



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2024 – 10:11 AM EDT

PDB ID : 8VA3  
Title : Crystal structure of CapGH3b enzyme retrieved from capybara gut metagenome  
Authors : Martins, M.P.; Morais, M.A.B.; Chinaglia, M.; Mandelli, F.; Lima, E.A.; Murakami, M.T.  
Deposited on : 2023-12-11  
Resolution : 1.80 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

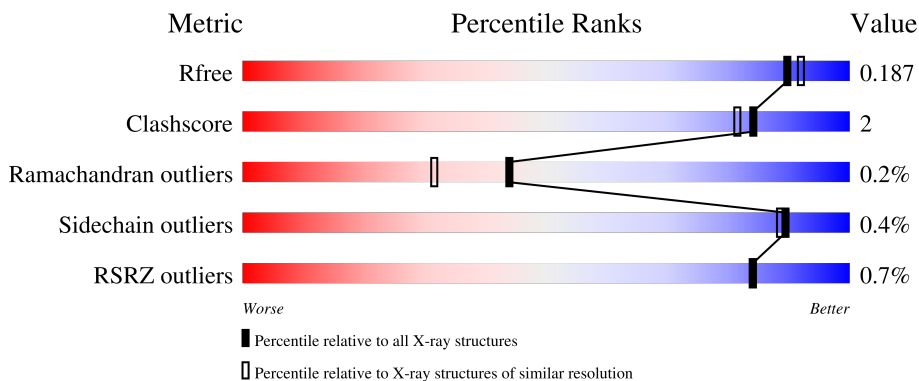
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

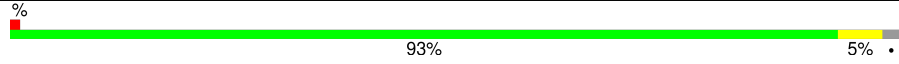
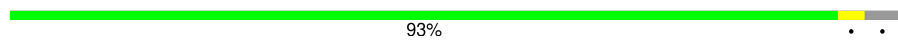
The reported resolution of this entry is 1.80 Å.

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))
$R_{free}$	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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  $\geq 3$ , 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	780	 93% 5%
1	B	780	 93%

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	PEG	A	801	-	-	X	-
4	GOL	B	809	-	-	X	-

## 2 Entry composition [i](#)

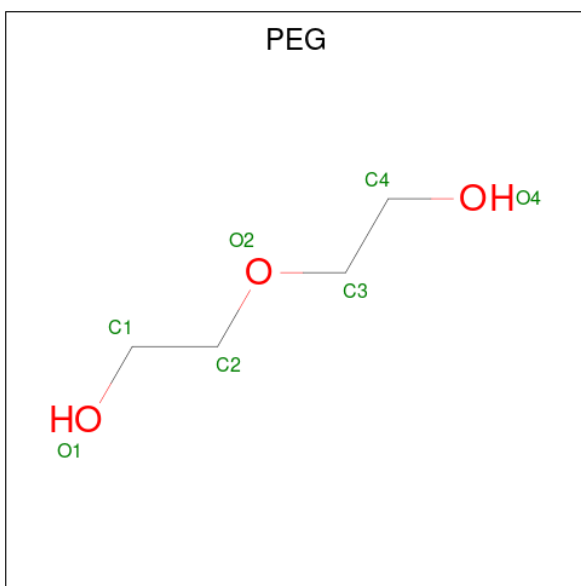
There are 9 unique types of molecules in this entry. The entry contains 13446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside hydrolase family 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	763	Total 5996	C 3774	N 1061	O 1133	S 28	0	6	0
1	B	752	Total 5885	C 3711	N 1038	O 1109	S 27	0	1	0

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

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

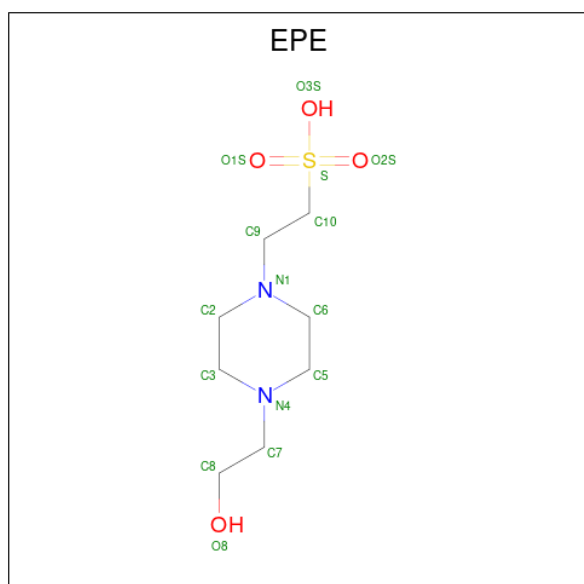
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

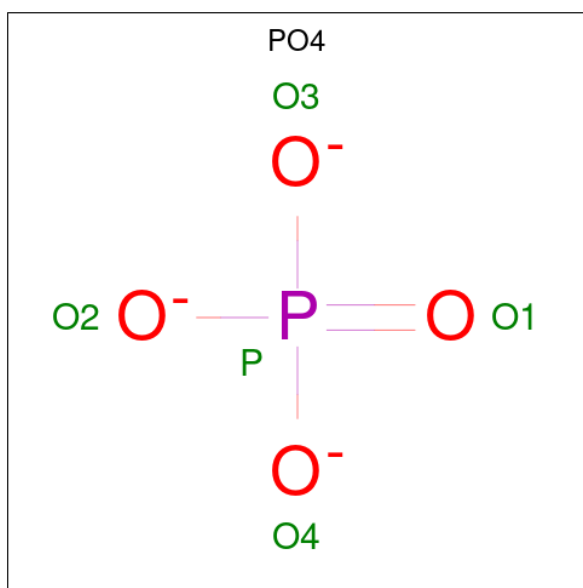
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 9 is water.

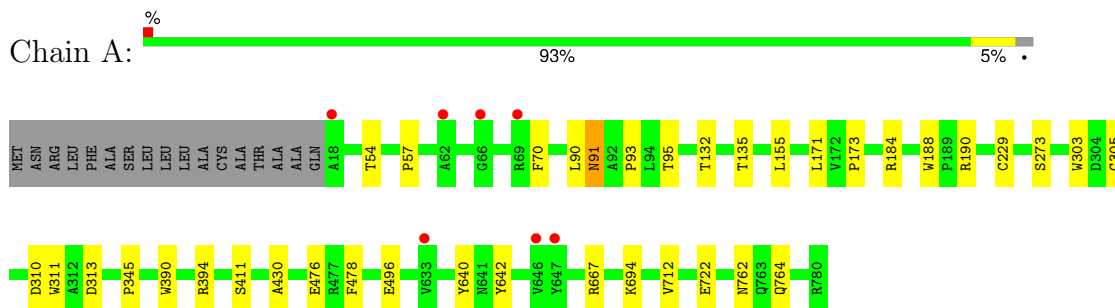
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	696	Total	O	0	0
			696	696		
9	B	658	Total	O	0	0
			658	658		



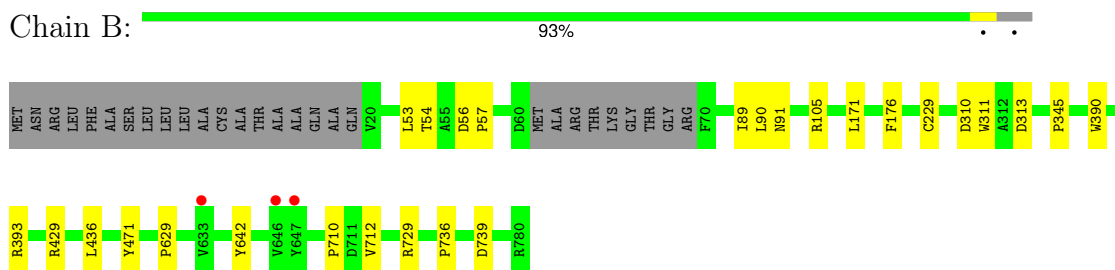
### 3 Residue-property plots [i](#)

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: Glycoside hydrolase family 3



- Molecule 1: Glycoside hydrolase family 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.06Å 105.35Å 190.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.07 – 1.80 47.07 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.07-1.80) 96.5 (47.07-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.79Å)	Xtrriage
Refinement program	PHENIX 1.20.1 4487:000	Depositor
R, $R_{free}$	0.155 , 0.187 0.155 , 0.187	Depositor DCC
$R_{free}$ test set	14586 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtrriage
Anisotropy	0.461	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, MG, EPE, PGE, PEG, 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	0.58	0/6133	0.70	0/8338
1	B	0.56	0/6018	0.69	0/8184
All	All	0.57	0/12151	0.70	0/16522

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

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	5996	0	5883	29	0
1	B	5885	0	5772	16	0
2	A	7	0	10	4	0
2	B	7	0	10	1	0
3	A	20	0	28	6	0
3	B	10	0	14	1	0
4	A	84	0	112	5	0
4	B	60	0	79	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	15	0	17	0	0
8	B	5	0	0	0	0
9	A	696	0	0	3	0
9	B	658	0	0	2	0
All	All	13446	0	11925	52	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 (52) 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:105:ARG:HH21	1:B:393:ARG:HH21	1.38	0.71
1:A:640:TYR:HD2	2:A:801:PEG:H32	1.61	0.65
1:B:54:THR:HG23	1:B:345:PRO:HB2	1.79	0.64
1:A:694:LYS:HG3	4:A:806:GOL:H32	1.83	0.61
1:A:764:GLN:HE22	2:A:801:PEG:H41	1.66	0.61
1:A:54:THR:O	1:A:57:PRO:HD2	2.04	0.58
4:B:809:GOL:H12	9:B:1364:HOH:O	2.05	0.56
1:A:54:THR:HG23	1:A:345:PRO:HB2	1.87	0.56
1:B:739:ASP:OD2	4:B:809:GOL:H32	2.06	0.56
1:B:54:THR:HG21	1:B:311:TRP:CH2	2.42	0.54
1:A:54:THR:HG21	1:A:311:TRP:CH2	2.42	0.54
1:B:105:ARG:HH21	1:B:393:ARG:NH2	2.06	0.54
1:A:722:GLU:OE2	4:A:806:GOL:H11	2.07	0.54
1:A:762:ASN:H	3:A:802:PGE:H52	1.73	0.53
1:B:54:THR:O	1:B:57:PRO:HD2	2.07	0.53
4:B:809:GOL:H31	9:B:1416:HOH:O	2.09	0.53
1:A:476:GLU:HG3	9:A:959:HOH:O	2.10	0.52
1:B:310:ASP:HB3	1:B:313:ASP:OD2	2.09	0.52
1:A:91:ASN:HD21	3:A:803:PGE:H22	1.77	0.50
1:A:171:LEU:HA	1:A:390:TRP:CZ2	2.47	0.50
1:A:70:PHE:CE1	1:A:93:PRO:HB3	2.47	0.49
1:B:105:ARG:NH2	1:B:393:ARG:HH21	2.09	0.49
1:A:478:PHE:CD2	4:A:807:GOL:H31	2.48	0.48
1:A:310:ASP:HB3	1:A:313:ASP:OD2	2.13	0.48
1:B:436:LEU:CD1	1:B:471:TYR:HA	2.43	0.48
1:A:640:TYR:CD2	2:A:801:PEG:H32	2.47	0.48
1:A:95:THR:HG21	3:A:803:PGE:O1	2.14	0.47
1:A:394:ARG:HG3	9:A:1420:HOH:O	2.14	0.46
1:A:762:ASN:CG	3:A:802:PGE:H6	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:813:GOL:O1	4:A:813:GOL:O3	2.19	0.46
2:B:802:PEG:H41	2:B:802:PEG:H21	1.75	0.46
1:A:155:LEU:HD13	1:A:411[A]:SER:HA	1.98	0.46
1:A:188:TRP:CZ2	1:A:190:ARG:HB2	2.52	0.45
1:A:91:ASN:HD21	3:A:803:PGE:C2	2.30	0.45
1:A:155:LEU:HD13	1:A:411[B]:SER:HA	1.98	0.45
2:A:801:PEG:H41	2:A:801:PEG:H21	1.40	0.44
1:B:171:LEU:HA	1:B:390:TRP:CZ2	2.53	0.44
1:A:430:ALA:N	4:A:807:GOL:H32	2.33	0.44
1:B:736:PRO:HD2	4:B:809:GOL:H32	2.00	0.43
1:A:303:TRP:CZ2	1:A:305:GLY:HA3	2.53	0.43
3:B:803:PGE:H32	3:B:803:PGE:H5	1.70	0.42
1:A:229:CYS:HA	1:A:273:SER:O	2.19	0.42
1:A:642:TYR:CD2	1:A:712:VAL:HB	2.54	0.42
1:A:132:THR:HB	1:A:135:THR:HB	2.01	0.42
1:B:642:TYR:CD2	1:B:712:VAL:HB	2.55	0.42
1:A:496:GLU:HG2	9:A:1344:HOH:O	2.19	0.42
1:A:184:ARG:HA	1:A:184:ARG:HD2	1.92	0.41
1:B:53:LEU:O	1:B:89:ILE:HA	2.20	0.41
1:B:629:PRO:HD3	1:B:710:PRO:O	2.21	0.40
1:B:176:PHE:HA	1:B:229:CYS:HB3	2.03	0.40
3:A:802:PGE:H12	3:A:802:PGE:H32	1.74	0.40
1:B:56:ASP:HB2	1:B:57:PRO:HD3	2.02	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	767/780 (98%)	745 (97%)	20 (3%)	2 (0%)	37 25
1	B	749/780 (96%)	729 (97%)	19 (2%)	1 (0%)	48 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1516/1560 (97%)	1474 (97%)	39 (3%)	3 (0%)	44 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	B	91	ASN
1	A	173	PRO

### 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	631/637 (99%)	629 (100%)	2 (0%)	91 90
1	B	619/637 (97%)	616 (100%)	3 (0%)	86 86
All	All	1250/1274 (98%)	1245 (100%)	5 (0%)	89 88

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	667	ARG
1	B	90	LEU
1	B	429	ARG
1	B	729	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 3 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	B	812	-	5,5,5	1.03	0	5,5,5	1.36	1 (20%)
3	PGE	B	803	-	9,9,9	0.37	0	8,8,8	0.32	0
4	GOL	B	806	-	5,5,5	0.88	0	5,5,5	1.26	1 (20%)
4	GOL	B	810	-	5,5,5	1.18	0	5,5,5	1.05	0
3	PGE	A	803	-	9,9,9	0.28	0	8,8,8	0.71	0
4	GOL	B	811	-	5,5,5	0.86	0	5,5,5	1.09	0
4	GOL	B	813	-	5,5,5	1.54	2 (40%)	5,5,5	0.70	0
4	GOL	B	808	-	5,5,5	1.07	0	5,5,5	1.10	0
4	GOL	A	804	-	5,5,5	1.25	0	5,5,5	1.16	0
4	GOL	A	812	-	5,5,5	1.11	0	5,5,5	1.21	1 (20%)
4	GOL	B	807	-	5,5,5	1.27	1 (20%)	5,5,5	0.79	0
4	GOL	B	804	-	5,5,5	0.63	0	5,5,5	1.25	0
2	PEG	B	802	-	6,6,6	0.21	0	5,5,5	0.07	0
4	GOL	A	810	-	5,5,5	0.76	0	5,5,5	1.14	1 (20%)
4	GOL	A	811	-	5,5,5	0.95	0	5,5,5	1.04	0
4	GOL	A	807	-	5,5,5	1.00	0	5,5,5	1.02	0
4	GOL	A	808	-	5,5,5	1.47	1 (20%)	5,5,5	1.14	0
4	GOL	A	813	-	5,5,5	1.12	0	5,5,5	1.02	0
4	GOL	B	805	-	5,5,5	0.81	0	5,5,5	1.13	0
7	EPE	B	801	-	15,15,15	0.79	1 (6%)	19,20,20	2.51	8 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PO4	B	815	-	4,4,4	0.62	0	6,6,6	1.35	1 (16%)
4	GOL	A	809	-	5,5,5	1.07	0	5,5,5	0.84	0
4	GOL	A	805	-	5,5,5	1.04	0	5,5,5	1.21	1 (20%)
4	GOL	A	817	-	5,5,5	1.13	0	5,5,5	1.17	1 (20%)
4	GOL	A	814	-	5,5,5	1.03	0	5,5,5	1.02	1 (20%)
3	PGE	A	802	-	9,9,9	0.40	0	8,8,8	0.61	0
2	PEG	A	801	-	6,6,6	0.39	0	5,5,5	0.24	0
4	GOL	A	816	-	5,5,5	1.04	0	5,5,5	0.74	0
4	GOL	B	809	-	5,5,5	1.08	0	5,5,5	1.35	0
4	GOL	A	815	-	5,5,5	0.69	0	5,5,5	1.46	1 (20%)
4	GOL	A	806	-	5,5,5	1.31	1 (20%)	5,5,5	1.42	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
4	GOL	B	812	-	-	2/4/4/4	-
3	PGE	B	803	-	-	4/7/7/7	-
4	GOL	B	806	-	-	3/4/4/4	-
4	GOL	B	810	-	-	2/4/4/4	-
3	PGE	A	803	-	-	6/7/7/7	-
4	GOL	B	811	-	-	2/4/4/4	-
4	GOL	B	813	-	-	0/4/4/4	-
4	GOL	B	808	-	-	0/4/4/4	-
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	A	812	-	-	0/4/4/4	-
4	GOL	B	807	-	-	2/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
2	PEG	B	802	-	-	2/4/4/4	-
4	GOL	A	810	-	-	2/4/4/4	-
4	GOL	A	811	-	-	0/4/4/4	-
4	GOL	A	807	-	-	3/4/4/4	-
4	GOL	A	808	-	-	4/4/4/4	-
4	GOL	A	813	-	-	2/4/4/4	-
4	GOL	B	805	-	-	0/4/4/4	-
7	EPE	B	801	-	-	4/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	809	-	-	2/4/4/4	-
4	GOL	A	805	-	-	0/4/4/4	-
4	GOL	A	817	-	-	2/4/4/4	-
4	GOL	A	814	-	-	2/4/4/4	-
3	PGE	A	802	-	-	5/7/7/7	-
2	PEG	A	801	-	-	3/4/4/4	-
4	GOL	A	816	-	-	1/4/4/4	-
4	GOL	B	809	-	-	2/4/4/4	-
4	GOL	A	815	-	-	2/4/4/4	-
4	GOL	A	806	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	801	EPE	C10-S	2.40	1.81	1.77
4	B	813	GOL	C1-C2	2.30	1.60	1.51
4	A	808	GOL	O2-C2	-2.13	1.37	1.43
4	B	807	GOL	O2-C2	-2.08	1.37	1.43
4	B	813	GOL	O2-C2	-2.08	1.37	1.43
4	A	806	GOL	C3-C2	2.01	1.59	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	801	EPE	O2S-S-C10	5.87	115.60	106.73
7	B	801	EPE	C7-N4-C3	4.79	124.00	111.24
7	B	801	EPE	C5-N4-C3	3.77	116.95	108.84
7	B	801	EPE	O3S-S-C10	-3.40	99.36	106.00
7	B	801	EPE	O1S-S-C10	3.17	111.52	106.73
7	B	801	EPE	C9-N1-C6	-2.41	104.81	111.24
4	A	805	GOL	C3-C2-C1	-2.28	103.42	111.80
8	B	815	PO4	O2-P-O1	2.27	118.99	110.95
7	B	801	EPE	C5-C6-N1	2.27	115.22	110.65
4	A	810	GOL	C3-C2-C1	-2.20	103.72	111.80
4	B	812	GOL	C3-C2-C1	-2.17	103.83	111.80
4	B	806	GOL	C3-C2-C1	-2.16	103.88	111.80
4	A	812	GOL	C3-C2-C1	-2.13	103.97	111.80
4	A	815	GOL	C3-C2-C1	-2.12	104.01	111.80
4	A	814	GOL	C3-C2-C1	-2.06	104.25	111.80
7	B	801	EPE	C7-N4-C5	2.05	116.70	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	817	GOL	C3-C2-C1	-2.02	104.38	111.80

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	808	GOL	O1-C1-C2-C3
4	A	808	GOL	C1-C2-C3-O3
4	A	809	GOL	O1-C1-C2-C3
4	A	814	GOL	C1-C2-C3-O3
4	A	814	GOL	O2-C2-C3-O3
4	B	806	GOL	C1-C2-C3-O3
4	B	810	GOL	C1-C2-C3-O3
7	B	801	EPE	C8-C7-N4-C3
7	B	801	EPE	C9-C10-S-O1S
7	B	801	EPE	C9-C10-S-O2S
7	B	801	EPE	C9-C10-S-O3S
3	A	802	PGE	C1-C2-O2-C3
2	A	801	PEG	C4-C3-O2-C2
3	B	803	PGE	C3-C4-O3-C5
4	A	815	GOL	O1-C1-C2-O2
3	A	803	PGE	C1-C2-O2-C3
3	B	803	PGE	C4-C3-O2-C2
2	A	801	PEG	O1-C1-C2-O2
2	B	802	PEG	O1-C1-C2-O2
3	A	802	PGE	O3-C5-C6-O4
4	A	810	GOL	O1-C1-C2-C3
4	A	813	GOL	O1-C1-C2-C3
4	A	815	GOL	O1-C1-C2-C3
4	A	817	GOL	C1-C2-C3-O3
4	B	807	GOL	O1-C1-C2-C3
4	B	811	GOL	O1-C1-C2-C3
4	B	812	GOL	O1-C1-C2-C3
3	A	803	PGE	O1-C1-C2-O2
4	A	808	GOL	O2-C2-C3-O3
4	A	809	GOL	O1-C1-C2-O2
4	A	810	GOL	O1-C1-C2-O2
4	A	817	GOL	O2-C2-C3-O3
4	B	806	GOL	O2-C2-C3-O3
4	B	807	GOL	O1-C1-C2-O2
3	A	803	PGE	O2-C3-C4-O3
3	A	802	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	A	807	GOL	O2-C2-C3-O3
4	A	808	GOL	O1-C1-C2-O2
4	B	810	GOL	O2-C2-C3-O3
4	A	807	GOL	O1-C1-C2-O2
4	A	813	GOL	O1-C1-C2-O2
4	B	806	GOL	O1-C1-C2-O2
4	A	816	GOL	O2-C2-C3-O3
3	A	802	PGE	C6-C5-O3-C4
3	A	803	PGE	C4-C3-O2-C2
3	B	803	PGE	C6-C5-O3-C4
3	A	802	PGE	C4-C3-O2-C2
2	B	802	PEG	C4-C3-O2-C2
3	A	803	PGE	C6-C5-O3-C4
4	B	811	GOL	O1-C1-C2-O2
4	B	812	GOL	O1-C1-C2-O2
2	A	801	PEG	C1-C2-O2-C3
4	A	807	GOL	C1-C2-C3-O3
4	B	809	GOL	O1-C1-C2-C3
4	A	806	GOL	O1-C1-C2-O2
4	B	809	GOL	O2-C2-C3-O3
3	B	803	PGE	O2-C3-C4-O3
3	A	803	PGE	C3-C4-O3-C5

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	PGE	1	0
3	A	803	PGE	3	0
2	B	802	PEG	1	0
4	A	807	GOL	2	0
4	A	813	GOL	1	0
3	A	802	PGE	3	0
2	A	801	PEG	4	0
4	B	809	GOL	4	0
4	A	806	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	763/780 (97%)	-0.57	7 (0%) 81 80	10, 23, 41, 80	6 (0%)
1	B	752/780 (96%)	-0.52	3 (0%) 89 88	12, 25, 41, 75	1 (0%)
All	All	1515/1560 (97%)	-0.55	10 (0%) 84 84	10, 24, 41, 80	7 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	633	VAL	4.6
1	B	633	VAL	4.6
1	A	646	VAL	4.4
1	A	647	TYR	4.2
1	B	647	TYR	3.7
1	B	646	VAL	3.2
1	A	62	ALA	3.1
1	A	18	ALA	2.6
1	A	66	GLY	2.4
1	A	69	ARG	2.3

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PGE	A	803	10/10	0.73	0.17	34,47,56,58	0
4	GOL	B	811	6/6	0.76	0.17	42,47,54,56	0
3	PGE	B	803	10/10	0.80	0.16	39,47,57,57	0
4	GOL	A	813	6/6	0.82	0.12	25,44,57,62	0
2	PEG	B	802	7/7	0.83	0.14	48,54,60,63	0
4	GOL	A	816	6/6	0.84	0.14	35,43,49,52	0
3	PGE	A	802	10/10	0.84	0.16	24,47,55,59	0
2	PEG	A	801	7/7	0.85	0.15	35,45,54,57	0
4	GOL	A	814	6/6	0.85	0.14	45,51,56,59	0
4	GOL	B	810	6/6	0.86	0.13	29,40,54,59	0
4	GOL	B	809	6/6	0.87	0.12	33,48,53,54	0
4	GOL	B	807	6/6	0.89	0.09	35,40,46,50	0
4	GOL	A	812	6/6	0.89	0.12	29,32,40,46	0
4	GOL	B	812	6/6	0.90	0.11	26,36,44,47	0
4	GOL	A	817	6/6	0.91	0.11	31,42,48,52	0
4	GOL	A	804	6/6	0.91	0.10	27,37,38,39	0
4	GOL	A	810	6/6	0.91	0.11	31,37,47,53	0
7	EPE	B	801	15/15	0.91	0.12	29,39,47,48	0
4	GOL	A	807	6/6	0.92	0.09	35,39,43,43	0
4	GOL	A	809	6/6	0.92	0.10	29,32,39,44	0
4	GOL	A	815	6/6	0.92	0.10	25,42,44,53	0
4	GOL	A	805	6/6	0.92	0.09	27,30,38,40	0
4	GOL	A	806	6/6	0.92	0.11	21,29,32,50	0
4	GOL	B	804	6/6	0.92	0.09	29,37,38,43	0
4	GOL	B	808	6/6	0.94	0.09	26,32,41,41	0
4	GOL	B	805	6/6	0.94	0.09	31,35,38,40	0
4	GOL	B	813	6/6	0.94	0.08	25,30,40,42	0
4	GOL	A	808	6/6	0.94	0.07	25,34,38,39	0
4	GOL	A	811	6/6	0.95	0.07	24,35,38,40	0
4	GOL	B	806	6/6	0.95	0.07	27,37,39,41	0
6	NA	A	819	1/1	0.97	0.08	30,30,30,30	0
8	PO4	B	815	5/5	0.97	0.10	27,30,39,50	0
5	MG	B	814	1/1	0.99	0.02	24,24,24,24	0
5	MG	A	818	1/1	0.99	0.02	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.