



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:51 PM UTC

PDB ID : 3H7L / pdb_00003h7l
Title : CRYSTAL STRUCTURE OF ENDOGLUCANASE-RELATED PROTEIN
FROM *Vibrio parahaemolyticus*
Authors : Patskovsky, Y.; Toro, R.; Morano, C.; Rutter, M.; Chang, S.; Sauder, J.M.;
Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Ge-
nomics (NYSGXRC)
Deposited on : 2009-04-27
Resolution : 2.30 Å(reported)

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

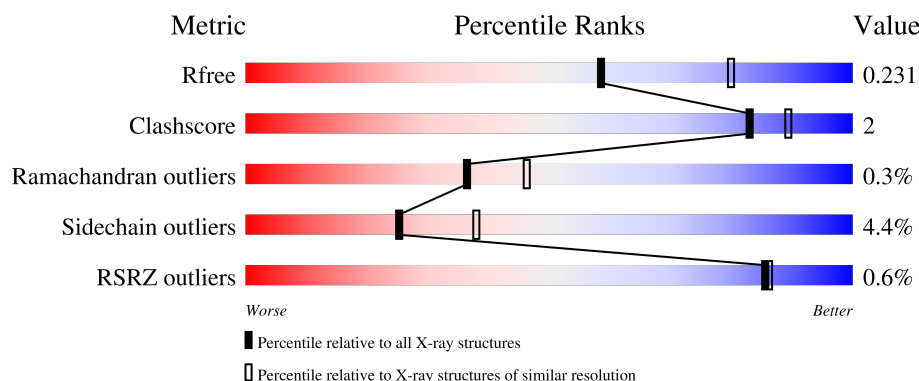
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	586	% 89% 9% ..
1	B	586	% 89% 9% ..
1	C	586	 88% 9% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14814 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 ENDOGLUCANASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	2	0
			4617	2924	789	886	18			
1	B	575	Total	C	N	O	S	0	4	0
			4622	2926	792	886	18			
1	C	575	Total	C	N	O	S	0	6	0
			4635	2934	793	890	18			

There are 36 discrepancies between the modelled and reference sequences:

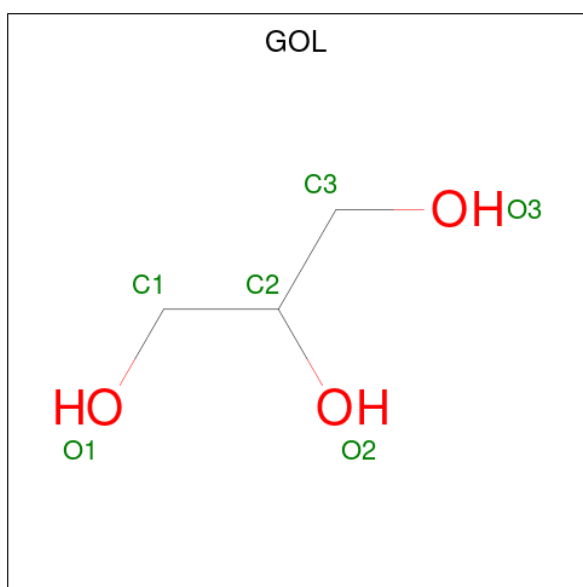
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q87LX4
A	1	SER	-	expression tag	UNP Q87LX4
A	87	THR	TYR	engineered mutation	UNP Q87LX4
A	132	ALA	VAL	engineered mutation	UNP Q87LX4
A	368	THR	GLY	engineered mutation	UNP Q87LX4
A	579	GLY	-	expression tag	UNP Q87LX4
A	580	HIS	-	expression tag	UNP Q87LX4
A	581	HIS	-	expression tag	UNP Q87LX4
A	582	HIS	-	expression tag	UNP Q87LX4
A	583	HIS	-	expression tag	UNP Q87LX4
A	584	HIS	-	expression tag	UNP Q87LX4
A	585	HIS	-	expression tag	UNP Q87LX4
B	0	MET	-	expression tag	UNP Q87LX4
B	1	SER	-	expression tag	UNP Q87LX4
B	87	THR	TYR	engineered mutation	UNP Q87LX4
B	132	ALA	VAL	engineered mutation	UNP Q87LX4
B	368	THR	GLY	engineered mutation	UNP Q87LX4
B	579	GLY	-	expression tag	UNP Q87LX4
B	580	HIS	-	expression tag	UNP Q87LX4
B	581	HIS	-	expression tag	UNP Q87LX4
B	582	HIS	-	expression tag	UNP Q87LX4
B	583	HIS	-	expression tag	UNP Q87LX4
B	584	HIS	-	expression tag	UNP Q87LX4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	585	HIS	-	expression tag	UNP Q87LX4
C	0	MET	-	expression tag	UNP Q87LX4
C	1	SER	-	expression tag	UNP Q87LX4
C	87	THR	TYR	engineered mutation	UNP Q87LX4
C	132	ALA	VAL	engineered mutation	UNP Q87LX4
C	368	THR	GLY	engineered mutation	UNP Q87LX4
C	579	GLY	-	expression tag	UNP Q87LX4
C	580	HIS	-	expression tag	UNP Q87LX4
C	581	HIS	-	expression tag	UNP Q87LX4
C	582	HIS	-	expression tag	UNP Q87LX4
C	583	HIS	-	expression tag	UNP Q87LX4
C	584	HIS	-	expression tag	UNP Q87LX4
C	585	HIS	-	expression tag	UNP Q87LX4

- 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	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

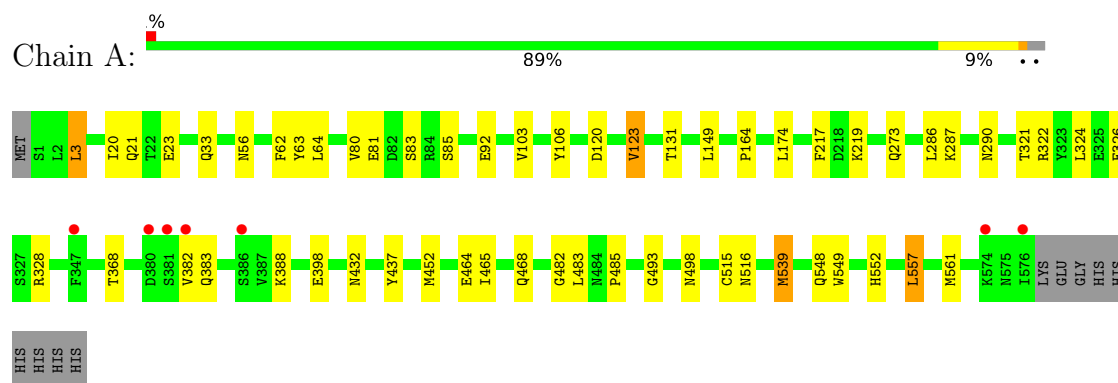
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total 203	O 203	0	0
3	B	334	Total 334	O 334	0	0
3	C	373	Total 373	O 373	0	0

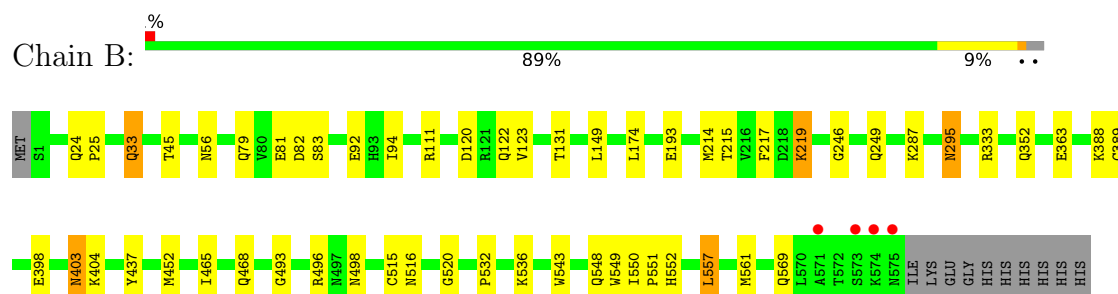
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

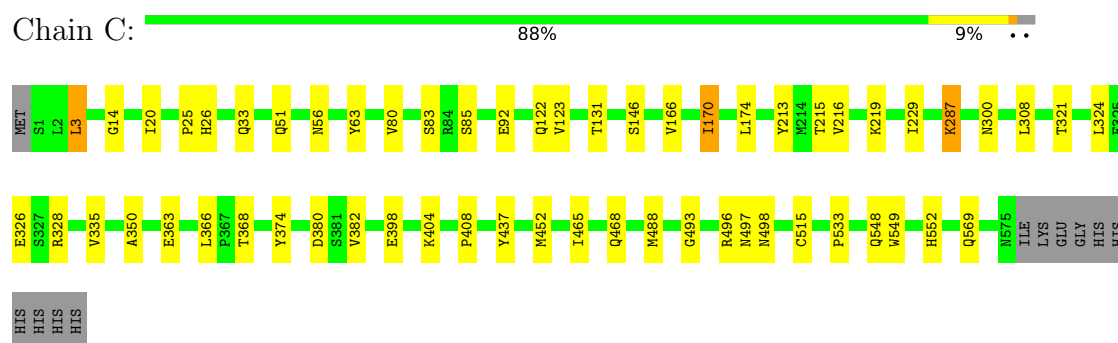
• Molecule 1: ENDOGLUCANASE



• Molecule 1: ENDOGLUCANASE



• Molecule 1: ENDOGLUCANASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	166.12Å 166.12Å 343.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 99.7 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.185 , 0.232 0.186 , 0.231	Depositor DCC
R_{free} test set	3734 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14814	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.60% 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

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	0.57	0/4741	0.95	1/6434 (0.0%)
1	B	0.58	0/4752	0.89	4/6448 (0.1%)
1	C	0.58	0/4768	0.89	3/6469 (0.0%)
All	All	0.58	0/14261	0.91	8/19351 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	GLY	N-CA-C	6.85	120.91	113.58
1	B	94	ILE	N-CA-C	5.55	115.75	110.42
1	C	363	GLU	N-CA-C	5.39	116.77	110.41
1	B	363	GLU	N-CA-C	5.38	116.76	110.41
1	B	532	PRO	O-C-N	5.19	123.59	121.15
1	C	14	GLY	CA-C-N	5.09	125.01	119.76
1	C	14	GLY	C-N-CA	5.09	125.01	119.76
1	B	520	GLY	N-CA-C	-5.05	106.08	112.54

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	4617	0	4362	21	0
1	B	4622	0	4370	23	0
1	C	4635	0	4382	22	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	12	0	16	1	0
3	A	203	0	0	0	0
3	B	334	0	0	1	0
3	C	373	0	0	0	0
All	All	14814	0	13154	64	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 2.

All (64) 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:557:LEU:HG	1:B:561:MET:HE2	1.62	0.81
1:A:557:LEU:HG	1:A:561:MET:HE2	1.66	0.78
1:B:246:GLY:H	1:B:249:GLN:HE21	1.34	0.74
1:B:246:GLY:H	1:B:249:GLN:NE2	1.91	0.69
1:C:493:GLY:H	1:C:498:ASN:ND2	1.96	0.63
1:C:465:ILE:HA	1:C:468:GLN:HE21	1.63	0.62
1:A:20:ILE:HB	1:A:63:TYR:HB2	1.82	0.62
1:A:21:GLN:HE22	1:A:485:PRO:HA	1.64	0.62
1:A:21:GLN:HE21	1:A:62:PHE:HE1	1.46	0.61
1:A:120:ASP:HA	1:A:123:VAL:HG22	1.83	0.59
1:A:20:ILE:HD11	1:A:80:VAL:HG21	1.85	0.59
1:B:493:GLY:H	1:B:498:ASN:ND2	2.02	0.58
1:A:515:CYS:HA	1:A:548:GLN:HA	1.86	0.57
1:B:549:TRP:HB3	1:B:552:HIS:CD2	2.40	0.56
1:C:3:LEU:HG	1:C:85:SER:HB3	1.87	0.55
1:C:20:ILE:HD11	1:C:80:VAL:HG21	1.86	0.55
1:C:515:CYS:HA	1:C:548:GLN:HA	1.87	0.55
1:C:166:VAL:O	1:C:170:ILE:HG12	2.07	0.54
1:A:493:GLY:H	1:A:498:ASN:ND2	2.06	0.54
1:A:465:ILE:HA	1:A:468:GLN:HE21	1.73	0.54
1:B:120:ASP:HA	1:B:123:VAL:CG2	2.38	0.53
1:C:549:TRP:HB3	1:C:552:HIS:CD2	2.44	0.53
1:B:295:ASN:HD22	1:B:295:ASN:H	1.56	0.51
1:C:493:GLY:H	1:C:498:ASN:HD21	1.56	0.51
1:C:488:MET:HG3	1:C:497:ASN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:GLN:HE22	1:C:25:PRO:HB2	1.75	0.51
1:C:20:ILE:HB	1:C:63:TYR:HB2	1.93	0.50
1:A:549:TRP:HB3	1:A:552:HIS:CD2	2.46	0.50
1:B:398:GLU:HG3	1:B:452:MET:HE1	1.94	0.49
1:B:515:CYS:HA	1:B:548:GLN:HA	1.93	0.49
1:A:368:THR:HB	1:A:452:MET:HG3	1.93	0.49
1:B:516:ASN:HA	1:B:552:HIS:NE2	2.27	0.49
1:B:465:ILE:HA	1:B:468:GLN:HE21	1.78	0.48
1:C:308:LEU:HD11	1:C:374:TYR:HB2	1.96	0.48
1:A:516:ASN:HA	1:A:552:HIS:NE2	2.29	0.48
1:C:398:GLU:HG3	1:C:452:MET:HE1	1.97	0.46
1:A:103:VAL:O	1:A:106:TYR:HB3	2.16	0.46
1:B:403:ASN:HD22	1:B:403:ASN:N	2.15	0.45
1:A:398:GLU:HG3	1:A:452:MET:HE1	1.98	0.44
1:B:333:ARG:HD3	1:C:26:HIS:ND1	2.32	0.44
1:A:3:LEU:HG	1:A:85:SER:HB3	1.98	0.44
1:A:217:PHE:CZ	1:A:219:LYS:HA	2.52	0.44
1:C:368:THR:HB	1:C:452:MET:HG3	2.01	0.43
1:B:217:PHE:CZ	1:B:219:LYS:HA	2.54	0.43
1:C:300:ASN:HB2	1:C:350:ALA:O	2.18	0.43
1:C:146:SER:HB3	1:C:216:VAL:O	2.18	0.43
1:A:286:LEU:O	1:A:290:ASN:HB2	2.19	0.42
1:B:516:ASN:ND2	1:B:543:TRP:O	2.52	0.42
1:C:533:PRO:HD2	2:C:587:GOL:H31	2.01	0.42
1:A:322:ARG:O	1:A:326:GLU:HG2	2.20	0.42
1:C:51:GLN:HG3	1:C:408:PRO:HB3	2.02	0.42
1:B:549:TRP:CG	1:B:551:PRO:HD2	2.55	0.42
1:B:33:GLN:HG2	1:B:79:GLN:HB3	2.02	0.42
1:B:550:ILE:HG13	1:B:551:PRO:HD3	2.02	0.42
1:C:324:LEU:O	1:C:328:ARG:HG3	2.20	0.42
1:B:111:ARG:HH22	1:B:193:GLU:HG2	1.85	0.42
1:C:213:TYR:CD1	1:C:229:ILE:HG21	2.55	0.42
1:A:324:LEU:O	1:A:328:ARG:HG3	2.20	0.41
1:B:120:ASP:HA	1:B:123:VAL:HG23	2.01	0.41
1:A:149:LEU:HG	1:A:164:PRO:HG3	2.01	0.41
1:A:539:MET:HE2	1:A:539:MET:HB3	1.81	0.41
1:B:24:GLN:HA	1:B:25:PRO:HD2	1.93	0.41
1:B:214:MET:HE1	3:B:836:HOH:O	2.20	0.41
1:C:287:LYS:HD2	1:C:326:GLU:OE2	2.22	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	576/586 (98%)	551 (96%)	23 (4%)	2 (0%)	36	46
1	B	577/586 (98%)	553 (96%)	22 (4%)	2 (0%)	36	46
1	C	579/586 (99%)	550 (95%)	28 (5%)	1 (0%)	43	55
All	All	1732/1758 (98%)	1654 (96%)	73 (4%)	5 (0%)	36	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	C	437	TYR
1	B	81	GLU
1	A	437	TYR
1	B	437	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/490 (99%)	462 (96%)	21 (4%)	26	39
1	B	484/490 (99%)	462 (96%)	22 (4%)	24	37
1	C	486/490 (99%)	464 (96%)	22 (4%)	24	37
All	All	1453/1470 (99%)	1388 (96%)	65 (4%)	25	37

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	23	GLU
1	A	33	GLN
1	A	56	ASN
1	A	64	LEU
1	A	83	SER
1	A	92	GLU
1	A	123	VAL
1	A	131	THR
1	A	174	LEU
1	A	273	GLN
1	A	287	LYS
1	A	321	THR
1	A	382	VAL
1	A	383	GLN
1	A	388	LYS
1	A	432	ASN
1	A	464	GLU
1	A	483	LEU
1	A	539	MET
1	A	557	LEU
1	B	33	GLN
1	B	45	THR
1	B	56	ASN
1	B	82	ASP
1	B	83	SER
1	B	92	GLU
1	B	122	GLN
1	B	131	THR
1	B	149	LEU
1	B	174	LEU
1	B	215	THR
1	B	219	LYS
1	B	287	LYS
1	B	295	ASN
1	B	388	LYS
1	B	389	CYS
1	B	403	ASN
1	B	404	LYS
1	B	496	ARG
1	B	536	LYS
1	B	557	LEU
1	B	569	GLN

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Mol	Chain	Res	Type
1	C	3	LEU
1	C	33	GLN
1	C	56	ASN
1	C	83	SER
1	C	92	GLU
1	C	122[A]	GLN
1	C	122[B]	GLN
1	C	123	VAL
1	C	131	THR
1	C	170	ILE
1	C	174	LEU
1	C	215	THR
1	C	219	LYS
1	C	287	LYS
1	C	321	THR
1	C	335	VAL
1	C	366	LEU
1	C	380	ASP
1	C	382	VAL
1	C	404	LYS
1	C	496	ARG
1	C	569	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	33	GLN
1	A	105	HIS
1	A	110	GLN
1	A	277	ASN
1	A	295	ASN
1	A	383	GLN
1	A	403	ASN
1	A	468	GLN
1	A	474	GLN
1	A	497	ASN
1	A	498	ASN
1	A	565	GLN
1	A	569	GLN
1	B	33	GLN
1	B	249	GLN

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Mol	Chain	Res	Type
1	B	277	ASN
1	B	289	HIS
1	B	292	GLN
1	B	295	ASN
1	B	332	GLN
1	B	352	GLN
1	B	403	ASN
1	B	457	GLN
1	B	466	GLN
1	B	468	GLN
1	B	498	ASN
1	B	531	ASN
1	B	566	HIS
1	C	33	GLN
1	C	56	ASN
1	C	79	GLN
1	C	161	GLN
1	C	277	ASN
1	C	332	GLN
1	C	392	ASN
1	C	432	ASN
1	C	459	HIS
1	C	468	GLN
1	C	498	ASN
1	C	531	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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	586	-	5,5,5	0.39	0	5,5,5	0.81	0
2	GOL	A	586	-	5,5,5	0.32	0	5,5,5	0.64	0
2	GOL	C	586	-	5,5,5	0.44	0	5,5,5	0.66	0
2	GOL	B	587	-	5,5,5	0.30	0	5,5,5	0.53	0
2	GOL	C	587	-	5,5,5	0.56	0	5,5,5	0.54	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	586	-	-	4/4/4/4	-
2	GOL	A	586	-	-	4/4/4/4	-
2	GOL	C	586	-	-	4/4/4/4	-
2	GOL	B	587	-	-	3/4/4/4	-
2	GOL	C	587	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	586	GOL	O1-C1-C2-O2
2	A	586	GOL	C1-C2-C3-O3
2	A	586	GOL	O2-C2-C3-O3
2	B	586	GOL	O1-C1-C2-C3
2	B	586	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	587	GOL	O1-C1-C2-C3
2	C	586	GOL	C1-C2-C3-O3
2	C	587	GOL	O1-C1-C2-C3
2	B	586	GOL	O2-C2-C3-O3
2	C	586	GOL	O2-C2-C3-O3
2	A	586	GOL	O1-C1-C2-C3
2	B	587	GOL	C1-C2-C3-O3
2	C	586	GOL	O1-C1-C2-C3
2	B	586	GOL	O1-C1-C2-O2
2	B	587	GOL	O1-C1-C2-O2
2	C	587	GOL	O1-C1-C2-O2
2	C	586	GOL	O1-C1-C2-O2
2	C	587	GOL	C1-C2-C3-O3
2	C	587	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	587	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	576/586 (98%)	-0.00	7 (1%) 76 77	22, 43, 73, 114	2 (0%)
1	B	575/586 (98%)	-0.68	4 (0%) 84 85	9, 27, 58, 115	4 (0%)
1	C	575/586 (98%)	-0.76	0 100 100	11, 26, 52, 100	6 (1%)
All	All	1726/1758 (98%)	-0.48	11 (0%) 85 86	9, 32, 66, 115	12 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	ILE	5.3
1	B	574	LYS	3.3
1	A	380	ASP	3.2
1	A	382	VAL	2.9
1	B	573	SER	2.6
1	B	575	ASN	2.5
1	A	386	SER	2.1
1	A	574	LYS	2.1
1	B	571	ALA	2.1
1	A	347	PHE	2.1
1	A	381	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	586	6/6	0.91	0.11	40,54,58,59	0
2	GOL	C	587	6/6	0.91	0.11	24,30,35,40	0
2	GOL	B	587	6/6	0.94	0.10	27,41,43,44	0
2	GOL	B	586	6/6	0.94	0.09	30,35,39,42	0
2	GOL	C	586	6/6	0.96	0.07	22,29,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.