

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	3H7L
Title	:	CRYSTAL STRUCTURE OF ENDOGLUCANASE-RELATED PROTEIN
		FROM Vibrio parahaemolyticus
Authors	:	Patskovsky, Y.; Toro, R.; Morano, C.; Rutter, M.; Chang, S.; Sauder, J.M.;
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		nomics (NYSGXRC)
Deposited on	:	2009-04-27
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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.



Motria	Whole archive	Similar resolution
Metric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	А	586	89%	9%	•••
1	В	586	90%	8%	•••
1	С	586	90%	8%	•



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	576	Total	С	Ν	0	\mathbf{S}	0	2	0
	A	570	4617	2924	789	886	18	0	2	0
1	Р	575	Total	С	Ν	0	S	0	1	0
	D	575	4622	2926	792	886	18	0	4	0
1	C	575	Total	С	Ν	0	S	0	6	0
		575	4635	2934	793	890	18	U	U	0

• Molecule 1 is a protein called ENDOGLUCANASE.

There are 36 discrepancies between	the modelled and ref	erence sequences:
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Chain	Residue	Modelled	Actual Comment		Reference
А	0	MET	-	expression tag	UNP Q87LX4
А	1	SER	-	expression tag	UNP Q87LX4
А	87	THR	TYR	engineered mutation	UNP Q87LX4
А	132	ALA	VAL	engineered mutation	UNP Q87LX4
А	368	THR	GLY	engineered mutation	UNP Q87LX4
A	579	GLY	-	expression tag	UNP Q87LX4
А	580	HIS	-	expression tag	UNP Q87LX4
А	581	HIS	-	expression tag	UNP Q87LX4
А	582	HIS	-	expression tag	UNP Q87LX4
А	583	HIS	-	expression tag	UNP Q87LX4
А	584	HIS	-	expression tag	UNP Q87LX4
А	585	HIS	-	expression tag	UNP Q87LX4
В	0	MET	-	expression tag	UNP Q87LX4
В	1	SER	-	expression tag	UNP Q87LX4
В	87	THR	TYR	engineered mutation	UNP Q87LX4
В	132	ALA	VAL	engineered mutation	UNP Q87LX4
В	368	THR	GLY	engineered mutation	UNP Q87LX4
В	579	GLY	-	expression tag	UNP Q87LX4
В	580	HIS	-	expression tag	UNP Q87LX4
В	581	HIS	-	expression tag	UNP Q87LX4
В	582	HIS	-	expression tag	UNP $Q87LX4$
В	583	HIS	-	expression tag	UNP Q87LX4
В	584	HIS	-	expression tag	UNP Q87LX4



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

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	203	Total O 203 203	0	0
3	В	334	Total O 334 334	0	0
3	С	373	Total O 373 373	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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants	166.12Å 166.12Å 343.53Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution(A)	20.00 - 2.30	Depositor
Resolution (A)	31.39 - 2.30	EDS
% Data completeness	100.0 (20.00-2.30)	Depositor
(in resolution range)	99.9 (31.39-2.30)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) > 1$	$2.06 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
D D	0.185 , 0.232	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.186 , 0.231	DCC
R_{free} test set	3734 reflections $(3.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	25.4	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33, 41.8	EDS
L-test for twinning ²	$ L > = 0.46, < L^2 > = 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.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.47	0/4741	0.61	0/6434	
1	В	0.51	0/4752	0.61	0/6448	
1	С	0.51	0/4768	0.62	0/6469	
All	All	0.50	0/14261	0.61	0/19351	

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	А	4617	0	4362	19	0
1	В	4622	0	4370	23	0
1	С	4635	0	4382	21	0
2	А	6	0	8	0	0
2	В	12	0	16	0	0
2	С	12	0	16	1	0
3	А	203	0	0	0	0
3	В	334	0	0	1	0
3	С	373	0	0	0	0
All	All	14814	0	13154	61	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 (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
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:B:557:LEU:HG	1:B:561:MET:HE1	1.88	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	
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: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:B:173:GLY:HA3	1:B:561:MET:HE3	1.95	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:A:557:LEU:HG	1:A:561:MET:HE1	1.97	0.47	
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	



A + 1	A + 9	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:B:214:MET:HE1	3:B:836:HOH:O	2.16	0.45	
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:B:24:GLN:HA	1:B:25:PRO:HD2	1.93	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	А	576/586~(98%)	551 (96%)	23~(4%)	2~(0%)	41 50	



0 0									
Mol	Chain	Analysed	Favoured Allowed		Outliers	Percentiles			
1	В	577/586~(98%)	553~(96%)	22~(4%)	2~(0%)	41	50		
1	С	579/586~(99%)	550~(95%)	28~(5%)	1 (0%)	47	58		
All	All	1732/1758~(98%)	1654 (96%)	73 (4%)	5~(0%)	41	50		

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	81	GLU
1	С	437	TYR
1	В	81	GLU
1	А	437	TYR
1	В	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 C		Outliers	Percenti	\mathbf{es}
1	А	483/490~(99%)	460 (95%)	23~(5%)	25 36	;
1	В	484/490~(99%)	465 (96%)	19 (4%)	32 46	i
1	С	486/490~(99%)	470 (97%)	16 (3%)	38 53	;
All	All	1453/1470~(99%)	1395~(96%)	58 (4%)	31 44	:

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	LEU
1	А	23	GLU
1	А	33	GLN
1	А	56	ASN
1	А	64	LEU
1	А	81	GLU
1	А	83	SER
1	А	84	ARG
1	А	92	GLU



1 A 122 GLN 1 A 123 VAL 1 A 131 THR 1 A 174 LEU 1 A 273 GLN 1 A 273 GLN 1 A 287 LYS 1 A 383 GLN 1 A 432 ASN 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 131 THR 1 B 131 THR 1 B 131 <th>Mol</th> <th>Chain</th> <th>Res</th> <th>Type</th>	Mol	Chain	Res	Type
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 321 THR 1 A 383 GLN 1 A 432 ASN 1 A 539 MET 1 A 565 GLN 1 B 33 GLN 1 B 83 SER 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 287 <td>1</td> <td>А</td> <td>122</td> <td>GLN</td>	1	А	122	GLN
1 A 131 THR 1 A 174 LEU 1 A 273 GLN 1 A 287 LYS 1 A 321 THR 1 A 383 GLN 1 A 432 ASN 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 83 SER 1 B 131 THR 1 <t< td=""><td>1</td><td>А</td><td>123</td><td>VAL</td></t<>	1	А	123	VAL
1 A 174 LEU 1 A 273 GLN 1 A 287 LYS 1 A 321 THR 1 A 383 GLN 1 A 388 LYS 1 A 432 ASN 1 A 539 MET 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 83 SER 1 B 83 SER 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 295 ASN 1 B 388 LYS 1 <td< td=""><td>1</td><td>А</td><td>131</td><td>THR</td></td<>	1	А	131	THR
1 A 273 GLN 1 A 287 LYS 1 A 321 THR 1 A 383 GLN 1 A 432 ASN 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 82 ASP 1 B 83 SER 1 B 131 THR 1 B 131 THR 1 B 287 LYS 1 B 295 ASN 1 B 3897 PHE	1	А	174	LEU
1 A 287 LYS 1 A 321 THR 1 A 383 GLN 1 A 383 LYS 1 A 383 LYS 1 A 432 ASN 1 A 432 ASN 1 A 433 LEU 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 82 ASP 1 B 83 SER 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 397 PHE 1	1	А	273	GLN
1 A 321 THR 1 A 383 GLN 1 A 388 LYS 1 A 432 ASN 1 A 432 ASN 1 A 432 ASN 1 A 432 ASN 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 33 GLN 1 B 82 ASP 1 B 83 SER 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 388 LYS 1 B 389 CYS 1 B	1	А	287	LYS
1A383GLN1A388LYS1A432ASN1A432ASN1A433LEU1A539MET1A557LEU1A565GLN1B33GLN1B56ASN1B82ASP1B83SER1B131THR1B131THR1B215THR1B287LYS1B388LYS1B389CYS1B397PHE1B403ASN1B404LYS1B406ARG1B536LYS1B557LEU	1	А	321	THR
1 A 388 LYS 1 A 432 ASN 1 A 483 LEU 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 82 ASP 1 B 82 ASP 1 B 82 ASP 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B	1	А	383	GLN
1 A 432 ASN 1 A 483 LEU 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 82 ASP 1 B 83 SER 1 B 83 SER 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 288 LYS 1 B 389 CYS 1 B 389 CYS 1 B 403 ASN 1 B 404 LYS 1 B 406 ARG 1 B 536 LYS 1 B	1	А	388	LYS
1 A 483 LEU 1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 82 ASP 1 B 82 ASP 1 B 122 GLN 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	А	432	ASN
1 A 539 MET 1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 33 GLN 1 B 33 GLN 1 B 56 ASN 1 B 82 ASP 1 B 83 SER 1 B 122 GLN 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 389 CYS 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B<	1	А	483	LEU
1 A 557 LEU 1 A 565 GLN 1 B 33 GLN 1 B 56 ASN 1 B 82 ASP 1 B 83 SER 1 B 122 GLN 1 B 122 GLN 1 B 131 THR 1 B 131 THR 1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	А	539	MET
1 A 565 GLN 1 B 33 GLN 1 B 56 ASN 1 B 82 ASP 1 B 82 ASP 1 B 122 GLN 1 B 122 GLN 1 B 122 GLN 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	А	557	LEU
1 B 33 GLN 1 B 56 ASN 1 B 82 ASP 1 B 83 SER 1 B 122 GLN 1 B 131 THR 1 B 131 THR 1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	А	565	GLN
1 B 56 ASN 1 B 82 ASP 1 B 83 SER 1 B 122 GLN 1 B 131 THR 1 B 131 THR 1 B 131 THR 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	33	GLN
1 B 82 ASP 1 B 83 SER 1 B 122 GLN 1 B 131 THR 1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 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	В	56	ASN
1 B 83 SER 1 B 122 GLN 1 B 131 THR 1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	82	ASP
1 B 122 GLN 1 B 131 THR 1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 406 ARG 1 B 536 LYS 1 B 557 LEU	1	В	83	SER
1 B 131 THR 1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	122	GLN
1 B 174 LEU 1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 406 ARG 1 B 536 LYS 1 B 557 LEU	1	В	131	THR
1 B 215 THR 1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	174	LEU
1 B 287 LYS 1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 406 ARG 1 B 536 LYS 1 B 557 LEU	1	В	215	THR
1 B 295 ASN 1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	287	LYS
1 B 388 LYS 1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 406 ARG 1 B 536 LYS 1 B 557 LEU	1	В	295	ASN
1 B 389 CYS 1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	388	LYS
1 B 397 PHE 1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	389	CYS
1 B 403 ASN 1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	397	PHE
1 B 404 LYS 1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	403	ASN
1 B 496 ARG 1 B 536 LYS 1 B 557 LEU	1	В	404	LYS
1 B 536 LYS 1 B 557 LEU	1	В	496	ARG
1 B 557 LEU	1	В	536	LYS
	1	В	557	LEU
1 B 569 GLN	1	В	569	GLN
1 C 3 LEU	1	С	3	LEU
1 C 33 GLN	1	С	33	GLN
1 C 56 ASN	1	С	56	ASN
1 C 81 GLU	1	С	81	GLU
1 C 83 SER	1	С	83	SER
1 C 122[A] GLN	1	С	122[A]	GLN
1 C 122[B] GLN	1	С	122[B]	GLN
1 C 131 THR	1	С	131	THR
1 C 174 LEU	1	С	174	LEU



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Mol	Chain	Res	Type
1	С	215	THR
1	С	219	LYS
1	С	287	LYS
1	С	380	ASP
1	С	404	LYS
1	С	496	ARG
1	Ċ	569	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	21	GLN
1	А	105	HIS
1	А	277	ASN
1	А	295	ASN
1	А	383	GLN
1	А	403	ASN
1	А	468	GLN
1	А	498	ASN
1	А	565	GLN
1	А	569	GLN
1	В	33	GLN
1	В	93	HIS
1	В	98	GLN
1	В	249	GLN
1	В	277	ASN
1	В	292	GLN
1	В	295	ASN
1	В	332	GLN
1	В	343	GLN
1	В	352	GLN
1	В	403	ASN
1	В	468	GLN
1	В	498	ASN
1	С	33	GLN
1	С	277	ASN
1	С	332	GLN
1	С	343	GLN
1	С	468	GLN
1	С	498	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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).

Mal	Mal Tuna (Dec	Tink	B	Bond lengths			Bond angles		
	Moi Type	Unain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
2	GOL	В	586	-	5,5,5	0.38	0	$5,\!5,\!5$	0.74	0	
2	GOL	С	586	-	5,5,5	0.43	0	$5,\!5,\!5$	0.60	0	
2	GOL	В	587	-	5,5,5	0.30	0	$5,\!5,\!5$	0.49	0	
2	GOL	С	587	-	5,5,5	0.54	0	$5,\!5,\!5$	0.52	0	
2	GOL	А	586	-	5,5,5	0.32	0	$5,\!5,\!5$	0.59	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	В	586	-	-	4/4/4/4	-
2	GOL	С	586	-	-	4/4/4/4	-
2	GOL	В	587	-	-	3/4/4/4	-
2	GOL	С	587	-	-	4/4/4/4	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	А	586	-	-	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	А	586	GOL	O1-C1-C2-O2
2	А	586	GOL	C1-C2-C3-O3
2	А	586	GOL	O2-C2-C3-O3
2	В	586	GOL	O1-C1-C2-C3
2	В	586	GOL	C1-C2-C3-O3
2	В	587	GOL	O1-C1-C2-C3
2	С	586	GOL	C1-C2-C3-O3
2	С	587	GOL	O1-C1-C2-C3
2	В	586	GOL	O2-C2-C3-O3
2	С	586	GOL	O2-C2-C3-O3
2	А	586	GOL	O1-C1-C2-C3
2	В	587	GOL	C1-C2-C3-O3
2	С	586	GOL	O1-C1-C2-C3
2	В	586	GOL	O1-C1-C2-O2
2	В	587	GOL	O1-C1-C2-O2
2	С	587	GOL	O1-C1-C2-O2
2	С	586	GOL	O1-C1-C2-O2
2	С	587	GOL	C1-C2-C3-O3
2	С	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	С	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, 95^{th} 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	А	576/586~(98%)	0.00	22 (3%) 40 47	22, 43, 73, 114	0
1	В	575/586~(98%)	-0.47	8 (1%) 75 80	9, 27, 58, 115	0
1	С	575/586~(98%)	-0.53	7 (1%) 79 83	11, 26, 52, 100	0
All	All	1726/1758~(98%)	-0.34	37 (2%) 63 70	9, 32, 66, 115	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	576	ILE	7.5
1	В	574	LYS	5.4
1	В	573	SER	4.7
1	В	575	ASN	4.6
1	А	572	THR	4.3
1	С	575	ASN	3.7
1	А	128	ALA	3.3
1	А	575	ASN	3.3
1	В	43	VAL	3.1
1	А	574	LYS	3.1
1	С	572	THR	3.0
1	А	464	GLU	2.9
1	С	573	SER	2.7
1	А	465	ILE	2.6
1	А	225	ALA	2.6
1	А	461	ALA	2.6
1	А	381	SER	2.5
1	А	250	GLY	2.5
1	В	41	GLN	2.5
1	А	342	GLU	2.5
1	А	39	SER	2.4
1	A	240	PHE	2.4
1	А	208	GLU	2.3



Mol	Chain	Res	Type	RSRZ
1	А	573	SER	2.3
1	А	379	ASP	2.3
1	С	379	ASP	2.3
1	А	420	ASN	2.3
1	А	462	SER	2.3
1	А	129	ASN	2.2
1	С	461	ALA	2.2
1	С	464	GLU	2.1
1	С	82	ASP	2.1
1	А	41	GLN	2.1
1	В	572	THR	2.1
1	В	461	ALA	2.1
1	А	382	VAL	2.1
1	В	39	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 monosaccharides 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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q < 0.9
2	GOL	С	587	6/6	0.91	0.17	24,30,35,40	0
2	GOL	А	586	6/6	0.94	0.15	$40,\!54,\!58,\!59$	0
2	GOL	В	587	6/6	0.95	0.16	27,41,43,44	0
2	GOL	В	586	6/6	0.95	0.17	30,35,39,42	0
2	GOL	С	586	6/6	0.98	0.13	22,29,31,35	0

6.5 Other polymers (i)

There are no such residues in this entry.

