



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:45 am GMT

PDB ID : 1YA0  
Title : Crystal structure of the N-terminal domain of human SMG7  
Authors : Fukuhara, N.; Ebert, J.; Unterholzner, L.; Lindner, D.; Izaurralde, E.; Conti, E.  
Deposited on : 2004-12-17  
Resolution : 2.55 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

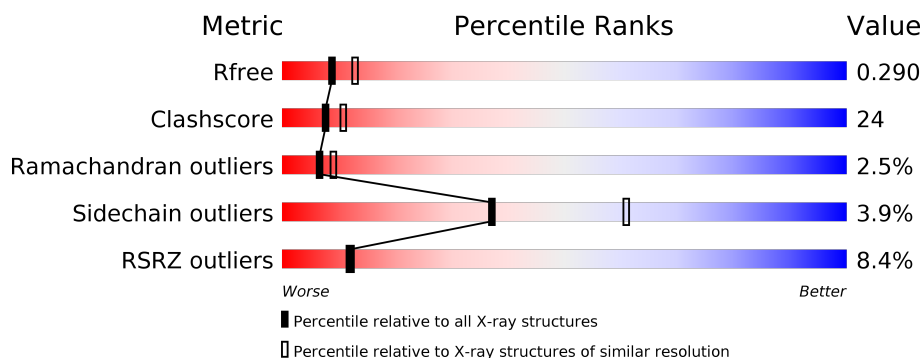
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	<div> <div>10%</div> <div>49%</div> <div>39%</div> <div>8%</div> </div>
1	B	497	<div> <div>6%</div> <div>55%</div> <div>34%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7854 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 SMG-7 transcript variant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	186	0	0
			3737	2384	646	693	14			
1	B	464	Total	C	N	O	S	102	0	0
			3783	2417	650	701	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total 131	O 131	0	0
3	B	188	Total 188	O 188	0	0

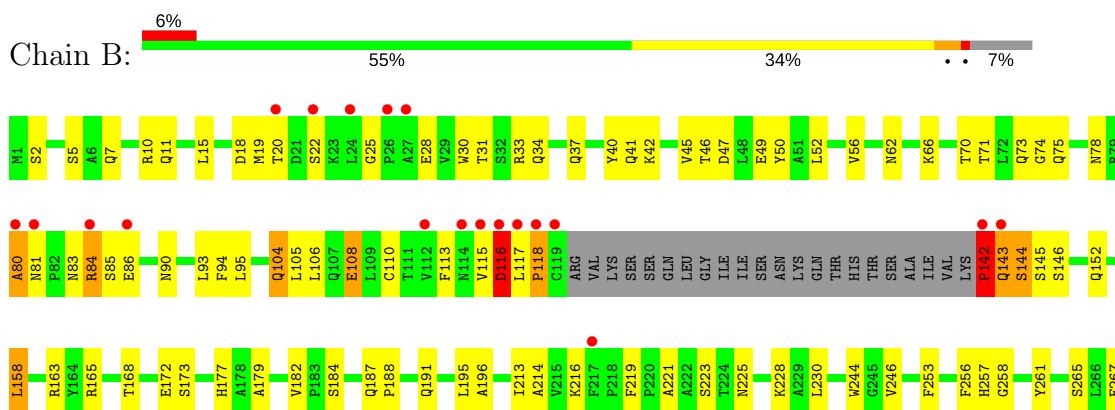
### 3 Residue-property plots

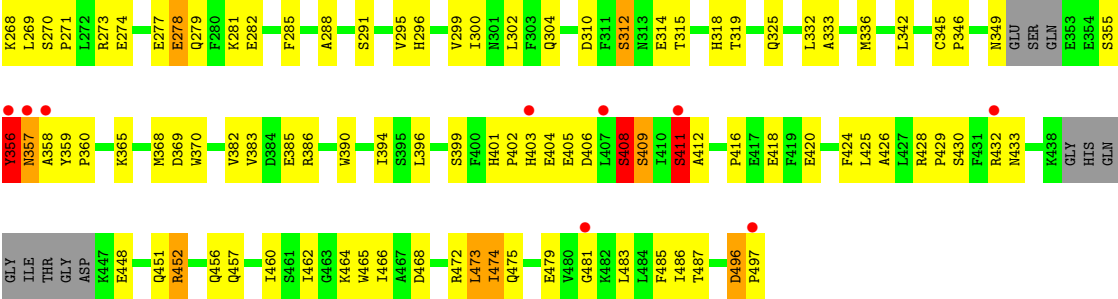
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: SMG-7 transcript variant 2



#### • Molecule 1: SMG-7 transcript variant 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.02Å 100.05Å 208.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55 48.65 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.55) 99.3 (48.65-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.246 , 0.287 0.249 , 0.290	Depositor DCC
$R_{free}$ test set	2219 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7854	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.42	0/3820	0.70	4/5165 (0.1%)
1	B	0.52	5/3869 (0.1%)	0.83	10/5236 (0.2%)
All	All	0.48	5/7689 (0.1%)	0.77	14/10401 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	SER	C-N	-14.03	1.01	1.34
1	B	408	SER	C-N	-9.95	1.11	1.34
1	B	356	TYR	C-N	-6.58	1.19	1.34
1	B	409	SER	C-N	-6.37	1.19	1.34
1	B	357	ASN	C-N	-5.42	1.21	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	SER	O-C-N	-18.34	93.35	122.70
1	B	411	SER	C-N-CA	15.74	161.04	121.70
1	B	408	SER	O-C-N	-14.32	99.78	122.70
1	B	411	SER	CA-C-N	14.12	148.26	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	SER	O-C-N	-11.54	104.23	122.70
1	B	408	SER	C-N-CA	10.95	149.07	121.70
1	B	408	SER	CA-C-N	9.55	138.21	117.20
1	A	496	ASP	N-CA-C	7.70	131.79	111.00
1	B	357	ASN	O-C-N	6.90	133.74	122.70
1	A	78	ASN	C-N-CA	6.87	138.88	121.70
1	B	80	ALA	N-CA-C	-6.60	93.19	111.00
1	A	21	ASP	CA-C-N	-5.95	104.12	117.20
1	A	84	ARG	O-C-N	-5.88	113.30	122.70
1	B	142	PRO	CA-C-N	-5.62	104.83	117.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	84	ARG	Mainchain
1	B	408	SER	Mainchain,Peptide
1	B	409	SER	Mainchain,Peptide
1	B	411	SER	Peptide

## 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	3737	0	3697	180	0
1	B	3783	0	3743	169	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
3	A	131	0	0	20	0
3	B	188	0	0	32	0
All	All	7854	0	7440	347	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 24.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ASN:HB2	1:B:356:TYR:CD1	1.78	1.18
1:B:349:ASN:HB2	1:B:356:TYR:HD1	1.03	1.11
1:A:81:ASN:HB3	1:A:84:ARG:HB3	1.22	1.11
1:B:257:HIS:HD2	1:B:304:GLN:HG3	0.98	1.07
1:B:257:HIS:CD2	1:B:304:GLN:HG3	1.91	1.05
1:B:93:LEU:HB2	3:B:648:HOH:O	1.59	1.01
1:A:81:ASN:CB	1:A:84:ARG:HB3	1.92	1.00
1:A:475:GLN:NE2	1:A:487:THR:HA	1.81	0.95
1:A:475:GLN:HE21	1:A:487:THR:HA	1.31	0.95
1:B:33:ARG:HH21	1:B:37:GLN:HE22	1.07	0.94
1:B:472:ARG:HB2	3:B:639:HOH:O	1.67	0.93
1:A:354:GLU:O	1:A:357:ASN:OD1	1.89	0.90
1:B:33:ARG:HE	1:B:37:GLN:NE2	1.71	0.89
1:A:344:LYS:HE3	1:A:348:GLN:HE21	1.38	0.88
1:A:257:HIS:ND1	1:A:304:GLN:HG3	1.88	0.87
1:A:344:LYS:HE3	1:A:348:GLN:NE2	1.89	0.87
1:A:351:SER:O	1:A:353:GLU:N	2.08	0.86
1:B:143:GLN:O	1:B:144:SER:HB3	1.77	0.85
1:A:405:GLU:C	1:A:407:LEU:H	1.81	0.83
1:A:448:GLU:HG3	1:A:449:GLY:H	1.42	0.83
1:A:352:GLN:HB2	1:A:355:SER:HB3	1.59	0.83
1:A:447:LYS:O	1:A:451:GLN:HG3	1.80	0.82
1:B:333:ALA:HB2	1:B:382:VAL:HG11	1.61	0.81
1:A:69:ILE:O	1:A:73:GLN:HG3	1.80	0.81
1:A:475:GLN:HG2	1:A:486:ILE:HG13	1.64	0.80
1:B:172:GLU:HG2	1:B:195:LEU:HD23	1.62	0.80
1:B:270:SER:HB3	1:B:271:PRO:HD3	1.64	0.79
1:B:300:ILE:HD12	3:B:536:HOH:O	1.81	0.79
1:A:110:CYS:HB3	1:A:151:CYS:SG	2.23	0.79
1:B:33:ARG:NH2	1:B:37:GLN:HE22	1.78	0.79
1:A:480:VAL:HG12	1:A:480:VAL:O	1.81	0.78
1:B:261:TYR:HB2	1:B:304:GLN:HE22	1.46	0.78
1:B:404:GLU:OE1	1:B:481:GLY:HA2	1.83	0.78
1:B:143:GLN:O	1:B:144:SER:CB	2.33	0.77
1:B:33:ARG:HE	1:B:37:GLN:HE21	1.30	0.77
1:B:74:GLY:N	3:B:517:HOH:O	2.17	0.77
1:B:365:LYS:HE3	1:B:369:ASP:OD2	1.86	0.76
1:B:71:THR:C	3:B:517:HOH:O	2.24	0.74
1:B:246:VAL:HG22	1:B:288:ALA:HB1	1.68	0.74
1:B:452:ARG:O	1:B:456:GLN:HG3	1.86	0.74
1:A:60:LEU:O	1:A:64:ALA:HB3	1.87	0.73
1:A:180:GLN:HG2	3:A:617:HOH:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:ND1	3:A:502:HOH:O	2.22	0.72
1:A:404:GLU:HA	1:A:404:GLU:OE1	1.89	0.72
1:A:10:ARG:O	1:A:14:VAL:HG23	1.89	0.72
1:B:214:ALA:O	1:B:425:LEU:HG	1.89	0.72
1:A:359:TYR:N	1:A:360:PRO:CD	2.53	0.72
1:B:2:SER:HA	3:B:558:HOH:O	1.89	0.72
1:A:30:TRP:CZ3	1:A:33:ARG:HD3	2.25	0.71
1:B:406:ASP:HA	1:B:457:GLN:HE21	1.55	0.71
1:B:403:HIS:HB3	3:B:664:HOH:O	1.91	0.71
1:A:31:THR:O	3:A:501:HOH:O	2.10	0.70
1:B:310:ASP:OD2	1:B:312:SER:HB3	1.90	0.70
1:A:285:PHE:HE2	1:A:348:GLN:NE2	1.91	0.69
1:B:117:LEU:HD12	1:B:118:PRO:HD2	1.74	0.69
1:A:452:ARG:O	1:A:456:GLN:HG3	1.93	0.69
1:A:405:GLU:O	1:A:407:LEU:N	2.26	0.68
1:A:359:TYR:CD2	1:A:360:PRO:HD3	2.28	0.67
1:A:185:ASN:HB3	3:A:535:HOH:O	1.94	0.67
1:A:410:ILE:O	1:A:412:ALA:N	2.27	0.67
1:A:172:GLU:O	1:A:176:ARG:HG2	1.94	0.67
1:B:278:GLU:HG3	1:B:279:GLN:N	2.08	0.67
1:A:322:GLN:HB3	3:A:592:HOH:O	1.96	0.66
1:A:401:HIS:N	1:A:402:PRO:HD3	2.10	0.66
1:A:407:LEU:C	1:A:409:SER:HB3	2.15	0.66
1:A:19:MET:HE1	1:A:33:ARG:HB2	1.78	0.65
1:A:359:TYR:H	1:A:360:PRO:HD3	1.62	0.65
1:A:365:LYS:HD3	1:A:369:ASP:OD2	1.95	0.65
1:A:344:LYS:CE	1:A:348:GLN:HE21	2.08	0.65
1:A:344:LYS:HD2	1:A:392:TRP:CE2	2.32	0.65
1:B:19:MET:CE	1:B:33:ARG:HG3	2.26	0.65
1:A:109:LEU:HD13	1:A:150:ILE:HD13	1.78	0.65
1:A:107:GLN:O	1:A:111:THR:HB	1.97	0.65
1:A:76:ALA:HB2	1:A:87:VAL:HG12	1.79	0.65
1:B:368:MET:HB3	1:B:462:ILE:HG21	1.79	0.64
1:B:486:ILE:CG2	1:B:487:THR:N	2.60	0.64
1:B:349:ASN:HB2	1:B:356:TYR:CE1	2.33	0.64
1:A:344:LYS:CE	1:A:348:GLN:NE2	2.61	0.63
1:A:456:GLN:O	1:A:460:ILE:HG12	1.98	0.63
1:B:62:ASN:HA	1:B:66:LYS:HB3	1.81	0.63
1:A:394:ILE:CD1	1:A:487:THR:HB	2.29	0.62
1:A:416:PRO:HD2	3:A:563:HOH:O	1.99	0.62
1:B:416:PRO:HG2	1:B:451:GLN:HE22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:SER:O	1:A:177:HIS:HD2	1.82	0.62
1:A:270:SER:HB3	1:A:271:PRO:HD3	1.81	0.62
1:A:314:GLU:OE1	1:A:375:PRO:HD2	2.00	0.61
1:A:63:HIS:HA	1:A:67:ASN:ND2	2.15	0.61
1:B:382:VAL:HG13	1:B:386:ARG:NH1	2.15	0.61
1:A:361:LEU:HB3	1:A:455:ARG:HD2	1.82	0.61
1:A:18:ASP:O	1:A:21:ASP:HB2	1.98	0.61
1:A:102:TYR:HB2	1:A:158:LEU:HD13	1.83	0.61
1:A:405:GLU:C	1:A:407:LEU:N	2.50	0.61
1:A:448:GLU:O	1:A:451:GLN:N	2.28	0.61
1:A:16:LYS:HD3	1:A:63:HIS:CE1	2.36	0.60
1:A:344:LYS:HD2	1:A:392:TRP:CZ2	2.36	0.60
1:B:401:HIS:N	1:B:402:PRO:HD3	2.17	0.60
1:B:315:THR:O	1:B:315:THR:HG22	2.00	0.60
1:B:333:ALA:CB	1:B:382:VAL:HG11	2.31	0.60
1:A:5:SER:HB3	1:A:50:TYR:CD2	2.35	0.60
1:A:44:LEU:HD22	1:A:150:ILE:HD12	1.84	0.59
1:A:34:GLN:N	3:A:501:HOH:O	2.35	0.59
1:B:318:HIS:CD2	1:B:319:THR:H	2.20	0.59
1:A:359:TYR:N	1:A:360:PRO:HD3	2.17	0.59
1:B:281:LYS:O	1:B:285:PHE:HD1	1.86	0.59
1:B:110:CYS:SG	1:B:117:LEU:HD23	2.43	0.59
1:B:474:ILE:HD11	1:B:485:PHE:HD2	1.68	0.59
1:B:318:HIS:HD2	1:B:319:THR:H	1.51	0.59
1:A:285:PHE:CE2	1:A:348:GLN:NE2	2.70	0.58
1:A:344:LYS:HG3	1:A:392:TRP:CD2	2.39	0.58
1:B:196:ALA:HA	3:B:579:HOH:O	2.04	0.58
1:B:265:SER:HA	1:B:267:GLU:OE2	2.04	0.58
1:B:456:GLN:O	1:B:460:ILE:HG12	2.03	0.58
1:A:273:ARG:NH2	1:A:274:GLU:OE2	2.35	0.58
1:B:465:TRP:CE3	1:B:466:ILE:HD13	2.39	0.58
1:A:48:LEU:O	1:A:52:LEU:HD13	2.04	0.58
1:B:191:GLN:NE2	3:B:671:HOH:O	2.30	0.58
1:B:33:ARG:NE	1:B:37:GLN:NE2	2.47	0.58
1:B:219:PHE:CE2	1:B:221:ALA:HB3	2.39	0.57
1:B:382:VAL:HG13	1:B:386:ARG:HH12	1.68	0.57
1:A:57:GLU:HG3	1:A:58:GLN:HG3	1.86	0.57
1:B:349:ASN:CB	1:B:356:TYR:CD1	2.72	0.57
1:B:465:TRP:HE3	1:B:466:ILE:HD13	1.68	0.57
1:A:416:PRO:HD3	1:A:451:GLN:NE2	2.19	0.57
1:B:496:ASP:HB3	1:B:497:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PHE:HE2	1:A:348:GLN:HE22	1.51	0.57
1:B:33:ARG:NE	3:B:568:HOH:O	2.38	0.57
1:A:345:CYS:HB3	1:A:346:PRO:HD3	1.86	0.57
1:B:173:SER:O	1:B:177:HIS:HD2	1.88	0.57
1:B:345:CYS:HB3	1:B:346:PRO:HD3	1.85	0.56
1:B:31:THR:HG22	3:B:510:HOH:O	2.03	0.56
1:A:359:TYR:O	3:A:525:HOH:O	2.18	0.56
1:B:113:PHE:O	1:B:115:VAL:HG23	2.06	0.56
1:B:486:ILE:HG22	1:B:487:THR:N	2.19	0.56
1:A:313:ASN:ND2	1:A:320:TYR:OH	2.39	0.56
1:A:219:PHE:CE2	1:A:221:ALA:HB3	2.40	0.56
1:A:480:VAL:O	1:A:480:VAL:CG1	2.54	0.55
1:A:347:LEU:HD12	3:A:554:HOH:O	2.05	0.55
1:A:414:PRO:HB2	1:A:419:PHE:CD1	2.41	0.55
1:A:42:LYS:O	1:A:46:THR:HB	2.07	0.55
1:B:349:ASN:CB	1:B:356:TYR:HD1	1.97	0.55
1:A:63:HIS:HA	1:A:67:ASN:HD22	1.72	0.55
1:B:359:TYR:CG	1:B:360:PRO:HD3	2.42	0.55
1:A:32:SER:C	3:A:501:HOH:O	2.46	0.55
1:B:356:TYR:N	1:B:356:TYR:CD2	2.75	0.55
1:B:7:GLN:O	1:B:11:GLN:HG3	2.07	0.55
1:A:496:ASP:O	1:A:497:PRO:O	2.25	0.55
1:B:40:TYR:CD2	1:B:56:VAL:HG13	2.42	0.54
1:B:253:PHE:CZ	1:B:257:HIS:HE1	2.24	0.54
1:A:439:GLY:O	1:A:440:HIS:HB2	2.07	0.54
1:A:57:GLU:HG3	1:A:58:GLN:N	2.21	0.54
1:B:432:ARG:HG3	1:B:433:ASN:N	2.22	0.54
1:B:428:ARG:HB2	1:B:429:PRO:HD3	1.89	0.53
1:B:71:THR:O	1:B:75:GLN:HG3	2.07	0.53
1:A:40:TYR:CD2	1:A:56:VAL:HG13	2.43	0.53
1:A:17:ALA:N	3:A:499:HOH:O	2.41	0.53
1:A:232:LYS:O	1:A:235:GLU:HB2	2.09	0.53
1:A:368:MET:HB3	1:A:462:ILE:HG21	1.90	0.53
1:A:353:GLU:O	1:A:354:GLU:HB2	2.08	0.53
1:B:81:ASN:HD22	1:B:84:ARG:N	2.06	0.53
1:A:410:ILE:C	1:A:412:ALA:N	2.62	0.53
1:A:365:LYS:NZ	1:A:418:GLU:HG2	2.24	0.53
1:B:172:GLU:HB3	3:B:650:HOH:O	2.09	0.53
1:A:36:LEU:HD22	1:A:40:TYR:CE1	2.45	0.52
1:A:431:PHE:O	1:A:433:ASN:N	2.40	0.52
1:B:273:ARG:NH2	1:B:274:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:CZ	3:B:568:HOH:O	2.56	0.52
1:A:237:ARG:NH1	1:A:268:LYS:NZ	2.58	0.52
1:B:19:MET:HE2	1:B:33:ARG:HG3	1.89	0.52
1:B:416:PRO:HG2	1:B:451:GLN:NE2	2.24	0.52
1:B:382:VAL:CG1	1:B:386:ARG:NH1	2.71	0.52
1:B:475:GLN:HA	3:B:665:HOH:O	2.08	0.52
1:A:286:GLN:O	1:A:287:LYS:HB2	2.09	0.52
1:A:246:VAL:CG2	1:A:288:ALA:HB1	2.40	0.52
1:A:448:GLU:HG3	1:A:449:GLY:N	2.17	0.52
1:A:44:LEU:HD22	1:A:150:ILE:CD1	2.40	0.52
1:B:163:ARG:NH2	2:B:498:SO4:O1	2.43	0.52
1:B:253:PHE:CZ	1:B:257:HIS:CE1	2.98	0.52
1:B:282:GLU:CD	3:B:601:HOH:O	2.48	0.52
1:A:321:SER:HB3	1:A:324:GLU:HG3	1.91	0.51
1:A:40:TYR:HD2	1:A:43:MET:CE	2.22	0.51
1:B:214:ALA:C	1:B:425:LEU:HG	2.30	0.51
1:B:33:ARG:NH1	1:B:94:PHE:CE2	2.78	0.51
1:A:4:GLN:HG3	1:A:8:TYR:CE1	2.45	0.51
1:B:244:TRP:CD2	1:B:279:GLN:HG3	2.46	0.51
1:B:273:ARG:HD2	1:B:333:ALA:HB3	1.93	0.51
1:A:396:LEU:O	1:A:399:SER:HB3	2.10	0.50
1:A:414:PRO:HB2	1:A:419:PHE:HD1	1.76	0.50
1:B:187:GLN:HB3	1:B:188:PRO:HD3	1.92	0.50
1:B:268:LYS:O	1:B:271:PRO:HD2	2.11	0.50
1:A:180:GLN:NE2	3:A:616:HOH:O	2.43	0.50
1:B:47:ASP:HB3	3:B:509:HOH:O	2.11	0.50
1:A:307:HIS:HE1	3:A:620:HOH:O	1.95	0.50
1:B:19:MET:HE1	1:B:33:ARG:HG3	1.92	0.50
1:B:356:TYR:N	1:B:356:TYR:HD2	2.09	0.50
1:B:296:HIS:C	3:B:536:HOH:O	2.50	0.49
1:B:355:SER:O	1:B:359:TYR:CD2	2.66	0.49
1:B:93:LEU:HD23	3:B:636:HOH:O	2.12	0.49
1:A:417:GLU:OE2	1:A:455:ARG:NH1	2.46	0.49
1:A:144:SER:HB3	1:A:147:CYS:HB2	1.93	0.49
1:B:146:SER:HB2	3:B:679:HOH:O	2.13	0.49
1:A:102:TYR:CB	1:A:158:LEU:HD13	2.43	0.49
1:A:218:PRO:O	1:A:220:PRO:HD3	2.13	0.48
1:A:239:GLU:HG3	3:A:586:HOH:O	2.13	0.48
1:A:40:TYR:HD2	1:A:43:MET:HE3	1.78	0.48
1:A:394:ILE:HD13	1:A:487:THR:HB	1.95	0.48
1:B:45:VAL:HG21	1:B:108:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:TYR:H	1:A:360:PRO:CD	2.20	0.48
1:B:152:GLN:NE2	1:B:182:VAL:HB	2.28	0.48
1:B:78:ASN:O	1:B:80:ALA:N	2.45	0.48
1:A:18:ASP:N	3:A:499:HOH:O	2.46	0.48
1:A:19:MET:CE	1:A:33:ARG:HB2	2.42	0.48
1:B:106:LEU:HD21	1:B:117:LEU:HD21	1.96	0.48
1:A:57:GLU:OE1	1:A:149:TYR:HE2	1.96	0.48
1:A:257:HIS:HE2	1:A:301:ASN:ND2	2.12	0.48
1:A:410:ILE:O	1:A:411:SER:C	2.51	0.48
1:B:281:LYS:O	1:B:285:PHE:CD1	2.66	0.48
1:A:175:TYR:CZ	1:A:191:GLN:HB3	2.48	0.47
1:A:244:TRP:HB3	1:A:248:ASP:HB2	1.96	0.47
1:B:267:GLU:CD	1:B:267:GLU:H	2.17	0.47
1:B:90:ASN:O	3:B:648:HOH:O	2.20	0.47
1:B:221:ALA:O	1:B:225:ASN:ND2	2.47	0.47
1:A:182:VAL:HG11	1:A:185:ASN:ND2	2.29	0.47
1:B:115:VAL:C	1:B:117:LEU:H	2.17	0.47
1:B:116:ASP:O	1:B:117:LEU:C	2.52	0.47
1:A:400:PHE:HD1	1:A:460:ILE:HD11	1.78	0.47
1:A:316:GLU:HG3	1:A:318:HIS:CE1	2.50	0.47
1:B:216:LYS:HG2	3:B:581:HOH:O	2.14	0.47
1:B:448:GLU:O	1:B:451:GLN:HG2	2.15	0.47
1:A:313:ASN:HD22	1:A:318:HIS:HD2	1.61	0.47
1:B:10:ARG:NH2	3:B:561:HOH:O	2.43	0.47
1:A:79:ARG:O	1:A:80:ALA:HB3	2.15	0.47
1:A:449:GLY:O	1:A:453:ARG:HB2	2.15	0.47
1:B:33:ARG:NH1	1:B:94:PHE:HE2	2.13	0.47
1:A:268:LYS:O	1:A:271:PRO:HD2	2.14	0.46
1:A:401:HIS:N	1:A:402:PRO:CD	2.77	0.46
1:B:5:SER:HB3	1:B:50:TYR:CD2	2.50	0.46
1:A:405:GLU:HA	1:A:407:LEU:CD1	2.45	0.46
1:A:455:ARG:NH1	1:A:455:ARG:HB2	2.31	0.46
1:A:232:LYS:HA	1:A:235:GLU:OE2	2.16	0.46
1:A:388:TYR:O	1:A:391:PRO:HD2	2.16	0.46
1:A:412:ALA:O	1:A:414:PRO:HD3	2.16	0.46
1:B:41:GLN:HG3	1:B:105:LEU:CD1	2.46	0.46
1:A:257:HIS:CE1	1:A:301:ASN:HD22	2.32	0.46
1:B:396:LEU:O	1:B:399:SER:HB3	2.16	0.46
1:A:411:SER:C	1:A:413:THR:H	2.20	0.46
1:B:359:TYR:N	1:B:360:PRO:CD	2.79	0.46
3:A:602:HOH:O	1:B:267:GLU:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ASN:O	1:B:358:ALA:HB3	2.16	0.45
1:B:405:GLU:HA	1:B:408:SER:OG	2.17	0.45
1:B:342:LEU:O	1:B:346:PRO:HD3	2.17	0.45
1:A:455:ARG:NH2	3:A:563:HOH:O	2.45	0.45
1:A:215:VAL:O	1:A:218:PRO:HD3	2.17	0.45
1:A:362:PRO:O	1:A:366:VAL:HG23	2.16	0.45
1:A:437:SER:OG	1:A:438:LYS:N	2.48	0.45
1:A:1:MET:O	1:A:3:LEU:N	2.49	0.45
1:B:230:LEU:HD13	1:B:258:GLY:HA2	1.97	0.45
1:A:173:SER:O	1:A:177:HIS:CD2	2.66	0.44
1:B:314:GLU:HB3	3:B:607:HOH:O	2.17	0.44
1:B:95:LEU:HD13	1:B:165:ARG:HG3	1.99	0.44
1:A:290:ASN:OD1	1:A:292:GLN:HB3	2.16	0.44
1:A:490:PRO:HD2	1:B:271:PRO:HG2	2.00	0.44
1:B:253:PHE:CE1	1:B:257:HIS:HE1	2.35	0.44
1:B:291:SER:HB3	1:B:359:TYR:HA	2.00	0.44
1:A:474:ILE:HG22	1:A:475:GLN:N	2.33	0.44
1:B:168:THR:O	1:B:172:GLU:HG3	2.17	0.44
1:B:256:PHE:CE1	1:B:269:LEU:HD22	2.52	0.44
1:A:372:ARG:HD3	3:A:532:HOH:O	2.17	0.44
1:B:424:PHE:O	1:B:428:ARG:HG3	2.17	0.44
1:A:385:GLU:OE2	1:B:385:GLU:OE1	2.36	0.44
1:A:458:ARG:O	1:A:462:ILE:HG13	2.18	0.44
1:B:142:PRO:HB2	1:B:143:GLN:H	1.26	0.44
1:A:103:THR:O	1:A:107:GLN:HG3	2.17	0.43
1:A:154:CYS:O	1:A:158:LEU:HB2	2.17	0.43
1:A:234:LEU:HD12	1:A:262:LEU:HD12	1.99	0.43
1:A:79:ARG:O	1:A:80:ALA:C	2.56	0.43
1:B:390:TRP:O	1:B:394:ILE:HD13	2.18	0.43
1:B:497:PRO:HB3	3:B:668:HOH:O	2.18	0.43
1:B:277:GLU:OE1	3:B:656:HOH:O	2.20	0.43
1:B:30:TRP:O	1:B:34:GLN:HG2	2.18	0.43
1:A:152:GLN:HG3	1:A:178:ALA:O	2.19	0.43
1:A:316:GLU:H	1:A:316:GLU:HG2	1.63	0.43
1:A:359:TYR:CG	1:A:360:PRO:HD3	2.54	0.43
1:B:172:GLU:CG	1:B:195:LEU:HD23	2.41	0.43
1:B:325:GLN:HG2	3:B:685:HOH:O	2.17	0.43
1:B:33:ARG:CZ	1:B:37:GLN:HE22	2.31	0.43
1:B:302:LEU:HD22	1:B:370:TRP:CG	2.54	0.43
1:B:70:THR:O	3:B:517:HOH:O	2.21	0.43
1:A:466:ILE:HG21	1:A:474:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLY:O	1:B:28:GLU:HB2	2.18	0.43
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.87	0.42
1:B:390:TRP:CD1	1:B:473:LEU:HG	2.54	0.42
1:B:474:ILE:CD1	1:B:485:PHE:HD2	2.32	0.42
1:B:464:LYS:HE3	1:B:468:ASP:OD2	2.20	0.42
1:B:104:GLN:HB3	1:B:104:GLN:HE21	1.68	0.42
1:A:273:ARG:HD3	1:A:330:GLN:OE1	2.19	0.42
1:A:1:MET:C	1:A:3:LEU:H	2.23	0.42
1:A:450:GLN:O	1:A:454:ILE:HG13	2.19	0.42
1:B:83:ASN:O	1:B:86:GLU:HG2	2.19	0.42
1:A:244:TRP:CD2	1:A:279:GLN:HG3	2.54	0.42
1:B:219:PHE:HE2	1:B:221:ALA:HB3	1.83	0.42
1:B:33:ARG:HH11	1:B:94:PHE:HE2	1.67	0.42
1:B:402:PRO:HB2	1:B:483:LEU:HB2	2.01	0.42
1:A:57:GLU:CG	1:A:58:GLN:N	2.83	0.42
1:A:464:LYS:HD2	1:A:468:ASP:OD2	2.20	0.42
1:A:157:HIS:HD2	1:A:160:ASP:OD2	2.02	0.42
1:B:246:VAL:CG2	1:B:288:ALA:HB1	2.45	0.42
1:B:420:GLU:HB3	3:B:626:HOH:O	2.19	0.42
1:B:355:SER:O	1:B:359:TYR:CE2	2.72	0.42
1:A:155:LEU:HD12	1:A:181:LEU:HD12	2.02	0.41
1:A:393:LEU:O	1:A:396:LEU:HB3	2.20	0.41
1:B:15:LEU:O	1:B:18:ASP:HB2	2.20	0.41
1:B:20:THR:O	1:B:20:THR:HG22	2.20	0.41
1:A:8:TYR:CZ	1:A:42:LYS:HE3	2.55	0.41
1:B:49:GLU:HB2	3:B:559:HOH:O	2.20	0.41
1:B:15:LEU:HA	1:B:15:LEU:HD23	1.89	0.41
1:B:336:MET:HG3	1:B:383:VAL:HG22	2.02	0.41
1:B:370:TRP:CD1	1:B:426:ALA:HB1	2.55	0.41
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.90	0.41
1:B:83:ASN:O	1:B:85:SER:N	2.53	0.41
1:A:213:ILE:HD11	1:A:223:SER:HA	2.02	0.41
1:A:389:ILE:HG13	1:A:390:TRP:N	2.34	0.41
1:A:495:GLU:O	1:A:497:PRO:HD2	2.20	0.41
1:A:455:ARG:NH1	3:A:563:HOH:O	2.47	0.41
1:B:295:VAL:O	1:B:299:VAL:HG23	2.20	0.41
1:A:51:ALA:O	1:A:56:VAL:HG23	2.21	0.41
1:A:66:LYS:HE2	1:A:164:TYR:OH	2.20	0.41
1:B:394:ILE:HD11	1:B:474:ILE:HB	2.02	0.41
1:A:31:THR:C	3:A:501:HOH:O	2.55	0.41
1:B:496:ASP:HB3	1:B:497:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:GLU:OE1	1:A:417:GLU:N	2.48	0.41
1:B:213:ILE:HD11	1:B:223:SER:HA	2.03	0.41
1:B:34:GLN:HG3	3:B:567:HOH:O	2.20	0.41
1:A:30:TRP:HZ3	1:A:33:ARG:HD3	1.81	0.41
1:B:152:GLN:HE22	1:B:182:VAL:HB	1.86	0.41
1:B:30:TRP:CZ3	1:B:33:ARG:NH1	2.89	0.41
1:A:175:TYR:HB3	1:A:192:LEU:HG	2.03	0.41
1:A:1:MET:C	1:A:3:LEU:N	2.73	0.41
1:B:179:ALA:HA	3:B:526:HOH:O	2.21	0.41
1:B:42:LYS:O	1:B:46:THR:HG23	2.21	0.41
1:B:73:GLN:N	3:B:517:HOH:O	2.53	0.41
1:A:41:GLN:O	1:A:45:VAL:HG23	2.21	0.40
1:A:470:GLN:N	1:A:471:PRO:HD3	2.37	0.40
1:A:394:ILE:HD11	1:A:474:ILE:HG12	2.03	0.40
1:A:193:ALA:HB2	1:A:208:TYR:CB	2.51	0.40
1:A:57:GLU:HG3	1:A:58:GLN:H	1.84	0.40
1:B:365:LYS:NZ	1:B:418:GLU:HG3	2.37	0.40
1:A:328:TRP:O	1:A:332:LEU:HB2	2.22	0.40







There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	448/497 (90%)	399 (89%)	36 (8%)	13 (3%)		
1	B	456/497 (92%)	413 (91%)	33 (7%)	10 (2%)		
All	All	904/994 (91%)	812 (90%)	69 (8%)	23 (2%)		

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	352	GLN
1	A	411	SER
1	A	432	ARG
1	A	437	SER
1	B	84	ARG
1	B	118	PRO
1	B	412	ALA
1	A	496	ASP
1	B	22	SER
1	B	116	ASP
1	B	143	GLN
1	B	479	GLU
1	A	2	SER
1	A	353	GLU
1	A	406	ASP
1	A	25	GLY
1	A	82	PRO
1	A	439	GLY
1	B	144	SER
1	B	411	SER
1	A	346	PRO
1	B	496	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	412/447 (92%)	396 (96%)	16 (4%)	37	61
1	B	419/447 (94%)	403 (96%)	16 (4%)	38	62
All	All	831/894 (93%)	799 (96%)	32 (4%)	37	61

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU

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Mol	Chain	Res	Type
1	A	18	ASP
1	A	21	ASP
1	A	36	LEU
1	A	46	THR
1	A	53	ASP
1	A	104	GLN
1	A	166	ASN
1	A	224	THR
1	A	237	ARG
1	A	332	LEU
1	A	413	THR
1	A	419	PHE
1	A	475	GLN
1	A	496	ASP
1	A	497	PRO
1	B	104	GLN
1	B	108	GLU
1	B	116	ASP
1	B	142	PRO
1	B	145	SER
1	B	158	LEU
1	B	184	SER
1	B	228	LYS
1	B	278	GLU
1	B	312	SER
1	B	332	LEU
1	B	356	TYR
1	B	430	SER
1	B	452	ARG
1	B	473	LEU
1	B	474	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	GLN
1	A	67	ASN
1	A	73	GLN
1	A	104	GLN
1	A	153	HIS
1	A	157	HIS

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Mol	Chain	Res	Type
1	A	177	HIS
1	A	301	ASN
1	A	304	GLN
1	A	313	ASN
1	A	318	HIS
1	A	348	GLN
1	A	387	GLN
1	A	422	GLN
1	A	475	GLN
1	B	11	GLN
1	B	37	GLN
1	B	58	GLN
1	B	81	ASN
1	B	177	HIS
1	B	190	ASN
1	B	257	HIS
1	B	292	GLN
1	B	301	ASN
1	B	304	GLN
1	B	318	HIS
1	B	451	GLN
1	B	457	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	SO4	A	498	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	B	498	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	B	499	-	4,4,4	0.32	0	6,6,6	0.07	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
2	SO4	A	498	-	-	0/0/0/0	0/0/0/0
2	SO4	B	498	-	-	0/0/0/0	0/0/0/0
2	SO4	B	499	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	498	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	458/497 (92%)	0.49	49 (10%) <b>7</b> <b>6</b>	24, 45, 86, 92	54 (11%)
1	B	464/497 (93%)	0.40	28 (6%) <b>23</b> <b>24</b>	19, 38, 74, 109	30 (6%)
All	All	922/994 (92%)	0.44	77 (8%) <b>12</b> <b>12</b>	19, 41, 82, 109	84 (9%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ASN	8.9
1	B	118	PRO	8.7
1	B	356	TYR	6.8
1	A	81	ASN	5.9
1	A	358	ALA	5.6
1	A	352	GLN	5.5
1	A	497	PRO	5.3
1	A	353	GLU	5.2
1	A	440	HIS	5.1
1	B	116	ASP	4.8
1	A	496	ASP	4.8
1	A	407	LEU	4.8
1	A	481	GLY	4.7
1	A	351	SER	4.7
1	B	20	THR	4.4
1	B	497	PRO	4.3
1	A	357	ASN	4.3
1	B	80	ALA	4.3
1	A	354	GLU	4.2
1	A	409	SER	4.2
1	B	119	CYS	4.1
1	B	481	GLY	4.1
1	A	316	GLU	4.0
1	A	410	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	358	ALA	3.9
1	A	143	GLN	3.9
1	A	21	ASP	3.7
1	A	439	GLY	3.7
1	A	80	ALA	3.7
1	A	356	TYR	3.6
1	A	22	SER	3.6
1	A	26	PRO	3.4
1	A	355	SER	3.3
1	A	23	LYS	3.3
1	A	83	ASN	3.3
1	A	315	THR	3.2
1	A	27	ALA	3.1
1	B	22	SER	3.0
1	A	24	LEU	3.0
1	A	82	PRO	3.0
1	A	50	TYR	2.9
1	B	407	LEU	2.9
1	B	26	PRO	2.9
1	A	25	GLY	2.9
1	A	19	MET	2.8
1	B	24	LEU	2.8
1	A	449	GLY	2.8
1	B	143	GLN	2.8
1	A	2	SER	2.8
1	B	117	LEU	2.7
1	B	142	PRO	2.7
1	A	480	VAL	2.7
1	A	448	GLU	2.6
1	A	348	GLN	2.6
1	A	447	LYS	2.6
1	A	411	SER	2.6
1	A	17	ALA	2.6
1	B	112	VAL	2.6
1	B	411	SER	2.5
1	A	87	VAL	2.4
1	A	1	MET	2.4
1	B	403	HIS	2.4
1	A	349	ASN	2.4
1	B	27	ALA	2.4
1	A	77	LYS	2.3
1	B	217	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	84	ARG	2.3
1	A	403	HIS	2.3
1	B	357	ASN	2.3
1	B	86	GLU	2.3
1	A	240	VAL	2.2
1	A	453	ARG	2.2
1	B	115	VAL	2.2
1	B	114	ASN	2.2
1	A	48	LEU	2.1
1	B	432	ARG	2.1
1	B	81	ASN	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	499	5/5	0.95	0.20	1.05	78,78,79,79	0
2	SO4	A	498	5/5	0.94	0.15	-0.25	64,66,68,68	0
2	SO4	B	498	5/5	0.97	0.10	-	53,54,56,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.