



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:12 AM UTC

PDB ID : 4B4B / pdb_00004b4b
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

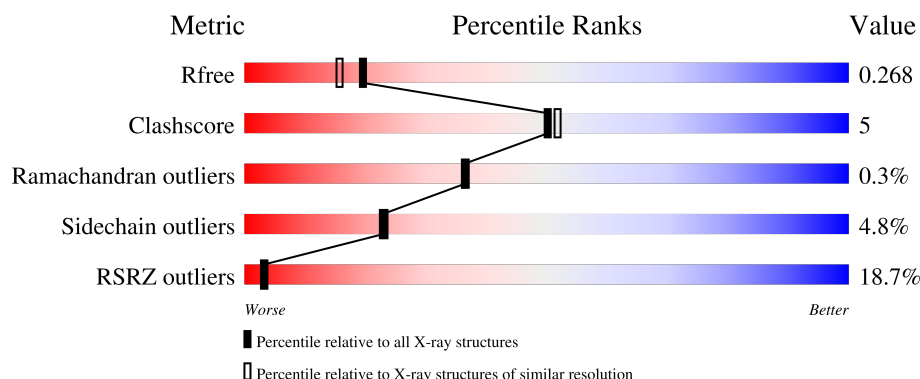
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of 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 $\leq 5\%$. 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	15% 88% 9% ..
1	B	303	13% 83% 11% ..
1	C	303	17% 86% 10% ..
1	D	303	28% 84% 12% ..

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:

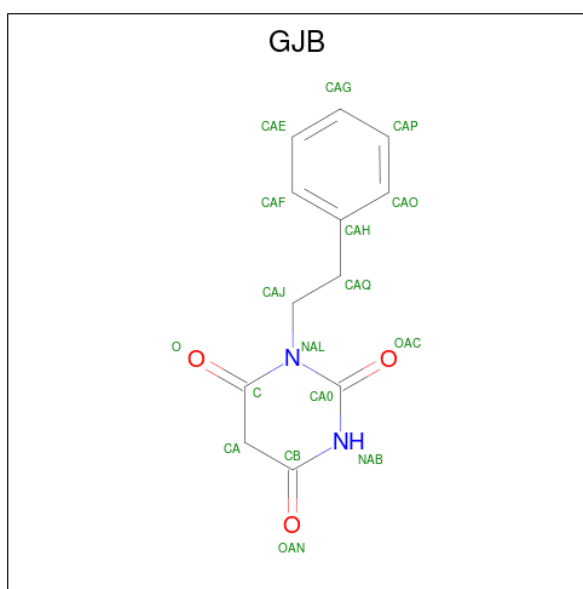
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP Q9HU22
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	GLY	-	expression tag	UNP 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 (CCD ID: GJB) (formula: C₁₂H₁₂N₂O₃).



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

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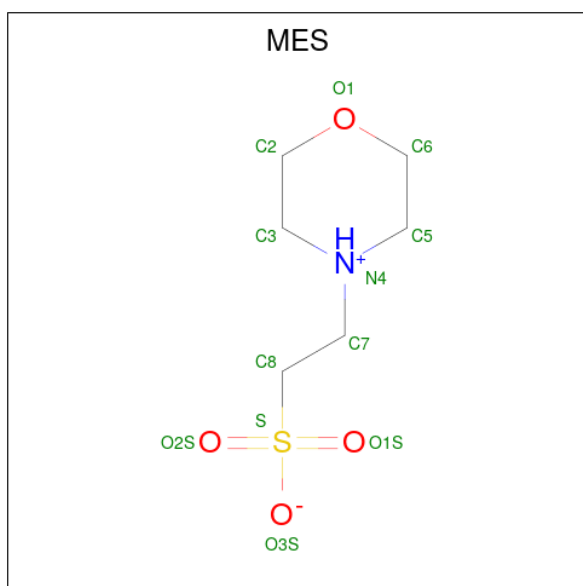
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			17	12	2	3		
2	C	1	Total	C	N	O	0	0
			17	12	2	3		
2	D	1	Total	C	N	O	0	0
			17	12	2	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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		

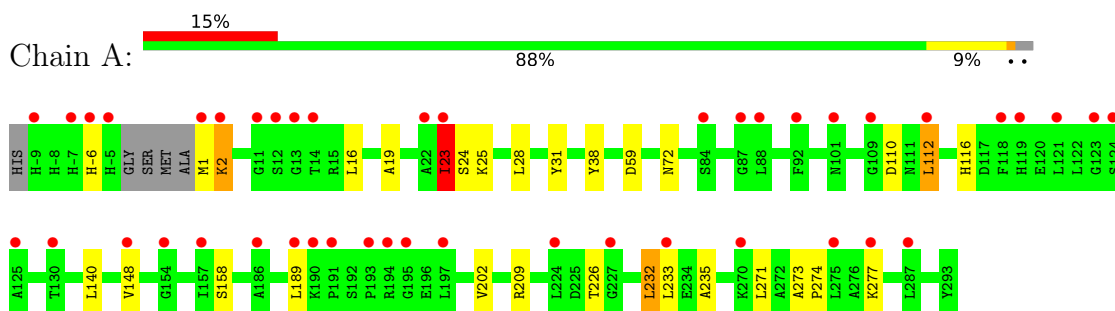
- Molecule 5 is water.

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		

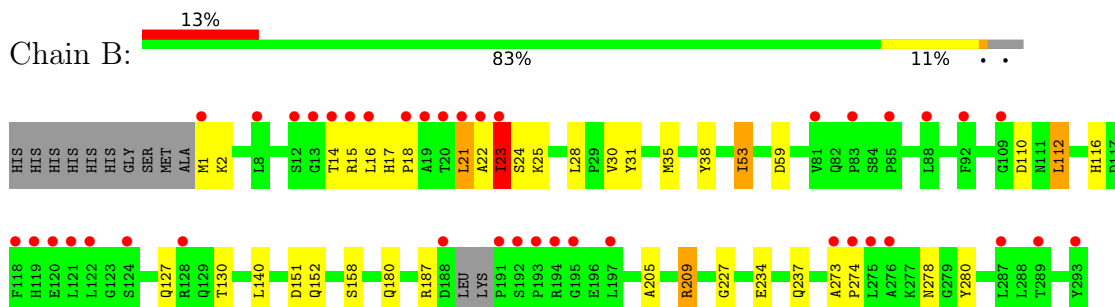
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

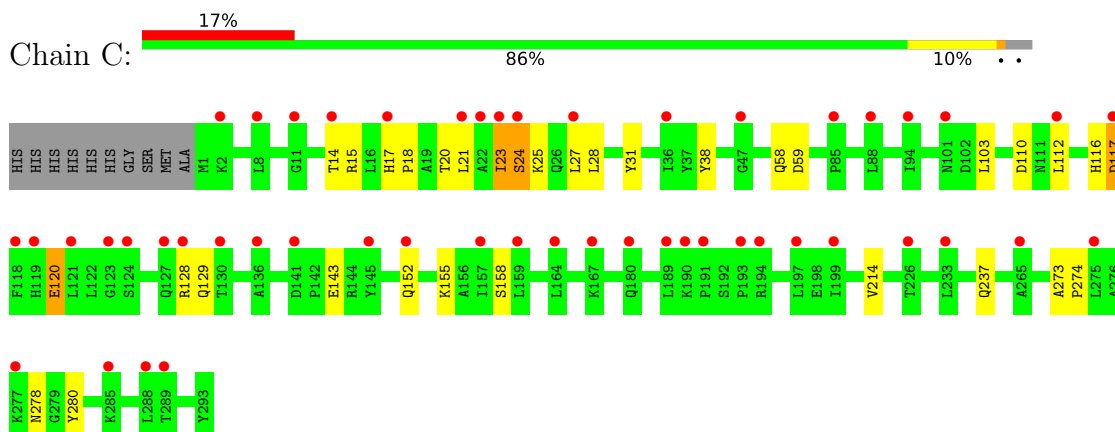
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



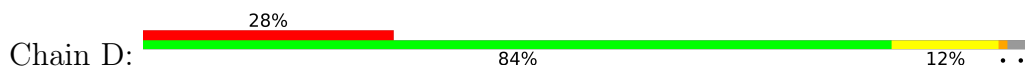
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

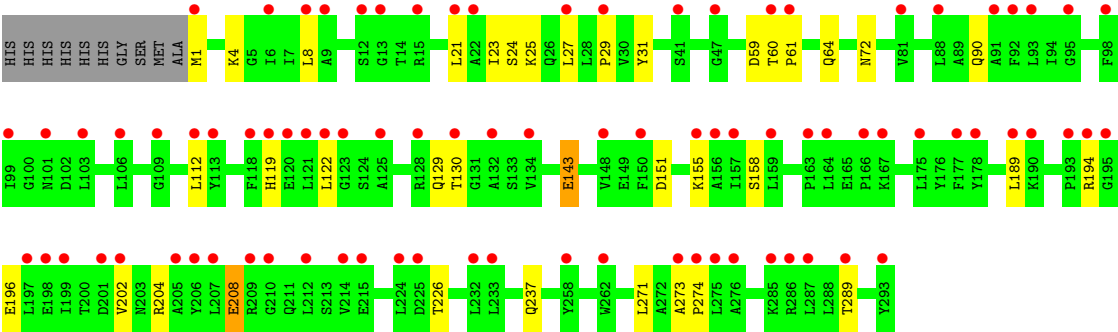


• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.226 , 0.266 0.230 , 0.268	Depositor DCC
R_{free} test set	3646 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, GJB, 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	0.97	1/2406 (0.0%)	0.89	1/3262 (0.0%)
1	B	0.91	0/2334	0.88	2/3164 (0.1%)
1	C	0.80	1/2352 (0.0%)	0.87	0/3190
1	D	0.78	0/2352	0.86	0/3190
All	All	0.87	2/9444 (0.0%)	0.88	3/12806 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ALA	CA-C	6.04	1.60	1.52
1	C	17	HIS	CG-CD2	5.05	1.41	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ILE	CB-CA-C	-8.62	103.64	111.74
1	A	23	ILE	CB-CA-C	-6.41	102.36	111.40
1	B	23	ILE	N-CA-C	6.34	115.43	107.70

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	2349	0	2329	16	0
1	B	2282	0	2268	49	0
1	C	2299	0	2292	38	0
1	D	2299	0	2292	23	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	99	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 (99) 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	1.36	0.91
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:CD	2.36	0.68
1:B:237[A]:GLN:OE1	1:C:237[A]:GLN:CG	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:GLU:HA	1:D:208:GLU:OE1	1.94	0.66
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: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:HD12	1:A:23:ILE:O	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:237[A]:GLN:CD	1:C:237[A]:GLN:OE1	2.45	0.59
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:B:24:SER:HB2	1:B:59:ASP:CG	2.28	0.57
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: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:25:LYS:NZ	1:B:110:ASP:OD2	2.35	0.53
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.90	0.53
1:B:1:MET:SD	1:B:180:GLN:NE2	2.82	0.53
1:B:14:THR:O	1:C:278:ASN:ND2	2.42	0.52
1:B:23:ILE:HD11	1:C:23:ILE:CD1	2.40	0.52
1:B:53:ILE:N	1:B:53:ILE:CD1	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:B:112:LEU:C	1:B:112:LEU:HD12	2.38	0.49
1:C:25:LYS:NZ	1:C:110:ASP:OD2	2.46	0.48
1:B:1:MET:HE1	1:B:180:GLN:HE22	1.79	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:B:25:LYS:NZ	1:B:227:GLY:HA2	2.20	0.47
1:A:25:LYS:NZ	1:A:110:ASP:OD2	2.44	0.46
1:C:24:SER:HB3	1:C:59:ASP:CG	2.40	0.46
1:C:117:ASP:O	1:C:120:GLU:HG3	2.16	0.46
1:C:58:GLN:CD	1:C:58:GLN:N	2.75	0.45
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:A:233:LEU:HD21	1:D:237[B]:GLN:HA	1.99	0.44
1:D:8:LEU:C	1:D:8:LEU:HD23	2.43	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:D:1:MET:HE3	1:D:129:GLN:OE1	2.20	0.42
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:D:143:GLU:H	1:D:143:GLU:CD	2.28	0.42
1:B:17:HIS:CD2	1:B:21:LEU:HG	2.54	0.42
1:B:278:ASN:ND2	1:C:14:THR:O	2.53	0.42
1:B:151:ASP:OD1	1:B:151:ASP:C	2.62	0.42
1:D:60:THR:HG22	1:D:64:GLN:OE1	2.21	0.41
1:D:151:ASP:OD1	1:D:151:ASP:C	2.63	0.41
1:B:23:ILE:CD1	1:C:23:ILE:HD11	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	36
1	B	288/303 (95%)	282 (98%)	5 (2%)	1 (0%)	36	36
1	C	292/303 (96%)	286 (98%)	5 (2%)	1 (0%)	36	36
1	D	292/303 (96%)	287 (98%)	4 (1%)	1 (0%)	36	36
All	All	1167/1212 (96%)	1143 (98%)	20 (2%)	4 (0%)	36	36

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%)	235 (96%)	11 (4%)	24	25
1	B	239/248 (96%)	227 (95%)	12 (5%)	22	22
1	C	241/248 (97%)	231 (96%)	10 (4%)	27	29
1	D	241/248 (97%)	228 (95%)	13 (5%)	20	18
All	All	967/992 (98%)	921 (95%)	46 (5%)	23	23

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	HIS
1	A	1	MET
1	A	2	LYS
1	A	23	ILE
1	A	112	LEU
1	A	140	LEU
1	A	148	VAL
1	A	158	SER
1	A	209	ARG
1	A	232	LEU
1	A	277	LYS
1	B	15	ARG
1	B	21	LEU
1	B	23	ILE
1	B	53	ILE
1	B	112	LEU
1	B	127	GLN
1	B	130	THR
1	B	140	LEU
1	B	152	GLN
1	B	158	SER
1	B	187	ARG
1	B	209	ARG
1	C	21	LEU
1	C	23	ILE
1	C	24	SER
1	C	117	ASP
1	C	120	GLU
1	C	128	ARG
1	C	143	GLU
1	C	152	GLN
1	C	155	LYS
1	C	158	SER

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Mol	Chain	Res	Type
1	D	4	LYS
1	D	21	LEU
1	D	90	GLN
1	D	112	LEU
1	D	119	HIS
1	D	122	LEU
1	D	130	THR
1	D	143	GLU
1	D	155	LYS
1	D	158	SER
1	D	204	ARG
1	D	208	GLU
1	D	289	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	211	GLN
1	A	229	HIS
1	B	82	GLN
1	B	90	GLN
1	B	101	ASN
1	B	138	HIS
1	C	78	GLN
1	C	119	HIS
1	C	181	GLN
1	C	211	GLN
1	D	138	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	GJB	B	400	-	18,18,18	0.77	1 (5%)	23,24,24	3.32	10 (43%)
2	GJB	C	400	-	18,18,18	1.23	3 (16%)	23,24,24	3.07	10 (43%)
2	GJB	D	400	-	18,18,18	1.24	1 (5%)	23,24,24	2.91	8 (34%)
4	MES	A	1295	-	12,12,12	1.83	1 (8%)	15,16,16	1.68	3 (20%)
2	GJB	A	400	-	18,18,18	0.85	0	23,24,24	2.79	8 (34%)
4	MES	B	1295	-	12,12,12	2.05	1 (8%)	15,16,16	1.51	1 (6%)
4	MES	C	1295	-	12,12,12	2.00	1 (8%)	15,16,16	1.32	2 (13%)

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	GJB	B	400	-	-	2/5/21/21	0/2/2/2
2	GJB	C	400	-	-	2/5/21/21	0/2/2/2
2	GJB	D	400	-	-	3/5/21/21	0/2/2/2
4	MES	A	1295	-	-	3/6/14/14	0/1/1/1
2	GJB	A	400	-	-	2/5/21/21	0/2/2/2
4	MES	B	1295	-	-	1/6/14/14	0/1/1/1
4	MES	C	1295	-	-	2/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1295	MES	C8-S	-6.58	1.68	1.77
4	C	1295	MES	C8-S	-6.45	1.68	1.77
4	A	1295	MES	C8-S	-5.70	1.69	1.77
2	C	400	GJB	CB-NAB	3.22	1.43	1.37
2	C	400	GJB	CA0-NAB	2.22	1.41	1.38
2	D	400	GJB	C-NAL	2.17	1.43	1.39
2	C	400	GJB	C-NAL	2.15	1.43	1.39
2	B	400	GJB	CB-NAB	2.03	1.41	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	GJB	CA-C-NAL	9.86	124.32	117.12
2	C	400	GJB	CA-C-NAL	8.14	123.07	117.12
2	A	400	GJB	CA-C-NAL	8.05	123.00	117.12
2	D	400	GJB	CA-C-NAL	7.47	122.58	117.12
2	D	400	GJB	CA-CB-NAB	6.76	123.13	116.81
2	B	400	GJB	CA-CB-NAB	6.00	122.42	116.81
2	A	400	GJB	CA-CB-NAB	5.93	122.35	116.81
2	C	400	GJB	CA-CB-NAB	5.63	122.07	116.81
2	D	400	GJB	C-NAL-CA0	-5.34	120.16	125.10
2	C	400	GJB	C-NAL-CA0	-5.10	120.38	125.10
2	B	400	GJB	C-NAL-CA0	-4.81	120.66	125.10
2	B	400	GJB	CAQ-CAJ-NAL	-4.75	104.80	112.13
2	A	400	GJB	C-NAL-CA0	-4.75	120.71	125.10
2	B	400	GJB	CAJ-NAL-CA0	4.57	122.55	117.31
4	A	1295	MES	O2S-S-C8	4.36	113.31	106.73
4	B	1295	MES	O3S-S-C8	4.35	114.52	106.00
2	D	400	GJB	CB-CA-C	-4.05	110.07	117.28
2	C	400	GJB	OAC-CA0-NAL	-3.97	117.14	122.32
2	C	400	GJB	CAJ-NAL-C	3.90	121.24	118.01
2	C	400	GJB	CAQ-CAJ-NAL	-3.88	106.14	112.13
2	B	400	GJB	CB-CA-C	-3.85	110.42	117.28
2	C	400	GJB	NAB-CA0-NAL	3.74	122.17	115.45
2	D	400	GJB	CAJ-NAL-C	3.60	121.00	118.01
2	D	400	GJB	NAB-CA0-NAL	3.59	121.90	115.45
2	A	400	GJB	CB-CA-C	-3.45	111.14	117.28
2	C	400	GJB	CB-CA-C	-3.45	111.15	117.28
4	A	1295	MES	O3S-S-C8	3.42	112.69	106.00
2	A	400	GJB	CAQ-CAJ-NAL	-3.00	107.50	112.13
4	C	1295	MES	O3S-S-C8	2.95	111.78	106.00
2	C	400	GJB	OAN-CB-CA	-2.93	118.01	122.78
2	B	400	GJB	O-C-NAL	-2.75	116.40	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	GJB	NAB-CA0-NAL	2.74	120.38	115.45
2	A	400	GJB	CAJ-NAL-C	2.60	120.16	118.01
2	B	400	GJB	NAB-CA0-NAL	2.60	120.11	115.45
2	B	400	GJB	OAN-CB-CA	-2.59	118.56	122.78
2	A	400	GJB	OAN-CB-CA	-2.56	118.61	122.78
2	D	400	GJB	OAN-CB-NAB	-2.54	116.39	120.30
2	C	400	GJB	CAJ-CAQ-CAH	2.34	118.75	112.15
2	D	400	GJB	OAC-CA0-NAB	-2.30	117.24	121.49
4	C	1295	MES	O3S-S-O2S	-2.14	106.03	111.40
4	A	1295	MES	O2S-S-O1S	-2.09	107.02	113.82
2	B	400	GJB	CAJ-CAQ-CAH	2.08	118.02	112.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1295	MES	C7-C8-S-O1S
4	A	1295	MES	C7-C8-S-O3S
2	A	400	GJB	CAO-CAH-CAQ-CAJ
4	C	1295	MES	C8-C7-N4-C3
2	A	400	GJB	CAF-CAH-CAQ-CAJ
2	C	400	GJB	CAF-CAH-CAQ-CAJ
2	B	400	GJB	CAF-CAH-CAQ-CAJ
2	C	400	GJB	CAO-CAH-CAQ-CAJ
2	B	400	GJB	CAO-CAH-CAQ-CAJ
4	A	1295	MES	C7-C8-S-O2S
2	D	400	GJB	CAF-CAH-CAQ-CAJ
2	D	400	GJB	CAO-CAH-CAQ-CAJ
4	B	1295	MES	C8-C7-N4-C5
4	C	1295	MES	C8-C7-N4-C5
2	D	400	GJB	CAQ-CAJ-NAL-C

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, 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(Å ²)	Q<0.9
1	A	298/303 (98%)	0.92	44 (14%)	5 6	24, 55, 94, 115	2 (0%)
1	B	291/303 (96%)	1.01	40 (13%)	6 7	25, 56, 93, 130	3 (1%)
1	C	293/303 (96%)	1.34	50 (17%)	4 4	28, 65, 97, 131	2 (0%)
1	D	293/303 (96%)	1.64	86 (29%)	1 1	28, 67, 95, 121	4 (1%)
All	All	1175/1212 (96%)	1.23	220 (18%)	3 3	24, 62, 95, 131	11 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	ILE	7.6
1	D	118	PHE	6.2
1	B	23	ILE	5.9
1	B	194	ARG	5.6
1	C	128	ARG	5.6
1	C	118	PHE	5.6
1	A	194	ARG	5.4
1	D	119	HIS	5.3
1	B	191	PRO	5.2
1	C	22	ALA	4.9
1	D	122	LEU	4.7
1	D	121	LEU	4.4
1	D	128	ARG	4.3
1	B	14	THR	4.3
1	D	92	PHE	4.2
1	C	193	PRO	4.1
1	A	2	LYS	4.0
1	B	22	ALA	4.0
1	B	118	PHE	4.0
1	D	22	ALA	3.8
1	A	118	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	164	LEU	3.7
1	B	193	PRO	3.7
1	A	13	GLY	3.6
1	D	232	LEU	3.6
1	C	130	THR	3.6
1	D	91	ALA	3.6
1	A	88	LEU	3.6
1	D	125	ALA	3.5
1	D	1	MET	3.5
1	B	21	LEU	3.5
1	B	88	LEU	3.5
1	A	-6	HIS	3.4
1	C	119	HIS	3.4
1	C	88	LEU	3.4
1	D	88	LEU	3.4
1	D	159	LEU	3.4
1	A	193	PRO	3.4
1	B	275	LEU	3.4
1	D	12	SER	3.3
1	D	166	PRO	3.3
1	D	212	LEU	3.3
1	D	193	PRO	3.2
1	D	112	LEU	3.2
1	A	189	LEU	3.2
1	C	141	ASP	3.2
1	D	156	ALA	3.2
1	C	112	LEU	3.2
1	B	128	ARG	3.2
1	C	14	THR	3.2
1	D	210	GLY	3.2
1	D	274	PRO	3.2
1	B	188	ASP	3.1
1	D	275	LEU	3.1
1	D	27	LEU	3.1
1	D	164	LEU	3.1
1	D	224	LEU	3.1
1	D	195	GLY	3.0
1	A	119	HIS	3.0
1	A	1	MET	3.0
1	D	134	VAL	3.0
1	D	233	LEU	3.0
1	B	1	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	12	SER	3.0
1	D	93	LEU	3.0
1	D	130	THR	3.0
1	A	-5	HIS	3.0
1	B	18	PRO	2.9
1	B	92	PHE	2.9
1	B	19	ALA	2.9
1	D	167	LYS	2.9
1	A	275	LEU	2.8
1	C	21	LEU	2.8
1	C	288	LEU	2.8
1	A	130	THR	2.8
1	B	124	SER	2.8
1	C	121	LEU	2.8
1	D	103	LEU	2.8
1	C	191	PRO	2.8
1	A	191	PRO	2.8
1	B	119	HIS	2.8
1	D	205	ALA	2.8
1	D	197	LEU	2.8
1	D	81	VAL	2.7
1	A	-7	HIS	2.7
1	D	123	GLY	2.7
1	C	189	LEU	2.7
1	D	15	ARG	2.7
1	D	207	LEU	2.7
1	D	202	VAL	2.7
1	A	224	LEU	2.6
1	C	24	SER	2.6
1	D	276	ALA	2.6
1	A	101	ASN	2.6
1	D	289	THR	2.6
1	D	61	PRO	2.6
1	D	190	LYS	2.6
1	B	289	THR	2.6
1	D	215	GLU	2.5
1	D	206	TYR	2.5
1	D	258	TYR	2.5
1	C	265	ALA	2.5
1	B	121	LEU	2.5
1	C	17	HIS	2.5
1	B	83	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	41	SER	2.5
1	D	199	ILE	2.5
1	A	14	THR	2.5
1	A	84	SER	2.5
1	C	289	THR	2.5
1	A	22	ALA	2.5
1	B	287	LEU	2.5
1	D	209	ARG	2.5
1	A	227	GLY	2.5
1	D	95	GLY	2.5
1	D	99	ILE	2.5
1	A	121	LEU	2.4
1	C	167	LYS	2.4
1	A	12	SER	2.4
1	D	273	ALA	2.4
1	C	27	LEU	2.4
1	B	195	GLY	2.4
1	D	13	GLY	2.4
1	C	94	ILE	2.4
1	D	6	ILE	2.4
1	B	192	SER	2.4
1	B	274	PRO	2.4
1	A	186	ALA	2.4
1	B	197	LEU	2.4
1	C	197	LEU	2.4
1	C	275	LEU	2.4
1	D	8	LEU	2.4
1	C	101	ASN	2.4
1	D	101	ASN	2.4
1	C	199	ILE	2.4
1	A	124	SER	2.4
1	C	277	LYS	2.4
1	D	113	TYR	2.3
1	B	122	LEU	2.3
1	C	159	LEU	2.3
1	D	120	GLU	2.3
1	A	195	GLY	2.3
1	B	16	LEU	2.3
1	C	11	GLY	2.3
1	D	225	ASP	2.3
1	C	190	LYS	2.3
1	C	124	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	198	GLU	2.3
1	B	276	ALA	2.3
1	D	132	ALA	2.3
1	A	154	GLY	2.3
1	B	109	GLY	2.3
1	B	293	TYR	2.3
1	D	287	LEU	2.3
1	A	92	PHE	2.3
1	D	148	VAL	2.3
1	D	201	ASP	2.3
1	D	21	LEU	2.3
1	C	145	TYR	2.3
1	D	150	PHE	2.2
1	D	163	PRO	2.2
1	C	194	ARG	2.2
1	A	277	LYS	2.2
1	D	155	LYS	2.2
1	A	125	ALA	2.2
1	C	123	GLY	2.2
1	A	287	LEU	2.2
1	D	175	LEU	2.2
1	A	157	ILE	2.2
1	D	47	GLY	2.2
1	D	9	ALA	2.2
1	A	197	LEU	2.2
1	C	180	GLN	2.2
1	D	29	PRO	2.2
1	B	120	GLU	2.2
1	C	47	GLY	2.2
1	C	2	LYS	2.2
1	C	285	LYS	2.2
1	A	23	ILE	2.1
1	D	177	PHE	2.1
1	D	214	VAL	2.1
1	B	273	ALA	2.1
1	A	233	LEU	2.1
1	C	8	LEU	2.1
1	D	189	LEU	2.1
1	D	286	ARG	2.1
1	D	293	TYR	2.1
1	D	60	THR	2.1
1	D	178	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	87	GLY	2.1
1	B	13	GLY	2.1
1	D	285	LYS	2.1
1	C	136	ALA	2.1
1	C	152	GLN	2.1
1	A	-9	HIS	2.1
1	B	15	ARG	2.1
1	D	194	ARG	2.1
1	D	109	GLY	2.1
1	A	148	VAL	2.1
1	B	81	VAL	2.1
1	D	98	PHE	2.1
1	A	112	LEU	2.0
1	C	233	LEU	2.0
1	D	106	LEU	2.0
1	C	127	GLN	2.0
1	B	85	PRO	2.0
1	C	226	THR	2.0
1	A	190	LYS	2.0
1	A	270	LYS	2.0
1	A	11	GLY	2.0
1	A	123	GLY	2.0
1	C	36	ILE	2.0
1	C	157	ILE	2.0
1	D	157	ILE	2.0
1	D	262	TRP	2.0
1	B	8	LEU	2.0
1	C	117	ASP	2.0
1	B	20	THR	2.0
1	C	85	PRO	2.0
1	A	109	GLY	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	GJB	D	400	17/17	0.81	0.15	59,72,76,77	0
4	MES	B	1295	12/12	0.85	0.18	72,85,88,91	0
2	GJB	C	400	17/17	0.86	0.13	55,62,71,76	0
3	CL	B	1294	1/1	0.89	0.18	64,64,64,64	0
4	MES	A	1295	12/12	0.89	0.13	68,83,93,93	0
2	GJB	A	400	17/17	0.89	0.12	49,51,66,66	0
4	MES	C	1295	12/12	0.89	0.13	76,85,90,91	0
2	GJB	B	400	17/17	0.90	0.13	50,53,59,63	0
3	CL	D	1294	1/1	0.93	0.11	84,84,84,84	0
3	CL	A	1294	1/1	0.95	0.10	62,62,62,62	0
3	CL	C	1294	1/1	0.95	0.12	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.