



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:49 PM EDT

PDB ID : 4FNA / pdb_00004fna
Title : Structure of unliganded FhuD2 from Staphylococcus Aureus
Authors : Shilton, B.H.; Heinrichs, D.E.
Deposited on : 2012-06-19
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

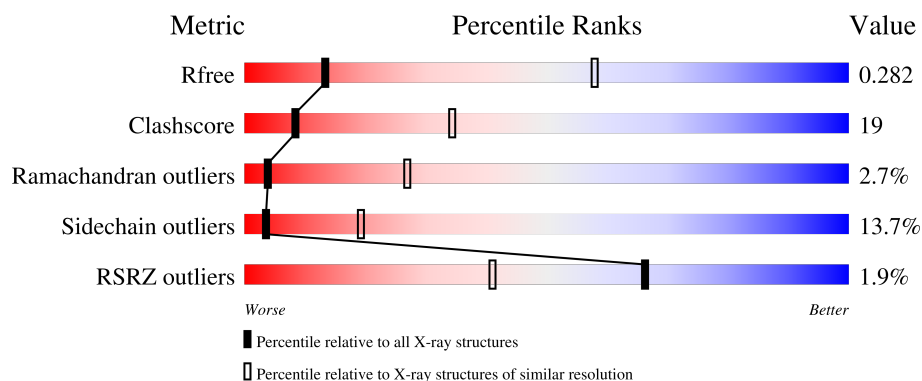
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	280	2% 59% 32% 7% ..
1	B	280	2% 55% 33% 10% ..
1	C	280	2% 51% 36% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6683 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 Ferric hydroxamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2216	1417	367	427	5			
1	B	278	Total	C	N	O	S	0	0	0
			2216	1417	367	427	5			
1	C	274	Total	C	N	O	S	0	0	0
			2186	1400	360	421	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q7BGA5
A	24	SER	-	expression tag	UNP Q7BGA5
B	23	GLY	-	expression tag	UNP Q7BGA5
B	24	SER	-	expression tag	UNP Q7BGA5
C	23	GLY	-	expression tag	UNP Q7BGA5
C	24	SER	-	expression tag	UNP Q7BGA5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

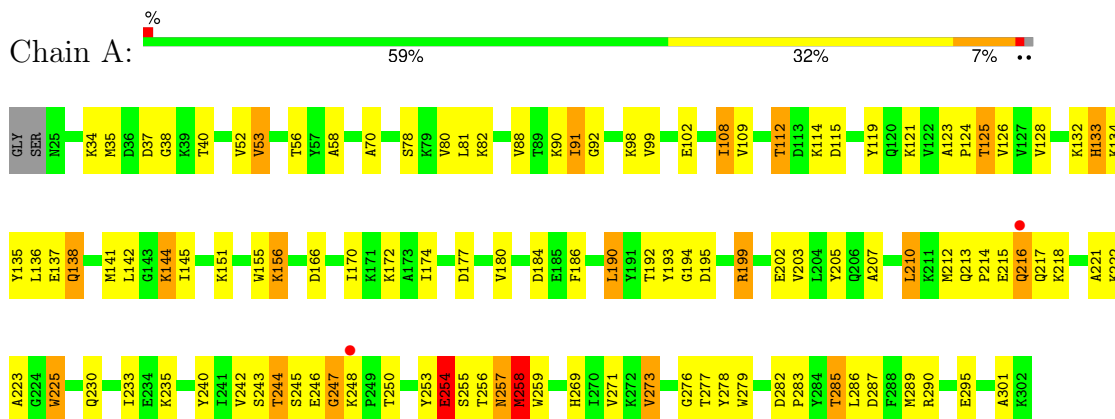


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

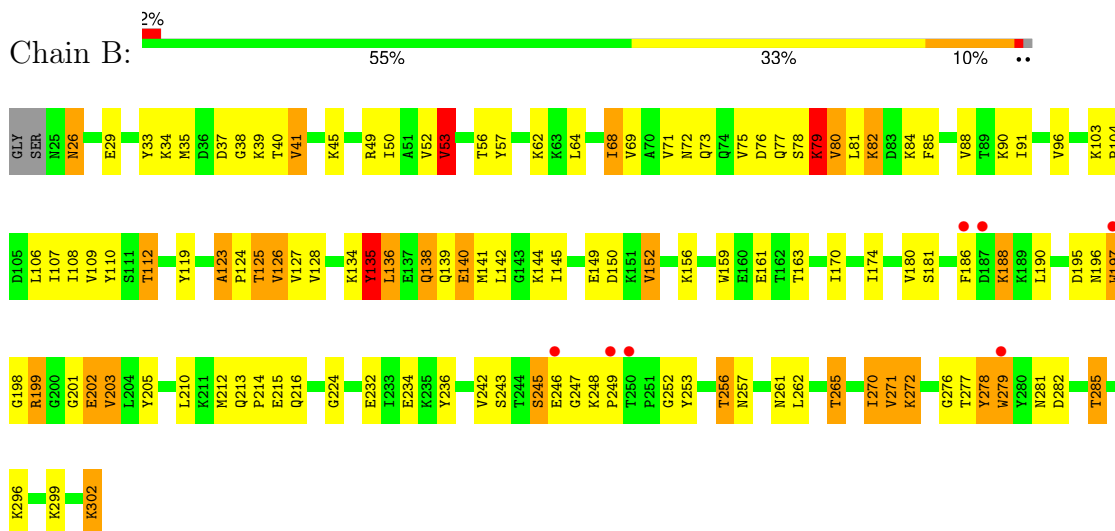
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

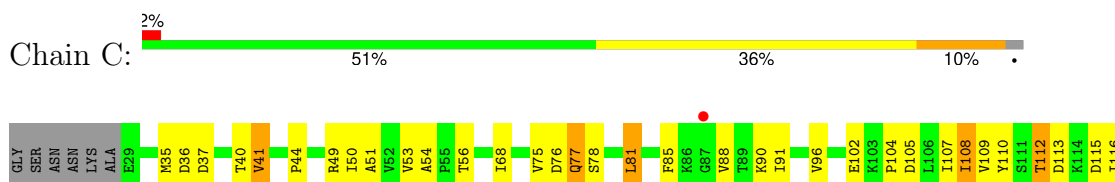
• Molecule 1: Ferric hydroxamate receptor 2

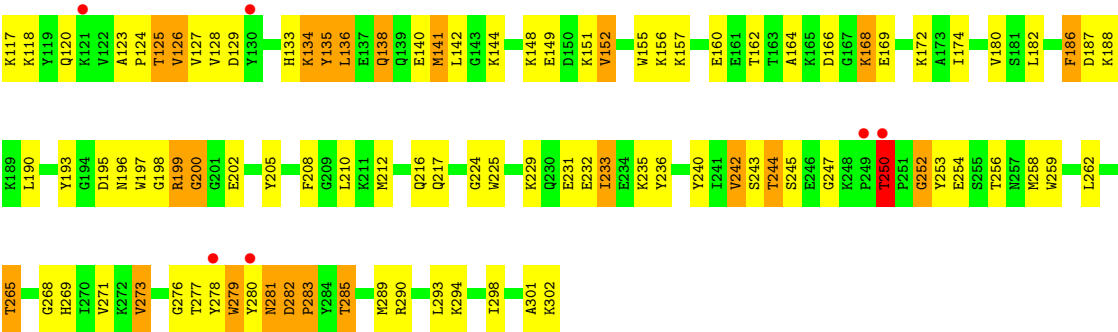


• Molecule 1: Ferric hydroxamate receptor 2



• Molecule 1: Ferric hydroxamate receptor 2





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	207.51Å 207.51Å 162.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.71 – 3.50 24.71 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.71-3.50) 97.5 (24.71-3.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.31 (at 3.54Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.220 , 0.281 0.224 , 0.282	Depositor DCC
R_{free} test set	1078 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 115.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6683	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0/2258	1.14	12/3033 (0.4%)
1	B	0.72	0/2258	1.19	10/3033 (0.3%)
1	C	0.60	0/2228	1.10	10/2993 (0.3%)
All	All	0.66	0/6744	1.14	32/9059 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ARG	N-CA-C	-9.67	99.80	111.69
1	C	54	ALA	CA-C-N	8.42	128.15	119.56
1	C	54	ALA	C-N-CA	8.42	128.15	119.56
1	B	135	TYR	N-CA-C	8.07	121.24	111.40
1	B	53	VAL	N-CA-C	-7.76	105.15	112.83
1	C	53	VAL	N-CA-C	-7.38	105.53	112.83
1	B	136	LEU	N-CA-C	-6.62	103.25	112.45
1	A	53	VAL	N-CA-C	-6.43	106.25	112.29
1	C	282	ASP	CA-C-N	6.41	127.85	119.84
1	C	282	ASP	C-N-CA	6.41	127.85	119.84
1	C	273	VAL	N-CA-C	-6.28	99.33	108.87
1	A	216	GLN	N-CA-C	-6.15	104.48	112.23
1	A	82	LYS	N-CA-C	-6.07	104.57	111.07
1	A	277	THR	N-CA-C	-5.98	104.14	112.45
1	A	145	ILE	N-CA-C	5.88	116.09	110.74
1	B	282	ASP	CA-C-N	5.75	127.03	119.84
1	B	282	ASP	C-N-CA	5.75	127.03	119.84
1	B	123	ALA	CA-C-N	-5.70	113.91	119.90
1	B	123	ALA	C-N-CA	-5.70	113.91	119.90
1	A	258	MET	N-CA-C	-5.50	105.93	113.30
1	C	250	THR	CA-C-N	-5.48	112.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	THR	C-N-CA	-5.48	112.99	119.84
1	A	282	ASP	CA-C-N	5.45	126.65	119.84
1	A	282	ASP	C-N-CA	5.45	126.65	119.84
1	B	45	LYS	N-CA-C	-5.37	105.51	111.36
1	C	242	VAL	N-CA-C	5.34	115.54	107.75
1	A	133	HIS	N-CA-C	5.30	116.84	107.61
1	B	203	VAL	CB-CA-C	-5.28	105.10	112.02
1	A	273	VAL	CB-CA-C	-5.16	104.62	111.80
1	A	92	GLY	N-CA-C	-5.16	104.31	112.66
1	A	108	ILE	N-CA-C	5.08	115.22	108.11
1	C	268	GLY	N-CA-C	-5.03	107.34	115.08

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	2216	0	2254	79	0
1	B	2216	0	2254	87	1
1	C	2186	0	2224	95	0
2	A	10	0	0	1	0
2	B	50	0	0	0	1
2	C	5	0	0	0	0
All	All	6683	0	6732	256	1

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 19.

All (256) 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:C:35:MET:HE2	1:C:126:VAL:HA	1.42	0.98
1:B:197:TRP:HB3	1:B:201:GLY:HA3	1.55	0.87
1:C:51:ALA:HB3	1:C:107:ILE:HG22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:HG13	1:C:125:THR:HB	1.62	0.81
1:C:56:THR:HG22	1:C:138:GLN:HE22	1.46	0.80
1:C:186:PHE:HD2	1:C:187:ASP:N	1.79	0.79
1:A:246:GLU:O	1:A:248:LYS:N	2.15	0.79
1:C:198:GLY:O	1:C:200:GLY:N	2.16	0.78
1:B:186:PHE:HE2	1:B:245:SER:HB3	1.48	0.77
1:C:188:LYS:HG3	1:C:253:TYR:HE2	1.49	0.77
1:A:56:THR:HG22	1:A:138:GLN:HE22	1.50	0.76
1:A:184:ASP:HB2	1:A:225:TRP:CH2	2.21	0.76
1:B:213:GLN:HE21	1:B:215:GLU:HB2	1.51	0.75
1:A:136:LEU:HD13	1:A:156:LYS:HG3	1.70	0.73
1:C:115:ASP:HB3	1:C:118:LYS:HB2	1.70	0.73
1:C:208:PHE:HB3	1:C:210:LEU:HD13	1.70	0.72
1:A:194:GLY:HA3	1:A:221:ALA:HB3	1.71	0.71
1:B:246:GLU:HB2	1:B:272:LYS:HD2	1.71	0.71
1:B:78:SER:HB3	1:B:81:LEU:HB2	1.73	0.70
1:A:193:TYR:HA	1:A:225:TRP:HB3	1.73	0.69
1:A:276:GLY:HA2	1:A:279:TRP:CE2	2.27	0.69
1:C:253:TYR:HD1	1:C:256:THR:H	1.40	0.69
1:A:137:GLU:HG2	1:C:302:LYS:HG2	1.75	0.68
1:A:52:VAL:HG12	1:A:108:ILE:HB	1.74	0.67
1:B:107:ILE:HB	1:B:125:THR:HB	1.75	0.67
1:A:193:TYR:HA	1:A:225:TRP:CB	2.23	0.67
1:B:136:LEU:HD13	1:B:156:LYS:HG3	1.76	0.67
1:A:186:PHE:HA	1:A:247:GLY:CA	2.26	0.66
1:A:133:HIS:HB3	1:A:138:GLN:HB2	1.79	0.65
1:A:285:THR:O	1:A:289:MET:HG3	1.96	0.65
1:C:35:MET:HG2	1:C:126:VAL:HG23	1.77	0.65
1:A:193:TYR:CE2	1:A:195:ASP:HB3	2.31	0.65
1:A:193:TYR:HD1	1:A:225:TRP:CD2	2.16	0.65
1:C:240:TYR:HA	1:C:269:HIS:HB3	1.78	0.64
1:C:78:SER:HB3	1:C:81:LEU:HB2	1.79	0.64
1:B:26:ASN:OD1	1:B:26:ASN:N	2.31	0.64
1:B:180:VAL:HG21	1:B:210:LEU:HD13	1.80	0.64
1:C:281:ASN:H	1:C:281:ASN:ND2	1.94	0.64
1:C:44:PRO:HG2	1:C:105:ASP:HB3	1.80	0.63
1:C:294:LYS:O	1:C:298:ILE:HG13	1.98	0.63
1:B:142:LEU:HA	1:B:145:ILE:HD12	1.80	0.63
1:A:246:GLU:C	1:A:248:LYS:N	2.58	0.62
1:A:257:ASN:CG	1:A:258:MET:H	2.07	0.62
1:C:195:ASP:OD1	1:C:196:ASN:N	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LYS:HG2	1:B:253:TYR:HD2	1.65	0.61
1:B:214:PRO:HG3	1:C:217:GLN:HE21	1.64	0.61
1:B:253:TYR:HD1	1:B:256:THR:H	1.49	0.61
1:A:192:THR:O	1:A:225:TRP:HB2	2.01	0.61
1:C:78:SER:HB2	1:C:280:TYR:HE2	1.66	0.60
1:C:140:GLU:HA	1:C:152:VAL:HG11	1.83	0.60
1:B:134:LYS:O	1:B:138:GLN:HB3	2.02	0.60
1:B:50:ILE:HG12	1:B:106:LEU:HD23	1.82	0.60
1:C:133:HIS:HB3	1:C:138:GLN:HB2	1.83	0.60
1:A:286:LEU:HA	1:A:289:MET:HE2	1.85	0.59
1:C:78:SER:HB2	1:C:280:TYR:CE2	2.39	0.58
1:A:174:ILE:HG22	1:A:301:ALA:HB2	1.86	0.58
1:C:199:ARG:HB2	1:C:279:TRP:CD2	2.38	0.58
1:A:88:VAL:O	1:A:90:LYS:HG2	2.04	0.57
1:A:119:TYR:HB3	1:A:125:THR:HG21	1.86	0.57
1:A:221:ALA:HB1	1:A:223:ALA:O	2.04	0.57
1:B:53:VAL:HG13	1:B:91:ILE:HD12	1.86	0.57
1:C:244:THR:HG22	1:C:245:SER:H	1.68	0.57
1:B:281:ASN:OD1	1:B:281:ASN:N	2.25	0.57
1:C:77:GLN:HE22	1:C:278:TYR:HB2	1.69	0.57
1:B:53:VAL:HG23	1:B:108:ILE:O	2.05	0.56
1:B:199:ARG:O	1:B:202:GLU:HB2	2.04	0.56
1:A:174:ILE:HB	1:A:240:TYR:CE2	2.40	0.56
1:C:49:ARG:NH1	1:C:102:GLU:O	2.38	0.56
1:A:221:ALA:HA	1:A:222:LYS:C	2.30	0.56
1:A:202:GLU:OE1	1:A:202:GLU:N	2.33	0.56
1:B:35:MET:HE2	1:B:127:VAL:H	1.71	0.56
1:B:195:ASP:OD1	1:B:196:ASN:N	2.35	0.56
1:C:35:MET:HE3	1:C:41:VAL:HG21	1.88	0.55
1:A:193:TYR:HE2	1:A:195:ASP:HB3	1.71	0.55
1:B:37:ASP:CG	1:B:38:GLY:H	2.13	0.55
1:C:229:LYS:HB2	1:C:232:GLU:HG2	1.89	0.55
1:A:70:ALA:HB1	1:A:91:ILE:HD11	1.88	0.55
1:B:35:MET:CE	1:B:126:VAL:HA	2.37	0.55
1:C:199:ARG:H	1:C:199:ARG:HD2	1.72	0.55
1:A:166:ASP:O	1:A:170:ILE:HG13	2.07	0.54
1:C:199:ARG:HB2	1:C:279:TRP:CG	2.42	0.54
1:B:78:SER:O	1:B:80:VAL:N	2.40	0.54
1:B:78:SER:O	1:B:81:LEU:N	2.40	0.54
1:C:182:LEU:HD12	1:C:242:VAL:O	2.07	0.54
1:C:205:TYR:CD1	1:C:212:MET:HG2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:TRP:H	1:C:225:TRP:CD1	2.25	0.54
1:B:119:TYR:HB3	1:B:125:THR:HG21	1.90	0.54
1:C:244:THR:HG23	1:C:273:VAL:HB	1.89	0.54
1:C:112:THR:O	1:C:112:THR:OG1	2.24	0.53
1:C:104:PRO:HG2	1:C:123:ALA:HB2	1.90	0.53
1:B:77:GLN:HB3	1:B:278:TYR:HE1	1.73	0.53
1:B:62:LYS:O	1:B:62:LYS:HG3	2.07	0.53
1:C:250:THR:C	1:C:252:GLY:H	2.17	0.53
1:C:281:ASN:H	1:C:281:ASN:HD22	1.57	0.53
1:B:57:TYR:CZ	1:B:128:VAL:HG21	2.43	0.53
1:A:133:HIS:CE1	1:A:141:MET:HE3	2.44	0.52
1:B:49:ARG:HG2	1:B:69:VAL:HG11	1.90	0.52
1:B:52:VAL:CG2	1:B:71:VAL:HG23	2.39	0.52
1:C:188:LYS:HG3	1:C:253:TYR:CE2	2.39	0.52
1:A:166:ASP:OD2	1:A:290:ARG:HD2	2.10	0.52
1:C:186:PHE:C	1:C:186:PHE:CD2	2.86	0.52
1:A:186:PHE:HA	1:A:247:GLY:HA3	1.92	0.52
1:A:134:LYS:O	1:A:138:GLN:HB3	2.09	0.52
1:B:37:ASP:OD1	1:B:37:ASP:N	2.42	0.52
1:C:186:PHE:HD2	1:C:186:PHE:C	2.18	0.52
1:C:285:THR:O	1:C:289:MET:HG3	2.10	0.51
1:A:112:THR:O	1:A:112:THR:OG1	2.28	0.51
1:B:110:TYR:HB3	1:B:112:THR:HG23	1.91	0.51
1:A:78:SER:HB3	1:A:81:LEU:HB2	1.93	0.51
1:B:34:LYS:HG3	1:B:39:LYS:HG3	1.92	0.51
1:B:253:TYR:CG	1:B:257:ASN:HB2	2.45	0.51
1:A:230:GLN:HB3	1:A:258:MET:SD	2.51	0.51
1:B:135:TYR:CD2	1:B:202:GLU:HG2	2.45	0.51
1:A:180:VAL:HG21	1:A:210:LEU:HD23	1.93	0.51
1:C:109:VAL:HG23	1:C:127:VAL:HG12	1.94	0.50
1:A:244:THR:OG1	1:A:245:SER:N	2.44	0.50
1:C:56:THR:CG2	1:C:281:ASN:HD21	2.24	0.50
1:A:254:GLU:O	1:A:254:GLU:HG2	2.11	0.50
1:C:37:ASP:OD1	1:C:37:ASP:N	2.41	0.50
1:C:148:LYS:HB3	1:C:151:LYS:HG3	1.93	0.50
1:B:35:MET:HE2	1:B:126:VAL:HA	1.94	0.49
1:C:51:ALA:O	1:C:107:ILE:HA	2.12	0.49
1:C:135:TYR:CZ	1:C:136:LEU:HD22	2.46	0.49
1:A:35:MET:HG2	1:A:126:VAL:HG13	1.95	0.49
1:C:141:MET:HG3	1:C:142:LEU:N	2.28	0.49
1:A:37:ASP:CG	1:A:38:GLY:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD11	1:A:259:TRP:HZ3	1.77	0.49
1:B:159:TRP:CE2	1:B:163:THR:HG21	2.48	0.49
1:A:213:GLN:HB3	1:A:216:GLN:HB3	1.95	0.49
1:A:132:LYS:O	1:A:133:HIS:ND1	2.46	0.48
1:A:123:ALA:HB1	1:A:124:PRO:HD2	1.93	0.48
1:A:155:TRP:CZ2	1:A:283:PRO:HB3	2.48	0.48
1:B:80:VAL:HG21	1:B:285:THR:HG23	1.93	0.48
1:A:99:VAL:HG11	1:A:119:TYR:HE1	1.78	0.48
1:A:203:VAL:CG2	1:A:289:MET:HE3	2.43	0.48
1:A:242:VAL:HA	1:A:271:VAL:HG22	1.95	0.48
1:C:164:ALA:O	1:C:168:LYS:HG3	2.13	0.48
1:B:149:GLU:O	1:B:152:VAL:HG12	2.13	0.48
1:C:174:ILE:HG22	1:C:301:ALA:HB2	1.94	0.48
1:A:203:VAL:HG21	1:A:289:MET:HE3	1.95	0.48
1:B:135:TYR:CG	1:B:202:GLU:HG2	2.49	0.48
1:C:259:TRP:HB3	1:C:265:THR:HG21	1.96	0.48
1:B:33:TYR:N	1:B:41:VAL:O	2.44	0.47
1:B:186:PHE:CE2	1:B:249:PRO:HG2	2.49	0.47
1:B:243:SER:OG	1:B:272:LYS:HG3	2.13	0.47
1:C:262:LEU:HB2	1:C:265:THR:OG1	2.14	0.47
1:A:286:LEU:HD23	1:A:289:MET:HE2	1.96	0.47
1:B:214:PRO:HG3	1:C:217:GLN:NE2	2.29	0.47
1:B:140:GLU:OE2	1:B:156:LYS:NZ	2.44	0.47
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.75	0.47
1:C:180:VAL:HG21	1:C:210:LEU:HD23	1.96	0.47
1:B:186:PHE:CZ	1:B:249:PRO:HG2	2.50	0.47
1:A:37:ASP:OD1	1:A:37:ASP:N	2.47	0.47
1:B:71:VAL:HG11	1:B:85:PHE:HD2	1.79	0.47
1:B:198:GLY:HA2	1:B:279:TRP:CH2	2.50	0.47
1:A:102:GLU:N	1:A:102:GLU:OE2	2.47	0.47
1:A:170:ILE:O	1:A:174:ILE:HG12	2.15	0.47
1:A:193:TYR:HA	1:A:225:TRP:HB2	1.95	0.47
1:A:199:ARG:HA	1:A:278:TYR:O	2.15	0.46
1:B:170:ILE:O	1:B:174:ILE:HG12	2.15	0.46
1:C:35:MET:HE3	1:C:41:VAL:CG2	2.46	0.46
1:B:109:VAL:HG23	1:B:127:VAL:HG12	1.97	0.46
1:B:213:GLN:CG	1:B:216:GLN:HB2	2.46	0.46
1:C:174:ILE:HB	1:C:240:TYR:CZ	2.50	0.46
1:C:186:PHE:CE2	1:C:187:ASP:HB2	2.51	0.46
1:B:56:THR:HG22	1:B:138:GLN:HE22	1.80	0.46
1:C:169:GLU:HA	1:C:172:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LYS:HE2	1:C:236:TYR:CE2	2.51	0.46
1:B:34:LYS:HD2	1:B:39:LYS:HE3	1.98	0.45
1:A:218:LYS:NZ	2:A:401:SO4:O3	2.47	0.45
1:A:286:LEU:HD23	1:A:289:MET:CE	2.45	0.45
1:B:88:VAL:O	1:B:90:LYS:HD3	2.17	0.45
1:A:172:LYS:HD3	1:B:161:GLU:HA	1.98	0.45
1:C:156:LYS:HE3	1:C:160:GLU:OE2	2.16	0.45
1:C:242:VAL:HG22	1:C:271:VAL:HB	1.99	0.45
1:A:214:PRO:HA	1:A:217:GLN:HE21	1.82	0.45
1:A:246:GLU:HB2	1:A:248:LYS:HE3	1.98	0.45
1:B:188:LYS:HG2	1:B:253:TYR:CD2	2.49	0.45
1:B:197:TRP:CD1	1:B:205:TYR:HD2	2.34	0.45
1:C:110:TYR:HB3	1:C:112:THR:HG23	1.99	0.45
1:B:139:GLN:HG3	1:B:152:VAL:CG2	2.47	0.45
1:A:138:GLN:O	1:A:138:GLN:HG3	2.16	0.45
1:B:72:ASN:OD1	1:B:73:GLN:N	2.50	0.45
1:C:252:GLY:C	1:C:254:GLU:H	2.24	0.45
1:A:215:GLU:HG2	1:A:235:LYS:HG2	1.99	0.44
1:B:78:SER:C	1:B:80:VAL:N	2.74	0.44
1:A:259:TRP:CD1	1:A:259:TRP:O	2.70	0.44
1:B:71:VAL:HG21	1:B:85:PHE:CE2	2.53	0.44
1:B:159:TRP:O	1:B:163:THR:HG23	2.17	0.44
1:B:271:VAL:CG1	1:B:296:LYS:HB3	2.46	0.44
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.79	0.44
1:A:193:TYR:CE1	1:A:199:ARG:HG3	2.52	0.44
1:A:240:TYR:CD1	1:A:269:HIS:HB3	2.53	0.44
1:C:138:GLN:O	1:C:142:LEU:HD13	2.18	0.44
1:C:281:ASN:HD22	1:C:281:ASN:N	2.15	0.44
1:B:49:ARG:HB3	1:B:104:PRO:HA	1.99	0.44
1:C:166:ASP:OD2	1:C:290:ARG:HD2	2.18	0.44
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.39	0.44
1:C:231:GLU:C	1:C:233:ILE:H	2.26	0.44
1:B:123:ALA:HB1	1:B:124:PRO:HD2	1.99	0.44
1:C:144:LYS:HA	1:C:149:GLU:HG2	2.00	0.44
1:B:199:ARG:HD2	1:B:281:ASN:HB3	2.00	0.43
1:A:177:ASP:HB3	1:B:212:MET:HE2	2.00	0.43
1:C:49:ARG:O	1:C:105:ASP:N	2.47	0.43
1:C:190:LEU:HD22	1:C:233:ILE:HD11	2.00	0.43
1:B:52:VAL:HG23	1:B:71:VAL:HG23	1.99	0.43
1:B:77:GLN:HB3	1:B:278:TYR:CE1	2.52	0.43
1:A:253:TYR:C	1:A:255:SER:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:HD3	1:B:103:LYS:O	2.18	0.43
1:C:197:TRP:HB2	1:C:198:GLY:H	1.50	0.43
1:B:262:LEU:HB2	1:B:265:THR:OG1	2.19	0.43
1:A:53:VAL:CG1	1:A:109:VAL:HG12	2.48	0.43
1:A:144:LYS:HE3	1:A:144:LYS:HB2	1.77	0.43
1:C:50:ILE:CG2	1:C:108:ILE:HD11	2.49	0.42
1:C:75:VAL:HG21	1:C:85:PHE:HD2	1.84	0.42
1:C:208:PHE:HB3	1:C:210:LEU:CD1	2.45	0.42
1:C:190:LEU:CD2	1:C:233:ILE:HD11	2.49	0.42
1:B:84:LYS:C	1:B:85:PHE:HD1	2.28	0.42
1:B:246:GLU:CB	1:B:272:LYS:HD2	2.47	0.42
1:B:190:LEU:HA	1:B:190:LEU:HD12	1.82	0.42
1:B:242:VAL:HG22	1:B:271:VAL:HG23	2.00	0.42
1:C:186:PHE:CD2	1:C:187:ASP:HB2	2.55	0.42
1:C:155:TRP:CZ2	1:C:283:PRO:HB3	2.55	0.42
1:A:205:TYR:CE1	1:A:212:MET:HG2	2.55	0.42
1:C:117:LYS:HA	1:C:120:GLN:OE1	2.20	0.42
1:A:156:LYS:HZ3	1:A:156:LYS:HG2	1.74	0.42
1:B:186:PHE:HE2	1:B:245:SER:CB	2.23	0.41
1:B:270:ILE:H	1:B:270:ILE:HG13	1.55	0.41
1:C:193:TYR:CZ	1:C:216:GLN:HG2	2.54	0.41
1:B:50:ILE:O	1:B:68:ILE:HA	2.19	0.41
1:C:108:ILE:HG23	1:C:126:VAL:HG13	2.00	0.41
1:C:136:LEU:HD12	1:C:136:LEU:HA	1.82	0.41
1:A:114:LYS:HG2	1:A:115:ASP:OD1	2.20	0.41
1:A:203:VAL:HA	1:A:207:ALA:HB3	2.02	0.41
1:C:36:ASP:OD2	1:C:129:ASP:N	2.48	0.41
1:C:135:TYR:CE2	1:C:136:LEU:HD22	2.55	0.41
1:A:273:VAL:HB	1:A:278:TYR:CE2	2.55	0.41
1:B:213:GLN:HG2	1:B:236:TYR:O	2.20	0.41
1:C:113:ASP:O	1:C:116:ILE:HG23	2.20	0.41
1:B:64:LEU:HD21	1:B:152:VAL:HG23	2.02	0.41
1:B:76:ASP:C	1:B:82:LYS:HG2	2.45	0.41
1:C:282:ASP:CG	1:C:285:THR:HG1	2.29	0.41
1:C:76:ASP:OD2	1:C:90:LYS:HE3	2.20	0.41
1:C:199:ARG:HG3	1:C:281:ASN:HB3	2.02	0.41
1:C:293:LEU:HA	1:C:293:LEU:HD23	1.86	0.41
1:A:80:VAL:HG12	1:A:81:LEU:HD12	2.03	0.41
1:C:35:MET:HG3	1:C:41:VAL:HG21	2.02	0.40
1:C:123:ALA:HB1	1:C:124:PRO:HD2	2.03	0.40
1:A:186:PHE:HA	1:A:247:GLY:HA2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LYS:CD	1:B:39:LYS:HG3	2.52	0.40
1:B:75:VAL:C	1:B:77:GLN:H	2.28	0.40
1:B:199:ARG:O	1:B:203:VAL:HG23	2.21	0.40
1:A:212:MET:HE2	1:A:216:GLN:HG2	2.02	0.40
1:C:235:LYS:HB3	1:C:236:TYR:HD2	1.87	0.40
1:C:113:ASP:HB3	1:C:116:ILE:CG2	2.51	0.40
1:C:136:LEU:HG	1:C:156:LYS:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:NH2	2:B:410:SO4:O4[15_454]	2.14	0.06

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	276/280 (99%)	239 (87%)	32 (12%)	5 (2%)	6	34
1	B	276/280 (99%)	239 (87%)	29 (10%)	8 (3%)	3	26
1	C	272/280 (97%)	231 (85%)	32 (12%)	9 (3%)	3	23
All	All	824/840 (98%)	709 (86%)	93 (11%)	22 (3%)	4	27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	TRP
1	C	199	ARG
1	C	250	THR
1	A	247	GLY
1	A	257	ASN

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Mol	Chain	Res	Type
1	B	224	GLY
1	B	247	GLY
1	B	252	GLY
1	C	247	GLY
1	C	252	GLY
1	A	254	GLU
1	B	79	LYS
1	B	279	TRP
1	A	250	THR
1	C	134	LYS
1	C	200	GLY
1	C	224	GLY
1	A	58	ALA
1	B	245	SER
1	B	276	GLY
1	C	276	GLY
1	C	283	PRO

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	235/236 (100%)	209 (89%)	26 (11%)	6	25
1	B	235/236 (100%)	198 (84%)	37 (16%)	2	15
1	C	232/236 (98%)	199 (86%)	33 (14%)	3	18
All	All	702/708 (99%)	606 (86%)	96 (14%)	3	19

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	40	THR
1	A	91	ILE
1	A	98	LYS
1	A	112	THR

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Mol	Chain	Res	Type
1	A	121	LYS
1	A	125	THR
1	A	128	VAL
1	A	135	TYR
1	A	138	GLN
1	A	144	LYS
1	A	151	LYS
1	A	156	LYS
1	A	190	LEU
1	A	199	ARG
1	A	210	LEU
1	A	225	TRP
1	A	233	ILE
1	A	243	SER
1	A	244	THR
1	A	254	GLU
1	A	256	THR
1	A	258	MET
1	A	285	THR
1	A	287	ASP
1	A	295	GLU
1	B	26	ASN
1	B	29	GLU
1	B	40	THR
1	B	41	VAL
1	B	53	VAL
1	B	68	ILE
1	B	79	LYS
1	B	80	VAL
1	B	82	LYS
1	B	96	VAL
1	B	112	THR
1	B	125	THR
1	B	126	VAL
1	B	135	TYR
1	B	138	GLN
1	B	140	GLU
1	B	141	MET
1	B	144	LYS
1	B	150	ASP
1	B	152	VAL
1	B	181	SER

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Mol	Chain	Res	Type
1	B	188	LYS
1	B	202	GLU
1	B	232	GLU
1	B	234	GLU
1	B	248	LYS
1	B	256	THR
1	B	261	ASN
1	B	265	THR
1	B	270	ILE
1	B	271	VAL
1	B	272	LYS
1	B	277	THR
1	B	278	TYR
1	B	285	THR
1	B	299	LYS
1	B	302	LYS
1	C	40	THR
1	C	41	VAL
1	C	68	ILE
1	C	77	GLN
1	C	81	LEU
1	C	88	VAL
1	C	91	ILE
1	C	96	VAL
1	C	108	ILE
1	C	112	THR
1	C	125	THR
1	C	126	VAL
1	C	128	VAL
1	C	134	LYS
1	C	135	TYR
1	C	136	LEU
1	C	138	GLN
1	C	141	MET
1	C	152	VAL
1	C	157	LYS
1	C	162	THR
1	C	168	LYS
1	C	186	PHE
1	C	202	GLU
1	C	233	ILE
1	C	243	SER

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Mol	Chain	Res	Type
1	C	244	THR
1	C	258	MET
1	C	265	THR
1	C	277	THR
1	C	279	TRP
1	C	281	ASN
1	C	285	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	74	GLN
1	A	138	GLN
1	A	269	HIS
1	B	74	GLN
1	B	138	GLN
1	B	213	GLN
1	B	217	GLN
1	C	77	GLN
1	C	138	GLN
1	C	213	GLN
1	C	217	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	B	404	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	401	-	4,4,4	0.25	0	6,6,6	0.22	0
2	SO4	B	406	-	4,4,4	0.33	0	6,6,6	0.23	0
2	SO4	B	407	-	4,4,4	0.31	0	6,6,6	0.26	0
2	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	B	409	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	B	408	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.26	0
2	SO4	B	403	-	4,4,4	0.32	0	6,6,6	0.46	0
2	SO4	B	410	-	4,4,4	0.24	0	6,6,6	0.60	0
2	SO4	B	402	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.16	0
2	SO4	B	405	-	4,4,4	0.26	0	6,6,6	0.10	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	SO4	0	1
2	A	401	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	278/280 (99%)	-0.12	2 (0%) 84 63	77, 135, 213, 331	0
1	B	278/280 (99%)	-0.06	7 (2%) 58 35	72, 118, 201, 282	0
1	C	274/280 (97%)	0.09	7 (2%) 57 33	82, 157, 239, 352	0
All	All	830/840 (98%)	-0.03	16 (1%) 66 41	72, 133, 223, 352	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	250	THR	5.1
1	B	186	PHE	4.0
1	B	197	TRP	3.5
1	A	248	LYS	3.3
1	B	250	THR	2.6
1	C	280	TYR	2.6
1	B	187	ASP	2.6
1	C	249	PRO	2.6
1	C	278	TYR	2.5
1	B	246	GLU	2.4
1	B	249	PRO	2.3
1	C	130	TYR	2.2
1	B	279	TRP	2.2
1	A	216	GLN	2.2
1	C	121	LYS	2.2
1	C	87	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	401	5/5	0.58	0.13	236,236,236,236	0
2	SO4	B	409	5/5	0.68	0.16	211,211,211,211	0
2	SO4	B	405	5/5	0.71	0.18	204,204,204,204	0
2	SO4	B	407	5/5	0.75	0.11	183,183,183,183	0
2	SO4	B	408	5/5	0.77	0.18	204,204,204,204	0
2	SO4	B	406	5/5	0.81	0.11	154,154,154,154	0
2	SO4	B	401	5/5	0.85	0.16	156,156,156,156	0
2	SO4	B	402	5/5	0.88	0.17	192,192,192,192	0
2	SO4	B	404	5/5	0.90	0.11	197,197,197,197	0
2	SO4	A	402	5/5	0.91	0.14	185,185,185,185	0
2	SO4	B	403	5/5	0.92	0.13	115,115,115,115	0
2	SO4	C	401	5/5	0.93	0.11	129,129,129,129	0
2	SO4	B	410	5/5	0.94	0.08	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.