



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 PM GMT

PDB ID : 4GPH
Title : Structure of HmuO, heme oxygenase from *Corynebacterium diphtheriae*, in complex with the putative reaction intermediates between Fe³⁺-biliverdin and biliverdin (data set IV)
Authors : Unno, M.; Ikeda-Saito, M.
Deposited on : 2012-08-21
Resolution : 1.70 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 ⓘ symbol.

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

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

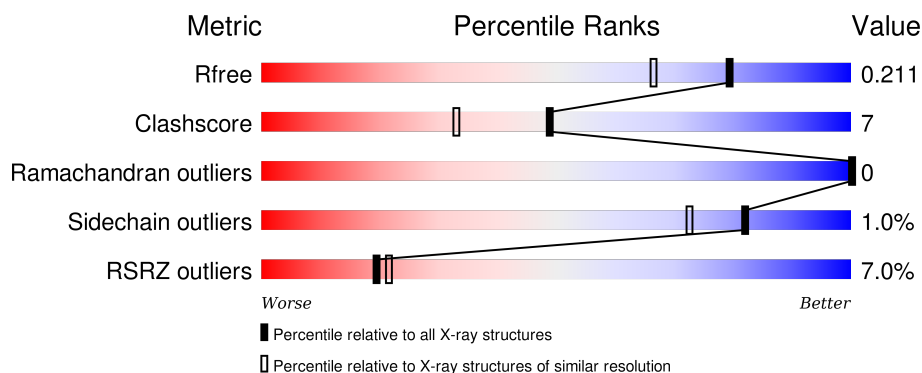
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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 $\leq 5\%$. 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	215	<div> <div>11%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
1	B	215	<div> <div>3%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
1	C	215	<div> <div>7%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>

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	BLA	A	3002[A]	-	-	-	X
3	BLA	A	3002[B]	-	-	-	X
3	BLA	B	601	-	-	-	X
4	SO4	A	3003	-	-	-	X
4	SO4	B	603	-	-	-	X
4	SO4	C	904	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5733 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.

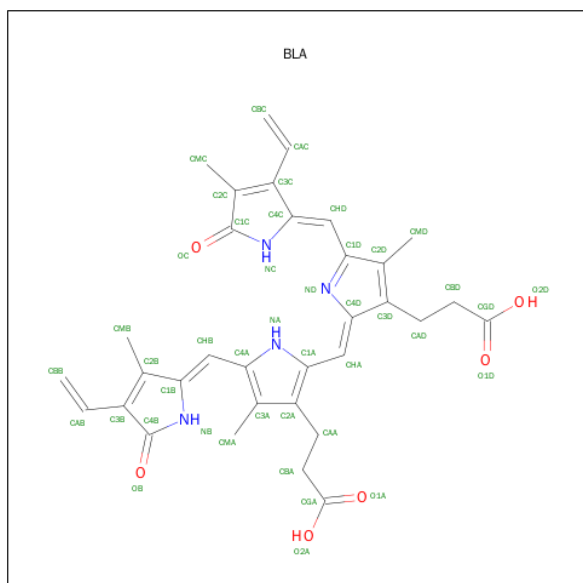
- Molecule 1 is a protein called Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	2	0
			1659	1044	296	316	3			
1	B	209	Total	C	N	O	S	0	3	0
			1657	1045	295	314	3			
1	C	212	Total	C	N	O	S	0	3	0
			1675	1053	299	320	3			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

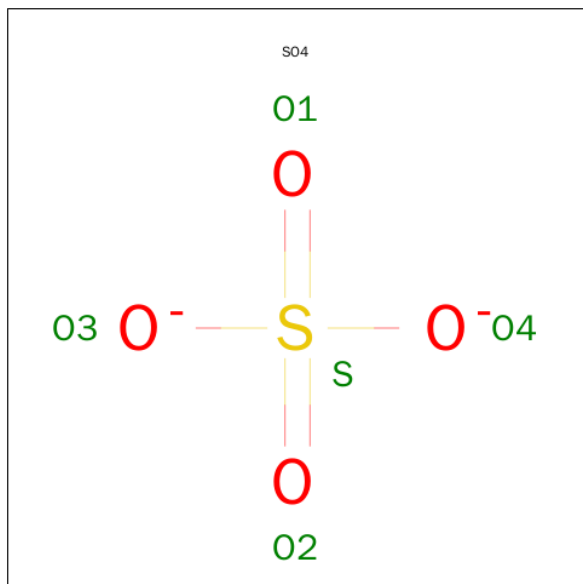
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	1
			1	1		
2	C	1	Total	Fe	0	1
			1	1		

- Molecule 3 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C₃₃H₃₄N₄O₆).



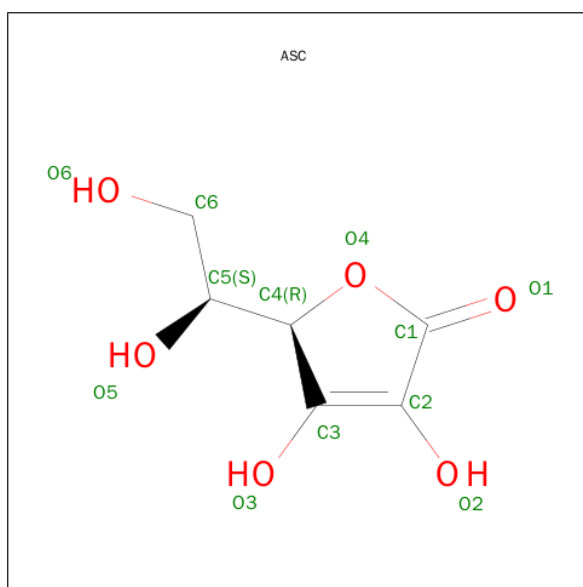
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			86	66	8	12		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	1
			86	66	8	12		

- 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	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ASCORBIC ACID (three-letter code: ASC) (formula: C₆H₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			12	6	6		

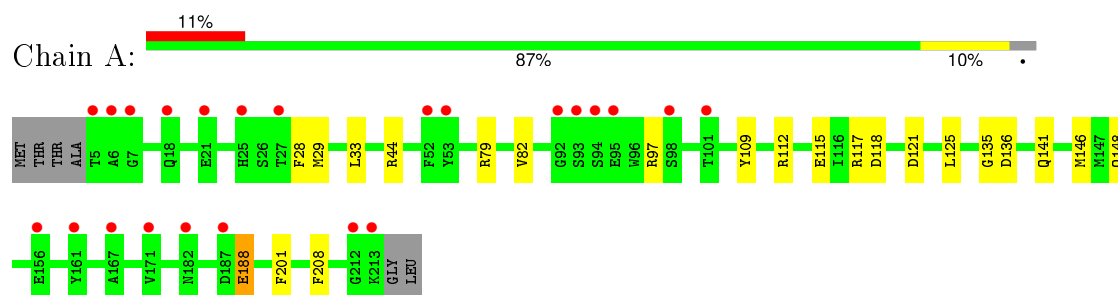
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	91	Total	O	0	1
			91	91		
6	B	195	Total	O	0	0
			195	195		
6	C	187	Total	O	0	0
			187	187		

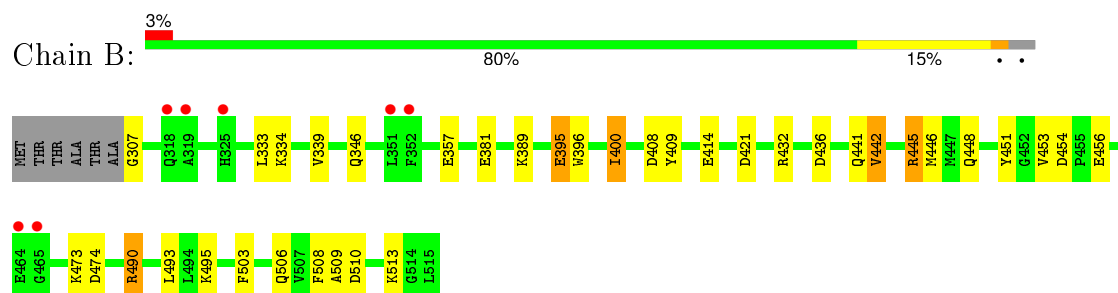
3 Residue-property plots [i](#)

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.

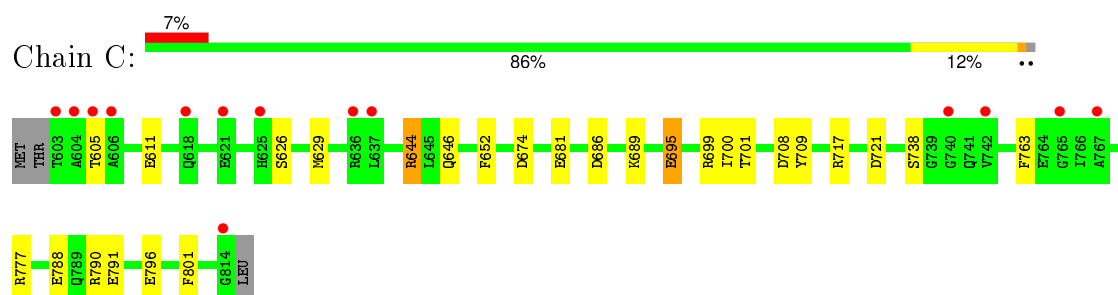
- Molecule 1: Heme oxygenase



- Molecule 1: Heme oxygenase



- Molecule 1: Heme oxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.06 Å 62.97 Å 107.73 Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.78 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-1.70) 98.6 (30.78-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.165 , 0.205 0.172 , 0.211	Depositor DCC
R_{free} test set	7806 reflections (11.23%)	DCC
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 77300 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5733	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ASC, BLA, FE, 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	1.16	3/1702 (0.2%)	1.04	6/2301 (0.3%)
1	B	1.46	9/1705 (0.5%)	1.33	17/2304 (0.7%)
1	C	1.48	9/1722 (0.5%)	1.34	16/2329 (0.7%)
All	All	1.38	21/5129 (0.4%)	1.24	39/6934 (0.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	681	GLU	CD-OE1	10.92	1.37	1.25
1	B	432	ARG	CZ-NH2	8.80	1.44	1.33
1	B	381	GLU	CD-OE1	8.67	1.35	1.25
1	B	409	TYR	CD1-CE1	8.34	1.51	1.39
1	C	681	GLU	CG-CD	7.40	1.63	1.51
1	C	791	GLU	CG-CD	7.25	1.62	1.51
1	B	395	GLU	CB-CG	6.42	1.64	1.52
1	B	381	GLU	CG-CD	6.08	1.61	1.51
1	B	503	PHE	CD1-CE1	5.55	1.50	1.39
1	B	432	ARG	CG-CD	5.53	1.65	1.51
1	A	79	ARG	CG-CD	5.50	1.65	1.51
1	C	796	GLU	CD-OE1	5.46	1.31	1.25
1	B	414	GLU	CB-CG	5.38	1.62	1.52
1	C	763	PHE	CE1-CZ	5.29	1.47	1.37
1	A	188	GLU	CG-CD	5.28	1.59	1.51
1	A	201	PHE	CD1-CE1	5.26	1.49	1.39
1	C	709	TYR	CG-CD2	5.23	1.46	1.39
1	C	695	GLU	CG-CD	5.12	1.59	1.51
1	B	396	TRP	CG-CD1	5.10	1.43	1.36
1	C	699	ARG	CB-CG	-5.04	1.39	1.52
1	C	788	GLU	CB-CG	5.02	1.61	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	699	ARG	NE-CZ-NH1	-10.92	114.84	120.30
1	B	490	ARG	NE-CZ-NH2	-9.23	115.68	120.30
1	B	445	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	B	454	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	445	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	C	629	MET	CG-SD-CE	-8.21	87.06	100.20
1	C	777	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	B	490	ARG	CG-CD-NE	-8.07	94.84	111.80
1	C	721	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	B	421	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	C	708[A]	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	C	708[B]	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	A	44	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	C	652	PHE	CB-CG-CD2	-7.18	115.78	120.80
1	C	708[A]	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	708[B]	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	109	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	B	409	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	C	717	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	B	408	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	C	644	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	490	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	510	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	436	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	97	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	381	GLU	CG-CD-OE1	5.90	130.10	118.30
1	C	796	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	C	686	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	117	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	674	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	432	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	C	709	TYR	CB-CG-CD1	5.58	124.35	121.00
1	C	709	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	121	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	136	ASP	CB-CG-OD1	-5.47	113.37	118.30
1	B	400	ILE	CB-CG1-CD1	-5.36	98.88	113.90
1	B	381	GLU	CG-CD-OE2	-5.35	107.59	118.30
1	B	357	GLU	CA-CB-CG	-5.29	101.76	113.40
1	B	510	ASP	CB-CG-OD2	-5.23	113.59	118.30

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	1659	0	1595	18	1
1	B	1657	0	1607	27	0
1	C	1675	0	1606	11	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	86	0	61	18	0
3	B	43	0	32	8	0
3	C	86	0	62	5	0
4	A	5	0	0	0	0
4	B	25	0	0	1	0
4	C	10	0	0	0	0
5	C	12	0	5	0	0
6	A	91	0	0	2	0
6	B	195	0	0	8	1
6	C	187	0	0	3	0
All	All	5733	0	4968	74	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 7.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ILE:CG1	1:B:400:ILE:CD1	1.74	1.61
3:A:3002[A]:BLA:OC	3:A:3002[A]:BLA:C4B	1.97	1.13
1:A:33:LEU:HD11	3:A:3002[B]:BLA:HMC1	1.25	1.10
3:A:3002[A]:BLA:HMB1	3:A:3002[A]:BLA:CBB	1.79	1.10
3:A:3002[A]:BLA:CMB	3:A:3002[A]:BLA:HBB1	1.78	1.08
3:A:3002[A]:BLA:HMB1	3:A:3002[A]:BLA:HBB1	1.05	1.03
1:A:118:ASP:OD2	1:B:445:ARG:NH2	1.95	1.00
1:B:333:LEU:HD11	3:B:601:BLA:HMC1	1.45	0.98
1:B:400:ILE:CD1	1:B:400:ILE:CB	2.44	0.95
3:A:3002[A]:BLA:OC	3:A:3002[A]:BLA:OB	1.87	0.93
3:A:3002[A]:BLA:C1C	3:A:3002[A]:BLA:OB	2.19	0.90
1:C:695:GLU:HG2	6:C:1146:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:902[A]:BLA:OB	3:C:902[A]:BLA:HBB1	1.83	0.77
1:B:389:LYS:HD2	1:B:456:GLU:O	1.87	0.75
3:A:3002[B]:BLA:HMB1	3:A:3002[B]:BLA:HBB1	1.70	0.73
1:A:208:PHE:CE2	3:A:3002[B]:BLA:HBB2	2.24	0.71
3:A:3002[A]:BLA:C1C	3:A:3002[A]:BLA:C4B	2.64	0.71
1:B:509:ALA:O	1:B:513:LYS:HG3	1.93	0.69
1:B:400:ILE:CD1	1:B:400:ILE:HB	2.22	0.69
3:A:3002[A]:BLA:CMB	3:A:3002[A]:BLA:CBB	2.55	0.69
3:B:601:BLA:HHD	3:B:601:BLA:CBC	2.23	0.68
1:B:441:GLN:O	1:B:445:ARG:HG3	1.94	0.68
1:A:208:PHE:HE2	3:A:3002[B]:BLA:HBB2	1.60	0.65
1:A:82:VAL:HG23	6:A:3167:HOH:O	1.96	0.65
1:A:28:PHE:CD2	1:A:29:MET:HE2	2.34	0.62
3:B:601:BLA:HHD	3:B:601:BLA:HBC1	1.82	0.62
1:B:442:VAL:HG13	1:B:446:MET:HE3	1.81	0.61
1:B:490:ARG:HD3	6:B:873:HOH:O	2.01	0.61
1:A:28:PHE:HD2	1:A:29:MET:HE2	1.65	0.60
1:B:333:LEU:CD1	3:B:601:BLA:HMC1	2.27	0.59
1:A:33:LEU:HD11	3:A:3002[A]:BLA:HMC1	1.83	0.58
1:C:611:GLU:OE1	1:C:790[A]:ARG:NH2	2.32	0.57
3:C:902[A]:BLA:OB	3:C:902[A]:BLA:CBB	2.51	0.57
1:A:28:PHE:HD2	1:A:29:MET:CE	2.18	0.57
1:C:644:ARG:HD3	6:C:1144:HOH:O	2.06	0.56
1:B:334:LYS:HE3	6:B:845:HOH:O	2.06	0.55
1:B:495:LYS:HG3	6:B:813:HOH:O	2.07	0.54
1:A:112[A]:ARG:NH2	1:A:115:GLU:OE1	2.39	0.54
1:B:473:LYS:NZ	4:B:605:SO4:O1	2.34	0.54
1:C:801:PHE:CE2	3:C:902[B]:BLA:HAC	2.43	0.53
1:C:738:SER:HB3	3:C:902[B]:BLA:HBA1	1.91	0.53
3:A:3002[A]:BLA:OC	3:A:3002[A]:BLA:C3B	2.55	0.53
1:B:448:GLN:HG2	1:B:453:VAL:O	2.10	0.52
1:B:346:GLN:HE21	1:B:346:GLN:HA	1.75	0.52
1:B:441:GLN:HG3	6:B:798:HOH:O	2.09	0.52
1:A:146:MET:CE	1:A:146:MET:HA	2.40	0.51
1:B:506[A]:GLN:NE2	6:B:853:HOH:O	2.43	0.51
1:B:307:GLY:N	6:B:895:HOH:O	2.44	0.50
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.27	0.50
1:B:490:ARG:NE	6:B:848:HOH:O	2.39	0.48
3:B:601:BLA:CHD	3:B:601:BLA:HBC1	2.44	0.48
1:C:738:SER:HB3	3:C:902[A]:BLA:HBA1	1.95	0.47
1:A:28:PHE:CD2	1:A:29:MET:CE	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:LYS:HE2	6:C:1156:HOH:O	2.14	0.46
1:A:135:GLY:HA2	3:A:3002[A]:BLA:C4A	2.46	0.45
1:B:474[A]:ASP:OD1	6:B:862:HOH:O	2.21	0.45
1:B:339[B]:VAL:HG13	1:B:451:TYR:HB3	1.97	0.45
1:A:125:LEU:HD13	1:A:125:LEU:C	2.37	0.45
1:B:339[A]:VAL:HG22	1:B:451:TYR:HB3	2.00	0.44
1:C:646:GLN:HA	1:C:646:GLN:NE2	2.33	0.43
1:A:148:GLN:NE2	6:A:3146:HOH:O	2.52	0.43
3:A:3002[B]:BLA:HMB1	3:A:3002[B]:BLA:CBB	2.45	0.42
1:C:611:GLU:OE1	1:C:790[A]:ARG:NE	2.52	0.42
3:B:601:BLA:HHA	3:B:601:BLA:HAA2	1.70	0.42
1:C:646:GLN:HA	1:C:646:GLN:HE21	1.85	0.41
1:A:188:GLU:H	1:A:188:GLU:CD	2.23	0.41
1:B:400:ILE:HG21	1:B:400:ILE:HD13	2.03	0.41
1:C:700:ILE:HD13	1:C:700:ILE:HG21	1.83	0.41
1:B:508:PHE:CE2	3:B:601:BLA:HBB2	2.55	0.41
3:B:601:BLA:HB	3:B:601:BLA:HA	1.69	0.41
1:A:29:MET:HA	1:A:29:MET:HE2	2.03	0.40
1:B:493:LEU:HD23	1:B:493:LEU:C	2.41	0.40
1:A:208:PHE:HE2	3:A:3002[B]:BLA:CBB	2.31	0.40
3:A:3002[B]:BLA:HHA	3:A:3002[B]:BLA:HAA2	1.85	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:A:141:GLN:NE2	6:B:881:HOH:O[2_645]	1.88	0.32

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	209/215 (97%)	205 (98%)	4 (2%)	0	100	100
1	B	210/215 (98%)	206 (98%)	4 (2%)	0	100	100
1	C	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
All	All	632/645 (98%)	618 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	169/175 (97%)	169 (100%)	0	100	100
1	B	170/175 (97%)	168 (99%)	2 (1%)	78	65
1	C	170/175 (97%)	167 (98%)	3 (2%)	66	49
All	All	509/525 (97%)	504 (99%)	5 (1%)	82	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	395	GLU
1	B	442	VAL
1	C	605	THR
1	C	626	SER
1	C	701	THR

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	78	ASN
1	A	148	GLN
1	A	182	ASN
1	B	346	GLN
1	B	378	ASN

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Mol	Chain	Res	Type
1	C	625	HIS
1	C	646	GLN
1	C	678	ASN
1	C	741	GLN
1	C	782	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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	BLA	A	3002[A]	2	35,46,46	1.99	6 (17%)	43,67,67	2.60	16 (37%)
3	BLA	A	3002[B]	-	35,46,46	1.93	5 (14%)	43,67,67	2.84	18 (41%)
4	SO4	A	3003	-	4,4,4	0.19	0	6,6,6	0.24	0
3	BLA	B	601	-	35,46,46	1.91	5 (14%)	43,67,67	3.40	23 (53%)
4	SO4	B	602	-	4,4,4	0.17	0	6,6,6	0.51	0
4	SO4	B	603	-	4,4,4	0.81	0	6,6,6	0.69	0
4	SO4	B	604	-	4,4,4	0.38	0	6,6,6	0.72	0
4	SO4	B	605	-	4,4,4	0.48	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	606	-	4,4,4	0.13	0	6,6,6	0.33	0
3	BLA	C	902[A]	2	35,46,46	2.01	4 (11%)	43,67,67	2.84	20 (46%)
3	BLA	C	902[B]	-	35,46,46	2.18	6 (17%)	43,67,67	3.04	17 (39%)
5	ASC	C	903	2	12,12,12	3.00	5 (41%)	17,17,17	3.15	9 (52%)
4	SO4	C	904	-	4,4,4	1.05	1 (25%)	6,6,6	0.63	0
4	SO4	C	905	-	4,4,4	0.68	0	6,6,6	0.73	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	BLA	A	3002[A]	2	-	0/22/74/74	0/4/4/4
3	BLA	A	3002[B]	-	-	0/22/74/74	0/4/4/4
4	SO4	A	3003	-	-	0/0/0/0	0/0/0/0
3	BLA	B	601	-	-	0/22/74/74	0/4/4/4
4	SO4	B	602	-	-	0/0/0/0	0/0/0/0
4	SO4	B	603	-	-	0/0/0/0	0/0/0/0
4	SO4	B	604	-	-	0/0/0/0	0/0/0/0
4	SO4	B	605	-	-	0/0/0/0	0/0/0/0
4	SO4	B	606	-	-	0/0/0/0	0/0/0/0
3	BLA	C	902[A]	2	-	0/22/74/74	0/4/4/4
3	BLA	C	902[B]	-	-	0/22/74/74	0/4/4/4
5	ASC	C	903	2	-	0/6/22/22	0/1/1/1
4	SO4	C	904	-	-	0/0/0/0	0/0/0/0
4	SO4	C	905	-	-	0/0/0/0	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	903	ASC	O6-C6	-6.46	1.14	1.42
5	C	903	ASC	C5-C4	-2.20	1.50	1.53
3	C	902[B]	BLA	C1C-C2C	-2.15	1.41	1.47
4	C	904	SO4	O2-S	2.00	1.54	1.47
3	C	902[B]	BLA	C1B-C2B	2.11	1.49	1.45
3	A	3002[A]	BLA	CAC-C3C	2.11	1.54	1.47
3	B	601	BLA	CAC-C3C	2.26	1.54	1.47
3	A	3002[B]	BLA	CAC-C3C	2.42	1.55	1.47
3	A	3002[A]	BLA	CHB-C1B	2.66	1.40	1.34
5	C	903	ASC	O4-C4	2.78	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002[B]	BLA	CHB-C1B	2.92	1.40	1.34
3	B	601	BLA	CHB-C1B	3.05	1.41	1.34
3	C	902[A]	BLA	CHB-C1B	3.65	1.42	1.34
3	A	3002[A]	BLA	CBD-CAD	3.70	1.71	1.52
5	C	903	ASC	C4-C3	3.72	1.55	1.50
3	C	902[B]	BLA	CHB-C1B	4.09	1.43	1.34
3	C	902[B]	BLA	CBC-CAC	4.64	1.53	1.30
3	A	3002[B]	BLA	CBB-CAB	5.04	1.55	1.30
3	C	902[B]	BLA	CBB-CAB	5.12	1.55	1.30
3	C	902[A]	BLA	CBB-CAB	5.12	1.55	1.30
3	A	3002[A]	BLA	CBB-CAB	5.14	1.55	1.30
3	B	601	BLA	CBB-CAB	5.18	1.56	1.30
3	C	902[A]	BLA	CBC-CAC	5.31	1.56	1.30
3	A	3002[A]	BLA	CBC-CAC	5.31	1.56	1.30
3	A	3002[B]	BLA	CBC-CAC	5.32	1.56	1.30
3	B	601	BLA	CBC-CAC	5.42	1.57	1.30
5	C	903	ASC	O4-C1	5.93	1.45	1.35
3	A	3002[B]	BLA	CHA-C4D	6.64	1.41	1.35
3	B	601	BLA	CHA-C4D	6.69	1.41	1.35
3	A	3002[A]	BLA	CHA-C4D	6.84	1.41	1.35
3	C	902[A]	BLA	CHA-C4D	7.41	1.41	1.35
3	C	902[B]	BLA	CHA-C4D	8.31	1.42	1.35

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	BLA	CAA-C2A-C1A	-12.62	113.31	127.01
3	A	3002[B]	BLA	CAA-C2A-C1A	-9.14	117.08	127.01
3	A	3002[A]	BLA	CHA-C4D-ND	-6.85	116.42	128.67
3	C	902[A]	BLA	CHD-C4C-NC	-6.35	112.41	126.16
3	C	902[A]	BLA	CAA-C2A-C1A	-6.25	120.22	127.01
3	B	601	BLA	CHA-C4D-ND	-6.15	117.67	128.67
3	A	3002[B]	BLA	CHA-C4D-ND	-6.01	117.92	128.67
3	C	902[B]	BLA	CHD-C4C-NC	-5.86	113.47	126.16
3	C	902[B]	BLA	CAA-C2A-C1A	-5.86	120.65	127.01
3	B	601	BLA	CHD-C1D-ND	-5.85	113.77	124.91
3	C	902[B]	BLA	C4C-NC-C1C	-5.78	102.27	110.73
3	B	601	BLA	C4C-NC-C1C	-5.64	102.48	110.73
5	C	903	ASC	O1-C1-C2	-5.59	121.88	129.44
3	C	902[A]	BLA	C4C-NC-C1C	-5.59	102.55	110.73
3	B	601	BLA	CHD-C4C-NC	-5.24	114.82	126.16
3	A	3002[A]	BLA	C1B-NB-C4B	-5.20	103.13	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903	ASC	O5-C5-C4	-4.87	102.12	110.35
3	C	902[A]	BLA	CAD-C3D-C4D	-4.81	116.47	125.06
3	C	902[B]	BLA	CBC-CAC-C3C	-4.72	103.05	127.01
3	A	3002[A]	BLA	C4C-NC-C1C	-4.61	103.99	110.73
3	A	3002[B]	BLA	CHD-C4C-NC	-4.55	116.31	126.16
3	A	3002[B]	BLA	CHD-C1D-ND	-4.53	116.29	124.91
3	C	902[B]	BLA	CAD-C3D-C4D	-4.47	117.08	125.06
3	A	3002[B]	BLA	C4C-NC-C1C	-4.46	104.20	110.73
3	A	3002[A]	BLA	CHD-C4C-NC	-4.41	116.61	126.16
3	C	902[A]	BLA	CHA-C4D-ND	-4.14	121.27	128.67
3	B	601	BLA	CAD-C3D-C4D	-4.10	117.73	125.06
3	A	3002[A]	BLA	CBB-CAB-C3B	-4.09	106.25	127.01
3	A	3002[A]	BLA	CHD-C1D-ND	-4.07	117.16	124.91
3	A	3002[B]	BLA	C1B-NB-C4B	-3.79	105.18	110.73
3	C	902[B]	BLA	CHA-C4D-ND	-3.73	121.99	128.67
3	A	3002[A]	BLA	CAD-C3D-C2D	-3.64	121.66	128.01
3	C	902[B]	BLA	C1D-C2D-C3D	-3.62	102.17	106.50
3	B	601	BLA	C1B-NB-C4B	-3.31	105.89	110.73
3	B	601	BLA	CHB-C1B-NB	-3.30	118.64	130.87
3	A	3002[A]	BLA	CBC-CAC-C3C	-3.22	110.66	127.01
3	C	902[A]	BLA	CBB-CAB-C3B	-3.18	110.86	127.01
3	A	3002[A]	BLA	CHB-C1B-C2B	-3.15	120.42	126.94
5	C	903	ASC	O3-C3-C2	-3.12	122.81	132.38
3	C	902[A]	BLA	C1D-C2D-C3D	-3.03	102.87	106.50
5	C	903	ASC	C4-O4-C1	-2.98	106.21	109.29
3	C	902[A]	BLA	CAC-C3C-C4C	-2.95	116.80	124.80
3	B	601	BLA	CAD-CBD-CGD	-2.82	107.58	112.75
3	B	601	BLA	C1D-C2D-C3D	-2.80	103.15	106.50
3	C	902[A]	BLA	OC-C1C-C2C	-2.75	114.97	128.97
3	B	601	BLA	CBB-CAB-C3B	-2.73	113.13	127.01
3	A	3002[B]	BLA	CAD-C3D-C2D	-2.70	123.29	128.01
3	B	601	BLA	CBC-CAC-C3C	-2.69	113.35	127.01
3	C	902[B]	BLA	CAC-C3C-C4C	-2.69	117.51	124.80
3	C	902[A]	BLA	CHD-C1D-ND	-2.64	119.88	124.91
3	B	601	BLA	CMD-C2D-C1D	-2.49	121.01	125.06
3	C	902[A]	BLA	OB-C4B-C3B	-2.42	123.77	129.82
3	A	3002[B]	BLA	CBC-CAC-C3C	-2.31	115.31	127.01
3	A	3002[B]	BLA	C1D-C2D-C3D	-2.21	103.86	106.50
3	C	902[B]	BLA	C3D-C4D-ND	-2.17	106.49	109.86
3	A	3002[B]	BLA	CBB-CAB-C3B	-2.13	116.18	127.01
3	A	3002[A]	BLA	CAA-C2A-C1A	-2.10	124.72	127.01
3	B	601	BLA	CHA-C4D-C3D	2.11	130.50	125.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902[A]	BLA	OC-C1C-NC	2.11	130.75	125.14
3	C	902[B]	BLA	CMC-C2C-C3C	2.17	134.30	128.48
3	C	902[A]	BLA	CMC-C2C-C3C	2.22	134.44	128.48
3	A	3002[B]	BLA	CAA-C2A-C3A	2.30	135.57	129.00
3	A	3002[A]	BLA	CAB-C3B-C4B	2.31	131.25	123.49
3	C	902[B]	BLA	CHA-C4D-C3D	2.34	131.03	125.55
5	C	903	ASC	O3-C3-C4	2.35	124.79	118.06
3	A	3002[B]	BLA	CHD-C1D-C2D	2.46	130.88	124.88
3	A	3002[A]	BLA	CHD-C1D-C2D	2.48	130.94	124.88
3	A	3002[B]	BLA	CBA-CAA-C2A	2.59	117.17	112.53
3	B	601	BLA	CMB-C2B-C1B	2.60	127.67	124.20
3	B	601	BLA	CMA-C3A-C2A	2.66	130.80	125.24
3	C	902[A]	BLA	C2C-C1C-NC	2.71	114.06	106.27
3	A	3002[B]	BLA	CMC-C2C-C3C	2.74	135.83	128.48
3	A	3002[B]	BLA	CHA-C4D-C3D	2.76	132.03	125.55
3	B	601	BLA	CHD-C1D-C2D	2.86	131.86	124.88
3	B	601	BLA	CMC-C2C-C3C	2.93	136.34	128.48
3	C	902[A]	BLA	C4D-C3D-C2D	2.93	110.09	106.81
3	B	601	BLA	C2B-C1B-NB	2.95	111.27	107.00
3	B	601	BLA	CAA-C2A-C3A	3.02	137.63	129.00
3	C	902[A]	BLA	CAD-C3D-C2D	3.09	133.41	128.01
3	A	3002[A]	BLA	CAD-C3D-C4D	3.11	130.62	125.06
3	C	902[B]	BLA	C2C-C1C-NC	3.26	115.65	106.27
3	A	3002[B]	BLA	C2B-C1B-NB	3.30	111.78	107.00
5	C	903	ASC	C6-C5-C4	3.31	117.54	111.95
3	B	601	BLA	CMD-C2D-C3D	3.41	135.84	125.94
3	A	3002[A]	BLA	CHA-C4D-C3D	3.43	133.59	125.55
3	A	3002[B]	BLA	CMA-C3A-C2A	3.53	132.62	125.24
3	B	601	BLA	CAD-C3D-C2D	3.70	134.47	128.01
3	C	902[A]	BLA	CMA-C3A-C2A	3.77	133.13	125.24
3	C	902[B]	BLA	CMA-C3A-C2A	3.78	133.15	125.24
5	C	903	ASC	O6-C6-C5	3.97	119.72	111.10
3	A	3002[A]	BLA	C2B-C1B-NB	4.15	113.02	107.00
3	C	902[A]	BLA	CAD-CBD-CGD	4.37	120.76	112.75
3	C	902[B]	BLA	C4D-C3D-C2D	4.48	111.82	106.81
3	C	902[A]	BLA	C4C-CHD-C1D	4.49	139.68	128.06
5	C	903	ASC	O4-C1-O1	4.58	126.68	121.29
3	C	902[B]	BLA	C4C-CHD-C1D	4.70	140.21	128.06
3	A	3002[A]	BLA	C4C-CHD-C1D	4.99	140.97	128.06
3	B	601	BLA	C4C-CHD-C1D	5.00	141.00	128.06
5	C	903	ASC	C5-C4-C3	5.41	121.79	114.14
3	C	902[A]	BLA	CBA-CAA-C2A	5.75	122.84	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3002[B]	BLA	C4C-CHD-C1D	6.23	144.17	128.06
3	C	902[B]	BLA	CAD-CBD-CGD	6.89	125.38	112.75
3	C	902[B]	BLA	CBA-CAA-C2A	7.60	126.16	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002[A]	BLA	11	0
3	A	3002[B]	BLA	7	0
3	B	601	BLA	8	0
4	B	605	SO4	1	0
3	C	902[A]	BLA	3	0
3	C	902[B]	BLA	2	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	209/215 (97%)	0.46	23 (11%) 7 8	21, 33, 51, 62	0
1	B	209/215 (97%)	0.20	7 (3%) 50 54	14, 24, 42, 51	0
1	C	212/215 (98%)	0.34	14 (6%) 22 23	15, 23, 44, 72	0
All	All	630/645 (97%)	0.33	44 (6%) 19 21	14, 27, 47, 72	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	814	GLY	7.3
1	A	6	ALA	6.7
1	C	605	THR	6.7
1	C	604	ALA	6.3
1	C	606	ALA	4.8
1	C	765	GLY	4.0
1	A	5	THR	3.6
1	B	319	ALA	3.6
1	B	325	HIS	3.5
1	C	603	THR	3.4
1	C	618	GLN	3.4
1	C	767	ALA	3.3
1	A	94	SER	3.3
1	A	93	SER	3.2
1	C	625	HIS	3.2
1	A	213	LYS	3.0
1	C	636	ARG	3.0
1	A	25	HIS	2.9
1	A	18	GLN	2.8
1	A	101	THR	2.7
1	A	98	SER	2.7
1	C	621	GLU	2.7
1	A	52	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLY	2.6
1	A	92	GLY	2.5
1	A	156	GLU	2.5
1	A	21	GLU	2.4
1	A	7	GLY	2.4
1	B	465	GLY	2.4
1	B	351	LEU	2.4
1	A	167	ALA	2.4
1	A	27	THR	2.4
1	C	740	GLY	2.3
1	A	95	GLU	2.3
1	A	171	VAL	2.3
1	C	637	LEU	2.2
1	C	742	VAL	2.2
1	B	352	PHE	2.2
1	A	161	TYR	2.2
1	B	318	GLN	2.0
1	A	53	TYR	2.0
1	B	464	GLU	2.0
1	A	187	ASP	2.0
1	A	182	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	B	603	5/5	0.84	0.16	3.43	22,28,37,37	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	3003	5/5	0.95	0.35	3.22	69,71,72,73	0
4	SO4	C	904	5/5	0.84	0.18	3.20	25,27,31,34	5
3	BLA	A	3002[A]	43/43	0.88	0.19	2.93	17,46,99,111	43
3	BLA	A	3002[B]	43/43	0.88	0.19	2.89	29,62,105,120	43
3	BLA	B	601	43/43	0.73	0.24	2.56	54,85,130,159	0
4	SO4	B	605	5/5	0.97	0.17	1.83	44,46,47,48	5
4	SO4	B	602	5/5	0.91	0.22	1.20	82,82,83,83	0
3	BLA	C	902[A]	43/43	0.91	0.15	0.94	25,30,41,48	43
3	BLA	C	902[B]	43/43	0.91	0.15	0.94	26,34,47,52	43
4	SO4	B	604	5/5	0.97	0.10	-0.30	27,30,31,35	5
4	SO4	B	606	5/5	0.86	0.13	-0.44	100,101,102,103	0
2	FE	C	901[A]	1/1	0.92	0.22	-	54,54,54,54	1
4	SO4	C	905	5/5	0.97	0.10	-	27,27,28,31	5
2	FE	A	3001[A]	1/1	0.95	0.10	-	49,49,49,49	1
5	ASC	C	903	12/12	0.91	0.14	-	29,39,51,54	0

6.5 Other polymers

There are no such residues in this entry.