



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:37 PM BST

PDB ID : 3ITB
Title : Crystal structure of Penicillin-Binding Protein 6 (PBP6) from E. coli in complex with a substrate fragment
Authors : Chen, Y.; Zhang, W.; Shi, Q.; Heseck, D.; Lee, M.; Mobashery, S.; Shoichet, B.K.
Deposited on : 2009-08-27
Resolution : 1.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

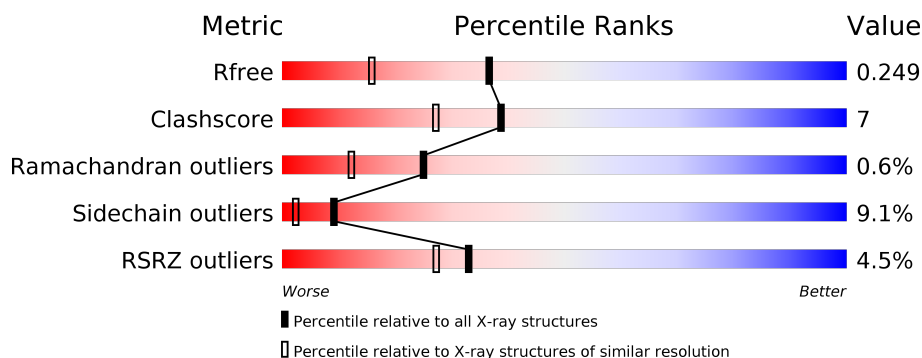
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 ≥ 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	352	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	352	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• • •</div> </div> </div>
1	C	352	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>• •</div> </div> </div>
1	D	352	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>•</div> </div> </div>
2	L	6	<div> <div></div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
3	E	2	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11444 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 D-alanyl-D-alanine carboxypeptidase dacC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	2	0
			2644	1673	454	507	10			
1	B	346	Total	C	N	O	S	0	4	0
			2666	1686	458	512	10			
1	C	347	Total	C	N	O	S	0	1	0
			2645	1670	455	510	10			
1	D	351	Total	C	N	O	S	0	2	0
			2683	1692	463	518	10			

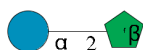
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P08506
B	1	MET	-	initiating methionine	UNP P08506
C	1	MET	-	initiating methionine	UNP P08506
D	1	MET	-	initiating methionine	UNP P08506

- Molecule 2 is a protein called Peptidoglycan substrate (AMV)A(FGA)K(DAL)(DAL).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	L	6	Total	C	N	O	0	0	0
			54	32	7	15			

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

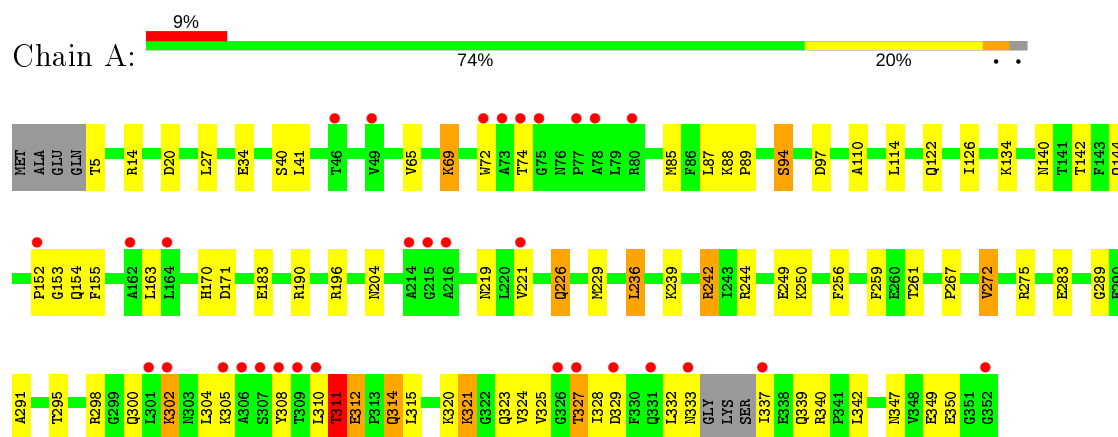
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	182	Total	O	0	0
			182	182		
5	C	161	Total	O	0	0
			161	161		
5	D	184	Total	O	0	0
			184	184		
5	L	2	Total	O	0	0
			2	2		

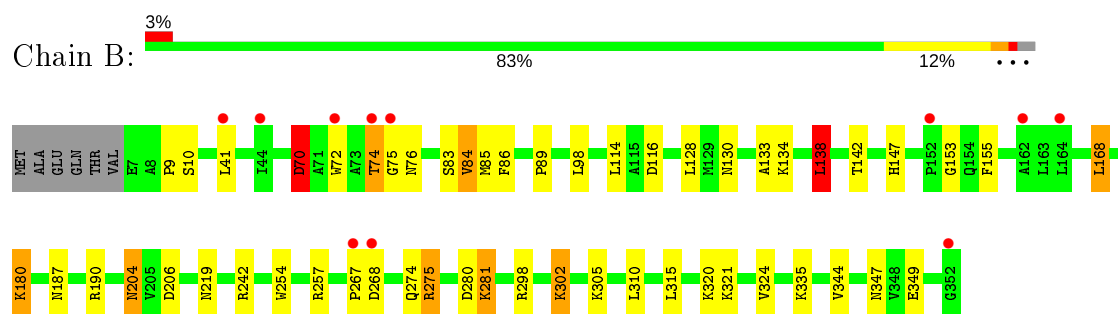
3 Residue-property plots [i](#)

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.

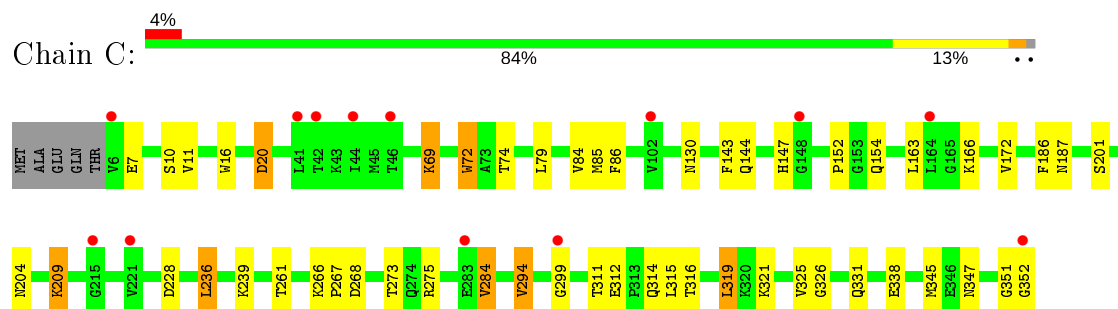
- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC



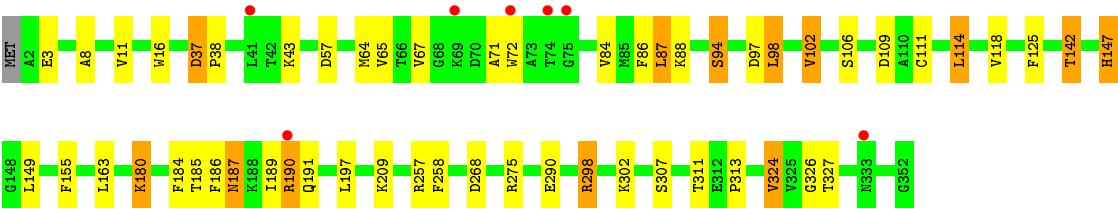
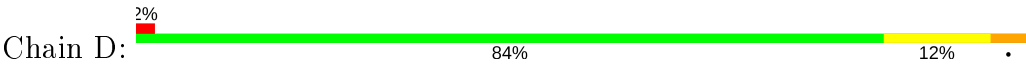
- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC



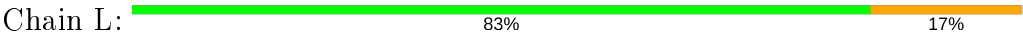
- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC



- Molecule 1: D-alanyl-D-alanine carboxypeptidase dacC



- Molecule 2: Peptidoglycan substrate (AMV)A(FGA)K(DAL)(DAL)



- Molecule 3: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.53Å 185.35Å 82.33Å 90.00° 100.99° 90.00°	Depositor
Resolution (Å)	40.20 – 1.80 34.32 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.8 (40.20-1.80) 87.8 (34.32-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.254 0.203 , 0.249	Depositor DCC
R_{free} test set	6831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11444	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, GLC, SO4, FRU, FGA, AMV

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	0.45	0/2692	0.87	4/3642 (0.1%)
1	B	0.45	0/2712	0.84	3/3667 (0.1%)
1	C	0.43	0/2690	0.82	1/3640 (0.0%)
1	D	0.47	0/2731	0.84	3/3695 (0.1%)
2	L	0.63	0/12	1.21	0/12
All	All	0.45	0/10837	0.84	11/14656 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	MET	CG-SD-CE	-5.99	90.61	100.20
1	D	37	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	84	VAL	CG1-CB-CG2	5.83	120.22	110.90
1	A	114	LEU	CA-CB-CG	5.66	128.32	115.30
1	D	102	VAL	CG1-CB-CG2	5.53	119.74	110.90
1	B	138	LEU	CB-CG-CD1	5.47	120.30	111.00
1	D	257	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	196	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	168	LEU	CA-CB-CG	5.24	127.36	115.30
1	C	236	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	236	LEU	CB-CG-CD1	5.01	119.52	111.00

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	2644	0	2668	71	0
1	B	2666	0	2691	39	0
1	C	2645	0	2667	22	0
1	D	2683	0	2706	30	0
2	L	54	0	50	1	0
3	E	23	0	21	0	0
4	A	5	0	0	0	0
4	B	15	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	170	0	0	2	0
5	B	182	0	0	4	0
5	C	161	0	0	3	0
5	D	184	0	0	4	0
5	L	2	0	0	0	0
All	All	11444	0	10803	161	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 7.

All (161) 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:332:LEU:HB2	1:A:337:ILE:HD13	1.32	1.10
1:A:332:LEU:HB2	1:A:337:ILE:CD1	1.80	1.09
1:D:8:ALA:HB2	5:D:411:HOH:O	1.61	0.98
1:A:332:LEU:CB	1:A:337:ILE:CD1	2.41	0.97
1:B:275:ARG:HG3	1:B:275:ARG:HH11	1.30	0.95
1:A:321:LYS:H	1:A:347:ASN:ND2	1.64	0.94
1:D:84:VAL:HG12	1:D:86:PHE:H	1.31	0.92
1:B:321:LYS:H	1:B:347:ASN:ND2	1.72	0.86
1:B:274:GLN:HE21	1:B:310:LEU:HD11	1.41	0.86
1:B:187:ASN:ND2	1:C:7:GLU:HG2	1.94	0.83
1:C:130:ASN:HD21	1:C:143:PHE:H	1.29	0.80
1:B:274:GLN:NE2	1:B:310:LEU:HD11	1.99	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:HIS:HD2	1:A:171:ASP:OD1	1.66	0.77
1:B:134[B]:LYS:N	1:B:134[B]:LYS:HD3	1.98	0.77
1:A:332:LEU:HB3	1:A:337:ILE:HD11	1.67	0.76
1:B:267:PRO:O	1:B:268:ASP:HB2	1.87	0.74
1:B:280:ASP:CG	1:B:349:GLU:HG2	2.09	0.72
1:A:94:SER:HB3	1:A:97:ASP:H	1.55	0.71
1:D:302:LYS:HE2	5:D:764:HOH:O	1.89	0.71
1:A:327:THR:HG22	1:A:327:THR:O	1.89	0.70
1:B:320:LYS:HA	1:B:347:ASN:HD22	1.57	0.70
1:D:149:LEU:CD2	2:L:501:AMV:H6C1	2.20	0.70
1:C:267:PRO:O	1:C:268:ASP:HB2	1.91	0.70
1:C:321:LYS:H	1:C:347:ASN:ND2	1.89	0.69
1:A:283:GLU:N	1:A:283:GLU:OE1	2.25	0.69
1:A:332:LEU:CB	1:A:337:ILE:HD11	2.23	0.68
1:D:118:VAL:HG21	1:D:125:PHE:CE1	2.29	0.67
1:A:204:ASN:HB3	5:A:368:HOH:O	1.94	0.67
1:A:88:LYS:NZ	1:A:88:LYS:HB2	2.10	0.66
1:B:281[B]:LYS:HE3	1:B:347:ASN:O	1.96	0.66
1:D:187:ASN:O	1:D:189:ILE:HG13	1.97	0.65
1:B:133:ALA:HA	1:B:138:LEU:HD22	1.80	0.64
1:D:142:THR:HG23	1:D:155:PHE:CE1	2.33	0.63
1:B:130:ASN:O	1:B:134[B]:LYS:HE2	1.97	0.63
1:D:84:VAL:HG13	1:D:109:ASP:OD2	1.98	0.63
1:A:144:GLN:H	1:A:154:GLN:HE21	1.48	0.62
1:D:142:THR:HG23	1:D:155:PHE:CZ	2.35	0.62
1:A:314:GLN:HA	1:A:314:GLN:NE2	2.15	0.61
1:D:190:ARG:HD2	5:D:410:HOH:O	2.00	0.61
1:A:314:GLN:HA	1:A:314:GLN:HE21	1.66	0.60
1:A:88:LYS:HZ2	1:A:88:LYS:HB2	1.68	0.59
1:D:118:VAL:HG21	1:D:125:PHE:HE1	1.67	0.59
1:C:311:THR:HG23	1:C:326:GLY:HA2	1.85	0.59
1:A:27:LEU:HD21	1:A:295:THR:HG21	1.84	0.59
1:B:190:ARG:NH1	4:B:355:SO4:O2	2.36	0.59
1:D:94:SER:HB3	1:D:97:ASP:H	1.68	0.59
1:A:41:LEU:HD22	1:A:221:VAL:HG23	1.84	0.58
1:A:332:LEU:N	1:A:337:ILE:HD12	2.17	0.58
1:C:186:PHE:O	1:C:187[B]:ASN:HB2	2.02	0.58
1:B:275:ARG:HG3	1:B:275:ARG:NH1	2.08	0.58
1:A:41:LEU:HD11	1:A:219:ASN:HB3	1.85	0.57
1:A:320:LYS:O	1:A:323:GLN:HB3	2.04	0.57
1:B:275:ARG:CG	1:B:275:ARG:HH11	2.09	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLN:HE21	1:B:310:LEU:CD1	2.14	0.57
1:D:186:PHE:O	1:D:187:ASN:CB	2.51	0.57
1:A:142:THR:HG22	1:A:155[A]:PHE:CE2	2.40	0.56
1:D:186:PHE:O	1:D:187:ASN:HB2	2.05	0.56
1:B:70:ASP:OD2	1:B:116:ASP:OD2	2.24	0.55
1:C:186:PHE:O	1:C:187[B]:ASN:CB	2.50	0.55
1:B:280:ASP:OD1	1:B:349:GLU:HG2	2.06	0.55
1:A:332:LEU:CB	1:A:337:ILE:HD13	2.16	0.55
1:B:180:LYS:HG3	1:B:206:ASP:HB2	1.88	0.55
1:A:142:THR:CG2	1:A:155[A]:PHE:CE2	2.90	0.54
1:D:67:VAL:HG13	1:D:71:ALA:HB3	1.90	0.54
1:A:72:TRP:CE3	1:A:89:PRO:CG	2.91	0.53
1:A:291:ALA:HB1	1:A:340:ARG:HD2	1.90	0.53
1:A:320:LYS:HA	1:A:347:ASN:HD22	1.73	0.53
1:A:321:LYS:H	1:A:347:ASN:HD22	1.49	0.53
1:C:20:ASP:OD2	1:C:261:THR:OG1	2.23	0.52
1:A:88:LYS:CB	1:A:88:LYS:NZ	2.72	0.52
1:A:72:TRP:CE3	1:A:89:PRO:HG2	2.45	0.52
1:B:305:LYS:NZ	5:B:425:HOH:O	2.42	0.52
1:A:250:LYS:NZ	5:A:794:HOH:O	2.43	0.51
1:A:272:VAL:HG11	1:A:308:TYR:OH	2.11	0.51
1:A:142:THR:HG22	1:A:155[A]:PHE:CZ	2.46	0.51
1:A:14:ARG:NH2	1:A:34:GLU:OE1	2.44	0.51
1:D:37:ASP:OD2	1:D:38:PRO:HD2	2.12	0.50
1:B:72:TRP:CG	1:B:89:PRO:HD3	2.47	0.50
1:A:328:ILE:HG13	1:A:342:LEU:HB2	1.94	0.50
1:A:300:GLN:HA	1:A:300:GLN:NE2	2.26	0.50
1:C:69:LYS:NZ	5:C:765:HOH:O	2.44	0.50
1:A:142:THR:CG2	1:A:153:GLY:O	2.59	0.50
1:B:275:ARG:CG	1:B:275:ARG:NH1	2.71	0.50
1:B:302:LYS:HD2	5:B:752:HOH:O	2.11	0.49
1:D:11:VAL:HG22	1:D:16:TRP:CE3	2.47	0.49
1:A:332:LEU:H	1:A:337:ILE:HD12	1.78	0.49
1:C:11:VAL:HG13	1:C:16:TRP:CE2	2.48	0.49
1:D:118:VAL:CG2	1:D:125:PHE:CD1	2.95	0.49
1:A:308:TYR:CE2	1:A:310:LEU:HG	2.48	0.49
1:B:41:LEU:HD11	1:B:219:ASN:HB3	1.95	0.49
1:D:98:LEU:HB3	1:D:114:LEU:HD22	1.94	0.49
1:A:69:LYS:HZ3	1:A:72:TRP:HZ3	1.60	0.48
1:A:329:ASP:HA	1:A:339:GLN:HG2	1.95	0.48
1:A:72:TRP:CE2	1:A:74:THR:HB	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASP:HB2	1:A:339:GLN:HG2	1.95	0.48
1:C:321:LYS:H	1:C:347:ASN:HD22	1.60	0.48
1:B:142[A]:THR:CG2	1:B:153:GLY:O	2.62	0.48
1:C:299:GLY:HA2	5:C:376:HOH:O	2.14	0.47
1:A:308:TYR:HE2	1:A:310:LEU:HG	1.78	0.47
1:A:72:TRP:CZ3	1:A:89:PRO:HG2	2.50	0.47
1:D:258:PHE:C	1:D:298:ARG:HG3	2.35	0.47
1:A:142:THR:HG23	1:A:153:GLY:O	2.15	0.47
1:A:304:LEU:HB2	1:A:332:LEU:HD13	1.98	0.46
1:B:321:LYS:H	1:B:347:ASN:HD21	1.58	0.46
1:D:180:LYS:HE2	1:D:180:LYS:HB2	1.63	0.46
1:C:72:TRP:CE2	1:C:74:THR:HB	2.50	0.46
1:B:320:LYS:HA	1:B:347:ASN:ND2	2.29	0.46
1:A:325:VAL:O	1:A:325:VAL:HG23	2.15	0.46
1:D:118:VAL:HG21	1:D:125:PHE:CD1	2.50	0.46
1:D:67:VAL:HG21	1:D:87:LEU:HG	1.97	0.46
1:A:27:LEU:HD21	1:A:295:THR:CG2	2.45	0.46
1:D:118:VAL:CG2	1:D:125:PHE:HD1	2.29	0.45
1:A:20:ASP:OD2	1:A:261:THR:OG1	2.32	0.45
1:A:259:PHE:O	1:A:298[B]:ARG:NE	2.48	0.45
1:A:69:LYS:NZ	1:A:72:TRP:HZ3	2.14	0.45
1:B:280:ASP:OD2	1:B:349:GLU:HG2	2.16	0.45
1:D:147:HIS:CE1	1:D:149:LEU:HD12	2.51	0.45
1:B:180:LYS:HB3	1:B:180:LYS:HE2	1.48	0.45
1:B:142[A]:THR:CG2	1:B:155[A]:PHE:CE2	3.01	0.44
1:C:294:VAL:HG13	1:C:338:GLU:CD	2.38	0.44
1:C:69:LYS:HE3	5:C:765:HOH:O	2.18	0.44
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.87	0.44
1:A:85:MET:SD	1:A:110:ALA:HB2	2.58	0.43
1:C:144:GLN:HG2	1:C:152:PRO:O	2.18	0.43
1:C:144:GLN:HB2	1:C:154:GLN:HB2	2.00	0.43
1:B:98:LEU:HB3	1:B:114:LEU:HD22	2.00	0.43
1:A:311:THR:HB	1:A:312:GLU:H	1.57	0.43
1:A:72:TRP:CD2	1:A:89:PRO:HD3	2.54	0.43
1:B:142[A]:THR:O	1:B:142[A]:THR:HG23	2.17	0.43
1:A:142:THR:CG2	1:A:155[A]:PHE:CZ	3.02	0.42
1:A:226:GLN:HB3	1:A:256:PHE:CD1	2.54	0.42
1:A:332:LEU:O	1:A:333:ASN:C	2.56	0.42
1:A:312:GLU:C	1:A:314:GLN:H	2.22	0.42
1:D:311:THR:HG23	1:D:326:GLY:HA2	2.00	0.42
1:B:204:ASN:ND2	5:B:433:HOH:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASP:OD2	1:B:349:GLU:CG	2.68	0.42
1:A:140:ASN:O	1:A:155[A]:PHE:HD1	2.03	0.42
1:C:209:LYS:HA	1:C:209:LYS:HE2	1.99	0.42
1:B:142[A]:THR:HG21	1:B:153:GLY:O	2.20	0.42
1:A:142:THR:HG21	1:A:155[A]:PHE:CE2	2.55	0.42
1:D:43:LYS:HG2	1:D:111:CYS:SG	2.60	0.42
1:A:302:LYS:HE2	1:A:302:LYS:HB2	1.65	0.42
1:C:172:VAL:O	1:C:172:VAL:HG23	2.20	0.42
1:A:122:GLN:O	1:A:126:ILE:HD12	2.20	0.41
1:A:41:LEU:HD22	1:A:221:VAL:CG2	2.50	0.41
1:A:140:ASN:O	1:A:155[A]:PHE:CD1	2.73	0.41
1:D:324:VAL:HG13	5:D:407:HOH:O	2.20	0.41
1:A:242:ARG:HH21	1:A:242:ARG:CG	2.33	0.41
1:A:267:PRO:HA	1:A:289:GLY:O	2.21	0.41
1:C:351:GLY:HA3	1:C:352:GLY:HA2	1.91	0.41
1:A:144:GLN:H	1:A:154:GLN:NE2	2.14	0.41
1:C:284:VAL:HG21	1:C:319:LEU:HD23	2.02	0.41
1:C:321:LYS:HE2	1:C:345:MET:O	2.21	0.41
1:B:10:SER:HA	5:B:397:HOH:O	2.21	0.41
1:B:85:MET:O	1:B:86:PHE:HB2	2.21	0.41
1:B:142[A]:THR:HG22	1:B:155[A]:PHE:CZ	2.56	0.40
1:B:9:PRO:HG3	1:B:254:TRP:CD2	2.56	0.40
1:D:102:VAL:O	1:D:106:SER:HA	2.21	0.40
1:A:183:GLU:OE2	1:A:190:ARG:HD2	2.21	0.40
1:A:329:ASP:CG	1:A:339:GLN:HE21	2.25	0.40
1:A:321:LYS:N	1:A:347:ASN:ND2	2.49	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	343/352 (97%)	329 (96%)	11 (3%)	3 (1%)	17	6
1	B	348/352 (99%)	332 (95%)	12 (3%)	4 (1%)	14	4
1	C	346/352 (98%)	334 (96%)	11 (3%)	1 (0%)	41	27
1	D	351/352 (100%)	340 (97%)	11 (3%)	0	100	100
All	All	1388/1408 (99%)	1335 (96%)	45 (3%)	8 (1%)	25	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	311	THR
1	B	70	ASP
1	B	74	THR
1	B	75	GLY
1	A	152	PRO
1	C	86	PHE
1	A	302	LYS
1	B	76	ASN

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	282/285 (99%)	256 (91%)	26 (9%)	9	2
1	B	284/285 (100%)	263 (93%)	21 (7%)	13	4
1	C	282/285 (99%)	254 (90%)	28 (10%)	8	2
1	D	286/285 (100%)	258 (90%)	28 (10%)	8	2
2	L	1/1 (100%)	1 (100%)	0	100	100
All	All	1135/1141 (100%)	1032 (91%)	103 (9%)	9	2

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	SER
1	A	65	VAL
1	A	69	LYS
1	A	87	LEU
1	A	94	SER
1	A	134	LYS
1	A	163	LEU
1	A	226	GLN
1	A	236	LEU
1	A	239	LYS
1	A	242	ARG
1	A	244	ARG
1	A	249	GLU
1	A	272	VAL
1	A	275	ARG
1	A	305	LYS
1	A	311	THR
1	A	312	GLU
1	A	314	GLN
1	A	315	LEU
1	A	321	LYS
1	A	324	VAL
1	A	327	THR
1	A	349	GLU
1	A	350	GLU
1	B	70	ASP
1	B	74	THR
1	B	83	SER
1	B	84	VAL
1	B	128	LEU
1	B	138	LEU
1	B	147	HIS
1	B	168	LEU
1	B	180	LYS
1	B	204	ASN
1	B	242	ARG
1	B	257	ARG
1	B	275	ARG
1	B	281[A]	LYS
1	B	281[B]	LYS
1	B	298	ARG
1	B	302	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	315	LEU
1	B	324	VAL
1	B	335	LYS
1	B	344	VAL
1	C	10	SER
1	C	20	ASP
1	C	69	LYS
1	C	72	TRP
1	C	79	LEU
1	C	84	VAL
1	C	85	MET
1	C	147	HIS
1	C	163	LEU
1	C	166	LYS
1	C	201	SER
1	C	204	ASN
1	C	209	LYS
1	C	228	ASP
1	C	236	LEU
1	C	239	LYS
1	C	266	LYS
1	C	273	THR
1	C	275	ARG
1	C	284	VAL
1	C	294	VAL
1	C	312	GLU
1	C	314	GLN
1	C	315	LEU
1	C	316	THR
1	C	319	LEU
1	C	325	VAL
1	C	331	GLN
1	D	3	GLU
1	D	57	ASP
1	D	64	MET
1	D	65	VAL
1	D	72	TRP
1	D	87	LEU
1	D	88	LYS
1	D	94	SER
1	D	98	LEU
1	D	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	142	THR
1	D	147	HIS
1	D	163	LEU
1	D	180	LYS
1	D	184	PHE
1	D	185	THR
1	D	187	ASN
1	D	190	ARG
1	D	191	GLN
1	D	209	LYS
1	D	268	ASP
1	D	275	ARG
1	D	290	GLU
1	D	298	ARG
1	D	307	SER
1	D	313	PRO
1	D	324	VAL
1	D	327	THR

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	99	ASN
1	A	105	GLN
1	A	154	GLN
1	A	170	HIS
1	A	187	ASN
1	A	226	GLN
1	A	300	GLN
1	A	314	GLN
1	A	333	ASN
1	A	339	GLN
1	A	347	ASN
1	B	105	GLN
1	B	144	GLN
1	B	187	ASN
1	B	202	ASN
1	B	204	ASN
1	B	274	GLN
1	B	285	ASN
1	B	303	ASN
1	B	347	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	130	ASN
1	C	191	GLN
1	C	204	ASN
1	C	285	ASN
1	C	303	ASN
1	C	339	GLN
1	C	347	ASN
1	D	99	ASN
1	D	285	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	AMV	L	501	2	19,20,21	0.66	1 (5%)	22,27,29	1.79	7 (31%)
2	FGA	L	503	2	4,8,9	0.45	0	2,9,11	1.12	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	AMV	L	501	2	-	2/12/34/36	0/1/1/1
2	FGA	L	503	2	-	0/3/8/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	501	AMV	O1-C1	2.14	1.43	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	AMV	C1-C2-N2	-3.84	104.40	111.00
2	L	501	AMV	C1-O5-C5	3.48	120.51	113.69
2	L	501	AMV	C3-C2-N2	-2.72	106.40	110.91
2	L	501	AMV	O5-C5-C4	2.44	114.13	109.69
2	L	501	AMV	O5-C5-C6	2.12	111.71	106.44
2	L	501	AMV	O5-C1-C2	2.11	114.70	110.58
2	L	501	AMV	C3-C4-C5	2.06	114.04	109.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	501	AMV	O5-C5-C6-O6
2	L	501	AMV	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	501	AMV	1	0

5.5 Carbohydrates ⓘ

2 monosaccharides 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	$\# Z > 2$
3	GLC	E	1	3	11,11,12	0.34	0	15,15,17	2.14	3 (20%)
3	FRU	E	2	3	11,12,12	0.52	0	10,18,18	0.71	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
3	GLC	E	1	3	-	0/2/19/22	0/1/1/1
3	FRU	E	2	3	-	0/5/24/24	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	GLC	C1-O5-C5	6.99	121.66	112.19
3	E	1	GLC	O5-C1-C2	-2.67	106.65	110.77
3	E	1	GLC	C6-C5-C4	-2.04	108.22	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
4	SO4	C	353	-	4,4,4	0.21	0	6,6,6	0.52	0
4	SO4	D	353	-	4,4,4	0.16	0	6,6,6	0.51	0
4	SO4	A	353	-	4,4,4	0.14	0	6,6,6	0.41	0
4	SO4	B	355	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	B	354	-	4,4,4	0.14	0	6,6,6	0.34	0
4	SO4	B	353	-	4,4,4	0.17	0	6,6,6	0.46	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
4	B	355	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, 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	345/352 (98%)	0.35	31 (8%) 9 7	24, 35, 64, 77	0
1	B	346/352 (98%)	0.00	11 (3%) 47 41	23, 34, 54, 72	0
1	C	347/352 (98%)	0.17	13 (3%) 41 36	26, 39, 56, 69	0
1	D	351/352 (99%)	0.07	7 (1%) 65 61	22, 35, 55, 70	0
2	L	2/6 (33%)	0.89	0 100 100	42, 42, 42, 48	0
All	All	1391/1414 (98%)	0.15	62 (4%) 33 27	22, 36, 57, 77	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	GLY	6.0
1	A	352	GLY	5.2
1	A	337	ILE	5.0
1	A	310	LEU	4.7
1	A	309	THR	4.6
1	A	305	LYS	4.4
1	B	75	GLY	4.2
1	A	216	ALA	4.2
1	A	80	ARG	4.1
1	A	214	ALA	4.0
1	A	307	SER	3.8
1	A	152	PRO	3.8
1	A	331	GLN	3.8
1	A	75	GLY	3.6
1	A	327	THR	3.6
1	D	72	TRP	3.4
1	C	46	THR	3.4
1	C	41	LEU	3.3
1	A	73	ALA	3.2
1	B	74	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	333	ASN	3.1
1	A	77	PRO	3.0
1	A	72	TRP	3.0
1	D	74	THR	2.9
1	D	75	GLY	2.9
1	A	302	LYS	2.9
1	A	74	THR	2.8
1	A	333	ASN	2.7
1	C	44	ILE	2.7
1	D	41	LEU	2.7
1	A	49	VAL	2.7
1	A	326	GLY	2.7
1	B	164	LEU	2.6
1	C	164	LEU	2.6
1	B	72	TRP	2.6
1	A	306	ALA	2.6
1	C	6	VAL	2.5
1	A	164	LEU	2.5
1	A	301	LEU	2.4
1	B	352	GLY	2.4
1	C	299	GLY	2.4
1	B	162	ALA	2.4
1	C	148	GLY	2.3
1	B	268	ASP	2.3
1	D	190	ARG	2.3
1	A	215	GLY	2.3
1	C	215	GLY	2.2
1	B	267	PRO	2.2
1	C	283	GLU	2.2
1	A	329	ASP	2.2
1	C	102	VAL	2.2
1	B	44	ILE	2.1
1	B	41	LEU	2.1
1	A	221	VAL	2.1
1	A	78	ALA	2.1
1	A	308	TYR	2.1
1	D	69	LYS	2.1
1	C	221	VAL	2.1
1	C	42	THR	2.0
1	A	162	ALA	2.0
1	B	152	PRO	2.0
1	A	46	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	AMV	L	501	20/21	0.91	0.14	40,51,64,65	0
2	FGA	L	503	9/10	0.91	0.19	48,49,62,62	0
2	DAL	L	505	5/6	0.92	0.12	35,37,39,40	0
2	DAL	L	506	6/6	0.94	0.17	35,40,45,45	0

6.3 Carbohydrates [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
3	FRU	E	2	12/12	0.90	0.12	28,35,42,43	12
3	GLC	E	1	11/12	0.94	0.10	25,31,34,39	11

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
4	SO4	B	355	5/5	0.86	0.16	87,88,90,93	0
4	SO4	B	353	5/5	0.96	0.08	43,53,56,59	0
4	SO4	D	353	5/5	0.97	0.09	33,56,57,58	0
4	SO4	B	354	5/5	0.98	0.19	63,69,71,72	0
4	SO4	A	353	5/5	0.98	0.08	34,46,49,57	0
4	SO4	C	353	5/5	0.99	0.12	37,38,44,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.