Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2018 – 10:08 PM EST

PDB ID	:	4B42
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	:	2012-07-27
Resolution	:	2.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030736

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 2.50 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.
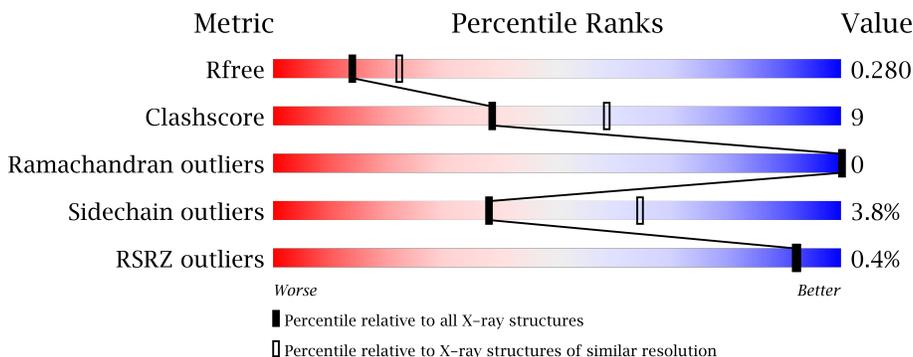
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	81% 13% • •
1	B	303	82% 14% • •
1	C	303	80% 16% • •
1	D	303	.% 83% 11% • •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	1295	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9527 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	293	Total 2299	C 1471	N 387	O 436	S 5	0	1	0
1	B	291	Total 2283	C 1460	N 384	O 434	S 5	0	1	0
1	C	293	Total 2299	C 1471	N 387	O 436	S 5	0	1	0
1	D	291	Total 2284	C 1463	N 382	O 434	S 5	0	1	0

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 N-[6-azanyl-1-butyl-2,4-bis(oxidanylidene)pyrimidin-5-yl]-N-methyl-benzamide (three-letter code: 942) (formula: $C_{16}H_{20}N_4O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	4	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 23	C 16	N 4	O 3	0	0
2	C	1	Total 23	C 16	N 4	O 3	0	0
2	D	1	Total 23	C 16	N 4	O 3	0	0

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

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
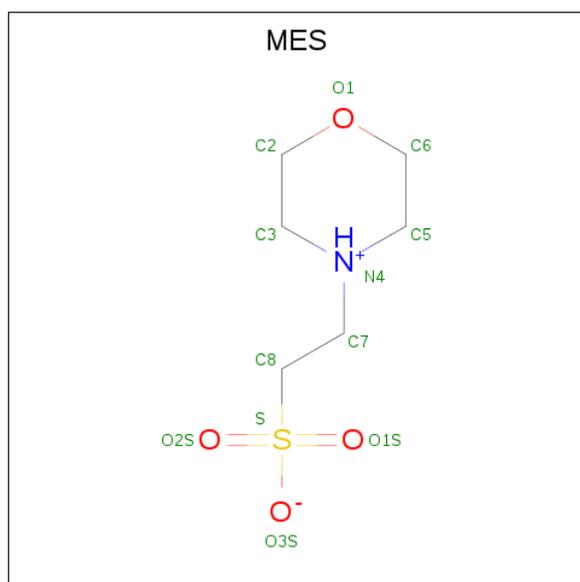
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 12	C 6	N 1	O 4	S 1	0	0
4	B	1	Total 12	C 6	N 1	O 4	S 1	0	0

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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		
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	64	Total	O	0	0
			64	64		
5	B	55	Total	O	0	0
			55	55		
5	C	56	Total	O	0	0
			56	56		
5	D	43	Total	O	0	0
			43	43		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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
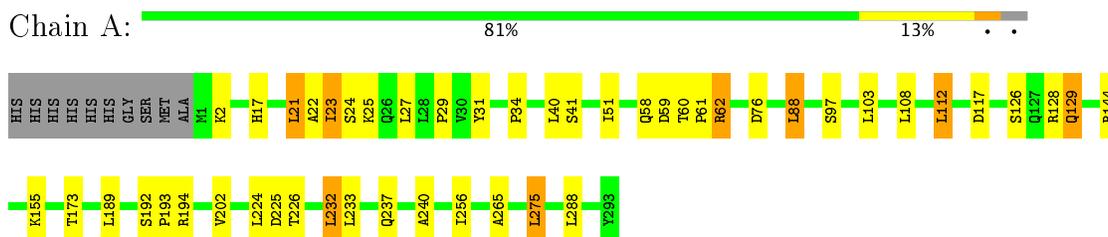
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE
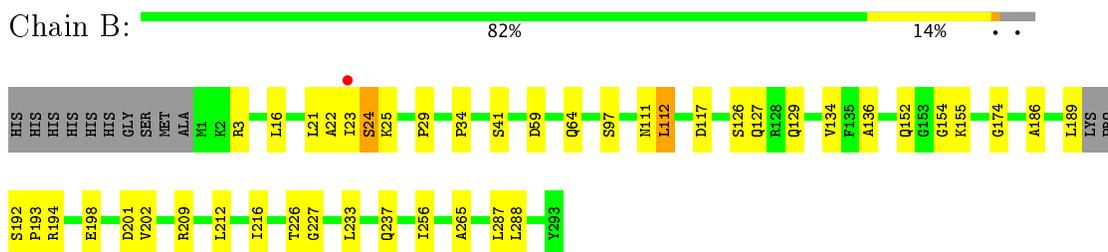
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE
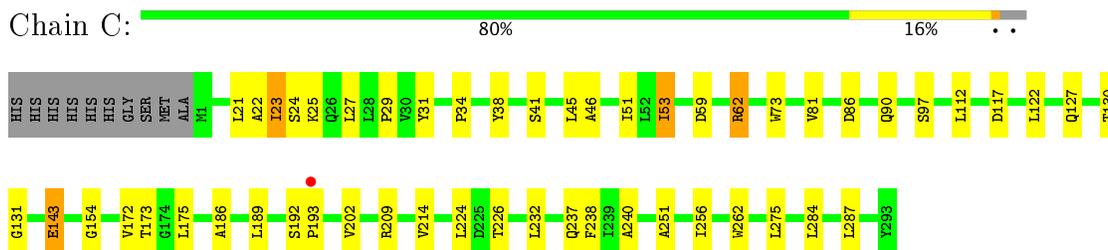
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE
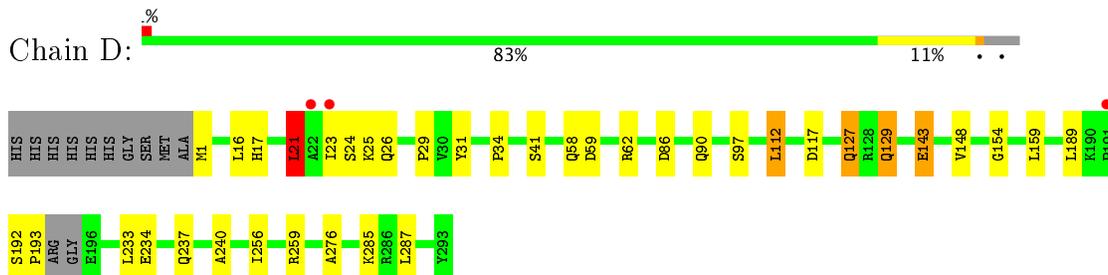
4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.15Å 153.40Å 134.67Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	34.79 – 2.50 34.79 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.2 (34.79-2.50) 97.2 (34.79-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.223 , 0.283 0.222 , 0.280	Depositor DCC
R_{free} test set	2181 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 18.9	EDS
L-test for twinning[2]	$<\vert L\vert> = 0.49, <L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9527	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<\vert L\vert>$, $<L^2>$ 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: 942, 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	0.81	0/2352	0.92	9/3190 (0.3%)
1	B	0.80	0/2334	0.88	3/3164 (0.1%)
1	C	0.72	2/2352 (0.1%)	0.87	3/3190 (0.1%)
1	D	0.72	0/2336	0.82	3/3168 (0.1%)
All	All	0.76	2/9374 (0.0%)	0.87	18/12712 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	TRP	CD2-CE2	5.23	1.47	1.41
1	C	73	TRP	CD2-CE2	5.12	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	LEU	CA-CB-CG	8.99	135.97	115.30
1	C	62	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	275	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	A	62	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	A	62	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	112	LEU	CA-CB-CG	6.16	129.48	115.30
1	A	224	LEU	CB-CG-CD2	6.00	121.20	111.00
1	C	112	LEU	CA-CB-CG	5.77	128.57	115.30
1	A	88	LEU	CB-CG-CD2	5.75	120.77	111.00
1	A	128	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	232	LEU	CB-CG-CD1	-5.68	101.35	111.00
1	D	143	GLU	CB-CA-C	-5.54	99.32	110.40
1	A	225	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	21	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	209	ARG	NE-CZ-NH1	5.21	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	112	LEU	CB-CG-CD1	5.18	119.81	111.00
1	B	3	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	143	GLU	CB-CA-C	-5.00	100.39	110.40

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	2299	0	2292	40	0
1	B	2283	0	2271	59	0
1	C	2299	0	2292	49	0
1	D	2284	0	2275	55	0
2	A	23	0	20	5	0
2	B	23	0	20	1	0
2	C	23	0	20	3	0
2	D	23	0	20	4	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	1	0
4	C	12	0	13	4	0
4	D	12	0	13	2	0
5	A	64	0	0	1	0
5	B	55	0	0	3	0
5	C	56	0	0	2	0
5	D	43	0	0	2	0
All	All	9527	0	9262	160	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 9.

All (160) 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:A:237[A]:GLN:OE1	1:C:237[A]:GLN:NE2	1.95	0.97
1:B:23:ILE:CD1	1:D:23:ILE:HD12	1.96	0.95
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:OE1	1.85	0.95
1:B:23:ILE:HD12	1:D:23:ILE:CD1	1.99	0.92
1:B:23:ILE:CD1	1:D:23:ILE:CD1	2.48	0.92
1:B:23:ILE:HG21	1:D:23:ILE:HD12	1.54	0.90
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:HG2	1.76	0.86
1:B:287:LEU:HD23	5:B:2054:HOH:O	1.79	0.82
1:A:237[A]:GLN:OE1	1:C:237[A]:GLN:HG2	1.82	0.79
1:A:256:ILE:HD11	2:A:1294:942:HAE	1.66	0.77
1:B:23:ILE:HD12	1:D:23:ILE:HD12	1.60	0.77
1:B:23:ILE:HG21	1:D:23:ILE:CD1	2.13	0.77
1:A:237[A]:GLN:CD	1:C:237[A]:GLN:HE21	1.87	0.76
1:C:154:GLY:O	4:C:1296:MES:H32	1.88	0.73
2:A:1294:942:HAF	2:A:1294:942:CAI	2.19	0.73
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:CG	2.37	0.72
1:B:23:ILE:HD13	1:D:23:ILE:CD1	2.18	0.72
1:A:237[A]:GLN:HG2	1:C:237[A]:GLN:NE2	2.03	0.72
1:A:17:HIS:CD2	1:A:21:LEU:HD13	2.25	0.72
1:B:237[A]:GLN:HG2	1:D:237[A]:GLN:OE1	1.90	0.71
1:B:23:ILE:CG2	1:D:23:ILE:HD12	2.18	0.71
1:C:186:ALA:HA	1:C:189:LEU:HD12	1.73	0.70
1:D:154:GLY:O	4:D:1296:MES:C7	2.40	0.70
1:A:144:ARG:NH2	5:A:2029:HOH:O	2.24	0.70
1:B:23:ILE:HD12	1:D:23:ILE:HG21	1.73	0.70
1:B:23:ILE:CD1	1:D:23:ILE:HG21	2.22	0.69
1:B:23:ILE:HD12	1:D:23:ILE:CB	2.23	0.69
1:D:154:GLY:O	4:D:1296:MES:H72	1.93	0.68
1:B:23:ILE:CD1	1:D:23:ILE:HD13	2.24	0.67
1:A:23:ILE:HB	1:C:23:ILE:HD13	1.76	0.67
1:A:256:ILE:CD1	2:A:1294:942:HAE	2.25	0.66
1:C:53:ILE:HD12	1:C:53:ILE:N	2.11	0.66
1:D:127:GLN:O	1:D:129:GLN:NE2	2.27	0.66
1:C:154:GLY:O	4:C:1296:MES:C3	2.44	0.65
1:C:53:ILE:CD1	1:C:53:ILE:N	2.60	0.65
1:C:86:ASP:HB2	1:C:90:GLN:OE1	1.97	0.65
1:B:112:LEU:CD1	1:B:226:THR:HG21	2.26	0.64
1:B:154:GLY:O	4:B:1296:MES:H32	1.97	0.64
1:B:23:ILE:HD12	1:D:23:ILE:CG2	2.28	0.64
1:B:237[A]:GLN:CG	1:D:237[A]:GLN:OE1	2.46	0.63
1:B:41:SER:HB3	1:B:256:ILE:HD12	1.79	0.63
1:A:237[A]:GLN:CG	1:C:237[A]:GLN:NE2	2.61	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HB3	1:A:256:ILE:HD12	1.81	0.62
1:B:23:ILE:HD13	1:D:23:ILE:HD13	1.81	0.62
1:C:284:LEU:HA	1:C:287:LEU:HD12	1.82	0.62
1:B:237[A]:GLN:OE1	1:D:237[A]:GLN:CD	2.37	0.61
1:B:41:SER:HB3	1:B:256:ILE:CD1	2.30	0.61
1:B:23:ILE:HD13	1:D:23:ILE:HD12	1.81	0.61
1:B:22:ALA:O	1:D:62:ARG:NH2	2.34	0.60
1:D:86:ASP:HB2	1:D:90:GLN:OE1	2.01	0.60
1:A:23:ILE:HD13	1:C:23:ILE:HB	1.83	0.60
2:A:1294:942:CAF	2:A:1294:942:CAI	2.79	0.59
1:B:23:ILE:CB	1:D:23:ILE:HD12	2.32	0.59
1:B:233:LEU:HD21	1:D:237[B]:GLN:HA	1.85	0.59
1:A:237[A]:GLN:OE1	1:C:237[A]:GLN:CG	2.49	0.58
1:A:31:TYR:CD1	1:A:240:ALA:HB2	2.38	0.58
1:C:41:SER:HB3	1:C:256:ILE:CD1	2.33	0.58
1:D:41:SER:HB3	1:D:256:ILE:HD12	1.85	0.58
1:A:256:ILE:HD11	2:A:1294:942:CAE	2.33	0.58
1:A:237[A]:GLN:CD	1:C:237[A]:GLN:NE2	2.51	0.58
1:C:41:SER:HB3	1:C:256:ILE:HD12	1.86	0.57
1:B:237[A]:GLN:HG3	1:D:233:LEU:HD11	1.87	0.56
1:D:17:HIS:CD2	1:D:21:LEU:HD13	2.41	0.56
1:B:237[A]:GLN:CD	1:D:237[A]:GLN:OE1	2.43	0.56
1:A:27:LEU:HD13	1:C:22:ALA:HB1	1.88	0.55
1:A:24:SER:HB3	1:A:59:ASP:OD2	2.06	0.55
1:B:111:ASN:ND2	1:B:174:GLY:HA3	2.22	0.55
1:C:189:LEU:HD11	1:C:202:VAL:HG22	1.88	0.55
1:D:259:ARG:HD2	2:D:1294:942:HAV2	1.89	0.55
1:D:26:GLN:NE2	5:D:2007:HOH:O	2.34	0.55
1:B:189:LEU:HD11	1:B:202:VAL:HG22	1.89	0.54
1:A:61:PRO:HD3	1:B:64:GLN:NE2	2.22	0.54
1:C:24:SER:HB3	1:C:59:ASP:OD2	2.07	0.54
1:D:41:SER:HB3	1:D:256:ILE:CD1	2.38	0.54
1:B:112:LEU:CD1	1:B:226:THR:CG2	2.86	0.54
1:C:25:LYS:NZ	1:C:226:THR:O	2.40	0.54
1:B:23:ILE:HD12	1:D:23:ILE:HB	1.89	0.53
1:C:51:ILE:HG22	1:C:53:ILE:HD12	1.90	0.53
1:A:76:ASP:OD1	1:D:58:GLN:HA	2.09	0.53
1:B:233:LEU:HD21	1:D:237[A]:GLN:HA	1.89	0.52
1:D:276:ALA:HB2	1:D:285:LYS:HZ1	1.73	0.52
1:A:31:TYR:CG	1:A:240:ALA:HB2	2.45	0.51
1:D:234:GLU:HA	1:D:237[A]:GLN:HE21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LYS:NZ	1:B:227:GLY:HA2	2.26	0.50
1:A:233:LEU:HD21	1:C:237[B]:GLN:HA	1.93	0.50
1:B:194:ARG:NH1	1:B:198:GLU:OE2	2.44	0.50
1:C:45:LEU:CD1	2:C:1294:942:HAW2	2.41	0.50
1:A:22:ALA:CB	1:C:27:LEU:HD22	2.41	0.50
2:C:1294:942:CAI	2:C:1294:942:CAF	2.89	0.50
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.94	0.49
1:D:24:SER:HB3	1:D:59:ASP:OD1	2.12	0.49
1:D:16:LEU:HD12	1:D:25:LYS:HD3	1.95	0.49
1:D:234:GLU:HA	1:D:237[A]:GLN:NE2	2.26	0.49
1:C:214:VAL:O	4:C:1296:MES:H82	2.13	0.49
1:D:189:LEU:HD23	5:D:2031:HOH:O	2.13	0.49
1:C:31:TYR:CD1	1:C:240:ALA:HB2	2.48	0.48
1:A:25:LYS:NZ	1:A:226:THR:O	2.43	0.48
1:D:31:TYR:CD1	1:D:240:ALA:HB2	2.48	0.48
2:D:1294:942:CAI	2:D:1294:942:CAF	2.91	0.48
1:C:172:VAL:HG12	1:C:173:THR:O	2.15	0.47
2:C:1294:942:CAI	2:C:1294:942:HAF	2.44	0.47
1:A:62:ARG:NH1	1:C:62:ARG:HD2	2.30	0.47
1:A:189:LEU:HD11	1:A:202:VAL:HG22	1.97	0.47
1:A:233:LEU:HD21	1:C:237[A]:GLN:HA	1.97	0.47
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.96	0.47
1:B:152:GLN:HB2	5:B:2030:HOH:O	2.14	0.47
1:B:111:ASN:HD21	1:B:174:GLY:HA3	1.80	0.46
1:C:189:LEU:HD11	1:C:202:VAL:CG2	2.45	0.46
1:B:112:LEU:HD13	1:B:226:THR:CG2	2.46	0.46
1:B:189:LEU:HD21	1:B:201:ASP:HB3	1.98	0.46
1:B:134:VAL:HG13	1:B:212:LEU:HD11	1.98	0.46
2:D:1294:942:HAF	2:D:1294:942:CAR	2.46	0.46
1:B:186:ALA:HA	1:B:189:LEU:HD12	1.97	0.46
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.98	0.45
1:D:1:MET:HE2	1:D:129:GLN:HG2	1.98	0.45
1:B:16:LEU:HD12	1:B:25:LYS:HD3	1.99	0.44
1:A:265:ALA:HB1	1:A:288:LEU:HD22	1.99	0.44
1:D:259:ARG:NH2	1:D:287:LEU:HD22	2.33	0.44
1:D:276:ALA:HB2	1:D:285:LYS:NZ	2.33	0.44
1:C:209:ARG:NE	5:C:2039:HOH:O	2.51	0.44
1:C:23:ILE:HD11	1:C:27:LEU:HD13	1.99	0.44
1:B:265:ALA:HB1	1:B:288:LEU:HD22	2.00	0.43
1:C:224:LEU:HD11	1:C:238:PHE:CD1	2.52	0.43
1:B:23:ILE:HD12	1:D:23:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:SER:HB3	1:B:59:ASP:OD1	2.18	0.43
1:A:237[A]:GLN:HG2	1:C:237[A]:GLN:HE22	1.81	0.43
1:A:60:THR:N	1:A:61:PRO:HD2	2.34	0.43
1:B:237[B]:GLN:HA	1:D:233:LEU:HD21	2.00	0.43
1:A:29:PRO:HA	1:A:34:PRO:HA	2.00	0.42
1:D:148:VAL:HA	1:D:159:LEU:HD23	2.00	0.42
1:B:25:LYS:HZ3	1:B:227:GLY:HA2	1.84	0.42
1:A:22:ALA:HB1	1:C:27:LEU:HD13	2.00	0.42
1:C:130:THR:HG22	1:C:131:GLY:N	2.34	0.42
1:C:154:GLY:O	4:C:1296:MES:H31	2.16	0.42
1:A:88:LEU:HD13	1:A:108:LEU:HD21	2.01	0.42
1:B:136:ALA:HB3	1:B:216:ILE:HD13	2.02	0.42
1:C:29:PRO:HA	1:C:34:PRO:HA	2.00	0.42
1:D:29:PRO:HA	1:D:34:PRO:HA	2.01	0.42
1:B:29:PRO:HA	1:B:34:PRO:HA	2.00	0.42
1:A:23:ILE:HD13	1:C:23:ILE:CD1	2.49	0.42
1:C:81:VAL:HG22	5:C:2016:HOH:O	2.20	0.42
2:D:1294:942:CAI	2:D:1294:942:HAF	2.49	0.42
1:D:16:LEU:CD1	1:D:25:LYS:HD3	2.49	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.75	0.42
1:C:38:TYR:CD1	1:C:251:ALA:HB3	2.54	0.42
1:A:22:ALA:HB2	1:C:27:LEU:HD22	2.02	0.42
1:B:127:GLN:O	1:B:129:GLN:HG2	2.20	0.41
1:C:122:LEU:CD2	1:C:175:LEU:HD21	2.50	0.41
1:C:41:SER:CB	1:C:256:ILE:HD12	2.50	0.41
1:D:192:SER:HB2	1:D:193:PRO:HD2	2.02	0.41
1:B:16:LEU:CD1	1:B:25:LYS:HD2	2.51	0.41
1:B:112:LEU:HD11	1:B:226:THR:HG21	2.00	0.41
1:A:103:LEU:HD11	1:A:129:GLN:HG3	2.02	0.41
1:A:40:LEU:CD1	1:A:51:ILE:HD13	2.51	0.41
2:B:1294:942:HAL	5:B:2007:HOH:O	2.19	0.41
1:B:41:SER:CB	1:B:256:ILE:HD12	2.50	0.40
1:C:46:ALA:HB2	1:C:122:LEU:HD13	2.03	0.40
1:A:17:HIS:CG	1:A:21:LEU:HD13	2.57	0.40
1:C:122:LEU:HD21	1:C:175:LEU:HD21	2.03	0.40
1:B:237[A]:GLN:HA	1:D:233:LEU:HD21	2.02	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	292/303 (96%)	284 (97%)	8 (3%)	0	100	100
1	B	288/303 (95%)	277 (96%)	11 (4%)	0	100	100
1	C	292/303 (96%)	282 (97%)	10 (3%)	0	100	100
1	D	288/303 (95%)	277 (96%)	11 (4%)	0	100	100
All	All	1160/1212 (96%)	1120 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	241/248 (97%)	227 (94%)	14 (6%)	23	43
1	B	239/248 (96%)	233 (98%)	6 (2%)	53	79
1	C	241/248 (97%)	232 (96%)	9 (4%)	39	66
1	D	240/248 (97%)	233 (97%)	7 (3%)	48	75
All	All	961/992 (97%)	925 (96%)	36 (4%)	38	66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	21	LEU

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Mol	Chain	Res	Type
1	A	23	ILE
1	A	58	GLN
1	A	97	SER
1	A	112	LEU
1	A	117	ASP
1	A	126	SER
1	A	129	GLN
1	A	155	LYS
1	A	173	THR
1	A	194	ARG
1	A	232	LEU
1	A	275	LEU
1	B	21	LEU
1	B	24	SER
1	B	97	SER
1	B	117	ASP
1	B	126	SER
1	B	155	LYS
1	C	21	LEU
1	C	23	ILE
1	C	53	ILE
1	C	97	SER
1	C	117	ASP
1	C	127	GLN
1	C	143	GLU
1	C	232	LEU
1	C	275	LEU
1	D	21	LEU
1	D	97	SER
1	D	112	LEU
1	D	117	ASP
1	D	127	GLN
1	D	129	GLN
1	D	143	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	129	GLN
1	B	111	ASN
1	C	111	ASN

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Mol	Chain	Res	Type
1	C	119	HIS
1	D	17	HIS

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 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	#$|Z| > 2$
2	942	A	1294	-	21,24,24	2.36	3 (14%)	21,33,33	2.28	8 (38%)
4	MES	A	1296	-	12,12,12	1.77	1 (8%)	14,16,16	3.67	5 (35%)
2	942	B	1294	-	21,24,24	2.41	4 (19%)	21,33,33	2.73	10 (47%)
4	MES	B	1296	-	12,12,12	1.95	1 (8%)	14,16,16	3.79	5 (35%)
2	942	C	1294	-	21,24,24	2.25	5 (23%)	21,33,33	2.85	8 (38%)
4	MES	C	1296	-	12,12,12	2.04	2 (16%)	14,16,16	2.36	3 (21%)
2	942	D	1294	-	21,24,24	2.66	5 (23%)	21,33,33	2.80	8 (38%)
4	MES	D	1296	-	12,12,12	2.21	1 (8%)	14,16,16	3.39	5 (35%)

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	942	A	1294	-	-	0/16/16/16	0/2/2/2
4	MES	A	1296	-	-	0/6/14/14	0/1/1/1
2	942	B	1294	-	-	0/16/16/16	0/2/2/2
4	MES	B	1296	-	-	0/6/14/14	0/1/1/1
2	942	C	1294	-	-	0/16/16/16	0/2/2/2
4	MES	C	1296	-	-	0/6/14/14	0/1/1/1
2	942	D	1294	-	-	0/16/16/16	0/2/2/2
4	MES	D	1296	-	-	0/6/14/14	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1294	942	CAI-NAJ	-7.79	1.31	1.45
2	A	1294	942	CAN-CAK	-7.03	1.39	1.50
2	D	1294	942	CAI-NAJ	-6.96	1.33	1.45
2	D	1294	942	CAN-CAK	-6.80	1.39	1.50
4	D	1296	MES	C8-S	-6.78	1.67	1.77
4	C	1296	MES	C8-S	-6.42	1.67	1.77
2	C	1294	942	CAN-CAK	-6.16	1.40	1.50
4	B	1296	MES	C8-S	-6.12	1.68	1.77
4	A	1296	MES	C8-S	-5.53	1.69	1.77
2	C	1294	942	CAI-NAJ	-4.92	1.36	1.45
2	B	1294	942	CAN-CAK	-4.91	1.42	1.50
2	A	1294	942	CAI-NAJ	-4.89	1.36	1.45
2	C	1294	942	CAH-CAI	-3.05	1.37	1.41
2	D	1294	942	CAK-NAJ	-2.90	1.30	1.36
2	D	1294	942	CAH-CAI	-2.70	1.38	1.41
2	B	1294	942	CAB-NAJ	2.10	1.50	1.46
4	C	1296	MES	O2S-S	2.16	1.51	1.45
2	C	1294	942	CAB-NAJ	2.87	1.51	1.46
2	B	1294	942	CAH-NAG	3.90	1.40	1.33
2	C	1294	942	CAH-NAG	4.44	1.41	1.33
2	A	1294	942	CAH-NAG	4.75	1.41	1.33
2	D	1294	942	CAH-NAG	4.78	1.41	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1296	MES	O1S-S-C8	-4.28	103.12	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1294	942	CAI-CAH-NAG	-4.24	116.71	123.37
4	B	1296	MES	O2S-S-O1S	-4.06	99.79	113.86
2	C	1294	942	CAI-CAH-NAG	-3.76	117.47	123.37
2	A	1294	942	CAB-NAJ-CAK	-3.65	111.57	118.69
4	A	1296	MES	O2S-S-C8	-3.64	103.67	106.79
2	D	1294	942	CAI-CAH-NAG	-3.64	117.67	123.37
2	B	1294	942	OAT-CAK-NAJ	-3.57	116.15	121.54
2	C	1294	942	OAT-CAK-NAJ	-3.51	116.23	121.54
2	C	1294	942	CAB-NAJ-CAK	-3.36	112.13	118.69
2	B	1294	942	NAS-CAR-NAQ	-3.06	118.56	120.67
4	A	1296	MES	O2S-S-O1S	-3.02	103.40	113.86
2	B	1294	942	CAB-NAJ-CAK	-2.80	113.23	118.69
4	C	1296	MES	O1-C2-C3	-2.46	106.32	111.83
2	D	1294	942	CAI-CAR-NAS	-2.41	112.29	123.49
2	A	1294	942	CAI-CAH-NAG	-2.41	119.59	123.37
2	D	1294	942	CAB-NAJ-CAK	-2.22	114.35	118.69
2	A	1294	942	OAT-CAK-NAJ	-2.16	118.28	121.54
2	D	1294	942	OAT-CAK-NAJ	-2.11	118.35	121.54
4	D	1296	MES	O3S-S-O2S	-2.01	106.77	111.37
2	C	1294	942	CAL-CAM-CAN	2.02	122.73	120.35
2	B	1294	942	CAL-CAM-CAN	2.10	122.82	120.35
4	B	1296	MES	C6-C5-N4	2.14	113.11	110.11
2	A	1294	942	CAI-NAJ-CAK	2.19	128.07	122.69
2	C	1294	942	CAB-NAJ-CAI	2.24	120.72	115.18
2	D	1294	942	CAF-CAN-CAK	2.31	126.06	120.27
2	A	1294	942	CAD-CAL-CAM	2.36	123.45	120.21
2	B	1294	942	CAE-CAF-CAN	2.49	123.28	120.35
4	C	1296	MES	C6-C5-N4	2.49	113.59	110.11
2	B	1294	942	CAI-NAJ-CAK	2.54	128.93	122.69
4	A	1296	MES	O3S-S-C8	2.61	109.27	106.06
4	D	1296	MES	C2-C3-N4	3.01	114.33	110.11
2	C	1294	942	NAS-CAR-NAQ	3.31	122.94	120.67
2	A	1294	942	CAH-NAG-CAP	3.38	118.11	115.16
4	A	1296	MES	C2-C3-N4	3.41	114.89	110.11
2	B	1294	942	CAN-CAK-NAJ	3.52	123.86	118.59
2	A	1294	942	NAS-CAR-NAQ	3.94	123.38	120.67
4	D	1296	MES	O3S-S-C8	4.13	111.14	106.06
2	C	1294	942	CAH-CAI-CAR	4.99	119.36	114.57
2	B	1294	942	CAH-CAI-CAR	5.21	119.56	114.57
2	A	1294	942	CAH-CAI-CAR	5.59	119.93	114.57
2	D	1294	942	CAH-CAI-CAR	5.89	120.22	114.57
2	B	1294	942	CAH-NAG-CAP	6.11	120.51	115.16

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1294	942	NAS-CAR-NAQ	6.26	124.98	120.67
2	D	1294	942	CAH-NAG-CAP	6.33	120.69	115.16
4	B	1296	MES	C2-C3-N4	7.09	120.04	110.11
4	C	1296	MES	O2S-S-C8	7.21	112.99	106.79
4	B	1296	MES	O2S-S-C8	7.45	113.19	106.79
4	B	1296	MES	O1S-S-C8	7.72	113.42	106.79
2	C	1294	942	CAH-NAG-CAP	8.24	122.37	115.16
4	D	1296	MES	O2S-S-C8	10.07	115.44	106.79
4	A	1296	MES	O1S-S-C8	12.00	117.10	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1294	942	5	0
2	B	1294	942	1	0
4	B	1296	MES	1	0
2	C	1294	942	3	0
4	C	1296	MES	4	0
2	D	1294	942	4	0
4	D	1296	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	293/303 (96%)	-0.60	0	100	100	21, 38, 66, 81	3 (1%)
1	B	291/303 (96%)	-0.51	1 (0%)	93	94	19, 40, 74, 103	3 (1%)
1	C	293/303 (96%)	-0.40	1 (0%)	93	94	29, 46, 74, 88	4 (1%)
1	D	291/303 (96%)	-0.36	3 (1%)	82	83	26, 52, 79, 110	3 (1%)
All	All	1168/1212 (96%)	-0.47	5 (0%)	92	92	19, 44, 74, 110	13 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	ALA	3.7
1	D	23	ILE	3.2
1	B	23	ILE	3.0
1	D	191	PRO	2.8
1	C	193	PRO	2.3

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, 95th 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(Å^2)	Q<0.9
3	CL	B	1295	1/1	0.93	0.18	<mark>3.56</mark>	43,43,43,43	0
4	MES	C	1296	12/12	0.89	0.17	1.49	58,73,87,90	0
2	942	D	1294	23/23	0.95	0.15	1.02	36,41,48,49	0
2	942	C	1294	23/23	0.96	0.13	0.51	32,41,49,51	0
4	MES	D	1296	12/12	0.92	0.16	0.44	49,56,59,67	0
4	MES	B	1296	12/12	0.97	0.13	0.03	44,57,61,64	0
2	942	B	1294	23/23	0.97	0.10	-0.42	24,29,36,37	0
4	MES	A	1296	12/12	0.96	0.13	-0.45	39,45,57,57	0
2	942	A	1294	23/23	0.97	0.10	-0.69	23,33,40,43	0
3	CL	C	1295	1/1	0.97	0.08	-1.25	62,62,62,62	0
3	CL	D	1295	1/1	0.98	0.08	-1.35	48,48,48,48	0
3	CL	A	1295	1/1	0.97	0.09	-1.67	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.