W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2024 – 12:55 AM EST

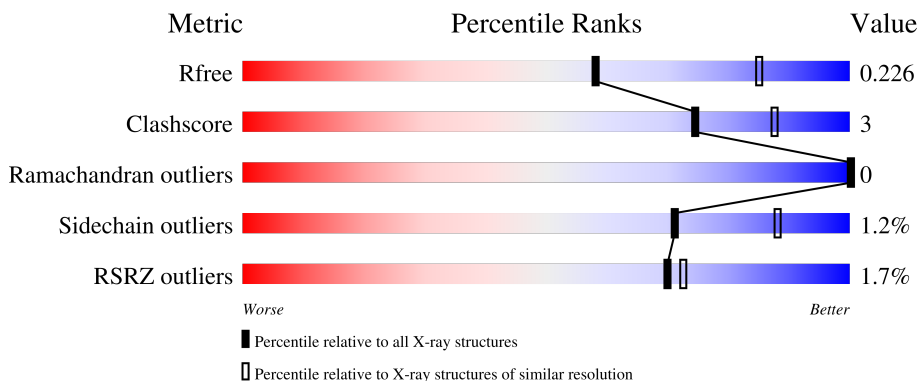|		
PDB ID	:	6O6M
Title	:	The Structure of EgtB (Cabther)
Authors	:	Irani, S.; Zhang, Y.
Deposited on	:	2019-03-07
Resolution	:	2.51 Å(reported)

1 Overall quality at a glance ⓘ

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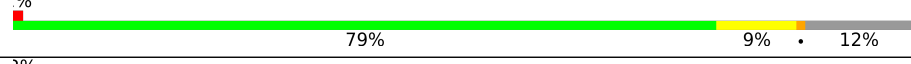*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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	Percentile Ranks	Value
Rfree		0.226
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		1.2%
RSRZ outliers		1.7%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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	462	2% / 82% 6% 12%
1	B	462	.% / 79% 9% · 12%
1	C	462	2% / 80% 7% 12%
1	D	462	2% / 80% 7% 12%

2   Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13597 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 EgtB (Cabther).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3281	2108	586	577	10			
1	B	406	Total	C	N	O	S	0	0	0
			3275	2105	585	575	10			
1	C	405	Total	C	N	O	S	0	0	0
			3268	2100	584	574	10			
1	D	405	Total	C	N	O	S	0	0	0
			3265	2098	583	574	10			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP G2LET6
A	-5	GLY	-	expression tag	UNP G2LET6
A	-4	ASP	-	expression tag	UNP G2LET6
A	-3	ARG	-	expression tag	UNP G2LET6
A	-2	GLY	-	expression tag	UNP G2LET6
A	-1	PRO	-	expression tag	UNP G2LET6
A	0	GLU	-	expression tag	UNP G2LET6
A	1	PHE	-	expression tag	UNP G2LET6
A	435	LEU	-	expression tag	UNP G2LET6
A	436	GLU	-	expression tag	UNP G2LET6
A	437	VAL	-	expression tag	UNP G2LET6
A	438	ASP	-	expression tag	UNP G2LET6
A	439	LEU	-	expression tag	UNP G2LET6
A	440	GLN	-	expression tag	UNP G2LET6
A	441	GLY	-	expression tag	UNP G2LET6
A	442	ASP	-	expression tag	UNP G2LET6
A	443	HIS	-	expression tag	UNP G2LET6
A	444	GLY	-	expression tag	UNP G2LET6
A	445	LEU	-	expression tag	UNP G2LET6
A	446	SER	-	expression tag	UNP G2LET6
A	447	ALA	-	expression tag	UNP G2LET6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	448	TRP	-	expression tag	UNP G2LET6
A	449	SER	-	expression tag	UNP G2LET6
A	450	HIS	-	expression tag	UNP G2LET6
A	451	PRO	-	expression tag	UNP G2LET6
A	452	GLN	-	expression tag	UNP G2LET6
A	453	PHE	-	expression tag	UNP G2LET6
A	454	GLU	-	expression tag	UNP G2LET6
A	455	LYS	-	expression tag	UNP G2LET6
B	-6	MET	-	initiating methionine	UNP G2LET6
B	-5	GLY	-	expression tag	UNP G2LET6
B	-4	ASP	-	expression tag	UNP G2LET6
B	-3	ARG	-	expression tag	UNP G2LET6
B	-2	GLY	-	expression tag	UNP G2LET6
B	-1	PRO	-	expression tag	UNP G2LET6
B	0	GLU	-	expression tag	UNP G2LET6
B	1	PHE	-	expression tag	UNP G2LET6
B	435	LEU	-	expression tag	UNP G2LET6
B	436	GLU	-	expression tag	UNP G2LET6
B	437	VAL	-	expression tag	UNP G2LET6
B	438	ASP	-	expression tag	UNP G2LET6
B	439	LEU	-	expression tag	UNP G2LET6
B	440	GLN	-	expression tag	UNP G2LET6
B	441	GLY	-	expression tag	UNP G2LET6
B	442	ASP	-	expression tag	UNP G2LET6
B	443	HIS	-	expression tag	UNP G2LET6
B	444	GLY	-	expression tag	UNP G2LET6
B	445	LEU	-	expression tag	UNP G2LET6
B	446	SER	-	expression tag	UNP G2LET6
B	447	ALA	-	expression tag	UNP G2LET6
B	448	TRP	-	expression tag	UNP G2LET6
B	449	SER	-	expression tag	UNP G2LET6
B	450	HIS	-	expression tag	UNP G2LET6
B	451	PRO	-	expression tag	UNP G2LET6
B	452	GLN	-	expression tag	UNP G2LET6
B	453	PHE	-	expression tag	UNP G2LET6
B	454	GLU	-	expression tag	UNP G2LET6
B	455	LYS	-	expression tag	UNP G2LET6
C	-6	MET	-	initiating methionine	UNP G2LET6
C	-5	GLY	-	expression tag	UNP G2LET6
C	-4	ASP	-	expression tag	UNP G2LET6
C	-3	ARG	-	expression tag	UNP G2LET6
C	-2	GLY	-	expression tag	UNP G2LET6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	PRO	-	expression tag	UNP G2LET6
C	0	GLU	-	expression tag	UNP G2LET6
C	1	PHE	-	expression tag	UNP G2LET6
C	435	LEU	-	expression tag	UNP G2LET6
C	436	GLU	-	expression tag	UNP G2LET6
C	437	VAL	-	expression tag	UNP G2LET6
C	438	ASP	-	expression tag	UNP G2LET6
C	439	LEU	-	expression tag	UNP G2LET6
C	440	GLN	-	expression tag	UNP G2LET6
C	441	GLY	-	expression tag	UNP G2LET6
C	442	ASP	-	expression tag	UNP G2LET6
C	443	HIS	-	expression tag	UNP G2LET6
C	444	GLY	-	expression tag	UNP G2LET6
C	445	LEU	-	expression tag	UNP G2LET6
C	446	SER	-	expression tag	UNP G2LET6
C	447	ALA	-	expression tag	UNP G2LET6
C	448	TRP	-	expression tag	UNP G2LET6
C	449	SER	-	expression tag	UNP G2LET6
C	450	HIS	-	expression tag	UNP G2LET6
C	451	PRO	-	expression tag	UNP G2LET6
C	452	GLN	-	expression tag	UNP G2LET6
C	453	PHE	-	expression tag	UNP G2LET6
C	454	GLU	-	expression tag	UNP G2LET6
C	455	LYS	-	expression tag	UNP G2LET6
D	-6	MET	-	initiating methionine	UNP G2LET6
D	-5	GLY	-	expression tag	UNP G2LET6
D	-4	ASP	-	expression tag	UNP G2LET6
D	-3	ARG	-	expression tag	UNP G2LET6
D	-2	GLY	-	expression tag	UNP G2LET6
D	-1	PRO	-	expression tag	UNP G2LET6
D	0	GLU	-	expression tag	UNP G2LET6
D	1	PHE	-	expression tag	UNP G2LET6
D	435	LEU	-	expression tag	UNP G2LET6
D	436	GLU	-	expression tag	UNP G2LET6
D	437	VAL	-	expression tag	UNP G2LET6
D	438	ASP	-	expression tag	UNP G2LET6
D	439	LEU	-	expression tag	UNP G2LET6
D	440	GLN	-	expression tag	UNP G2LET6
D	441	GLY	-	expression tag	UNP G2LET6
D	442	ASP	-	expression tag	UNP G2LET6
D	443	HIS	-	expression tag	UNP G2LET6
D	444	GLY	-	expression tag	UNP G2LET6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	445	LEU	-	expression tag	UNP G2LET6
D	446	SER	-	expression tag	UNP G2LET6
D	447	ALA	-	expression tag	UNP G2LET6
D	448	TRP	-	expression tag	UNP G2LET6
D	449	SER	-	expression tag	UNP G2LET6
D	450	HIS	-	expression tag	UNP G2LET6
D	451	PRO	-	expression tag	UNP G2LET6
D	452	GLN	-	expression tag	UNP G2LET6
D	453	PHE	-	expression tag	UNP G2LET6
D	454	GLU	-	expression tag	UNP G2LET6
D	455	LYS	-	expression tag	UNP G2LET6

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Fe 1	0	0
2	B	1	Total 1	Fe 1	0	0
2	C	1	Total 1	Fe 1	0	0
2	D	1	Total 1	Fe 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
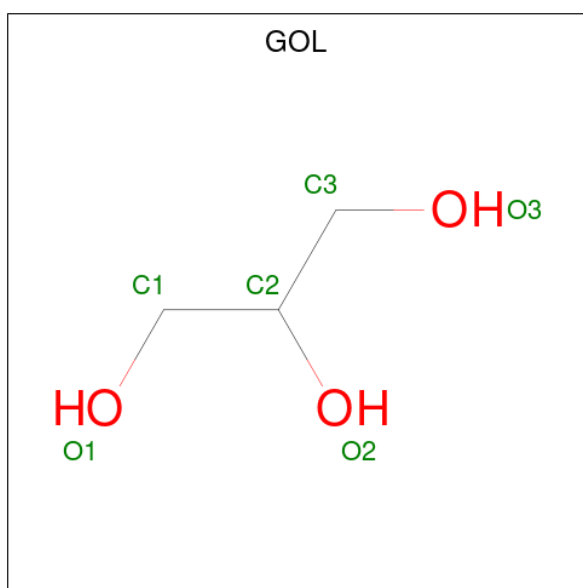
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total 130	O 130	0	0
4	B	128	Total 128	O 128	0	0
4	C	124	Total 124	O 124	0	0
4	D	110	Total 110	O 110	0	0

3 Residue-property plots ⓘ

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.
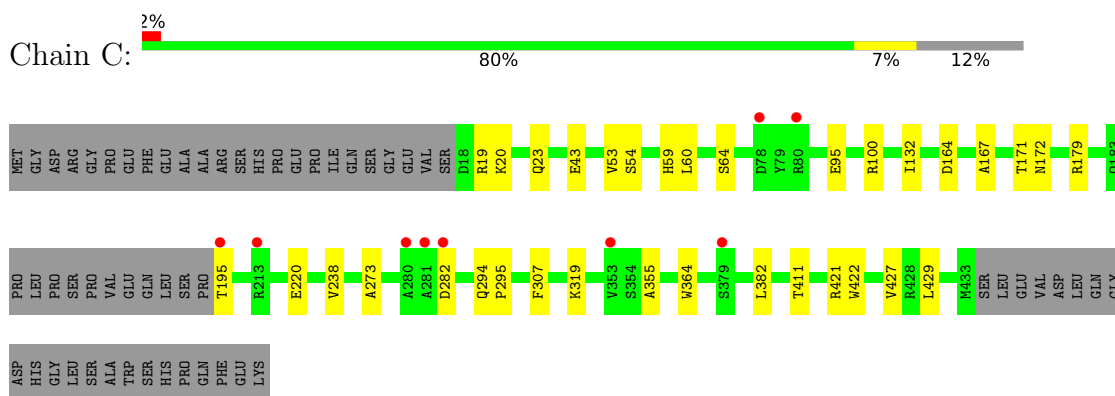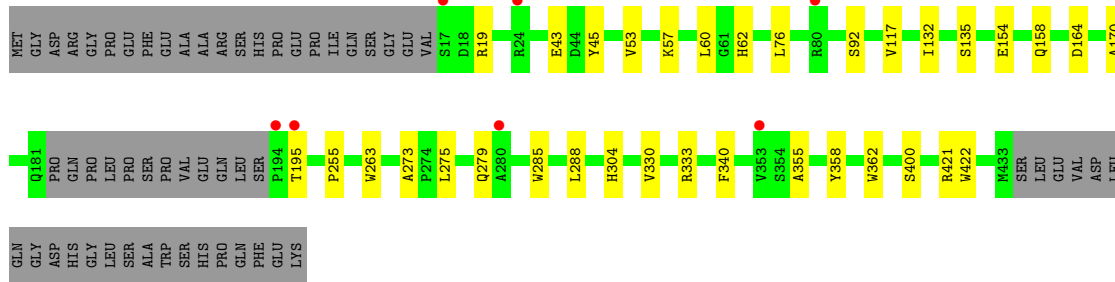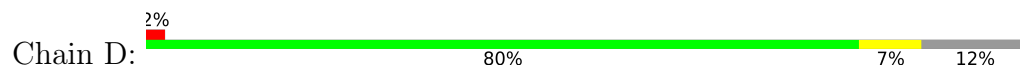
• Molecule 1: EgtB (Cabther)

• Molecule 1: EgtB (Cabther)

• Molecule 1: EgtB (Cabther)

• Molecule 1: EgtB (Cabther)

Chain D:
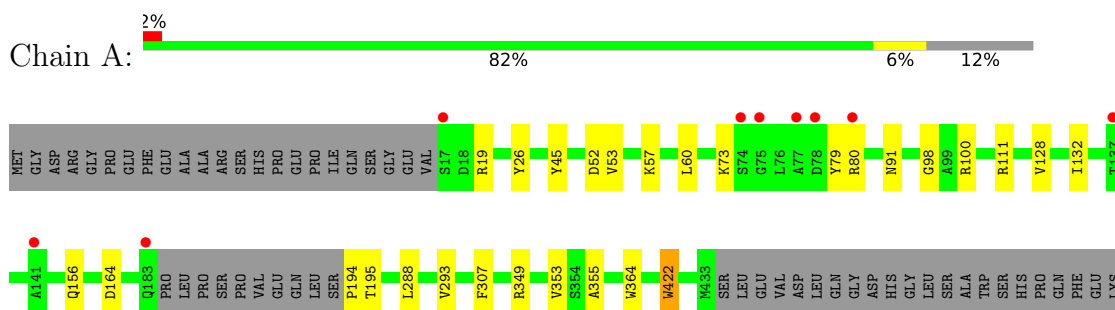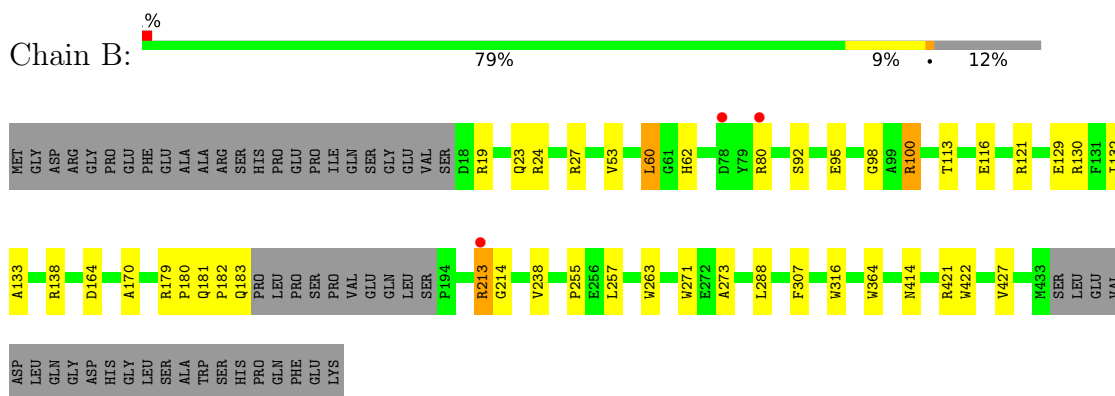
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	85.29Å 137.31Å 85.39Å	Depositor
a, b, c, α, β, γ	90.00° 92.43° 90.00°	
Resolution (Å)	45.85 – 2.51	Depositor
	45.86 – 2.51	EDS
% Data completeness	99.7 (45.85-2.51)	Depositor
(in resolution range)	99.7 (45.86-2.51)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.185 , 0.226	Depositor
	0.185 , 0.226	DCC
R_{free} test set	1978 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.3	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.001 for l,k,-h	Xtriage
	0.025 for h,-k,-l	
	0.021 for l,-k,h	
F_o,F_c correlation	0.93	EDS
Total number of atoms	13597	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FE

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	0.28	0/3399	0.46	0/4647
1	B	0.27	0/3393	0.48	1/4639 (0.0%)
1	C	0.27	0/3385	0.46	0/4628
1	D	0.27	0/3382	0.46	0/4623
All	All	0.27	0/13559	0.46	1/18537 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	213	ARG	NE-CZ-NH1	6.54	123.57	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3281	0	3118	17	0
1	B	3275	0	3113	30	0
1	C	3268	0	3105	18	0
1	D	3265	0	3103	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
4	A	130	0	0	1	0
4	B	128	0	0	2	0
4	C	124	0	0	0	0
4	D	110	0	0	0	0
All	All	13597	0	12455	81	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 3.

The worst 5 of 81 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:213:ARG:CD	1:B:214:GLY:H	2.03	0.72
1:B:213:ARG:HD2	1:B:214:GLY:H	1.54	0.71
1:B:181:GLN:NE2	4:B:602:HOH:O	2.23	0.67
1:A:349:ARG:NH2	4:A:602:HOH:O	2.28	0.66
1:D:19:ARG:HD3	1:D:132:ILE:O	1.98	0.64

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/462 (87%)	393 (98%)	10 (2%)	0	100	100
1	B	402/462 (87%)	396 (98%)	6 (2%)	0	100	100
1	C	401/462 (87%)	392 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	401/462 (87%)	392 (98%)	9 (2%)	0	100	100
All	All	1607/1848 (87%)	1573 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/379 (88%)	329 (99%)	3 (1%)	78	92
1	B	331/379 (87%)	325 (98%)	6 (2%)	59	81
1	C	330/379 (87%)	325 (98%)	5 (2%)	65	85
1	D	330/379 (87%)	328 (99%)	2 (1%)	86	95
All	All	1323/1516 (87%)	1307 (99%)	16 (1%)	71	88

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	60	LEU
1	C	422	TRP
1	B	422	TRP
1	C	382	LEU
1	B	138	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	23	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	B	502	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	A	502	-	5,5,5	0.35	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	502	-	-	4/4/4/4	-
3	GOL	A	502	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	GOL	O1-C1-C2-O2
3	B	502	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	A	502	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	GOL	1	0
3	A	502	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	407/462 (88%)	-0.37	9 (2%)	62	65	7, 14, 42, 69	0
1	B	406/462 (87%)	-0.46	3 (0%)	87	89	8, 15, 34, 64	0
1	C	405/462 (87%)	-0.34	9 (2%)	62	65	7, 15, 33, 63	0
1	D	405/462 (87%)	-0.36	7 (1%)	70	72	8, 16, 41, 66	0
All	All	1623/1848 (87%)	-0.38	28 (1%)	70	72	7, 15, 39, 69	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	17	SER	5.3
1	D	194	PRO	4.7
1	A	183	GLN	3.5
1	A	77	ALA	3.4
1	C	280	ALA	3.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	GOL	A	502	6/6	0.92	0.16	9,13,19,25	0
3	GOL	B	502	6/6	0.97	0.15	13,15,17,21	0
2	FE	C	501	1/1	0.99	0.08	19,19,19,19	0
2	FE	A	501	1/1	0.99	0.04	22,22,22,22	0
2	FE	B	501	1/1	0.99	0.02	14,14,14,14	0
2	FE	D	501	1/1	1.00	0.04	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.