Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 08:27 AM EST

PDB ID	:	3S03
Title	:	The crystal structure of the periplasmic domain of Helicobacter pylori MotB (residues 97-256, P43).
Authors	:	Roujeinikova, A.R.
Deposited on	:	2011-05-13
Resolution	:	2.50 Å(reported)

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

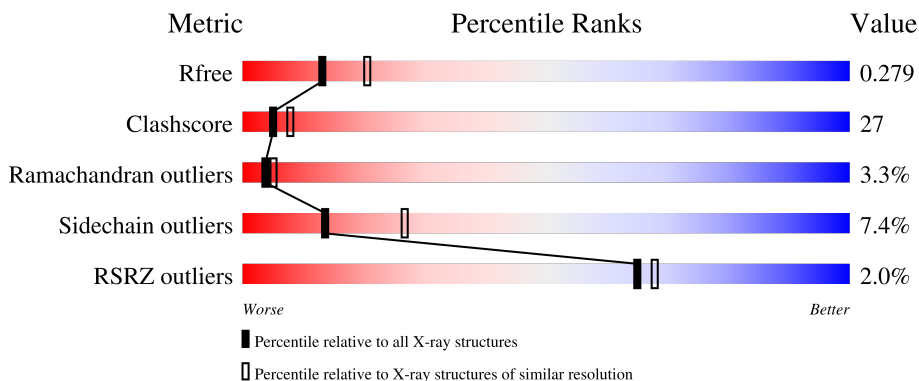|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	Percentile Ranks	Value
Rfree		0.279
Clashscore		27
Ramachandran outliers		3.3%
Sidechain outliers		7.4%
RSRZ outliers		2.0%

Worse — *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	166	46% 37% ·· 13%
1	B	166	2% 43% 34% · 19%
1	C	166	3% 33% 52% · 12%
1	D	166	2% 37% 39% 5% 18%

WORLDWIDE PDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4664 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	145	Total	C	N	O	S	0	0	0
			1160	732	203	221	4			
1	B	135	Total	C	N	O	S	0	0	0
			1077	683	188	203	3			
1	C	146	Total	C	N	O	S	0	0	0
			1159	730	203	223	3			
1	D	136	Total	C	N	O	S	0	0	0
			1088	688	191	206	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	GLY	-	expression tag	UNP P56427
A	92	ILE	-	expression tag	UNP P56427
A	93	ASP	-	expression tag	UNP P56427
A	94	PRO	-	expression tag	UNP P56427
A	95	PHE	-	expression tag	UNP P56427
A	96	THR	-	expression tag	UNP P56427
B	91	GLY	-	expression tag	UNP P56427
B	92	ILE	-	expression tag	UNP P56427
B	93	ASP	-	expression tag	UNP P56427
B	94	PRO	-	expression tag	UNP P56427
B	95	PHE	-	expression tag	UNP P56427
B	96	THR	-	expression tag	UNP P56427
C	91	GLY	-	expression tag	UNP P56427
C	92	ILE	-	expression tag	UNP P56427
C	93	ASP	-	expression tag	UNP P56427
C	94	PRO	-	expression tag	UNP P56427
C	95	PHE	-	expression tag	UNP P56427
C	96	THR	-	expression tag	UNP P56427
D	91	GLY	-	expression tag	UNP P56427
D	92	ILE	-	expression tag	UNP P56427
D	93	ASP	-	expression tag	UNP P56427

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	PRO	-	expression tag	UNP P56427
D	95	PHE	-	expression tag	UNP P56427
D	96	THR	-	expression tag	UNP P56427

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
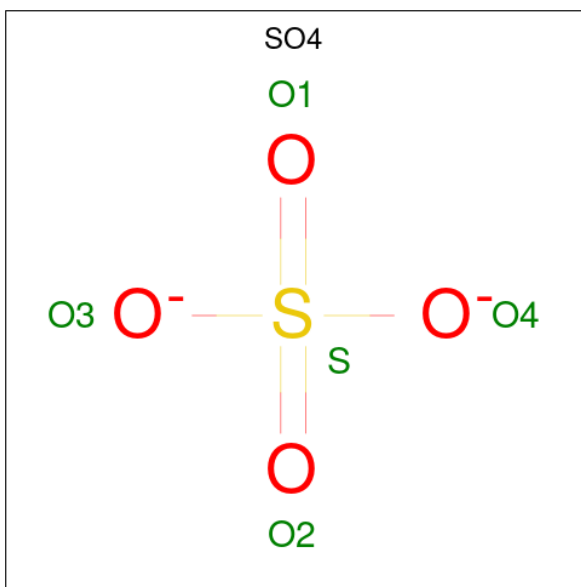
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	38	Total 38	O 38	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	42	Total O 42 42		0	0
3	C	41	Total O 41 41		0	0
3	D	24	Total O 24 24		0	0

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.
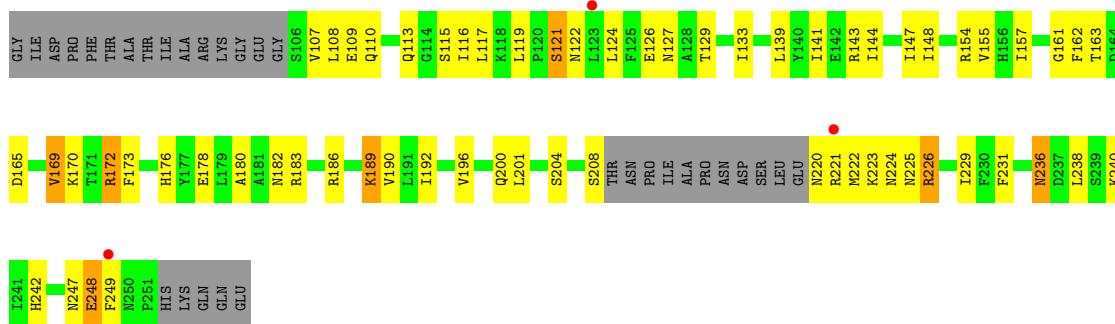
• Molecule 1: Motility protein B

Chain A:
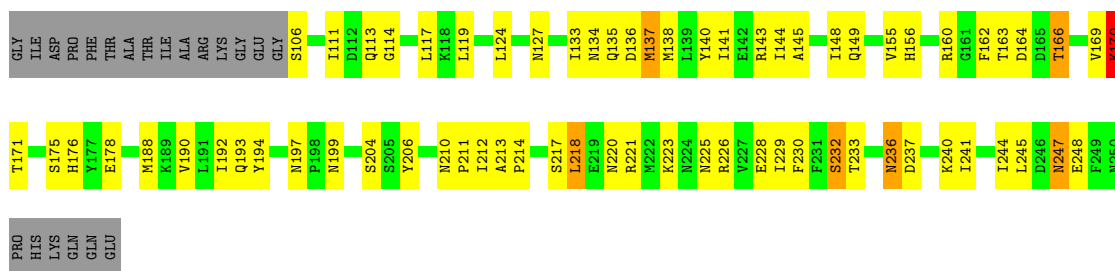
• Molecule 1: Motility protein B

Chain B:

• Molecule 1: Motility protein B

Chain C:

R226 V227 E228 I229 F230 F231 N236 D237 I241 H242 L245 D246 N250 P251 HIS LYS GLN GLU

• Molecule 1: Motility protein B

Chain D:

GLY ILE ASP PRO PHE THR ALA THR ILE ALA ARG LYS G103 S106 V107 L108 E109 Q110 I111 I116 L117 K118 L119 P120 S121 L124 F125 E126 T129 S130 D131 A132 I133 M137 I141 E142 I147 I148 L151 P152 K153 R154 V155 H156 I157 N158 V159 R160 D164 D165 T166

P167 L168 V169 K170 T171 K174 E178 L179 A180 A181 N182 R183 A184 Y185 R186 V187 M188 K189 V190 L191 I192 Q193 Y194 G195 V196 N197 P198 N199 Q200 L201 S202 F203 S204 S205 Y206 GLY SER THR ASN PRO ILE ALA PRO ASN ASP SER LEU GLU N220 R221 N224 N225 R226 V227 E228 I229 F230

F231 S232 L238 S239 K240 I241 H242 S243 N247 E248 F249 N250 P251 HIS LYS GLN GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	71.67Å　71.67Å　126.24Å 90.00°　90.00°　90.00°	Depositor
Resolution (Å)	71.67　–　2.50 28.88　–　2.50	Depositor EDS
% Data completeness (in resolution range)	84.2 (71.67-2.50) 84.2 (28.88-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.225　,　0.284 0.221　,　0.279	Depositor DCC
R_{free} test set	981 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å^2)	44.8	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 29.4	EDS
L-test for twinning[2]	$< |L| > = 0.37, < L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.348 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4664	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.53	0/1180	0.63	0/1596
1	B	0.50	0/1095	0.59	0/1479
1	C	0.43	0/1180	0.55	0/1598
1	D	0.46	0/1106	0.62	0/1492
All	All	0.48	0/4561	0.60	0/6165

There are no bond length outliers.

There are no bond angle outliers.

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	1160	0	1156	64	0
1	B	1077	0	1069	52	0
1	C	1159	0	1142	79	0
1	D	1088	0	1079	67	0
2	A	10	0	0	1	0
2	B	10	0	0	1	0
2	C	15	0	0	0	0
3	A	38	0	0	6	0
3	B	42	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	41	0	0	2	0
3	D	24	0	0	2	0
All	All	4664	0	4446	244	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 27.

All (244) 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:204:SER:OG	1:B:204:SER:HB3	1.60	1.01
1:B:248:GLU:HG2	1:C:147:ILE:HG21	1.49	0.94
1:C:141:ILE:HG23	1:C:191:LEU:HD23	1.53	0.90
1:D:221:ARG:HA	1:D:224:ASN:HD22	1.41	0.86
1:C:126:GLU:HG3	1:C:127:ASN:H	1.43	0.83
1:A:144:ILE:O	1:A:148:ILE:HG13	1.80	0.82
1:A:169:VAL:HG13	1:A:170:LYS:HD3	1.60	0.82
1:D:106:SER:HB3	1:D:118:LYS:O	1.79	0.80
1:B:148:ILE:HD12	1:B:196:VAL:HG21	1.62	0.80
1:D:187:VAL:HG21	1:D:227:VAL:HG21	1.63	0.78
1:C:151:LEU:HB3	1:C:155:VAL:HG21	1.65	0.78
1:C:147:ILE:HG22	1:C:150:LYS:HE3	1.66	0.78
1:A:164:ASP:OD1	1:A:166:THR:HB	1.84	0.77
1:B:139:LEU:O	1:B:143:ARG:HG2	1.84	0.77
1:B:119:LEU:CD1	1:B:229:ILE:HD11	2.17	0.75
1:A:221:ARG:O	1:A:225:ASN:ND2	2.21	0.74
1:B:162:PHE:HB2	1:B:226:ARG:HD3	1.70	0.72
1:D:137:MET:O	1:D:141:ILE:HG12	1.89	0.72
1:D:154:ARG:NH1	3:D:261:HOH:O	2.20	0.72
1:D:131:ASP:CB	1:D:183:ARG:HG3	2.20	0.72
1:C:138:MET:O	1:C:142:GLU:HG3	1.91	0.71
1:C:219:GLU:O	1:C:223:LYS:HG3	1.91	0.70
1:B:121:SER:HB2	1:B:183:ARG:HH22	1.55	0.70
1:C:213:ALA:HB2	3:C:33:HOH:O	1.92	0.69
1:D:157:ILE:HB	1:D:201:LEU:HD23	1.76	0.68
1:C:141:ILE:HG23	1:C:191:LEU:CD2	2.22	0.68
3:B:80:HOH:O	1:C:108:LEU:HD11	1.92	0.68
1:A:113:GLN:NE2	1:B:113:GLN:HA	2.08	0.68
1:A:236:ASN:HD21	1:A:240:LYS:HE2	1.59	0.67
1:C:116:ILE:HG23	1:C:230:PHE:HD1	1.59	0.67
1:A:113:GLN:HE21	1:B:113:GLN:HA	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HB	1:B:201:LEU:HD23	1.76	0.67
1:B:119:LEU:HD11	1:B:229:ILE:HD11	1.77	0.67
1:D:158:ASN:HA	1:D:202:SER:O	1.94	0.67
1:B:154:ARG:HG2	2:B:5:SO4:O1	1.94	0.67
1:D:156:HIS:C	1:D:157:ILE:HD13	2.16	0.66
1:D:187:VAL:HG11	1:D:227:VAL:HG11	1.79	0.65
1:B:157:ILE:N	1:B:157:ILE:HD12	2.11	0.65
1:C:113:GLN:HE21	1:C:113:GLN:HA	1.61	0.65
1:A:117:LEU:HB3	1:A:229:ILE:HB	1.79	0.64
1:C:145:ALA:HA	1:C:148:ILE:HD12	1.78	0.64
1:A:164:ASP:OD1	1:A:166:THR:N	2.27	0.64
1:A:143:ARG:NH1	1:D:248:GLU:O	2.31	0.64
1:D:142:GLU:HG3	1:D:194:TYR:CD1	2.33	0.64
1:A:124:LEU:O	1:A:137:MET:HG3	1.99	0.63
1:D:166:THR:HG22	1:D:168:LEU:HG	1.78	0.63
1:D:170:LYS:HE3	1:D:171:THR:HG23	1.79	0.63
1:D:181:ALA:N	1:D:205:SER:HB2	2.14	0.63
1:C:136:ASP:HB2	3:C:90:HOH:O	1.99	0.62
1:C:143:ARG:HA	1:C:146:LYS:HD2	1.80	0.62
1:D:197:ASN:ND2	1:D:199:ASN:HB2	2.15	0.62
1:A:213:ALA:HB1	1:A:214:PRO:CD	2.29	0.62
1:A:247:ASN:N	1:A:247:ASN:HD22	1.96	0.62
1:D:187:VAL:HG21	1:D:227:VAL:HG11	1.81	0.62
1:C:250:ASN:N	1:C:250:ASN:HD22	1.98	0.62
1:C:116:ILE:HG23	1:C:230:PHE:CD1	2.35	0.61
1:C:141:ILE:HG21	1:C:190:VAL:HG12	1.81	0.61
1:D:116:ILE:HG23	1:D:228:GLU:HG2	1.82	0.61
1:D:178:GLU:HG3	1:D:182:ASN:ND2	2.15	0.61
1:B:172:ARG:H	1:B:172:ARG:HD3	1.65	0.60
1:C:115:SER:O	1:C:231:PHE:HD2	1.85	0.59
1:A:137:MET:HG2	1:A:141:ILE:HD11	1.84	0.59
1:B:236:ASN:HD22	1:B:236:ASN:N	2.01	0.59
1:D:221:ARG:HA	1:D:224:ASN:ND2	2.15	0.59
1:C:189:LYS:HA	1:C:192:ILE:HD12	1.84	0.59
1:C:157:ILE:HB	1:C:201:LEU:HD23	1.84	0.59
1:D:131:ASP:HB3	1:D:183:ARG:HG3	1.83	0.59
1:C:126:GLU:HG3	1:C:127:ASN:N	2.17	0.58
1:D:197:ASN:HD21	1:D:199:ASN:HB2	1.68	0.58
1:A:236:ASN:ND2	1:A:240:LYS:HE2	2.18	0.58
1:C:175:SER:OG	1:C:178:GLU:HG3	2.04	0.57
1:C:188:MET:HG2	1:C:201:LEU:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLY:HA2	1:D:238:LEU:HD22	1.85	0.57
1:A:170:LYS:HD3	1:A:170:LYS:H	1.69	0.57
1:D:130:SER:O	1:D:183:ARG:HD2	2.04	0.57
1:A:133:ILE:HD12	1:A:133:ILE:C	2.24	0.57
1:A:156:HIS:HB2	3:A:83:HOH:O	2.03	0.57
1:A:135:GLN:HG3	1:A:136:ASP:H	1.70	0.56
1:A:244:ILE:HG23	3:A:267:HOH:O	2.03	0.56
1:B:117:LEU:O	1:B:229:ILE:HD12	2.05	0.56
1:C:166:THR:HG23	1:C:167:PRO:HD2	1.86	0.56
1:C:190:VAL:HA	1:C:193:GLN:HE21	1.69	0.56
1:B:229:ILE:HD12	1:B:229:ILE:H	1.70	0.56
1:A:169:VAL:HG13	1:A:170:LYS:H	1.70	0.56
1:B:223:LYS:O	1:B:226:ARG:HD2	2.06	0.56
1:A:210:ASN:ND2	3:A:12:HOH:O	2.31	0.56
1:A:213:ALA:HB1	1:A:214:PRO:HD2	1.86	0.56
1:C:179:LEU:O	1:C:183:ARG:HG3	2.05	0.56
1:D:129:THR:OG1	1:D:168:LEU:HD13	2.06	0.55
1:B:157:ILE:HD13	1:B:200:GLN:HB3	1.89	0.55
1:A:138:MET:HB3	1:A:194:TYR:OH	2.07	0.55
1:A:164:ASP:CG	1:A:166:THR:HB	2.27	0.55
1:B:161:GLY:O	1:B:180:ALA:HB1	2.07	0.55
1:B:236:ASN:HD22	1:B:236:ASN:H	1.54	0.55
1:B:176:HIS:ND1	1:B:208:SER:HB3	2.22	0.55
1:C:127:ASN:N	1:C:127:ASN:HD22	2.03	0.54
1:C:213:ALA:HB1	1:C:214:PRO:HD2	1.90	0.54
1:C:173:PHE:HE1	1:C:182:ASN:ND2	2.06	0.54
1:B:141:ILE:HG21	1:B:190:VAL:HG12	1.89	0.54
1:C:188:MET:HA	1:C:191:LEU:HD12	1.90	0.54
1:D:188:MET:SD	1:D:203:PHE:HB3	2.48	0.53
1:C:226:ARG:NE	1:C:228:GLU:OE2	2.40	0.53
1:B:178:GLU:O	1:B:182:ASN:ND2	2.40	0.53
1:C:214:PRO:HB2	1:C:216:ASP:OD1	2.08	0.53
1:C:124:LEU:HD21	1:C:187:VAL:HG22	1.90	0.53
1:B:155:VAL:HG22	1:C:241:ILE:HD11	1.91	0.53
1:A:188:MET:O	1:A:192:ILE:HG13	2.08	0.53
1:B:157:ILE:CD1	1:B:200:GLN:HB3	2.39	0.53
1:A:137:MET:O	1:A:141:ILE:HD12	2.09	0.52
1:A:237:ASP:O	1:A:241:ILE:HG13	2.09	0.52
1:C:122:ASN:HB3	1:C:222:MET:SD	2.50	0.52
1:A:106:SER:N	3:A:24:HOH:O	2.41	0.52
1:D:190:VAL:O	1:D:193:GLN:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:HIS:O	1:C:246:ASP:HB2	2.09	0.52
1:D:156:HIS:O	1:D:157:ILE:HD13	2.09	0.52
1:D:190:VAL:HA	1:D:193:GLN:HE21	1.74	0.52
1:A:217:SER:O	1:A:218:LEU:C	2.47	0.51
1:A:245:LEU:CD2	1:D:147:ILE:HG21	2.40	0.51
1:B:124:LEU:O	1:B:133:ILE:HD12	2.10	0.51
1:C:127:ASN:H	1:C:127:ASN:HD22	1.57	0.51
1:B:162:PHE:O	1:B:225:ASN:HA	2.11	0.51
1:B:108:LEU:HD21	1:C:245:LEU:HB3	1.93	0.51
1:D:121:SER:HB2	1:D:125:PHE:HD2	1.75	0.51
1:D:148:ILE:HA	1:D:151:LEU:HD12	1.93	0.51
1:A:210:ASN:N	1:A:211:PRO:HD3	2.26	0.51
1:A:163:THR:OG1	1:A:176:HIS:HB3	2.12	0.50
1:D:240:LYS:NZ	1:D:240:LYS:HB3	2.27	0.50
1:A:137:MET:HG2	1:A:141:ILE:CD1	2.40	0.50
1:C:141:ILE:CG2	1:C:191:LEU:HD23	2.31	0.50
1:A:236:ASN:H	1:A:236:ASN:HD22	1.58	0.50
1:C:106:SER:N	1:C:120:PRO:HD3	2.27	0.50
1:C:152:PRO:HB2	1:C:154:ARG:HG2	1.92	0.50
1:B:148:ILE:CD1	1:B:196:VAL:HG21	2.36	0.50
1:A:230:PHE:CE2	1:A:232:SER:HB3	2.47	0.49
1:B:108:LEU:HD12	1:B:116:ILE:O	2.11	0.49
1:B:115:SER:O	1:B:231:PHE:HD2	1.95	0.49
1:B:173:PHE:HE1	1:B:182:ASN:ND2	2.10	0.49
1:A:162:PHE:HE2	1:A:228:GLU:HB2	1.76	0.49
1:C:164:ASP:O	1:C:208:SER:HB3	2.13	0.49
1:C:174:LYS:HB2	1:C:178:GLU:OE2	2.12	0.49
1:A:145:ALA:O	1:A:149:GLN:HG2	2.13	0.49
1:C:151:LEU:HD13	1:C:155:VAL:HG11	1.94	0.49
1:D:230:PHE:CE2	1:D:232:SER:HB3	2.48	0.49
1:B:141:ILE:HG21	1:B:190:VAL:CG1	2.42	0.48
1:A:199:ASN:ND2	3:A:266:HOH:O	2.44	0.48
1:C:109:GLU:HG2	1:C:110:GLN:H	1.78	0.48
1:C:148:ILE:HG22	1:C:149:GLN:HE21	1.77	0.48
1:D:190:VAL:HG12	1:D:194:TYR:CD2	2.48	0.48
1:D:203:PHE:CD1	1:D:203:PHE:C	2.86	0.48
1:D:130:SER:OG	1:D:131:ASP:N	2.47	0.48
1:C:106:SER:HA	1:C:118:LYS:O	2.14	0.48
1:D:119:LEU:HD13	1:D:124:LEU:HD11	1.94	0.48
1:B:189:LYS:NZ	1:B:192:ILE:HD12	2.29	0.48
1:C:145:ALA:HB1	1:C:194:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ILE:CG2	1:D:228:GLU:HG2	2.42	0.48
1:B:221:ARG:C	1:B:223:LYS:H	2.16	0.47
1:A:175:SER:HB2	2:A:1:SO4:O2	2.14	0.47
1:C:250:ASN:N	1:C:250:ASN:ND2	2.62	0.47
3:A:271:HOH:O	1:B:113:GLN:HG2	2.13	0.47
1:A:141:ILE:HG21	1:A:190:VAL:CG1	2.45	0.47
1:A:164:ASP:N	1:A:225:ASN:OD1	2.41	0.47
1:B:110:GLN:HE22	1:D:110:GLN:HE22	1.62	0.47
1:D:178:GLU:HG3	1:D:182:ASN:HD22	1.77	0.47
1:A:141:ILE:HG21	1:A:190:VAL:HG12	1.96	0.47
1:D:121:SER:OG	1:D:225:ASN:HB3	2.14	0.47
1:A:247:ASN:N	1:A:247:ASN:ND2	2.63	0.47
1:D:131:ASP:HB2	1:D:183:ARG:HG3	1.93	0.46
1:C:236:ASN:HB3	1:D:111:ILE:HG22	1.98	0.46
1:A:223:LYS:O	1:A:226:ARG:HD3	2.16	0.46
1:B:144:ILE:HA	1:B:147:ILE:HD12	1.98	0.46
1:C:159:VAL:HG11	1:C:187:VAL:HB	1.96	0.46
1:C:209:THR:HB	1:D:199:ASN:ND2	2.30	0.46
1:A:197:ASN:ND2	1:A:199:ASN:HB2	2.31	0.46
1:A:140:TYR:CE2	1:A:144:ILE:HD11	2.51	0.46
1:A:111:ILE:HD11	1:A:230:PHE:HE1	1.81	0.46
1:C:129:THR:O	1:C:171:THR:HG21	2.16	0.46
1:A:217:SER:OG	1:A:220:ASN:ND2	2.44	0.45
1:B:189:LYS:N	1:B:189:LYS:HD2	2.26	0.45
1:D:125:PHE:CZ	1:D:183:ARG:HG2	2.51	0.45
1:D:183:ARG:HH22	1:D:225:ASN:ND2	2.14	0.45
1:C:197:ASN:HD21	1:C:199:ASN:HB2	1.82	0.45
1:C:197:ASN:HD21	1:C:199:ASN:HD22	1.64	0.45
1:B:107:VAL:HG12	1:B:108:LEU:N	2.32	0.45
1:C:217:SER:HB2	1:C:220:ASN:ND2	2.31	0.45
1:A:117:LEU:HG	1:A:119:LEU:HD21	1.98	0.45
1:B:127:ASN:ND2	1:B:129:THR:H	2.14	0.45
1:D:148:ILE:HB	1:D:196:VAL:HG22	1.98	0.45
1:A:190:VAL:HA	1:A:193:GLN:HE21	1.82	0.45
1:D:159:VAL:HB	1:D:188:MET:HB2	1.99	0.44
1:B:189:LYS:HD2	1:B:189:LYS:HA	1.67	0.44
1:A:155:VAL:HG22	1:D:241:ILE:HD11	1.99	0.44
1:B:169:VAL:O	1:B:170:LYS:HG3	2.18	0.44
1:A:134:ASN:OD1	1:A:137:MET:HB2	2.17	0.44
1:B:186:ARG:HA	1:B:186:ARG:HD3	1.76	0.44
1:B:242:HIS:HA	3:B:80:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASN:HD21	1:C:130:SER:HB3	1.83	0.44
1:D:180:ALA:O	1:D:181:ALA:C	2.56	0.44
1:C:134:ASN:O	1:C:137:MET:N	2.48	0.44
1:C:157:ILE:HG22	1:C:158:ASN:N	2.33	0.44
1:C:164:ASP:HB2	1:C:215:ASN:ND2	2.33	0.44
1:B:236:ASN:O	1:B:240:LYS:HG3	2.18	0.43
1:D:220:ASN:O	1:D:224:ASN:ND2	2.51	0.43
1:A:206:TYR:HB3	1:A:210:ASN:HD22	1.83	0.43
1:C:107:VAL:O	1:C:117:LEU:HD12	2.18	0.43
1:D:221:ARG:CA	1:D:224:ASN:HD22	2.23	0.43
1:C:166:THR:CG2	1:C:167:PRO:HD2	2.48	0.43
1:C:197:ASN:ND2	1:C:199:ASN:HB2	2.34	0.43
1:C:117:LEU:O	1:C:228:GLU:HA	2.18	0.43
1:D:185:TYR:CD1	1:D:203:PHE:CE2	3.06	0.43
1:A:137:MET:SD	1:A:141:ILE:HD13	2.59	0.42
1:D:190:VAL:HG13	1:D:193:GLN:HE21	1.83	0.42
1:C:168:LEU:HD23	1:C:179:LEU:HD22	2.01	0.42
1:C:127:ASN:H	1:C:127:ASN:ND2	2.16	0.42
1:D:148:ILE:HG21	1:D:196:VAL:CG1	2.50	0.42
1:C:139:LEU:O	1:C:142:GLU:HB2	2.19	0.42
1:B:249:PHE:HZ	1:C:144:ILE:HG12	1.85	0.42
1:C:149:GLN:H	1:C:149:GLN:HG2	1.66	0.42
1:C:153:LYS:HA	1:C:200:GLN:OE1	2.19	0.41
1:A:248:GLU:HG2	1:D:147:ILE:HD11	2.02	0.41
1:A:197:ASN:HD21	1:A:199:ASN:HB2	1.85	0.41
1:C:129:THR:HG21	1:C:170:LYS:HE3	2.01	0.41
1:B:155:VAL:O	1:B:200:GLN:OE1	2.38	0.41
1:C:185:TYR:CD1	1:C:203:PHE:CE2	3.09	0.41
1:D:190:VAL:HG12	1:D:194:TYR:HD2	1.84	0.41
1:A:169:VAL:C	1:A:171:THR:H	2.23	0.41
1:A:248:GLU:OE2	1:D:147:ILE:HD11	2.20	0.41
1:D:121:SER:HB2	1:D:125:PHE:CD2	2.54	0.41
1:C:175:SER:HG	1:C:178:GLU:HG3	1.85	0.41
1:D:109:GLU:HB3	1:D:116:ILE:HB	2.03	0.41
1:D:192:ILE:HG23	1:D:198:PRO:HG3	2.03	0.41
1:D:247:ASN:O	1:D:249:PHE:N	2.52	0.41
1:A:212:ILE:HG21	1:A:223:LYS:HD3	2.03	0.41
1:C:188:MET:HG3	1:C:201:LEU:HD22	2.02	0.41
1:D:121:SER:HA	1:D:124:LEU:HB2	2.02	0.41
1:D:154:ARG:NH2	3:D:264:HOH:O	2.53	0.41
1:D:181:ALA:CA	1:D:205:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HD22	1:C:114:GLY:HA2	2.02	0.41
1:A:223:LYS:O	1:A:226:ARG:HB3	2.20	0.40
1:D:152:PRO:O	1:D:154:ARG:N	2.54	0.40
1:A:236:ASN:HD22	1:A:236:ASN:N	2.16	0.40
1:B:110:GLN:HB2	1:C:242:HIS:CE1	2.55	0.40
1:B:163:THR:OG1	1:B:176:HIS:HB3	2.21	0.40
1:C:220:ASN:O	1:C:223:LYS:N	2.55	0.40
1:C:125:PHE:HB2	1:C:183:ARG:HH21	1.85	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	143/166 (86%)	125 (87%)	15 (10%)	3 (2%)	7	11
1	B	131/166 (79%)	111 (85%)	16 (12%)	4 (3%)	4	5
1	C	144/166 (87%)	121 (84%)	22 (15%)	1 (1%)	22	39
1	D	132/166 (80%)	111 (84%)	11 (8%)	10 (8%)	1	1
All	All	550/664 (83%)	468 (85%)	64 (12%)	18 (3%)	4	5

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	164	ASP
1	D	168	LEU
1	C	135	GLN
1	D	153	LYS
1	D	247	ASN
1	D	248	GLU
1	A	218	LEU

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Mol	Chain	Res	Type
1	A	170	LYS
1	B	222	MET
1	D	126	GLU
1	D	250	ASN
1	B	121	SER
1	D	174	LYS
1	A	232	SER
1	B	169	VAL
1	B	224	ASN
1	D	133	ILE
1	D	196	VAL

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	131/149 (88%)	122 (93%)	9 (7%)	15	30
1	B	120/149 (80%)	109 (91%)	11 (9%)	9	18
1	C	130/149 (87%)	123 (95%)	7 (5%)	22	42
1	D	121/149 (81%)	111 (92%)	10 (8%)	11	22
All	All	502/596 (84%)	465 (93%)	37 (7%)	13	27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	137	MET
1	A	160	ARG
1	A	166	THR
1	A	170	LYS
1	A	178	GLU
1	A	233	THR
1	A	236	ASN
1	A	247	ASN
1	B	109	GLU

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Mol	Chain	Res	Type
1	B	122	ASN
1	B	126	GLU
1	B	165	ASP
1	B	172	ARG
1	B	189	LYS
1	B	220	ASN
1	B	226	ARG
1	B	236	ASN
1	B	247	ASN
1	B	248	GLU
1	C	113	GLN
1	C	124	LEU
1	C	127	ASN
1	C	134	ASN
1	C	168	LEU
1	C	237	ASP
1	C	250	ASN
1	D	108	LEU
1	D	119	LEU
1	D	129	THR
1	D	160	ARG
1	D	164	ASP
1	D	170	LYS
1	D	186	ARG
1	D	199	ASN
1	D	226	ARG
1	D	243	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	182	ASN
1	A	193	GLN
1	A	199	ASN
1	A	210	ASN
1	A	236	ASN
1	A	247	ASN
1	B	113	GLN
1	B	127	ASN
1	B	135	GLN
1	B	149	GLN

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Mol	Chain	Res	Type
1	B	156	HIS
1	B	193	GLN
1	B	199	ASN
1	B	236	ASN
1	C	113	GLN
1	C	149	GLN
1	C	156	HIS
1	C	158	ASN
1	C	182	ASN
1	C	193	GLN
1	C	199	ASN
1	C	215	ASN
1	C	220	ASN
1	C	242	HIS
1	C	247	ASN
1	C	250	ASN
1	D	110	GLN
1	D	193	GLN
1	D	197	ASN
1	D	199	ASN
1	D	220	ASN
1	D	224	ASN
1	D	242	HIS
1	D	250	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	3	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	B	5	-	4,4,4	0.14	0	6,6,6	0.25	0
2	SO4	C	2	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	C	4	-	4,4,4	0.09	0	6,6,6	0.32	0
2	SO4	B	7	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	A	1	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	A	6	-	4,4,4	0.19	0	6,6,6	0.15	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	5	SO4	1	0
2	A	1	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 ⓘ

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	145/166 (87%)	-0.50	0 100	100	17, 36, 65, 78	0
1	B	135/166 (81%)	-0.34	3 (2%) 62	65	19, 45, 82, 93	0
1	C	146/166 (87%)	-0.09	5 (3%) 45	48	26, 55, 89, 99	0
1	D	136/166 (81%)	-0.13	3 (2%) 62	65	34, 54, 84, 97	0
All	All	562/664 (84%)	-0.26	11 (1%) 65	68	17, 48, 84, 99	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	106	SER	3.7
1	B	249	PHE	3.5
1	C	169	VAL	3.1
1	C	170	LYS	3.0
1	D	168	LEU	2.4
1	B	221	ARG	2.2
1	C	213	ALA	2.2
1	B	123	LEU	2.2
1	D	148	ILE	2.1
1	C	137	MET	2.1
1	C	190	VAL	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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	C	3	5/5	0.90	0.18	95,101,104,113	0
2	SO4	C	2	5/5	0.96	0.09	73,74,95,95	0
2	SO4	A	6	5/5	0.96	0.12	65,82,85,96	0
2	SO4	C	4	5/5	0.97	0.10	39,43,47,48	0
2	SO4	A	1	5/5	0.99	0.12	34,37,41,41	0
2	SO4	B	5	5/5	0.99	0.04	48,49,64,64	0
2	SO4	B	7	5/5	0.99	0.09	44,47,49,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.