



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 2, 2026 – 04:18 PM UTC

PDB ID : 8U5F / pdb_00008u5f
Title : Crystal Structure of Trypsinized Clostridium perfringens Enterotoxin
Authors : Kapoor, S.; Ogbu, C.P.; Vecchio, A.J.
Deposited on : 2023-09-12
Resolution : 2.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

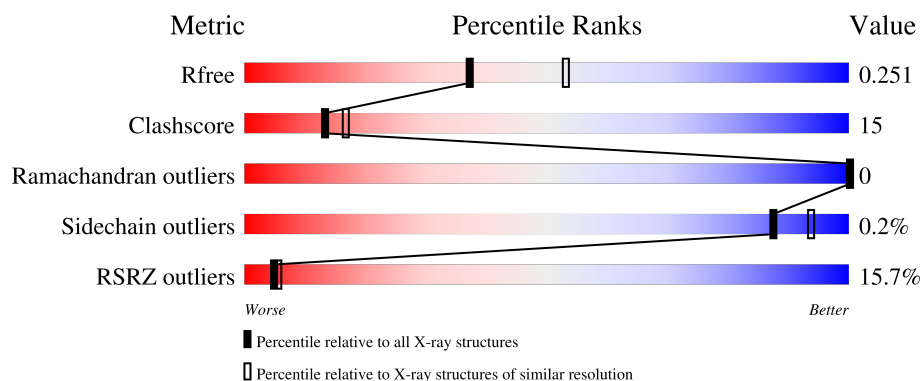
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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.



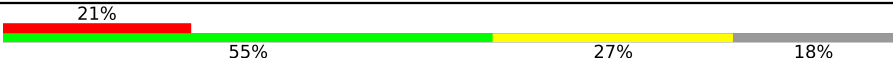
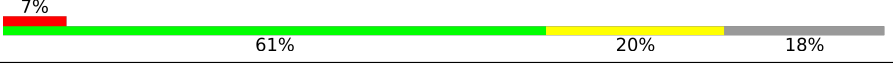
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	348	11% 63% 19% 18%
1	B	348	5% 64% 18% 18%
1	C	348	7% 63% 20% 18%
1	D	348	7% 61% 21% 18%
1	E	348	12% 60% 23% 18%

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Mol	Chain	Length	Quality of chain
1	F	348	
1	G	348	
1	H	348	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	420	-	-	-	X
3	GOL	B	412	-	-	X	-
3	GOL	B	419	-	-	X	-
3	GOL	E	408	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19218 atoms, of which 369 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 Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2220	1407	363	448	2			
1	B	286	Total	C	N	O	S	0	0	0
			2223	1408	364	449	2			
1	C	286	Total	C	N	O	S	0	0	0
			2230	1415	364	449	2			
1	D	286	Total	C	N	O	S	0	0	0
			2230	1415	364	449	2			
1	E	287	Total	C	N	O	S	0	1	0
			2242	1423	366	451	2			
1	F	286	Total	C	N	O	S	0	0	0
			2219	1405	364	448	2			
1	G	285	Total	C	N	O	S	0	0	0
			2223	1410	363	448	2			
1	H	285	Total	C	N	O	S	0	0	0
			2223	1410	363	448	2			

There are 232 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP P01558
A	321	LEU	-	expression tag	UNP P01558
A	322	VAL	-	expression tag	UNP P01558
A	323	PRO	-	expression tag	UNP P01558
A	324	ARG	-	expression tag	UNP P01558
A	325	GLY	-	expression tag	UNP P01558
A	326	SER	-	expression tag	UNP P01558
A	327	GLY	-	expression tag	UNP P01558
A	328	GLY	-	expression tag	UNP P01558
A	329	GLY	-	expression tag	UNP P01558
A	330	GLY	-	expression tag	UNP P01558
A	331	SER	-	expression tag	UNP P01558
A	332	GLY	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
A	333	GLY	-	expression tag	UNP P01558
A	334	GLY	-	expression tag	UNP P01558
A	335	GLY	-	expression tag	UNP P01558
A	336	SER	-	expression tag	UNP P01558
A	337	GLY	-	expression tag	UNP P01558
A	338	GLY	-	expression tag	UNP P01558
A	339	HIS	-	expression tag	UNP P01558
A	340	HIS	-	expression tag	UNP P01558
A	341	HIS	-	expression tag	UNP P01558
A	342	HIS	-	expression tag	UNP P01558
A	343	HIS	-	expression tag	UNP P01558
A	344	HIS	-	expression tag	UNP P01558
A	345	HIS	-	expression tag	UNP P01558
A	346	HIS	-	expression tag	UNP P01558
A	347	HIS	-	expression tag	UNP P01558
A	348	HIS	-	expression tag	UNP P01558
B	320	GLY	-	expression tag	UNP P01558
B	321	LEU	-	expression tag	UNP P01558
B	322	VAL	-	expression tag	UNP P01558
B	323	PRO	-	expression tag	UNP P01558
B	324	ARG	-	expression tag	UNP P01558
B	325	GLY	-	expression tag	UNP P01558
B	326	SER	-	expression tag	UNP P01558
B	327	GLY	-	expression tag	UNP P01558
B	328	GLY	-	expression tag	UNP P01558
B	329	GLY	-	expression tag	UNP P01558
B	330	GLY	-	expression tag	UNP P01558
B	331	SER	-	expression tag	UNP P01558
B	332	GLY	-	expression tag	UNP P01558
B	333	GLY	-	expression tag	UNP P01558
B	334	GLY	-	expression tag	UNP P01558
B	335	GLY	-	expression tag	UNP P01558
B	336	SER	-	expression tag	UNP P01558
B	337	GLY	-	expression tag	UNP P01558
B	338	GLY	-	expression tag	UNP P01558
B	339	HIS	-	expression tag	UNP P01558
B	340	HIS	-	expression tag	UNP P01558
B	341	HIS	-	expression tag	UNP P01558
B	342	HIS	-	expression tag	UNP P01558
B	343	HIS	-	expression tag	UNP P01558
B	344	HIS	-	expression tag	UNP P01558
B	345	HIS	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
B	346	HIS	-	expression tag	UNP P01558
B	347	HIS	-	expression tag	UNP P01558
B	348	HIS	-	expression tag	UNP P01558
C	320	GLY	-	expression tag	UNP P01558
C	321	LEU	-	expression tag	UNP P01558
C	322	VAL	-	expression tag	UNP P01558
C	323	PRO	-	expression tag	UNP P01558
C	324	ARG	-	expression tag	UNP P01558
C	325	GLY	-	expression tag	UNP P01558
C	326	SER	-	expression tag	UNP P01558
C	327	GLY	-	expression tag	UNP P01558
C	328	GLY	-	expression tag	UNP P01558
C	329	GLY	-	expression tag	UNP P01558
C	330	GLY	-	expression tag	UNP P01558
C	331	SER	-	expression tag	UNP P01558
C	332	GLY	-	expression tag	UNP P01558
C	333	GLY	-	expression tag	UNP P01558
C	334	GLY	-	expression tag	UNP P01558
C	335	GLY	-	expression tag	UNP P01558
C	336	SER	-	expression tag	UNP P01558
C	337	GLY	-	expression tag	UNP P01558
C	338	GLY	-	expression tag	UNP P01558
C	339	HIS	-	expression tag	UNP P01558
C	340	HIS	-	expression tag	UNP P01558
C	341	HIS	-	expression tag	UNP P01558
C	342	HIS	-	expression tag	UNP P01558
C	343	HIS	-	expression tag	UNP P01558
C	344	HIS	-	expression tag	UNP P01558
C	345	HIS	-	expression tag	UNP P01558
C	346	HIS	-	expression tag	UNP P01558
C	347	HIS	-	expression tag	UNP P01558
C	348	HIS	-	expression tag	UNP P01558
D	320	GLY	-	expression tag	UNP P01558
D	321	LEU	-	expression tag	UNP P01558
D	322	VAL	-	expression tag	UNP P01558
D	323	PRO	-	expression tag	UNP P01558
D	324	ARG	-	expression tag	UNP P01558
D	325	GLY	-	expression tag	UNP P01558
D	326	SER	-	expression tag	UNP P01558
D	327	GLY	-	expression tag	UNP P01558
D	328	GLY	-	expression tag	UNP P01558
D	329	GLY	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
D	330	GLY	-	expression tag	UNP P01558
D	331	SER	-	expression tag	UNP P01558
D	332	GLY	-	expression tag	UNP P01558
D	333	GLY	-	expression tag	UNP P01558
D	334	GLY	-	expression tag	UNP P01558
D	335	GLY	-	expression tag	UNP P01558
D	336	SER	-	expression tag	UNP P01558
D	337	GLY	-	expression tag	UNP P01558
D	338	GLY	-	expression tag	UNP P01558
D	339	HIS	-	expression tag	UNP P01558
D	340	HIS	-	expression tag	UNP P01558
D	341	HIS	-	expression tag	UNP P01558
D	342	HIS	-	expression tag	UNP P01558
D	343	HIS	-	expression tag	UNP P01558
D	344	HIS	-	expression tag	UNP P01558
D	345	HIS	-	expression tag	UNP P01558
D	346	HIS	-	expression tag	UNP P01558
D	347	HIS	-	expression tag	UNP P01558
D	348	HIS	-	expression tag	UNP P01558
E	320	GLY	-	expression tag	UNP P01558
E	321	LEU	-	expression tag	UNP P01558
E	322	VAL	-	expression tag	UNP P01558
E	323	PRO	-	expression tag	UNP P01558
E	324	ARG	-	expression tag	UNP P01558
E	325	GLY	-	expression tag	UNP P01558
E	326	SER	-	expression tag	UNP P01558
E	327	GLY	-	expression tag	UNP P01558
E	328	GLY	-	expression tag	UNP P01558
E	329	GLY	-	expression tag	UNP P01558
E	330	GLY	-	expression tag	UNP P01558
E	331	SER	-	expression tag	UNP P01558
E	332	GLY	-	expression tag	UNP P01558
E	333	GLY	-	expression tag	UNP P01558
E	334	GLY	-	expression tag	UNP P01558
E	335	GLY	-	expression tag	UNP P01558
E	336	SER	-	expression tag	UNP P01558
E	337	GLY	-	expression tag	UNP P01558
E	338	GLY	-	expression tag	UNP P01558
E	339	HIS	-	expression tag	UNP P01558
E	340	HIS	-	expression tag	UNP P01558
E	341	HIS	-	expression tag	UNP P01558
E	342	HIS	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	expression tag	UNP P01558
E	344	HIS	-	expression tag	UNP P01558
E	345	HIS	-	expression tag	UNP P01558
E	346	HIS	-	expression tag	UNP P01558
E	347	HIS	-	expression tag	UNP P01558
E	348	HIS	-	expression tag	UNP P01558
F	320	GLY	-	expression tag	UNP P01558
F	321	LEU	-	expression tag	UNP P01558
F	322	VAL	-	expression tag	UNP P01558
F	323	PRO	-	expression tag	UNP P01558
F	324	ARG	-	expression tag	UNP P01558
F	325	GLY	-	expression tag	UNP P01558
F	326	SER	-	expression tag	UNP P01558
F	327	GLY	-	expression tag	UNP P01558
F	328	GLY	-	expression tag	UNP P01558
F	329	GLY	-	expression tag	UNP P01558
F	330	GLY	-	expression tag	UNP P01558
F	331	SER	-	expression tag	UNP P01558
F	332	GLY	-	expression tag	UNP P01558
F	333	GLY	-	expression tag	UNP P01558
F	334	GLY	-	expression tag	UNP P01558
F	335	GLY	-	expression tag	UNP P01558
F	336	SER	-	expression tag	UNP P01558
F	337	GLY	-	expression tag	UNP P01558
F	338	GLY	-	expression tag	UNP P01558
F	339	HIS	-	expression tag	UNP P01558
F	340	HIS	-	expression tag	UNP P01558
F	341	HIS	-	expression tag	UNP P01558
F	342	HIS	-	expression tag	UNP P01558
F	343	HIS	-	expression tag	UNP P01558
F	344	HIS	-	expression tag	UNP P01558
F	345	HIS	-	expression tag	UNP P01558
F	346	HIS	-	expression tag	UNP P01558
F	347	HIS	-	expression tag	UNP P01558
F	348	HIS	-	expression tag	UNP P01558
G	320	GLY	-	expression tag	UNP P01558
G	321	LEU	-	expression tag	UNP P01558
G	322	VAL	-	expression tag	UNP P01558
G	323	PRO	-	expression tag	UNP P01558
G	324	ARG	-	expression tag	UNP P01558
G	325	GLY	-	expression tag	UNP P01558
G	326	SER	-	expression tag	UNP P01558

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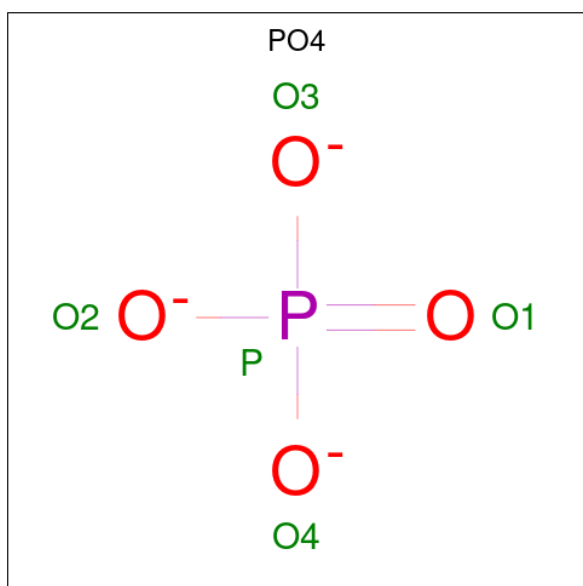
Chain	Residue	Modelled	Actual	Comment	Reference
G	327	GLY	-	expression tag	UNP P01558
G	328	GLY	-	expression tag	UNP P01558
G	329	GLY	-	expression tag	UNP P01558
G	330	GLY	-	expression tag	UNP P01558
G	331	SER	-	expression tag	UNP P01558
G	332	GLY	-	expression tag	UNP P01558
G	333	GLY	-	expression tag	UNP P01558
G	334	GLY	-	expression tag	UNP P01558
G	335	GLY	-	expression tag	UNP P01558
G	336	SER	-	expression tag	UNP P01558
G	337	GLY	-	expression tag	UNP P01558
G	338	GLY	-	expression tag	UNP P01558
G	339	HIS	-	expression tag	UNP P01558
G	340	HIS	-	expression tag	UNP P01558
G	341	HIS	-	expression tag	UNP P01558
G	342	HIS	-	expression tag	UNP P01558
G	343	HIS	-	expression tag	UNP P01558
G	344	HIS	-	expression tag	UNP P01558
G	345	HIS	-	expression tag	UNP P01558
G	346	HIS	-	expression tag	UNP P01558
G	347	HIS	-	expression tag	UNP P01558
G	348	HIS	-	expression tag	UNP P01558
H	320	GLY	-	expression tag	UNP P01558
H	321	LEU	-	expression tag	UNP P01558
H	322	VAL	-	expression tag	UNP P01558
H	323	PRO	-	expression tag	UNP P01558
H	324	ARG	-	expression tag	UNP P01558
H	325	GLY	-	expression tag	UNP P01558
H	326	SER	-	expression tag	UNP P01558
H	327	GLY	-	expression tag	UNP P01558
H	328	GLY	-	expression tag	UNP P01558
H	329	GLY	-	expression tag	UNP P01558
H	330	GLY	-	expression tag	UNP P01558
H	331	SER	-	expression tag	UNP P01558
H	332	GLY	-	expression tag	UNP P01558
H	333	GLY	-	expression tag	UNP P01558
H	334	GLY	-	expression tag	UNP P01558
H	335	GLY	-	expression tag	UNP P01558
H	336	SER	-	expression tag	UNP P01558
H	337	GLY	-	expression tag	UNP P01558
H	338	GLY	-	expression tag	UNP P01558
H	339	HIS	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
H	340	HIS	-	expression tag	UNP P01558
H	341	HIS	-	expression tag	UNP P01558
H	342	HIS	-	expression tag	UNP P01558
H	343	HIS	-	expression tag	UNP P01558
H	344	HIS	-	expression tag	UNP P01558
H	345	HIS	-	expression tag	UNP P01558
H	346	HIS	-	expression tag	UNP P01558
H	347	HIS	-	expression tag	UNP P01558
H	348	HIS	-	expression tag	UNP P01558

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



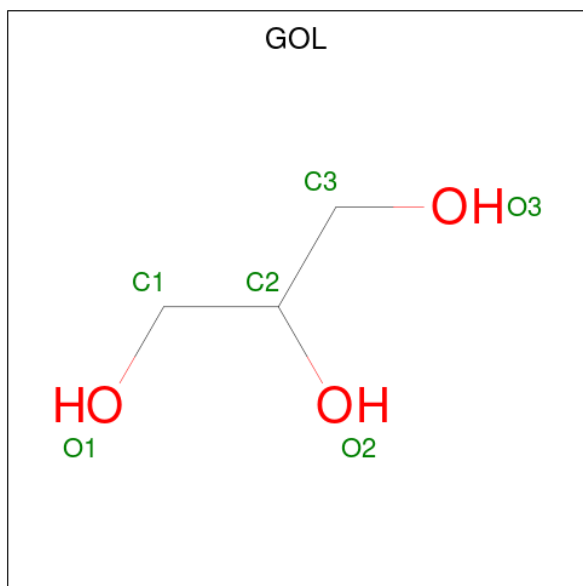
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	O		0	0
			6	3	3			
3	E	1	Total	C	O		0	0
			6	3	3			
3	E	1	Total	C	O		0	0
			6	3	3			
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	O		0	0
			6	3	3			

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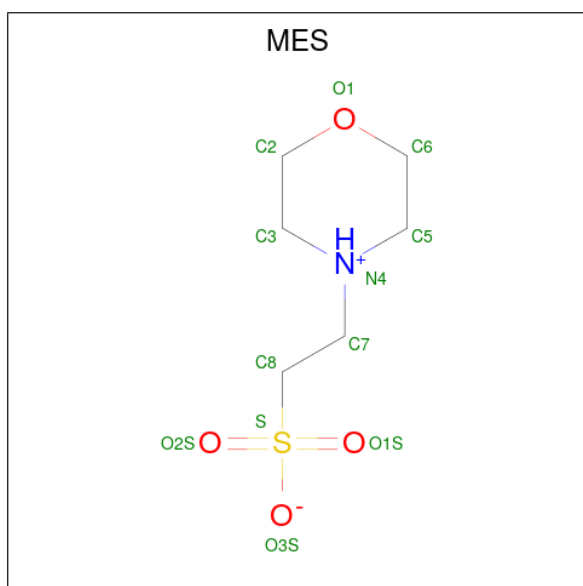
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	O		0	0
			6	3	3			
3	F	1	Total	C	O		0	0
			6	3	3			
3	F	1	Total	C	O		0	0
			6	3	3			
3	F	1	Total	C	O		0	0
			6	3	3			
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	H	O	0	0
			14	3	8	3		
3	F	1	Total	C	O		0	0
			6	3	3			
3	G	1	Total	C	O		0	0
			6	3	3			
3	G	1	Total	C	O		0	0
			6	3	3			
3	G	1	Total	C	O		0	0
			6	3	3			
3	G	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	G	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	G	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

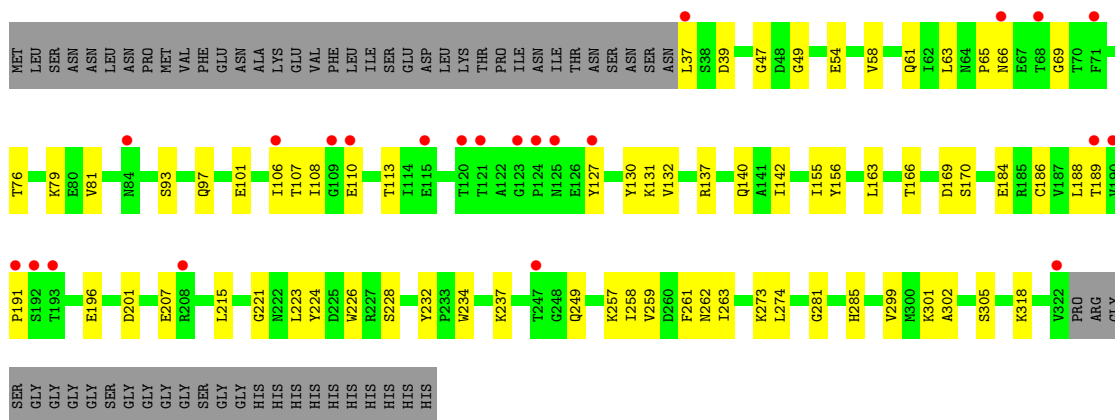
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		

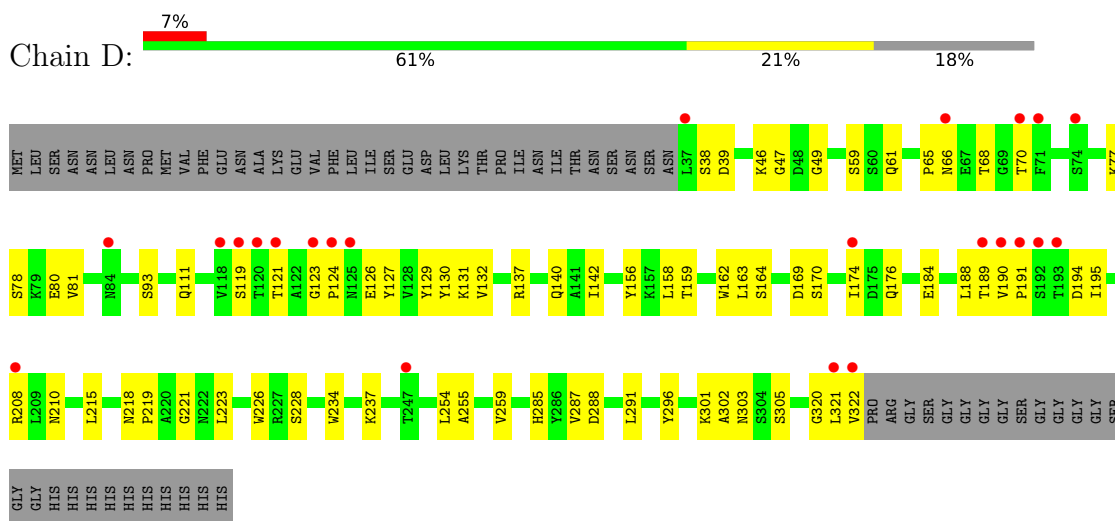
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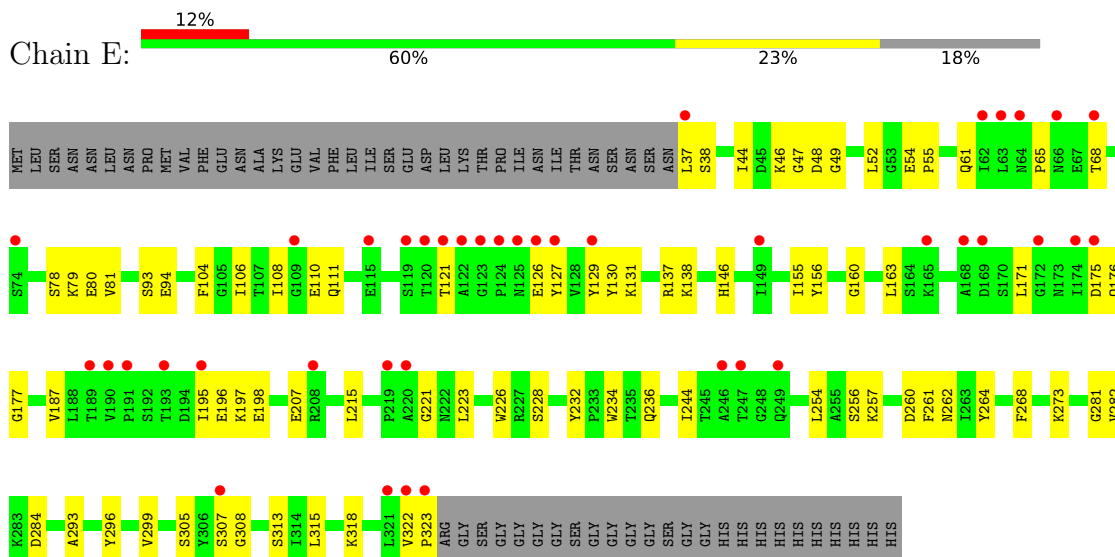
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	58	Total 58	O 58	0	0
5	C	53	Total 53	O 53	0	0
5	D	62	Total 62	O 62	0	0
5	E	38	Total 38	O 38	0	0
5	F	28	Total 28	O 28	0	0
5	G	54	Total 54	O 54	0	0
5	H	21	Total 21	O 21	0	0



- Molecule 1: Heat-labile enterotoxin B chain

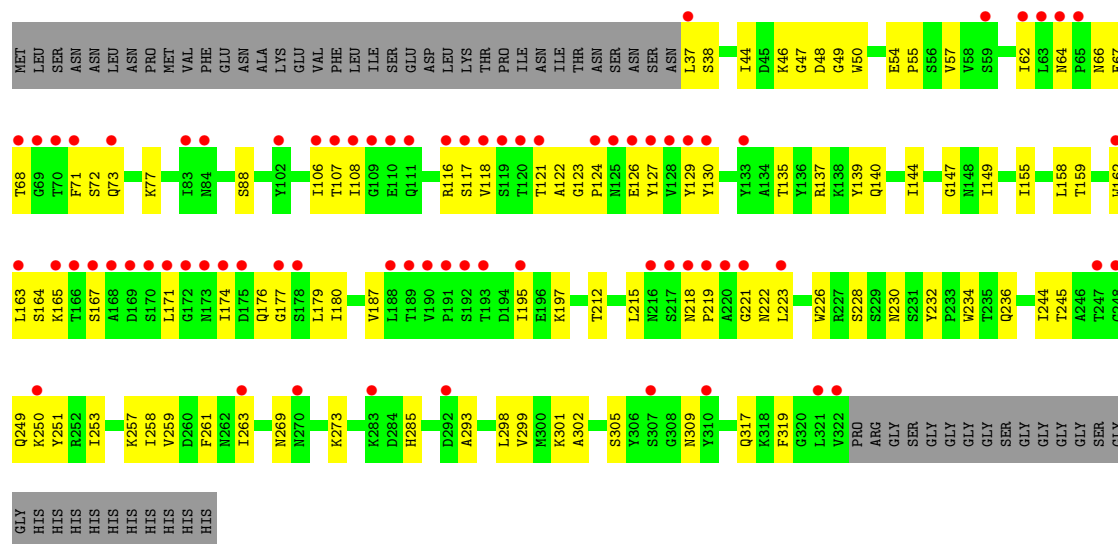


- Molecule 1: Heat-labile enterotoxin B chain

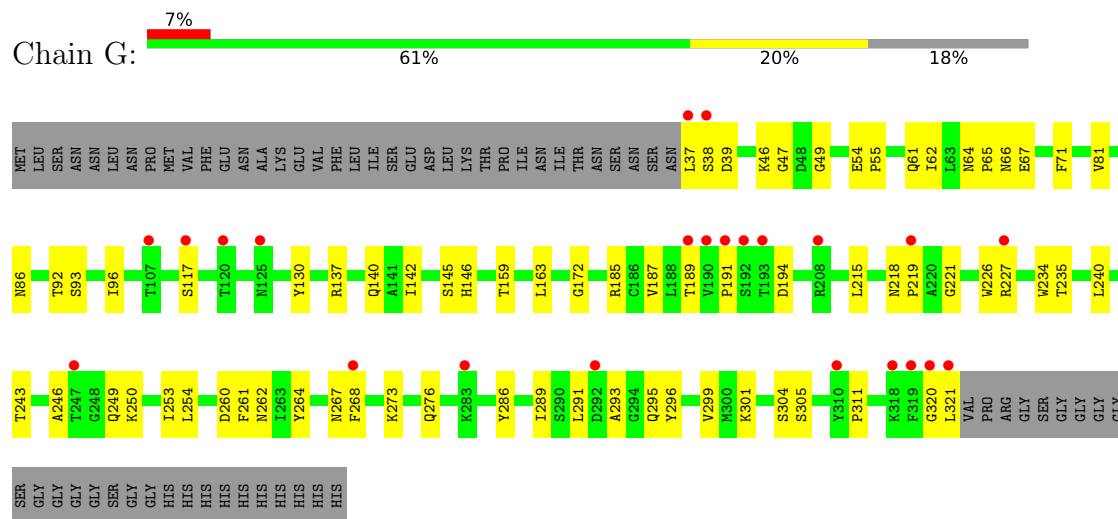


- Molecule 1: Heat-labile enterotoxin B chain

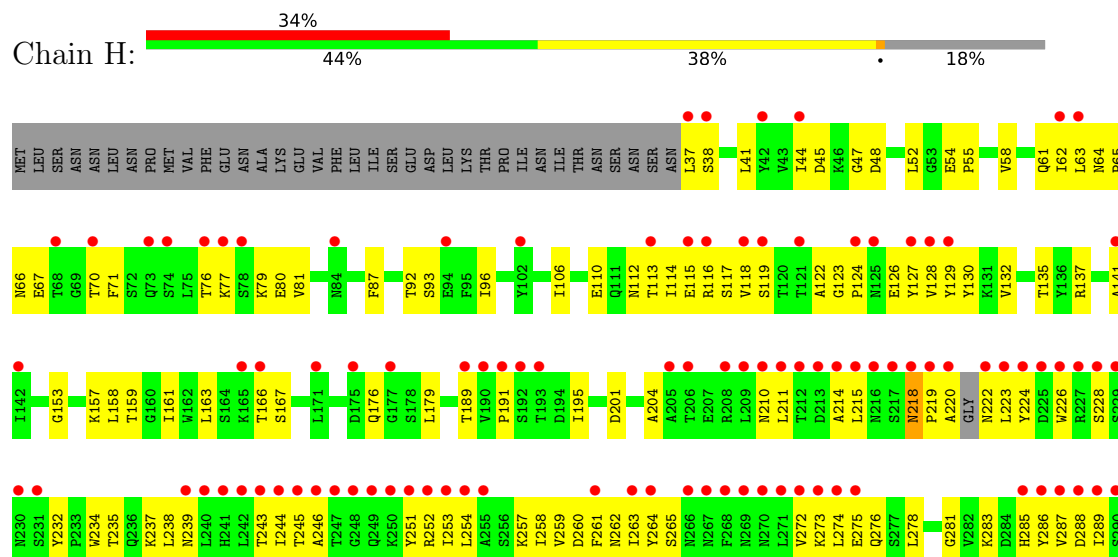




● Molecule 1: Heat-labile enterotoxin B chain



● Molecule 1: Heat-labile enterotoxin B chain



L291	D292	A293	G294	Q295	Y296	V297	L298	V299	M300	K301	S304	S305	Y306	N309	Y310	P311	Y312	S313	I314	L315	F316	Q317	K318	F319	G320	L321	V322	PRO	ARG	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	SER	GLY	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	200.33Å 200.33Å 254.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.78 – 2.32 66.78 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.6 (66.78-2.32) 86.1 (66.78-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.37 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.224 , 0.248 0.230 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (0.90%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19218	wwPDB-VP
Average B, all atoms (Å ²)	77.0	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 20.75 % 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 8.1179e-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: MES, GOL, PO4

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	0.20	0/2264	0.41	0/3077
1	B	0.19	0/2267	0.39	0/3080
1	C	0.15	0/2274	0.35	0/3091
1	D	0.21	0/2274	0.41	0/3091
1	E	0.18	0/2290	0.38	0/3114
1	F	0.16	0/2262	0.37	0/3073
1	G	0.12	0/2267	0.33	0/3081
1	H	0.17	0/2266	0.41	1/3079 (0.0%)
All	All	0.18	0/18164	0.38	1/24686 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	218	ASN	CB-CA-C	-6.87	102.18	110.08

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	2220	0	2161	60	0
1	B	2223	0	2161	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2230	0	2179	46	0
1	D	2230	0	2179	63	0
1	E	2242	0	2192	62	0
1	F	2219	0	2163	79	0
1	G	2223	0	2170	52	0
1	H	2223	0	2166	131	0
2	A	20	0	0	1	0
2	B	20	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	10	0	0	0	0
2	F	5	0	0	1	0
2	G	10	0	0	0	0
2	H	5	0	0	0	0
3	A	96	56	128	9	0
3	B	102	48	136	18	0
3	C	72	40	95	6	0
3	D	78	40	104	18	0
3	E	42	32	56	5	0
3	F	66	40	88	5	0
3	G	66	48	88	11	0
3	H	12	0	16	3	0
4	B	12	13	13	0	0
4	E	24	26	25	3	0
4	G	12	13	13	2	0
4	H	12	13	13	0	0
5	A	51	0	0	2	0
5	B	58	0	0	0	0
5	C	53	0	0	1	0
5	D	62	0	0	1	0
5	E	38	0	0	1	0
5	F	28	0	0	0	0
5	G	54	0	0	2	0
5	H	21	0	0	3	0
All	All	18849	369	18146	543	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 15.

The worst 5 of 543 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:D:320:GLY:C	1:D:321:LEU:HD12	1.35	1.51
1:D:320:GLY:C	1:D:321:LEU:CD1	2.14	1.19
1:D:320:GLY:O	1:D:321:LEU:HD12	1.00	1.16
1:D:320:GLY:O	1:D:321:LEU:CD1	1.95	1.13
1:H:38:SER:HB2	1:H:273:LYS:HE3	1.40	1.00

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	283/348 (81%)	278 (98%)	5 (2%)	0	100	100
1	B	284/348 (82%)	280 (99%)	4 (1%)	0	100	100
1	C	284/348 (82%)	278 (98%)	6 (2%)	0	100	100
1	D	284/348 (82%)	277 (98%)	7 (2%)	0	100	100
1	E	286/348 (82%)	278 (97%)	8 (3%)	0	100	100
1	F	284/348 (82%)	273 (96%)	11 (4%)	0	100	100
1	G	283/348 (81%)	278 (98%)	5 (2%)	0	100	100
1	H	281/348 (81%)	271 (96%)	10 (4%)	0	100	100
All	All	2269/2784 (82%)	2213 (98%)	56 (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	247/299 (83%)	246 (100%)	1 (0%)	84	91
1	B	247/299 (83%)	247 (100%)	0	100	100
1	C	249/299 (83%)	249 (100%)	0	100	100
1	D	249/299 (83%)	248 (100%)	1 (0%)	84	91
1	E	251/299 (84%)	250 (100%)	1 (0%)	84	91
1	F	247/299 (83%)	247 (100%)	0	100	100
1	G	248/299 (83%)	248 (100%)	0	100	100
1	H	248/299 (83%)	247 (100%)	1 (0%)	84	91
All	All	1986/2392 (83%)	1982 (100%)	4 (0%)	87	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	D	190	VAL
1	E	197	LYS
1	H	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	218	ASN
1	G	125	ASN
1	H	266	ASN
1	G	64	ASN
1	G	295	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

110 ligands are modelled in this entry.

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	A	410	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	D	410	-	5,5,5	0.87	0	5,5,5	1.05	0
3	GOL	C	409	-	5,5,5	0.97	0	5,5,5	0.89	0
3	GOL	A	409	-	5,5,5	0.98	0	5,5,5	1.03	0
3	GOL	B	418	-	5,5,5	1.00	0	5,5,5	1.24	1 (20%)
3	GOL	B	411	-	5,5,5	0.94	0	5,5,5	1.09	0
3	GOL	F	410	-	5,5,5	1.09	0	5,5,5	1.31	1 (20%)
3	GOL	A	405	-	5,5,5	0.90	0	5,5,5	1.08	0
2	PO4	B	401	-	4,4,4	0.97	0	6,6,6	0.45	0
3	GOL	F	411	-	5,5,5	1.08	0	5,5,5	1.24	1 (20%)
2	PO4	A	404	-	4,4,4	0.97	0	6,6,6	0.46	0
3	GOL	D	407	-	5,5,5	0.97	0	5,5,5	1.05	0
3	GOL	C	407	-	5,5,5	0.93	0	5,5,5	1.07	0
3	GOL	D	413	-	5,5,5	0.93	0	5,5,5	1.04	0
2	PO4	F	401	-	4,4,4	0.97	0	6,6,6	0.47	0
3	GOL	D	404	-	5,5,5	0.91	0	5,5,5	1.05	0
3	GOL	A	418	-	5,5,5	1.04	0	5,5,5	1.27	1 (20%)
3	GOL	C	411	-	5,5,5	0.93	0	5,5,5	1.03	0
3	GOL	B	408	-	5,5,5	0.92	0	5,5,5	1.11	0
2	PO4	B	404	-	4,4,4	0.99	0	6,6,6	0.47	0
3	GOL	D	411	-	5,5,5	0.97	0	5,5,5	1.13	0
3	GOL	A	411	-	5,5,5	0.96	0	5,5,5	1.06	0
3	GOL	E	408	-	5,5,5	1.15	1 (20%)	5,5,5	1.27	1 (20%)
3	GOL	A	407	-	5,5,5	0.90	0	5,5,5	1.13	0
3	GOL	H	402	-	5,5,5	0.90	0	5,5,5	1.09	0
3	GOL	A	416	-	5,5,5	0.96	0	5,5,5	1.27	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	417	-	5,5,5	1.01	0	5,5,5	1.28	1 (20%)
3	GOL	B	406	-	5,5,5	0.90	0	5,5,5	1.08	0
3	GOL	D	414	-	5,5,5	0.92	0	5,5,5	1.07	0
2	PO4	E	401	-	4,4,4	0.99	0	6,6,6	0.46	0
3	GOL	C	405	-	5,5,5	0.91	0	5,5,5	1.07	0
3	GOL	D	405	-	5,5,5	0.99	0	5,5,5	1.03	0
3	GOL	D	412	-	5,5,5	0.91	0	5,5,5	1.12	0
3	GOL	F	407	-	5,5,5	0.96	0	5,5,5	1.11	0
2	PO4	G	401	-	4,4,4	0.98	0	6,6,6	0.47	0
2	PO4	C	401	-	4,4,4	0.97	0	6,6,6	0.45	0
3	GOL	D	403	-	5,5,5	0.96	0	5,5,5	1.08	0
3	GOL	G	407	-	5,5,5	0.97	0	5,5,5	1.15	1 (20%)
3	GOL	H	403	-	5,5,5	0.91	0	5,5,5	1.09	0
3	GOL	F	402	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	A	417	-	5,5,5	0.95	0	5,5,5	1.16	1 (20%)
3	GOL	E	404	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	F	405	-	5,5,5	0.94	0	5,5,5	1.10	0
3	GOL	G	408	-	5,5,5	1.13	1 (20%)	5,5,5	1.25	1 (20%)
3	GOL	A	420	-	5,5,5	1.02	0	5,5,5	1.24	1 (20%)
4	MES	E	410	-	12,12,12	2.29	1 (8%)	15,16,16	1.66	3 (20%)
3	GOL	G	411	-	5,5,5	1.18	1 (20%)	5,5,5	1.37	1 (20%)
4	MES	G	414	-	12,12,12	2.27	1 (8%)	15,16,16	1.63	3 (20%)
3	GOL	E	403	-	5,5,5	1.03	0	5,5,5	1.04	0
3	GOL	B	421	-	5,5,5	0.92	0	5,5,5	1.06	0
3	GOL	G	409	-	5,5,5	1.02	0	5,5,5	1.22	1 (20%)
3	GOL	G	406	-	5,5,5	0.94	0	5,5,5	1.06	0
3	GOL	C	413	-	5,5,5	0.88	0	5,5,5	1.08	0
2	PO4	H	401	-	4,4,4	0.97	0	6,6,6	0.48	0
3	GOL	E	406	-	5,5,5	0.97	0	5,5,5	1.24	1 (20%)
2	PO4	A	401	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	A	403	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	D	401	-	4,4,4	0.98	0	6,6,6	0.47	0
3	GOL	B	414	-	5,5,5	0.89	0	5,5,5	1.37	1 (20%)
3	GOL	E	405	-	5,5,5	0.88	0	5,5,5	1.05	0
3	GOL	E	409	-	5,5,5	0.91	0	5,5,5	1.05	0
3	GOL	B	416	-	5,5,5	1.15	0	5,5,5	1.40	1 (20%)
3	GOL	F	409	-	5,5,5	1.09	0	5,5,5	1.30	1 (20%)
3	GOL	G	405	-	5,5,5	0.94	0	5,5,5	1.06	0
3	GOL	B	409	-	5,5,5	0.91	0	5,5,5	1.08	0
3	GOL	F	406	-	5,5,5	0.90	0	5,5,5	1.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	H	404	-	12,12,12	2.28	1 (8%)	15,16,16	1.40	2 (13%)
3	GOL	C	412	-	5,5,5	1.33	1 (20%)	5,5,5	1.58	1 (20%)
4	MES	B	422	-	12,12,12	2.29	1 (8%)	15,16,16	1.67	2 (13%)
3	GOL	A	419	-	5,5,5	1.05	0	5,5,5	1.14	1 (20%)
3	GOL	C	406	-	5,5,5	0.95	0	5,5,5	1.02	0
3	GOL	D	406	-	5,5,5	0.94	0	5,5,5	1.04	0
3	GOL	D	402	-	5,5,5	0.92	0	5,5,5	1.07	0
2	PO4	E	402	-	4,4,4	0.98	0	6,6,6	0.48	0
3	GOL	A	412	-	5,5,5	0.88	0	5,5,5	1.08	0
3	GOL	B	415	-	5,5,5	1.05	0	5,5,5	1.23	1 (20%)
4	MES	E	411	-	12,12,12	2.26	1 (8%)	15,16,16	1.87	3 (20%)
3	GOL	G	413	-	5,5,5	0.93	0	5,5,5	1.07	0
3	GOL	B	413	-	5,5,5	0.93	0	5,5,5	1.08	0
3	GOL	F	404	-	5,5,5	0.97	0	5,5,5	1.06	0
2	PO4	B	403	-	4,4,4	0.98	0	6,6,6	0.46	0
3	GOL	B	410	-	5,5,5	0.90	0	5,5,5	1.09	0
3	GOL	G	404	-	5,5,5	0.94	0	5,5,5	1.07	0
3	GOL	A	406	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	C	404	-	5,5,5	0.91	0	5,5,5	1.07	0
3	GOL	A	414	-	5,5,5	0.80	0	5,5,5	1.03	0
3	GOL	A	415	-	5,5,5	0.92	0	5,5,5	1.16	1 (20%)
2	PO4	B	402	-	4,4,4	0.87	0	6,6,6	0.50	0
3	GOL	A	408	-	5,5,5	1.02	0	5,5,5	1.02	0
3	GOL	G	410	-	5,5,5	1.06	0	5,5,5	1.22	1 (20%)
3	GOL	C	410	-	5,5,5	1.00	0	5,5,5	1.17	1 (20%)
3	GOL	C	402	-	5,5,5	1.00	0	5,5,5	1.09	0
3	GOL	B	420	-	5,5,5	0.99	0	5,5,5	1.05	0
3	GOL	F	403	-	5,5,5	0.96	0	5,5,5	1.05	0
3	GOL	B	405	-	5,5,5	0.90	0	5,5,5	1.08	0
3	GOL	B	412	-	5,5,5	0.95	0	5,5,5	1.08	0
2	PO4	G	402	-	4,4,4	0.92	0	6,6,6	0.46	0
3	GOL	C	408	-	5,5,5	1.02	0	5,5,5	1.38	1 (20%)
3	GOL	G	403	-	5,5,5	0.93	0	5,5,5	1.11	0
3	GOL	B	419	-	5,5,5	0.96	0	5,5,5	1.17	1 (20%)
3	GOL	C	403	-	5,5,5	0.92	0	5,5,5	1.10	0
3	GOL	D	408	-	5,5,5	0.89	0	5,5,5	1.11	0
3	GOL	E	407	-	5,5,5	1.04	0	5,5,5	1.19	1 (20%)
3	GOL	D	409	-	5,5,5	1.14	1 (20%)	5,5,5	1.31	1 (20%)
2	PO4	A	402	-	4,4,4	0.97	0	6,6,6	0.45	0
3	GOL	G	412	-	5,5,5	1.09	0	5,5,5	1.15	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	412	-	5,5,5	0.90	0	5,5,5	1.04	0
3	GOL	A	413	-	5,5,5	0.89	0	5,5,5	1.13	0
3	GOL	F	408	-	5,5,5	1.22	1 (20%)	5,5,5	1.52	1 (20%)
3	GOL	B	407	-	5,5,5	0.94	0	5,5,5	1.09	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	A	410	-	-	0/4/4/4	-
3	GOL	D	410	-	-	0/4/4/4	-
3	GOL	C	409	-	-	0/4/4/4	-
3	GOL	A	409	-	-	1/4/4/4	-
3	GOL	B	418	-	-	0/4/4/4	-
3	GOL	B	411	-	-	0/4/4/4	-
3	GOL	F	410	-	-	2/4/4/4	-
3	GOL	A	405	-	-	0/4/4/4	-
3	GOL	F	411	-	-	0/4/4/4	-
3	GOL	D	407	-	-	0/4/4/4	-
3	GOL	C	407	-	-	3/4/4/4	-
3	GOL	D	413	-	-	0/4/4/4	-
3	GOL	D	404	-	-	0/4/4/4	-
3	GOL	A	418	-	-	0/4/4/4	-
3	GOL	C	411	-	-	2/4/4/4	-
3	GOL	B	408	-	-	0/4/4/4	-
3	GOL	D	411	-	-	1/4/4/4	-
3	GOL	A	411	-	-	0/4/4/4	-
3	GOL	E	408	-	-	4/4/4/4	-
3	GOL	A	407	-	-	0/4/4/4	-
3	GOL	H	402	-	-	0/4/4/4	-
3	GOL	A	416	-	-	0/4/4/4	-
3	GOL	B	417	-	-	0/4/4/4	-
3	GOL	B	406	-	-	0/4/4/4	-
3	GOL	D	414	-	-	0/4/4/4	-
3	GOL	C	405	-	-	0/4/4/4	-
3	GOL	D	405	-	-	0/4/4/4	-
3	GOL	D	412	-	-	2/4/4/4	-
3	GOL	F	407	-	-	0/4/4/4	-
3	GOL	D	403	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	H	403	-	-	0/4/4/4	-
3	GOL	G	407	-	-	2/4/4/4	-
3	GOL	F	402	-	-	0/4/4/4	-
3	GOL	A	417	-	-	2/4/4/4	-
3	GOL	E	404	-	-	0/4/4/4	-
3	GOL	F	405	-	-	0/4/4/4	-
3	GOL	G	408	-	-	0/4/4/4	-
3	GOL	A	420	-	-	0/4/4/4	-
4	MES	E	410	-	-	0/6/14/14	0/1/1/1
3	GOL	G	411	-	-	1/4/4/4	-
4	MES	G	414	-	-	3/6/14/14	0/1/1/1
3	GOL	B	421	-	-	0/4/4/4	-
3	GOL	E	403	-	-	0/4/4/4	-
3	GOL	G	409	-	-	1/4/4/4	-
3	GOL	G	406	-	-	0/4/4/4	-
3	GOL	C	413	-	-	0/4/4/4	-
3	GOL	E	406	-	-	0/4/4/4	-
3	GOL	B	414	-	-	1/4/4/4	-
3	GOL	E	405	-	-	2/4/4/4	-
3	GOL	E	409	-	-	2/4/4/4	-
3	GOL	B	416	-	-	0/4/4/4	-
3	GOL	F	409	-	-	1/4/4/4	-
3	GOL	G	405	-	-	0/4/4/4	-
3	GOL	B	409	-	-	0/4/4/4	-
3	GOL	F	406	-	-	0/4/4/4	-
4	MES	H	404	-	-	0/6/14/14	0/1/1/1
3	GOL	C	412	-	-	0/4/4/4	-
4	MES	B	422	-	-	0/6/14/14	0/1/1/1
3	GOL	A	419	-	-	1/4/4/4	-
3	GOL	C	406	-	-	2/4/4/4	-
3	GOL	D	406	-	-	0/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	A	412	-	-	2/4/4/4	-
3	GOL	B	415	-	-	0/4/4/4	-
4	MES	E	411	-	-	4/6/14/14	0/1/1/1
3	GOL	G	413	-	-	0/4/4/4	-
3	GOL	B	413	-	-	0/4/4/4	-
3	GOL	F	404	-	-	0/4/4/4	-
3	GOL	B	410	-	-	0/4/4/4	-
3	GOL	G	404	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	406	-	-	1/4/4/4	-
3	GOL	C	404	-	-	1/4/4/4	-
3	GOL	A	414	-	-	0/4/4/4	-
3	GOL	A	415	-	-	1/4/4/4	-
3	GOL	A	408	-	-	0/4/4/4	-
3	GOL	G	410	-	-	2/4/4/4	-
3	GOL	C	410	-	-	2/4/4/4	-
3	GOL	C	402	-	-	2/4/4/4	-
3	GOL	B	420	-	-	0/4/4/4	-
3	GOL	F	403	-	-	0/4/4/4	-
3	GOL	B	405	-	-	0/4/4/4	-
3	GOL	B	412	-	-	0/4/4/4	-
3	GOL	G	403	-	-	0/4/4/4	-
3	GOL	C	408	-	-	1/4/4/4	-
3	GOL	B	419	-	-	2/4/4/4	-
3	GOL	C	403	-	-	0/4/4/4	-
3	GOL	D	408	-	-	0/4/4/4	-
3	GOL	E	407	-	-	2/4/4/4	-
3	GOL	D	409	-	-	3/4/4/4	-
3	GOL	G	412	-	-	1/4/4/4	-
3	GOL	F	412	-	-	2/4/4/4	-
3	GOL	A	413	-	-	0/4/4/4	-
3	GOL	F	408	-	-	0/4/4/4	-
3	GOL	B	407	-	-	0/4/4/4	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	410	MES	C8-S	-7.66	1.66	1.77
4	B	422	MES	C8-S	-7.65	1.66	1.77
4	H	404	MES	C8-S	-7.63	1.66	1.77
4	G	414	MES	C8-S	-7.61	1.66	1.77
4	E	411	MES	C8-S	-7.55	1.67	1.77

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	411	MES	C2-C3-N4	-3.89	104.21	110.12
4	E	411	MES	C5-N4-C3	3.67	116.74	108.84
4	B	422	MES	C2-C3-N4	-3.40	104.95	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	410	MES	C2-C3-N4	-3.21	105.24	110.12
3	C	412	GOL	C3-C2-C1	-3.14	100.27	111.80

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	419	GOL	C1-C2-C3-O3
3	C	410	GOL	C1-C2-C3-O3
3	C	411	GOL	C1-C2-C3-O3
3	F	410	GOL	C1-C2-C3-O3
3	G	407	GOL	C1-C2-C3-O3

There are no ring outliers.

52 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	GOL	2	0
3	D	410	GOL	1	0
3	B	411	GOL	1	0
3	A	405	GOL	1	0
3	D	407	GOL	1	0
3	D	413	GOL	3	0
2	F	401	PO4	1	0
3	D	404	GOL	3	0
2	B	404	PO4	1	0
3	D	411	GOL	3	0
3	H	402	GOL	1	0
3	B	417	GOL	3	0
3	D	414	GOL	2	0
3	D	412	GOL	1	0
3	D	403	GOL	3	0
3	G	407	GOL	2	0
3	H	403	GOL	2	0
3	A	417	GOL	1	0
3	E	404	GOL	1	0
3	G	408	GOL	2	0
3	A	420	GOL	2	0
4	E	410	MES	1	0
4	G	414	MES	2	0
3	G	406	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	413	GOL	2	0
3	E	406	GOL	2	0
2	A	403	PO4	1	0
3	E	409	GOL	1	0
3	B	416	GOL	2	0
3	F	409	GOL	2	0
3	G	405	GOL	2	0
3	A	419	GOL	1	0
3	D	406	GOL	1	0
3	B	415	GOL	1	0
4	E	411	MES	2	0
3	B	413	GOL	1	0
3	F	404	GOL	1	0
3	B	410	GOL	2	0
3	C	404	GOL	1	0
3	A	414	GOL	2	0
3	G	410	GOL	1	0
3	C	410	GOL	2	0
3	C	402	GOL	1	0
3	B	420	GOL	1	0
3	F	403	GOL	1	0
3	B	412	GOL	4	0
3	G	403	GOL	2	0
3	B	419	GOL	4	0
3	D	408	GOL	1	0
3	E	407	GOL	1	0
3	G	412	GOL	1	0
3	F	408	GOL	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	285/348 (81%)	0.82	39 (13%) 6 7	30, 66, 113, 125	0
1	B	286/348 (82%)	0.45	16 (5%) 30 32	46, 61, 87, 171	0
1	C	286/348 (82%)	0.70	23 (8%) 18 20	46, 63, 110, 138	0
1	D	286/348 (82%)	0.62	23 (8%) 18 20	45, 59, 104, 147	0
1	E	287/348 (82%)	0.99	41 (14%) 6 7	42, 68, 125, 159	1 (0%)
1	F	286/348 (82%)	1.40	74 (25%) 1 2	55, 80, 138, 179	0
1	G	285/348 (81%)	0.73	23 (8%) 18 20	51, 68, 101, 138	0
1	H	285/348 (81%)	2.13	120 (42%) 0 0	62, 91, 131, 258	0
All	All	2286/2784 (82%)	0.98	359 (15%) 5 5	30, 69, 121, 258	1 (0%)

The worst 5 of 359 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	190	VAL	10.6
1	B	322	VAL	10.2
1	H	322	VAL	10.1
1	H	321	LEU	9.9
1	G	321	LEU	9.8

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 ⓘ

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	G	407	6/6	0.54	0.22	125,150,163,170	0
3	GOL	D	410	6/6	0.58	0.22	134,161,172,178	0
2	PO4	E	402	5/5	0.62	0.22	162,167,170,189	0
2	PO4	A	404	5/5	0.64	0.18	182,184,188,193	0
2	PO4	C	401	5/5	0.65	0.29	156,165,168,171	0
3	GOL	E	406	6/6	0.67	0.22	118,142,159,170	0
2	PO4	B	403	5/5	0.68	0.16	154,157,170,176	0
3	GOL	C	402	6/6	0.69	0.33	79,84,103,109	0
2	PO4	B	401	5/5	0.70	0.22	173,176,178,185	0
2	PO4	D	401	5/5	0.72	0.29	158,164,168,175	0
3	GOL	C	409	6/6	0.73	0.26	79,123,141,157	0
4	MES	E	410	12/12	0.73	0.39	165,204,223,245	0
3	GOL	B	417	6/6	0.74	0.22	103,131,164,164	0
3	GOL	D	407	6/6	0.74	0.29	90,103,108,110	0
3	GOL	G	408	6/6	0.74	0.33	109,134,162,162	0
3	GOL	A	417	6/6	0.74	0.23	100,129,154,156	0
3	GOL	C	412	6/6	0.75	0.30	76,100,120,120	0
3	GOL	B	407	6/6	0.75	0.29	121,123,127,129	0
3	GOL	F	404	6/6	0.75	0.35	105,111,118,120	0
3	GOL	G	412	6/6	0.76	0.22	121,145,154,157	0
3	GOL	G	405	6/6	0.76	0.27	111,115,121,122	0
3	GOL	D	413	6/6	0.78	0.25	78,115,138,138	0
3	GOL	F	403	6/6	0.78	0.31	100,123,126,127	0
3	GOL	B	420	6/6	0.79	0.30	101,117,131,141	0
3	GOL	B	415	6/6	0.79	0.27	103,132,158,159	0
3	GOL	G	413	6/6	0.79	0.28	94,103,107,109	0
3	GOL	A	420	6/6	0.79	0.41	117,154,172,196	0
4	MES	E	411	12/12	0.79	0.38	167,200,219,234	0
4	MES	H	404	12/12	0.79	0.37	141,192,218,232	0
3	GOL	D	411	6/6	0.80	0.32	86,126,151,179	0
3	GOL	F	402	6/6	0.80	0.29	77,96,112,115	0
2	PO4	A	402	5/5	0.80	0.20	138,144,161,169	0
3	GOL	F	410	6/6	0.81	0.21	83,119,143,145	0
3	GOL	E	407	6/6	0.81	0.21	94,119,143,143	0
2	PO4	E	401	5/5	0.81	0.22	162,162,165,179	0
3	GOL	B	418	6/6	0.82	0.20	123,148,163,163	0
3	GOL	C	406	6/6	0.82	0.33	116,121,122,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	F	408	6/6	0.82	0.32	119,142,167,171	0
3	GOL	H	402	6/6	0.82	0.26	81,102,107,121	0
3	GOL	D	408	6/6	0.82	0.29	76,93,109,115	0
3	GOL	D	409	6/6	0.82	0.29	83,118,142,157	0
4	MES	G	414	12/12	0.82	0.34	145,190,236,245	0
2	PO4	G	401	5/5	0.82	0.15	138,139,142,146	0
3	GOL	E	408	6/6	0.83	0.31	97,134,152,166	0
3	GOL	A	419	6/6	0.83	0.22	88,118,142,162	0
2	PO4	F	401	5/5	0.84	0.17	157,161,162,165	0
2	PO4	H	401	5/5	0.84	0.34	171,176,181,193	0
3	GOL	B	419	6/6	0.84	0.25	102,125,155,155	0
3	GOL	A	408	6/6	0.84	0.32	100,107,115,123	0
3	GOL	A	410	6/6	0.84	0.20	93,102,108,112	0
4	MES	B	422	12/12	0.84	0.34	132,164,196,200	0
3	GOL	F	405	6/6	0.84	0.24	90,107,109,113	0
3	GOL	C	405	6/6	0.84	0.26	111,113,115,120	0
3	GOL	B	412	6/6	0.84	0.26	81,114,119,119	0
3	GOL	A	413	6/6	0.84	0.29	94,101,105,107	0
3	GOL	B	421	6/6	0.85	0.26	99,111,117,125	0
3	GOL	B	413	6/6	0.85	0.23	85,106,112,112	0
3	GOL	B	408	6/6	0.85	0.28	93,108,116,116	0
3	GOL	G	411	6/6	0.85	0.27	108,129,139,142	0
2	PO4	B	404	5/5	0.86	0.16	158,161,163,174	0
3	GOL	C	403	6/6	0.86	0.23	97,101,103,110	0
3	GOL	G	410	6/6	0.86	0.28	115,139,150,155	0
3	GOL	F	409	6/6	0.86	0.19	104,125,142,150	0
3	GOL	A	418	6/6	0.86	0.25	107,129,138,139	0
3	GOL	D	404	6/6	0.86	0.26	101,105,112,112	0
3	GOL	F	411	6/6	0.87	0.18	92,117,138,141	0
3	GOL	E	403	6/6	0.87	0.22	76,90,109,120	0
3	GOL	E	404	6/6	0.87	0.21	93,103,104,106	0
3	GOL	D	403	6/6	0.87	0.25	73,91,102,108	0
3	GOL	C	408	6/6	0.87	0.19	94,117,143,152	0
3	GOL	A	406	6/6	0.87	0.22	69,75,99,108	0
3	GOL	C	407	6/6	0.87	0.28	91,104,108,112	0
3	GOL	E	409	6/6	0.88	0.20	83,87,104,105	0
3	GOL	D	405	6/6	0.88	0.23	96,120,130,131	0
3	GOL	C	410	6/6	0.88	0.24	84,117,147,147	0
3	GOL	A	415	6/6	0.88	0.17	84,108,130,141	0
3	GOL	G	409	6/6	0.88	0.22	104,135,159,163	0
3	GOL	C	404	6/6	0.89	0.24	88,92,99,115	0
3	GOL	A	411	6/6	0.89	0.19	77,104,105,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	416	6/6	0.89	0.21	87,108,136,141	0
3	GOL	F	412	6/6	0.89	0.16	70,76,91,96	0
3	GOL	G	404	6/6	0.89	0.22	85,100,103,106	0
3	GOL	B	405	6/6	0.89	0.18	91,99,106,113	0
3	GOL	G	406	6/6	0.89	0.19	92,97,105,120	0
3	GOL	F	406	6/6	0.89	0.18	100,102,105,105	0
3	GOL	F	407	6/6	0.89	0.16	98,118,135,136	0
3	GOL	D	402	6/6	0.89	0.19	78,86,91,108	0
3	GOL	A	409	6/6	0.90	0.17	80,87,91,102	0
3	GOL	A	412	6/6	0.90	0.21	72,86,92,98	0
3	GOL	B	414	6/6	0.90	0.21	85,118,142,156	0
3	GOL	C	411	6/6	0.90	0.16	84,101,116,135	0
2	PO4	A	401	5/5	0.90	0.14	121,127,132,136	0
3	GOL	B	410	6/6	0.90	0.18	82,90,101,112	0
3	GOL	B	416	6/6	0.91	0.20	100,120,135,142	0
3	GOL	B	409	6/6	0.91	0.20	75,83,86,89	0
3	GOL	B	411	6/6	0.91	0.22	88,98,103,106	0
3	GOL	G	403	6/6	0.91	0.21	101,104,105,107	0
3	GOL	D	406	6/6	0.91	0.18	94,107,110,115	0
3	GOL	D	414	6/6	0.92	0.16	71,78,89,110	0
3	GOL	C	413	6/6	0.92	0.15	71,79,91,109	0
3	GOL	A	407	6/6	0.92	0.19	71,87,92,94	0
3	GOL	E	405	6/6	0.92	0.16	79,104,111,124	0
3	GOL	D	412	6/6	0.92	0.17	85,109,144,144	0
2	PO4	A	403	5/5	0.92	0.18	125,135,143,146	0
2	PO4	B	402	5/5	0.93	0.11	85,90,98,110	0
3	GOL	A	414	6/6	0.93	0.17	97,117,132,140	0
3	GOL	H	403	6/6	0.94	0.14	84,93,104,110	0
2	PO4	G	402	5/5	0.94	0.12	85,86,98,109	0
3	GOL	A	405	6/6	0.95	0.11	82,90,91,96	0
3	GOL	B	406	6/6	0.95	0.16	79,90,92,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.