Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:48 AM GMT

PDB ID	:	2IU8
Title	:	CHLAMYDIA TRACHOMATIS LPXD WITH 25MM UDPGLCNAC (COMPLEX I)
Authors	:	Buetow, L.; Smith, T.K.; Dawson, A.; Fyffe, S.; Hunter, W.N.
Deposited on	:	2006-05-30
Resolution	:	2.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

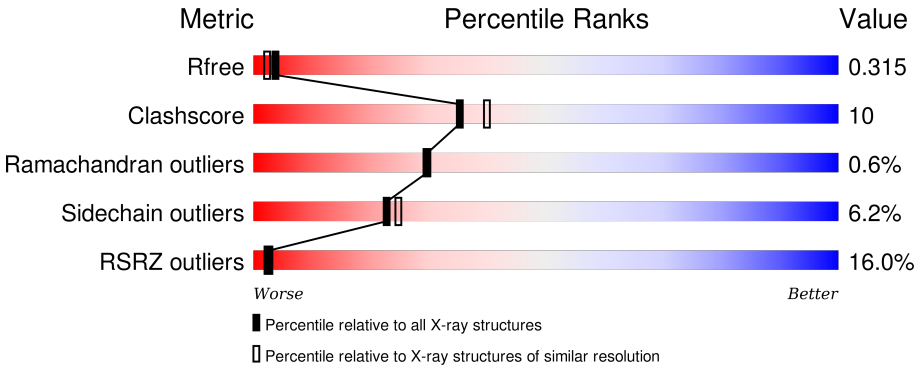
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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 <=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	374	13% 73% 17% • 7%
1	B	374	12% 72% 17% • 8%
1	C	374	20% 75% 16% • 7%

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
3	PLM	B	1349[A]	-	-	-	X
3	PLM	B	1349[B]	-	-	-	X
6	UD1	B	1348	-	-	-	X

2 Entry composition

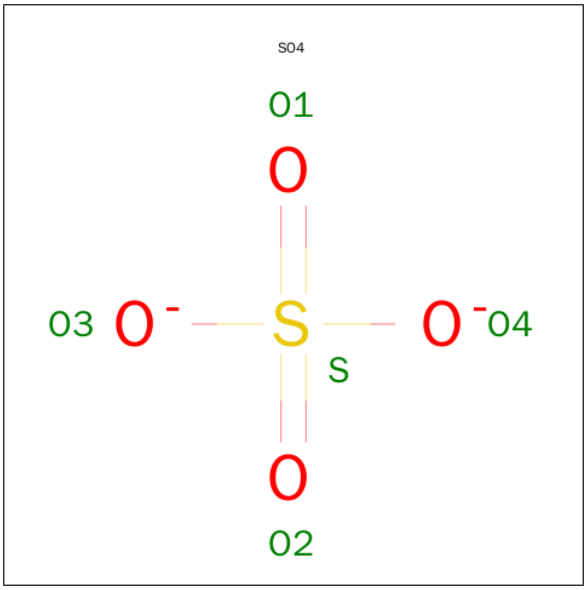
There are 7 unique types of molecules in this entry. The entry contains 8688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	12	0
			2695	1700	485	498	12			
1	B	345	Total	C	N	O	S	0	9	0
			2676	1689	479	498	10			
1	C	346	Total	C	N	O	S	0	8	0
			2680	1693	481	496	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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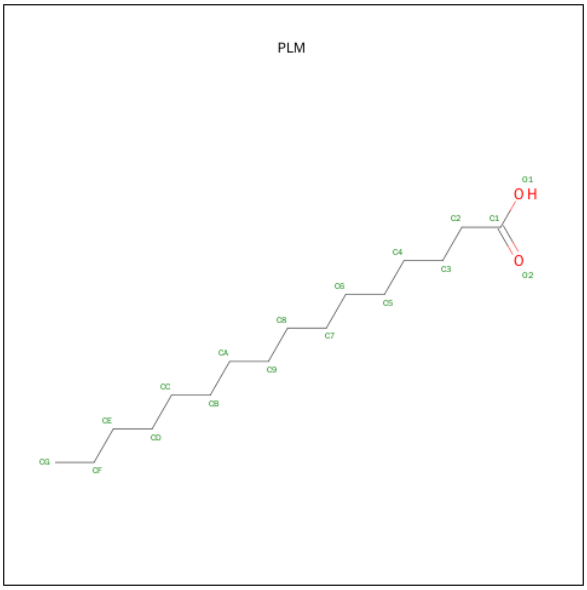
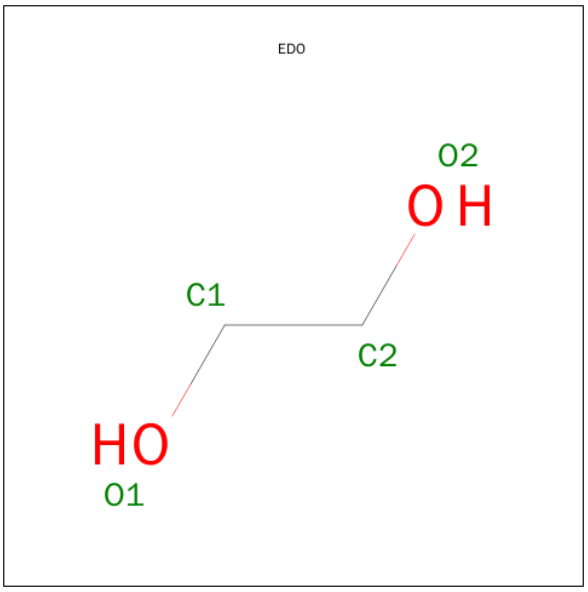
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



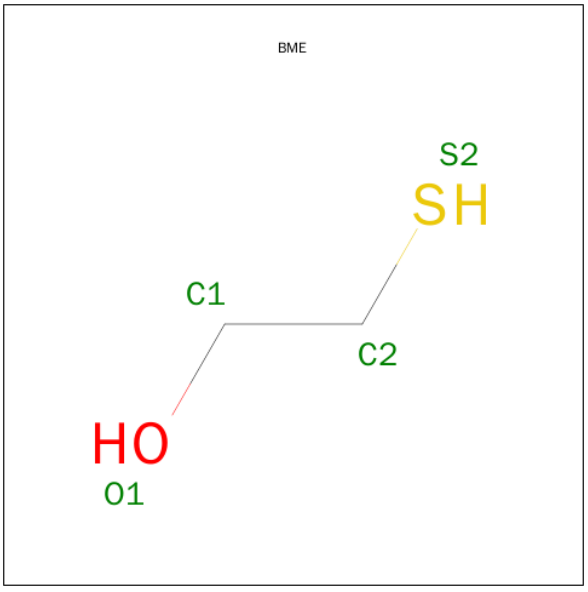
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 18 16 2	0	0
3	B	1	Total C O 25 23 2	0	1
3	C	1	Total C O 18 16 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



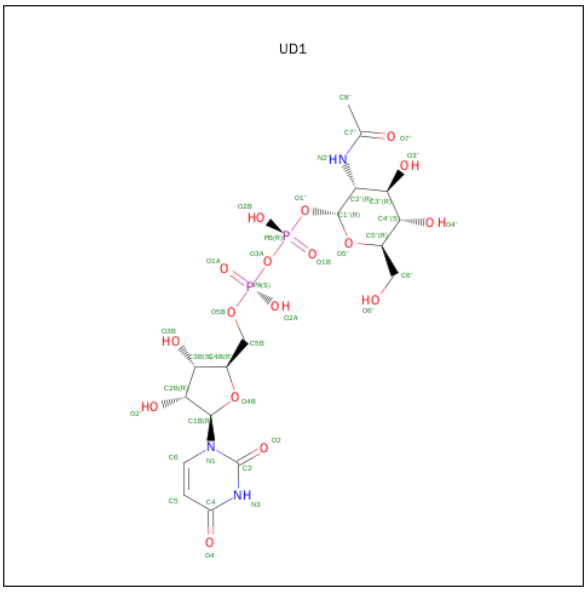
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	8	4	2	2	0	1

- Molecule 6 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 7 is water.

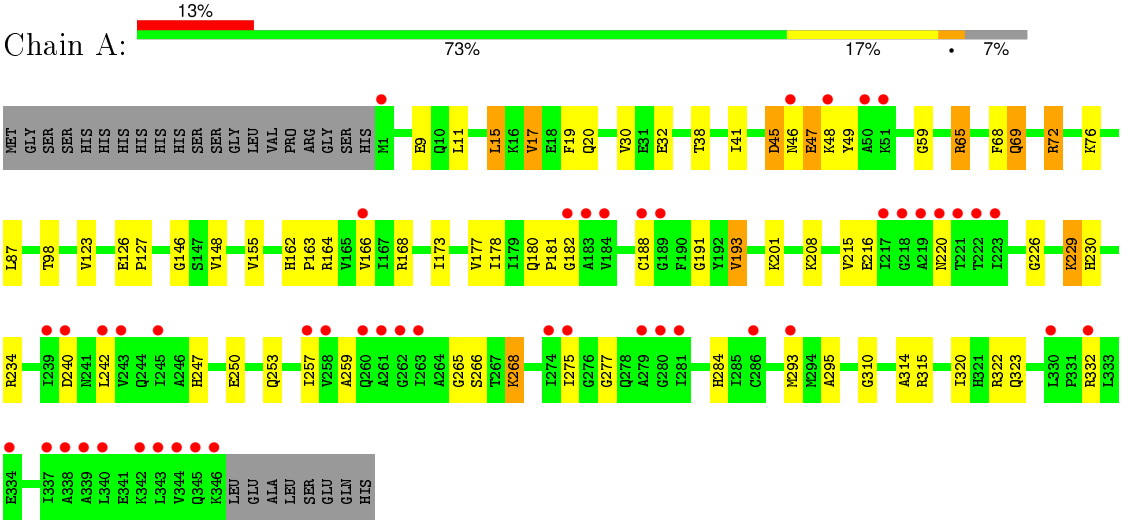
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	147	Total	O	0	0
			147	147		
7	C	139	Total	O	0	0
			139	139		

3 Residue-property plots (i)

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.

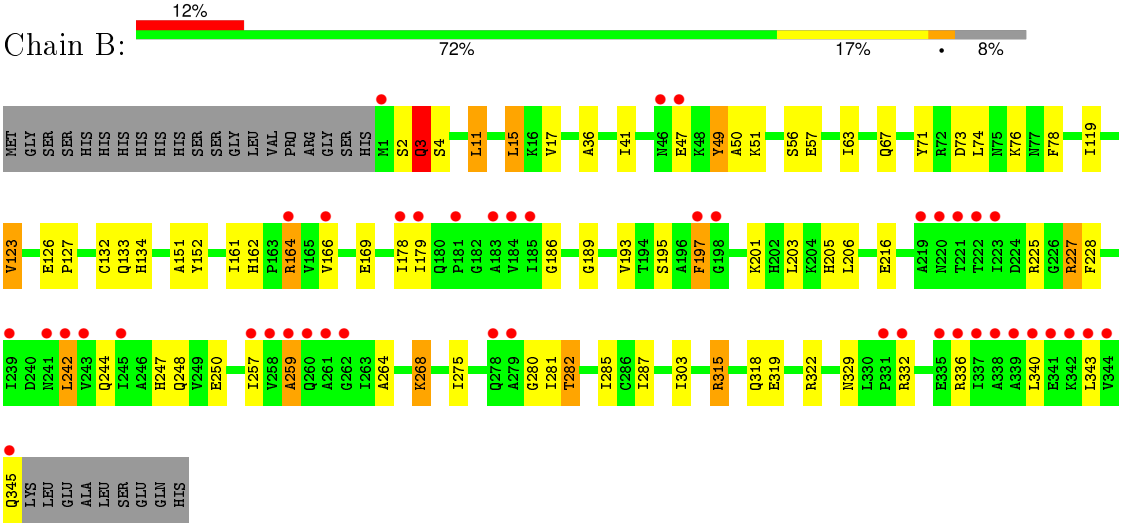
• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE

Chain A:



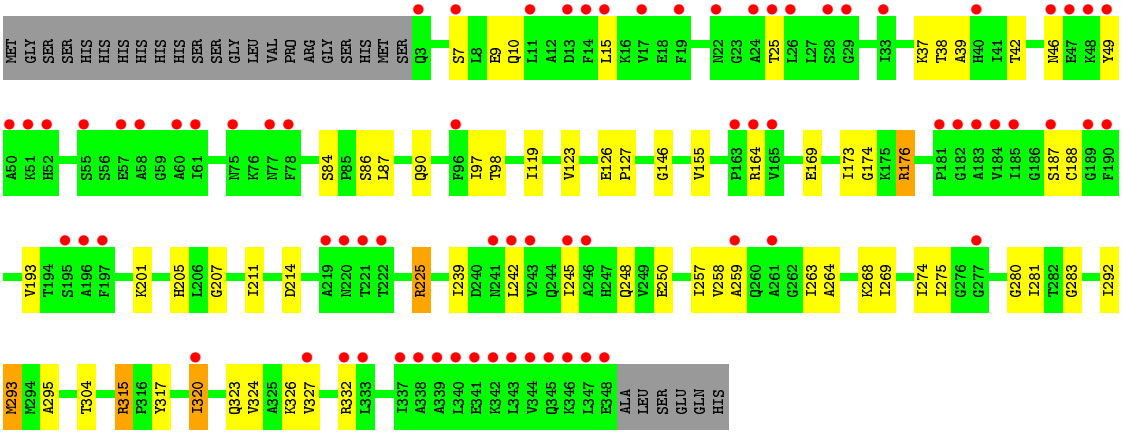
• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE

Chain B:



• Molecule 1: UDP-3-O-[3-HYDROXYMYRISTOYL] GLUCOSAMINE N-ACYLTRANSFERASE

Chain C:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER Q8 S7 L8 E9 Q10 L11 A12 D13 F14 L15 K16 V17 E18 F19 M22 G23 A24 T25 L26 L27 S28 G29 I33 K37 T38 A39 H40 I41 T42 N46 E47 K48 Y49
A50 K51 H52 S55 S56 E57 A58 G59 A60 I61 N75 K76 N77 F78 S84 P85 S86 L87 Q90 F96 I97 T98 I119 V123 E126 P127 G146 V155 P163 R164 V165 E169 I173 G174 K175 R176 P181 G182 A183 V184 I185 G186 S187 C188 G189 F190
V193 T194 S195 A196 F197 K201 H205 L206 G207 I211 D214 A219 N220 T221 T222 R225 I239 D240 N241 L242 V243 Q244 I245 A246 H247 Q248 V249 E250 I257 V258 A259 Q260 A261 G262 I263 A264 K268 I269 I274 I275 G276 G277 G280 I281 T282 G283 I292
M293 M294 A295 T304 R315 P316 Y317 I320 Q323 V324 A325 K326 V327 R332 L333 I337 A338 A339 L340 E341 K342 L343 V344 Q345 K346 I347 E348 ALA LEU SER GLU GLN HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.81Å 98.81Å 283.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.72 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (50.00-2.20) 90.3 (49.72-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.256 0.273 , 0.315	Depositor DCC
R_{free} test set	3302 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 65171 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8688	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PLM, SO4, UD1, EDO, BME

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	0.66	4/2796 (0.1%)	0.68	3/3778 (0.1%)
1	B	0.61	2/2763 (0.1%)	0.70	3/3737 (0.1%)
1	C	0.52	2/2763 (0.1%)	0.59	0/3736
All	All	0.60	8/8322 (0.1%)	0.66	6/11251 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLU	CD-OE1	14.81	1.42	1.25
1	A	47	GLU	CD-OE2	14.46	1.41	1.25
1	C	9	GLU	CD-OE2	12.83	1.39	1.25
1	A	47	GLU	CG-CD	9.44	1.66	1.51
1	B	195	SER	CB-OG	9.02	1.53	1.42
1	A	45	ASP	CG-OD2	8.78	1.45	1.25
1	C	9	GLU	CD-OE1	8.56	1.35	1.25
1	B	132	CYS	CB-SG	5.01	1.90	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	45	ASP	CB-CG-OD2	-9.38	109.85	118.30
1	A	45	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	197	PHE	CB-CG-CD2	7.24	125.87	120.80
1	B	197	PHE	CG-CD2-CE2	5.58	126.94	120.80
1	A	47	GLU	CG-CD-OE2	5.57	129.43	118.30
1	B	242	LEU	CA-CB-CG	5.15	127.14	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2695	0	2716	66	0
1	B	2676	0	2694	61	0
1	C	2680	0	2702	52	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
3	A	18	0	31	1	0
3	B	25	0	34	1	0
3	C	18	0	31	8	0
4	A	4	0	6	0	0
5	A	8	0	11	3	0
6	B	39	0	25	6	0
7	A	209	0	0	3	0
7	B	147	0	0	4	0
7	C	139	0	0	4	0
All	All	8688	0	8250	162	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (162) 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:164[A]:ARG:HD2	1:C:164[A]:ARG:CG	1.74	1.16
1:A:65:ARG:HH11	1:A:65:ARG:HG3	1.18	1.06
1:B:164[B]:ARG:HH11	1:B:164[B]:ARG:HG2	1.11	1.06
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:HG2	1.91	1.01
1:A:164[A]:ARG:HD2	1:C:164[A]:ARG:HG2	0.95	0.94
1:A:164[B]:ARG:NE	1:C:164[B]:ARG:NH1	2.15	0.89
1:A:164[B]:ARG:HE	1:C:164[B]:ARG:NH1	1.69	0.88
1:A:148:VAL:HG23	1:B:164[B]:ARG:HH21	1.39	0.86
1:B:164[A]:ARG:HB2	1:C:164[A]:ARG:HD2	1.58	0.85
1:B:164[B]:ARG:HH11	1:B:164[B]:ARG:CG	1.89	0.84
1:A:164[B]:ARG:NH1	1:B:164[B]:ARG:NE	2.22	0.81
1:A:164[B]:ARG:NE	1:C:164[B]:ARG:HH12	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HB	1:A:216:GLU:HG2	1.67	0.77
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:HD2	1.67	0.77
3:A:1349:PLM:H21	1:B:259:ALA:HB3	1.68	0.75
1:A:9:GLU:HG3	1:A:19:PHE:CE2	2.22	0.74
1:B:164[B]:ARG:NH1	1:B:164[B]:ARG:HG2	1.92	0.71
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.00	0.71
1:B:319[A]:GLU:OE2	7:B:2143:HOH:O	2.12	0.68
6:B:1348:UD1:H3B	6:B:1348:UD1:O1A	1.94	0.68
1:A:295:ALA:CB	3:C:1351:PLM:H91	2.27	0.65
1:B:11:LEU:HD21	1:B:41:ILE:HD11	1.77	0.65
1:B:250[A]:GLU:OE2	1:B:268:LYS:HD3	1.97	0.64
1:B:257:ILE:HG12	1:B:275:ILE:HD12	1.79	0.64
1:A:193:VAL:HG23	1:A:201:LYS:HB2	1.81	0.63
1:A:65:ARG:HG3	1:A:65:ARG:NH1	1.99	0.62
1:A:259:ALA:HB3	3:C:1351:PLM:H32	1.81	0.62
1:A:126:GLU:HB3	1:A:127:PRO:HD2	1.82	0.61
1:A:164[A]:ARG:HG2	1:B:164[A]:ARG:CD	2.29	0.61
1:B:282:THR:HG23	7:C:2046:HOH:O	2.00	0.61
7:A:2206:HOH:O	6:B:1348:UD1:H8'2	2.01	0.59
1:B:126:GLU:HB3	1:B:127:PRO:HD2	1.85	0.58
1:C:146:GLY:O	1:C:164[B]:ARG:NH1	2.37	0.58
1:B:247:HIS:H	1:B:247:HIS:CD2	2.22	0.58
1:A:164[B]:ARG:HH12	1:B:164[B]:ARG:NE	1.97	0.57
1:B:315[A]:ARG:HH22	1:C:324:VAL:HG13	1.69	0.57
1:A:47:GLU:HB2	1:A:49:TYR:CE1	2.38	0.57
1:B:11:LEU:HD12	1:B:15:LEU:HD22	1.85	0.57
1:C:7:SER:OG	1:C:10:GLN:HB2	2.05	0.57
1:C:119:ILE:HG22	1:C:123:VAL:HG11	1.87	0.57
1:A:188[B]:CYS:HB2	5:A:1351[B]:BME:S2	2.44	0.57
1:A:32:GLU:OE1	1:A:32:GLU:HA	2.04	0.57
1:B:189:GLY:HA3	1:B:205:HIS:CE1	2.40	0.57
1:B:3:GLN:O	7:B:2003:HOH:O	2.17	0.57
1:A:162:HIS:HB3	1:A:163:PRO:HD2	1.88	0.56
1:C:239:ILE:HG12	1:C:257:ILE:HD12	1.86	0.56
1:A:315:ARG:HB2	1:A:320:ILE:HG23	1.87	0.56
6:B:1348:UD1:PA	6:B:1348:UD1:H3B	2.45	0.56
1:C:207:GLY:O	1:C:225:ARG:NH1	2.40	0.55
1:A:164[B]:ARG:CD	1:C:164[B]:ARG:HH12	2.18	0.55
1:A:257:ILE:HG12	1:A:275:ILE:HD12	1.89	0.55
1:C:46:ASN:HB2	1:C:49:TYR:HB2	1.88	0.55
1:B:227:ARG:NH2	1:C:86:SER:OG	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HD12	1:B:179:ILE:HD12	1.88	0.54
1:C:275:ILE:HG12	1:C:293:MET:CE	2.37	0.54
1:B:164[A]:ARG:HE	1:C:164[A]:ARG:NE	2.04	0.54
1:C:263:ILE:HD13	1:C:269:ILE:HD13	1.89	0.54
1:A:247:HIS:HD2	7:A:2155:HOH:O	1.91	0.54
1:C:245:ILE:HD13	1:C:263:ILE:HD12	1.91	0.53
3:B:1349[B]:PLM:HC2	1:C:295:ALA:HB3	1.91	0.53
1:A:38:THR:O	1:A:59:GLY:HA3	2.09	0.53
1:C:176:ARG:HG3	1:C:214:ASP:OD1	2.09	0.52
1:B:178:ILE:HB	1:B:216:GLU:HG2	1.91	0.52
1:A:146:GLY:O	1:A:164[B]:ARG:NH1	2.41	0.52
1:B:227:ARG:HB3	1:B:228:PHE:HD2	1.74	0.51
1:A:162:HIS:HB3	1:A:163:PRO:CD	2.40	0.51
1:A:164[A]:ARG:CG	1:B:164[A]:ARG:HD2	2.40	0.51
1:B:343:LEU:HD13	1:B:345:GLN:HB2	1.93	0.51
1:C:245:ILE:CD1	1:C:263:ILE:HD12	2.41	0.51
1:A:126:GLU:HB3	1:A:127:PRO:CD	2.41	0.50
1:C:126:GLU:HB3	1:C:127:PRO:CD	2.41	0.50
1:A:47:GLU:HB2	1:A:49:TYR:HE1	1.76	0.50
1:A:65:ARG:NH1	2:A:1347:SO4:O1	2.44	0.49
1:B:49:TYR:O	1:B:51:LYS:N	2.35	0.49
1:B:2:SER:C	1:B:4:SER:H	2.15	0.49
1:A:188[B]:CYS:SG	5:A:1351[B]:BME:S2	3.11	0.49
1:A:166:VAL:CG2	1:B:164[A]:ARG:HG2	2.43	0.49
1:C:248:GLN:NE2	7:C:2101:HOH:O	2.46	0.49
1:B:71:TYR:HB3	1:B:74:LEU:HD12	1.94	0.48
1:C:84:SER:HB3	1:C:87:LEU:HD12	1.94	0.48
1:B:164[B]:ARG:NH1	1:B:164[B]:ARG:CG	2.58	0.48
1:B:227:ARG:HD3	1:C:90:GLN:OE1	2.13	0.48
1:B:186:GLY:O	1:B:225:ARG:NH1	2.46	0.48
1:C:257:ILE:HG12	1:C:275:ILE:HD12	1.94	0.48
1:B:133:GLN:HG3	1:B:134:HIS:HD2	1.78	0.47
1:C:174:GLY:N	1:C:211:ILE:O	2.45	0.47
1:C:315:ARG:NH1	7:C:2125:HOH:O	2.48	0.47
1:B:36:ALA:HB3	7:B:2027:HOH:O	2.14	0.47
1:B:166:VAL:CG2	1:C:164[B]:ARG:HG2	2.44	0.46
1:B:11:LEU:HD21	1:B:41:ILE:CD1	2.43	0.46
1:C:126:GLU:HB3	1:C:127:PRO:HD2	1.97	0.46
1:A:191:GLY:HA2	6:B:1348:UD1:O4'	2.15	0.46
1:A:47:GLU:C	1:A:49:TYR:H	2.18	0.46
1:B:287:ILE:HD12	1:B:303:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:HG23	1:B:285:ILE:HD11	1.98	0.46
1:A:182:GLY:O	1:A:220:ASN:HA	2.15	0.46
1:A:11:LEU:HG	1:A:15:LEU:HD22	1.98	0.46
1:C:250:GLU:HB3	1:C:268:LYS:HG3	1.98	0.46
1:C:280:GLY:HA3	3:C:1351:PLM:H81	1.98	0.45
1:A:275:ILE:HG12	1:A:293:MET:CE	2.47	0.45
1:B:119:ILE:HG22	1:B:123:VAL:HG11	1.98	0.45
1:C:274:ILE:HD12	1:C:292:ILE:HG12	1.97	0.45
1:A:277:GLY:HA3	3:C:1351:PLM:H71	1.98	0.45
1:A:226:GLY:HA3	1:A:229:LYS:O	2.17	0.45
1:B:193:VAL:HG23	1:B:203:LEU:HD21	1.98	0.45
1:A:295:ALA:HB3	3:C:1351:PLM:H91	1.99	0.44
1:B:151:ALA:O	1:B:152:TYR:HB2	2.17	0.44
5:A:1351[A]:BME:H21	1:B:162:HIS:HE1	1.82	0.44
1:C:275:ILE:HG23	1:C:293:MET:HE3	2.00	0.44
1:A:15:LEU:HB3	1:A:17:VAL:HB	1.99	0.44
1:A:208:LYS:HG3	1:A:230:HIS:CE1	2.53	0.44
1:C:37:LYS:HE3	1:C:39:ALA:HB3	2.00	0.44
1:A:47:GLU:O	1:A:49:TYR:N	2.49	0.44
1:C:317:TYR:HA	1:C:320:ILE:HD11	1.98	0.43
1:C:7:SER:HA	1:C:25:THR:O	2.19	0.43
1:B:76:LYS:HB2	1:B:78:PHE:CZ	2.53	0.43
1:C:205:HIS:O	1:C:225:ARG:HD3	2.17	0.43
1:A:20:GLN:HG3	1:A:68:PHE:CZ	2.54	0.43
1:C:188:CYS:HB2	2:C:1350:SO4:O4	2.18	0.43
1:A:69[B]:GLN:HE22	1:A:72[B]:ARG:HH12	1.66	0.43
3:C:1351:PLM:HF2	3:C:1351:PLM:HC1	1.57	0.43
1:A:320:ILE:HA	1:A:323:GLN:HB2	2.00	0.43
1:C:258:VAL:HG12	1:C:259:ALA:N	2.34	0.43
1:B:169:GLU:O	1:B:225:ARG:NH2	2.51	0.43
1:B:49:TYR:CD1	1:B:49:TYR:N	2.87	0.42
1:C:264:ALA:HB2	3:C:1351:PLM:H41	2.01	0.42
1:C:264:ALA:HB3	1:C:283:GLY:N	2.33	0.42
1:B:247:HIS:O	1:B:248:GLN:HB2	2.19	0.42
1:A:155:VAL:HA	1:A:173:ILE:HB	2.02	0.42
1:A:164[A]:ARG:NE	1:C:164[A]:ARG:HE	2.17	0.42
1:C:193:VAL:HB	1:C:201:LYS:HB2	2.00	0.42
1:C:155:VAL:HA	1:C:173:ILE:HB	2.02	0.42
1:A:30:VAL:HG12	1:A:41:ILE:HB	2.02	0.42
1:A:295:ALA:HB1	3:C:1351:PLM:H91	2.00	0.42
1:A:265:GLY:O	6:B:1348:UD1:O7'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164[A]:ARG:CD	1:C:164[A]:ARG:CG	2.69	0.41
1:C:281:ILE:HD11	1:C:293:MET:HE1	2.02	0.41
1:B:247:HIS:H	1:B:247:HIS:HD2	1.65	0.41
1:A:180:GLN:HB3	1:A:181:PRO:CD	2.50	0.41
1:A:250[A]:GLU:HB2	1:A:268:LYS:HG3	2.01	0.41
1:A:310:GLY:O	1:A:314:ALA:HA	2.20	0.41
1:C:323:GLN:O	1:C:327:VAL:HG23	2.21	0.41
1:B:63:ILE:HG12	1:B:67:GLN:HB2	2.03	0.41
1:A:234[B]:ARG:HD3	1:A:253:GLN:HG3	2.03	0.41
1:B:329:ASN:OD1	1:B:332:ARG:HD3	2.21	0.41
1:A:177:VAL:HG13	1:A:215:VAL:O	2.21	0.40
1:A:240:ASP:HB3	1:A:259:ALA:N	2.36	0.40
1:C:275:ILE:HG12	1:C:293:MET:HE2	2.03	0.40
1:A:284:HIS:CD2	6:B:1348:UD1:O7'	2.74	0.40
1:A:247:HIS:CD2	7:A:2155:HOH:O	2.72	0.40
1:B:332:ARG:HH12	1:B:336:ARG:HH11	1.69	0.40
1:B:205:HIS:O	1:B:206:LEU:HD23	2.21	0.40
1:B:56:SER:OG	7:B:2027:HOH:O	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	356/374 (95%)	336 (94%)	19 (5%)	1 (0%)	46 50
1	B	352/374 (94%)	333 (95%)	14 (4%)	5 (1%)	14 10
1	C	352/374 (94%)	333 (95%)	19 (5%)	0	100 100
All	All	1060/1122 (94%)	1002 (94%)	52 (5%)	6 (1%)	30 29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	B	3	GLN
1	B	49	TYR
1	B	50	ALA
1	B	197	PHE
1	B	259	ALA

5.3.2 Protein sidechains (i)

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	297/309 (96%)	276 (93%)	21 (7%)	18	19
1	B	293/309 (95%)	272 (93%)	21 (7%)	18	18
1	C	293/309 (95%)	277 (94%)	16 (6%)	27	30
All	All	883/927 (95%)	825 (93%)	58 (7%)	23	22

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	17	VAL
1	A	45	ASP
1	A	46	ASN
1	A	65	ARG
1	A	69[A]	GLN
1	A	69[B]	GLN
1	A	72[A]	ARG
1	A	72[B]	ARG
1	A	76	LYS
1	A	87	LEU
1	A	98	THR
1	A	123	VAL
1	A	168	ARG
1	A	193	VAL
1	A	229	LYS
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	266	SER
1	A	268	LYS
1	A	322	ARG
1	A	332	ARG
1	B	3	GLN
1	B	11	LEU
1	B	15	LEU
1	B	17	VAL
1	B	47	GLU
1	B	57[A]	GLU
1	B	57[B]	GLU
1	B	73	ASP
1	B	123	VAL
1	B	164[A]	ARG
1	B	164[B]	ARG
1	B	201	LYS
1	B	227	ARG
1	B	242	LEU
1	B	268	LYS
1	B	282	THR
1	B	315[A]	ARG
1	B	315[B]	ARG
1	B	318	GLN
1	B	322	ARG
1	B	340	LEU
1	C	15	LEU
1	C	38	THR
1	C	42	THR
1	C	97	ILE
1	C	98	THR
1	C	169	GLU
1	C	176	ARG
1	C	187	SER
1	C	225	ARG
1	C	242	LEU
1	C	293	MET
1	C	304	THR
1	C	315	ARG
1	C	320	ILE
1	C	326	LYS
1	C	332	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	247	HIS
1	A	253	GLN
1	A	345	GLN
1	B	134	HIS
1	B	162	HIS
1	B	199	GLN
1	B	247	HIS
1	B	318	GLN
1	C	345	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)

14 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	1347	-	4,4,4	0.24	0	6,6,6	0.40	0
2	SO4	A	1348	-	4,4,4	0.18	0	6,6,6	0.22	0
3	PLM	A	1349	-	14,17,17	0.35	0	14,17,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	1350	-	3,3,3	0.49	0	2,2,2	0.32	0
5	BME	A	1351[A]	-	3,3,3	0.61	0	2,2,2	0.45	0
5	BME	A	1351[B]	-	3,3,3	0.54	0	2,2,2	0.15	0
2	SO4	B	1346	-	4,4,4	0.29	0	6,6,6	0.14	0
2	SO4	B	1347	-	4,4,4	0.17	0	6,6,6	0.21	0
6	UD1	B	1348	-	32,41,41	1.50	4 (12%)	46,62,62	1.72	8 (17%)
3	PLM	B	1349[A]	-	14,17,17	0.35	0	14,17,17	0.44	0
3	PLM	B	1349[B]	-	14,17,17	0.33	0	14,17,17	0.52	0
2	SO4	C	1349	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	C	1350	-	4,4,4	0.22	0	6,6,6	0.27	0
3	PLM	C	1351	-	14,17,17	0.35	0	14,17,17	0.39	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	1347	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1348	-	-	0/0/0/0	0/0/0/0
3	PLM	A	1349	-	-	0/13/15/15	0/0/0/0
4	EDO	A	1350	-	-	0/1/1/1	0/0/0/0
5	BME	A	1351[A]	-	-	0/1/1/1	0/0/0/0
5	BME	A	1351[B]	-	-	0/1/1/1	0/0/0/0
2	SO4	B	1346	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1347	-	-	0/0/0/0	0/0/0/0
6	UD1	B	1348	-	-	0/22/63/63	0/3/3/3
3	PLM	B	1349[A]	-	-	0/13/15/15	0/0/0/0
3	PLM	B	1349[B]	-	-	0/13/15/15	0/0/0/0
2	SO4	C	1349	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1350	-	-	0/0/0/0	0/0/0/0
3	PLM	C	1351	-	-	0/13/15/15	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1348	UD1	O4B-C1B	2.63	1.44	1.41
6	B	1348	UD1	O5'-C1'	2.63	1.48	1.41
6	B	1348	UD1	C4-N3	4.20	1.40	1.33
6	B	1348	UD1	C6-N1	4.28	1.41	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1348	UD1	PB-O3A-PA	-4.85	119.11	132.73
6	B	1348	UD1	C4B-O4B-C1B	-3.06	106.36	109.72
6	B	1348	UD1	C3'-C2'-N2'	-2.69	105.09	110.66
6	B	1348	UD1	O4'-C4'-C3'	-2.57	104.56	110.34
6	B	1348	UD1	C5B-C4B-C3B	-2.32	106.00	115.21
6	B	1348	UD1	O5'-C1'-O1'	2.92	115.21	111.36
6	B	1348	UD1	C4'-C3'-C2'	3.17	114.83	110.43
6	B	1348	UD1	C4-N3-C2	5.85	119.94	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1347	SO4	1	0
3	A	1349	PLM	1	0
5	A	1351[A]	BME	1	0
5	A	1351[B]	BME	2	0
6	B	1348	UD1	6	0
3	B	1349[B]	PLM	1	0
2	C	1350	SO4	1	0
3	C	1351	PLM	8	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^{th} 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	346/374 (92%)	0.81	48 (13%)	4 3	54, 62, 66, 72	1 (0%)
1	B	345/374 (92%)	0.68	44 (12%)	5 4	53, 61, 65, 78	0
1	C	346/374 (92%)	1.06	74 (21%)	1 1	53, 62, 65, 72	0
All	All	1037/1122 (92%)	0.85	166 (16%)	3 2	53, 61, 66, 78	1 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188[A]	CYS	7.5
1	C	347	LEU	6.5
1	C	340	LEU	5.8
1	C	344	VAL	5.8
1	A	337	ILE	5.7
1	B	340	LEU	5.6
1	C	345	GLN	5.6
1	C	242	LEU	5.3
1	B	345	GLN	5.3
1	C	48	LYS	5.3
1	B	338	ALA	5.3
1	A	48	LYS	5.1
1	B	46	ASN	4.9
1	A	339	ALA	4.8
1	A	340	LEU	4.8
1	A	344	VAL	4.6
1	C	342	LYS	4.5
1	C	343	LEU	4.4
1	B	344	VAL	4.4
1	C	26	LEU	4.3
1	B	339	ALA	4.3
1	B	242	LEU	4.3
1	C	96	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	338	ALA	4.2
1	A	346	LYS	4.2
1	C	337	ILE	4.1
1	C	19	PHE	4.1
1	C	15	LEU	4.0
1	B	243	VAL	4.0
1	A	243	VAL	4.0
1	A	51	LYS	3.9
1	B	197	PHE	3.9
1	B	184	VAL	3.9
1	C	243	VAL	3.9
1	A	262	GLY	3.8
1	A	330	LEU	3.8
1	C	259	ALA	3.7
1	A	245	ILE	3.7
1	C	24	ALA	3.6
1	C	49	TYR	3.6
1	C	181	PRO	3.6
1	B	337	ILE	3.6
1	B	342	LYS	3.6
1	A	50	ALA	3.5
1	C	75	ASN	3.5
1	A	222	THR	3.5
1	C	51	LYS	3.5
1	C	47	GLU	3.5
1	A	343	LEU	3.4
1	C	183	ALA	3.4
1	A	184	VAL	3.4
1	A	342	LYS	3.4
1	C	196	ALA	3.4
1	A	223	ILE	3.4
1	C	219	ALA	3.3
1	A	46	ASN	3.3
1	C	50	ALA	3.3
1	C	339	ALA	3.3
1	C	333	LEU	3.2
1	C	13	ASP	3.2
1	C	33	ILE	3.2
1	C	22	ASN	3.2
1	C	197	PHE	3.2
1	C	182	GLY	3.1
1	B	1	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	239	ILE	3.1
1	A	338	ALA	3.0
1	A	263	ILE	3.0
1	A	1	MET	3.0
1	A	189	GLY	3.0
1	B	164[A]	ARG	3.0
1	C	61	ILE	3.0
1	C	190	PHE	3.0
1	A	217	ILE	2.9
1	B	336	ARG	2.9
1	C	220	ASN	2.9
1	A	281	ILE	2.9
1	A	280	GLY	2.9
1	C	40	HIS	2.9
1	A	257	ILE	2.9
1	A	242	LEU	2.9
1	B	183	ALA	2.9
1	C	46	ASN	2.9
1	B	198	GLY	2.8
1	C	14	PHE	2.8
1	A	221	THR	2.8
1	B	221	THR	2.8
1	C	348	GLU	2.8
1	C	245	ILE	2.8
1	A	219	ALA	2.8
1	B	332	ARG	2.8
1	A	258	VAL	2.8
1	C	184	VAL	2.8
1	C	327	VAL	2.7
1	C	185	ILE	2.7
1	A	261	ALA	2.7
1	B	262	GLY	2.7
1	B	223	ILE	2.7
1	B	245	ILE	2.7
1	C	60	ALA	2.7
1	C	55	SER	2.7
1	B	341	GLU	2.7
1	B	239	ILE	2.7
1	B	343	LEU	2.7
1	C	346	LYS	2.7
1	A	345	GLN	2.7
1	C	164[A]	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	246	ALA	2.7
1	C	222	THR	2.7
1	C	3	GLN	2.6
1	C	57	GLU	2.6
1	C	241	ASN	2.6
1	B	258	VAL	2.6
1	C	11	LEU	2.6
1	B	331	PRO	2.5
1	C	7	SER	2.5
1	C	221	THR	2.5
1	A	274	ILE	2.5
1	A	166	VAL	2.5
1	C	165	VAL	2.5
1	A	332	ARG	2.5
1	B	185	ILE	2.5
1	B	181	PRO	2.5
1	B	220	ASN	2.5
1	B	179	ILE	2.5
1	A	334	GLU	2.5
1	B	241	ASN	2.4
1	B	47	GLU	2.4
1	C	189	GLY	2.4
1	B	259	ALA	2.4
1	A	286[A]	CYS	2.4
1	A	182	GLY	2.4
1	C	163	PRO	2.4
1	A	279	ALA	2.4
1	B	222	THR	2.4
1	C	25	THR	2.4
1	C	78	PHE	2.4
1	C	320	ILE	2.3
1	C	277	GLY	2.3
1	B	219	ALA	2.3
1	B	261	ALA	2.3
1	C	195	SER	2.3
1	A	275	ILE	2.3
1	A	240	ASP	2.3
1	C	17	VAL	2.3
1	C	29	GLY	2.3
1	C	52	HIS	2.2
1	C	77	ASN	2.2
1	C	332	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	183	ALA	2.2
1	C	261	ALA	2.2
1	A	218	GLY	2.2
1	C	341	GLU	2.2
1	A	293	MET	2.2
1	C	28	SER	2.2
1	B	166	VAL	2.2
1	C	58	ALA	2.2
1	A	260	GLN	2.1
1	C	187	SER	2.1
1	B	279	ALA	2.1
1	B	260	GLN	2.1
1	B	278	GLN	2.1
1	B	257	ILE	2.1
1	A	220	ASN	2.0
1	B	335	GLU	2.0
1	B	178	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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^{th} 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^2)	Q<0.9
3	PLM	B	1349[B]	18/18	0.74	0.32	4.72	57,60,69,70	7
3	PLM	B	1349[A]	18/18	0.74	0.32	3.43	52,60,69,70	7
6	UD1	B	1348	39/39	0.79	0.38	2.81	56,70,73,74	39
3	PLM	C	1351	18/18	0.80	0.28	1.27	70,72,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BME	A	1351[A]	4/4	0.94	0.31	0.40	37,40,41,46	4
5	BME	A	1351[B]	4/4	0.94	0.31	0.14	73,75,76,77	4
2	SO4	B	1346	5/5	0.96	0.12	-0.30	79,79,80,80	0
3	PLM	A	1349	18/18	0.84	0.20	-0.77	54,61,69,69	0
2	SO4	C	1350	5/5	0.97	0.16	-0.91	71,72,72,73	5
2	SO4	A	1347	5/5	0.97	0.09	-1.28	70,70,71,72	0
2	SO4	C	1349	5/5	0.98	0.07	-1.38	77,78,78,78	0
4	EDO	A	1350	4/4	0.93	0.13	-1.73	61,63,65,66	0
2	SO4	B	1347	5/5	0.97	0.13	-3.64	49,49,50,50	5
2	SO4	A	1348	5/5	0.86	0.24	-	66,67,68,68	5

6.5 Other polymers (i)

There are no such residues in this entry.