



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:40 AM UTC

PDB ID : 8AJQ / pdb_00008ajq
Title : Crystal structure of PA2722 from Pseudomonas aeruginosa PAO1
Authors : Popp, M.A.; Blankenfeldt, W.
Deposited on : 2022-07-28
Resolution : 1.25 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

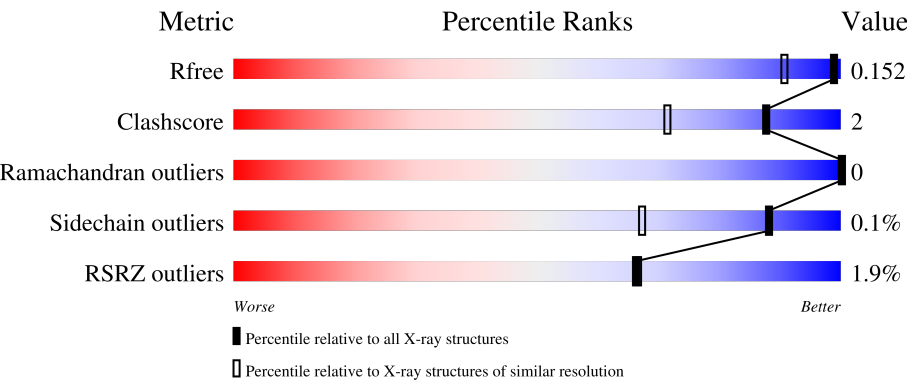
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	132	2% 95% 5%
1	B	132	2% 97% .
1	C	132	3% 97% .
1	D	132	2% 95% 5%
1	E	132	2% 94% 6%

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Mol	Chain	Length	Quality of chain
1	F	132	% 90% 10%
1	G	132	2% 94% 6%
1	H	132	2% 94% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19682 atoms, of which 8886 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 CENP-V/GFA domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	132	Total	C	H	N	O	S	0	11	0
			2150	687	1059	202	193	9			
1	B	132	Total	C	H	N	O	S	0	12	0
			2192	699	1081	204	199	9			
1	C	132	Total	C	H	N	O	S	0	23	0
			2267	718	1114	218	208	9			
1	D	132	Total	C	H	N	O	S	0	12	0
			2165	692	1069	200	195	9			
1	E	132	Total	C	H	N	O	S	0	14	0
			2217	702	1097	210	200	8			
1	F	132	Total	C	H	N	O	S	0	16	0
			2232	710	1092	211	210	9			
1	G	132	Total	C	H	N	O	S	0	5	0
			2089	671	1020	199	191	8			
1	H	132	Total	C	H	N	O	S	0	17	0
			2232	711	1103	210	199	9			

There are 16 discrepancies between the modelled and reference sequences:

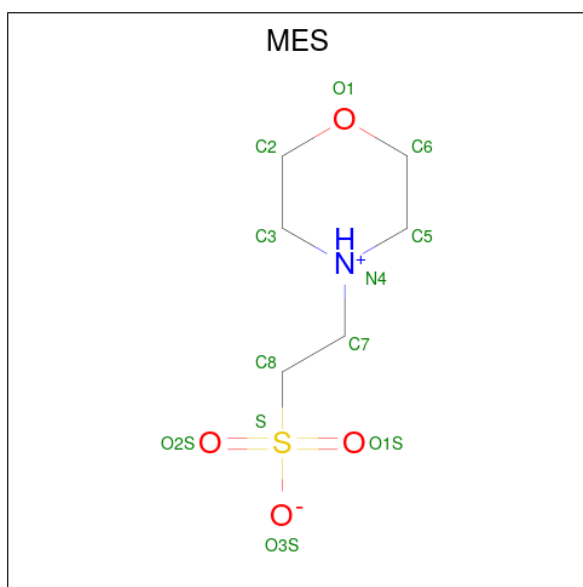
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9I0C0
A	0	HIS	-	expression tag	UNP Q9I0C0
B	-1	GLY	-	expression tag	UNP Q9I0C0
B	0	HIS	-	expression tag	UNP Q9I0C0
C	-1	GLY	-	expression tag	UNP Q9I0C0
C	0	HIS	-	expression tag	UNP Q9I0C0
D	-1	GLY	-	expression tag	UNP Q9I0C0
D	0	HIS	-	expression tag	UNP Q9I0C0
E	-1	GLY	-	expression tag	UNP Q9I0C0
E	0	HIS	-	expression tag	UNP Q9I0C0
F	-1	GLY	-	expression tag	UNP Q9I0C0
F	0	HIS	-	expression tag	UNP Q9I0C0
G	-1	GLY	-	expression tag	UNP Q9I0C0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q9I0C0
H	-1	GLY	-	expression tag	UNP Q9I0C0
H	0	HIS	-	expression tag	UNP Q9I0C0

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



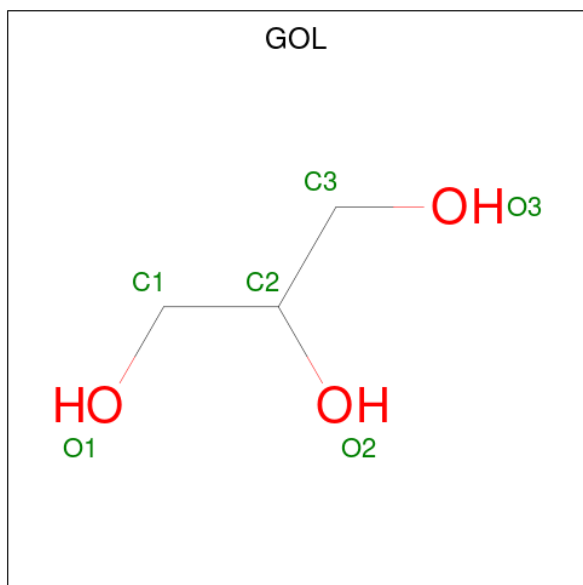
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	C	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	E	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	E	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	F	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	G	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	0
2	H	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	0
2	H	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			14	3	8	3	0	0
3	A	1	Total	C	H	O		
			14	3	8	3	0	0
3	A	1	Total	C	H	O		
			14	3	8	3	0	0
3	B	1	Total	C	H	O		
			14	3	8	3	0	0
3	C	1	Total	C	H	O		
			14	3	8	3	0	1
3	D	1	Total	C	H	O		
			28	6	16	6	0	1
3	E	1	Total	C	H	O		
			14	3	8	3	0	0
3	F	1	Total	C	H	O		
			13	3	7	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	G	1	Total	C	H	O	0	0
			14	3	8	3		
3	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	E	2	Total	Zn	0	0
			2	2		
4	F	2	Total	Zn	0	0
			2	2		
4	G	2	Total	Zn	0	0
			2	2		
4	H	2	Total	Zn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	216	Total	O	0	2
			216	216		
5	B	226	Total	O	0	5
			226	226		
5	C	211	Total	O	0	3
			211	211		
5	D	199	Total	O	0	2
			199	199		
5	E	183	Total	O	0	4
			183	183		
5	F	205	Total	O	0	5
			207	207		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	197	Total 197	O 197	0	3
5	H	216	Total 216	O 216	0	2

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: CENP-V/GFA domain-containing protein



- Molecule 1: CENP-V/GFA domain-containing protein



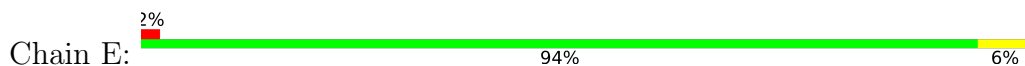
- Molecule 1: CENP-V/GFA domain-containing protein



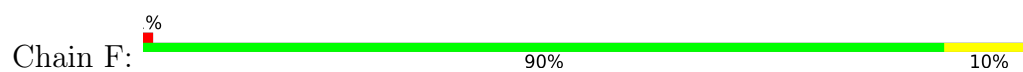
- Molecule 1: CENP-V/GFA domain-containing protein



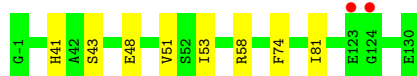
- Molecule 1: CENP-V/GFA domain-containing protein



- Molecule 1: CENP-V/GFA domain-containing protein



- Molecule 1: CENP-V/GFA domain-containing protein



- Molecule 1: CENP-V/GFA domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.57Å 86.24Å 172.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.79 – 1.25 47.79 – 1.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.79-1.25) 99.7 (47.79-1.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.25Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.138 , 0.152 0.138 , 0.152	Depositor DCC
R_{free} test set	17489 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	19682	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1227e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, MES, GOL

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	0.37	0/1154	0.56	0/1552
1	B	0.38	0/1182	0.57	0/1590
1	C	0.37	0/1251	0.56	0/1680
1	D	0.38	0/1160	0.59	0/1561
1	E	0.36	0/1193	0.58	0/1604
1	F	0.33	0/1203	0.54	0/1617
1	G	0.34	0/1110	0.55	0/1495
1	H	0.34	0/1216	0.52	0/1636
All	All	0.36	0/9469	0.56	0/12735

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1091	1059	1049	4	1
1	B	1111	1081	1081	3	0
1	C	1153	1114	1064	2	0
1	D	1096	1069	1063	3	1
1	E	1120	1097	1073	7	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1140	1092	1088	9	1
1	G	1069	1020	1019	6	0
1	H	1129	1103	1081	6	1
2	A	12	13	13	0	0
2	B	24	26	25	0	0
2	C	12	13	13	0	0
2	D	12	13	13	0	0
2	E	24	26	26	1	0
2	F	12	13	13	0	0
2	G	24	26	26	0	0
2	H	24	26	25	0	0
3	A	18	24	24	2	0
3	B	6	8	8	1	0
3	C	6	8	8	0	0
3	D	12	16	16	0	0
3	E	6	8	8	0	0
3	F	12	15	15	1	0
3	G	6	8	8	0	0
3	H	6	8	8	0	0
4	A	2	0	0	0	1
4	B	2	0	0	0	1
4	C	2	0	0	0	1
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	1
4	H	2	0	0	0	1
5	A	216	0	0	0	0
5	B	226	0	0	0	0
5	C	211	0	0	0	0
5	D	199	0	0	0	0
5	E	183	0	0	0	0
5	F	207	0	0	0	0
5	G	197	0	0	0	0
5	H	216	0	0	0	0
All	All	10796	8886	8767	36	5

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 2.

All (36) 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:H:45:ILE:HG12	1:H:82[B]:GLU:HG3	1.70	0.74
1:F:30:LEU:HD12	3:F:202:GOL:H31	1.78	0.63
1:H:45:ILE:HG12	1:H:82[B]:GLU:CG	2.34	0.58
1:A:58:ARG:HH12	1:B:58[A]:ARG:HH12	1.55	0.55
1:C:45:ILE:HG12	1:C:82[B]:GLU:HG2	1.93	0.51
1:G:58:ARG:HH12	1:H:58:ARG:HH12	1.58	0.51
1:A:30[A]:LEU:HB2	3:A:203:GOL:H2	1.94	0.50
1:E:103[B]:VAL:HG23	1:E:119:GLU:HB3	1.93	0.50
1:H:118:TYR:OH	1:H:129:GLU:OE2	2.29	0.49
1:F:118:TYR:CD1	1:F:122[A]:ARG:HA	2.49	0.47
1:F:51:VAL:CG2	1:F:81[B]:ILE:HG21	2.45	0.47
1:E:58[A]:ARG:HH12	1:F:58:ARG:HH12	1.63	0.46
1:E:103[B]:VAL:HG12	1:E:104[B]:ARG:NH1	2.30	0.46
1:B:53[A]:ILE:HD13	3:B:203:GOL:H11	1.96	0.45
1:B:36:HIS:CE1	1:B:41[A]:HIS:CE1	3.04	0.45
1:G:51:VAL:CG2	1:G:81[B]:ILE:HG21	2.47	0.45
1:G:41[B]:HIS:CE1	1:G:43:SER:HB3	2.53	0.43
1:A:30[B]:LEU:HB2	3:A:203:GOL:H2	2.00	0.43
1:H:41[B]:HIS:NE2	1:H:82[B]:GLU:OE2	2.46	0.43
1:C:36:HIS:CE1	1:C:41:HIS:CE1	3.07	0.43
1:D:36:HIS:CE1	1:D:41:HIS:CE1	3.07	0.43
1:E:58[B]:ARG:HH12	1:F:58:ARG:HH12	1.67	0.43
1:E:101:TRP:CZ2	2:E:202:MES:H31	2.54	0.42
1:D:35:HIS:CD2	1:D:63:ARG:HD3	2.55	0.42
1:E:103[B]:VAL:CG2	1:E:119:GLU:HB3	2.50	0.41
1:F:118:TYR:CE1	1:F:122[A]:ARG:HA	2.55	0.41
1:G:53[B]:ILE:HD13	1:G:74:PHE:CZ	2.56	0.41
1:A:36:HIS:CE1	1:A:41:HIS:CE1	3.08	0.41
1:D:15[B]:LEU:HD11	1:D:83:VAL:HG22	2.03	0.41
1:F:45:ILE:HG12	1:F:82[A]:GLU:HG2	2.02	0.41
1:H:36:HIS:CE1	1:H:41[A]:HIS:CE1	3.09	0.41
1:E:36:HIS:CE1	1:E:41:HIS:CE1	3.09	0.41
1:G:48:GLU:HA	1:G:81[B]:ILE:HG22	2.02	0.40
1:F:35:HIS:CD2	1:F:63:ARG:HD3	2.55	0.40
1:F:36:HIS:CE1	1:F:41:HIS:CE1	3.10	0.40
1:G:53[B]:ILE:HD11	1:G:81[B]:ILE:CD1	2.51	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:0:HIS:HE2	4:B:204:ZN:ZN[4_566]	1.31	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:0:HIS:HE2	4:C:203:ZN:ZN[3_656]	1.31	0.29
1:H:0:HIS:HE2	4:A:205:ZN:ZN[4_466]	1.32	0.28
1:A:0:HIS:HE2	4:H:205:ZN:ZN[1_545]	1.34	0.26
1:E:0:HIS:HE2	4:G:204:ZN:ZN[3_546]	1.39	0.21

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	141/132 (107%)	138 (98%)	3 (2%)	0	100	100
1	B	144/132 (109%)	139 (96%)	5 (4%)	0	100	100
1	C	153/132 (116%)	150 (98%)	3 (2%)	0	100	100
1	D	142/132 (108%)	139 (98%)	3 (2%)	0	100	100
1	E	144/132 (109%)	140 (97%)	4 (3%)	0	100	100
1	F	147/132 (111%)	144 (98%)	3 (2%)	0	100	100
1	G	135/132 (102%)	133 (98%)	2 (2%)	0	100	100
1	H	150/132 (114%)	147 (98%)	3 (2%)	0	100	100
All	All	1156/1056 (110%)	1130 (98%)	26 (2%)	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	115/107 (108%)	114 (99%)	1 (1%)	70	39
1	B	119/107 (111%)	119 (100%)	0	100	100
1	C	124/107 (116%)	124 (100%)	0	100	100
1	D	116/107 (108%)	116 (100%)	0	100	100
1	E	121/107 (113%)	121 (100%)	0	100	100
1	F	121/107 (113%)	121 (100%)	0	100	100
1	G	110/107 (103%)	110 (100%)	0	100	100
1	H	122/107 (114%)	122 (100%)	0	100	100
All	All	948/856 (111%)	947 (100%)	1 (0%)	88	67

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 40 ligands modelled in this entry, 16 are monoatomic - leaving 24 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	MES	G	202[A]	-	12,12,12	2.26	1 (8%)	15,16,16	1.56	3 (20%)
3	GOL	A	204	-	5,5,5	0.64	0	5,5,5	0.96	0
3	GOL	F	202	-	5,5,5	1.17	1 (20%)	5,5,5	0.92	0
3	GOL	F	203	-	5,5,5	0.64	0	5,5,5	0.88	0
3	GOL	D	202[A]	-	5,5,5	0.87	0	5,5,5	0.98	0
3	GOL	B	203	-	5,5,5	0.82	0	5,5,5	1.10	0
2	MES	H	201	-	12,12,12	1.56	1 (8%)	15,16,16	0.80	0
2	MES	G	201	-	12,12,12	1.62	1 (8%)	15,16,16	0.90	1 (6%)
2	MES	D	201	-	12,12,12	1.73	1 (8%)	15,16,16	1.05	1 (6%)
2	MES	B	202	-	12,12,12	2.03	1 (8%)	15,16,16	1.71	3 (20%)
2	MES	A	201	-	12,12,12	1.42	1 (8%)	15,16,16	0.78	0
3	GOL	A	202	-	5,5,5	0.91	0	5,5,5	1.08	0
3	GOL	G	203	-	5,5,5	0.97	0	5,5,5	1.15	0
2	MES	C	201	-	12,12,12	1.23	1 (8%)	15,16,16	0.79	1 (6%)
2	MES	H	202	-	12,12,12	2.44	1 (8%)	15,16,16	1.98	3 (20%)
3	GOL	C	202[B]	-	5,5,5	0.79	0	5,5,5	0.82	0
2	MES	E	201	-	12,12,12	1.66	1 (8%)	15,16,16	1.08	1 (6%)
3	GOL	D	202[B]	-	5,5,5	0.85	0	5,5,5	0.77	0
3	GOL	A	203	-	5,5,5	0.79	0	5,5,5	1.12	0
2	MES	E	202	-	12,12,12	2.27	1 (8%)	15,16,16	1.40	3 (20%)
2	MES	B	201	-	12,12,12	1.36	1 (8%)	15,16,16	0.78	0
2	MES	F	201	-	12,12,12	1.73	1 (8%)	15,16,16	0.70	0
3	GOL	E	203	-	5,5,5	0.67	0	5,5,5	1.00	0
3	GOL	H	203	-	5,5,5	0.91	0	5,5,5	0.80	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
2	MES	G	202[A]	-	-	1/6/14/14	0/1/1/1
3	GOL	A	204	-	-	1/4/4/4	-
3	GOL	F	202	-	-	4/4/4/4	-
3	GOL	F	203	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	202[A]	-	-	0/4/4/4	-
3	GOL	B	203	-	-	0/4/4/4	-
2	MES	H	201	-	-	0/6/14/14	0/1/1/1
2	MES	G	201	-	-	0/6/14/14	0/1/1/1
2	MES	D	201	-	-	0/6/14/14	0/1/1/1
2	MES	B	202	-	-	2/6/14/14	0/1/1/1
2	MES	A	201	-	-	0/6/14/14	0/1/1/1
3	GOL	A	202	-	-	0/4/4/4	-
3	GOL	G	203	-	-	4/4/4/4	-
2	MES	C	201	-	-	0/6/14/14	0/1/1/1
2	MES	H	202	-	-	1/6/14/14	0/1/1/1
3	GOL	C	202[B]	-	-	0/4/4/4	-
2	MES	E	201	-	-	0/6/14/14	0/1/1/1
3	GOL	D	202[B]	-	-	2/4/4/4	-
3	GOL	A	203	-	-	3/4/4/4	-
2	MES	E	202	-	-	0/6/14/14	0/1/1/1
2	MES	B	201	-	-	0/6/14/14	0/1/1/1
2	MES	F	201	-	-	0/6/14/14	0/1/1/1
3	GOL	E	203	-	-	0/4/4/4	-
3	GOL	H	203	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	202	MES	C8-S	-8.22	1.66	1.77
2	E	202	MES	C8-S	-7.62	1.66	1.77
2	G	202[A]	MES	C8-S	-7.47	1.67	1.77
2	B	202	MES	C8-S	-6.73	1.68	1.77
2	D	201	MES	C8-S	-5.66	1.69	1.77
2	F	201	MES	C8-S	-5.54	1.69	1.77
2	E	201	MES	C8-S	-5.48	1.69	1.77
2	H	201	MES	C8-S	-5.17	1.70	1.77
2	G	201	MES	C8-S	-5.13	1.70	1.77
2	A	201	MES	C8-S	-4.61	1.71	1.77
2	B	201	MES	C8-S	-4.29	1.71	1.77
2	C	201	MES	C8-S	-3.87	1.72	1.77
3	F	202	GOL	O2-C2	-2.25	1.36	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	202	MES	C5-N4-C3	4.70	118.96	108.84
2	H	202	MES	C6-C5-N4	-3.82	104.31	110.12
2	G	202[A]	MES	O1S-S-C8	3.77	112.43	106.73
2	B	202	MES	C6-C5-N4	-3.59	104.67	110.12
2	B	202	MES	O3S-S-C8	3.55	112.95	106.00
2	H	202	MES	C2-C3-N4	-2.82	105.83	110.12
2	G	201	MES	C5-N4-C3	2.74	114.73	108.84
2	B	202	MES	C7-N4-C5	2.64	118.29	111.24
2	G	202[A]	MES	C6-C5-N4	-2.46	106.38	110.12
2	E	202	MES	C6-C5-N4	-2.45	106.39	110.12
2	E	201	MES	C5-N4-C3	2.43	114.08	108.84
2	G	202[A]	MES	C2-C3-N4	-2.40	106.47	110.12
2	D	201	MES	C5-N4-C3	2.36	113.92	108.84
2	E	202	MES	C5-N4-C3	2.36	113.92	108.84
2	E	202	MES	O3S-S-C8	2.20	110.32	106.00
2	C	201	MES	C5-N4-C3	2.07	113.29	108.84

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	202	MES	C8-C7-N4-C5
3	A	203	GOL	C1-C2-C3-O3
3	D	202[B]	GOL	C1-C2-C3-O3
3	F	202	GOL	O1-C1-C2-C3
3	F	203	GOL	O1-C1-C2-C3
3	G	203	GOL	C1-C2-C3-O3
3	F	202	GOL	O1-C1-C2-O2
3	A	203	GOL	O1-C1-C2-C3
3	F	202	GOL	C1-C2-C3-O3
3	G	203	GOL	O1-C1-C2-C3
3	A	203	GOL	O2-C2-C3-O3
3	F	203	GOL	O1-C1-C2-O2
3	G	203	GOL	O1-C1-C2-O2
3	D	202[B]	GOL	O2-C2-C3-O3
3	G	203	GOL	O2-C2-C3-O3
2	B	202	MES	C8-C7-N4-C3
2	H	202	MES	C8-C7-N4-C3
3	F	202	GOL	O2-C2-C3-O3
2	G	202[A]	MES	C8-C7-N4-C5
3	A	204	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	202	GOL	1	0
3	B	203	GOL	1	0
3	A	203	GOL	2	0
2	E	202	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 ⓘ

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	132/132 (100%)	-0.51	2 (1%) 72 72	6, 14, 25, 67	10 (7%)
1	B	132/132 (100%)	-0.50	3 (2%) 61 62	6, 13, 27, 54	12 (9%)
1	C	132/132 (100%)	-0.41	4 (3%) 52 55	5, 14, 25, 51	18 (13%)
1	D	132/132 (100%)	-0.42	2 (1%) 72 72	6, 14, 34, 63	11 (8%)
1	E	132/132 (100%)	-0.26	3 (2%) 61 62	7, 15, 33, 70	12 (9%)
1	F	132/132 (100%)	-0.39	1 (0%) 82 83	7, 14, 25, 48	15 (11%)
1	G	132/132 (100%)	-0.40	2 (1%) 72 72	7, 15, 31, 73	5 (3%)
1	H	132/132 (100%)	-0.38	3 (2%) 61 62	6, 15, 29, 58	14 (10%)
All	All	1056/1056 (100%)	-0.41	20 (1%) 66 66	5, 14, 30, 73	97 (9%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	123[A]	GLU	6.1
1	E	124	GLY	4.6
1	A	123	GLU	4.4
1	A	124	GLY	4.4
1	H	123	GLU	3.6
1	C	124[A]	GLY	3.3
1	C	123[A]	GLU	3.3
1	D	124	GLY	3.2
1	B	-1	GLY	3.1
1	B	123	GLU	3.0
1	G	123	GLU	2.8
1	E	125	ASP	2.8
1	C	-1	GLY	2.7
1	G	124	GLY	2.7
1	E	-1	GLY	2.6
1	H	124	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	125[A]	ASP	2.4
1	D	123	GLU	2.2
1	B	124	GLY	2.0
1	H	-1	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
3	GOL	G	203	6/6	0.81	0.26	18,24,35,42	14
3	GOL	D	202[B]	6/6	0.82	0.12	14,25,30,30	14
3	GOL	D	202[A]	6/6	0.82	0.12	21,28,33,39	14
3	GOL	F	203	6/6	0.86	0.22	20,28,33,39	14
3	GOL	A	202	6/6	0.88	0.14	21,26,29,35	14
3	GOL	F	202	6/6	0.88	0.15	16,30,36,36	13
3	GOL	H	203	6/6	0.88	0.12	21,26,40,40	14
3	GOL	A	204	6/6	0.89	0.13	15,24,33,40	14
3	GOL	E	203	6/6	0.89	0.12	18,24,28,28	14
2	MES	H	202	12/12	0.89	0.15	14,30,47,50	25
2	MES	B	202	12/12	0.91	0.15	13,30,40,46	25
3	GOL	B	203	6/6	0.91	0.10	20,25,33,33	0
2	MES	G	202[A]	12/12	0.91	0.13	14,27,33,34	25
3	GOL	A	203	6/6	0.92	0.15	12,27,44,44	14
3	GOL	C	202[B]	6/6	0.92	0.10	14,17,20,21	14
2	MES	E	202	12/12	0.92	0.13	15,29,34,36	25
2	MES	G	201	12/12	0.97	0.08	15,19,27,32	0
2	MES	D	201	12/12	0.98	0.06	12,16,22,24	0
2	MES	E	201	12/12	0.98	0.07	15,19,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	A	201	12/12	0.99	0.05	11,14,16,17	0
2	MES	H	201	12/12	0.99	0.04	12,15,17,18	0
2	MES	C	201	12/12	0.99	0.03	10,13,14,14	0
2	MES	F	201	12/12	0.99	0.04	11,14,16,17	0
2	MES	B	201	12/12	0.99	0.04	11,13,15,17	0
4	ZN	A	205	1/1	0.99	0.02	9,9,9,9	0
4	ZN	A	206	1/1	0.99	0.02	10,10,10,10	0
4	ZN	C	204	1/1	0.99	0.02	9,9,9,9	0
4	ZN	E	204	1/1	0.99	0.02	11,11,11,11	0
4	ZN	E	205	1/1	0.99	0.02	10,10,10,10	0
4	ZN	F	204	1/1	0.99	0.02	10,10,10,10	0
4	ZN	F	205	1/1	0.99	0.03	11,11,11,11	0
4	ZN	G	204	1/1	0.99	0.02	11,11,11,11	0
4	ZN	G	205	1/1	0.99	0.02	10,10,10,10	0
4	ZN	H	204	1/1	0.99	0.02	11,11,11,11	0
4	ZN	B	204	1/1	1.00	0.01	9,9,9,9	0
4	ZN	D	203	1/1	1.00	0.02	10,10,10,10	0
4	ZN	D	204	1/1	1.00	0.02	9,9,9,9	0
4	ZN	B	205	1/1	1.00	0.02	9,9,9,9	0
4	ZN	C	203	1/1	1.00	0.01	9,9,9,9	0
4	ZN	H	205	1/1	1.00	0.01	10,10,10,10	0

6.5 Other polymers

There are no such residues in this entry.