



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:56 AM GMT

PDB ID : 2EYU  
Title : The Crystal Structure of the C-terminal Domain of Aquifex aeolicus PilT  
Authors : Satyshur, K.A.; Worzalla, G.A.; Meyer, L.S.; Heiniger, E.K.; Aukema, K.G.; Forest, K.T.  
Deposited on : 2005-11-09  
Resolution : 1.87 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

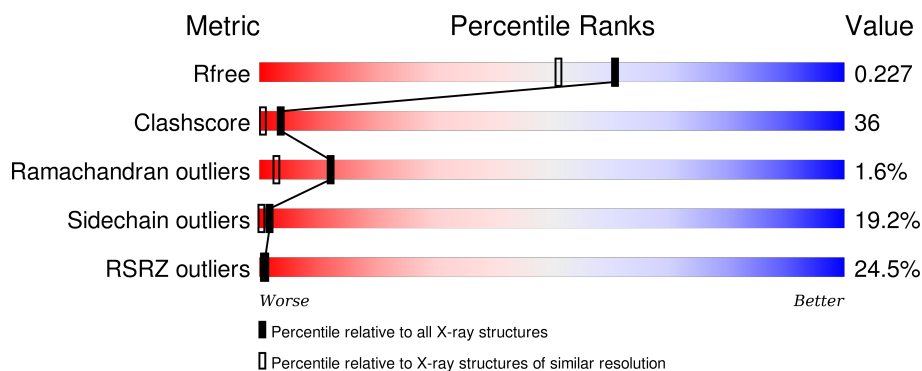
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	261	
1	B	261	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	2800	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3920 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 twitching motility protein PilT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	Se	0	0	0
			1949	1236	338	366	1	8			
1	B	247	Total	C	N	O	S	Se	0	0	0
			1949	1236	338	366	1	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	MSE	-	CLONING ARTIFACT	GB 15606134
A	136	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	156	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	218	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	294	GLY	GLU	ENGINEERED	GB 15606134
A	318	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	327	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	330	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	349	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	361	MSE	MET	MODIFIED RESIDUE	GB 15606134
A	367	HIS	-	EXPRESSION TAG	GB 15606134
A	368	HIS	-	EXPRESSION TAG	GB 15606134
A	369	HIS	-	EXPRESSION TAG	GB 15606134
A	370	HIS	-	EXPRESSION TAG	GB 15606134
A	371	HIS	-	EXPRESSION TAG	GB 15606134
A	372	HIS	-	EXPRESSION TAG	GB 15606134
B	112	MSE	-	CLONING ARTIFACT	GB 15606134
B	136	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	156	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	218	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	294	GLY	GLU	ENGINEERED	GB 15606134
B	318	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	327	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	330	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	349	MSE	MET	MODIFIED RESIDUE	GB 15606134

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Chain	Residue	Modelled	Actual	Comment	Reference
B	361	MSE	MET	MODIFIED RESIDUE	GB 15606134
B	367	HIS	-	EXPRESSION TAG	GB 15606134
B	368	HIS	-	EXPRESSION TAG	GB 15606134
B	369	HIS	-	EXPRESSION TAG	GB 15606134
B	370	HIS	-	EXPRESSION TAG	GB 15606134
B	371	HIS	-	EXPRESSION TAG	GB 15606134
B	372	HIS	-	EXPRESSION TAG	GB 15606134

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



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

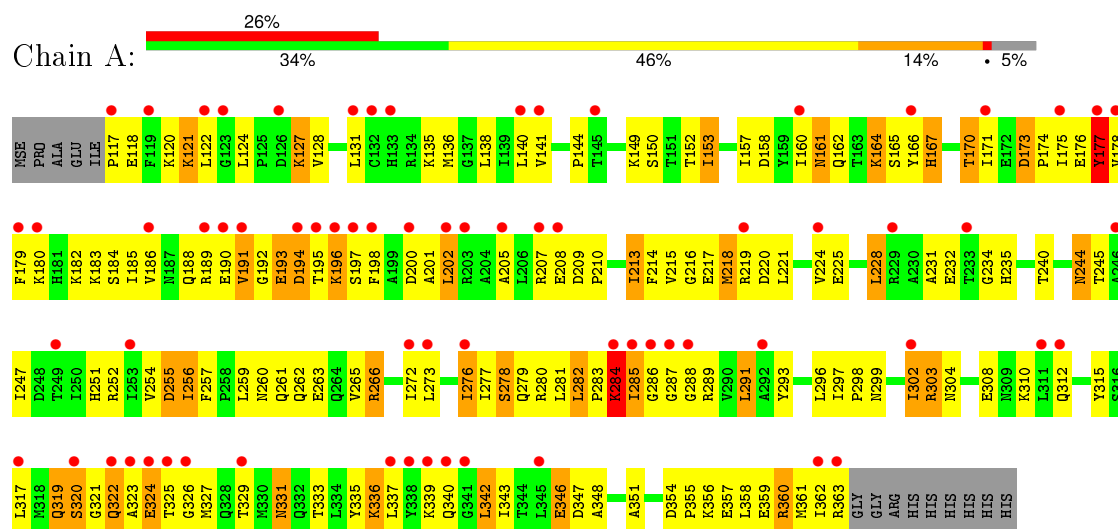
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	9	Total	O	0	0
			9	9		

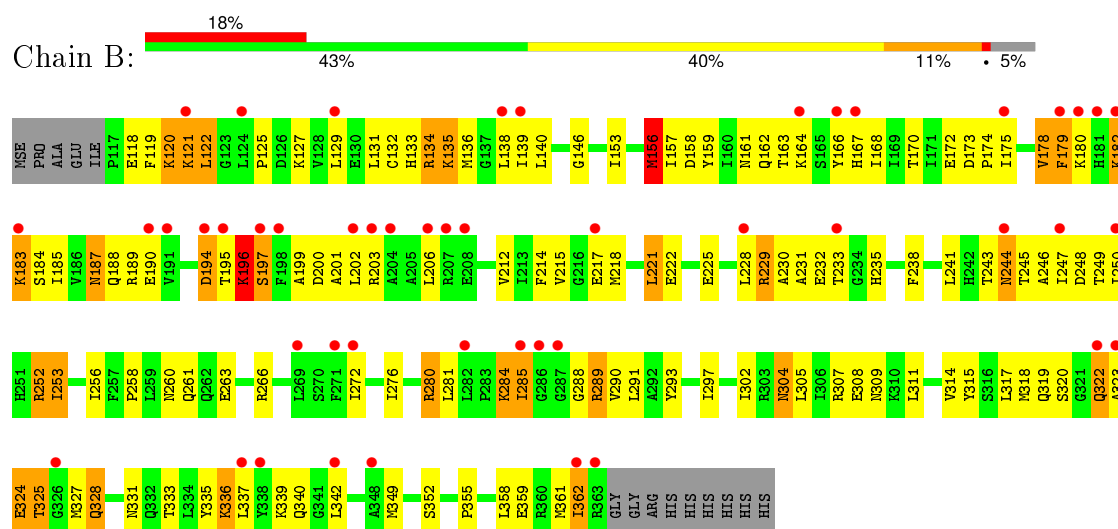
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: twitching motility protein PilT



#### • Molecule 1: twitching motility protein PilT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.15Å 89.15Å 70.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.87 34.71 – 1.87	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-1.87) 98.8 (34.71-1.87)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 1.87Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.170 , (Not available) 0.159 , 0.227	Depositor DCC
$R_{free}$ test set	2222 reflections (5.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 98.2	EDS
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 45210 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	3920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/1970	1.17	7/2646 (0.3%)
1	B	0.39	0/1970	1.24	11/2646 (0.4%)
All	All	0.39	0/3940	1.20	18/5292 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	B	324	GLU	C-N-CA	9.67	145.88	121.70
1	A	177	TYR	CA-CB-CG	9.51	131.47	113.40
1	A	303	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	B	156	MSE	CA-CB-CG	7.55	126.13	113.30
1	A	303	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	B	134	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	B	134	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	177	TYR	CB-CG-CD2	6.46	124.88	121.00
1	B	293	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	B	252	ARG	CD-NE-CZ	6.22	132.30	123.60
1	A	303	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	156	MSE	CG-SE-CE	-5.82	86.09	98.90
1	A	219	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	189	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	B	146	GLY	C-N-CA	-5.52	107.91	121.70
1	A	266	ARG	CD-NE-CZ	5.27	130.98	123.60
1	B	134	ARG	CD-NE-CZ	-5.04	116.55	123.60

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	1949	0	2015	165	0
1	B	1949	0	2014	122	0
2	B	5	0	0	0	0
3	A	8	0	0	1	0
3	B	9	0	0	0	0
All	All	3920	0	4029	284	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 36.

All (284) 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:296:LEU:HA	1:A:327:MSE:SE	1.50	1.61
1:A:296:LEU:CA	1:A:327:MSE:SE	2.38	1.21
1:B:195:THR:HG21	1:B:201:ALA:HB2	1.44	0.98
1:A:284:LYS:HG2	1:A:343:ILE:HA	1.43	0.97
1:B:125:PRO:HB2	1:B:324:GLU:HG3	1.44	0.96
1:B:314:VAL:HG12	1:B:318:MSE:HE2	1.48	0.95
1:B:302:ILE:HD11	1:B:327:MSE:HE1	1.51	0.93
1:A:167:HIS:HA	1:A:185:ILE:HG23	1.48	0.93
1:A:302:ILE:HD12	1:A:327:MSE:HE2	1.49	0.92
1:B:175:ILE:HG13	1:B:190:GLU:HG3	1.56	0.86
1:A:298:PRO:HA	1:A:302:ILE:HG13	1.57	0.86
1:B:245:THR:HG22	1:B:248:ASP:HB2	1.60	0.84
1:A:175:ILE:HD11	1:A:178:VAL:HG12	1.60	0.83
1:B:315:TYR:HA	1:B:318:MSE:HE3	1.60	0.83
1:A:136:MSE:HE2	1:A:234:GLY:HA2	1.60	0.80
1:B:159:TYR:O	1:B:163:THR:HG22	1.82	0.80
1:A:196:LYS:HE3	1:A:197:SER:OG	1.83	0.79
1:B:166:TYR:H	1:B:184:SER:HB3	1.47	0.78
1:B:221:LEU:O	1:B:225:GLU:HG3	1.83	0.78
1:B:182:LYS:O	1:B:183:LYS:HE3	1.83	0.77
1:B:250:ILE:HD11	1:B:311:LEU:HD11	1.65	0.77
1:A:252:ARG:O	1:A:256:ILE:HD13	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLN:HG2	1:A:291:LEU:HD21	1.69	0.74
1:B:127:LYS:HB2	1:B:324:GLU:HG2	1.69	0.74
1:B:252:ARG:O	1:B:256:ILE:HG23	1.88	0.73
1:B:323:ALA:HB2	1:B:328:GLN:OE1	1.88	0.73
1:A:171:ILE:HD11	1:A:213:ILE:HD11	1.71	0.72
1:A:358:LEU:O	1:A:362:ILE:HG12	1.89	0.72
1:B:336:LYS:HD2	1:B:337:LEU:HD22	1.71	0.72
1:B:333:THR:O	1:B:336:LYS:HG3	1.88	0.72
1:B:153:ILE:O	1:B:157:ILE:HG22	1.89	0.72
1:A:193:GLU:O	1:B:288:GLY:HA3	1.89	0.72
1:A:197:SER:OG	1:A:200:ASP:HB2	1.91	0.71
1:B:170:THR:HG23	1:B:214:PHE:HD2	1.53	0.70
1:A:195:THR:HG21	1:A:201:ALA:HB2	1.72	0.70
1:A:252:ARG:O	1:A:256:ILE:HG23	1.92	0.70
1:A:131:LEU:HD11	1:A:297:ILE:HD13	1.73	0.69
1:A:179:PHE:H	1:A:188:GLN:HE22	1.41	0.69
1:A:357:GLU:O	1:A:361:MSE:HG3	1.92	0.69
1:B:166:TYR:O	1:B:184:SER:HB2	1.93	0.69
1:B:133:HIS:HA	1:B:164:LYS:NZ	2.08	0.69
1:B:335:TYR:HB2	1:B:361:MSE:HE1	1.74	0.69
1:A:299:ASN:O	1:A:303:ARG:HG3	1.92	0.69
1:B:156:MSE:HG2	1:B:238:PHE:HE2	1.58	0.68
1:A:322:GLN:HA	3:A:612:HOH:O	1.93	0.67
1:A:117:PRO:HD2	1:A:177:TYR:HE1	1.60	0.67
1:A:179:PHE:H	1:A:188:GLN:NE2	1.93	0.66
1:A:220:ASP:O	1:A:224:VAL:HG23	1.96	0.65
1:B:317:LEU:HA	1:B:320:SER:OG	1.97	0.65
1:B:157:ILE:HD11	1:B:168:ILE:HG21	1.79	0.65
1:B:168:ILE:HD12	1:B:212:VAL:HB	1.79	0.65
1:A:122:LEU:HD23	1:A:124:LEU:HD12	1.78	0.65
1:B:132:CYS:SG	1:B:156:MSE:HG3	2.37	0.65
1:A:118:GLU:OE2	1:A:121:LYS:HE3	1.96	0.65
1:B:258:PRO:HG2	1:B:261:GLN:OE1	1.96	0.65
1:A:170:THR:OG1	1:A:188:GLN:HA	1.97	0.65
1:B:118:GLU:OE2	1:B:120:LYS:HE2	1.96	0.65
1:A:245:THR:HG22	1:A:247:ILE:H	1.62	0.64
1:A:251:HIS:O	1:A:255:ASP:HB2	1.96	0.64
1:A:284:LYS:HA	1:A:284:LYS:HZ3	1.62	0.64
1:B:158:ASP:O	1:B:161:ASN:HB3	1.97	0.64
1:A:315:TYR:OH	1:A:329:THR:HG21	1.96	0.64
1:B:229:ARG:O	1:B:232:GLU:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HA	1:A:360:ARG:NH1	2.12	0.64
1:B:331:ASN:HD21	1:B:352:SER:HB3	1.63	0.63
1:A:144:PRO:HD3	1:A:244:ASN:ND2	2.13	0.63
1:A:331:ASN:HB3	1:A:361:MSE:HE1	1.81	0.63
1:B:284:LYS:HE3	1:B:290:VAL:HG13	1.80	0.62
1:A:120:LYS:HG2	1:A:121:LYS:NZ	2.14	0.62
1:A:325:THR:O	1:A:325:THR:HG22	1.99	0.62
1:A:360:ARG:HH22	1:A:363:ARG:HD3	1.63	0.62
1:A:289:ARG:HB2	1:A:289:ARG:NH1	2.14	0.62
1:A:191:VAL:HG13	1:A:196:LYS:O	2.00	0.61
1:A:196:LYS:HE3	1:A:200:ASP:HB2	1.83	0.61
1:B:302:ILE:CD1	1:B:327:MSE:HE1	2.27	0.61
1:A:360:ARG:HH12	1:A:363:ARG:CG	2.13	0.61
1:B:247:ILE:HG13	1:B:318:MSE:HE1	1.82	0.60
1:B:358:LEU:O	1:B:362:ILE:HG12	2.00	0.60
1:A:297:ILE:N	1:A:327:MSE:SE	2.84	0.60
1:B:284:LYS:HD3	1:B:342:LEU:HD22	1.83	0.60
1:A:336:LYS:O	1:A:340:GLN:HG3	2.01	0.60
1:B:119:PHE:HA	1:B:122:LEU:HD22	1.82	0.60
1:A:308:GLU:HB3	1:A:310:LYS:NZ	2.17	0.60
1:B:127:LYS:NZ	1:B:297:ILE:HG21	2.17	0.59
1:A:158:ASP:O	1:A:162:GLN:HG3	2.03	0.59
1:B:162:GLN:O	1:B:183:LYS:HD2	2.03	0.59
1:A:153:ILE:HG21	1:A:214:PHE:CZ	2.37	0.59
1:B:197:SER:HB2	1:B:200:ASP:OD1	2.01	0.59
1:A:297:ILE:H	1:A:327:MSE:SE	2.36	0.58
1:A:299:ASN:H	1:A:302:ILE:CG1	2.17	0.58
1:A:360:ARG:NH2	1:A:363:ARG:HD3	2.18	0.58
1:A:224:VAL:O	1:A:228:LEU:HD12	2.03	0.58
1:A:171:ILE:CD1	1:A:213:ILE:HD11	2.34	0.58
1:B:284:LYS:HD2	1:B:285:ILE:O	2.03	0.58
1:B:229:ARG:HA	1:B:232:GLU:HG2	1.86	0.58
1:A:173:ASP:O	1:A:190:GLU:HG2	2.05	0.57
1:B:199:ALA:O	1:B:203:ARG:HG2	2.04	0.57
1:B:315:TYR:CA	1:B:318:MSE:HE3	2.33	0.57
1:B:170:THR:HG23	1:B:214:PHE:CD2	2.37	0.57
1:B:156:MSE:HG2	1:B:238:PHE:CE2	2.38	0.57
1:A:189:ARG:NH2	1:A:205:ALA:HB2	2.20	0.57
1:A:333:THR:O	1:A:337:LEU:HG	2.05	0.57
1:A:283:PRO:O	1:A:284:LYS:HB2	2.03	0.57
1:A:299:ASN:OD1	1:A:302:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ILE:CD1	1:B:315:TYR:HB2	2.36	0.56
1:A:284:LYS:CA	1:A:284:LYS:HZ3	2.18	0.56
1:A:164:LYS:HD3	1:A:166:TYR:CZ	2.39	0.56
1:A:127:LYS:HD3	1:A:326:GLY:HA2	1.88	0.56
1:B:247:ILE:CG1	1:B:318:MSE:HE1	2.36	0.56
1:A:170:THR:OG1	1:A:188:GLN:HG2	2.06	0.55
1:B:250:ILE:HD11	1:B:311:LEU:HD21	1.88	0.55
1:A:144:PRO:HD3	1:A:244:ASN:HD21	1.71	0.55
1:A:173:ASP:OD2	1:A:198:PHE:HE1	1.90	0.55
1:A:190:GLU:HB3	1:A:194:ASP:OD2	2.06	0.55
1:B:245:THR:HG23	1:B:248:ASP:H	1.72	0.55
1:A:261:GLN:O	1:A:265:VAL:HG23	2.07	0.55
1:A:343:ILE:HD13	1:A:348:ALA:HB2	1.89	0.55
1:A:296:LEU:CB	1:A:327:MSE:SE	3.05	0.54
1:A:281:LEU:CD2	1:A:291:LEU:HD12	2.37	0.54
1:A:162:GLN:HG2	1:A:182:LYS:HD3	1.88	0.54
1:B:246:ALA:HA	1:B:276:ILE:HG21	1.90	0.54
1:B:221:LEU:HD22	1:B:225:GLU:OE1	2.08	0.54
1:A:121:LYS:HE2	1:A:121:LYS:N	2.23	0.53
1:A:284:LYS:O	1:A:288:GLY:O	2.26	0.53
1:A:174:PRO:HD2	1:A:176:GLU:OE2	2.08	0.53
1:B:131:LEU:HB3	1:B:139:ILE:CD1	2.39	0.53
1:B:247:ILE:HD12	1:B:315:TYR:HB2	1.89	0.53
1:A:131:LEU:HD11	1:A:297:ILE:CD1	2.38	0.52
1:B:199:ALA:HB1	1:B:222:GLU:HG3	1.91	0.52
1:A:247:ILE:HD11	1:A:315:TYR:CD1	2.43	0.52
1:A:174:PRO:O	1:A:176:GLU:OE2	2.27	0.52
1:A:281:LEU:HD21	1:A:291:LEU:HD12	1.91	0.52
1:A:289:ARG:HH11	1:A:289:ARG:HB2	1.74	0.52
1:A:173:ASP:O	1:A:190:GLU:OE2	2.28	0.52
1:A:284:LYS:NZ	1:A:284:LYS:HA	2.25	0.52
1:A:127:LYS:O	1:A:131:LEU:HD13	2.10	0.52
1:A:196:LYS:HD2	1:A:197:SER:HB3	1.92	0.52
1:B:199:ALA:CB	1:B:222:GLU:HG3	2.40	0.52
1:A:215:VAL:HG11	1:A:218:MSE:HE1	1.91	0.51
1:B:120:LYS:HG3	1:B:121:LYS:HD2	1.92	0.51
1:A:127:LYS:HE3	1:A:297:ILE:HG21	1.92	0.51
1:B:322:GLN:O	1:B:328:GLN:HB2	2.10	0.51
1:A:331:ASN:HB3	1:A:361:MSE:CE	2.39	0.51
1:B:119:PHE:O	1:B:122:LEU:HB2	2.09	0.51
1:A:210:PRO:O	1:A:235:HIS:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:HIS:HE1	1:B:187:ASN:HB2	1.75	0.51
1:B:218:MSE:O	1:B:218:MSE:HG3	2.10	0.51
1:A:175:ILE:CD1	1:A:178:VAL:HG12	2.38	0.51
1:A:279:GLN:HG2	1:A:291:LEU:CD2	2.40	0.51
1:A:218:MSE:HB2	1:A:224:VAL:HG22	1.93	0.50
1:A:231:ALA:HB3	1:A:272:ILE:HD12	1.93	0.50
1:A:118:GLU:HB3	1:A:121:LYS:HG2	1.93	0.50
1:A:138:LEU:HD21	1:A:140:LEU:HD21	1.92	0.50
1:A:215:VAL:HG13	1:A:215:VAL:O	2.11	0.50
1:A:152:THR:HG21	1:A:279:GLN:NE2	2.27	0.50
1:A:273:LEU:HD11	1:A:276:ILE:HG22	1.93	0.50
1:B:355:PRO:O	1:B:359:GLU:OE2	2.30	0.50
1:A:186:VAL:HG13	1:A:186:VAL:O	2.12	0.50
1:A:207:ARG:HG3	1:A:207:ARG:HH11	1.77	0.50
1:A:191:VAL:O	1:A:191:VAL:HG12	2.12	0.49
1:A:319:GLN:OE1	1:A:357:GLU:OE1	2.29	0.49
1:A:299:ASN:H	1:A:302:ILE:HG12	1.77	0.49
1:B:157:ILE:HD11	1:B:168:ILE:CG2	2.41	0.49
1:B:284:LYS:HG2	1:B:342:LEU:O	2.13	0.49
1:B:190:GLU:O	1:B:194:ASP:OD1	2.30	0.49
1:B:222:GLU:O	1:B:222:GLU:OE2	2.30	0.49
1:A:164:LYS:HD3	1:A:166:TYR:CE1	2.48	0.49
1:A:360:ARG:CZ	1:A:360:ARG:HA	2.42	0.49
1:B:339:LYS:HE2	1:B:339:LYS:HA	1.93	0.49
1:A:161:ASN:HA	1:A:184:SER:HB2	1.95	0.49
1:A:216:GLY:O	1:A:240:THR:OG1	2.31	0.49
1:B:233:THR:HG22	1:B:233:THR:O	2.11	0.49
1:B:333:THR:O	1:B:337:LEU:HD23	2.12	0.49
1:B:135:LYS:O	1:B:136:MSE:HB3	2.11	0.49
1:B:178:VAL:HA	1:B:188:GLN:HE22	1.78	0.49
1:A:152:THR:CB	1:A:279:GLN:HE22	2.26	0.49
1:A:198:PHE:O	1:A:202:LEU:HB2	2.13	0.49
1:B:250:ILE:HD11	1:B:311:LEU:CD1	2.37	0.49
1:A:213:ILE:HG13	1:A:214:PHE:N	2.28	0.49
1:B:134:ARG:HH11	1:B:134:ARG:HA	1.77	0.48
1:B:247:ILE:HG23	1:B:311:LEU:HD13	1.95	0.48
1:B:284:LYS:NZ	1:B:284:LYS:HB3	2.28	0.48
1:A:276:ILE:HG13	1:A:276:ILE:O	2.12	0.48
1:A:221:LEU:HD11	1:A:257:PHE:CD2	2.49	0.48
1:B:131:LEU:HB3	1:B:139:ILE:HD13	1.95	0.48
1:B:175:ILE:HG13	1:B:190:GLU:CG	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD22	1:B:272:ILE:HD11	1.96	0.47
1:B:161:ASN:O	1:B:183:LYS:HB2	2.14	0.47
1:A:360:ARG:HH12	1:A:363:ARG:CB	2.27	0.47
1:A:127:LYS:HG3	1:A:127:LYS:O	2.13	0.47
1:B:337:LEU:HD13	1:B:340:GLN:NE2	2.30	0.47
1:B:133:HIS:CG	1:B:164:LYS:HZ1	2.32	0.47
1:B:337:LEU:HD13	1:B:340:GLN:HE22	1.80	0.47
1:B:195:THR:HG23	1:B:196:LYS:N	2.30	0.47
1:A:173:ASP:HB3	1:A:174:PRO:HD3	1.95	0.47
1:B:304:ASN:O	1:B:308:GLU:HG3	2.15	0.47
1:B:318:MSE:HA	1:B:327:MSE:HE3	1.96	0.47
1:B:166:TYR:H	1:B:184:SER:CB	2.22	0.47
1:A:127:LYS:CD	1:A:326:GLY:HA2	2.45	0.46
1:B:195:THR:OG1	1:B:200:ASP:OD2	2.30	0.46
1:B:302:ILE:HD11	1:B:327:MSE:CE	2.33	0.46
1:B:358:LEU:HD12	1:B:361:MSE:HE2	1.97	0.46
1:A:158:ASP:HB2	1:A:179:PHE:HE2	1.81	0.46
1:B:249:THR:O	1:B:253:ILE:HG13	2.15	0.46
1:B:263:GLU:OE1	1:B:266:ARG:NH1	2.48	0.46
1:A:232:GLU:HG2	1:A:232:GLU:O	2.16	0.46
1:A:193:GLU:HG2	1:B:289:ARG:N	2.31	0.46
1:A:282:LEU:CD1	1:A:347:ASP:HB3	2.45	0.46
1:A:296:LEU:C	1:A:327:MSE:SE	3.02	0.46
1:A:320:SER:O	1:A:322:GLN:N	2.49	0.46
1:A:360:ARG:HH12	1:A:363:ARG:HB2	1.80	0.46
1:B:175:ILE:CG1	1:B:190:GLU:HG3	2.39	0.46
1:A:120:LYS:HG2	1:A:121:LYS:HZ3	1.78	0.45
1:A:304:ASN:ND2	1:A:308:GLU:OE1	2.49	0.45
1:A:308:GLU:HB3	1:A:310:LYS:HZ3	1.81	0.45
1:B:322:GLN:O	1:B:328:GLN:NE2	2.50	0.45
1:A:356:LYS:O	1:A:359:GLU:HG2	2.17	0.45
1:A:278:SER:O	1:A:293:TYR:HA	2.17	0.45
1:B:244:ASN:OD1	1:B:280:ARG:NH1	2.50	0.45
1:A:170:THR:HG22	1:A:214:PHE:HB3	1.98	0.45
1:A:282:LEU:HD12	1:A:347:ASP:HB3	1.97	0.45
1:B:200:ASP:OD2	1:B:201:ALA:N	2.50	0.45
1:B:190:GLU:O	1:B:194:ASP:N	2.50	0.45
1:A:192:GLY:N	1:A:195:THR:O	2.50	0.45
1:A:284:LYS:HB3	1:A:285:ILE:H	1.40	0.45
1:A:360:ARG:HH12	1:A:363:ARG:CD	2.30	0.45
1:B:281:LEU:HD23	1:B:291:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HH22	1:A:363:ARG:CD	2.30	0.45
1:A:335:TYR:HE1	1:A:339:LYS:HZ2	1.65	0.45
1:A:324:GLU:O	1:A:327:MSE:O	2.35	0.45
1:B:361:MSE:HB2	1:B:361:MSE:HE2	1.69	0.45
1:B:173:ASP:HB3	1:B:174:PRO:HD3	1.98	0.45
1:A:136:MSE:CE	1:A:234:GLY:HA2	2.38	0.44
1:B:194:ASP:N	1:B:194:ASP:OD1	2.50	0.44
1:A:141:VAL:HG12	1:A:149:LYS:HB2	2.00	0.44
1:A:308:GLU:HB3	1:A:310:LYS:HZ2	1.82	0.44
1:A:323:ALA:O	1:A:324:GLU:CB	2.66	0.44
1:A:153:ILE:HG21	1:A:214:PHE:CE2	2.53	0.44
1:A:195:THR:OG1	1:A:196:LYS:N	2.50	0.44
1:B:258:PRO:HB2	1:B:260:ASN:OD1	2.18	0.44
1:B:215:VAL:O	1:B:215:VAL:HG13	2.18	0.44
1:A:128:VAL:CG1	1:A:277:ILE:HD11	2.48	0.43
1:A:280:ARG:HD2	1:A:351:ALA:HB1	2.00	0.43
1:A:217:GLU:OE2	1:A:240:THR:OG1	2.30	0.43
1:A:128:VAL:O	1:A:131:LEU:HB2	2.18	0.43
1:B:284:LYS:HD2	1:B:285:ILE:C	2.38	0.43
1:B:140:LEU:HD22	1:B:241:LEU:CD1	2.48	0.43
1:A:284:LYS:HA	1:A:284:LYS:CE	2.49	0.43
1:B:361:MSE:HB3	1:B:361:MSE:HE3	1.75	0.43
1:B:231:ALA:HB3	1:B:272:ILE:HD12	2.01	0.43
1:A:285:ILE:HG23	1:A:286:GLY:N	2.33	0.42
1:A:122:LEU:HD21	1:A:152:THR:HA	2.01	0.42
1:B:323:ALA:HA	1:B:328:GLN:HB2	2.00	0.42
1:A:245:THR:HG22	1:A:247:ILE:N	2.30	0.42
1:B:127:LYS:NZ	1:B:297:ILE:HD12	2.34	0.42
1:B:319:GLN:HE21	1:B:319:GLN:HB3	1.27	0.42
1:A:346:GLU:H	1:A:346:GLU:HG3	1.53	0.42
1:A:221:LEU:HD12	1:A:221:LEU:HA	1.83	0.42
1:A:337:LEU:O	1:A:342:LEU:HB2	2.19	0.42
1:B:202:LEU:O	1:B:206:LEU:HD13	2.19	0.42
1:A:323:ALA:O	1:A:324:GLU:HB2	2.20	0.42
1:B:245:THR:CG2	1:B:248:ASP:H	2.31	0.42
1:A:158:ASP:O	1:A:162:GLN:OE1	2.37	0.42
1:B:276:ILE:HD13	1:B:276:ILE:HG21	1.76	0.42
1:A:302:ILE:HG21	1:A:302:ILE:HD12	1.82	0.41
1:B:284:LYS:HG2	1:B:285:ILE:H	1.85	0.41
1:A:354:ASP:HA	1:A:355:PRO:HD2	1.90	0.41
1:A:218:MSE:HB3	1:A:218:MSE:HE3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD11	1:A:257:PHE:CE2	2.56	0.41
1:B:230:ALA:O	1:B:235:HIS:HD2	2.02	0.41
1:A:157:ILE:HA	1:A:160:ILE:HD12	2.02	0.41
1:B:129:LEU:HA	1:B:129:LEU:HD23	1.81	0.41
1:B:157:ILE:HG23	1:B:179:PHE:CE2	2.56	0.41
1:B:228:LEU:O	1:B:232:GLU:HB3	2.20	0.41
1:A:194:ASP:N	1:A:194:ASP:OD2	2.49	0.41
1:A:254:VAL:CG1	1:A:262:GLN:HB3	2.51	0.41
1:A:120:LYS:HG2	1:A:121:LYS:HZ1	1.85	0.40
1:A:298:PRO:CA	1:A:302:ILE:HG13	2.40	0.40
1:A:196:LYS:HD2	1:A:197:SER:N	2.37	0.40
1:A:193:GLU:HA	1:B:288:GLY:HA3	2.04	0.40
1:A:335:TYR:HE1	1:A:339:LYS:NZ	2.19	0.40
1:B:349:MSE:HE3	1:B:349:MSE:HB3	1.96	0.40
1:A:284:LYS:HG2	1:A:343:ILE:CA	2.32	0.40
1:A:360:ARG:NH1	1:A:363:ARG:HD3	2.35	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	245/261 (94%)	215 (88%)	25 (10%)	5 (2%)	9	2
1	B	245/261 (94%)	226 (92%)	16 (6%)	3 (1%)	16	5
All	All	490/522 (94%)	441 (90%)	41 (8%)	8 (2%)	12	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	LYS
1	A	322	GLN

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Mol	Chain	Res	Type
1	A	324	GLU
1	B	197	SER
1	B	325	THR
1	A	321	GLY
1	B	196	LYS
1	A	287	GLY

### 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	216/218 (99%)	168 (78%)	48 (22%)	1	0
1	B	216/218 (99%)	181 (84%)	35 (16%)	3	0
All	All	432/436 (99%)	349 (81%)	83 (19%)	2	0

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LYS
1	A	127	LYS
1	A	135	LYS
1	A	150	SER
1	A	153	ILE
1	A	161	ASN
1	A	164	LYS
1	A	165	SER
1	A	167	HIS
1	A	170	THR
1	A	173	ASP
1	A	177	TYR
1	A	180	LYS
1	A	183	LYS
1	A	191	VAL
1	A	193	GLU
1	A	194	ASP

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Mol	Chain	Res	Type
1	A	196	LYS
1	A	202	LEU
1	A	208	GLU
1	A	209	ASP
1	A	213	ILE
1	A	218	MSE
1	A	225	GLU
1	A	228	LEU
1	A	244	ASN
1	A	255	ASP
1	A	256	ILE
1	A	259	LEU
1	A	260	ASN
1	A	263	GLU
1	A	266	ARG
1	A	276	ILE
1	A	278	SER
1	A	282	LEU
1	A	284	LYS
1	A	285	ILE
1	A	291	LEU
1	A	302	ILE
1	A	312	GLN
1	A	317	LEU
1	A	319	GLN
1	A	320	SER
1	A	331	ASN
1	A	336	LYS
1	A	342	LEU
1	A	346	GLU
1	A	360	ARG
1	B	120	LYS
1	B	121	LYS
1	B	122	LEU
1	B	135	LYS
1	B	138	LEU
1	B	156	MSE
1	B	172	GLU
1	B	178	VAL
1	B	179	PHE
1	B	180	LYS
1	B	182	LYS

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Mol	Chain	Res	Type
1	B	183	LYS
1	B	185	ILE
1	B	187	ASN
1	B	194	ASP
1	B	196	LYS
1	B	217	GLU
1	B	221	LEU
1	B	229	ARG
1	B	243	THR
1	B	244	ASN
1	B	253	ILE
1	B	280	ARG
1	B	284	LYS
1	B	285	ILE
1	B	289	ARG
1	B	304	ASN
1	B	305	LEU
1	B	307	ARG
1	B	309	ASN
1	B	322	GLN
1	B	325	THR
1	B	328	GLN
1	B	336	LYS
1	B	362	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	HIS
1	A	161	ASN
1	A	188	GLN
1	A	235	HIS
1	A	244	ASN
1	A	261	GLN
1	A	262	GLN
1	A	279	GLN
1	A	319	GLN
1	A	331	ASN
1	A	340	GLN
1	B	161	ASN
1	B	188	GLN
1	B	235	HIS

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Mol	Chain	Res	Type
1	B	242	HIS
1	B	309	ASN
1	B	319	GLN
1	B	331	ASN
1	B	340	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](#)

1 ligand is 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	B	2800	-	4,4,4	2.25	4 (100%)	6,6,6	0.17	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	B	2800	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2800	SO4	O3-S	2.03	1.54	1.47
2	B	2800	SO4	O4-S	2.19	1.55	1.47
2	B	2800	SO4	O1-S	2.31	1.55	1.47
2	B	2800	SO4	O2-S	2.44	1.55	1.47

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, 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	239/261 (91%)	1.60	69 (28%) <b>1</b> <b>0</b>	12, 33, 63, 116	0
1	B	239/261 (91%)	1.47	48 (20%) <b>1</b> <b>1</b>	12, 30, 61, 94	0
All	All	478/522 (91%)	1.53	117 (24%) <b>1</b> <b>1</b>	12, 32, 62, 116	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	GLY	10.9
1	A	285	ILE	10.3
1	A	205	ALA	9.4
1	B	195	THR	9.4
1	B	191	VAL	7.6
1	B	286	GLY	7.5
1	B	194	ASP	7.4
1	A	288	GLY	6.4
1	A	286	GLY	6.3
1	B	287	GLY	6.1
1	A	340	GLN	5.8
1	B	167	HIS	5.7
1	B	285	ILE	5.0
1	B	181	HIS	5.0
1	A	323	ALA	4.7
1	B	207	ARG	4.0
1	A	338	TYR	4.0
1	B	247	ILE	3.9
1	A	325	THR	3.9
1	B	323	ALA	3.8
1	B	197	SER	3.8
1	B	206	LEU	3.8
1	B	203	ARG	3.8
1	A	123	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	312	GLN	3.6
1	B	322	GLN	3.6
1	A	132	CYS	3.5
1	B	180	LYS	3.4
1	B	198	PHE	3.4
1	B	338	TYR	3.3
1	B	244	ASN	3.3
1	A	284	LYS	3.2
1	A	141	VAL	3.2
1	A	208	GLU	3.2
1	B	204	ALA	3.2
1	B	228	LEU	3.1
1	A	126	ASP	3.1
1	A	337	LEU	3.1
1	A	229	ARG	3.1
1	A	233	THR	3.1
1	B	362	ILE	3.1
1	B	166	TYR	3.1
1	A	191	VAL	3.1
1	A	322	GLN	3.1
1	A	273	LEU	3.0
1	A	345	LEU	3.0
1	B	342	LEU	3.0
1	A	194	ASP	3.0
1	A	196	LYS	3.0
1	A	117	PRO	3.0
1	A	219	ARG	2.9
1	B	208	GLU	2.9
1	A	198	PHE	2.9
1	A	131	LEU	2.9
1	A	363	ARG	2.8
1	B	337	LEU	2.8
1	A	119	PHE	2.8
1	B	164	LYS	2.8
1	A	292	ALA	2.7
1	A	317	LEU	2.7
1	B	202	LEU	2.7
1	A	175	ILE	2.7
1	B	269	LEU	2.7
1	B	233	THR	2.7
1	B	129	LEU	2.7
1	A	171	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	189	ARG	2.6
1	A	179	PHE	2.6
1	A	302	ILE	2.6
1	A	160	ILE	2.6
1	B	139	ILE	2.6
1	B	138	LEU	2.5
1	B	271	PHE	2.5
1	A	324	GLU	2.5
1	A	362	ILE	2.5
1	B	250	ILE	2.5
1	A	246	ALA	2.5
1	A	207	ARG	2.5
1	A	195	THR	2.5
1	A	203	ARG	2.4
1	B	282	LEU	2.4
1	A	178	VAL	2.4
1	A	272	ILE	2.4
1	B	348	ALA	2.4
1	B	124	LEU	2.4
1	A	180	LYS	2.4
1	A	224	VAL	2.4
1	A	145	THR	2.4
1	B	121	LYS	2.3
1	A	140	LEU	2.3
1	A	186	VAL	2.3
1	A	197	SER	2.3
1	A	339	LYS	2.3
1	B	272	ILE	2.3
1	B	190	GLU	2.2
1	A	200	ASP	2.2
1	B	326	GLY	2.2
1	A	276	ILE	2.2
1	B	175	ILE	2.2
1	B	179	PHE	2.2
1	A	177	TYR	2.2
1	A	190	GLU	2.2
1	A	311	LEU	2.2
1	B	363	ARG	2.2
1	B	183	LYS	2.2
1	A	326	GLY	2.1
1	A	253	ILE	2.1
1	A	320	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	166	TYR	2.1
1	A	202	LEU	2.1
1	B	182	LYS	2.1
1	A	249	THR	2.1
1	A	329	THR	2.1
1	A	122	LEU	2.1
1	A	133	HIS	2.1
1	B	217	GLU	2.0
1	A	341	GLY	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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	2800	5/5	0.91	0.14	-0.30	30,31,41,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.