



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:42 pm GMT

PDB ID : 4B4B  
Title : Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor  
Authors : Alphey, M.S.; Pirrie, L.; Torrie, L.S.; Gardiner, M.; Sarkar, A.; Brenk, R.;  
Westwood, N.J.; Gray, D.; Naismith, J.H.  
Deposited on : 2012-07-30  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

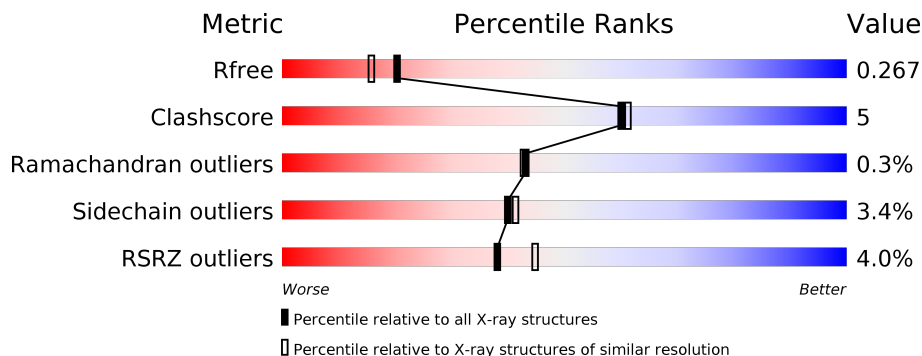
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	303	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	B	303	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div></div> </div> <div></div> </div>
1	C	303	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div></div> </div> <div></div> </div>
1	D	303	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> <div></div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9580 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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	1	0
			2349	1501	402	441	5			
1	B	291	Total	C	N	O	S	0	1	0
			2282	1459	384	434	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:

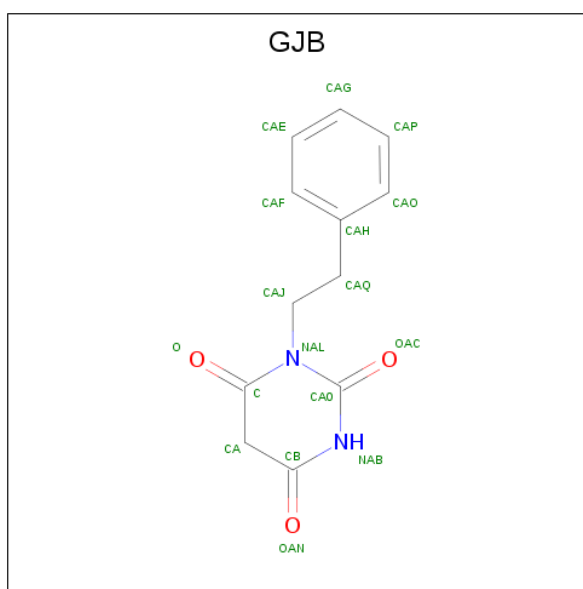
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP Q9HU22
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	GLY	-	expression tag	UNP 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 1-(2-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione (three-letter code: GJB) (formula: C<sub>12</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	12	2	3		

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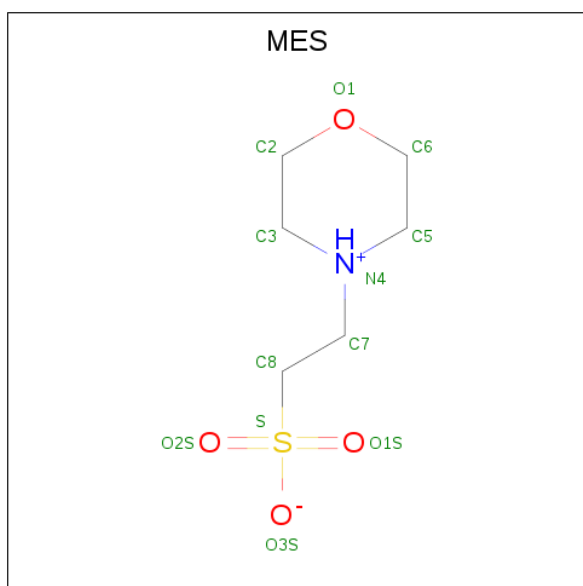
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			17	12	2	3		
2	C	1	Total	C	N	O	0	0
			17	12	2	3		
2	D	1	Total	C	N	O	0	0
			17	12	2	3		

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

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (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	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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

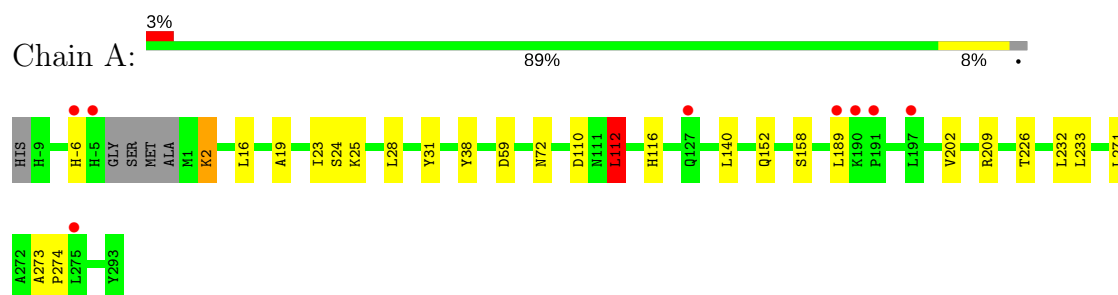
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	61	Total	O	0	0
			61	61		
5	C	52	Total	O	0	0
			52	52		
5	D	49	Total	O	0	0
			49	49		

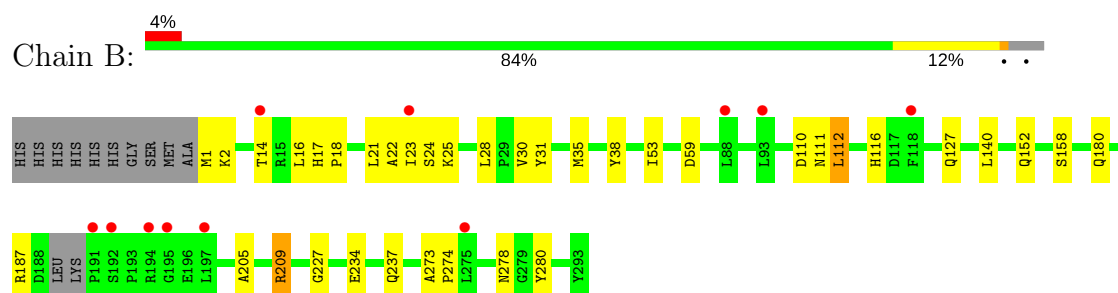
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

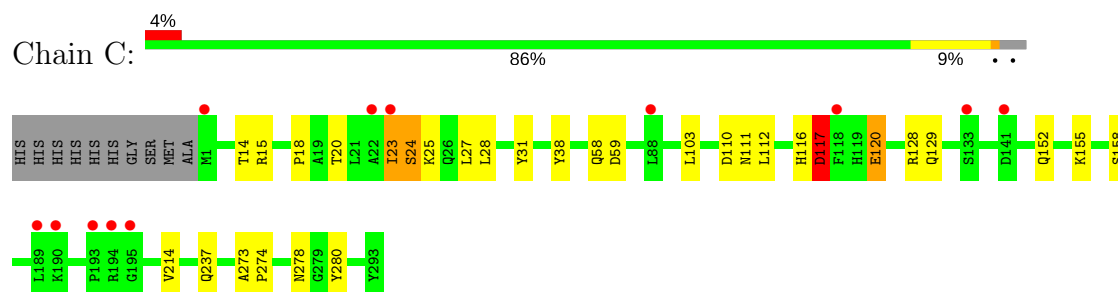
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



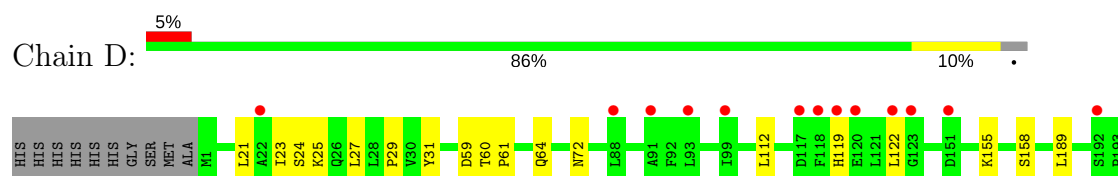
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

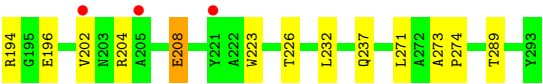


#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.06Å 154.24Å 134.85Å 90.00° 92.78° 90.00°	Depositor
Resolution (Å)	59.10 – 2.10 59.10 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (59.10-2.10) 94.9 (59.10-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.226 , 0.266 0.230 , 0.267	Depositor DCC
$R_{free}$ test set	3646 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.060 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9580	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GJB, 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	0.69	0/2406	0.75	1/3262 (0.0%)
1	B	0.67	0/2334	0.73	0/3164
1	C	0.58	0/2352	0.72	1/3190 (0.0%)
1	D	0.58	1/2352 (0.0%)	0.73	1/3190 (0.0%)
All	All	0.63	1/9444 (0.0%)	0.73	3/12806 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	TRP	CD2-CE2	5.37	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LEU	CA-CB-CG	6.72	130.77	115.30
1	D	232	LEU	CA-CB-CG	5.52	128.00	115.30
1	C	117	ASP	CB-CG-OD2	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2349	0	2329	16	0
1	B	2282	0	2268	47	0
1	C	2299	0	2292	38	0
1	D	2299	0	2292	19	0
2	A	17	0	12	0	0
2	B	17	0	12	0	0
2	C	17	0	12	0	0
2	D	17	0	12	0	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	12	0	13	0	0
4	B	12	0	13	0	0
4	C	12	0	13	1	0
5	A	81	0	0	0	0
5	B	61	0	0	4	0
5	C	52	0	0	0	0
5	D	49	0	0	0	0
All	All	9580	0	9268	93	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 5.

All (93) 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:B:23:ILE:HD11	1:B:28:LEU:HD23	1.41	1.02
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:OE1	1.82	0.97
1:B:25:LYS:HZ3	1:B:227:GLY:HA2	1.35	0.90
1:D:24:SER:HB2	1:D:59:ASP:OD2	1.73	0.88
1:C:24:SER:OG	1:C:27:LEU:HD12	1.74	0.87
1:C:23:ILE:HD12	1:C:28:LEU:HD23	1.59	0.84
1:A:226:THR:HB	1:A:232:LEU:HD12	1.61	0.83
1:B:23:ILE:HD11	1:B:28:LEU:CD2	2.08	0.83
1:A:116:HIS:ND1	3:A:1294:CL:CL	2.47	0.80
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:HG2	1.85	0.76
1:B:53:ILE:HD12	1:B:53:ILE:N	2.01	0.74
1:B:35:MET:CG	5:B:2011:HOH:O	2.35	0.73
1:B:23:ILE:HG12	1:C:23:ILE:HD13	1.73	0.69
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:CG	2.44	0.66
1:D:208:GLU:HA	1:D:208:GLU:OE1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HG12	1:C:23:ILE:CD1	2.27	0.65
1:B:35:MET:HG3	5:B:2011:HOH:O	1.96	0.65
1:B:23:ILE:CG1	1:C:23:ILE:HD13	2.27	0.65
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:CD	2.36	0.64
1:B:237[A]:GLN:HG2	1:C:237[A]:GLN:OE1	1.98	0.63
1:A:24:SER:OG	1:A:59:ASP:OD2	2.09	0.63
1:A:233:LEU:HD11	1:D:237[A]:GLN:HG3	1.82	0.62
1:D:194:ARG:NH2	1:D:196:GLU:OE1	2.33	0.61
1:A:23:ILE:O	1:A:23:ILE:HD12	2.00	0.61
1:C:24:SER:HB3	1:C:59:ASP:OD1	2.00	0.61
1:D:189:LEU:HD11	1:D:202:VAL:HG23	1.83	0.60
1:B:35:MET:HG2	5:B:2011:HOH:O	2.00	0.59
1:B:2:LYS:NZ	5:B:2002:HOH:O	2.36	0.58
1:B:24:SER:HB2	1:B:59:ASP:OD2	2.03	0.58
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.86	0.58
1:D:208:GLU:OE1	1:D:208:GLU:CA	2.51	0.58
1:C:117:ASP:HB3	1:C:120:GLU:HG3	1.87	0.57
1:C:116:HIS:ND1	3:C:1294:CL:CL	2.67	0.57
1:C:38:TYR:CB	1:C:112:LEU:HD22	2.36	0.56
1:B:205:ALA:O	1:B:209:ARG:HD3	2.06	0.56
1:B:23:ILE:HG12	1:C:23:ILE:CG1	2.36	0.56
1:B:116:HIS:ND1	3:B:1294:CL:CL	2.63	0.55
1:B:237[A]:GLN:CD	1:C:237[A]:GLN:OE1	2.45	0.55
1:B:23:ILE:CD1	1:B:28:LEU:CD2	2.84	0.54
1:B:237[A]:GLN:CG	1:C:237[A]:GLN:OE1	2.56	0.54
1:D:25:LYS:NZ	1:D:226:THR:O	2.41	0.53
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.90	0.53
1:B:24:SER:HB2	1:B:59:ASP:CG	2.28	0.53
1:B:1:MET:SD	1:B:180:GLN:NE2	2.82	0.53
1:B:25:LYS:NZ	1:B:110:ASP:OD2	2.35	0.52
1:B:23:ILE:HD11	1:C:23:ILE:CD1	2.40	0.52
1:B:14:THR:O	1:C:278:ASN:ND2	2.42	0.52
1:B:53:ILE:CD1	1:B:53:ILE:N	2.72	0.51
1:A:16:LEU:HD12	1:A:25:LYS:HD3	1.92	0.51
1:B:23:ILE:HG12	1:C:23:ILE:HG12	1.93	0.51
1:A:38:TYR:CG	1:A:112:LEU:HD22	2.47	0.50
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.92	0.50
1:B:22:ALA:O	1:B:23:ILE:HG23	2.12	0.50
1:B:23:ILE:HD11	1:C:23:ILE:HD11	1.94	0.49
1:A:28:LEU:HD22	1:D:29:PRO:CD	2.42	0.49
1:B:23:ILE:CD1	1:C:23:ILE:CD1	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LYS:NZ	1:C:110:ASP:OD2	2.46	0.48
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.95	0.48
1:A:2:LYS:HA	1:A:2:LYS:HE2	1.95	0.47
1:A:25:LYS:NZ	1:A:110:ASP:OD2	2.44	0.46
1:C:117:ASP:O	1:C:120:GLU:HG3	2.16	0.46
1:A:233:LEU:HD21	1:D:237[A]:GLN:HA	1.99	0.45
1:D:189:LEU:HD11	1:D:202:VAL:CG2	2.46	0.45
1:A:189:LEU:HD11	1:A:202:VAL:HG23	1.98	0.44
1:B:112:LEU:C	1:B:112:LEU:HD12	2.38	0.44
1:A:233:LEU:HD21	1:D:237[B]:GLN:HA	1.99	0.44
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.48	0.44
1:B:278:ASN:HB3	1:C:15:ARG:HA	2.00	0.43
1:C:20:THR:HA	1:C:23:ILE:O	2.19	0.43
1:A:19:ALA:HB1	1:D:29:PRO:HB3	2.00	0.43
1:D:23:ILE:HD11	1:D:27:LEU:CD1	2.48	0.43
1:D:23:ILE:HD11	1:D:27:LEU:HD12	1.99	0.43
1:C:237[A]:GLN:HE21	1:C:237[A]:GLN:HB2	1.65	0.43
1:B:234:GLU:HA	1:B:237[A]:GLN:HE21	1.85	0.42
1:D:72:ASN:HB3	1:D:271:LEU:HD21	2.00	0.42
1:B:17:HIS:CD2	1:B:21:LEU:HG	2.54	0.42
1:B:25:LYS:NZ	1:B:227:GLY:HA2	2.20	0.42
1:B:278:ASN:ND2	1:C:14:THR:O	2.53	0.42
1:D:60:THR:HG22	1:D:64:GLN:OE1	2.21	0.41
1:B:23:ILE:CD1	1:C:23:ILE:HD11	2.50	0.41
1:C:24:SER:HB3	1:C:59:ASP:CG	2.40	0.41
1:C:117:ASP:HB3	1:C:120:GLU:CG	2.49	0.41
1:B:18:PRO:HD3	1:C:280:TYR:CD2	2.56	0.41
1:B:280:TYR:CD2	1:C:18:PRO:HD3	2.55	0.41
1:A:72:ASN:HB3	1:A:271:LEU:HD21	2.02	0.41
1:B:16:LEU:N	1:B:16:LEU:HD12	2.37	0.40
1:B:23:ILE:CD1	1:B:28:LEU:HD23	2.29	0.40
1:B:23:ILE:CG1	1:C:23:ILE:CD1	2.92	0.40
1:C:103:LEU:HD11	1:C:129:GLN:HG2	2.03	0.40
1:C:214:VAL:O	4:C:1295:MES:H71	2.22	0.40
1:C:58:GLN:N	1:C:58:GLN:CD	2.75	0.40
1:D:60:THR:N	1:D:61:PRO:HD2	2.36	0.40
1:B:30:VAL:HB	1:B:38:TYR:CE1	2.56	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	295/303 (97%)	288 (98%)	6 (2%)	1 (0%)	43	43
1	B	288/303 (95%)	282 (98%)	5 (2%)	1 (0%)	43	43
1	C	292/303 (96%)	286 (98%)	5 (2%)	1 (0%)	43	43
1	D	292/303 (96%)	287 (98%)	4 (1%)	1 (0%)	43	43
All	All	1167/1212 (96%)	1143 (98%)	20 (2%)	4 (0%)	43	43

All (4) Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains [i](#)

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	246/248 (99%)	239 (97%)	7 (3%)	47	50
1	B	239/248 (96%)	231 (97%)	8 (3%)	41	43
1	C	241/248 (97%)	232 (96%)	9 (4%)	37	38
1	D	241/248 (97%)	232 (96%)	9 (4%)	37	38
All	All	967/992 (98%)	934 (97%)	33 (3%)	40	41

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	2	LYS
1	A	112	LEU
1	A	140	LEU
1	A	152	GLN
1	A	158	SER
1	A	209	ARG
1	B	111	ASN
1	B	112	LEU
1	B	127	GLN
1	B	140	LEU
1	B	152	GLN
1	B	158	SER
1	B	187	ARG
1	B	209	ARG
1	C	23	ILE
1	C	24	SER
1	C	111	ASN
1	C	117	ASP
1	C	120	GLU
1	C	128	ARG
1	C	152	GLN
1	C	155	LYS
1	C	158	SER
1	D	21	LEU
1	D	112	LEU
1	D	119	HIS
1	D	122	LEU
1	D	155	LYS
1	D	158	SER
1	D	204	ARG
1	D	208	GLU
1	D	289	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	C	78	GLN
1	D	82	GLN
1	D	90	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	1.78	1 (8%)	14,16,16	2.03	3 (21%)
2	GJB	A	400	-	18,18,18	0.84	0	24,24,24	2.88	9 (37%)
4	MES	B	1295	-	12,12,12	1.99	1 (8%)	14,16,16	1.80	1 (7%)
2	GJB	B	400	-	18,18,18	0.77	1 (5%)	24,24,24	3.37	10 (41%)
4	MES	C	1295	-	12,12,12	1.95	1 (8%)	14,16,16	1.54	4 (28%)
2	GJB	C	400	-	18,18,18	1.26	2 (11%)	24,24,24	3.22	11 (45%)
2	GJB	D	400	-	18,18,18	1.23	1 (5%)	24,24,24	2.97	9 (37%)

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	0/1/1/1
2	GJB	A	400	-	-	0/5/21/21	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	B	1295	-	-	0/6/14/14	0/1/1/1
2	GJB	B	400	-	-	0/5/21/21	0/2/2/2
4	MES	C	1295	-	-	0/6/14/14	0/1/1/1
2	GJB	C	400	-	-	0/5/21/21	0/2/2/2
2	GJB	D	400	-	-	0/5/21/21	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1295	MES	C8-S	-6.44	1.68	1.77
4	C	1295	MES	C8-S	-6.30	1.68	1.77
4	A	1295	MES	C8-S	-5.57	1.69	1.77
2	C	400	GJB	CA0-NAB	2.11	1.41	1.38
2	D	400	GJB	CA-CB	2.23	1.55	1.49
2	B	400	GJB	CB-NAB	2.28	1.41	1.37
2	C	400	GJB	CB-NAB	3.59	1.43	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	GJB	CB-NAB-CA0	-5.55	121.06	125.81
2	D	400	GJB	C-NAL-CA0	-5.29	120.16	125.23
2	C	400	GJB	C-NAL-CA0	-5.06	120.38	125.23
2	B	400	GJB	CAQ-CAJ-NAL	-4.80	104.80	112.18
2	B	400	GJB	C-NAL-CA0	-4.78	120.66	125.23
2	A	400	GJB	C-NAL-CA0	-4.72	120.71	125.23
2	B	400	GJB	CB-NAB-CA0	-4.71	121.78	125.81
2	D	400	GJB	CB-CA-C	-4.63	110.07	116.88
2	A	400	GJB	CB-NAB-CA0	-4.46	121.99	125.81
2	B	400	GJB	CB-CA-C	-4.39	110.42	116.88
2	D	400	GJB	CB-NAB-CA0	-4.29	122.13	125.81
2	C	400	GJB	CAQ-CAJ-NAL	-3.93	106.14	112.18
2	A	400	GJB	CB-CA-C	-3.91	111.14	116.88
2	C	400	GJB	CB-CA-C	-3.90	111.15	116.88
2	C	400	GJB	OAC-CA0-NAL	-3.84	117.14	122.41
2	C	400	GJB	OAN-CB-CA	-3.42	118.01	122.52
2	A	400	GJB	CAQ-CAJ-NAL	-3.05	107.50	112.18
2	B	400	GJB	OAN-CB-CA	-3.00	118.56	122.52
2	A	400	GJB	OAN-CB-CA	-2.96	118.61	122.52
2	D	400	GJB	OAN-CB-NAB	-2.65	116.39	120.38
2	B	400	GJB	O-C-NAL	-2.41	116.40	120.81
2	D	400	GJB	OAC-CA0-NAB	-2.23	117.24	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1295	MES	O3S-S-O2S	-2.15	106.03	111.27
4	A	1295	MES	O2S-S-O1S	-2.00	107.02	113.95
4	C	1295	MES	O2S-S-C8	2.00	109.33	106.92
4	C	1295	MES	C2-C3-N4	2.13	113.04	110.11
2	C	400	GJB	CAJ-CAQ-CAH	2.18	118.75	112.18
2	B	400	GJB	NAB-CA0-NAL	2.69	120.11	115.25
2	A	400	GJB	CAJ-NAL-C	2.73	120.16	117.96
2	A	400	GJB	NAB-CA0-NAL	2.84	120.38	115.25
2	D	400	GJB	NAB-CA0-NAL	3.68	121.90	115.25
4	C	1295	MES	O3S-S-C8	3.71	111.78	105.77
2	D	400	GJB	CAJ-NAL-C	3.76	121.00	117.96
2	C	400	GJB	NAB-CA0-NAL	3.83	122.17	115.25
2	C	400	GJB	CAJ-NAL-C	4.06	121.24	117.96
4	A	1295	MES	O3S-S-C8	4.28	112.69	105.77
2	B	400	GJB	CAJ-NAL-CA0	4.60	122.55	117.17
2	C	400	GJB	CA-CB-NAB	5.30	122.07	116.82
4	A	1295	MES	O2S-S-C8	5.31	113.31	106.92
4	B	1295	MES	O3S-S-C8	5.41	114.52	105.77
2	A	400	GJB	CA-CB-NAB	5.58	122.35	116.82
2	B	400	GJB	CA-CB-NAB	5.65	122.42	116.82
2	D	400	GJB	CA-CB-NAB	6.37	123.13	116.82
2	D	400	GJB	CA-C-NAL	7.34	122.58	117.12
2	A	400	GJB	CA-C-NAL	7.91	123.00	117.12
2	C	400	GJB	CA-C-NAL	8.01	123.07	117.12
2	B	400	GJB	CA-C-NAL	9.69	124.32	117.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1295	MES	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, 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	298/303 (98%)	0.26	8 (2%) 54 61	36, 55, 94, 115	1 (0%)
1	B	291/303 (96%)	0.34	11 (3%) 40 47	38, 56, 93, 130	2 (0%)
1	C	293/303 (96%)	0.46	12 (4%) 37 44	42, 66, 97, 131	1 (0%)
1	D	293/303 (96%)	0.54	16 (5%) 25 31	47, 68, 95, 121	3 (1%)
All	All	1175/1212 (96%)	0.40	47 (4%) 38 45	36, 62, 95, 131	7 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	PHE	9.7
1	B	195	GLY	5.9
1	A	-5	HIS	5.5
1	C	118	PHE	5.4
1	B	14	THR	4.9
1	D	205	ALA	4.6
1	D	123	GLY	4.5
1	D	122	LEU	4.4
1	A	-6	HIS	3.9
1	C	23	ILE	3.9
1	B	197	LEU	3.6
1	B	23	ILE	3.6
1	D	117	ASP	3.6
1	B	194	ARG	3.6
1	A	189	LEU	3.5
1	C	22	ALA	3.3
1	C	88	LEU	3.3
1	B	191	PRO	3.3
1	A	191	PRO	3.1
1	C	190	LYS	3.1
1	A	275	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	202	VAL	2.9
1	C	195	GLY	2.7
1	D	192	SER	2.6
1	C	133	SER	2.6
1	D	221	TYR	2.6
1	D	91	ALA	2.6
1	D	22	ALA	2.6
1	D	119	HIS	2.5
1	D	99	ILE	2.5
1	B	118	PHE	2.5
1	B	88	LEU	2.5
1	C	141	ASP	2.4
1	C	193	PRO	2.4
1	D	151	ASP	2.2
1	A	190	LYS	2.2
1	B	93	LEU	2.2
1	C	194	ARG	2.2
1	B	192	SER	2.2
1	D	93	LEU	2.2
1	D	88	LEU	2.1
1	A	197	LEU	2.1
1	A	127	GLN	2.1
1	B	275	LEU	2.0
1	C	1	MET	2.0
1	D	120	GLU	2.0
1	C	189	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MES	B	1295	12/12	0.87	0.20	72,85,88,91	0
2	GJB	D	400	17/17	0.87	0.12	59,72,76,77	0
3	CL	B	1294	1/1	0.88	0.12	64,64,64,64	0
4	MES	C	1295	12/12	0.89	0.16	76,85,90,91	0
2	GJB	C	400	17/17	0.90	0.12	55,62,71,76	0
3	CL	D	1294	1/1	0.90	0.09	84,84,84,84	0
4	MES	A	1295	12/12	0.91	0.16	68,83,93,93	0
2	GJB	A	400	17/17	0.92	0.14	49,51,66,66	0
2	GJB	B	400	17/17	0.93	0.13	50,53,59,63	0
3	CL	C	1294	1/1	0.95	0.11	76,76,76,76	0
3	CL	A	1294	1/1	0.96	0.18	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.