



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:03 AM UTC

PDB ID : 4B4B / pdb_00004b4b
Title : Pseudomonas aeruginosa RmlA in complex with allosteric inhibitor
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Deposited on : 2012-07-30
Resolution : 2.10 Å(reported)

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

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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

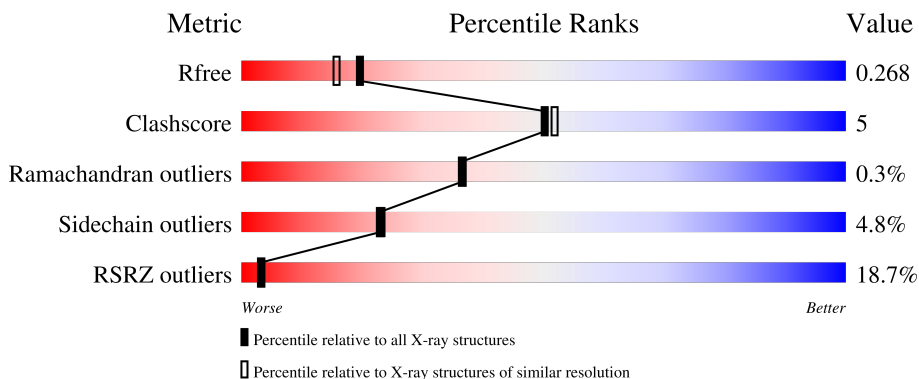
1 Overall quality at a glance

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
			Total	C	N	O	S			
1	A	298	Total 2349	C 1501	N 402	O 441	S 5	0	1	0
1	B	291	Total 2282	C 1459	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	293	Total 2299	C 1471	N 387	O 436	S 5	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

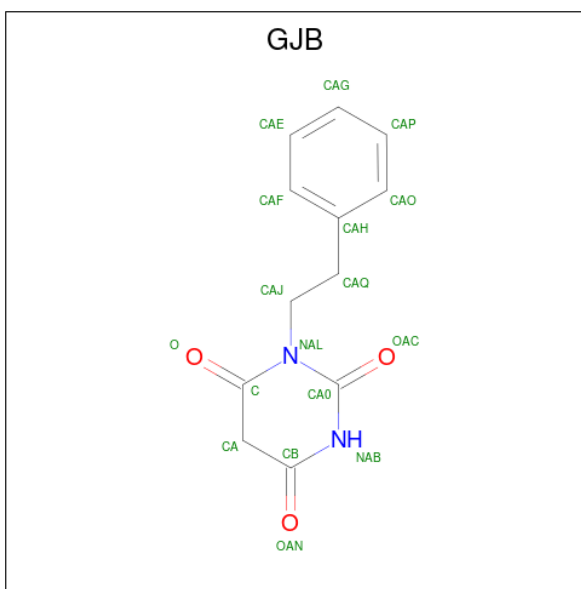
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	HIS	-	expression tag	UNP Q9HU22
A	-9	HIS	-	expression tag	UNP Q9HU22
A	-8	HIS	-	expression tag	UNP Q9HU22
A	-7	HIS	-	expression tag	UNP Q9HU22
A	-6	HIS	-	expression tag	UNP Q9HU22
A	-5	HIS	-	expression tag	UNP Q9HU22
A	-4	GLY	-	expression tag	UNP 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
			Total	C	N	O		
2	A	1	17	12	2	3	0	0

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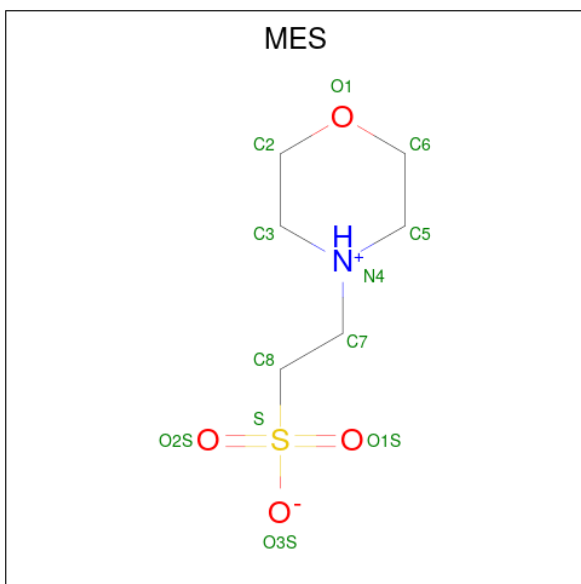
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	Total 17	C 12	N 2	O 3	0	0
2	C	1	Total 17	C 12	N 2	O 3	0	0
2	D	1	Total 17	C 12	N 2	O 3	0	0

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

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

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



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

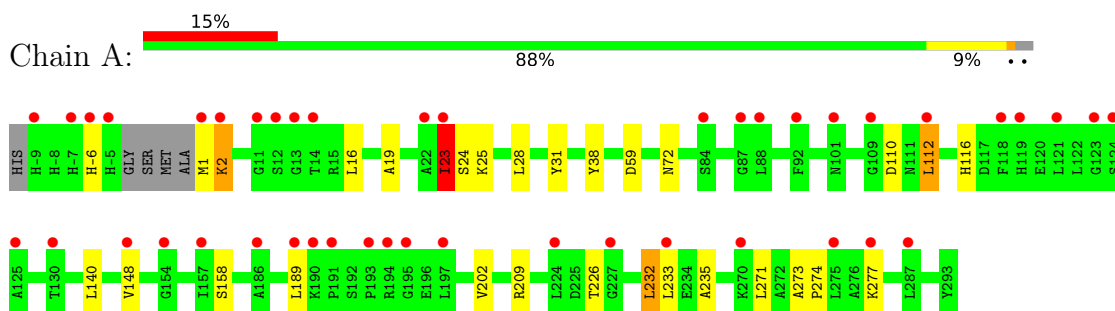
- Molecule 5 is water.

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

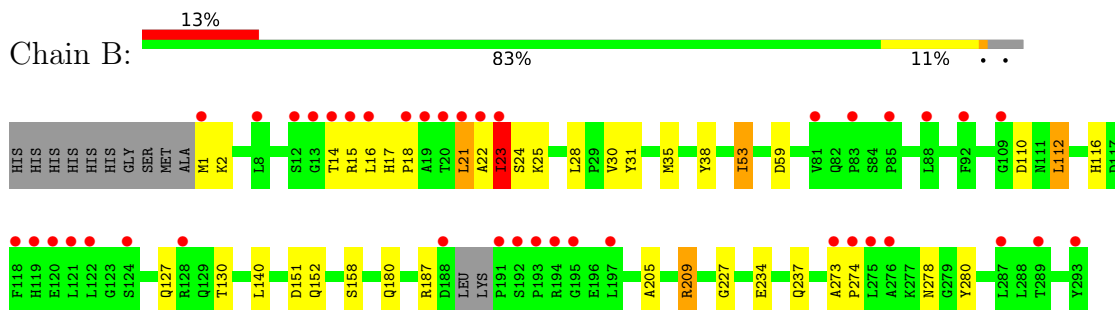
3 Residue-property plots [i](#)

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.

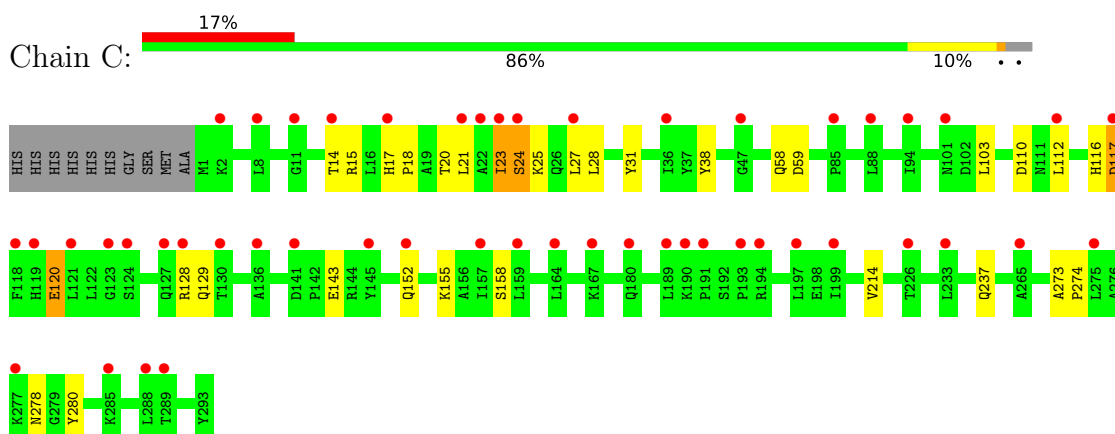
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



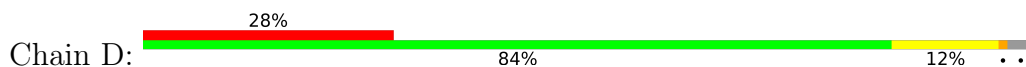
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

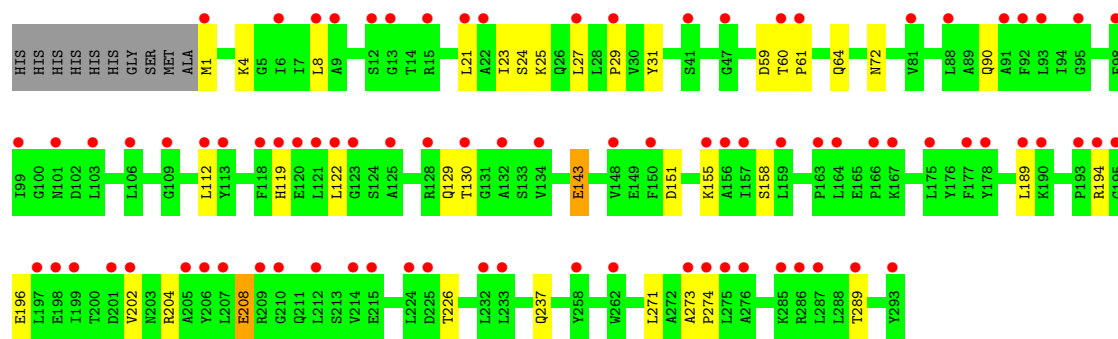


- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE



- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE





4 Data and refinement statistics i

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)	Xtrriage
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	Xtrriage
Anisotropy	0.376	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.060 for h,-k,-l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2349	0	2329	16	0
1	B	2282	0	2268	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.

The worst 5 of 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

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

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	128	ARG
1	D	90	GLN
1	C	143	GLU
1	C	158	SER

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Mol	Chain	Res	Type
1	D	119	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	GLN
1	C	119	HIS
1	D	138	HIS
1	C	181	GLN
1	B	82	GLN

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 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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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

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 [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(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%)

The worst 5 of 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

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(\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.