Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:34 pm BST

PDB ID	:	3ZLL
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	:	2013-02-01
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

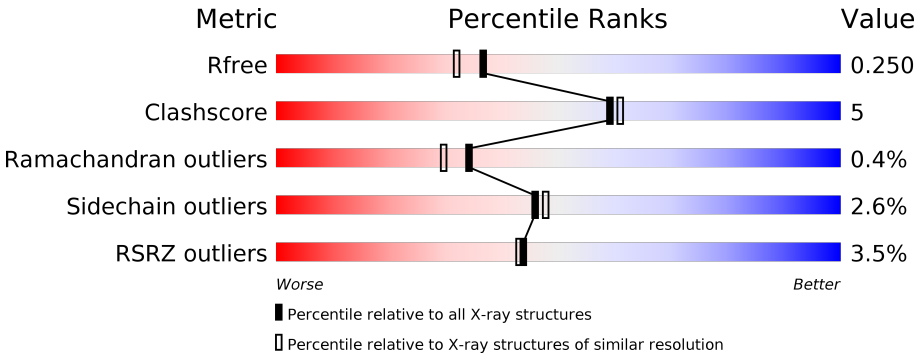
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 89% 9%
1	B	303	6% 86% 12%
1	C	303	2% 89% 7%
1	D	303	3% 86% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9858 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	297	Total	C	N	O	S	0	0	0
			2335	1492	400	439	4			
1	B	298	Total	C	N	O	S	0	1	0
			2349	1501	402	441	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	0	0
			2293	1467	386	435	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP G3XCK4
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	GLY	-	expression tag	UNP G3XCK4
A	-2	SER	-	expression tag	UNP G3XCK4
A	-1	MET	-	expression tag	UNP G3XCK4
A	0	ALA	-	expression tag	UNP G3XCK4
B	-9	HIS	-	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	GLY	-	expression tag	UNP G3XCK4
B	-2	SER	-	expression tag	UNP G3XCK4
B	-1	MET	-	expression tag	UNP G3XCK4
B	0	ALA	-	expression tag	UNP G3XCK4

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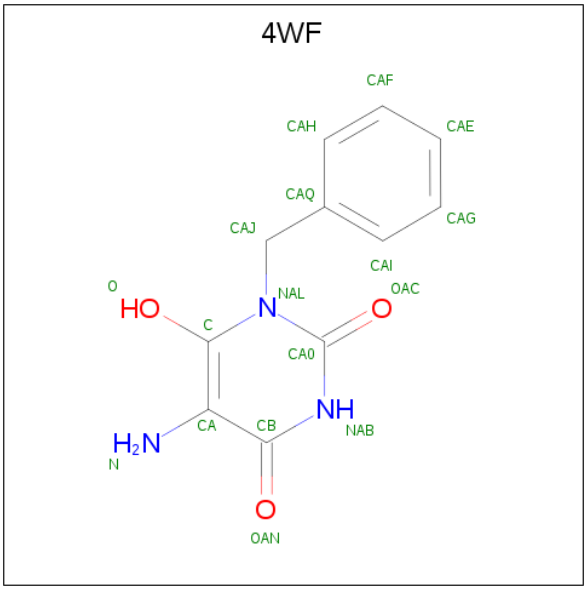
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	HIS	-	expression tag	UNP G3XCK4
C	-8	HIS	-	expression tag	UNP G3XCK4
C	-7	HIS	-	expression tag	UNP G3XCK4
C	-6	HIS	-	expression tag	UNP G3XCK4
C	-5	HIS	-	expression tag	UNP G3XCK4
C	-4	HIS	-	expression tag	UNP G3XCK4
C	-3	GLY	-	expression tag	UNP G3XCK4
C	-2	SER	-	expression tag	UNP G3XCK4
C	-1	MET	-	expression tag	UNP G3XCK4
C	0	ALA	-	expression tag	UNP G3XCK4
D	-9	HIS	-	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	GLY	-	expression tag	UNP G3XCK4
D	-2	SER	-	expression tag	UNP G3XCK4
D	-1	MET	-	expression tag	UNP G3XCK4
D	0	ALA	-	expression tag	UNP G3XCK4

- Molecule 2 is 5-azanyl-6-oxidanyl-1-(phenylmethyl)pyrimidine-2,4-dione (three-letter code: 4WF) (formula: $C_{11}H_{11}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	11	3	3		

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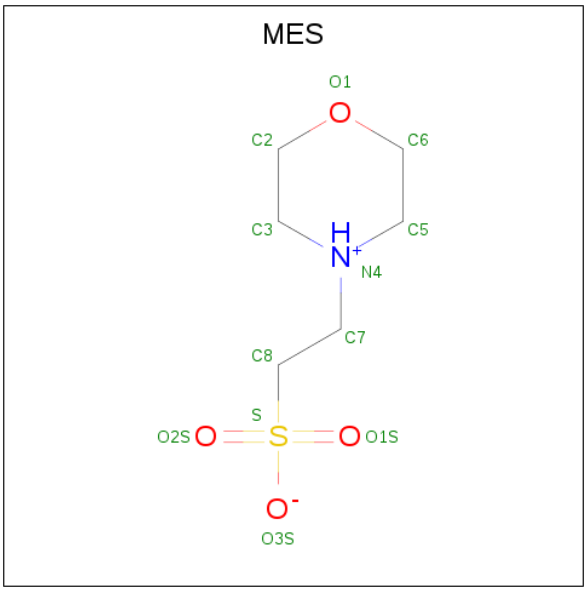
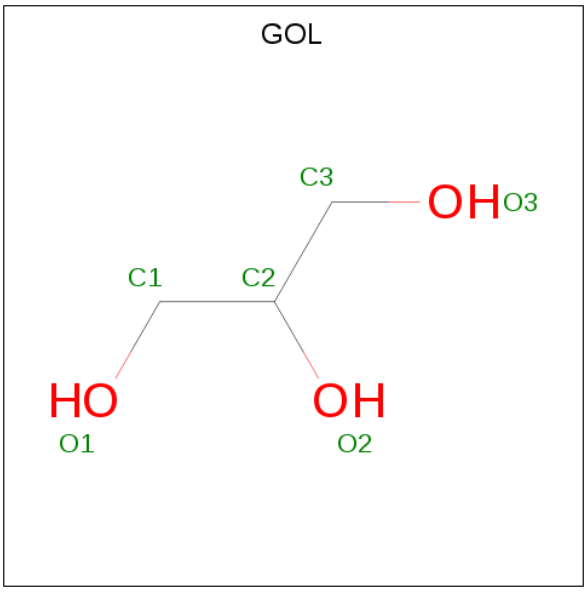
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 17 11 3 3	0	0
2	C	1	Total C N O 17 11 3 3	0	0
2	D	1	Total C N O 17 11 3 3	0	0

- 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 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0
3	C	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	151	Total O 151 151	0	0
6	B	119	Total O 119 119	0	0

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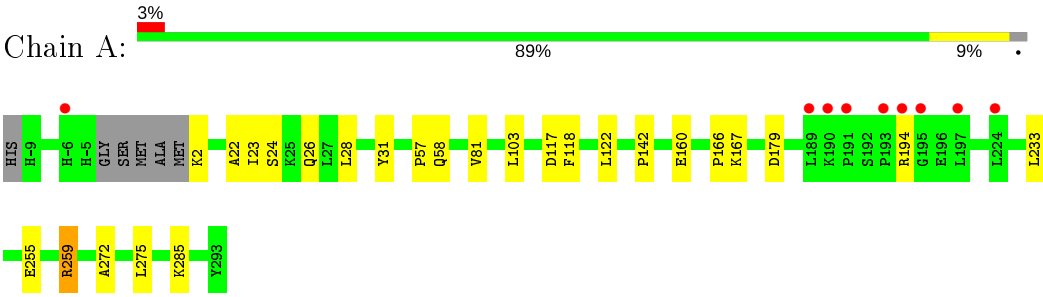
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	85	Total O 85 85	0	0
6	D	101	Total O 101 101	0	0

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.

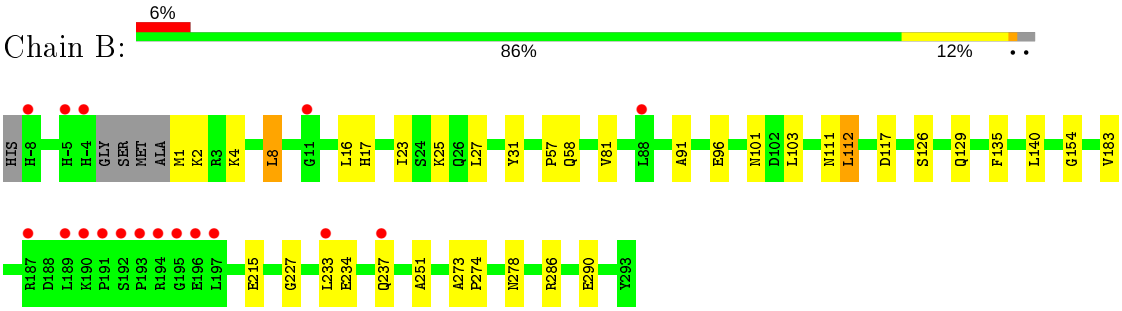
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



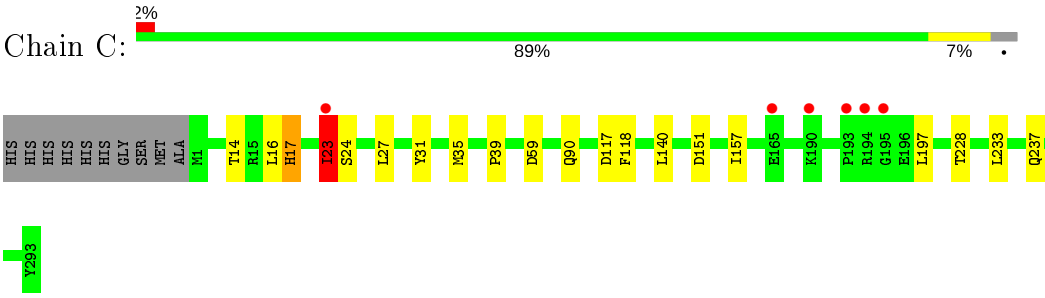
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



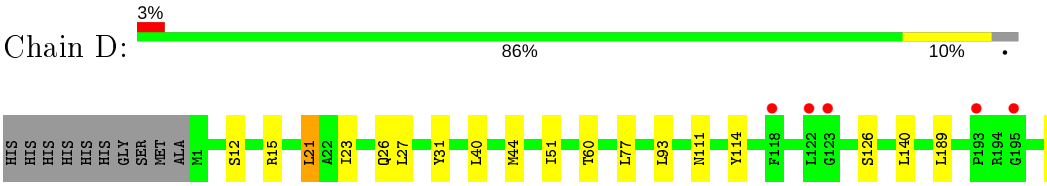
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain C:



- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain D:




Q237
F238
I239
L242
E255
R259
W262
A265
L268
A273
P274
L287
L288
T289
Y293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.09Å 154.11Å 134.67Å 90.00° 92.49° 90.00°	Depositor
Resolution (Å)	45.32 – 2.00 45.32 – 1.98	Depositor EDS
% Data completeness (in resolution range)	94.5 (45.32-2.00) 94.4 (45.32-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.199 , 0.245 0.202 , 0.250	Depositor DCC
R_{free} test set	4243 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9858	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 4WF, 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	0/2389	0.64	1/3240 (0.0%)
1	B	0.52	0/2406	0.63	0/3262
1	C	0.47	0/2352	0.59	0/3190
1	D	0.48	1/2343 (0.0%)	0.59	0/3178
All	All	0.51	1/9490 (0.0%)	0.61	1/12870 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	262	TRP	CD2-CE2	5.04	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ARG	NE-CZ-NH1	5.28	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2335	0	2309	19	0
1	B	2349	0	2329	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2299	0	2292	30	0
1	D	2293	0	2284	25	0
2	A	17	0	10	1	0
2	B	17	0	10	0	0
2	C	17	0	11	0	0
2	D	17	0	10	0	0
3	A	12	0	13	0	0
3	B	12	0	13	1	0
3	C	12	0	13	0	0
4	A	12	0	16	1	0
4	B	6	0	8	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	151	0	0	1	0
6	B	119	0	0	0	0
6	C	85	0	0	2	0
6	D	101	0	0	5	0
All	All	9858	0	9318	88	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 (88) 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:237[A]:GLN:OE1	1:C:237[A]:GLN:OE1	1.57	1.23
1:C:23:ILE:HD11	1:C:27:LEU:HB2	1.59	0.84
1:C:23:ILE:HD11	1:C:27:LEU:CB	2.10	0.81
1:B:237[A]:GLN:CD	1:C:237[A]:GLN:OE1	2.19	0.81
1:A:233:LEU:HD11	1:D:237:GLN:HG3	1.68	0.75
1:B:23:ILE:HG21	1:C:23:ILE:HG21	1.69	0.75
1:A:233:LEU:HD21	1:D:237:GLN:HG2	1.70	0.74
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:CD	2.26	0.73
1:B:237[A]:GLN:CG	1:C:237[A]:GLN:OE1	2.39	0.70
1:B:8:LEU:HD21	1:B:91:ALA:HB2	1.74	0.69
1:B:23:ILE:HD11	1:B:27:LEU:HD13	1.75	0.67
1:D:268:LEU:HD23	1:D:288:LEU:CD2	2.25	0.67
1:B:237[A]:GLN:HG2	1:C:237[A]:GLN:OE1	1.97	0.65
1:D:60:THR:HG23	6:D:2017:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LEU:HD23	1:D:288:LEU:HD21	1.80	0.63
1:B:25:LYS:NZ	1:B:227:GLY:HA2	2.15	0.62
1:A:251:ALA:HB2	4:A:1295:GOL:H31	1.83	0.61
1:D:255:GLU:O	1:D:259:ARG:HG3	2.02	0.59
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.33	0.58
1:B:8:LEU:CD2	1:B:91:ALA:HB2	2.34	0.58
1:A:57:PRO:HG3	1:A:81:VAL:HG11	1.86	0.57
1:D:51:ILE:HB	1:D:77:LEU:HD23	1.86	0.57
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.87	0.55
1:B:237[A]:GLN:HG3	1:C:233:LEU:HD11	1.88	0.55
1:D:265:ALA:HB2	6:D:2089:HOH:O	2.06	0.55
1:A:233:LEU:HD21	1:D:237:GLN:CG	2.35	0.55
1:D:21:LEU:O	1:D:21:LEU:HD13	2.06	0.55
1:A:23:ILE:HD11	1:A:28:LEU:HD23	1.89	0.55
1:A:24:SER:OG	1:A:26:GLN:OE1	2.26	0.54
1:A:118:PHE:CZ	1:A:122:LEU:HD11	2.43	0.54
1:B:57:PRO:HG3	1:B:81:VAL:HG11	1.90	0.54
1:B:112:LEU:C	1:B:112:LEU:HD12	2.30	0.51
1:C:23:ILE:CD1	1:C:27:LEU:HB2	2.37	0.51
1:C:255:GLU:O	1:C:259:ARG:HG3	2.11	0.51
1:C:259:ARG:NH2	6:C:2075:HOH:O	2.43	0.51
1:C:151:ASP:HB3	1:C:157:ILE:HD13	1.94	0.50
1:B:234:GLU:HA	1:B:237[A]:GLN:HE21	1.77	0.49
1:D:26:GLN:NE2	6:D:2006:HOH:O	2.44	0.49
1:B:25:LYS:HZ3	1:B:227:GLY:HA2	1.77	0.49
1:B:23:ILE:HG13	1:B:27:LEU:HB2	1.95	0.49
1:B:23:ILE:HG12	1:C:23:ILE:CG2	2.43	0.49
1:A:237:GLN:HA	1:D:233:LEU:HD21	1.95	0.48
1:A:22:ALA:CB	1:D:27:LEU:HD22	2.44	0.48
1:B:23:ILE:HD13	1:C:23:ILE:HB	1.95	0.47
1:B:251:ALA:HB2	4:B:1294:GOL:H32	1.95	0.47
1:C:14:THR:HG22	1:C:17:HIS:NE2	2.29	0.47
1:A:23:ILE:HG21	1:D:23:ILE:HG12	1.97	0.47
1:A:255:GLU:O	1:A:259:ARG:HG3	2.15	0.47
1:B:278:ASN:ND2	1:C:14:THR:O	2.45	0.46
1:D:268:LEU:HD23	1:D:288:LEU:HD23	1.96	0.46
1:B:237[B]:GLN:HA	1:C:233:LEU:HD21	1.97	0.46
1:A:272:ALA:HB1	1:A:285:LYS:HG3	1.97	0.46
1:D:259:ARG:NH2	6:D:2092:HOH:O	2.48	0.46
1:B:96:GLU:HG3	1:B:183:VAL:HG11	1.98	0.45
1:A:160:GLU:OE2	1:A:167:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD11	1:D:237:GLN:CG	2.44	0.45
1:C:23:ILE:HD11	1:C:27:LEU:HB3	1.96	0.45
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:CG	2.64	0.45
1:D:189:LEU:HD11	1:D:202:VAL:HG23	1.98	0.45
1:B:286:ARG:NH1	1:B:290:GLU:OE1	2.50	0.45
1:C:118:PHE:N	6:C:2036:HOH:O	2.51	0.44
1:D:114:TYR:CE1	1:D:242:LEU:HD13	2.52	0.44
1:B:23:ILE:HB	1:C:23:ILE:HG13	1.98	0.44
1:D:21:LEU:C	1:D:21:LEU:HD13	2.39	0.44
1:B:233:LEU:HD21	1:C:237[A]:GLN:HG2	1.99	0.43
1:A:23:ILE:HD13	1:D:23:ILE:HG21	2.00	0.43
1:B:237[A]:GLN:HA	1:C:233:LEU:HD21	2.00	0.43
1:C:35:MET:O	1:C:39:PRO:HD2	2.19	0.43
1:B:23:ILE:HG12	1:C:23:ILE:HG21	1.99	0.43
1:B:58:GLN:CD	1:B:58:GLN:H	2.22	0.43
1:C:24:SER:HB2	1:C:59:ASP:OD1	2.19	0.42
1:B:57:PRO:HG3	1:B:81:VAL:CG1	2.48	0.42
1:B:16:LEU:CD1	1:B:25:LYS:HD2	2.49	0.42
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:HG2	2.18	0.42
1:B:135:PHE:CE1	1:B:215:GLU:HG3	2.55	0.42
1:C:16:LEU:HD21	1:C:228:THR:HA	2.02	0.41
1:A:142:PRO:HG2	1:A:166:PRO:HG2	2.01	0.41
1:B:154:GLY:O	3:B:450:MES:H72	2.21	0.41
1:D:12:SER:HB3	6:D:2006:HOH:O	2.20	0.41
1:B:1:MET:HB2	1:B:129:GLN:OE1	2.21	0.41
1:D:255:GLU:HB2	1:D:287:LEU:HD11	2.02	0.41
1:A:103:LEU:HD22	1:A:179:ASP:HA	2.02	0.41
1:C:90:GLN:HG2	1:C:197:LEU:HD12	2.02	0.41
1:D:40:LEU:O	1:D:44:MET:HG3	2.22	0.40
1:A:57:PRO:HG3	1:A:81:VAL:CG1	2.51	0.40
1:D:273:ALA:HB3	1:D:274:PRO:HD3	2.03	0.40
1:B:140:LEU:O	1:B:140:LEU:HD13	2.22	0.40
2:A:400:4WF:HAG	6:A:2133:HOH:O	2.20	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%)	289 (99%)	3 (1%)	1 (0%)	41	37
1	B	295/303 (97%)	287 (97%)	7 (2%)	1 (0%)	41	37
1	C	292/303 (96%)	284 (97%)	6 (2%)	2 (1%)	22	16
1	D	291/303 (96%)	288 (99%)	2 (1%)	1 (0%)	41	37
All	All	1171/1212 (97%)	1148 (98%)	18 (2%)	5 (0%)	34	30

All (5) 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
1	C	23	ILE

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%)	239 (98%)	5 (2%)	55	58
1	B	246/248 (99%)	236 (96%)	10 (4%)	30	28
1	C	241/248 (97%)	237 (98%)	4 (2%)	60	65
1	D	240/248 (97%)	234 (98%)	6 (2%)	47	49
All	All	971/992 (98%)	946 (97%)	25 (3%)	46	48

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	58	GLN
1	A	117	ASP
1	A	194	ARG
1	A	275	LEU
1	B	2	LYS
1	B	4	LYS
1	B	8	LEU
1	B	17	HIS
1	B	101	ASN
1	B	103	LEU
1	B	111	ASN
1	B	112	LEU
1	B	117	ASP
1	B	126	SER
1	C	17	HIS
1	C	23	ILE
1	C	117	ASP
1	C	140	LEU
1	D	15	ARG
1	D	21	LEU
1	D	93	LEU
1	D	111	ASN
1	D	126	SER
1	D	140	LEU

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 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 (i)

Of 14 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	MES	B	450	-	12,12,12	2.26	1 (8%)	14,16,16	1.44	2 (14%)
3	MES	A	450	-	12,12,12	2.18	1 (8%)	14,16,16	1.73	2 (14%)
3	MES	C	450	-	12,12,12	2.06	1 (8%)	14,16,16	1.61	2 (14%)
4	GOL	B	1294	-	5,5,5	0.36	0	5,5,5	0.27	0
2	4WF	A	400	-	16,18,18	1.63	2 (12%)	13,25,25	2.40	3 (23%)
2	4WF	B	400	-	16,18,18	1.45	2 (12%)	13,25,25	2.85	3 (23%)
2	4WF	D	400	-	16,18,18	1.37	2 (12%)	13,25,25	2.34	2 (15%)
2	4WF	C	400	-	16,18,18	1.71	2 (12%)	13,25,25	1.98	2 (15%)
4	GOL	A	1294	-	5,5,5	0.38	0	5,5,5	0.24	0
4	GOL	A	1295	-	5,5,5	0.37	0	5,5,5	0.19	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
3	MES	B	450	-	-	1/6/14/14	0/1/1/1
3	MES	A	450	-	-	3/6/14/14	0/1/1/1
3	MES	C	450	-	-	3/6/14/14	0/1/1/1
4	GOL	B	1294	-	-	4/4/4/4	-
2	4WF	A	400	-	-	2/4/4/4	0/2/2/2
2	4WF	B	400	-	-	2/4/4/4	0/2/2/2
2	4WF	D	400	-	-	2/4/4/4	0/2/2/2
2	4WF	C	400	-	-	2/4/4/4	0/2/2/2
4	GOL	A	1294	-	-	2/4/4/4	-
4	GOL	A	1295	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	450	MES	C8-S	-7.38	1.67	1.77
3	A	450	MES	C8-S	-7.19	1.67	1.77
3	C	450	MES	C8-S	-6.79	1.67	1.77
2	A	400	4WF	CB-NAB	5.40	1.42	1.33
2	C	400	4WF	CB-NAB	5.40	1.42	1.33
2	B	400	4WF	CB-NAB	4.43	1.40	1.33
2	D	400	4WF	CB-NAB	4.08	1.40	1.33
2	B	400	4WF	C-NAL	3.07	1.42	1.38
2	C	400	4WF	C-NAL	2.89	1.42	1.38
2	D	400	4WF	C-NAL	2.64	1.42	1.38
2	A	400	4WF	C-NAL	2.23	1.41	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	4WF	CB-NAB-CA0	8.66	122.45	115.14
2	D	400	4WF	CB-NAB-CA0	7.30	121.31	115.14
2	A	400	4WF	CB-NAB-CA0	6.67	120.77	115.14
2	C	400	4WF	CB-NAB-CA0	6.16	120.34	115.14
3	A	450	MES	O1S-S-C8	5.25	113.23	106.92
3	C	450	MES	O1S-S-C8	4.14	111.90	106.92
2	A	400	4WF	CAQ-CAJ-NAL	3.79	118.51	112.63
3	B	450	MES	O3S-S-C8	3.70	111.75	105.77
2	B	400	4WF	CAQ-CAJ-NAL	3.21	117.61	112.63
3	C	450	MES	O3S-S-C8	3.12	110.81	105.77
2	C	400	4WF	CAJ-NAL-C	3.06	121.60	117.86
2	D	400	4WF	CAJ-NAL-C	2.66	121.11	117.86
2	B	400	4WF	CAJ-NAL-CA0	2.56	120.92	117.92
2	A	400	4WF	CAJ-NAL-C	2.56	120.99	117.86
3	A	450	MES	O3S-S-C8	2.49	109.80	105.77
3	B	450	MES	O2S-S-C8	2.38	109.78	106.92

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	450	MES	C8-C7-N4-C5
3	C	450	MES	C7-C8-S-O2S
4	B	1294	GOL	O1-C1-C2-C3
4	B	1294	GOL	C1-C2-C3-O3
4	A	1294	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	1295	GOL	O1-C1-C2-C3
4	B	1294	GOL	O2-C2-C3-O3
4	A	1294	GOL	O2-C2-C3-O3
4	A	1295	GOL	O1-C1-C2-O2
3	C	450	MES	C7-C8-S-O3S
4	B	1294	GOL	O1-C1-C2-O2
3	A	450	MES	C7-C8-S-O3S
2	A	400	4WF	NAL-CAJ-CAQ-CAH
2	B	400	4WF	NAL-CAJ-CAQ-CAH
2	A	400	4WF	NAL-CAJ-CAQ-CAI
2	B	400	4WF	NAL-CAJ-CAQ-CAI
2	D	400	4WF	NAL-CAJ-CAQ-CAI
3	A	450	MES	C7-C8-S-O1S
3	A	450	MES	C7-C8-S-O2S
3	C	450	MES	C7-C8-S-O1S
2	D	400	4WF	NAL-CAJ-CAQ-CAH
2	C	400	4WF	NAL-CAJ-CAQ-CAI
2	C	400	4WF	NAL-CAJ-CAQ-CAH

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	450	MES	1	0
4	B	1294	GOL	1	0
2	A	400	4WF	1	0
4	A	1295	GOL	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	297/303 (98%)	0.05	9 (3%) 50 49	28, 44, 70, 97	0
1	B	298/303 (98%)	0.19	17 (5%) 23 23	28, 46, 81, 110	0
1	C	293/303 (96%)	0.15	6 (2%) 65 63	32, 52, 79, 109	2 (0%)
1	D	293/303 (96%)	0.20	9 (3%) 49 48	39, 52, 73, 87	0
All	All	1181/1212 (97%)	0.15	41 (3%) 44 43	28, 49, 77, 110	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	LEU	6.3
1	B	191	PRO	5.5
1	B	195	GLY	5.4
1	B	194	ARG	4.6
1	C	23	ILE	4.5
1	A	194	ARG	4.3
1	B	190	LYS	4.2
1	A	189	LEU	4.2
1	B	197	LEU	4.2
1	B	11	GLY	4.1
1	B	-8	HIS	3.6
1	A	190	LYS	3.5
1	D	123	GLY	3.5
1	D	193	PRO	3.3
1	B	192	SER	3.1
1	C	195	GLY	3.1
1	C	190	LYS	3.1
1	C	193	PRO	2.9
1	D	233	LEU	2.9
1	A	193	PRO	2.8
1	B	193	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	2.7
1	D	289	THR	2.7
1	B	233	LEU	2.6
1	D	118	PHE	2.6
1	B	-5	HIS	2.5
1	A	191	PRO	2.5
1	B	-4	HIS	2.5
1	A	-6	HIS	2.5
1	D	232	LEU	2.4
1	B	88	LEU	2.4
1	D	122	LEU	2.4
1	B	196	GLU	2.3
1	C	194	ARG	2.3
1	B	187	ARG	2.1
1	B	237[A]	GLN	2.1
1	A	224	LEU	2.1
1	D	195	GLY	2.1
1	C	165	GLU	2.1
1	A	197	LEU	2.0
1	D	239	ILE	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	1294	6/6	0.80	0.19	56,61,64,65	0
2	4WF	D	400	17/17	0.80	0.20	61,70,78,78	0
4	GOL	A	1295	6/6	0.82	0.25	51,60,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	1294	6/6	0.84	0.12	59,63,65,65	0
2	4WF	C	400	17/17	0.85	0.16	54,64,72,72	0
3	MES	A	450	12/12	0.92	0.16	61,74,75,76	0
2	4WF	B	400	17/17	0.92	0.12	43,48,55,57	0
5	CL	B	1295	1/1	0.93	0.06	50,50,50,50	0
3	MES	B	450	12/12	0.93	0.20	58,68,72,73	0
2	4WF	A	400	17/17	0.93	0.11	43,54,59,61	0
3	MES	C	450	12/12	0.93	0.18	62,69,71,74	0
5	CL	C	1294	1/1	0.95	0.09	65,65,65,65	0
5	CL	D	1294	1/1	0.97	0.07	63,63,63,63	0
5	CL	A	1296	1/1	0.98	0.08	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.