



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 PM GMT

PDB ID : 4ARW  
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 : 2012-04-26  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

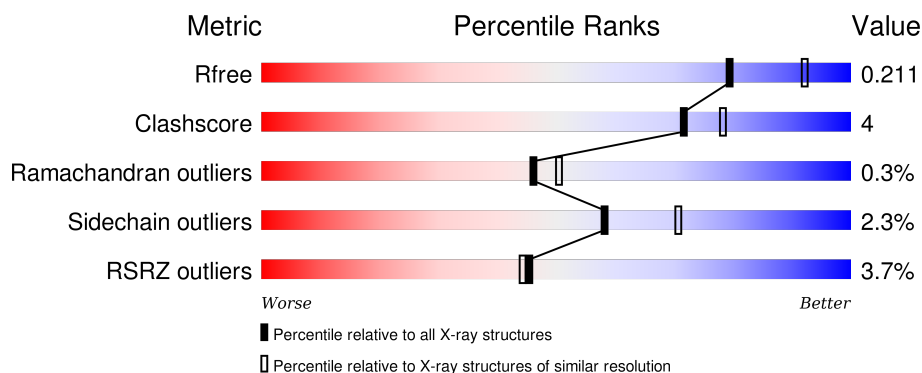
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	302	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	302	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	C	302	<div> <div>5%</div> <div>84%</div> <div>11%</div> <div>.</div> </div>
1	D	302	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>

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
3	MES	A	450	-	-	-	X
3	MES	C	450	-	-	-	X
4	CL	A	1294	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9848 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	294	Total	C	N	O	S	0	1	0
			2312	1478	393	437	4			
1	B	290	Total	C	N	O	S	0	1	0
			2273	1455	381	433	4			
1	C	289	Total	C	N	O	S	0	1	0
			2264	1449	379	432	4			
1	D	292	Total	C	N	O	S	0	1	0
			2291	1466	386	435	4			

There are 36 discrepancies between the modelled and reference sequences:

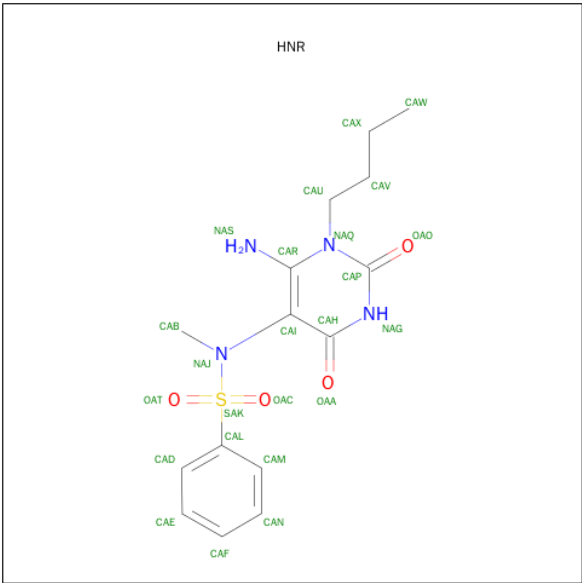
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	HIS	-	EXPRESSION TAG	UNP G3XCK4
A	-7	HIS	-	EXPRESSION TAG	UNP G3XCK4
A	-6	HIS	-	EXPRESSION TAG	UNP G3XCK4
A	-5	HIS	-	EXPRESSION TAG	UNP G3XCK4
A	-4	HIS	-	EXPRESSION TAG	UNP G3XCK4
A	-3	HIS	-	EXPRESSION TAG	UNP G3XCK4
A	-2	GLY	-	EXPRESSION TAG	UNP G3XCK4
A	-1	SER	-	EXPRESSION TAG	UNP G3XCK4
A	0	ALA	-	EXPRESSION TAG	UNP G3XCK4
B	-8	HIS	-	EXPRESSION TAG	UNP G3XCK4
B	-7	HIS	-	EXPRESSION TAG	UNP G3XCK4
B	-6	HIS	-	EXPRESSION TAG	UNP G3XCK4
B	-5	HIS	-	EXPRESSION TAG	UNP G3XCK4
B	-4	HIS	-	EXPRESSION TAG	UNP G3XCK4
B	-3	HIS	-	EXPRESSION TAG	UNP G3XCK4
B	-2	GLY	-	EXPRESSION TAG	UNP G3XCK4
B	-1	SER	-	EXPRESSION TAG	UNP G3XCK4
B	0	ALA	-	EXPRESSION TAG	UNP G3XCK4
C	-8	HIS	-	EXPRESSION TAG	UNP G3XCK4
C	-7	HIS	-	EXPRESSION TAG	UNP G3XCK4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	HIS	-	EXPRESSION TAG	UNP G3XCK4
C	-5	HIS	-	EXPRESSION TAG	UNP G3XCK4
C	-4	HIS	-	EXPRESSION TAG	UNP G3XCK4
C	-3	HIS	-	EXPRESSION TAG	UNP G3XCK4
C	-2	GLY	-	EXPRESSION TAG	UNP G3XCK4
C	-1	SER	-	EXPRESSION TAG	UNP G3XCK4
C	0	ALA	-	EXPRESSION TAG	UNP G3XCK4
D	-8	HIS	-	EXPRESSION TAG	UNP G3XCK4
D	-7	HIS	-	EXPRESSION TAG	UNP G3XCK4
D	-6	HIS	-	EXPRESSION TAG	UNP G3XCK4
D	-5	HIS	-	EXPRESSION TAG	UNP G3XCK4
D	-4	HIS	-	EXPRESSION TAG	UNP G3XCK4
D	-3	HIS	-	EXPRESSION TAG	UNP G3XCK4
D	-2	GLY	-	EXPRESSION TAG	UNP G3XCK4
D	-1	SER	-	EXPRESSION TAG	UNP G3XCK4
D	0	ALA	-	EXPRESSION TAG	UNP G3XCK4

- Molecule 2 is N-(6-AMINO-1-BUTYL-2,4-DIOXO-1,2,3,4-TETRAHYDOPYRIMIDIN-5-YL)-N-METHYL-BENZENESULFONAMIDE (three-letter code: HNR) (formula: C<sub>15</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>S).



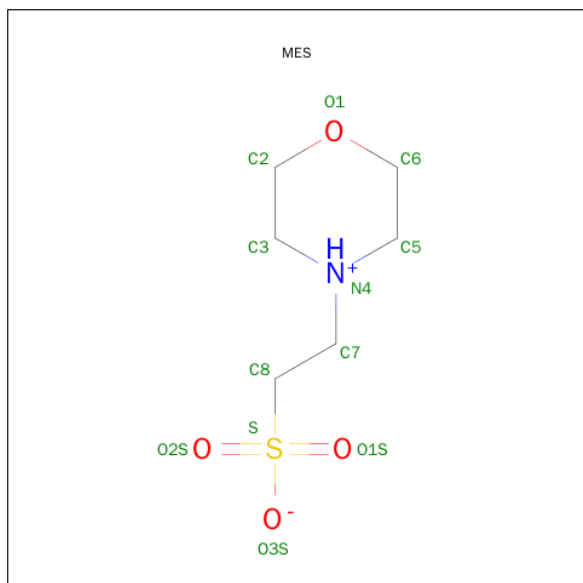
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			24	15	4	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			24	15	4	4	1		
2	D	1	Total	C	N	O	S	0	0
			24	15	4	4	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

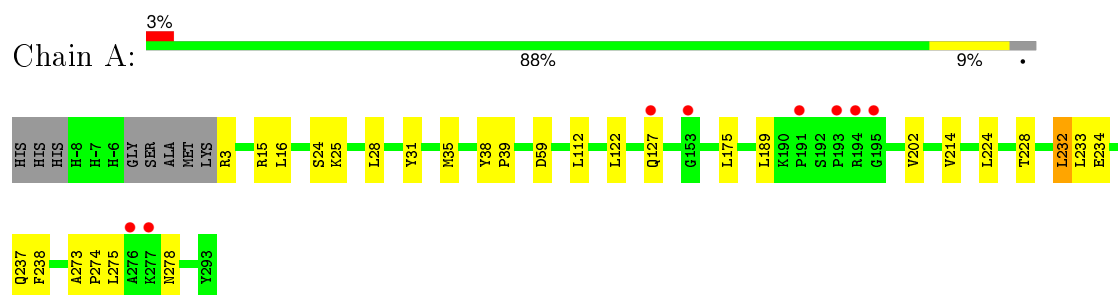
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	152	Total	O	0	0
			152	152		
6	B	127	Total	O	0	0
			127	127		
6	C	132	Total	O	0	0
			132	132		
6	D	136	Total	O	0	0
			136	136		

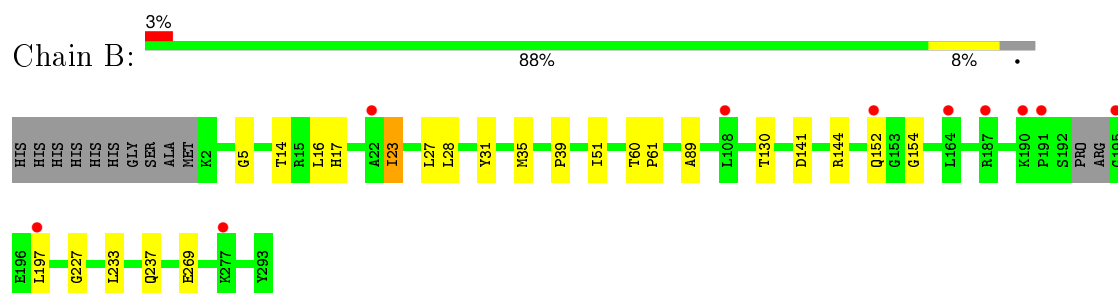
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

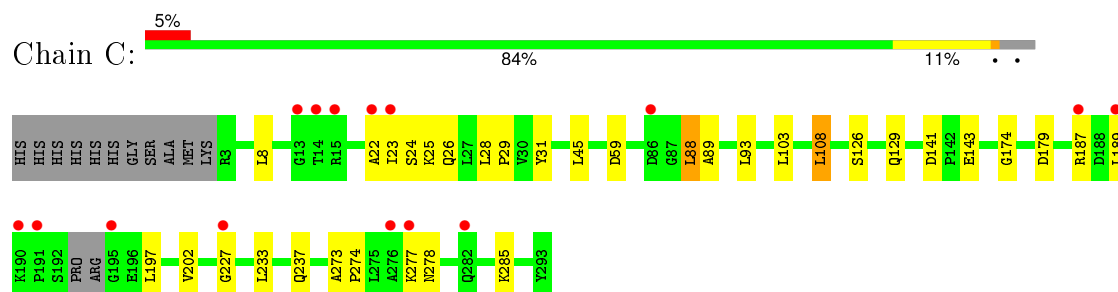
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



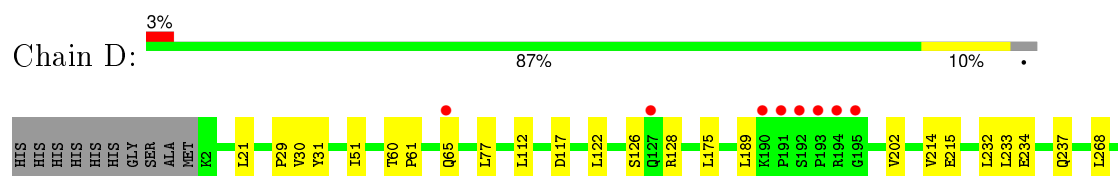
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



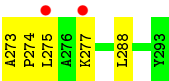
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE



#### • 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, $\alpha$ , $\beta$ , $\gamma$	63.99Å 153.76Å 134.65Å 90.00° 92.32° 90.00°	Depositor
Resolution (Å)	30.82 – 2.20 30.81 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.82-2.20) 96.2 (30.81-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.175 , 0.208 0.181 , 0.211	Depositor DCC
$R_{free}$ test set	3192 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.4	EDS
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 62911 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, HNR, 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	0.52	0/2367	0.62	0/3211
1	B	0.48	0/2324	0.59	0/3151
1	C	0.51	0/2315	0.65	0/3140
1	D	0.50	0/2344	0.61	0/3180
All	All	0.50	0/9350	0.62	0/12682

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	2312	0	2290	21	0
1	B	2273	0	2258	23	0
1	C	2264	0	2245	32	0
1	D	2291	0	2280	23	0
2	A	24	0	20	0	0
2	B	24	0	20	0	0
2	C	24	0	20	2	0
2	D	24	0	20	0	0
3	A	12	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	1	0
3	C	12	0	13	0	0
3	D	12	0	13	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	B	6	0	8	0	0
5	D	6	0	8	0	0
6	A	152	0	0	2	0
6	B	127	0	0	1	0
6	C	132	0	0	1	0
6	D	136	0	0	1	0
All	All	9848	0	9221	79	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 4.

All (79) 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:D:60:THR:HG23	1:D:61:PRO:HD3	1.37	1.03
1:B:23:ILE:HD12	1:C:23:ILE:HG12	1.50	0.94
1:D:60:THR:CG2	1:D:61:PRO:HD3	2.16	0.75
1:B:89:ALA:HB3	1:B:197:LEU:HB3	1.72	0.71
1:A:233:LEU:HD11	1:D:237[B]:GLN:HG3	1.72	0.70
1:A:234:GLU:HA	1:A:237[A]:GLN:HE21	1.55	0.68
1:C:8:LEU:HD23	1:C:88:LEU:HD12	1.78	0.65
1:D:60:THR:HG23	1:D:61:PRO:CD	2.21	0.65
1:B:23:ILE:HD12	1:C:23:ILE:CG1	2.25	0.63
1:B:23:ILE:HB	1:C:23:ILE:HD13	1.83	0.61
1:A:15:ARG:NH1	6:A:2009:HOH:O	2.35	0.59
1:A:275:LEU:HD22	1:A:278:ASN:HD21	1.67	0.58
1:B:154:GLY:O	3:B:450:MES:H82	2.04	0.58
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.86	0.58
1:D:268:LEU:HD23	1:D:288:LEU:HD23	1.86	0.57
1:B:16:LEU:HD21	1:B:227:GLY:O	2.05	0.56
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.88	0.55
1:B:27:LEU:HB3	1:C:22:ALA:HB1	1.89	0.55
1:D:189:LEU:HD11	1:D:202:VAL:HG23	1.91	0.53
1:D:234:GLU:HA	1:D:237[B]:GLN:HE21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASP:HB3	6:C:2056:HOH:O	2.09	0.53
1:D:122:LEU:CD2	1:D:175:LEU:HD21	2.39	0.53
1:C:24:SER:HB2	1:C:59:ASP:OD2	2.09	0.52
1:A:237[B]:GLN:HA	1:D:233:LEU:HD21	1.91	0.52
1:C:8:LEU:CD2	1:C:88:LEU:HD12	2.39	0.52
1:A:38:TYR:CB	1:A:112:LEU:HD22	2.40	0.51
1:C:103:LEU:HD23	1:C:179:ASP:HA	1.92	0.51
1:A:237[A]:GLN:HA	1:D:233:LEU:HD21	1.93	0.51
1:B:23:ILE:CG2	1:C:23:ILE:HD13	2.42	0.50
1:A:233:LEU:HD21	1:D:237[B]:GLN:CG	2.43	0.49
1:A:228:THR:O	1:A:232:LEU:HD12	2.13	0.49
1:A:28:LEU:HD22	1:D:29:PRO:HD2	1.95	0.48
1:D:60:THR:CG2	1:D:61:PRO:CD	2.88	0.48
1:A:35:MET:O	1:A:39:PRO:HD2	2.13	0.48
1:B:14:THR:O	1:C:278:ASN:ND2	2.46	0.48
1:B:23:ILE:CB	1:C:23:ILE:HD13	2.43	0.47
1:D:214:VAL:O	3:D:450:MES:H81	2.14	0.47
1:C:25:LYS:HZ1	1:C:227:GLY:HA2	1.80	0.47
1:D:275:LEU:HD11	6:D:2013:HOH:O	2.13	0.47
1:D:30:VAL:HG11	1:D:112:LEU:HD21	1.96	0.47
1:D:51:ILE:HB	1:D:77:LEU:HD23	1.96	0.47
1:B:233:LEU:HD21	1:C:237[A]:GLN:HA	1.96	0.47
1:B:141:ASP:OD2	1:B:144:ARG:HD3	2.15	0.47
1:A:214:VAL:O	3:A:450:MES:H71	2.15	0.46
1:B:35:MET:O	1:B:39:PRO:HD2	2.16	0.46
1:C:45:LEU:HD22	2:C:400:HNR:CAM	2.45	0.46
1:D:122:LEU:HD21	1:D:175:LEU:HD21	1.97	0.46
1:C:187:ARG:HG2	1:C:187:ARG:HH11	1.81	0.46
1:A:233:LEU:HD21	1:D:237[B]:GLN:HG2	1.97	0.45
1:B:233:LEU:HD21	1:C:237[B]:GLN:HA	1.98	0.45
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.47	0.45
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.98	0.45
1:C:45:LEU:HD22	2:C:400:HNR:HAM	1.99	0.45
3:D:450:MES:H82	3:D:450:MES:H51	1.64	0.45
1:C:189:LEU:HD11	1:C:202:VAL:HG23	1.99	0.45
1:A:189:LEU:HD11	1:A:202:VAL:CG2	2.48	0.44
1:B:237[B]:GLN:HE22	1:C:237[B]:GLN:HG2	1.57	0.44
1:C:23:ILE:HD11	1:C:28:LEU:HD23	1.99	0.44
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.83	0.44
1:B:23:ILE:HD12	1:C:23:ILE:CD1	2.47	0.44
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237[A]:GLN:HA	1:C:233:LEU:HD21	2.00	0.44
1:B:152:GLN:HG3	6:B:2074:HOH:O	2.18	0.44
1:A:24:SER:OG	1:A:59:ASP:OD2	2.25	0.44
1:A:38:TYR:HB2	1:A:112:LEU:HD22	2.00	0.44
1:C:108:LEU:HD22	1:C:174:GLY:HA3	2.00	0.43
1:C:103:LEU:CD2	1:C:179:ASP:HA	2.48	0.43
1:B:28:LEU:HD22	1:C:29:PRO:HG3	2.00	0.43
1:B:237[B]:GLN:HA	1:C:233:LEU:HD21	2.01	0.43
1:A:122:LEU:CD2	1:A:175:LEU:HD21	2.48	0.43
1:C:25:LYS:NZ	1:C:227:GLY:HA2	2.34	0.42
1:C:89:ALA:HB3	1:C:197:LEU:HB3	2.02	0.42
1:D:268:LEU:HD23	1:D:288:LEU:CD2	2.49	0.42
1:B:60:THR:HB	1:B:61:PRO:HD3	2.02	0.41
1:A:3:ARG:N	6:A:2001:HOH:O	2.53	0.41
1:B:5:GLY:O	1:B:51:ILE:HA	2.21	0.41
1:A:224:LEU:HD11	1:A:238:PHE:CD2	2.56	0.41
1:A:16:LEU:CD1	1:A:25:LYS:HD3	2.52	0.40
1:B:23:ILE:HG21	1:C:23:ILE:CD1	2.52	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	291/302 (96%)	286 (98%)	4 (1%)	1 (0%)	46	50
1	B	287/302 (95%)	282 (98%)	4 (1%)	1 (0%)	46	50
1	C	286/302 (95%)	281 (98%)	4 (1%)	1 (0%)	46	50
1	D	291/302 (96%)	287 (99%)	3 (1%)	1 (0%)	46	50
All	All	1155/1208 (96%)	1136 (98%)	15 (1%)	4 (0%)	46	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	31	TYR
1	C	31	TYR
1	A	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	242/247 (98%)	240 (99%)	2 (1%)	86	93
1	B	238/247 (96%)	234 (98%)	4 (2%)	68	81
1	C	237/247 (96%)	228 (96%)	9 (4%)	40	49
1	D	240/247 (97%)	233 (97%)	7 (3%)	50	62
All	All	957/988 (97%)	935 (98%)	22 (2%)	58	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	232	LEU
1	B	17	HIS
1	B	23	ILE
1	B	130	THR
1	B	269	GLU
1	C	26	GLN
1	C	88	LEU
1	C	93	LEU
1	C	108	LEU
1	C	126	SER
1	C	129	GLN
1	C	143	GLU
1	C	277	LYS
1	C	285	LYS
1	D	21	LEU
1	D	65	GLN
1	D	117	ASP

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Mol	Chain	Res	Type
1	D	126	SER
1	D	215	GLU
1	D	232	LEU
1	D	277	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	101	ASN
1	A	127	GLN
1	A	203	ASN
1	B	127	GLN
1	B	229	HIS
1	C	17	HIS
1	C	26	GLN
1	C	111	ASN
1	C	129	GLN
1	C	203	ASN

### 5.3.3 RNA [i](#)

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](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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
2	HNR	A	400	-	19,25,25	1.54	3 (15%)	24,36,36	2.64	7 (29%)
3	MES	A	450	-	11,12,12	0.98	0	14,16,16	1.05	1 (7%)
5	GOL	B	1295	-	5,5,5	0.28	0	5,5,5	0.40	0
2	HNR	B	400	-	19,25,25	1.99	4 (21%)	24,36,36	2.27	5 (20%)
3	MES	B	450	-	11,12,12	1.00	0	14,16,16	1.58	1 (7%)
2	HNR	C	400	-	19,25,25	1.66	3 (15%)	24,36,36	2.56	6 (25%)
3	MES	C	450	-	11,12,12	1.14	0	14,16,16	2.48	6 (42%)
5	GOL	D	1295	-	5,5,5	0.30	0	5,5,5	0.43	0
2	HNR	D	400	-	19,25,25	1.55	3 (15%)	24,36,36	2.46	6 (25%)
3	MES	D	450	-	11,12,12	1.07	0	14,16,16	1.75	1 (7%)

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	HNR	A	400	-	-	0/20/20/20	0/2/2/2
3	MES	A	450	-	-	0/6/14/14	0/1/1/1
5	GOL	B	1295	-	-	0/4/4/4	0/0/0/0
2	HNR	B	400	-	-	0/20/20/20	0/2/2/2
3	MES	B	450	-	-	0/6/14/14	0/1/1/1
2	HNR	C	400	-	-	0/20/20/20	0/2/2/2
3	MES	C	450	-	-	0/6/14/14	0/1/1/1
5	GOL	D	1295	-	-	0/4/4/4	0/0/0/0
2	HNR	D	400	-	-	0/20/20/20	0/2/2/2
3	MES	D	450	-	-	0/6/14/14	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	HNR	OAT-SAK	-2.16	1.40	1.43
2	D	400	HNR	CAR-NAQ	2.59	1.40	1.36
2	C	400	HNR	CAH-NAG	2.63	1.38	1.33
2	A	400	HNR	CAR-NAQ	3.00	1.41	1.36
2	D	400	HNR	CAH-NAG	3.20	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	HNR	CAH-NAG	3.29	1.39	1.33
2	C	400	HNR	CAR-NAQ	4.27	1.43	1.36
2	B	400	HNR	CAR-NAQ	4.32	1.43	1.36
2	D	400	HNR	OAC-SAK	4.55	1.49	1.43
2	B	400	HNR	OAC-SAK	4.64	1.49	1.43
2	C	400	HNR	OAC-SAK	4.80	1.49	1.43
2	A	400	HNR	OAC-SAK	4.81	1.49	1.43
2	B	400	HNR	CAH-NAG	5.23	1.42	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	HNR	OAC-SAK-OAT	-6.89	107.58	119.47
2	A	400	HNR	CAV-CAU-NAQ	-5.96	107.26	112.29
2	B	400	HNR	OAC-SAK-OAT	-5.42	110.12	119.47
2	D	400	HNR	OAC-SAK-OAT	-5.31	110.31	119.47
2	A	400	HNR	OAC-SAK-OAT	-5.03	110.79	119.47
2	D	400	HNR	CAV-CAU-NAQ	-4.55	108.45	112.29
3	C	450	MES	C7-N4-C3	-3.65	101.92	111.27
3	C	450	MES	C7-N4-C5	-3.59	102.07	111.27
2	A	400	HNR	NAS-CAR-NAQ	-2.43	118.87	120.66
2	C	400	HNR	OAT-SAK-CAL	2.00	110.61	108.00
3	A	450	MES	O1S-S-C8	2.11	108.70	106.91
2	C	400	HNR	OAT-SAK-NAJ	2.22	109.48	106.84
2	D	400	HNR	OAC-SAK-NAJ	2.62	109.96	106.84
3	C	450	MES	O2S-S-C8	2.65	109.17	106.91
3	C	450	MES	C6-O1-C2	2.68	118.92	109.89
3	C	450	MES	C5-N4-C3	2.74	114.83	108.90
2	B	400	HNR	OAC-SAK-NAJ	2.84	110.21	106.84
2	D	400	HNR	OAT-SAK-NAJ	2.85	110.23	106.84
2	A	400	HNR	OAT-SAK-NAJ	3.29	110.75	106.84
2	C	400	HNR	CAH-CAI-CAR	3.50	117.92	114.57
2	A	400	HNR	CAH-CAI-CAR	4.15	118.54	114.57
2	B	400	HNR	OAT-SAK-NAJ	4.16	111.78	106.84
2	C	400	HNR	OAC-SAK-NAJ	4.46	112.14	106.84
2	A	400	HNR	OAC-SAK-NAJ	4.74	112.47	106.84
2	D	400	HNR	CAH-CAI-CAR	4.82	119.18	114.57
3	B	450	MES	O1S-S-C8	4.95	111.13	106.91
2	B	400	HNR	CAH-CAI-CAR	5.01	119.37	114.57
2	B	400	HNR	CAH-NAG-CAP	5.05	119.61	115.25
3	C	450	MES	O1S-S-C8	5.05	111.21	106.91
3	D	450	MES	O1S-S-C8	5.46	111.57	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	HNR	CAH-NAG-CAP	6.03	120.46	115.25
2	D	400	HNR	CAH-NAG-CAP	6.10	120.52	115.25
2	C	400	HNR	CAH-NAG-CAP	7.21	121.48	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	450	MES	1	0
3	B	450	MES	1	0
2	C	400	HNR	2	0
3	D	450	MES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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	294/302 (97%)	-0.22	8 (2%) 58 57	25, 36, 58, 93	0
1	B	290/302 (96%)	-0.08	10 (3%) 49 47	27, 41, 61, 79	0
1	C	289/302 (95%)	-0.07	15 (5%) 31 30	23, 36, 69, 97	0
1	D	292/302 (96%)	-0.03	10 (3%) 49 47	30, 40, 60, 83	0
All	All	1165/1208 (96%)	-0.10	43 (3%) 45 44	23, 38, 62, 97	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	LYS	4.5
1	C	14	THR	4.2
1	D	193	PRO	4.0
1	C	191	PRO	3.9
1	A	127	GLN	3.9
1	C	277	LYS	3.3
1	D	194	ARG	3.2
1	C	15	ARG	3.2
1	C	187	ARG	3.2
1	D	195	GLY	3.1
1	B	22	ALA	2.9
1	C	189	LEU	2.9
1	C	195	GLY	2.8
1	D	65	GLN	2.6
1	D	190	LYS	2.6
1	D	277	LYS	2.6
1	C	276	ALA	2.6
1	C	13	GLY	2.6
1	A	276	ALA	2.6
1	B	152	GLN	2.6
1	D	191	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	153	GLY	2.6
1	C	23	ILE	2.6
1	A	195	GLY	2.5
1	D	192	SER	2.5
1	A	194	ARG	2.5
1	A	193	PRO	2.4
1	B	164	LEU	2.4
1	C	22	ALA	2.4
1	B	277	LYS	2.4
1	B	195	GLY	2.3
1	D	127	GLN	2.3
1	A	191	PRO	2.3
1	B	191	PRO	2.3
1	C	190	LYS	2.3
1	A	277	LYS	2.2
1	C	282	GLN	2.1
1	D	275	LEU	2.1
1	C	227	GLY	2.1
1	B	187	ARG	2.0
1	B	108	LEU	2.0
1	B	197	LEU	2.0
1	C	86	ASP	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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	A	1294	1/1	1.00	0.20	4.86	28,28,28,28	0
3	MES	C	450	12/12	0.93	0.20	3.04	46,47,49,51	0
3	MES	A	450	12/12	0.94	0.23	2.24	50,55,61,61	0
3	MES	D	450	12/12	0.91	0.21	1.70	57,59,65,72	0
3	MES	B	450	12/12	0.93	0.17	1.61	57,60,63,66	0
4	CL	B	1294	1/1	0.99	0.13	1.27	30,30,30,30	0
5	GOL	B	1295	6/6	0.79	0.15	1.19	57,59,61,63	0
4	CL	D	1294	1/1	1.00	0.13	0.47	35,35,35,35	0
4	CL	C	1294	1/1	0.98	0.16	0.46	29,29,29,29	0
5	GOL	D	1295	6/6	0.93	0.12	0.36	51,52,54,54	0
2	HNR	A	400	24/24	0.97	0.13	-0.00	27,29,34,40	0
2	HNR	C	400	24/24	0.97	0.13	-0.12	26,30,33,35	0
2	HNR	B	400	24/24	0.97	0.11	-0.63	31,35,42,44	0
2	HNR	D	400	24/24	0.96	0.11	-0.87	33,38,50,54	0
4	CL	C	1295	1/1	0.99	0.06	-	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.