



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:22 am BST

PDB ID : 4LD5
Title : Crystal structure of MepR Q18P mutant from multidrug resistant *S. aureus* clinical isolate
Authors : Birukou, I.; Brennan, R.G.
Deposited on : 2013-06-24
Resolution : 2.40 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

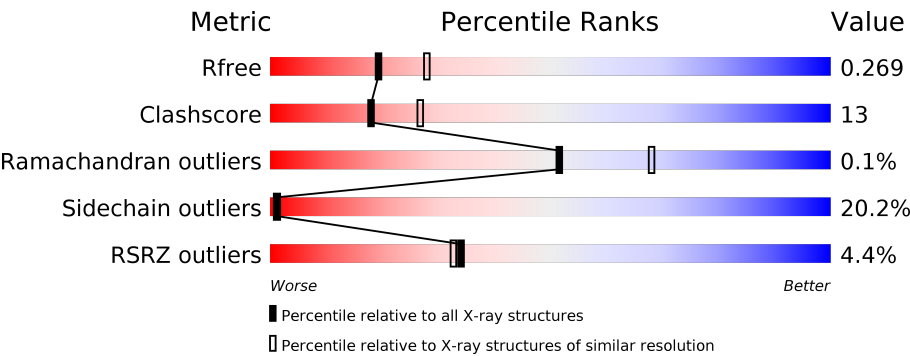
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	145	<div><div>%</div><div><div></div><div>61%</div><div>28%</div><div>6%</div><div>5%</div></div></div>
1	B	145	<div><div>12%</div><div><div></div><div>53%</div><div>26%</div><div>8%</div><div>13%</div></div></div>
1	C	145	<div><div></div><div><div></div><div>63%</div><div>30%</div><div>.</div><div>.</div></div></div>
1	D	145	<div><div>3%</div><div><div></div><div>67%</div><div>24%</div><div>5%</div><div>.</div></div></div>
1	E	145	<div><div>5%</div><div><div></div><div>56%</div><div>32%</div><div>7%</div><div>6%</div></div></div>
1	F	145	<div><div>9%</div><div><div></div><div>61%</div><div>28%</div><div>7%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	145	
1	H	145	

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
2	SO4	E	201	-	-	X	-
2	SO4	F	201	-	-	X	-
2	SO4	H	201	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8554 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 MepR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1035	653	178	199	5			
1	E	137	Total	C	N	O	S	0	0	0
			1039	648	185	201	5			
1	F	139	Total	C	N	O	S	0	0	0
			1012	639	173	195	5			
1	H	139	Total	C	N	O	S	0	0	0
			1108	693	193	217	5			
1	D	139	Total	C	N	O	S	0	0	0
			1054	661	179	209	5			
1	C	139	Total	C	N	O	S	0	0	0
			1106	694	190	217	5			
1	B	126	Total	C	N	O	S	0	0	0
			914	584	156	169	5			
1	G	139	Total	C	N	O	S	0	0	0
			1035	652	179	199	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
A	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
A	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
A	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
A	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
A	144	HIS	-	EXPRESSION TAG	UNP Q5Y812
A	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
E	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
E	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
E	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
E	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
E	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
E	144	HIS	-	EXPRESSION TAG	UNP Q5Y812

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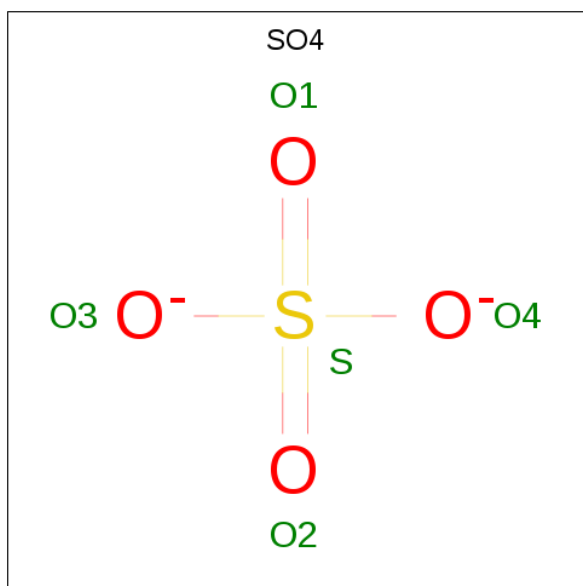
Chain	Residue	Modelled	Actual	Comment	Reference
E	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
F	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	144	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
H	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
H	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
H	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
H	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
H	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
H	144	HIS	-	EXPRESSION TAG	UNP Q5Y812
H	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
D	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
D	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
D	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
D	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
D	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
D	144	HIS	-	EXPRESSION TAG	UNP Q5Y812
D	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
C	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
C	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
C	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
C	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
C	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
C	144	HIS	-	EXPRESSION TAG	UNP Q5Y812
C	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
B	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
B	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
B	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
B	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
B	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
B	144	HIS	-	EXPRESSION TAG	UNP Q5Y812
B	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
G	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
G	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
G	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
G	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
G	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
G	144	HIS	-	EXPRESSION TAG	UNP Q5Y812

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Chain	Residue	Modelled	Actual	Comment	Reference
G	145	HIS	-	EXPRESSION TAG	UNP Q5Y812

- 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	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

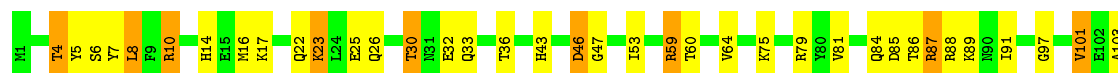
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	E	28	Total	O	0	0
			28	28		

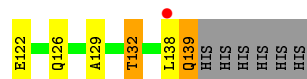
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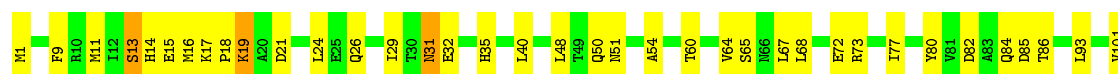
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	19	Total 19	O 19	0	0
3	H	47	Total 47	O 47	0	0
3	D	33	Total 33	O 33	0	0
3	C	53	Total 53	O 53	0	0
3	B	8	Total 8	O 8	0	0
3	G	16	Total 16	O 16	0	0



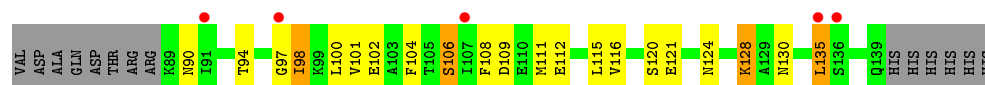
• Molecule 1: MepR



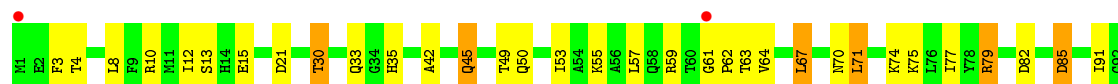
• Molecule 1: MepR



• Molecule 1: MepR



• Molecule 1: MepR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.84Å 45.84Å 210.06Å 90.00° 97.30° 90.00°	Depositor
Resolution (Å)	34.93 – 2.40 41.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.5 (34.93-2.40) 90.5 (41.96-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, R_{free}	0.211 , 0.268 0.211 , 0.269	Depositor DCC
R_{free} test set	1997 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8554	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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	0.48	0/1049	0.77	0/1422
1	B	0.43	0/926	0.72	0/1256
1	C	0.68	0/1121	0.82	1/1510 (0.1%)
1	D	0.59	0/1069	0.72	0/1449
1	E	0.55	0/1053	0.80	1/1424 (0.1%)
1	F	0.44	0/1027	0.72	1/1395 (0.1%)
1	G	0.50	0/1049	0.74	0/1420
1	H	0.69	0/1123	0.85	0/1513
All	All	0.56	0/8417	0.77	3/11389 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	LEU	CA-CB-CG	-6.80	99.66	115.30
1	C	67	LEU	CA-CB-CG	5.59	128.15	115.30
1	E	40	LEU	CB-CG-CD2	-5.24	102.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1	MET	Peptide
1	H	46	ASP	Peptide

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	1035	0	972	30	0
1	B	914	0	826	34	0
1	C	1106	0	1081	27	0
1	D	1054	0	986	26	0
1	E	1039	0	975	39	0
1	F	1012	0	919	25	0
1	G	1035	0	973	35	0
1	H	1108	0	1090	28	0
2	A	5	0	0	0	0
2	E	5	0	0	2	0
2	F	5	0	0	2	0
2	H	20	0	0	2	0
3	A	12	0	0	3	0
3	B	8	0	0	1	0
3	C	53	0	0	5	0
3	D	33	0	0	6	0
3	E	28	0	0	1	0
3	F	19	0	0	2	0
3	G	16	0	0	3	0
3	H	47	0	0	6	0
All	All	8554	0	7822	218	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 13.

All (218) 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:50:GLN:OE1	1:A:79:ARG:NH1	2.02	0.93
1:D:112:GLU:OE1	3:D:204:HOH:O	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:VAL:O	1:C:105:THR:HB	1.79	0.81
1:E:69:ARG:NH2	2:E:201:SO4:O4	2.13	0.81
1:G:59:ARG:NH1	3:G:203:HOH:O	2.15	0.80
1:B:16:MET:HE1	1:B:115:LEU:HD11	1.64	0.78
1:H:119:LEU:HB3	1:H:123:GLU:HB3	1.65	0.78
1:E:30:THR:HG22	1:E:32:GLU:H	1.49	0.78
1:G:10:ARG:O	3:G:210:HOH:O	2.03	0.77
2:H:201:SO4:O4	3:H:330:HOH:O	2.02	0.77
1:D:1:MET:N	3:D:229:HOH:O	2.19	0.76
1:H:79:ARG:HG2	1:H:91:ILE:HD13	1.68	0.76
1:E:5:TYR:HA	1:E:8:LEU:HD12	1.67	0.75
1:G:71:LEU:HB3	1:G:77:ILE:HG12	1.69	0.75
1:A:134:MET:HE3	1:B:115:LEU:HD22	1.67	0.75
1:C:19:LYS:O	3:C:253:HOH:O	2.05	0.74
1:E:70:ASN:OD1	1:E:74:LYS:NZ	2.20	0.74
1:E:69:ARG:NH2	2:E:201:SO4:S	2.61	0.73
1:G:114:THR:O	1:G:118:GLN:NE2	2.21	0.73
1:G:64:VAL:HA	1:G:67:LEU:HD23	1.71	0.73
1:G:120:SER:OG	1:G:123:GLU:HG3	1.90	0.71
1:H:85:ASP:OD1	1:H:87:ARG:HB2	1.90	0.71
1:G:30:THR:HG22	1:G:33:GLN:H	1.56	0.70
1:B:112:GLU:O	1:B:116:VAL:HG23	1.92	0.70
1:B:102:GLU:O	1:B:106:SER:HB2	1.92	0.69
1:E:98:ILE:O	1:E:102:GLU:HG3	1.93	0.69
1:G:116:VAL:HA	1:G:124:ASN:HD21	1.58	0.68
1:B:41:TYR:O	1:B:44:GLN:NE2	2.26	0.68
1:C:130:ASN:O	1:C:134:MET:HG3	1.94	0.68
1:D:79:ARG:NH2	3:D:216:HOH:O	2.25	0.68
1:G:139:GLN:O	3:G:201:HOH:O	2.12	0.67
1:A:79:ARG:HG2	1:A:91:ILE:HG12	1.76	0.67
1:H:138:LEU:O	1:H:139:GLN:HB2	1.94	0.67
1:A:98:ILE:O	1:A:102:GLU:HG3	1.95	0.66
1:D:60:THR:OG1	1:D:63:THR:OG1	2.09	0.66
1:D:82:ASP:OD2	3:D:232:HOH:O	2.11	0.66
1:E:40:LEU:HD21	1:E:53:ILE:HD11	1.76	0.66
1:B:30:THR:O	3:B:201:HOH:O	2.14	0.65
1:A:75:LYS:HB3	1:G:45:GLN:HG2	1.78	0.65
1:H:59:ARG:O	3:H:338:HOH:O	2.15	0.65
1:A:120:SER:O	1:A:124:ASN:ND2	2.30	0.64
1:E:50:GLN:OE1	1:E:79:ARG:NH1	2.31	0.64
1:C:108:PHE:HB2	3:C:241:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ARG:NE	3:D:223:HOH:O	1.95	0.63
1:A:103:ALA:O	1:A:107:ILE:HG23	1.98	0.63
1:H:118:GLN:O	1:G:133:LYS:HE3	1.99	0.62
1:E:46:ASP:OD1	1:E:46:ASP:N	2.27	0.62
1:H:14:HIS:CE1	1:G:35:HIS:HB2	2.34	0.62
1:H:128:LYS:O	1:H:132:THR:OG1	2.17	0.62
1:G:120:SER:O	1:G:124:ASN:HB2	2.00	0.62
1:B:37:LEU:HB3	1:B:101:VAL:HG22	1.82	0.61
1:E:50:GLN:HG3	1:E:91:ILE:HD11	1.82	0.60
1:A:130:ASN:O	1:A:134:MET:HG3	2.02	0.60
1:G:70:ASN:O	1:G:74:LYS:HG3	2.02	0.60
1:A:88:ARG:HG2	1:A:88:ARG:HH11	1.67	0.59
1:D:23:LYS:HD2	1:D:31:ASN:H	1.67	0.59
1:F:112:GLU:O	1:F:116:VAL:HG22	2.02	0.59
1:E:30:THR:HG22	1:E:32:GLU:N	2.16	0.59
1:E:130:ASN:O	1:E:134:MET:HG3	2.02	0.58
1:F:24:LEU:HD13	1:F:29:ILE:HG13	1.84	0.58
1:F:77:ILE:HG22	1:F:93:LEU:HD23	1.86	0.58
1:G:104:PHE:O	1:G:107:ILE:HG12	2.04	0.58
1:E:40:LEU:HD23	1:E:48:LEU:HD12	1.85	0.58
1:D:72:GLU:OE1	1:D:79:ARG:NH2	2.36	0.58
1:D:3:PHE:CD1	1:C:105:THR:HG23	2.38	0.56
1:E:53:ILE:O	1:E:57:LEU:HB2	2.06	0.56
1:E:82:ASP:HB3	1:E:85:ASP:O	2.04	0.56
1:G:74:LYS:NZ	1:G:74:LYS:HB3	2.20	0.56
1:E:128:LYS:O	1:E:132:THR:OG1	2.22	0.56
1:E:71:LEU:HB3	1:E:77:ILE:HG12	1.86	0.56
1:F:57:LEU:O	1:F:58:GLN:HG2	2.06	0.56
1:E:88:ARG:NH1	3:E:302:HOH:O	2.29	0.55
1:G:30:THR:HG22	1:G:33:GLN:HG3	1.87	0.55
1:A:102:GLU:O	1:A:106:SER:HB2	2.05	0.55
1:A:138:LEU:O	1:A:139:GLN:HG2	2.07	0.55
1:F:128:LYS:O	1:F:132:THR:OG1	2.25	0.54
1:A:4:THR:HG23	1:A:7:TYR:H	1.73	0.54
1:A:32:GLU:H	1:A:32:GLU:CD	2.11	0.54
1:A:23:LYS:HE3	1:B:10:ARG:HH22	1.72	0.54
1:A:88:ARG:HG2	1:A:88:ARG:NH1	2.23	0.54
1:B:48:LEU:O	1:B:90:ASN:HA	2.07	0.54
1:B:27:PHE:HB3	1:B:100:LEU:HD11	1.89	0.54
1:E:127:MET:HG3	1:E:131:LEU:HD12	1.90	0.53
1:E:69:ARG:HG2	1:E:73:ARG:HE	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HG2	1:B:71:LEU:HD21	1.90	0.53
3:H:333:HOH:O	1:G:4:THR:HG21	2.08	0.53
1:B:37:LEU:HD21	1:B:71:LEU:HD13	1.89	0.53
1:D:122:GLU:O	1:D:126:GLN:HG2	2.09	0.53
1:F:20:ALA:HB2	1:F:108:PHE:HZ	1.74	0.53
1:B:135:LEU:O	1:B:135:LEU:HD12	2.08	0.53
1:B:67:LEU:O	1:B:71:LEU:HG	2.10	0.52
1:H:32:GLU:HG3	1:H:59:ARG:HH12	1.74	0.52
1:D:60:THR:HB	1:D:62:PRO:HD2	1.91	0.52
1:H:43:HIS:O	1:H:47:GLY:HA2	2.09	0.52
1:H:138:LEU:HD21	1:G:115:LEU:HD21	1.92	0.52
1:B:37:LEU:HB3	1:B:101:VAL:CG2	2.40	0.52
1:A:77:ILE:HG22	1:A:93:LEU:HD23	1.91	0.51
1:H:30:THR:HG22	1:H:33:GLN:H	1.75	0.51
1:H:4:THR:HB	1:H:7:TYR:H	1.75	0.51
1:A:119:LEU:HB3	1:A:124:ASN:ND2	2.26	0.51
1:F:33:GLN:HG3	1:F:67:LEU:CD1	2.40	0.50
1:A:16:MET:HE1	1:B:9:PHE:HB2	1.93	0.50
1:D:63:THR:O	1:D:66:ASN:ND2	2.43	0.50
1:F:30:THR:HG22	1:F:33:GLN:HB2	1.92	0.50
1:B:15:GLU:OE1	1:B:15:GLU:HA	2.11	0.50
1:G:53:ILE:O	1:G:57:LEU:HD12	2.12	0.50
1:F:23:LYS:HE2	1:F:27:PHE:CZ	2.47	0.50
1:C:82:ASP:HB3	1:C:85:ASP:O	2.13	0.49
1:H:118:GLN:O	1:H:119:LEU:HD23	2.12	0.49
1:D:3:PHE:HD1	1:C:105:THR:HG23	1.77	0.49
1:E:112:GLU:OE2	1:F:6:SER:HB2	2.13	0.49
1:E:13:SER:OG	1:F:13:SER:HB3	2.13	0.49
3:A:302:HOH:O	1:B:112:GLU:HG2	2.12	0.49
1:D:11:MET:HE1	1:C:35:HIS:HA	1.95	0.49
1:D:33:GLN:NE2	3:D:212:HOH:O	2.45	0.49
1:F:10:ARG:NH2	2:F:201:SO4:O4	2.44	0.49
1:A:33:GLN:HG2	1:A:71:LEU:HD21	1.95	0.48
1:B:16:MET:HE1	1:B:115:LEU:CD1	2.39	0.48
1:A:75:LYS:NZ	3:A:308:HOH:O	2.45	0.48
1:H:60:THR:O	1:H:64:VAL:HG23	2.13	0.48
1:F:90:ASN:ND2	3:F:316:HOH:O	2.46	0.48
1:A:69:ARG:HD2	1:A:79:ARG:NH2	2.29	0.48
1:C:80:TYR:OH	3:C:232:HOH:O	2.14	0.48
1:H:88:ARG:HD3	2:H:201:SO4:O3	2.14	0.48
1:H:7:TYR:OH	1:G:42:ALA:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:LYS:O	1:E:21:ASP:HB2	2.15	0.47
1:E:33:GLN:NE2	1:E:71:LEU:HD13	2.29	0.47
1:E:9:PHE:HE1	1:F:131:LEU:HD11	1.80	0.47
1:A:4:THR:OG1	1:B:112:GLU:HG3	2.14	0.47
1:B:40:LEU:HD23	1:B:48:LEU:HD23	1.97	0.46
1:H:81:VAL:HG11	1:H:86:THR:HG22	1.96	0.46
1:H:97:GLY:O	1:H:101:VAL:HG12	2.15	0.46
1:B:9:PHE:O	1:B:13:SER:HB2	2.15	0.46
1:C:54:ALA:HA	1:C:64:VAL:HG21	1.98	0.46
1:H:36:THR:HG23	1:H:53:ILE:HD12	1.97	0.46
1:B:3:PHE:H	1:B:3:PHE:HD2	1.64	0.46
1:F:60:THR:O	1:F:63:THR:OG1	2.31	0.46
1:C:50:GLN:HG3	1:C:68:LEU:CD1	2.46	0.46
1:C:40:LEU:HD23	1:C:48:LEU:HD12	1.97	0.45
1:A:50:GLN:HB2	3:A:311:HOH:O	2.15	0.45
1:H:23:LYS:HD2	1:H:107:ILE:HG21	1.98	0.45
1:B:7:TYR:CZ	1:B:11:MET:HG2	2.52	0.45
1:C:109:ASP:H	1:C:112:GLU:HB3	1.82	0.45
1:E:110:GLU:O	1:E:113:GLN:HG2	2.16	0.45
1:B:16:MET:CE	1:B:115:LEU:HD11	2.42	0.45
1:D:7:TYR:CZ	1:D:11:MET:HG3	2.51	0.45
1:E:35:HIS:HE1	1:F:2:GLU:O	1.99	0.45
1:D:30:THR:HG22	1:D:32:GLU:N	2.32	0.44
1:F:60:THR:HB	1:F:62:PRO:HD2	1.99	0.44
1:G:8:LEU:O	1:G:12:ILE:HD12	2.17	0.44
1:D:129:ALA:O	1:D:132:THR:HG22	2.17	0.44
1:H:8:LEU:HD12	1:H:8:LEU:HA	1.55	0.44
1:H:128:LYS:HE2	1:G:3:PHE:O	2.18	0.44
1:C:109:ASP:HB3	1:C:112:GLU:H	1.81	0.44
1:A:24:LEU:HD23	1:A:31:ASN:HA	2.00	0.44
1:H:5:TYR:OH	1:G:124:ASN:OD1	2.18	0.44
1:H:5:TYR:OH	1:G:127:MET:HG2	2.18	0.44
1:A:12:ILE:O	1:A:16:MET:HB2	2.17	0.43
1:D:23:LYS:NZ	1:D:30:THR:HG23	2.33	0.43
1:C:17:LYS:N	1:C:18:PRO:HD2	2.33	0.43
1:C:19:LYS:HG3	3:C:253:HOH:O	2.17	0.43
1:F:43:HIS:HB2	1:F:48:LEU:CD1	2.48	0.43
1:H:14:HIS:ND1	1:G:35:HIS:HB2	2.33	0.43
1:E:30:THR:HG23	2:F:201:SO4:O3	2.18	0.43
1:F:75:LYS:HD3	1:F:75:LYS:HA	1.89	0.43
1:G:50:GLN:OE1	1:G:79:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:HD23	1:D:48:LEU:HD12	2.00	0.43
1:B:97:GLY:O	1:B:101:VAL:HG23	2.19	0.43
1:D:6:SER:O	1:D:10:ARG:HB3	2.18	0.43
1:G:61:GLY:N	1:G:62:PRO:HD2	2.34	0.43
1:C:9:PHE:O	1:C:13:SER:HB2	2.19	0.43
1:E:69:ARG:NH2	1:E:79:ARG:HH22	2.16	0.43
1:E:23:LYS:HD3	1:E:23:LYS:HA	1.57	0.43
1:F:107:ILE:HG13	1:F:108:PHE:N	2.33	0.43
1:H:103:ALA:O	1:H:106:SER:HB3	2.19	0.43
1:D:138:LEU:O	1:D:139:GLN:HB2	2.18	0.42
1:H:10:ARG:HB3	1:H:10:ARG:HE	1.65	0.42
1:F:70:ASN:ND2	3:F:314:HOH:O	2.36	0.42
1:C:24:LEU:HD22	1:C:29:ILE:HD11	2.01	0.42
1:A:138:LEU:HB3	1:B:15:GLU:HG2	2.02	0.42
3:H:333:HOH:O	1:G:4:THR:CG2	2.68	0.42
1:B:3:PHE:N	1:B:3:PHE:CD2	2.88	0.42
1:C:77:ILE:HG22	1:C:93:LEU:HD23	2.02	0.42
1:G:55:LYS:HB2	1:G:55:LYS:HE3	1.68	0.42
1:D:115:LEU:HG	1:C:134:MET:HE3	2.01	0.42
1:E:70:ASN:O	1:E:74:LYS:HG3	2.19	0.42
1:B:8:LEU:O	1:B:12:ILE:HG13	2.19	0.42
1:C:139:GLN:OE1	3:C:248:HOH:O	2.22	0.42
1:D:54:ALA:HA	1:D:64:VAL:HG21	2.02	0.41
1:G:49:THR:O	1:G:53:ILE:HG13	2.20	0.41
1:G:82:ASP:HB3	1:G:85:ASP:O	2.20	0.41
1:C:16:MET:HB3	1:C:16:MET:HE3	1.89	0.41
1:D:16:MET:HE1	1:C:9:PHE:HB2	2.01	0.41
1:E:108:PHE:HA	1:E:111:MET:CG	2.51	0.41
1:E:16:MET:HE1	1:F:9:PHE:CB	2.50	0.41
1:C:104:PHE:CD1	1:C:104:PHE:C	2.94	0.41
1:E:60:THR:OG1	1:E:63:THR:OG1	2.37	0.41
1:D:39:TYR:HE1	1:C:14:HIS:CE1	2.39	0.41
1:F:119:LEU:HD13	1:F:127:MET:CE	2.51	0.41
1:G:35:HIS:CD2	1:G:57:LEU:HD23	2.56	0.41
1:A:111:MET:O	1:A:114:THR:OG1	2.30	0.41
1:B:94:THR:O	1:B:98:ILE:HG23	2.20	0.41
1:E:50:GLN:HG2	1:E:68:LEU:CD1	2.51	0.41
1:B:64:VAL:O	1:B:68:LEU:HG	2.20	0.41
1:E:72:GLU:OE2	1:E:79:ARG:HG3	2.21	0.41
1:B:124:ASN:O	1:B:128:LYS:HB2	2.19	0.41
1:E:16:MET:HB2	1:E:16:MET:HE2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD21	1:B:9:PHE:CE1	2.56	0.41
1:F:8:LEU:O	1:F:12:ILE:HG13	2.21	0.41
1:A:108:PHE:HE1	1:A:116:VAL:HG21	1.86	0.40
1:C:19:LYS:HE2	1:C:111:MET:HB2	2.03	0.40
1:A:68:LEU:HD23	1:A:68:LEU:HA	1.79	0.40
1:E:45:GLN:NE2	3:H:312:HOH:O	2.55	0.40
1:E:112:GLU:OE1	1:F:5:TYR:HB2	2.22	0.40
1:G:61:GLY:HA2	1:G:64:VAL:HG12	2.04	0.40
1:B:3:PHE:HD1	1:B:7:TYR:CD1	2.39	0.40
1:C:21:ASP:OD1	1:C:31:ASN:ND2	2.54	0.40
3:H:333:HOH:O	1:G:4:THR:HB	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	136/145 (94%)	135 (99%)	1 (1%)	0	100	100
1	B	120/145 (83%)	117 (98%)	3 (2%)	0	100	100
1	C	137/145 (94%)	136 (99%)	1 (1%)	0	100	100
1	D	137/145 (94%)	125 (91%)	11 (8%)	1 (1%)	22	32
1	E	135/145 (93%)	134 (99%)	1 (1%)	0	100	100
1	F	137/145 (94%)	136 (99%)	1 (1%)	0	100	100
1	G	137/145 (94%)	137 (100%)	0	0	100	100
1	H	137/145 (94%)	137 (100%)	0	0	100	100
All	All	1076/1160 (93%)	1057 (98%)	18 (2%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	21	ASP

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	102/132 (77%)	81 (79%)	21 (21%)	1	1
1	B	82/132 (62%)	58 (71%)	24 (29%)	0	0
1	C	118/132 (89%)	100 (85%)	18 (15%)	2	3
1	D	107/132 (81%)	92 (86%)	15 (14%)	3	4
1	E	103/132 (78%)	85 (82%)	18 (18%)	2	2
1	F	94/132 (71%)	72 (77%)	22 (23%)	1	1
1	G	101/132 (76%)	80 (79%)	21 (21%)	1	1
1	H	120/132 (91%)	92 (77%)	28 (23%)	1	1
All	All	827/1056 (78%)	660 (80%)	167 (20%)	1	1

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	13	SER
1	A	16	MET
1	A	31	ASN
1	A	32	GLU
1	A	44	GLN
1	A	45	GLN
1	A	57	LEU
1	A	59	ARG
1	A	60	THR
1	A	67	LEU
1	A	69	ARG
1	A	73	ARG
1	A	89	LYS
1	A	95	THR

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Mol	Chain	Res	Type
1	A	106	SER
1	A	108	PHE
1	A	116	VAL
1	A	118	GLN
1	A	131	LEU
1	A	137	SER
1	E	4	THR
1	E	5	TYR
1	E	8	LEU
1	E	13	SER
1	E	19	LYS
1	E	21	ASP
1	E	22	GLN
1	E	26	GLN
1	E	46	ASP
1	E	63	THR
1	E	71	LEU
1	E	75	LYS
1	E	79	ARG
1	E	87	ARG
1	E	89	LYS
1	E	100	LEU
1	E	111	MET
1	E	123	GLU
1	F	6	SER
1	F	8	LEU
1	F	23	LYS
1	F	24	LEU
1	F	26	GLN
1	F	28	ASP
1	F	40	LEU
1	F	48	LEU
1	F	49	THR
1	F	60	THR
1	F	66	ASN
1	F	72	GLU
1	F	85	ASP
1	F	86	THR
1	F	90	ASN
1	F	91	ILE
1	F	95	THR
1	F	104	PHE

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Mol	Chain	Res	Type
1	F	124	ASN
1	F	127	MET
1	F	132	THR
1	F	137	SER
1	H	4	THR
1	H	6	SER
1	H	8	LEU
1	H	10	ARG
1	H	16	MET
1	H	17	LYS
1	H	22	GLN
1	H	23	LYS
1	H	25	GLU
1	H	26	GLN
1	H	30	THR
1	H	46	ASP
1	H	59	ARG
1	H	75	LYS
1	H	84	GLN
1	H	87	ARG
1	H	89	LYS
1	H	101	VAL
1	H	117	SER
1	H	121	GLU
1	H	122	GLU
1	H	123	GLU
1	H	126	GLN
1	H	127	MET
1	H	128	LYS
1	H	132	THR
1	H	136	SER
1	H	139	GLN
1	D	2	GLU
1	D	6	SER
1	D	10	ARG
1	D	22	GLN
1	D	44	GLN
1	D	45	GLN
1	D	58	GLN
1	D	66	ASN
1	D	67	LEU
1	D	73	ARG

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Mol	Chain	Res	Type
1	D	107	ILE
1	D	115	LEU
1	D	120	SER
1	D	132	THR
1	D	139	GLN
1	C	11	MET
1	C	13	SER
1	C	15	GLU
1	C	19	LYS
1	C	26	GLN
1	C	31	ASN
1	C	32	GLU
1	C	51	ASN
1	C	60	THR
1	C	65	SER
1	C	72	GLU
1	C	73	ARG
1	C	84	GLN
1	C	86	THR
1	C	104	PHE
1	C	105	THR
1	C	136	SER
1	C	138	LEU
1	B	3	PHE
1	B	11	MET
1	B	13	SER
1	B	15	GLU
1	B	16	MET
1	B	36	THR
1	B	44	GLN
1	B	45	GLN
1	B	67	LEU
1	B	73	ARG
1	B	75	LYS
1	B	79	ARG
1	B	80	TYR
1	B	98	ILE
1	B	104	PHE
1	B	106	SER
1	B	108	PHE
1	B	109	ASP
1	B	111	MET

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Mol	Chain	Res	Type
1	B	120	SER
1	B	121	GLU
1	B	128	LYS
1	B	130	ASN
1	B	135	LEU
1	G	13	SER
1	G	15	GLU
1	G	21	ASP
1	G	30	THR
1	G	45	GLN
1	G	63	THR
1	G	67	LEU
1	G	71	LEU
1	G	75	LYS
1	G	79	ARG
1	G	85	ASP
1	G	91	ILE
1	G	93	LEU
1	G	102	GLU
1	G	105	THR
1	G	109	ASP
1	G	112	GLU
1	G	117	SER
1	G	127	MET
1	G	136	SER
1	G	137	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	35	HIS
1	E	45	GLN
1	D	118	GLN
1	B	44	GLN
1	G	118	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	H	201	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	E	201	-	4,4,4	0.16	0	6,6,6	0.17	0
2	SO4	A	201	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	H	202	-	4,4,4	0.13	0	6,6,6	0.12	0
2	SO4	H	203	-	4,4,4	0.14	0	6,6,6	0.81	0
2	SO4	F	201	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	H	204	-	4,4,4	0.22	0	6,6,6	0.38	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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	201	SO4	2	0
2	E	201	SO4	2	0
2	F	201	SO4	2	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	138/145 (95%)	0.14	2 (1%) 75 73	39, 73, 100, 108	0
1	B	126/145 (86%)	0.59	17 (13%) 3 2	55, 85, 129, 152	0
1	C	139/145 (95%)	0.22	0 100 100	21, 43, 72, 82	0
1	D	139/145 (95%)	0.14	5 (3%) 42 42	22, 53, 102, 124	0
1	E	137/145 (94%)	0.17	7 (5%) 28 26	36, 60, 106, 117	0
1	F	139/145 (95%)	0.38	13 (9%) 8 7	47, 76, 114, 123	0
1	G	139/145 (95%)	-0.01	3 (2%) 62 60	34, 62, 106, 131	0
1	H	139/145 (95%)	0.11	1 (0%) 87 86	19, 43, 73, 88	0
All	All	1096/1160 (94%)	0.21	48 (4%) 34 33	19, 63, 107, 152	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	ALA	4.8
1	B	47	GLY	4.8
1	E	8	LEU	4.6
1	E	9	PHE	4.6
1	B	48	LEU	4.4
1	D	83	ALA	4.1
1	F	39	TYR	4.0
1	B	91	ILE	3.7
1	B	79	ARG	3.7
1	D	24	LEU	3.6
1	E	5	TYR	3.5
1	F	119	LEU	3.5
1	B	46	ASP	3.5
1	G	1	MET	3.4
1	B	107	ILE	3.2
1	E	12	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	56	ALA	2.9
1	F	5	TYR	2.8
1	F	62	PRO	2.8
1	B	36	THR	2.8
1	E	108	PHE	2.7
1	E	111	MET	2.7
1	G	104	PHE	2.6
1	D	84	GLN	2.6
1	A	108	PHE	2.5
1	F	108	PHE	2.5
1	G	61	GLY	2.5
1	B	44	GLN	2.4
1	F	48	LEU	2.4
1	F	131	LEU	2.4
1	F	38	GLY	2.4
1	F	8	LEU	2.4
1	F	37	LEU	2.3
1	B	135	LEU	2.3
1	A	107	ILE	2.3
1	B	97	GLY	2.2
1	F	109	ASP	2.2
1	B	136	SER	2.2
1	D	138	LEU	2.2
1	B	78	TYR	2.1
1	D	22	GLN	2.1
1	B	35	HIS	2.1
1	E	128	LYS	2.1
1	B	50	GLN	2.1
1	B	80	TYR	2.1
1	F	58	GLN	2.1
1	B	64	VAL	2.0
1	H	137	SER	2.0

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 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(Å ²)	Q<0.9
2	SO4	H	202	5/5	0.94	0.18	104,104,106,106	0
2	SO4	E	201	5/5	0.95	0.23	98,102,104,104	0
2	SO4	F	201	5/5	0.95	0.09	59,66,69,73	0
2	SO4	H	203	5/5	0.96	0.13	57,57,59,65	0
2	SO4	A	201	5/5	0.96	0.13	85,87,88,89	0
2	SO4	H	201	5/5	0.98	0.17	81,87,93,97	0
2	SO4	H	204	5/5	0.98	0.14	40,42,47,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.