



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:06 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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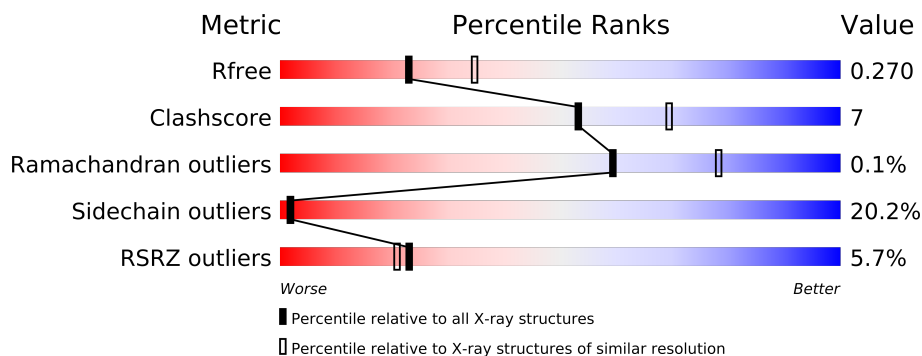
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	145	
1	B	145	
1	C	145	
1	D	145	
1	E	145	
1	F	145	
1	G	145	
1	H	145	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8554 atoms, of which 0 are hydrogen and 0 are deuterium.

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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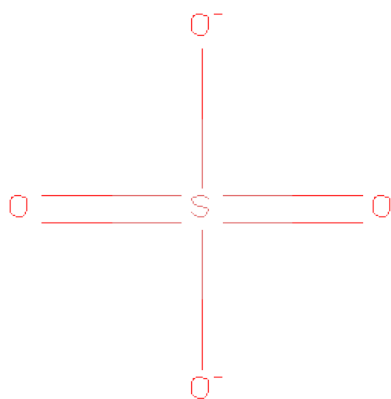
Chain	Residue	Modelled	Actual	Comment	Reference
E	145	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	18	PRO	GLN	ENGINEERED MUTATION	UNP Q5Y812
F	140	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	141	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	142	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	143	HIS	-	EXPRESSION TAG	UNP Q5Y812
F	144	HIS	-	EXPRESSION 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: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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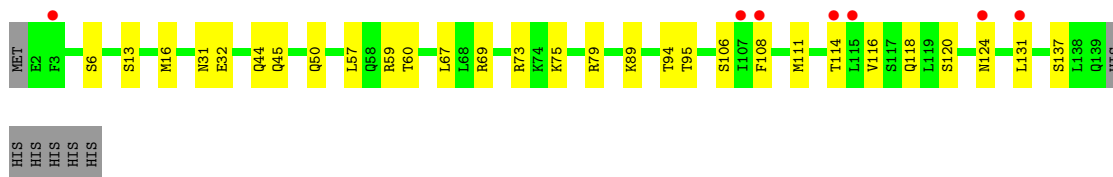
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	19	Total 19	O 19	0	0
3	H	47	Total 47	O 47	0	0
3	D	33	Total 33	O 33	0	0
3	C	53	Total 53	O 53	0	0
3	B	8	Total 8	O 8	0	0
3	G	16	Total 16	O 16	0	0

### 3 Residue-property plots

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.

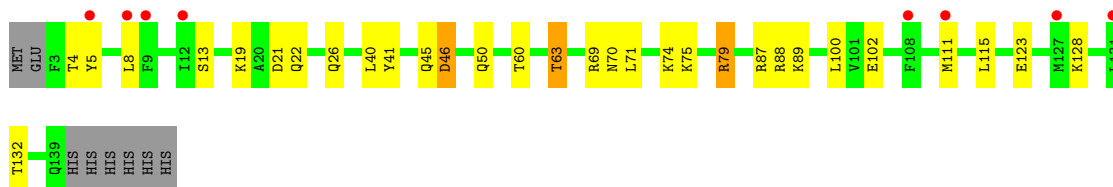
- Molecule 1: MepR

Chain A: 



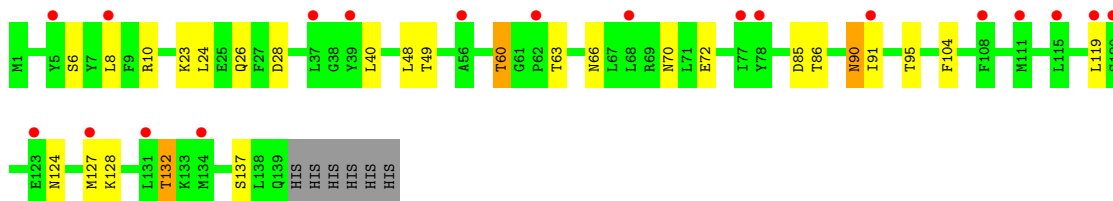
- Molecule 1: MepR

Chain E: 



- Molecule 1: MepR

Chain F: 



- Molecule 1: MepR

Chain H: 



- Molecule 1: MepR

Chain D: 



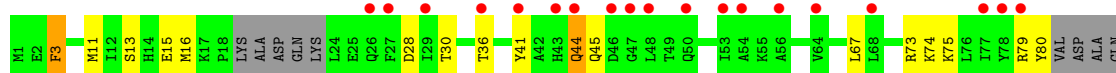
- Molecule 1: MepR

Chain C:



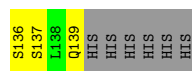
- Molecule 1: MepR

Chain B:



- Molecule 1: MepR

Chain G:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.211 , 0.268 0.212 , 0.270	Depositor DCC
$R_{free}$ test set	1958 reflections (3.90%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.4	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 51322 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1035	0	0	5	0
1	B	914	0	0	4	0
1	C	1106	0	0	6	0
1	D	1054	0	0	11	0
1	E	1039	0	0	12	0
1	F	1012	0	0	5	0
1	G	1035	0	0	10	0
1	H	1108	0	0	6	0
2	A	5	0	0	0	0
2	E	5	0	0	3	0
2	F	5	0	0	1	0
2	H	20	0	0	1	0
3	A	12	0	0	1	0
3	B	8	0	0	1	0
3	C	53	0	0	4	0
3	D	33	0	0	8	0
3	E	28	0	0	2	0
3	F	19	0	0	2	0
3	G	16	0	0	4	0
3	H	47	0	0	5	0
All	All	8554	0	0	58	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (58) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:73:ARG:NE	3:D:223:HOH:O	1.95	0.98
1:A:50:GLN:OE1	1:A:79:ARG:NH1	2.02	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:112:GLU:OE1	3:D:204:HOH:O	1.93	0.86
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: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:E:70:ASN:OD1	1:E:74:LYS:NZ	2.20	0.74
1:C:19:LYS:O	3:C:253:HOH:O	2.05	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:D:51:ASN:N	3:D:207:HOH:O	2.20	0.72
1:D:60:THR:OG1	1:D:63:THR:OG1	2.09	0.71
1:B:41:TYR:O	1:B:44:GLN:NE2	2.26	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:E:46:ASP:N	1:E:46:ASP:OD1	2.27	0.67
1:D:82:ASP:OD2	3:D:232:HOH:O	2.11	0.66
1:E:88:ARG:NH1	3:E:302:HOH:O	2.29	0.65
1:B:30:THR:O	3:B:201:HOH:O	2.14	0.65
1:G:48:LEU:N	3:G:205:HOH:O	2.30	0.65
1:A:120:SER:O	1:A:124:ASN:ND2	2.30	0.65
1:H:59:ARG:O	3:H:338:HOH:O	2.15	0.65
1:C:80:TYR:OH	3:C:232:HOH:O	2.14	0.64
1:E:50:GLN:OE1	1:E:79:ARG:NH1	2.31	0.64
1:H:5:TYR:N	1:G:112:GLU:OE1	2.31	0.63
1:H:128:LYS:O	1:H:132:THR:OG1	2.17	0.63
1:H:5:TYR:OH	1:G:124:ASN:OD1	2.18	0.61
1:C:108:PHE:N	3:C:241:HOH:O	2.34	0.60
1:F:70:ASN:ND2	3:F:314:HOH:O	2.36	0.58
1:D:72:GLU:OE1	1:D:79:ARG:NH2	2.36	0.58
1:E:128:LYS:O	1:E:132:THR:OG1	2.22	0.56
1:F:128:LYS:O	1:F:132:THR:OG1	2.25	0.54
1:D:63:THR:O	1:D:66:ASN:ND2	2.43	0.51
1:F:10:ARG:NH2	2:F:201:SO4:O4	2.44	0.50
1:A:111:MET:O	1:A:114:THR:OG1	2.30	0.49
1:D:33:GLN:NE2	3:D:212:HOH:O	2.45	0.49
1:F:60:THR:O	1:F:63:THR:OG1	2.31	0.48
1:A:75:LYS:NZ	3:A:308:HOH:O	2.45	0.48
1:F:90:ASN:ND2	3:F:316:HOH:O	2.46	0.48
1:E:69:ARG:NH2	2:E:201:SO4:O2	2.46	0.48
1:G:41:TYR:OH	1:G:102:GLU:OE1	2.33	0.47
1:H:89:LYS:NZ	3:H:311:HOH:O	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:10:ARG:NE	3:D:227:HOH:O	2.48	0.45
1:H:72:GLU:OE1	1:H:79:ARG:NH2	2.50	0.44
1:E:115:LEU:N	3:E:305:HOH:O	2.51	0.44
1:G:50:GLN:OE1	1:G:79:ARG:NH1	2.51	0.43
1:B:28:ASP:OD2	1:B:74:LYS:NZ	2.52	0.43
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:139:GLN:OE1	3:C:248:HOH:O	2.22	0.42
1:E:60:THR:OG1	1:E:63:THR:OG1	2.37	0.41
1:A:75:LYS:O	1:A:94:THR:OG1	2.38	0.41
1:C:21:ASP:OD1	1:C:31:ASN:ND2	2.54	0.41
1:C:104:PHE:C	1:C:104:PHE:CD1	2.94	0.41
1:E:41:TYR:OH	1:E:102:GLU:OE2	2.39	0.40
1:E:45:GLN:NE2	3:H:312:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 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	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%)	30	43
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%)	59	78

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%)	2	2
1	B	82/132 (62%)	58 (71%)	24 (29%)	0	0
1	C	118/132 (89%)	100 (85%)	18 (15%)	4	5
1	D	107/132 (81%)	92 (86%)	15 (14%)	5	6
1	E	103/132 (78%)	85 (82%)	18 (18%)	3	3
1	F	94/132 (71%)	72 (77%)	22 (23%)	1	1
1	G	101/132 (76%)	80 (79%)	21 (21%)	2	2
1	H	120/132 (91%)	92 (77%)	28 (23%)	1	1
All	All	827/1056 (78%)	660 (80%)	167 (20%)	2	2

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
1	A	106	SER
1	A	108	PHE

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Mol	Chain	Res	Type
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
1	F	124	ASN
1	F	127	MET

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Mol	Chain	Res	Type
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
1	D	107	ILE
1	D	115	LEU

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Mol	Chain	Res	Type
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
1	B	120	SER
1	B	121	GLU

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Mol	Chain	Res	Type
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. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	A	201	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	E	201	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	F	201	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	H	201	-	4,4,4	0.20	0	6,6,6	0.19	0
2	SO4	H	202	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	H	203	-	4,4,4	0.15	0	6,6,6	0.83	0
2	SO4	H	204	-	4,4,4	0.21	0	6,6,6	0.26	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
2	SO4	A	201	-	-	0/0/0/0	0/0/0/0
2	SO4	E	201	-	-	0/0/0/0	0/0/0/0
2	SO4	F	201	-	-	0/0/0/0	0/0/0/0
2	SO4	H	201	-	-	0/0/0/0	0/0/0/0
2	SO4	H	202	-	-	0/0/0/0	0/0/0/0
2	SO4	H	203	-	-	0/0/0/0	0/0/0/0
2	SO4	H	204	-	-	0/0/0/0	0/0/0/0

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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	138/145 (95%)	0.27	7 (5%) 27 25	39, 73, 100, 108	0
1	B	126/145 (86%)	0.70	22 (17%) 2 1	55, 85, 129, 152	0
1	C	139/145 (95%)	0.33	1 (0%) 84 84	21, 43, 72, 82	0
1	D	139/145 (95%)	0.17	2 (1%) 72 71	22, 53, 102, 124	0
1	E	137/145 (94%)	0.29	8 (5%) 22 20	36, 60, 106, 117	0
1	F	139/145 (95%)	0.56	19 (13%) 4 3	47, 76, 114, 123	0
1	G	139/145 (95%)	0.14	4 (2%) 49 47	34, 62, 106, 131	0
1	H	139/145 (95%)	0.14	0 100 100	19, 43, 73, 88	0
All	All	1096/1160 (94%)	0.32	63 (5%) 23 21	19, 63, 107, 152	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5	TYR	6.3
1	E	9	PHE	6.2
1	B	48	LEU	5.8
1	E	8	LEU	5.5
1	B	54	ALA	4.8
1	B	47	GLY	4.4
1	B	91	ILE	4.3
1	F	37	LEU	4.3
1	F	5	TYR	4.1
1	F	119	LEU	3.9
1	F	131	LEU	3.9
1	E	12	ILE	3.9
1	F	108	PHE	3.7
1	G	104	PHE	3.6
1	B	50	GLN	3.5
1	F	123	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	83	ALA	3.4
1	B	53	ILE	3.3
1	B	46	ASP	3.3
1	A	108	PHE	3.1
1	B	64	VAL	3.1
1	B	41	TYR	3.0
1	B	44	GLN	3.0
1	B	79	ARG	3.0
1	E	131	LEU	2.9
1	G	61	GLY	2.9
1	B	77	ILE	2.8
1	D	84	GLN	2.8
1	B	27	PHE	2.8
1	B	36	THR	2.8
1	B	43	HIS	2.8
1	G	1	MET	2.7
1	F	8	LEU	2.7
1	F	77	ILE	2.6
1	F	115	LEU	2.5
1	F	68	LEU	2.5
1	F	78	TYR	2.5
1	B	56	ALA	2.5
1	F	91	ILE	2.4
1	F	62	PRO	2.4
1	A	107	ILE	2.3
1	E	127	MET	2.3
1	B	68	LEU	2.3
1	A	3	PHE	2.3
1	F	39	TYR	2.3
1	F	127	MET	2.3
1	F	111	MET	2.3
1	E	108	PHE	2.2
1	B	29	ILE	2.2
1	A	124	ASN	2.1
1	B	107	ILE	2.1
1	G	62	PRO	2.1
1	F	134	MET	2.1
1	B	26	GLN	2.1
1	B	78	TYR	2.1
1	B	135	LEU	2.1
1	A	115	LEU	2.1
1	F	120	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	131	LEU	2.0
1	C	139	GLN	2.0
1	F	56	ALA	2.0
1	E	111	MET	2.0
1	A	114	THR	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 ⓘ

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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	E	201	5/5	0.15	-0.16	98,102,104,104	0
2	SO4	H	202	5/5	0.13	-0.74	104,104,106,106	0
2	SO4	H	201	5/5	0.15	-1.19	81,87,93,97	0
2	SO4	A	201	5/5	0.12	-1.52	85,87,88,89	0
2	SO4	H	203	5/5	0.13	-1.53	57,57,59,65	0
2	SO4	F	201	5/5	0.08	-1.57	59,66,69,73	0
2	SO4	H	204	5/5	0.14	-2.97	40,42,47,55	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.