



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:58 PM GMT

PDB ID : 4B4M  
Title : Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor  
Authors : Alphey, M.S.; Pirrie, L.; Torrie, L.S.; Gardiner, M.; Westwood, N.J.; Gray, D.; Naismith, J.H.  
Deposited on : 2012-07-31  
Resolution : 2.35 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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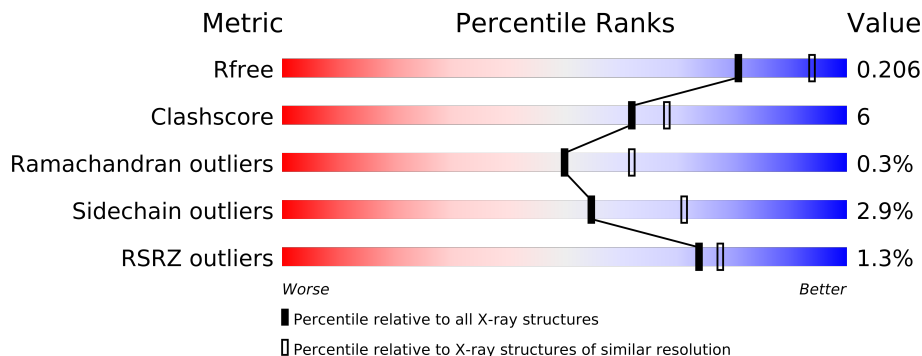
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	303	
1	B	303	
1	C	303	
1	D	303	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	A	1294	-	X
3	CL	C	1294	-	X
4	MES	A	1295	-	X
4	MES	B	1295	-	X
4	MES	C	1295	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9651 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	1	0
			2329	1489	396	439	5			
1	B	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			
1	C	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			
1	D	293	Total	C	N	O	S	0	1	0
			2299	1471	387	436	5			

There are 40 discrepancies between the modelled and reference sequences:

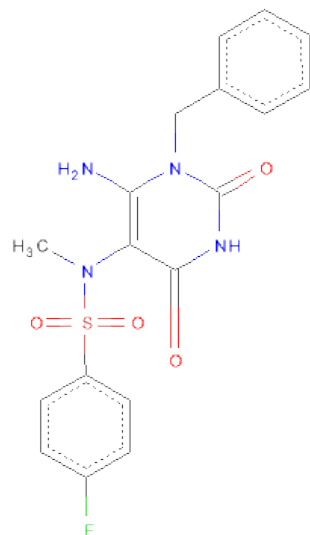
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	EXPRESSION TAG	UNP Q9HU22
A	-9	HIS	-	EXPRESSION TAG	UNP Q9HU22
A	-8	HIS	-	EXPRESSION TAG	UNP Q9HU22
A	-7	HIS	-	EXPRESSION TAG	UNP Q9HU22
A	-6	HIS	-	EXPRESSION TAG	UNP Q9HU22
A	-5	HIS	-	EXPRESSION TAG	UNP Q9HU22
A	-4	GLY	-	EXPRESSION TAG	UNP Q9HU22
A	-3	SER	-	EXPRESSION TAG	UNP Q9HU22
A	-2	MET	-	EXPRESSION TAG	UNP Q9HU22
A	-1	ALA	-	EXPRESSION TAG	UNP Q9HU22
B	-10	HIS	-	EXPRESSION TAG	UNP Q9HU22
B	-9	HIS	-	EXPRESSION TAG	UNP Q9HU22
B	-8	HIS	-	EXPRESSION TAG	UNP Q9HU22
B	-7	HIS	-	EXPRESSION TAG	UNP Q9HU22
B	-6	HIS	-	EXPRESSION TAG	UNP Q9HU22
B	-5	HIS	-	EXPRESSION TAG	UNP Q9HU22
B	-4	GLY	-	EXPRESSION TAG	UNP Q9HU22
B	-3	SER	-	EXPRESSION TAG	UNP Q9HU22
B	-2	MET	-	EXPRESSION TAG	UNP Q9HU22
B	-1	ALA	-	EXPRESSION TAG	UNP Q9HU22

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	EXPRESSION TAG	UNP Q9HU22
C	-9	HIS	-	EXPRESSION TAG	UNP Q9HU22
C	-8	HIS	-	EXPRESSION TAG	UNP Q9HU22
C	-7	HIS	-	EXPRESSION TAG	UNP Q9HU22
C	-6	HIS	-	EXPRESSION TAG	UNP Q9HU22
C	-5	HIS	-	EXPRESSION TAG	UNP Q9HU22
C	-4	GLY	-	EXPRESSION TAG	UNP Q9HU22
C	-3	SER	-	EXPRESSION TAG	UNP Q9HU22
C	-2	MET	-	EXPRESSION TAG	UNP Q9HU22
C	-1	ALA	-	EXPRESSION TAG	UNP Q9HU22
D	-10	HIS	-	EXPRESSION TAG	UNP Q9HU22
D	-9	HIS	-	EXPRESSION TAG	UNP Q9HU22
D	-8	HIS	-	EXPRESSION TAG	UNP Q9HU22
D	-7	HIS	-	EXPRESSION TAG	UNP Q9HU22
D	-6	HIS	-	EXPRESSION TAG	UNP Q9HU22
D	-5	HIS	-	EXPRESSION TAG	UNP Q9HU22
D	-4	GLY	-	EXPRESSION TAG	UNP Q9HU22
D	-3	SER	-	EXPRESSION TAG	UNP Q9HU22
D	-2	MET	-	EXPRESSION TAG	UNP Q9HU22
D	-1	ALA	-	EXPRESSION TAG	UNP Q9HU22

- Molecule 2 is N-(6-AMINO-1-BENZYL-2,4-DIOXO-1,2,3,4-TETRAHYDROPYRIMIDI N-5-YL)-4-FLUORO-N-METHYLBENZENESULFONAMIDE (three-letter code: JWT) (formula: C<sub>18</sub>H<sub>17</sub>FN<sub>4</sub>O<sub>4</sub>S).

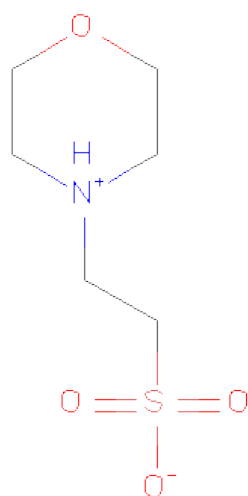


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	
			28	18	1	4	4	1	
2	B	1	Total	C	F	N	O	S	
			28	18	1	4	4	1	
2	C	1	Total	C	F	N	O	S	
			28	18	1	4	4	1	
2	D	1	Total	C	F	N	O	S	
			28	18	1	4	4	1	

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl		
			1	1	0	0
3	A	1	Total	Cl		
			1	1	0	0
3	D	1	Total	Cl		
			1	1	0	0
3	C	1	Total	Cl		
			1	1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S		
			12	6	1	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	63	Total	O	0	0
			63	63		
5	C	66	Total	O	0	0
			66	66		
5	D	51	Total	O	0	0
			51	51		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.16Å 153.96Å 134.75Å 90.00° 92.38° 90.00°	Depositor
Resolution (Å)	33.66 – 2.35 33.66 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.3 (33.66-2.35) 86.9 (33.66-2.34)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.183 , 0.237 0.183 , 0.206	Depositor DCC
$R_{free}$ test set	2743 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 21.0	EDS
Estimated twinning fraction	0.094 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 53967 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9651	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: JWT, MES, CL

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	0.56	2/2384 (0.1%)	0.65	0/3232
1	B	0.53	2/2352 (0.1%)	0.66	0/3190
1	C	0.54	0/2352	0.66	0/3190
1	D	0.52	1/2352 (0.0%)	0.63	1/3190 (0.0%)
All	All	0.54	5/9440 (0.1%)	0.65	1/12802 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	TRP	CD2-CE2	5.64	1.48	1.41
1	B	73	TRP	CD2-CE2	5.38	1.47	1.41
1	A	73	TRP	CD2-CE2	5.30	1.47	1.41
1	A	223	TRP	CD2-CE2	5.22	1.47	1.41
1	B	262	TRP	CD2-CE2	5.16	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	112	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2329	0	2315	28	0
1	B	2299	0	2292	35	0
1	C	2299	0	2292	22	0
1	D	2299	0	2292	45	0
2	A	28	0	17	0	0
2	B	28	0	17	0	0
2	C	28	0	17	1	0
2	D	28	0	17	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	13	3	0
4	C	12	0	13	0	0
4	D	12	0	13	5	0
5	A	81	0	0	4	0
5	B	63	0	0	2	0
5	C	66	0	0	1	0
5	D	51	0	0	3	0
All	All	9651	0	9311	107	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 6.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:OE1	1.80	1.00
1:C:23:ILE:HD13	1:D:23:ILE:HG12	1.50	0.94
1:D:58:GLN:HE21	1:D:58:GLN:H	1.19	0.91
1:C:23:ILE:HD12	1:C:28:LEU:HD23	1.54	0.88
1:B:4:LYS:HE3	1:B:98:PHE:O	1.74	0.86
1:D:154:GLY:O	4:D:1295:MES:H72	1.82	0.80
1:B:154:GLY:O	4:B:1295:MES:H32	1.89	0.72
1:A:30:VAL:HG11	1:A:112:LEU:HD21	1.73	0.71
1:A:2:LYS:HB3	5:A:2005:HOH:O	1.92	0.69
1:D:154:GLY:O	4:D:1295:MES:H32	1.93	0.68
1:C:23:ILE:HD12	1:C:28:LEU:CD2	2.23	0.68
1:D:24:SER:HB2	1:D:59:ASP:OD1	1.96	0.66
1:D:15:ARG:HB3	1:D:15:ARG:HH11	1.61	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:23:ILE:HG21	1:B:23:ILE:HG12	1.80	0.64
1:C:23:ILE:CD1	1:D:23:ILE:HG12	2.25	0.64
1:C:23:ILE:HG12	1:D:23:ILE:HG21	1.80	0.64
1:D:24:SER:CB	5:D:2007:HOH:O	2.46	0.63
1:B:234:GLU:HA	1:B:237[A]:GLN:HE21	1.65	0.62
1:B:12:SER:HB3	5:B:2006:HOH:O	2.01	0.60
1:D:58:GLN:NE2	1:D:58:GLN:H	1.97	0.59
1:B:189:LEU:HD11	1:B:202:VAL:HG23	1.85	0.58
1:A:2:LYS:HD2	5:A:2004:HOH:O	2.04	0.58
1:D:216:ILE:CG1	4:D:1295:MES:H21	2.32	0.58
1:A:234:GLU:HA	1:A:237[A]:GLN:HE21	1.69	0.58
1:A:23:ILE:HD13	1:B:23:ILE:HG12	1.86	0.57
1:A:2:LYS:CB	5:A:2005:HOH:O	2.52	0.57
1:B:23:ILE:HD13	1:B:28:LEU:HD21	1.86	0.57
1:C:25:LYS:NZ	1:C:110:ASP:OD2	2.34	0.56
1:B:284:LEU:HA	1:B:287:LEU:HD12	1.85	0.56
1:A:72:ASN:HB3	1:A:271:LEU:HD21	1.88	0.56
1:B:214:VAL:O	4:B:1295:MES:H81	2.05	0.55
1:D:58:GLN:HE21	1:D:58:GLN:N	1.97	0.55
1:A:19:ALA:HB1	1:B:29:PRO:HB3	1.89	0.54
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.89	0.53
1:B:122:LEU:CD2	1:B:175:LEU:HD21	2.39	0.53
1:A:233:LEU:HD11	1:B:237[A]:GLN:HG3	1.89	0.53
1:C:237[A]:GLN:HG2	1:D:237[A]:GLN:OE1	2.09	0.53
1:D:24:SER:HB3	5:D:2007:HOH:O	2.08	0.52
1:C:234:GLU:HA	1:C:237[A]:GLN:HE21	1.74	0.52
1:D:122:LEU:CD2	1:D:175:LEU:HD21	2.40	0.52
1:D:216:ILE:HG12	4:D:1295:MES:H21	1.92	0.51
1:A:2:LYS:HA	5:A:2004:HOH:O	2.11	0.50
1:A:26:GLN:OE1	1:A:26:GLN:N	2.39	0.50
1:B:127:GLN:HG3	1:B:128:ARG:N	2.26	0.50
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:HG2	2.12	0.49
1:D:122:LEU:HD21	1:D:175:LEU:HD21	1.94	0.49
1:D:24:SER:HB2	5:D:2007:HOH:O	2.11	0.49
1:A:23:ILE:HD11	1:B:28:LEU:HD23	1.94	0.49
1:D:23:ILE:HD12	1:D:23:ILE:H	1.78	0.49
1:B:1:MET:HB2	1:B:129:GLN:OE1	2.12	0.49
1:D:24:SER:HB2	1:D:59:ASP:CG	2.33	0.48
1:D:15:ARG:HB3	1:D:15:ARG:NH1	2.28	0.48
1:B:154:GLY:O	4:B:1295:MES:H71	2.13	0.48
1:A:28:LEU:HD22	1:B:29:PRO:CD	2.43	0.48
1:A:184:ASP:OD1	1:A:187:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:28:LEU:HD22	1:B:29:PRO:HD2	1.96	0.48
1:A:237[B]:GLN:HA	1:B:233:LEU:HD21	1.95	0.47
1:A:24:SER:HB3	1:A:59:ASP:OD2	2.14	0.47
1:B:55:SER:HB2	5:B:2005:HOH:O	2.13	0.47
1:A:233:LEU:HD21	1:B:237[A]:GLN:HA	1.95	0.47
1:B:30:VAL:HG11	1:B:112:LEU:HD11	1.97	0.47
1:A:233:LEU:HD21	1:B:237[B]:GLN:HA	1.96	0.47
1:A:142:PRO:HG3	1:A:169:ASN:HA	1.96	0.47
1:C:233:LEU:HD21	1:D:237[B]:GLN:HA	1.96	0.46
1:D:137:TYR:CD2	1:D:223:TRP:HE3	2.33	0.46
1:C:32:ASP:O	1:D:18:PRO:HD2	2.16	0.46
1:C:35:MET:O	1:C:39:PRO:HD2	2.15	0.46
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.97	0.45
1:D:283:TYR:O	1:D:287:LEU:HG	2.16	0.45
1:D:249:LYS:HD2	1:D:283:TYR:CD2	2.52	0.45
2:C:400:JWT:OAL	2:C:400:JWT:HAW	2.17	0.45
1:B:124:SER:HA	1:B:127:GLN:HG2	1.99	0.45
1:C:23:ILE:HG12	1:D:23:ILE:CG2	2.45	0.45
1:C:233:LEU:HD21	1:D:237[A]:GLN:HA	1.98	0.44
1:D:5:GLY:O	1:D:51:ILE:HA	2.18	0.44
1:B:38:TYR:CB	1:B:112:LEU:HD22	2.48	0.44
1:C:128:ARG:HD3	5:C:2027:HOH:O	2.18	0.44
1:D:133:SER:HB2	1:D:177:PHE:HB2	2.00	0.44
1:A:239:ILE:O	1:A:243:GLU:HG3	2.18	0.44
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:CD	2.51	0.43
1:B:141:ASP:OD2	1:B:144:ARG:HD3	2.18	0.43
1:D:162:LYS:HD2	1:D:194:ARG:HH22	1.83	0.43
1:A:237[A]:GLN:HA	1:B:233:LEU:HD21	2.00	0.43
1:B:23:ILE:HD12	1:B:23:ILE:H	1.83	0.43
1:C:237[A]:GLN:CD	1:D:237[A]:GLN:OE1	2.53	0.43
1:B:23:ILE:HD12	1:B:23:ILE:N	2.34	0.43
1:D:15:ARG:CB	1:D:15:ARG:HH11	2.27	0.42
1:D:54:ILE:HA	1:D:80:ALA:O	2.18	0.42
1:D:286:ARG:NH1	1:D:290:GLU:OE1	2.52	0.42
1:D:38:TYR:CG	1:D:112:LEU:HD22	2.54	0.42
1:A:35:MET:O	1:A:39:PRO:HD2	2.19	0.42
1:C:70:GLY:HA3	1:C:77:LEU:HG	2.01	0.42
1:B:54:ILE:HA	1:B:80:ALA:O	2.20	0.42
1:A:136:ALA:HA	1:A:171:ALA:O	2.19	0.42
1:A:105:ALA:HA	1:A:176:TYR:O	2.20	0.42
1:C:24:SER:HB2	1:C:59:ASP:CG	2.40	0.42
1:A:88:LEU:HD13	1:A:108:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:35:MET:O	1:D:39:PRO:HD2	2.20	0.41
1:D:234:GLU:HA	1:D:237[A]:GLN:HE21	1.85	0.41
1:B:249:LYS:HE3	1:B:280:TYR:CD2	2.55	0.41
1:D:216:ILE:HG13	4:D:1295:MES:H21	2.02	0.41
1:D:111:ASN:ND2	1:D:223:TRP:HE1	2.19	0.41
1:B:105:ALA:HA	1:B:176:TYR:O	2.21	0.41
1:C:237[A]:GLN:OE1	1:D:237[A]:GLN:CG	2.69	0.41
1:D:45:LEU:HD22	2:D:400:JWT:HAR	2.03	0.41
1:A:122:LEU:CD2	1:A:175:LEU:HD21	2.51	0.41
1:B:6:ILE:HD11	1:B:99:ILE:HD11	2.03	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	293/303 (97%)	284 (97%)	9 (3%)	0	100	100
1	B	292/303 (96%)	287 (98%)	4 (1%)	1 (0%)	50	62
1	C	292/303 (96%)	285 (98%)	6 (2%)	1 (0%)	50	62
1	D	292/303 (96%)	283 (97%)	8 (3%)	1 (0%)	50	62
All	All	1169/1212 (96%)	1139 (97%)	27 (2%)	3 (0%)	50	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	TYR
1	C	31	TYR
1	D	31	TYR

### 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	244/248 (98%)	237 (97%)	7 (3%)	55	71
1	B	241/248 (97%)	233 (97%)	8 (3%)	50	65
1	C	241/248 (97%)	235 (98%)	6 (2%)	60	76
1	D	241/248 (97%)	234 (97%)	7 (3%)	55	71
All	All	967/992 (98%)	939 (97%)	28 (3%)	55	71

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	111	ASN
1	A	126	SER
1	A	127	GLN
1	A	148	VAL
1	A	155	LYS
1	A	277	LYS
1	B	21	LEU
1	B	23	ILE
1	B	81	VAL
1	B	127	GLN
1	B	140	LEU
1	B	187	ARG
1	B	194	ARG
1	B	277	LYS
1	C	17	HIS
1	C	23	ILE
1	C	126	SER
1	C	127	GLN
1	C	130	THR
1	C	232	LEU
1	D	15	ARG
1	D	23	ILE
1	D	58	GLN
1	D	62	ARG
1	D	112	LEU

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Mol	Chain	Res	Type
1	D	126	SER
1	D	209	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	B	101	ASN
1	B	152	GLN
1	C	101	ASN
1	C	111	ASN
1	D	58	GLN
1	D	111	ASN
1	D	152	GLN

### 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 ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	MES	A	1295	-	12,12,12	1.87	1 (8%)	16,16,16	1.17	0
2	JWT	A	400	-	30,30,30	2.60	6 (20%)	40,44,44	2.12	11 (27%)
4	MES	B	1295	-	12,12,12	1.79	1 (8%)	16,16,16	2.58	4 (25%)
2	JWT	B	400	-	30,30,30	2.62	7 (23%)	40,44,44	2.46	11 (27%)
4	MES	C	1295	-	12,12,12	1.86	1 (8%)	16,16,16	1.59	4 (25%)
2	JWT	C	400	-	30,30,30	3.25	8 (26%)	40,44,44	2.54	12 (30%)
4	MES	D	1295	-	12,12,12	1.87	1 (8%)	16,16,16	1.57	3 (18%)
2	JWT	D	400	-	30,30,30	2.60	8 (26%)	40,44,44	2.14	9 (22%)

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
4	MES	A	1295	-	-	0/6/14/14	1/1/1/1
2	JWT	A	400	-	-	0/20/20/20	0/3/3/3
4	MES	B	1295	-	-	0/6/14/14	0/1/1/1
2	JWT	B	400	-	-	0/20/20/20	0/3/3/3
4	MES	C	1295	-	-	0/6/14/14	1/1/1/1
2	JWT	C	400	-	-	0/20/20/20	0/3/3/3
4	MES	D	1295	-	-	0/6/14/14	0/1/1/1
2	JWT	D	400	-	-	0/20/20/20	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	JWT	SAH-NAG	10.01	1.79	1.64
2	B	400	JWT	OAC-SAH	7.52	1.53	1.43
2	D	400	JWT	OAC-SAH	7.39	1.53	1.43
2	A	400	JWT	OAC-SAH	7.31	1.52	1.43
2	A	400	JWT	OAQ-SAH	7.13	1.52	1.43
2	B	400	JWT	CAF-NAG	-7.07	1.35	1.45
2	C	400	JWT	OAC-SAH	7.01	1.52	1.43
2	D	400	JWT	CAF-NAG	-6.99	1.35	1.45
2	A	400	JWT	CAF-NAG	-6.87	1.35	1.45
2	C	400	JWT	OAQ-SAH	6.63	1.52	1.43
2	C	400	JWT	FAM-CAT	-6.51	1.21	1.36
2	B	400	JWT	OAQ-SAH	6.42	1.51	1.43
2	C	400	JWT	CAF-NAG	-6.23	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	JWT	OAQ-SAH	5.94	1.51	1.43
4	D	1295	MES	C8-S	-5.86	1.67	1.78
4	A	1295	MES	C8-S	-5.77	1.68	1.78
4	C	1295	MES	C8-S	-5.61	1.68	1.78
4	B	1295	MES	C8-S	-5.54	1.68	1.78
2	A	400	JWT	SAH-NAG	4.49	1.71	1.64
2	D	400	JWT	CAU-CAV	-4.25	1.40	1.51
2	D	400	JWT	FAM-CAT	-3.52	1.28	1.36
2	C	400	JWT	CAU-CAV	-3.45	1.42	1.51
2	B	400	JWT	FAM-CAT	-3.36	1.28	1.36
2	C	400	JWT	CAM-NAN	-3.29	1.34	1.38
2	A	400	JWT	CAU-CAV	-3.23	1.43	1.51
2	B	400	JWT	SAH-NAG	3.14	1.69	1.64
2	B	400	JWT	CAU-CAV	-3.04	1.43	1.51
2	B	400	JWT	CAI-SAH	-3.03	1.71	1.76
2	D	400	JWT	CAM-NAN	-2.72	1.35	1.38
2	D	400	JWT	CAE-NAD	2.62	1.41	1.37
2	A	400	JWT	CAM-NAN	-2.52	1.35	1.38
2	D	400	JWT	CAM-NAD	2.50	1.42	1.37
2	C	400	JWT	CAE-NAD	2.16	1.40	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	JWT	OAC-SAH-OAQ	-7.66	105.72	119.38
2	C	400	JWT	CAM-NAN-CAO	-7.03	119.22	121.69
2	D	400	JWT	OAQ-SAH-NAG	6.84	114.97	106.84
4	B	1295	MES	C2-C3-N4	6.38	118.14	109.96
2	B	400	JWT	CAE-CAF-CAO	6.22	120.44	114.57
2	A	400	JWT	CAE-CAF-CAO	6.13	120.36	114.57
2	B	400	JWT	CAM-NAN-CAO	-6.03	119.58	121.69
2	D	400	JWT	CAE-CAF-CAO	6.02	120.26	114.57
2	C	400	JWT	OAQ-SAH-NAG	5.94	113.89	106.84
4	B	1295	MES	C6-C5-N4	5.58	117.12	109.96
2	A	400	JWT	OAC-SAH-OAQ	-5.38	109.78	119.38
2	B	400	JWT	OAC-SAH-NAG	5.32	113.17	106.84
2	D	400	JWT	OAC-SAH-OAQ	-5.16	110.17	119.38
2	C	400	JWT	CAE-CAF-CAO	4.99	119.28	114.57
2	B	400	JWT	OAC-SAH-OAQ	-4.93	110.59	119.38
2	A	400	JWT	OAQ-SAH-NAG	4.75	112.48	106.84
2	B	400	JWT	CAF-CAO-NAP	-4.44	116.03	124.61
2	B	400	JWT	CAU-NAN-CAM	4.42	121.33	117.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	JWT	CAF-CAO-NAP	-4.41	116.09	124.61
2	B	400	JWT	NAP-CAO-NAN	4.25	123.59	120.86
4	B	1295	MES	C5-N4-C3	4.13	117.93	109.75
2	C	400	JWT	OAC-SAH-NAG	3.96	111.55	106.84
4	D	1295	MES	C2-C3-N4	3.93	115.00	109.96
2	B	400	JWT	CAB-NAG-SAH	3.93	122.93	117.74
2	A	400	JWT	CAM-NAN-CAO	-3.80	120.36	121.69
2	D	400	JWT	CAF-CAO-NAP	-3.78	117.31	124.61
4	C	1295	MES	O2S-S-O1S	-3.65	105.39	112.44
2	A	400	JWT	CAF-CAO-NAP	-3.28	118.28	124.61
2	B	400	JWT	OAQ-SAH-NAG	2.99	110.40	106.84
4	C	1295	MES	O2S-S-C8	2.95	115.46	106.36
2	D	400	JWT	CAM-NAN-CAO	-2.93	120.66	121.69
2	A	400	JWT	OAC-SAH-NAG	2.88	110.27	106.84
2	C	400	JWT	CAF-NAG-SAH	2.76	123.70	118.91
2	D	400	JWT	CAE-NAD-CAM	-2.75	119.75	125.39
2	D	400	JWT	CAF-NAG-SAH	2.59	123.41	118.91
2	C	400	JWT	CAF-CAO-NAN	2.57	121.98	115.77
2	B	400	JWT	NAD-CAM-NAN	2.53	120.99	116.93
2	C	400	JWT	OAC-SAH-CAI	2.52	111.28	107.94
2	A	400	JWT	CAB-NAG-SAH	2.50	121.04	117.74
2	C	400	JWT	NAD-CAM-NAN	2.48	120.91	116.93
2	D	400	JWT	NAD-CAM-NAN	2.48	120.90	116.93
4	B	1295	MES	O3S-S-C8	2.35	112.07	105.99
2	A	400	JWT	CAE-NAD-CAM	-2.36	120.56	125.39
4	C	1295	MES	C2-C3-N4	2.33	112.95	109.96
2	B	400	JWT	CAE-NAD-CAM	-2.33	120.62	125.39
2	A	400	JWT	NAD-CAM-NAN	2.29	120.61	116.93
2	D	400	JWT	CAJ-CAK-CAT	2.27	120.73	118.33
2	A	400	JWT	CAF-NAG-SAH	2.21	122.75	118.91
4	C	1295	MES	C6-C5-N4	2.20	112.78	109.96
4	D	1295	MES	O1-C2-C3	2.19	113.95	111.34
2	C	400	JWT	CAB-NAG-SAH	2.16	120.60	117.74
4	D	1295	MES	O1S-S-C8	2.16	113.01	106.36
2	C	400	JWT	CAB-NAG-CAF	-2.08	115.12	117.12
2	A	400	JWT	OAC-SAH-CAI	2.05	110.67	107.94

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1295	MES	C2-C3-C5-C6-N4-O1
4	C	1295	MES	C2-C3-C5-C6-N4-O1

## 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	296/303 (97%)	-0.36	0 100 100	26, 39, 63, 87	3 (1%)
1	B	293/303 (96%)	-0.28	0 100 100	30, 43, 64, 80	2 (0%)
1	C	293/303 (96%)	-0.17	10 (3%) 43 47	26, 40, 79, 129	2 (0%)
1	D	293/303 (96%)	-0.27	5 (1%) 67 70	30, 45, 70, 98	2 (0%)
All	All	1175/1212 (96%)	-0.27	15 (1%) 74 77	26, 42, 69, 129	9 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	LEU	3.8
1	C	191	PRO	3.5
1	D	22	ALA	3.4
1	D	23	ILE	3.0
1	C	88	LEU	2.9
1	D	194	ARG	2.7
1	D	1	MET	2.6
1	C	193	PRO	2.5
1	C	195	GLY	2.4
1	C	21	LEU	2.4
1	C	1	MET	2.4
1	D	190	LYS	2.3
1	C	194	ARG	2.2
1	C	23	ILE	2.2
1	C	190	LYS	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 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
3	CL	A	1294	1/1	0.17	7.54	34,34,34,34	0
3	CL	C	1294	1/1	0.14	2.90	30,30,30,30	0
4	MES	B	1295	12/12	0.21	2.85	62,69,72,75	0
4	MES	C	1295	12/12	0.17	2.73	50,58,63,64	0
4	MES	A	1295	12/12	0.19	2.66	55,65,70,72	0
3	CL	D	1294	1/1	0.12	1.09	37,37,37,37	0
2	JWT	A	400	28/28	0.11	0.80	31,36,44,47	0
3	CL	B	1294	1/1	0.11	0.67	41,41,41,41	0
4	MES	D	1295	12/12	0.14	0.58	57,64,66,67	0
2	JWT	B	400	28/28	0.11	0.43	35,43,46,47	0
2	JWT	C	400	28/28	0.10	-0.46	28,34,38,42	0
2	JWT	D	400	28/28	0.09	-0.46	36,41,44,44	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.