



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:32 AM UTC

PDB ID : 8U5E / pdb_00008u5e
Title : Crystal Structure of C-terminal domain of Clostridium perfringens Enterotoxin
in Space Group P 21 21 21
Authors : Kapoor, S.; Vecchio, A.J.
Deposited on : 2023-09-12
Resolution : 1.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

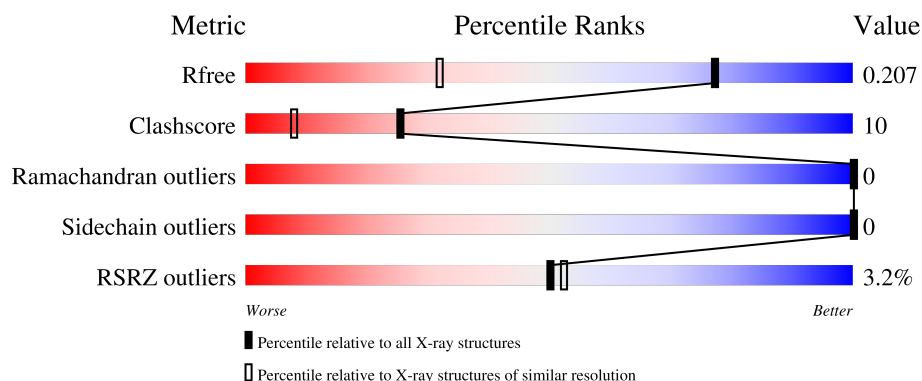
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	145	2% 71% 11% 18%
1	B	145	3% 74% 14% 12%
1	C	145	4% 79% 8% 12%
1	D	145	0% 74% 14% 12%

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
2	GOL	B	402	-	-	X	-
3	ACT	B	401	-	-	X	-
3	ACT	C	403	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4956 atoms, of which 38 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	119	Total	C	N	O	S	0	10	0
			1017	647	171	198	1			
1	B	127	Total	C	N	O	S	0	7	0
			1051	672	171	207	1			
1	C	127	Total	C	N	O	S	0	0	0
			1011	642	168	200	1			
1	D	128	Total	C	N	O	S	0	8	0
			1055	677	171	206	1			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	GLY	-	expression tag	UNP P01558
A	176	GLY	-	expression tag	UNP P01558
A	177	GLY	-	expression tag	UNP P01558
A	178	GLY	-	expression tag	UNP P01558
A	179	SER	-	expression tag	UNP P01558
A	180	GLY	-	expression tag	UNP P01558
A	181	GLY	-	expression tag	UNP P01558
A	182	GLY	-	expression tag	UNP P01558
A	183	GLY	-	expression tag	UNP P01558
A	184	SER	-	expression tag	UNP P01558
A	185	GLY	-	expression tag	UNP P01558
A	186	GLY	-	expression tag	UNP P01558
A	187	GLY	-	expression tag	UNP P01558
A	188	LEU	-	expression tag	UNP P01558
A	189	VAL	-	expression tag	UNP P01558
A	190	PRO	-	expression tag	UNP P01558
A	191	ARG	-	expression tag	UNP P01558
A	192	GLY	-	expression tag	UNP P01558
A	193	SER	-	expression tag	UNP P01558
B	175	GLY	-	expression tag	UNP P01558
B	176	GLY	-	expression tag	UNP P01558

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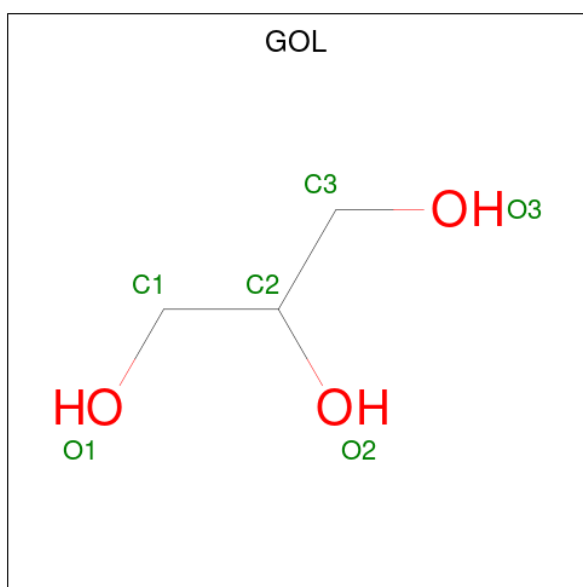
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	GLY	-	expression tag	UNP P01558
B	178	GLY	-	expression tag	UNP P01558
B	179	SER	-	expression tag	UNP P01558
B	180	GLY	-	expression tag	UNP P01558
B	181	GLY	-	expression tag	UNP P01558
B	182	GLY	-	expression tag	UNP P01558
B	183	GLY	-	expression tag	UNP P01558
B	184	SER	-	expression tag	UNP P01558
B	185	GLY	-	expression tag	UNP P01558
B	186	GLY	-	expression tag	UNP P01558
B	187	GLY	-	expression tag	UNP P01558
B	188	LEU	-	expression tag	UNP P01558
B	189	VAL	-	expression tag	UNP P01558
B	190	PRO	-	expression tag	UNP P01558
B	191	ARG	-	expression tag	UNP P01558
B	192	GLY	-	expression tag	UNP P01558
B	193	SER	-	expression tag	UNP P01558
C	175	GLY	-	expression tag	UNP P01558
C	176	GLY	-	expression tag	UNP P01558
C	177	GLY	-	expression tag	UNP P01558
C	178	GLY	-	expression tag	UNP P01558
C	179	SER	-	expression tag	UNP P01558
C	180	GLY	-	expression tag	UNP P01558
C	181	GLY	-	expression tag	UNP P01558
C	182	GLY	-	expression tag	UNP P01558
C	183	GLY	-	expression tag	UNP P01558
C	184	SER	-	expression tag	UNP P01558
C	185	GLY	-	expression tag	UNP P01558
C	186	GLY	-	expression tag	UNP P01558
C	187	GLY	-	expression tag	UNP P01558
C	188	LEU	-	expression tag	UNP P01558
C	189	VAL	-	expression tag	UNP P01558
C	190	PRO	-	expression tag	UNP P01558
C	191	ARG	-	expression tag	UNP P01558
C	192	GLY	-	expression tag	UNP P01558
C	193	SER	-	expression tag	UNP P01558
D	175	GLY	-	expression tag	UNP P01558
D	176	GLY	-	expression tag	UNP P01558
D	177	GLY	-	expression tag	UNP P01558
D	178	GLY	-	expression tag	UNP P01558
D	179	SER	-	expression tag	UNP P01558
D	180	GLY	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
D	181	GLY	-	expression tag	UNP P01558
D	182	GLY	-	expression tag	UNP P01558
D	183	GLY	-	expression tag	UNP P01558
D	184	SER	-	expression tag	UNP P01558
D	185	GLY	-	expression tag	UNP P01558
D	186	GLY	-	expression tag	UNP P01558
D	187	GLY	-	expression tag	UNP P01558
D	188	LEU	-	expression tag	UNP P01558
D	189	VAL	-	expression tag	UNP P01558
D	190	PRO	-	expression tag	UNP P01558
D	191	ARG	-	expression tag	UNP P01558
D	192	GLY	-	expression tag	UNP P01558
D	193	SER	-	expression tag	UNP P01558

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



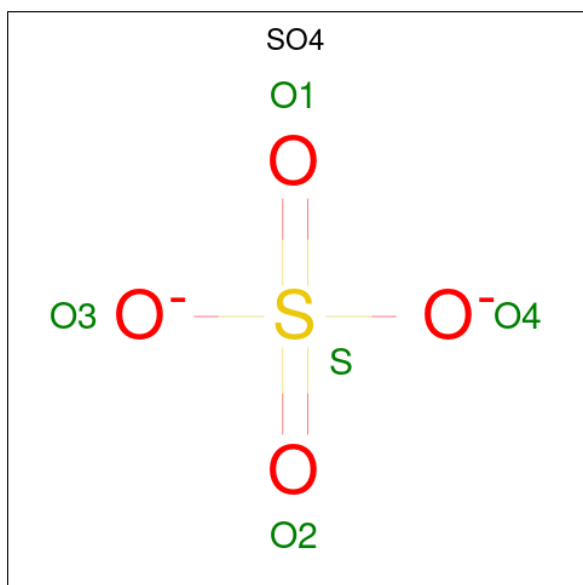
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 7 2 3 2	0	0
3	A	1	Total C H O 7 2 3 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

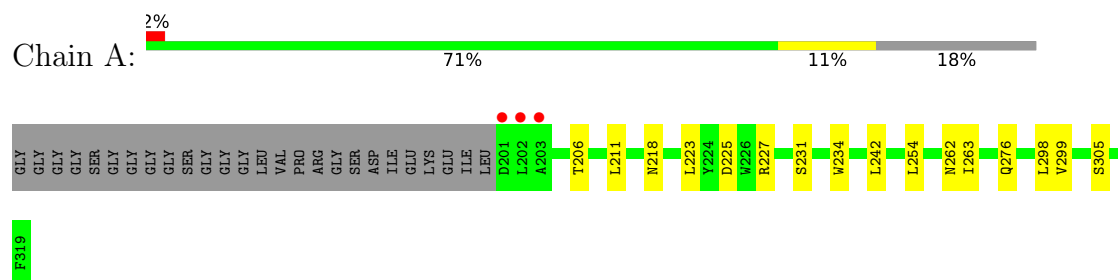
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	171	Total	O	0	0
			171	171		
5	C	170	Total	O	0	0
			170	170		
5	D	156	Total	O	0	0
			156	156		

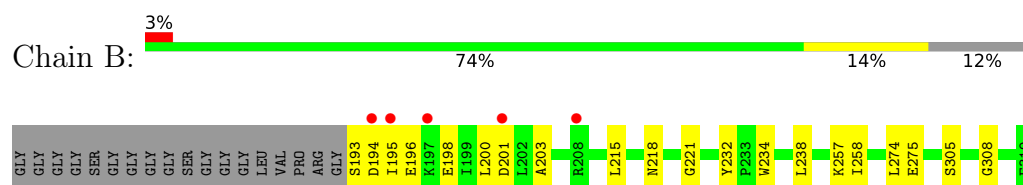
3 Residue-property plots [i](#)

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.

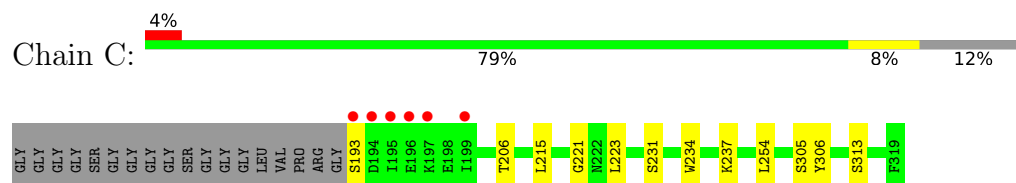
- Molecule 1: Heat-labile enterotoxin B chain



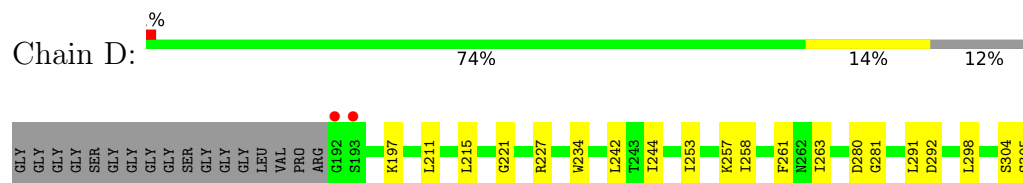
- Molecule 1: Heat-labile enterotoxin B chain



- Molecule 1: Heat-labile enterotoxin B chain



- Molecule 1: Heat-labile enterotoxin B chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.63Å 64.00Å 136.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.19 – 1.40 59.19 – 1.40	Depositor EDS
% Data completeness (in resolution range)	83.8 (59.19-1.40) 76.6 (59.19-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.31 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.161 , 0.205 0.164 , 0.207	Depositor DCC
R_{free} test set	1951 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4956	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, ACT

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	0.16	0/1044	0.39	0/1417
1	B	0.16	0/1088	0.40	0/1477
1	C	0.15	0/1032	0.40	0/1400
1	D	0.14	0/1098	0.37	0/1491
All	All	0.15	0/4262	0.39	0/5785

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	1017	0	989	22	0
1	B	1051	0	1036	18	0
1	C	1011	0	979	12	0
1	D	1055	0	1053	26	0
2	A	18	8	24	6	0
2	B	12	8	16	4	0
2	C	12	8	16	3	0
2	D	30	8	40	7	0
3	A	8	6	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	3	2	0
3	C	8	0	6	3	0
3	D	4	0	3	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	176	0	0	5	0
5	B	171	0	0	2	0
5	C	170	0	0	4	0
5	D	156	0	0	5	0
All	All	4918	38	4171	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 10.

All (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:A:211:LEU:HB2	1:A:242[B]:LEU:HD11	1.52	0.91
1:B:308:GLY:H	3:B:401:ACT:H3	1.43	0.81
1:B:258[B]:ILE:HG22	5:B:502:HOH:O	1.88	0.74
1:B:196:GLU:HB3	1:B:203:ALA:HB2	1.71	0.73
1:A:263[B]:ILE:HG12	1:A:298:LEU:CD1	2.20	0.71
1:A:211:LEU:HB2	1:A:242[B]:LEU:CD1	2.26	0.66
1:D:211:LEU:HB3	1:D:244[A]:ILE:CD1	2.26	0.65
1:D:211:LEU:HB3	1:D:244[A]:ILE:HD13	1.79	0.64
1:C:306:TYR:HA	2:C:404:GOL:H2	1.80	0.64
1:A:223:LEU:HB3	2:B:402:GOL:H11	1.80	0.63
1:B:195:ILE:HG12	4:B:404:SO4:O2	1.99	0.63
1:D:257:LYS:HG3	1:D:258[B]:ILE:HG12	1.80	0.62
2:D:404:GOL:H32	5:D:548:HOH:O	1.99	0.62
1:D:258[B]:ILE:HD11	5:D:510:HOH:O	2.01	0.61
1:C:237:LYS:HE2	3:C:403:ACT:CH3	2.31	0.60
1:C:193:SER:N	5:C:501:HOH:O	2.33	0.60
2:D:402:GOL:H32	5:D:625:HOH:O	2.02	0.60
1:C:237:LYS:HE2	3:C:403:ACT:H3	1.86	0.57
1:B:193:SER:OG	1:B:196:GLU:HG3	2.04	0.57
1:B:234:TRP:CD2	1:B:305:SER:HA	2.39	0.56
1:D:263:ILE:HG12	1:D:298[B]:LEU:CD2	2.35	0.56
1:D:215:LEU:O	1:D:221:GLY:HA2	2.07	0.55
1:D:242:LEU:HD11	1:D:298[B]:LEU:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HD23	2:A:402:GOL:H2	1.89	0.54
1:A:299:VAL:HG12	2:A:405:GOL:H31	1.89	0.54
1:C:234:TRP:CD2	1:C:305:SER:HA	2.43	0.53
2:A:401:GOL:H32	5:A:547:HOH:O	2.08	0.53
1:A:231:SER:HB2	1:C:231:SER:HB2	1.91	0.53
1:A:234:TRP:CD2	1:A:305[A]:SER:HA	2.44	0.53
1:B:218:ASN:HB3	5:B:523:HOH:O	2.08	0.52
1:A:223:LEU:HD22	2:B:402:GOL:H32	1.91	0.52
1:D:291:LEU:HA	2:D:406:GOL:H31	1.92	0.52
1:A:223:LEU:HB3	2:B:402:GOL:C1	2.41	0.51
1:B:215:LEU:O	1:B:221:GLY:HA2	2.10	0.51
1:D:261:PHE:CD1	1:D:298[A]:LEU:HD11	2.45	0.51
1:D:234:TRP:CD2	1:D:305:SER:HA	2.45	0.51
1:A:218:ASN:HB3	5:A:521:HOH:O	2.12	0.51
1:A:206[B]:THR:HG22	5:A:643:HOH:O	2.11	0.50
1:D:263:ILE:HG12	1:D:298[A]:LEU:CD1	2.41	0.50
1:A:234:TRP:CD2	1:A:305[B]:SER:HA	2.47	0.50
1:D:280:ASP:H	2:D:405:GOL:C3	2.25	0.50
1:D:258[B]:ILE:HD13	1:D:281:GLY:HA2	1.94	0.49
1:A:263[A]:ILE:HD13	1:A:298:LEU:HD13	1.93	0.49
1:B:232:TYR:CE2	1:B:238[B]:LEU:HD12	2.48	0.49
1:D:197:LYS:HD2	5:D:640:HOH:O	2.13	0.49
1:A:206[A]:THR:HG23	5:A:522:HOH:O	2.13	0.49
1:D:211:LEU:HD23	1:D:244[A]:ILE:HD12	1.94	0.48
1:B:257:LYS:HG3	1:B:258[B]:ILE:HG23	1.94	0.48
1:D:280:ASP:CG	2:D:405:GOL:H31	2.38	0.48
3:C:403:ACT:H2	5:C:600:HOH:O	2.12	0.48
1:A:223:LEU:CB	2:B:402:GOL:H11	2.43	0.48
1:C:313:SER:O	2:C:402:GOL:H31	2.14	0.47
1:D:263:ILE:HG12	1:D:298[B]:LEU:HD22	1.96	0.47
1:D:280:ASP:CB	2:D:405:GOL:H31	2.45	0.47
1:A:299:VAL:HG12	2:A:405:GOL:C3	2.44	0.46
1:B:308:GLY:N	3:B:401:ACT:H3	2.23	0.46
1:D:227:ARG:NH2	5:D:504:HOH:O	2.48	0.46
1:D:211:LEU:HD23	1:D:244[A]:ILE:CD1	2.45	0.46
1:C:254:LEU:C	1:C:254:LEU:HD23	2.41	0.45
1:C:313:SER:C	2:C:402:GOL:H31	2.42	0.44
1:B:200:LEU:O	1:B:201:ASP:HB2	2.17	0.44
1:B:194:ASP:O	1:B:198:GLU:HG3	2.17	0.43
1:B:234:TRP:CG	1:B:305:SER:HA	2.54	0.43
1:D:292:ASP:H	2:D:406:GOL:H31	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:561:HOH:O	1:D:257:LYS:HD3	2.19	0.43
1:A:262:ASN:OD1	1:A:276:GLN:HG3	2.18	0.43
1:A:299:VAL:CG1	2:A:405:GOL:H31	2.50	0.42
1:D:258[B]:ILE:HG23	1:D:304[B]:SER:OG	2.19	0.42
1:A:227[B]:ARG:NH2	5:A:510:HOH:O	2.53	0.42
1:A:263[B]:ILE:HG12	1:A:298:LEU:HD11	1.97	0.42
1:C:215:LEU:O	1:C:221:GLY:HA2	2.20	0.42
1:D:253:ILE:HD12	1:D:263:ILE:HD13	2.01	0.41
1:B:274:LEU:O	1:B:275:GLU:HG2	2.21	0.41
1:C:206:THR:HG22	5:C:635:HOH:O	2.20	0.41
1:A:225:ASP:OD1	2:A:402:GOL:H12	2.20	0.41
1:C:223:LEU:C	1:C:223:LEU:HD23	2.46	0.41
1:B:193:SER:HG	1:B:196:GLU:HG3	1.85	0.41
1:D:242:LEU:CD1	1:D:298[B]:LEU:HG	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	127/145 (88%)	126 (99%)	1 (1%)	0	100	100
1	B	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
1	C	125/145 (86%)	123 (98%)	2 (2%)	0	100	100
1	D	134/145 (92%)	132 (98%)	2 (2%)	0	100	100
All	All	518/580 (89%)	511 (99%)	7 (1%)	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	113/118 (96%)	113 (100%)	0	100	100
1	B	119/118 (101%)	119 (100%)	0	100	100
1	C	111/118 (94%)	111 (100%)	0	100	100
1	D	120/118 (102%)	120 (100%)	0	100	100
All	All	463/472 (98%)	463 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	A	239	ASN
1	A	249	GLN
1	A	262	ASN
1	A	269	ASN
1	A	276	GLN
1	A	309	ASN
1	C	249	GLN
1	C	269	ASN
1	D	309	ASN

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](#)

21 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	$\# Z > 2$
2	GOL	B	402	-	5,5,5	1.19	0	5,5,5	0.88	0
3	ACT	D	401	-	3,3,3	1.38	0	3,3,3	1.38	0
3	ACT	B	401	-	3,3,3	1.40	1 (33%)	3,3,3	1.33	0
4	SO4	C	405	-	4,4,4	0.23	0	6,6,6	0.08	0
2	GOL	C	404	-	5,5,5	0.76	0	5,5,5	1.06	0
2	GOL	B	403	-	5,5,5	0.79	0	5,5,5	1.00	0
2	GOL	D	402	-	5,5,5	0.98	0	5,5,5	1.12	0
2	GOL	A	405	-	5,5,5	0.10	0	5,5,5	0.25	0
3	ACT	A	404	-	3,3,3	1.14	0	3,3,3	1.50	0
2	GOL	D	405	-	5,5,5	1.04	0	5,5,5	1.42	1 (20%)
2	GOL	D	406	-	5,5,5	0.08	0	5,5,5	0.28	0
2	GOL	C	402	-	5,5,5	0.93	0	5,5,5	1.07	0
2	GOL	D	403	-	5,5,5	0.88	0	5,5,5	1.12	0
3	ACT	A	403	-	3,3,3	1.19	0	3,3,3	1.51	0
3	ACT	C	403	-	3,3,3	1.33	0	3,3,3	1.35	0
4	SO4	B	404	-	4,4,4	0.23	0	6,6,6	0.08	0
2	GOL	D	404	-	5,5,5	0.97	0	5,5,5	0.98	0
4	SO4	D	407	-	4,4,4	0.25	0	6,6,6	0.08	0
3	ACT	C	401	-	3,3,3	1.45	1 (33%)	3,3,3	1.45	0
2	GOL	A	402	-	5,5,5	0.96	0	5,5,5	1.12	1 (20%)
2	GOL	A	401	-	5,5,5	0.95	0	5,5,5	1.08	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	GOL	B	402	-	-	4/4/4/4	-
2	GOL	D	405	-	-	2/4/4/4	-
2	GOL	D	406	-	-	0/4/4/4	-
2	GOL	D	402	-	-	0/4/4/4	-
2	GOL	C	402	-	-	1/4/4/4	-
2	GOL	D	404	-	-	0/4/4/4	-
2	GOL	A	405	-	-	2/4/4/4	-
2	GOL	C	404	-	-	0/4/4/4	-
2	GOL	D	403	-	-	0/4/4/4	-
2	GOL	B	403	-	-	0/4/4/4	-
2	GOL	A	402	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	ACT	CH3-C	2.06	1.57	1.49
3	B	401	ACT	CH3-C	2.01	1.57	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	405	GOL	C3-C2-C1	-2.50	102.61	111.80
2	A	402	GOL	C3-C2-C1	-2.11	104.04	111.80

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	GOL	O1-C1-C2-C3
2	B	402	GOL	C1-C2-C3-O3
2	D	405	GOL	C1-C2-C3-O3
2	B	402	GOL	O1-C1-C2-O2
2	B	402	GOL	O2-C2-C3-O3
2	D	405	GOL	O2-C2-C3-O3
2	A	405	GOL	C1-C2-C3-O3
2	A	405	GOL	O2-C2-C3-O3
2	C	402	GOL	C1-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	GOL	4	0
3	B	401	ACT	2	0
2	C	404	GOL	1	0
2	D	402	GOL	1	0
2	A	405	GOL	3	0
2	D	405	GOL	3	0
2	D	406	GOL	2	0
2	C	402	GOL	2	0
3	C	403	ACT	3	0
4	B	404	SO4	1	0
2	D	404	GOL	1	0
2	A	402	GOL	2	0
2	A	401	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	119/145 (82%)	-0.29	3 (2%) 58 61	9, 21, 29, 108	10 (8%)
1	B	127/145 (87%)	-0.13	5 (3%) 43 45	11, 22, 41, 79	7 (5%)
1	C	127/145 (87%)	-0.05	6 (4%) 36 39	15, 22, 41, 120	0
1	D	128/145 (88%)	-0.03	2 (1%) 70 73	12, 24, 37, 82	8 (6%)
All	All	501/580 (86%)	-0.12	16 (3%) 50 52	9, 22, 40, 120	25 (4%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	195	ILE	5.9
1	B	195	ILE	5.7
1	A	202	LEU	5.2
1	C	193	SER	4.7
1	C	194	ASP	4.5
1	C	196	GLU	3.8
1	D	192	GLY	3.8
1	C	197	LYS	3.6
1	B	208	ARG	3.4
1	A	201	ASP	3.3
1	B	197	LYS	3.2
1	A	203	ALA	3.2
1	D	193	SER	2.9
1	B	201	ASP	2.8
1	C	199	ILE	2.3
1	B	194	ASP	2.1

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 ⓘ

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
2	GOL	A	405	6/6	0.61	0.17	20,20,20,20	0
2	GOL	C	404	6/6	0.64	0.19	71,110,135,145	0
3	ACT	A	403	4/4	0.69	0.22	58,71,100,100	0
3	ACT	B	401	4/4	0.69	0.21	49,51,54,56	0
2	GOL	B	403	6/6	0.78	0.21	38,62,116,140	0
2	GOL	D	402	6/6	0.81	0.19	49,62,68,71	0
2	GOL	D	406	6/6	0.81	0.18	47,87,149,179	0
4	SO4	B	404	5/5	0.81	0.12	91,92,92,92	0
2	GOL	B	402	6/6	0.84	0.17	32,36,37,39	0
2	GOL	D	404	6/6	0.84	0.19	62,63,66,70	0
2	GOL	D	403	6/6	0.86	0.15	52,53,54,57	0
3	ACT	A	404	4/4	0.86	0.17	31,44,53,80	0
3	ACT	D	401	4/4	0.87	0.12	45,51,52,53	0
2	GOL	C	402	6/6	0.88	0.15	49,55,58,60	0
4	SO4	C	405	5/5	0.88	0.11	70,75,75,77	0
3	ACT	C	403	4/4	0.89	0.16	50,50,52,53	0
4	SO4	D	407	5/5	0.89	0.11	64,66,67,67	0
2	GOL	A	402	6/6	0.91	0.16	31,36,43,51	0
2	GOL	A	401	6/6	0.91	0.13	43,46,47,51	0
3	ACT	C	401	4/4	0.92	0.11	31,34,36,42	0
2	GOL	D	405	6/6	0.92	0.12	23,33,39,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.