



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:49 am BST

PDB ID : 3S0H
Title : The crystal structure of the periplasmic domain of Helicobacter pylori MotB (residues 90-256).
Authors : Roujeinikova, A.R.
Deposited on : 2011-05-13
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

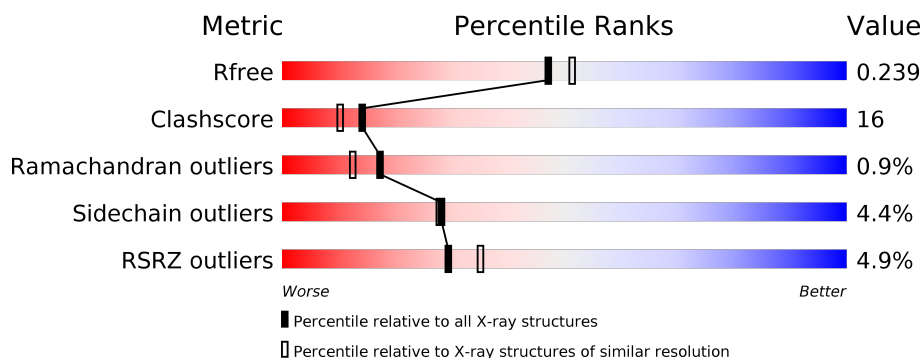
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	173	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>6%</div> </div> </div>
1	B	173	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>24%</div> <div>8%</div> </div> </div>
1	C	173	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• • •</div> </div> </div>
1	D	173	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>23%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6059 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 Motility protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	9	0
			1383	864	249	266	4			
1	B	160	Total	C	N	O	S	0	9	0
			1356	848	245	259	4			
1	C	169	Total	C	N	O	S	0	3	0
			1371	860	244	263	4			
1	D	159	Total	C	N	O	S	0	3	0
			1290	812	227	247	4			

There are 24 discrepancies between the modelled and reference sequences:

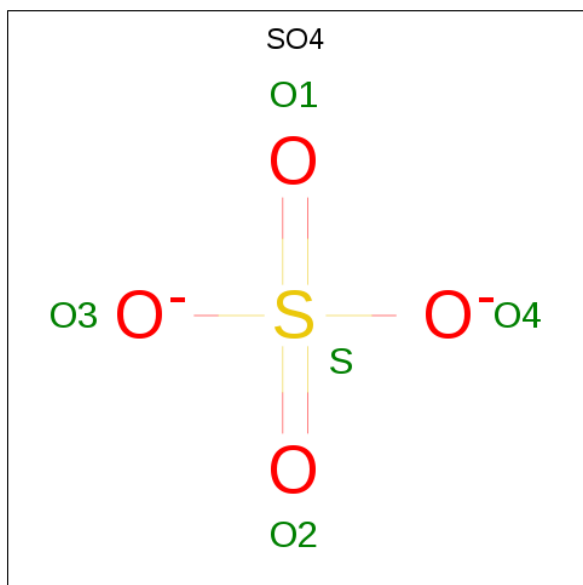
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	GLY	-	EXPRESSION TAG	UNP P56427
A	85	ILE	-	EXPRESSION TAG	UNP P56427
A	86	ASP	-	EXPRESSION TAG	UNP P56427
A	87	PRO	-	EXPRESSION TAG	UNP P56427
A	88	PHE	-	EXPRESSION TAG	UNP P56427
A	89	THR	-	EXPRESSION TAG	UNP P56427
B	84	GLY	-	EXPRESSION TAG	UNP P56427
B	85	ILE	-	EXPRESSION TAG	UNP P56427
B	86	ASP	-	EXPRESSION TAG	UNP P56427
B	87	PRO	-	EXPRESSION TAG	UNP P56427
B	88	PHE	-	EXPRESSION TAG	UNP P56427
B	89	THR	-	EXPRESSION TAG	UNP P56427
C	84	GLY	-	EXPRESSION TAG	UNP P56427
C	85	ILE	-	EXPRESSION TAG	UNP P56427
C	86	ASP	-	EXPRESSION TAG	UNP P56427
C	87	PRO	-	EXPRESSION TAG	UNP P56427
C	88	PHE	-	EXPRESSION TAG	UNP P56427
C	89	THR	-	EXPRESSION TAG	UNP P56427
D	84	GLY	-	EXPRESSION TAG	UNP P56427
D	85	ILE	-	EXPRESSION TAG	UNP P56427
D	86	ASP	-	EXPRESSION TAG	UNP P56427

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	87	PRO	-	EXPRESSION TAG	UNP P56427
D	88	PHE	-	EXPRESSION TAG	UNP P56427
D	89	THR	-	EXPRESSION TAG	UNP P56427

- Molecule 2 is SULFATE ION (three-letter code: 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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

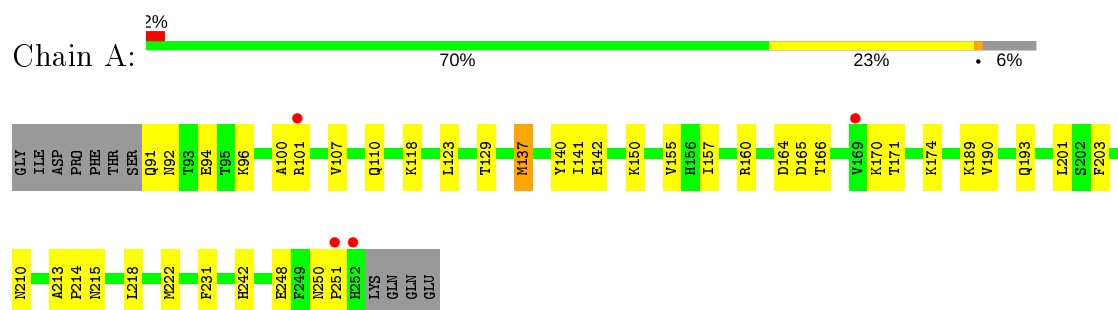
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total 156	O 156	0	0
3	B	162	Total 162	O 162	0	0
3	C	158	Total 158	O 158	0	0
3	D	138	Total 138	O 138	0	0

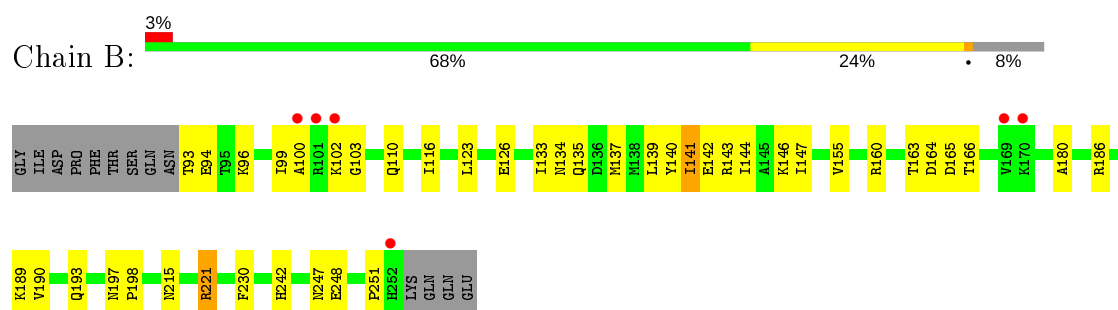
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

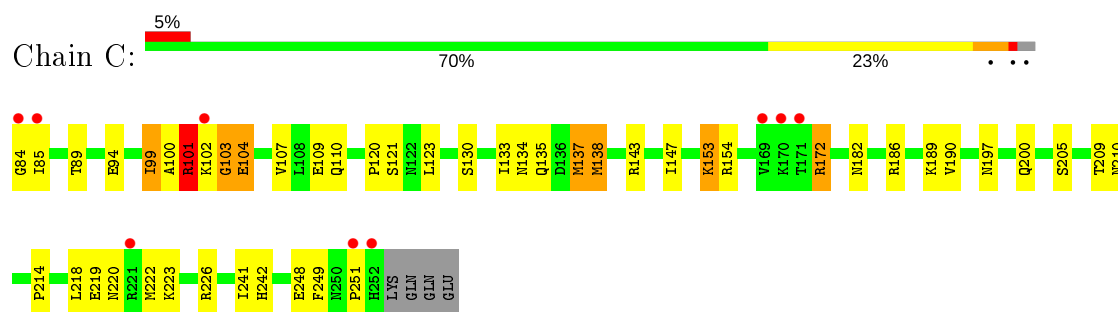
• Molecule 1: Motility protein B



• Molecule 1: Motility protein B

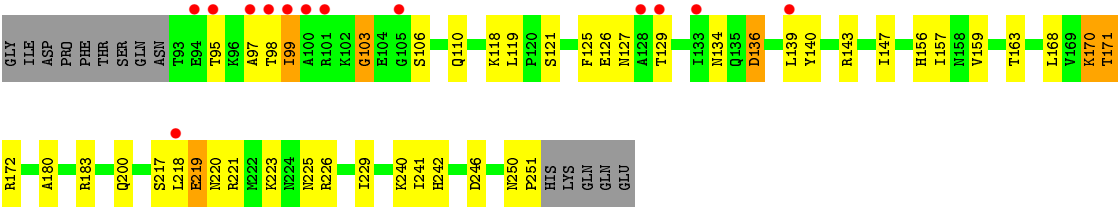


• Molecule 1: Motility protein B



• Molecule 1: Motility protein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	72.97 Å 72.97 Å 127.18 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.10) 97.5 (29.15-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.181 , 0.236 0.182 , 0.239	Depositor DCC
R_{free} test set	1903 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.219 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6059	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 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.63	0/1405	0.71	0/1897
1	B	0.71	0/1378	0.73	1/1861 (0.1%)
1	C	0.66	0/1395	0.73	0/1885
1	D	0.64	0/1311	0.73	1/1771 (0.1%)
All	All	0.66	0/5489	0.73	2/7414 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	119	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	141	ILE	CG1-CB-CG2	-5.05	100.28	111.40

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	1383	0	1376	44	0
1	B	1356	0	1355	49	0
1	C	1371	0	1370	57	0
1	D	1290	0	1301	43	0
2	A	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	0	0	0
2	C	15	0	0	1	0
2	D	5	0	0	0	0
3	A	156	0	0	8	0
3	B	162	0	0	5	0
3	C	158	0	0	5	0
3	D	138	0	0	3	0
All	All	6059	0	5402	170	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 16.

All (170) 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:248:GLU:HG2	1:D:147:ILE:HD11	1.18	1.14
1:B:221:ARG:HG2	1:B:221:ARG:HH11	1.02	1.11
1:C:137:MET:HE3	1:C:190:VAL:HG21	1.33	1.05
1:A:248:GLU:HG2	1:D:147:ILE:CD1	1.85	1.04
1:C:137:MET:CE	1:C:190:VAL:HG21	1.88	1.03
1:B:147[B]:ILE:HG21	1:C:248:GLU:HG2	1.40	1.03
1:A:248:GLU:CG	1:D:147:ILE:HD11	2.00	0.91
1:B:147[A]:ILE:HD12	1:C:248:GLU:HG2	1.52	0.90
1:B:221:ARG:HG2	1:B:221:ARG:NH1	1.80	0.88
1:B:147[B]:ILE:CG2	1:C:248:GLU:HG2	2.03	0.88
1:C:197:ASN:HD22	1:C:200:GLN:HE21	1.20	0.87
1:D:99:ILE:HG21	1:D:143:ARG:HG3	1.57	0.86
1:A:137:MET:SD	1:A:141[A]:ILE:HD12	2.16	0.85
1:C:133:ILE:CG2	1:C:137:MET:HG2	2.09	0.83
1:B:147[A]:ILE:HG13	1:C:249:PHE:CZ	2.14	0.82
1:B:221:ARG:CG	1:B:221:ARG:HH11	1.92	0.79
1:C:137:MET:HG3	1:C:138:MET:N	1.96	0.79
1:D:126:GLU:OE1	3:D:518:HOH:O	2.01	0.77
1:A:164:ASP:HB2	1:A:215:ASN:HD21	1.52	0.75
1:C:133:ILE:HG22	1:C:134:ASN:O	1.86	0.75
1:A:251:PRO:HD3	1:D:97:ALA:HA	1.69	0.74
1:D:97:ALA:HB3	1:D:106:SER:O	1.88	0.74
1:C:133:ILE:HG23	1:C:137:MET:HG2	1.70	0.73
1:B:141:ILE:HG21	1:B:190:VAL:HG12	1.69	0.73
1:B:160[B]:ARG:NH2	3:B:369:HOH:O	2.21	0.72
1:B:137:MET:SD	1:B:140:TYR:HE2	2.13	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:THR:OG1	1:C:210:ASN:ND2	2.25	0.70
1:D:168:LEU:HB3	1:D:171:THR:HG21	1.74	0.69
1:A:137:MET:SD	1:A:141[A]:ILE:CD1	2.81	0.68
1:C:133:ILE:HD11	1:C:186:ARG:HG2	1.75	0.68
1:C:102:LYS:O	1:C:104:GLU:N	2.27	0.68
1:D:129:THR:HG21	1:D:170:LYS:HE2	1.75	0.68
1:C:133:ILE:HG21	1:C:137:MET:HG2	1.74	0.67
1:B:110:GLN:HB2	1:C:242:HIS:CE1	2.30	0.67
1:C:133:ILE:HG23	1:C:137:MET:CB	2.26	0.66
1:A:137:MET:CE	1:A:141[A]:ILE:HD11	2.26	0.65
1:D:98:THR:HG22	1:D:99:ILE:N	2.12	0.65
1:B:143:ARG:O	1:B:147[A]:ILE:HG12	1.96	0.65
1:C:101:ARG:HG3	1:C:101:ARG:HH21	1.62	0.64
1:B:133:ILE:HG22	1:B:134[B]:ASN:O	1.98	0.64
1:A:137:MET:CE	1:A:141[A]:ILE:CD1	2.76	0.64
1:C:133:ILE:HG23	1:C:137:MET:CG	2.29	0.62
1:C:100:ALA:C	1:C:102:LYS:H	2.03	0.61
1:B:164:ASP:OD2	1:B:221:ARG:HD2	2.01	0.61
1:B:147[A]:ILE:CD1	1:C:248:GLU:HG2	2.28	0.61
1:B:102:LYS:O	1:B:140:TYR:HE1	1.84	0.61
1:B:189:LYS:O	1:B:193:GLN:HG3	2.01	0.60
1:A:92[B]:ASN:C	1:A:92[B]:ASN:OD1	2.39	0.60
1:B:133:ILE:HD11	1:B:186:ARG:HG3	1.83	0.59
1:C:84:GLY:O	1:C:85:ILE:HG13	2.03	0.59
1:C:133:ILE:HG23	1:C:137:MET:HB3	1.85	0.59
1:C:102:LYS:O	1:C:103:GLY:C	2.41	0.59
1:B:215:ASN:ND2	3:B:836:HOH:O	2.33	0.58
1:C:218:LEU:HB2	3:C:548:HOH:O	2.04	0.57
1:D:200:GLN:NE2	3:D:433:HOH:O	2.36	0.57
1:C:89:THR:HG21	3:C:810:HOH:O	2.04	0.57
1:B:100:ALA:HB2	1:B:143:ARG:HG3	1.86	0.57
1:C:137:MET:HE1	1:C:190:VAL:HG21	1.84	0.57
1:D:99:ILE:CG2	1:D:143:ARG:HG3	2.32	0.57
1:C:154:ARG:HG3	2:C:7:SO4:O1	2.04	0.57
1:A:137:MET:HE1	1:A:141[A]:ILE:CD1	2.34	0.57
1:D:168:LEU:HB3	1:D:171:THR:CG2	2.34	0.57
1:B:99:ILE:H	1:B:103:GLY:HA3	1.69	0.56
1:B:144:ILE:O	1:B:147[B]:ILE:HG13	2.05	0.56
1:C:94:GLU:HB2	1:C:107:VAL:CG2	2.35	0.56
1:B:221:ARG:CG	1:B:221:ARG:NH1	2.59	0.55
1:B:102:LYS:O	1:B:140:TYR:CE1	2.60	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:HIS:CE1	1:C:110:GLN:HB2	2.42	0.54
1:C:120:PRO:HD2	1:C:123[A]:LEU:CD1	2.38	0.54
1:A:96:LYS:HD3	1:A:107:VAL:HG12	1.90	0.53
1:C:137:MET:CE	1:C:190:VAL:CG2	2.77	0.53
1:D:157:ILE:N	1:D:157:ILE:HD12	2.23	0.53
1:C:84:GLY:C	1:C:85:ILE:HG13	2.28	0.53
1:B:248:GLU:HG3	1:C:147:ILE:HG23	1.91	0.52
1:C:101:ARG:NH2	1:C:101:ARG:HG3	2.19	0.52
1:D:139:LEU:O	1:D:143:ARG:HG2	2.09	0.52
1:A:110:GLN:HB2	1:D:242:HIS:CE1	2.45	0.52
1:B:133:ILE:HG22	1:B:134[A]:ASN:O	2.10	0.52
1:A:164:ASP:HB2	1:A:215:ASN:ND2	2.23	0.51
1:A:218:LEU:O	1:A:222:MET:HG2	2.10	0.51
1:C:121:SER:HB3	1:C:222:MET:HE1	1.92	0.51
1:A:174:LYS:HB2	3:A:540:HOH:O	2.09	0.51
1:B:147[A]:ILE:HD12	1:C:248:GLU:CG	2.34	0.51
1:A:94:GLU:OE2	1:A:118:LYS:NZ	2.44	0.50
1:D:99:ILE:HB	1:D:140:TYR:CD1	2.47	0.50
1:C:100:ALA:O	1:C:102:LYS:N	2.45	0.50
1:D:143:ARG:HD3	3:D:799:HOH:O	2.11	0.50
1:C:153:LYS:HG3	3:C:878:HOH:O	2.11	0.50
1:C:133:ILE:HD11	1:C:186:ARG:CG	2.42	0.49
1:A:248:GLU:OE2	1:D:99:ILE:HD11	2.12	0.49
1:B:94[B]:GLU:N	1:B:94[B]:GLU:OE1	2.43	0.49
1:B:123:LEU:O	1:B:137:MET:HB3	2.13	0.48
1:B:147[A]:ILE:HG13	1:C:249:PHE:HZ	1.72	0.48
1:B:147[B]:ILE:HG12	1:C:249:PHE:HZ	1.78	0.48
1:D:98:THR:CG2	1:D:99:ILE:N	2.76	0.48
1:A:101[B]:ARG:HB3	1:A:101[B]:ARG:HH11	1.78	0.48
1:C:220:ASN:O	1:C:223:LYS:HB2	2.13	0.48
1:A:142:GLU:OE2	3:A:398:HOH:O	2.20	0.48
1:A:92[B]:ASN:O	1:A:92[B]:ASN:OD1	2.31	0.47
1:A:123:LEU:HD22	1:A:140:TYR:CZ	2.50	0.47
1:D:139:LEU:HD12	1:D:139:LEU:O	2.15	0.47
1:A:91:GLN:HG3	1:A:92[B]:ASN:N	2.29	0.47
1:A:157[A]:ILE:HB	1:A:201:LEU:HD23	1.97	0.46
1:B:134[B]:ASN:HD22	1:B:137:MET:HG3	1.80	0.46
1:B:147[B]:ILE:HG12	1:C:249:PHE:CZ	2.50	0.46
1:A:157[A]:ILE:HD12	1:A:231:PHE:CD1	2.50	0.46
1:D:98:THR:HA	1:D:103:GLY:O	2.16	0.46
1:A:101[C]:ARG:HB2	3:A:500:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ARG:HA	1:C:101:ARG:HD2	1.55	0.46
1:B:142:GLU:O	1:B:146:LYS:HG3	2.16	0.46
1:B:93:THR:N	3:B:568:HOH:O	2.49	0.46
1:C:133:ILE:CG2	1:C:137:MET:HB3	2.45	0.46
1:D:156:HIS:C	1:D:157:ILE:HD12	2.37	0.46
1:D:218:LEU:HD12	1:D:221:ARG:HE	1.81	0.46
1:B:155[B]:VAL:HG22	1:C:241:ILE:HD11	1.98	0.45
1:B:93:THR:HG23	1:D:240:LYS:HG2	1.99	0.45
1:A:189:LYS:HE3	3:A:336:HOH:O	2.16	0.45
1:A:150:LYS:NZ	3:A:627:HOH:O	2.45	0.44
1:D:159:VAL:HG13	1:D:229[B]:ILE:CD1	2.46	0.44
1:A:129:THR:HG21	1:A:170:LYS:HE3	1.99	0.44
1:B:165:ASP:O	1:B:166:THR:C	2.55	0.44
3:A:870:HOH:O	1:D:240:LYS:HD2	2.16	0.44
1:D:99:ILE:HA	1:D:99:ILE:HD13	1.69	0.44
1:A:210:ASN:ND2	3:A:508:HOH:O	2.50	0.44
1:D:163:THR:HG23	1:D:180:ALA:HB2	1.99	0.44
1:A:101[B]:ARG:HB3	1:A:101[B]:ARG:NH1	2.33	0.44
1:A:190:VAL:HA	1:A:193:GLN:HE21	1.83	0.44
1:D:98:THR:HG22	1:D:99:ILE:H	1.80	0.43
1:B:135[A]:GLN:C	1:B:137:MET:H	2.21	0.43
1:B:247[B]:ASN:OD1	1:B:247[B]:ASN:C	2.56	0.43
1:C:172:ARG:HD2	1:C:172:ARG:H	1.82	0.43
1:D:250:ASN:HA	1:D:251:PRO:HD2	1.80	0.43
1:D:246:ASP:O	1:D:250:ASN:HB3	2.18	0.43
1:C:94:GLU:HB3	1:C:109:GLU:HB2	2.00	0.43
1:C:121:SER:HB3	1:C:222:MET:CE	2.49	0.43
1:D:125:PHE:CZ	1:D:183:ARG:HG2	2.54	0.43
1:D:106:SER:HB2	1:D:118:LYS:O	2.18	0.43
1:D:159:VAL:HG22	1:D:229[B]:ILE:HD12	2.00	0.43
1:A:155:VAL:HG22	1:D:241:ILE:HD11	2.01	0.43
1:C:214:PRO:O	1:C:220:ASN:HB3	2.19	0.43
1:D:217:SER:O	1:D:221:ARG:N	2.45	0.42
1:C:100:ALA:C	1:C:102:LYS:N	2.70	0.42
1:D:99:ILE:HB	1:D:140:TYR:CE1	2.55	0.42
1:A:203:PHE:CE2	1:C:205:SER:HB3	2.55	0.42
1:B:96:LYS:HE2	3:B:795:HOH:O	2.19	0.42
1:A:101[A]:ARG:NH2	3:A:694:HOH:O	2.53	0.42
1:B:126:GLU:OE2	1:B:134[A]:ASN:HA	2.19	0.42
1:C:130:SER:HB3	3:C:390:HOH:O	2.19	0.42
1:C:143:ARG:O	1:C:147:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165[B]:ASP:O	1:A:166:THR:C	2.58	0.42
1:B:197:ASN:HA	1:B:198:PRO:HD3	1.92	0.42
1:A:129:THR:HB	1:A:171:THR:HG21	2.02	0.41
1:B:163[B]:THR:HG23	1:B:180:ALA:HB2	2.01	0.41
1:D:217:SER:HB3	1:D:220:ASN:H	1.84	0.41
1:D:121:SER:HB2	1:D:225:ASN:O	2.20	0.41
1:A:164:ASP:OD1	1:A:164:ASP:C	2.59	0.41
1:A:242:HIS:CE1	1:D:110:GLN:HB2	2.55	0.41
1:B:133:ILE:HD13	3:B:378:HOH:O	2.20	0.41
1:C:220:ASN:ND2	3:C:498:HOH:O	2.52	0.41
1:A:164:ASP:CG	1:A:166:THR:HG1	2.23	0.41
1:C:133:ILE:CG2	1:C:137:MET:CG	2.87	0.41
1:D:134:ASN:OD1	1:D:136:ASP:HB2	2.21	0.41
1:B:100:ALA:H	1:B:143:ARG:CZ	2.33	0.41
1:B:116:ILE:HG12	1:B:230:PHE:HD1	1.87	0.40
1:A:213:ALA:HB1	1:A:214:PRO:HD2	2.03	0.40
1:B:163[A]:THR:HG23	1:B:180:ALA:HB2	2.02	0.40
1:D:219:GLU:O	1:D:223:LYS:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	170/173 (98%)	160 (94%)	10 (6%)	0	100	100
1	B	167/173 (96%)	159 (95%)	7 (4%)	1 (1%)	25	21
1	C	170/173 (98%)	162 (95%)	4 (2%)	4 (2%)	6	2
1	D	160/173 (92%)	150 (94%)	9 (6%)	1 (1%)	25	21
All	All	667/692 (96%)	631 (95%)	30 (4%)	6 (1%)	17	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	103	GLY
1	C	99	ILE
1	C	251	PRO
1	C	101	ARG
1	B	251	PRO
1	D	103	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/156 (100%)	153 (98%)	3 (2%)	57	63
1	B	153/156 (98%)	151 (99%)	2 (1%)	69	75
1	C	155/156 (99%)	143 (92%)	12 (8%)	13	9
1	D	146/156 (94%)	137 (94%)	9 (6%)	18	15
All	All	610/624 (98%)	584 (96%)	26 (4%)	28	29

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	MET
1	A	160	ARG
1	A	250	ASN
1	B	139	LEU
1	B	221	ARG
1	C	99	ILE
1	C	101	ARG
1	C	104	GLU
1	C	135	GLN
1	C	137	MET
1	C	138	MET
1	C	153	LYS
1	C	172	ARG
1	C	182	ASN
1	C	189	LYS
1	C	219	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	226	ARG
1	D	95	THR
1	D	99	ILE
1	D	127	ASN
1	D	136	ASP
1	D	170	LYS
1	D	171	THR
1	D	172	ARG
1	D	219	GLU
1	D	226	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	193	GLN
1	A	200	GLN
1	A	210	ASN
1	A	247	ASN
1	A	250	ASN
1	C	113	GLN
1	C	135	GLN
1	C	193	GLN
1	C	199	ASN
1	C	200	GLN
1	C	210	ASN
1	C	247	ASN
1	D	135	GLN
1	D	156	HIS
1	D	200	GLN
1	D	210	ASN
1	D	242	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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	C	9	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	A	1	-	4,4,4	0.18	0	6,6,6	0.50	0
2	SO4	B	4	-	4,4,4	0.20	0	6,6,6	0.26	0
2	SO4	C	7	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	B	3	-	4,4,4	0.29	0	6,6,6	0.26	0
2	SO4	B	6	-	4,4,4	0.19	0	6,6,6	0.68	0
2	SO4	D	2	-	4,4,4	0.17	0	6,6,6	0.31	0
2	SO4	A	8	-	4,4,4	0.16	0	6,6,6	0.12	0
2	SO4	C	10	-	4,4,4	0.17	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	7	SO4	1	0

5.7 Other polymers [i](#)

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 ⓘ

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	162/173 (93%)	-0.18	4 (2%) 57 62	10, 21, 46, 58	0
1	B	160/173 (92%)	-0.16	6 (3%) 40 46	11, 21, 49, 61	0
1	C	169/173 (97%)	-0.04	9 (5%) 26 32	11, 28, 59, 71	0
1	D	159/173 (91%)	0.18	13 (8%) 11 15	12, 29, 80, 86	0
All	All	650/692 (93%)	-0.05	32 (4%) 29 35	10, 24, 59, 86	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	98	THR	5.7
1	C	252	HIS	5.1
1	C	169	VAL	5.0
1	D	97	ALA	4.6
1	B	102	LYS	4.3
1	B	100	ALA	4.3
1	A	101[A]	ARG	4.2
1	A	252	HIS	4.2
1	C	85	ILE	4.2
1	D	100	ALA	3.9
1	A	251	PRO	3.8
1	B	169	VAL	3.6
1	D	218	LEU	3.3
1	D	95	THR	3.1
1	A	169	VAL	2.9
1	D	101	ARG	2.9
1	C	102	LYS	2.9
1	B	101	ARG	2.8
1	D	139	LEU	2.8
1	D	129	THR	2.7
1	B	252	HIS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	221[A]	ARG	2.6
1	C	170	LYS	2.6
1	C	84	GLY	2.6
1	D	105	GLY	2.6
1	D	133	ILE	2.5
1	D	94	GLU	2.4
1	D	128	ALA	2.4
1	C	171	THR	2.4
1	D	99	ILE	2.3
1	B	170	LYS	2.1
1	C	251	PRO	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. 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(\AA^2)	Q<0.9
2	SO4	C	9	5/5	0.82	0.28	81,81,82,82	0
2	SO4	C	7	5/5	0.95	0.12	73,73,73,74	0
2	SO4	B	3	5/5	0.97	0.11	29,32,34,35	0
2	SO4	A	8	5/5	0.97	0.10	57,57,58,58	0
2	SO4	B	6	5/5	0.98	0.08	19,22,24,25	0
2	SO4	D	2	5/5	0.98	0.06	48,50,50,50	0
2	SO4	B	4	5/5	0.98	0.10	37,40,40,41	0
2	SO4	C	10	5/5	0.98	0.08	48,48,50,52	0
2	SO4	A	1	5/5	0.99	0.08	25,26,28,28	0

6.5 Other polymers

There are no such residues in this entry.