:THR:CG2	2.80	0.59
2:B:1125:ASP:OD1	2:B:1126:ILE:N	2.36	0.59
1:A:568:LEU:HD12	1:A:594:VAL:HG11	1.85	0.59
2:B:336:LEU:CB	2:B:347:MET:HE1	2.21	0.59
3:C:84:ASN:O	3:C:84:ASN:ND2	2.29	0.59
2:B:79:LEU:O	2:B:83:ILE:HG13	2.03	0.59
2:B:674:THR:HG22	2:B:675:GLN:HG3	1.85	0.59
1:A:388:ASP:HB3	1:A:391:ASN:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:924:LYS:HG3	2:B:928:CYS:O	2.03	0.59
1:A:1128:VAL:HG11	1:A:1191:TYR:CE2	2.38	0.58
2:B:169:ILE:CD1	2:B:199:THR:HB	2.33	0.58
2:B:639:LEU:HD12	2:B:783:PHE:HE1	1.67	0.58
2:B:1082:ASN:ND2	2:B:1084:THR:O	2.36	0.58
2:B:1172:GLU:H	2:B:1174:HIS:H	1.50	0.58
3:C:30:GLY:HA2	3:C:71:ARG:CZ	2.34	0.58
1:A:1277:THR:HG21	2:B:341:LYS:HE3	1.85	0.58
1:A:1117:TYR:CD1	1:A:1277:THR:OG1	2.55	0.58
3:C:29:LEU:HD11	3:C:78:LEU:HB2	1.85	0.57
3:C:99:TYR:CD1	3:C:100:ARG:HB2	2.39	0.57
2:B:110:TYR:O	2:B:150:TYR:HD1	1.87	0.57
1:A:687:ASN:ND2	1:A:690:LEU:HD22	2.19	0.56
1:A:1228:ASP:OD2	1:A:1231:ILE:HB	2.05	0.56
2:B:238:PRO:HG3	2:B:287:TYR:CZ	2.40	0.56
2:B:281:TYR:OH	2:B:440:ARG:O	2.23	0.56
2:B:313:GLY:H	2:B:317:LYS:HZ2	1.52	0.56
1:A:1134:MET:HE1	1:A:1193:LEU:HD13	1.88	0.56
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.40	0.56
2:B:169:ILE:HD13	2:B:199:THR:HB	1.88	0.56
1:A:67:GLN:HG2	1:A:425:PHE:CE1	2.41	0.56
1:A:869:TYR:HD1	1:A:870:ILE:HD12	1.72	0.55
2:B:283:PHE:HA	2:B:434:TYR:OH	2.06	0.55
1:A:80:THR:HB	1:A:83:GLU:HG3	1.88	0.55
3:C:97:THR:HG21	3:C:108:GLY:HA2	1.89	0.55
1:A:648:TYR:O	1:A:651:ASP:HB2	2.07	0.55
1:A:49:ASP:OD1	1:A:52:THR:HB	2.06	0.55
1:A:1277:THR:O	1:A:1277:THR:HG23	2.05	0.55
1:A:553:TYR:CZ	1:A:572:VAL:HG21	2.42	0.54
1:A:35:ALA:HB2	1:A:45:ILE:HG12	1.88	0.54
1:A:322:LEU:HD12	1:A:341:LEU:HB2	1.89	0.54
1:A:1271:ILE:O	1:A:1271:ILE:HG22	2.07	0.54
2:B:361:LYS:NZ	6:B:1196:SO4:O4	2.30	0.54
2:B:1137:ASN:OD1	2:B:1139:ASN:HB2	2.07	0.54
3:C:13:GLN:HB3	3:C:14:PRO:HD2	1.89	0.54
2:B:112:TYR:CE1	2:B:149:GLY:HA3	2.42	0.54
1:A:42:ILE:HD13	1:A:151:LEU:HB3	1.90	0.54
1:A:61:PRO:HB3	1:A:419:PHE:CZ	2.43	0.54
3:C:18:LEU:HD22	3:C:20:LEU:CD1	2.36	0.54
1:A:763:ASN:O	1:A:937:MET:HE1	2.07	0.54
2:B:762:TYR:HB3	2:B:763:PRO:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:GLU:HA	3:C:21:SER:O	2.07	0.53
1:A:108:LEU:O	1:A:112:VAL:HG23	2.08	0.53
2:B:243:VAL:HG11	2:B:259:GLN:CD	2.33	0.53
1:A:565:ARG:HB2	1:A:749:TYR:CZ	2.43	0.53
1:A:1228:ASP:HB3	1:A:1232:THR:N	2.23	0.53
2:B:227:ILE:HD11	2:B:339:PHE:CE2	2.43	0.53
2:B:306:ILE:HG23	2:B:312:ILE:CD1	2.39	0.53
2:B:513:LYS:HD2	2:B:514:PHE:H	1.74	0.53
2:B:513:LYS:HD2	2:B:514:PHE:N	2.23	0.53
3:C:24:ALA:HB3	3:C:76:ASN:HD21	1.74	0.53
1:A:1122:TYR:OH	1:A:1137:LYS:HD2	2.09	0.52
1:A:1241:ASP:HB3	1:A:1247:ILE:HD11	1.91	0.52
2:B:329:ASN:O	2:B:333:GLU:HG2	2.10	0.52
2:B:528:ASP:HB2	2:B:529:LYS:C	2.35	0.52
1:A:67:GLN:O	1:A:460:TRP:CZ2	2.62	0.52
1:A:1137:LYS:HG2	1:A:1138:GLY:N	2.21	0.52
2:B:715:ILE:CG2	2:B:720:LEU:HD22	2.38	0.52
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.92	0.52
2:B:1043:ARG:HB3	2:B:1047:GLU:HA	1.92	0.52
1:A:1:MET:H1	1:A:2:PRO:HD3	1.74	0.52
1:A:115:ILE:HD11	1:A:512:PRO:HB2	1.92	0.52
1:A:207:LEU:HD11	1:A:1076:ASP:HB3	1.91	0.52
1:A:227:HIS:CE1	1:A:262:GLU:OE2	2.63	0.52
2:B:40:TRP:CD1	2:B:167:SER:HB2	2.45	0.52
3:C:37:VAL:HG23	3:C:46:GLU:O	2.10	0.52
1:A:1209:LEU:CD1	1:A:1217:LEU:HD13	2.40	0.52
1:A:1228:ASP:OD1	1:A:1234:LYS:HD2	2.09	0.52
2:B:341:LYS:HA	2:B:824:GLU:HG2	1.90	0.52
1:A:52:THR:HG22	1:A:53:ASN:N	2.25	0.52
2:B:266:LEU:O	2:B:335:ASN:HB3	2.10	0.52
2:B:887:ILE:HG23	2:B:1005:LEU:HB3	1.92	0.52
2:B:112:TYR:HE1	2:B:149:GLY:HA3	1.75	0.51
2:B:1058:LEU:HD23	2:B:1068:ILE:HG13	1.93	0.51
1:A:172:VAL:HG23	1:A:173:LEU:N	2.26	0.51
1:A:644:GLY:O	1:A:645:ASN:ND2	2.43	0.51
1:A:1278:LEU:HG	1:A:1280:CYS:SG	2.51	0.51
1:A:888:LEU:HB3	1:A:900:ILE:HD11	1.91	0.51
2:B:864:SER:HB2	2:B:867:ILE:HG13	1.93	0.51
1:A:699:LEU:HD22	1:A:844:THR:HG21	1.93	0.51
1:A:671:ILE:HG23	1:A:671:ILE:O	2.11	0.51
2:B:426:THR:CG2	2:B:428:ASP:OD2	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:TYR:OH	1:A:1148:ILE:O	2.28	0.51
1:A:864:SER:HA	1:A:867:THR:HB	1.93	0.51
3:C:67:PHE:CD1	3:C:67:PHE:N	2.77	0.51
1:A:729:ARG:HD2	1:A:785:ASN:OD1	2.11	0.50
2:B:227:ILE:HG22	2:B:267:VAL:HG22	1.92	0.50
3:C:10:GLY:HA2	3:C:18:LEU:CD1	2.41	0.50
1:A:1031:ILE:HG12	1:A:1036:ILE:HG13	1.92	0.50
2:B:1:MET:HG2	2:B:2:ASN:H	1.75	0.50
1:A:1096:ILE:O	1:A:1098:LYS:HE3	2.11	0.50
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.94	0.50
1:A:1238:ASN:HB2	1:A:1249:PHE:CE1	2.46	0.50
1:A:706:TRP:CE3	1:A:808:LEU:HD13	2.46	0.50
2:B:227:ILE:O	2:B:230:LEU:HB2	2.12	0.50
2:B:227:ILE:HD11	2:B:339:PHE:HE2	1.77	0.50
1:A:172:VAL:HG23	1:A:173:LEU:H	1.77	0.50
2:B:1172:GLU:H	2:B:1174:HIS:N	2.10	0.50
1:A:623:THR:HG23	6:A:1303:SO4:O1	2.12	0.49
1:A:177:ARG:HD3	1:A:238:ASN:HA	1.95	0.49
2:B:615:ILE:O	2:B:615:ILE:HG13	2.12	0.49
1:A:45:ILE:HB	1:A:154:ILE:HG22	1.94	0.49
1:A:599:GLU:HB2	1:A:602:MET:HE2	1.93	0.49
2:B:259:GLN:OE1	2:B:426:THR:O	2.31	0.49
3:C:92:VAL:HG13	3:C:94:TYR:HE2	1.78	0.49
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.95	0.49
3:C:18:LEU:HD23	3:C:19:ARG:H	1.74	0.49
2:B:874:ASN:HB2	2:B:1036:VAL:HG13	1.94	0.49
1:A:179:GLY:O	1:A:321:TYR:OH	2.28	0.49
1:A:688:LYS:HD3	1:A:833:GLN:NE2	2.27	0.49
2:B:326:ILE:HG23	2:B:327:ASN:N	2.28	0.48
2:B:374:ILE:HD12	2:B:375:ASN:N	2.27	0.48
2:B:1115:SER:HB2	2:B:1123:TYR:CD2	2.48	0.48
1:A:634:ILE:HD12	1:A:634:ILE:N	2.27	0.48
2:B:212:ASP:HB3	2:B:213:GLU:OE2	2.12	0.48
2:B:407:ASN:OD1	2:B:411:VAL:HG12	2.13	0.48
2:B:528:ASP:CB	2:B:530:SER:N	2.61	0.48
2:B:633:GLU:OE1	2:B:633:GLU:HA	2.12	0.48
1:A:23:LYS:HD2	3:C:33:TYR:OH	2.14	0.48
1:A:1186:VAL:HB	1:A:1191:TYR:CE1	2.49	0.48
1:A:532:PRO:O	1:A:534:ILE:HD12	2.14	0.47
1:A:179:GLY:CA	1:A:234:GLY:HA3	2.44	0.47
1:A:1164:LYS:NZ	1:A:1170:LYS:HA	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:ILE:HG22	2:B:317:LYS:N	2.29	0.47
2:B:320:LEU:HD12	2:B:320:LEU:HA	1.74	0.47
2:B:1123:TYR:HD1	2:B:1138:LYS:HA	1.80	0.47
1:A:565:ARG:HB2	1:A:749:TYR:CE2	2.50	0.47
2:B:914:ASP:OD2	2:B:916:ILE:HG23	2.14	0.47
2:B:1172:GLU:N	2:B:1173:ASN:HA	2.30	0.47
1:A:1014:TRP:CH2	1:A:1068:TRP:HB3	2.49	0.47
2:B:944:ILE:HB	2:B:950:GLU:HG3	1.95	0.47
2:B:1172:GLU:HB2	2:B:1173:ASN:C	2.39	0.47
1:A:858:ASP:N	1:A:858:ASP:OD1	2.47	0.47
2:B:1115:SER:HB2	2:B:1123:TYR:CE2	2.50	0.47
3:C:63:ALA:HA	3:C:66:ARG:HE	1.78	0.47
2:B:426:THR:CB	2:B:427:VAL:CA	2.69	0.47
2:B:1039:ASN:O	2:B:1040:SER:OG	2.33	0.47
1:A:525:ILE:HD12	1:A:525:ILE:N	2.23	0.47
2:B:272:ASP:N	2:B:273:PRO:HD2	2.29	0.47
2:B:528:ASP:CB	2:B:529:LYS:HA	2.40	0.47
2:B:966:ILE:HD12	2:B:966:ILE:N	2.30	0.47
2:B:902:PHE:HE1	2:B:904:ILE:HD11	1.80	0.46
1:A:590:TYR:O	1:A:594:VAL:HG12	2.15	0.46
2:B:238:PRO:HD2	2:B:263:VAL:CG2	2.45	0.46
3:C:90:THR:HG23	3:C:116:VAL:O	2.15	0.46
2:B:1039:ASN:O	2:B:1040:SER:CB	2.63	0.46
2:B:1144:MET:HE2	2:B:1144:MET:HB2	1.61	0.46
2:B:1166:CYS:HB3	2:B:1188:TYR:CD1	2.51	0.46
1:A:230:HIS:CE1	1:A:264:ARG:HD3	2.51	0.46
3:C:27:PHE:CE1	3:C:29:LEU:HD23	2.50	0.46
3:C:30:GLY:HA2	3:C:71:ARG:NH1	2.31	0.46
1:A:1125:VAL:HG22	1:A:1134:MET:HG2	1.98	0.46
2:B:892:ASP:O	2:B:895:GLU:HG2	2.15	0.46
1:A:97:ARG:HA	1:A:386:ILE:HG23	1.97	0.46
2:B:92:THR:HB	2:B:343:PHE:CZ	2.51	0.46
2:B:569:TYR:CE2	2:B:734:ILE:HG23	2.51	0.46
2:B:1129:ASP:OD1	2:B:1129:ASP:N	2.49	0.46
3:C:22:CYS:O	3:C:77:THR:HG23	2.16	0.46
1:A:80:THR:HG23	6:A:1306:SO4:O2	2.16	0.46
1:A:257:GLU:HG3	1:A:534:ILE:HG21	1.98	0.46
1:A:49:ASP:HB2	1:A:154:ILE:HD12	1.98	0.46
1:A:334:ASP:HB3	1:A:337:LYS:HB2	1.98	0.46
2:B:314:ASN:O	2:B:318:LEU:HB2	2.16	0.46
2:B:761:ILE:N	2:B:761:ILE:HD12	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:774:ASN:O	2:B:778:ILE:HG12	2.16	0.46
2:B:1070:GLU:CD	2:B:1077:ILE:HD11	2.40	0.46
1:A:504:LEU:O	2:B:1170:LYS:HB2	2.16	0.45
2:B:1114:ILE:HB	2:B:1124:ILE:HD12	1.98	0.45
1:A:26:ASN:HD21	1:A:54:PRO:HD3	1.81	0.45
2:B:587:LYS:HB3	2:B:587:LYS:HE2	1.67	0.45
2:B:636:ASN:HA	2:B:639:LEU:CD1	2.47	0.45
1:A:22:ILE:HD11	1:A:45:ILE:HD11	1.99	0.45
2:B:155:TYR:HA	2:B:165:TYR:O	2.16	0.45
1:A:838:LYS:HD3	8:A:1448:HOH:O	2.16	0.45
2:B:435:LYS:HA	2:B:628:ILE:HG23	1.98	0.45
2:B:842:ALA:HA	2:B:850:VAL:O	2.16	0.45
1:A:773:LEU:O	1:A:777:ILE:HG13	2.17	0.45
1:A:930:ASN:O	1:A:933:VAL:HG13	2.16	0.45
2:B:184:VAL:CG2	2:B:200:GLU:HB2	2.47	0.45
2:B:17:ASN:HD22	2:B:34:LYS:HE3	1.81	0.45
2:B:306:ILE:HG23	2:B:312:ILE:HD12	1.99	0.45
7:B:1204:MES:H52	7:B:1204:MES:H81	1.71	0.45
3:C:2:VAL:HG13	3:C:27:PHE:CE2	2.51	0.45
2:B:1080:THR:OG1	2:B:1081:ILE:N	2.49	0.45
1:A:140:PRO:O	3:C:97:THR:HG23	2.16	0.45
1:A:275:ASP:OD2	1:A:275:ASP:C	2.60	0.45
1:A:118:TRP:HB3	1:A:128:LYS:O	2.17	0.44
2:B:261:ASN:OD1	2:B:263:VAL:HG23	2.17	0.44
2:B:427:VAL:HA	2:B:428:ASP:HA	1.68	0.44
3:C:10:GLY:H	3:C:18:LEU:HD11	1.82	0.44
1:A:162:GLN:HE21	1:A:164:GLU:CD	2.25	0.44
1:A:125:THR:O	1:A:301:LYS:N	2.48	0.44
1:A:749:TYR:CD1	1:A:749:TYR:C	2.95	0.44
1:A:421:GLY:H	1:A:424:GLU:CG	2.18	0.44
1:A:1209:LEU:HD11	1:A:1217:LEU:HD13	1.99	0.44
2:B:406:LEU:HD11	2:B:494:ASN:HB3	1.99	0.44
1:A:1097:LEU:HD12	1:A:1225:SER:HB3	2.00	0.44
2:B:426:THR:HG1	2:B:427:VAL:HG22	1.82	0.44
1:A:1193:LEU:HD11	1:A:1206:LEU:HD13	2.00	0.44
2:B:1156:LEU:HD21	2:B:1192:PHE:CD2	2.53	0.44
1:A:149:LEU:HD11	1:A:183:THR:HG21	2.00	0.44
2:B:1167:LEU:HD12	2:B:1167:LEU:HA	1.81	0.44
1:A:1155:TYR:CD2	1:A:1293:GLU:HG3	2.53	0.44
2:B:105:ALA:HB3	2:B:233:LEU:HD13	2.00	0.44
2:B:293:LYS:HB2	2:B:293:LYS:NZ	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:841:TYR:CZ	2:B:852:GLY:HA3	2.53	0.44
1:A:1122:TYR:CD1	1:A:1157:GLY:HA2	2.53	0.43
2:B:34:LYS:HB2	2:B:40:TRP:CZ3	2.53	0.43
2:B:46:TYR:OH	2:B:200:GLU:OE2	2.23	0.43
2:B:154:ASN:HB2	2:B:167:SER:O	2.18	0.43
2:B:1123:TYR:CD1	2:B:1138:LYS:HA	2.53	0.43
3:C:27:PHE:HE1	3:C:29:LEU:HD23	1.83	0.43
1:A:43:TRP:CD1	1:A:149:LEU:HD22	2.54	0.43
1:A:501:GLN:HG3	2:B:1063:PHE:CE1	2.53	0.43
2:B:911:LEU:H	2:B:911:LEU:HG	1.68	0.43
2:B:967:THR:HB	2:B:980:PHE:HB2	2.00	0.43
3:C:99:TYR:CE1	3:C:100:ARG:HB2	2.54	0.43
1:A:1202:VAL:HG13	1:A:1203:GLU:OE2	2.18	0.43
2:B:184:VAL:HG22	2:B:200:GLU:HB2	2.01	0.43
2:B:626:MET:HE1	2:B:764:LYS:HB3	2.00	0.43
2:B:859:THR:HA	2:B:890:SER:O	2.18	0.43
1:A:128:LYS:HG2	1:A:304:VAL:HB	1.99	0.43
1:A:484:ASP:O	1:A:485:THR:C	2.61	0.43
1:A:711:LYS:HB3	1:A:711:LYS:HE2	1.80	0.43
2:B:762:TYR:O	2:B:765:PHE:HB3	2.19	0.43
2:B:1108:LYS:O	2:B:1109:LEU:HB2	2.19	0.43
3:C:14:PRO:HA	3:C:15:GLY:HA3	1.88	0.43
3:C:72:ASP:OD2	3:C:75:LYS:HG3	2.18	0.43
1:A:178:ASN:OD1	1:A:180:TYR:HB2	2.19	0.43
1:A:313:MET:HE1	1:A:515:ILE:HD13	1.99	0.43
2:B:426:THR:HB	2:B:428:ASP:HA	2.00	0.43
3:C:10:GLY:HA2	3:C:18:LEU:HD11	2.00	0.43
1:A:135:ILE:HD13	1:A:149:LEU:HD23	1.99	0.43
2:B:110:TYR:CE1	2:B:195:MET:HE2	2.54	0.43
1:A:135:ILE:HD13	1:A:149:LEU:HD21	2.01	0.43
2:B:249:ARG:NH1	2:B:256:GLU:OE2	2.52	0.43
2:B:567:ARG:NH1	2:B:973:LEU:O	2.52	0.43
1:A:195:GLY:HA2	1:A:213:PHE:O	2.19	0.43
1:A:600:ALA:HA	1:A:754:TYR:CZ	2.54	0.43
1:A:907:ASP:HB3	1:A:910:ASP:O	2.19	0.43
1:A:1271:ILE:HG13	2:B:854:ALA:CB	2.49	0.43
2:B:1100:ASN:HA	2:B:1101:PRO:HD2	1.85	0.43
1:A:67:GLN:HA	1:A:425:PHE:CZ	2.54	0.43
1:A:881:LEU:HD11	1:A:898:ILE:HG12	2.01	0.43
1:A:1023:ARG:NH1	1:A:1023:ARG:HB3	2.34	0.43
1:A:1030:TYR:O	1:A:1031:ILE:HD13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:518:SER:HB3	2:B:540:MET:HE1	2.00	0.43
3:C:1:GLN:HB3	3:C:3:GLN:OE1	2.19	0.43
3:C:20:LEU:HD13	3:C:82:MET:SD	2.58	0.43
3:C:63:ALA:HB1	3:C:67:PHE:CG	2.54	0.43
1:A:481:ILE:O	1:A:682:VAL:HG12	2.18	0.42
1:A:1293:GLU:O	1:A:1295:PRO:HD3	2.19	0.42
1:A:1114:LEU:C	1:A:1114:LEU:HD23	2.44	0.42
1:A:1188:ASN:HD22	1:A:1188:ASN:C	2.25	0.42
1:A:164:GLU:OE2	1:A:166:LYS:HE2	2.19	0.42
2:B:838:LEU:HD13	2:B:859:THR:HG21	2.01	0.42
2:B:1071:VAL:CG1	2:B:1176:TRP:HZ3	2.33	0.42
2:B:1173:ASN:O	2:B:1174:HIS:CD2	2.72	0.42
1:A:1135:TYR:HB2	1:A:1259:ALA:O	2.18	0.42
1:A:1188:ASN:O	1:A:1188:ASN:ND2	2.42	0.42
1:A:1245:ASN:ND2	2:B:846:PRO:HA	2.34	0.42
2:B:554:THR:OG1	2:B:557:LYS:HG3	2.19	0.42
1:A:135:ILE:CD1	1:A:149:LEU:HD23	2.50	0.42
1:A:788:LEU:HD23	1:A:788:LEU:HA	1.82	0.42
2:B:313:GLY:H	2:B:317:LYS:NZ	2.17	0.42
2:B:709:LEU:HD12	2:B:709:LEU:HA	1.86	0.42
2:B:871:TYR:CE2	2:B:1049:ARG:HD3	2.55	0.42
2:B:1123:TYR:HE1	2:B:1138:LYS:HB2	1.77	0.42
1:A:985:TRP:CE2	1:A:1019:ILE:HG21	2.55	0.42
1:A:1179:ARG:NH2	1:A:1240:GLN:OE1	2.50	0.42
1:A:1228:ASP:H	1:A:1232:THR:HA	1.85	0.42
2:B:636:ASN:HA	2:B:639:LEU:HD13	2.02	0.42
2:B:674:THR:HG22	2:B:675:GLN:N	2.35	0.42
2:B:700:ARG:NH1	8:B:1275:HOH:O	2.52	0.42
2:B:20:VAL:HG13	2:B:29:VAL:HG13	2.01	0.42
2:B:1031:SER:O	2:B:1035:GLU:CG	2.64	0.42
2:B:1052:TYR:CE1	2:B:1098:SER:HB2	2.54	0.42
1:A:1277:THR:HG21	2:B:341:LYS:CE	2.49	0.42
2:B:1084:THR:HB	2:B:1087:LEU:HB2	2.01	0.42
1:A:471:PHE:CE2	1:A:720:LYS:HE3	2.54	0.42
1:A:1159:LYS:HB2	1:A:1185:VAL:HB	2.01	0.42
1:A:1241:ASP:OD1	1:A:1241:ASP:C	2.63	0.41
2:B:638:MET:HE3	2:B:649:LYS:HB3	2.01	0.41
2:B:638:MET:HA	2:B:641:LEU:HD13	2.01	0.41
1:A:240:ASN:C	1:A:240:ASN:HD22	2.28	0.41
2:B:185:PHE:HB2	2:B:197:THR:HG21	2.01	0.41
2:B:330:ASP:HB3	2:B:453:SER:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:13:GLN:NE2	8:C:241:HOH:O	2.53	0.41
1:A:10:TYR:CE1	1:A:84:LYS:HD3	2.53	0.41
1:A:10:TYR:OH	1:A:84:LYS:HD3	2.20	0.41
2:B:105:ALA:O	2:B:106:ILE:C	2.64	0.41
2:B:368:TYR:HA	2:B:369:PRO:HA	1.62	0.41
2:B:426:THR:CB	2:B:427:VAL:CG2	2.97	0.41
2:B:906:PHE:HB3	2:B:1017:LEU:HA	2.02	0.41
1:A:688:LYS:O	1:A:692:VAL:HG23	2.21	0.41
2:B:1122:LYS:HB3	2:B:1134:LEU:HB3	2.00	0.41
2:B:40:TRP:HD1	2:B:167:SER:HB2	1.84	0.41
1:A:242:VAL:HG13	1:A:258:VAL:O	2.20	0.41
1:A:964:ILE:HD13	1:A:978:LEU:HG	2.03	0.41
2:B:624:LEU:HD12	2:B:624:LEU:HA	1.76	0.41
1:A:495:SER:OG	1:A:497:ASP:OD1	2.36	0.41
1:A:97:ARG:HD2	1:A:386:ILE:O	2.20	0.41
1:A:1023:ARG:NH2	1:A:1045:GLY:O	2.54	0.41
1:A:1111:TYR:CG	1:A:1284:PHE:HB3	2.56	0.41
2:B:177:ASN:ND2	2:B:180:GLU:HB2	2.36	0.41
2:B:514:PHE:CD1	2:B:514:PHE:C	2.99	0.41
2:B:648:GLU:O	2:B:648:GLU:HG2	2.19	0.41
2:B:1127:SER:OG	2:B:1128:GLU:N	2.54	0.41
3:C:4:LEU:O	3:C:111:GLY:HA2	2.20	0.41
2:B:579:ILE:O	2:B:585:ILE:HA	2.21	0.40
1:A:1:MET:N	1:A:2:PRO:CD	2.83	0.40
1:A:1:MET:O	1:A:1:MET:HG2	2.21	0.40
1:A:525:ILE:H	1:A:525:ILE:CD1	2.24	0.40
1:A:1120:ASN:O	1:A:1140:ARG:HG3	2.22	0.40
2:B:754:ILE:O	2:B:758:GLU:HG3	2.21	0.40
2:B:1152:ILE:CG2	2:B:1155:CYS:HB2	2.52	0.40
1:A:179:GLY:HA2	1:A:234:GLY:HA3	2.02	0.40
1:A:634:ILE:HA	1:A:635:PRO:HD3	1.84	0.40
2:B:639:LEU:CD1	2:B:783:PHE:HE1	2.32	0.40
3:C:46:GLU:OE2	3:C:62:SER:HB2	2.19	0.40
1:A:565:ARG:HD2	1:A:749:TYR:CE1	2.55	0.40
2:B:368:TYR:N	2:B:368:TYR:CD2	2.89	0.40
2:B:1130:ASN:HB3	2:B:1179:CYS:O	2.21	0.40
1:A:266:PHE:CE1	1:A:366:PHE:HB3	2.56	0.40
1:A:1277:THR:O	1:A:1277:THR:CG2	2.67	0.40
2:B:511:ASN:HB3	2:B:513:LYS:O	2.21	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	1276/1296 (98%)	1242 (97%)	34 (3%)	0	100	100
2	B	1144/1196 (96%)	1105 (97%)	38 (3%)	1 (0%)	48	73
3	C	117/152 (77%)	112 (96%)	5 (4%)	0	100	100
All	All	2537/2644 (96%)	2459 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	429	ASP

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	1162/1176 (99%)	1113 (96%)	49 (4%)	26	55
2	B	1076/1114 (97%)	993 (92%)	83 (8%)	12	30
3	C	94/123 (76%)	81 (86%)	13 (14%)	3	9
All	All	2332/2413 (97%)	2187 (94%)	145 (6%)	16	39

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	52	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	GLU
1	A	58	ASP
1	A	240	ASN
1	A	434	ILE
1	A	482	THR
1	A	484	ASP
1	A	485	THR
1	A	507	ASN
1	A	510	ASN
1	A	513	GLU
1	A	520	LEU
1	A	525	ILE
1	A	541	LYS
1	A	546	ASP
1	A	572	VAL
1	A	608	GLU
1	A	645	ASN
1	A	682	VAL
1	A	690	LEU
1	A	733	LYS
1	A	757	GLU
1	A	770	SER
1	A	806	LYS
1	A	819	LEU
1	A	858	ASP
1	A	871	LYS
1	A	909	ILE
1	A	933	VAL
1	A	948	ARG
1	A	958	LEU
1	A	988	GLN
1	A	1013	ARG
1	A	1027	SER
1	A	1087	LEU
1	A	1146	THR
1	A	1156	ARG
1	A	1169	ASN
1	A	1170	LYS
1	A	1188	ASN
1	A	1214	VAL
1	A	1226	LYS
1	A	1234	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1262	VAL
1	A	1271	ILE
1	A	1272	GLU
1	A	1274	SER
1	A	1278	LEU
2	B	3	ILE
2	B	7	LEU
2	B	29	VAL
2	B	50	SER
2	B	69	LEU
2	B	186	TYR
2	B	213	GLU
2	B	224	LYS
2	B	230	LEU
2	B	243	VAL
2	B	250	SER
2	B	251	GLU
2	B	253	GLU
2	B	279	ASP
2	B	284	THR
2	B	292	LYS
2	B	293	LYS
2	B	310	ASN
2	B	316	ILE
2	B	320	LEU
2	B	326	ILE
2	B	329	ASN
2	B	362	GLN
2	B	406	LEU
2	B	409	ASN
2	B	469	ILE
2	B	484	VAL
2	B	487	ILE
2	B	493	ILE
2	B	504	LEU
2	B	509	THR
2	B	511	ASN
2	B	528	ASP
2	B	550	SER
2	B	553	ASP
2	B	554	THR
2	B	583	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	585	ILE
2	B	590	THR
2	B	611	ASN
2	B	624	LEU
2	B	629	ILE
2	B	639	LEU
2	B	648	GLU
2	B	674	THR
2	B	703	GLN
2	B	709	LEU
2	B	712	ASN
2	B	716	SER
2	B	720	LEU
2	B	724	ASN
2	B	745	VAL
2	B	790	ILE
2	B	797	GLN
2	B	800	ASN
2	B	830	LYS
2	B	858	ASN
2	B	865	LYS
2	B	911	LEU
2	B	913	LYS
2	B	916	ILE
2	B	924	LYS
2	B	927	ASN
2	B	978	LEU
2	B	993	GLU
2	B	1024	THR
2	B	1026	SER
2	B	1048	GLU
2	B	1055	THR
2	B	1077	ILE
2	B	1083	ASN
2	B	1086	ASN
2	B	1089	LEU
2	B	1099	ILE
2	B	1115	SER
2	B	1117	LEU
2	B	1126	ILE
2	B	1128	GLU
2	B	1129	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1136	ASP
2	B	1142	LYS
2	B	1144	MET
2	B	1167	LEU
3	C	0	SER
3	C	5	VAL
3	C	11	LEU
3	C	12	VAL
3	C	28	THR
3	C	29	LEU
3	C	49	SER
3	C	51	ILE
3	C	59	ASP
3	C	76	ASN
3	C	84	ASN
3	C	88	GLU
3	C	114	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	GLN
1	A	205	ASN
1	A	400	ASN
1	A	500	GLN
1	A	573	ASN
1	A	578	ASN
1	A	748	ASN
1	A	753	GLN
1	A	859	ASN
1	A	905	ASN
1	A	915	GLN
1	A	970	ASN
1	A	1046	ASN
1	A	1245	ASN
2	B	2	ASN
2	B	38	ASN
2	B	322	GLN
2	B	375	ASN
2	B	379	ASN
2	B	410	ASN
2	B	417	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	694	GLN
2	B	858	ASN
2	B	961	ASN
2	B	1057	GLN
2	B	1139	ASN
3	C	76	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	B	1199	-	4,4,4	0.25	0	6,6,6	0.16	0
7	MES	B	1202	-	12,12,12	1.25	1 (8%)	15,16,16	1.88	5 (33%)
6	SO4	A	1305	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	1304	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	1201	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	A	1306	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	A	1300	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	B	1196	-	4,4,4	0.24	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	B	1200	-	4,4,4	0.22	0	6,6,6	0.17	0
6	SO4	B	1195	-	4,4,4	0.25	0	6,6,6	0.06	0
6	SO4	A	1301	-	4,4,4	0.23	0	6,6,6	0.12	0
6	SO4	A	1308	-	4,4,4	0.23	0	6,6,6	0.14	0
6	SO4	A	1309	-	4,4,4	0.24	0	6,6,6	0.06	0
7	MES	B	1204	-	12,12,12	1.32	2 (16%)	15,16,16	1.93	4 (26%)
6	SO4	B	1198	-	4,4,4	0.25	0	6,6,6	0.11	0
6	SO4	A	1299	-	4,4,4	0.25	0	6,6,6	0.10	0
6	SO4	B	1197	-	4,4,4	0.25	0	6,6,6	0.13	0
6	SO4	A	1303	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	C	144	-	4,4,4	0.26	0	6,6,6	0.06	0
6	SO4	A	1302	-	4,4,4	0.24	0	6,6,6	0.11	0
7	MES	B	1203	-	12,12,12	1.31	1 (8%)	15,16,16	1.85	4 (26%)
6	SO4	A	1310	-	4,4,4	0.26	0	6,6,6	0.11	0
7	MES	B	1205	-	12,12,12	1.32	2 (16%)	15,16,16	1.87	4 (26%)
6	SO4	A	1307	-	4,4,4	0.24	0	6,6,6	0.11	0

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
7	MES	B	1203	-	-	0/6/14/14	0/1/1/1
7	MES	B	1204	-	-	1/6/14/14	0/1/1/1
7	MES	B	1202	-	-	3/6/14/14	0/1/1/1
7	MES	B	1205	-	-	1/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1205	MES	C5-N4	-3.12	1.38	1.46
7	B	1203	MES	C5-N4	-3.10	1.38	1.46
7	B	1204	MES	C5-N4	-3.07	1.38	1.46
7	B	1202	MES	C5-N4	-2.90	1.39	1.46
7	B	1205	MES	C8-S	2.09	1.80	1.77
7	B	1204	MES	C8-S	2.00	1.80	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1204	MES	O3S-S-O2S	-4.26	100.73	111.40
7	B	1202	MES	O3S-S-O2S	-4.14	101.04	111.40
7	B	1205	MES	O3S-S-O2S	-4.12	101.09	111.40
7	B	1203	MES	O3S-S-O2S	-3.85	101.78	111.40
7	B	1204	MES	O2S-S-C8	3.33	111.76	106.73
7	B	1203	MES	O2S-S-C8	3.29	111.70	106.73
7	B	1205	MES	O2S-S-C8	3.07	111.36	106.73
7	B	1202	MES	O2S-S-C8	2.93	111.15	106.73
7	B	1205	MES	O1S-S-C8	2.89	111.09	106.73
7	B	1204	MES	O1S-S-C8	2.77	110.92	106.73
7	B	1202	MES	O3S-S-C8	2.65	111.19	106.00
7	B	1205	MES	O3S-S-C8	2.63	111.15	106.00
7	B	1202	MES	O1S-S-C8	2.61	110.68	106.73
7	B	1204	MES	O3S-S-C8	2.54	110.97	106.00
7	B	1203	MES	O3S-S-C8	2.25	110.41	106.00
7	B	1203	MES	O1S-S-C8	2.23	110.10	106.73
7	B	1202	MES	C5-N4-C3	2.02	113.20	108.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1202	MES	C8-C7-N4-C5
7	B	1204	MES	N4-C7-C8-S
7	B	1202	MES	C8-C7-N4-C3
7	B	1205	MES	C8-C7-N4-C5
7	B	1202	MES	C7-C8-S-O3S

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1306	SO4	1	0
6	B	1196	SO4	1	0
7	B	1204	MES	1	0
6	A	1303	SO4	1	0

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	1280/1296 (98%)	-0.42	17 (1%) 75 73	32, 56, 97, 170	10 (0%)
2	B	1150/1196 (96%)	-0.38	20 (1%) 69 67	29, 54, 109, 166	14 (1%)
3	C	119/152 (78%)	0.58	5 (4%) 40 37	66, 115, 158, 187	1 (0%)
All	All	2549/2644 (96%)	-0.35	42 (1%) 70 68	29, 56, 115, 187	25 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1230	GLY	5.2
1	A	1276	ARG	4.5
2	B	441	ALA	4.1
2	B	113	ILE	4.1
2	B	629	ILE	4.1
2	B	912	GLY	4.0
1	A	1278	LEU	3.7
1	A	434	ILE	3.6
1	A	1	MET	3.5
1	A	1277	THR	3.3
3	C	9	GLY	3.3
1	A	487	ILE	3.3
1	A	1275	SER	3.2
1	A	1232	THR	3.2
2	B	440	ARG	3.1
1	A	1231	ILE	3.0
1	A	647	LEU	3.0
2	B	1087	LEU	3.0
2	B	1119	ASN	3.0
2	B	1118	ASP	3.0
1	A	1295	PRO	2.9
3	C	12	VAL	2.9
1	A	1272	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	527	LYS	2.9
2	B	915	THR	2.8
1	A	450	LEU	2.6
2	B	359	TYR	2.6
2	B	452	SER	2.5
3	C	16	GLY	2.5
2	B	1120	MET	2.4
1	A	486	ASN	2.4
1	A	1226	LYS	2.4
2	B	628	ILE	2.3
2	B	526	SER	2.2
2	B	451	ASP	2.2
3	C	13	GLN	2.2
2	B	911	LEU	2.1
3	C	41	PRO	2.1
2	B	1	MET	2.1
2	B	858	ASN	2.0
2	B	281	TYR	2.0
1	A	648	TYR	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(Å ²)	Q<0.9
6	SO4	A	1307	5/5	0.50	0.20	172,173,174,176	0
6	SO4	A	1306	5/5	0.52	0.11	157,160,162,162	0
6	SO4	B	1201	5/5	0.61	0.14	151,152,155,160	0
6	SO4	C	144	5/5	0.70	0.09	161,162,165,165	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	1303	5/5	0.71	0.13	132,136,137,140	0
6	SO4	A	1310	5/5	0.73	0.12	133,139,139,142	0
6	SO4	A	1308	5/5	0.74	0.11	139,142,142,143	0
6	SO4	B	1197	5/5	0.74	0.12	129,131,132,135	0
6	SO4	B	1196	5/5	0.76	0.18	157,159,161,162	0
6	SO4	A	1309	5/5	0.76	0.14	159,159,160,160	0
7	MES	B	1204	12/12	0.76	0.16	82,100,176,178	0
7	MES	B	1205	12/12	0.77	0.15	105,116,150,150	0
6	SO4	A	1305	5/5	0.79	0.11	155,157,160,161	0
6	SO4	A	1304	5/5	0.79	0.10	136,137,138,139	0
6	SO4	A	1301	5/5	0.80	0.15	120,121,125,125	0
6	SO4	B	1199	5/5	0.81	0.13	122,125,128,130	0
7	MES	B	1202	12/12	0.81	0.21	88,96,189,190	0
6	SO4	A	1302	5/5	0.83	0.10	137,137,138,139	0
6	SO4	B	1200	5/5	0.88	0.08	112,117,119,121	0
6	SO4	B	1198	5/5	0.91	0.15	86,94,105,105	0
7	MES	B	1203	12/12	0.92	0.10	74,79,111,112	0
6	SO4	A	1300	5/5	0.94	0.08	98,103,108,110	0
6	SO4	B	1195	5/5	0.95	0.09	96,102,104,104	0
6	SO4	A	1299	5/5	0.95	0.10	97,99,101,103	0
4	ZN	A	1297	1/1	1.00	0.02	62,62,62,62	0
5	CA	A	1298	1/1	1.00	0.04	67,67,67,67	1

6.5 Other polymers [i](#)

There are no such residues in this entry.