Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2024 – 10:09 AM EDT

PDB ID	:	8VA7
Title	:	Crystal structure of CapGH3a enzyme retrieved from capybara gut metagenome
Authors	:	Martins, M.P.; Vieira, P.S.; Morais, M.A.B.; Mandelli, F.; Chinaglia, M.; Lima, E.A.; Murakami, M.T.
Deposited on	:	2023-12-11
Resolution	:	2.60 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:

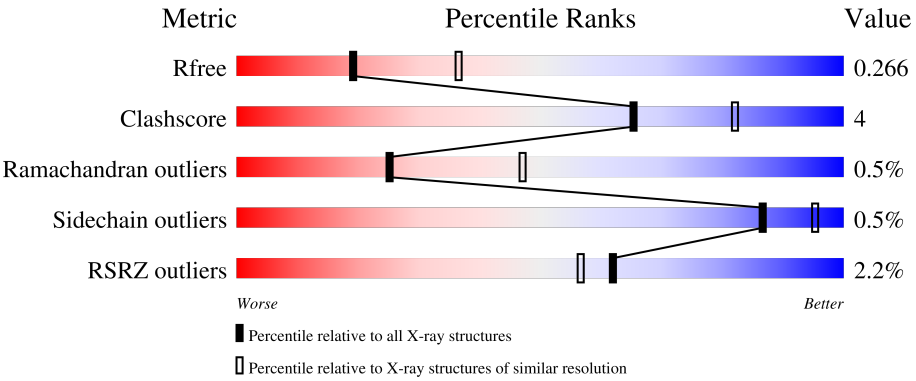
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

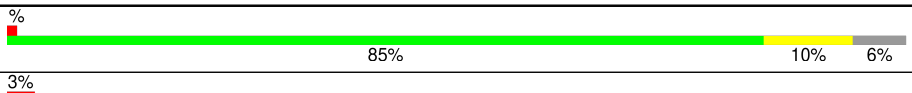
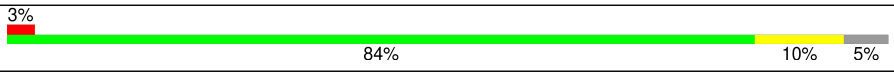
The reported resolution of this entry is 2.60 Å.

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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	A	745	
1	B	745	

2 Entry composition

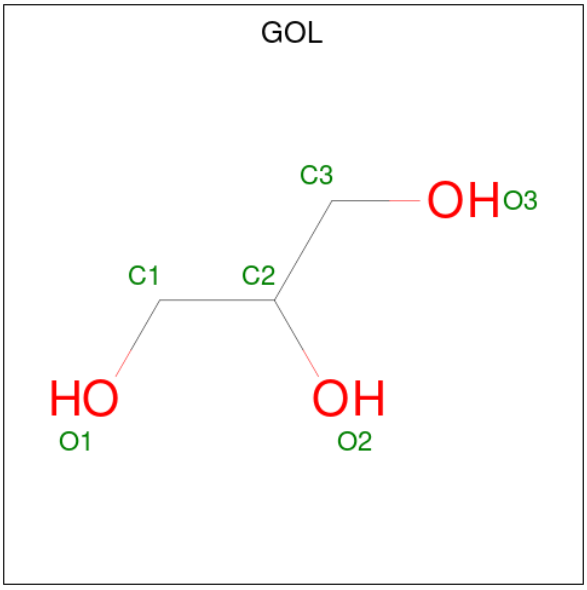
There are 6 unique types of molecules in this entry. The entry contains 11327 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

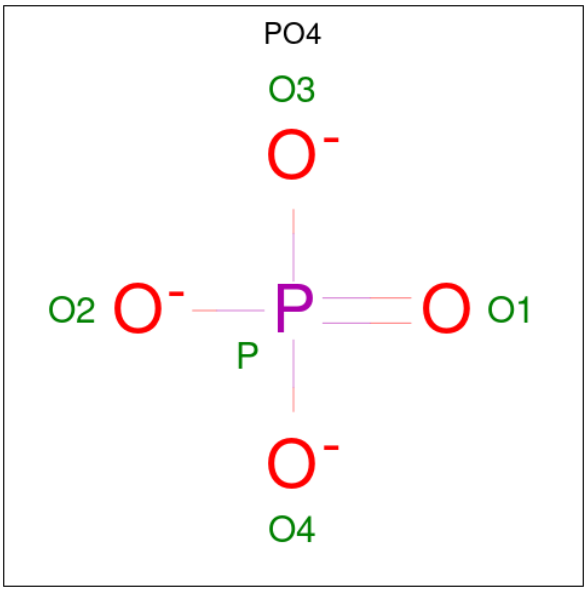
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	0	2	0
			5549	3487	1004	1039	19			
1	B	709	Total	C	N	O	S	0	1	0
			5574	3502	1013	1039	20			

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



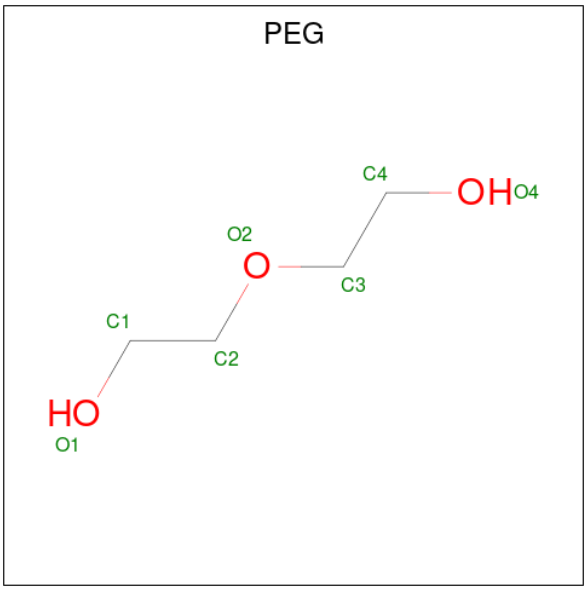
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



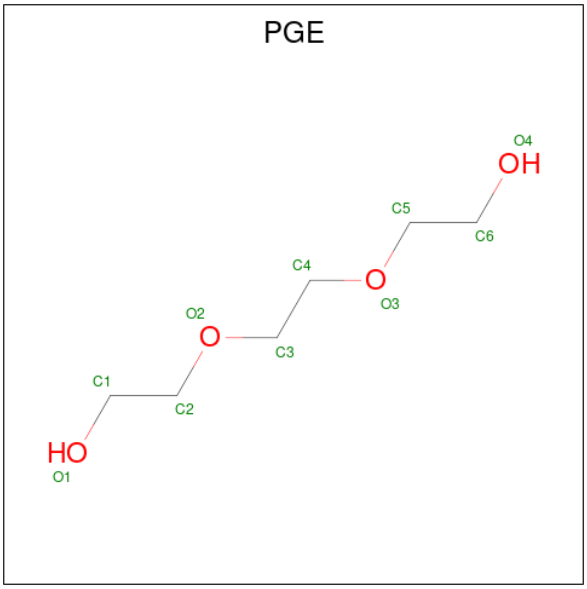
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 6 is water.

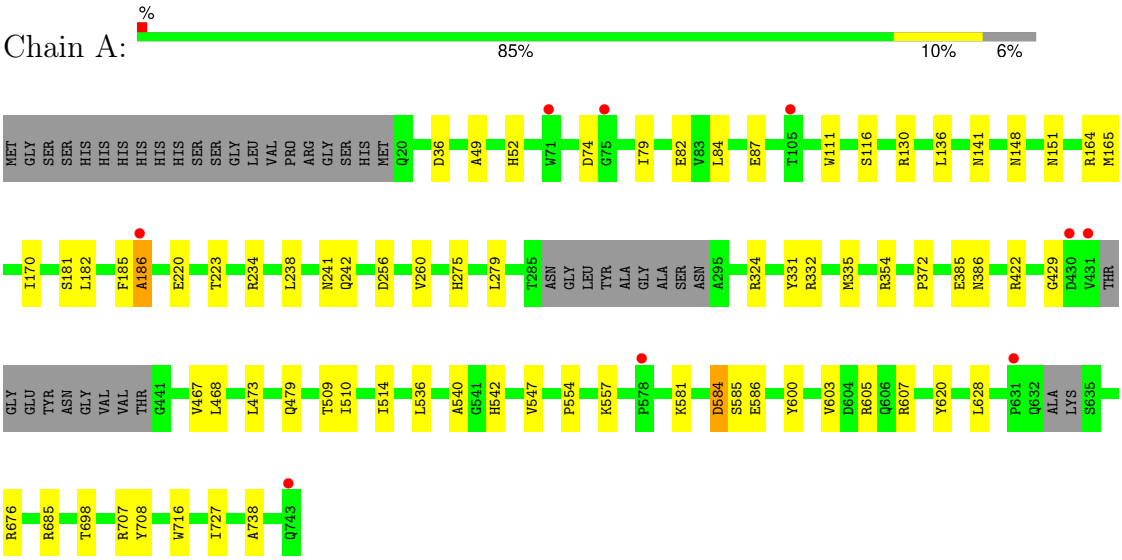
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	87	Total O 87 87	0	0
6	B	68	Total O 68 68	0	0

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.

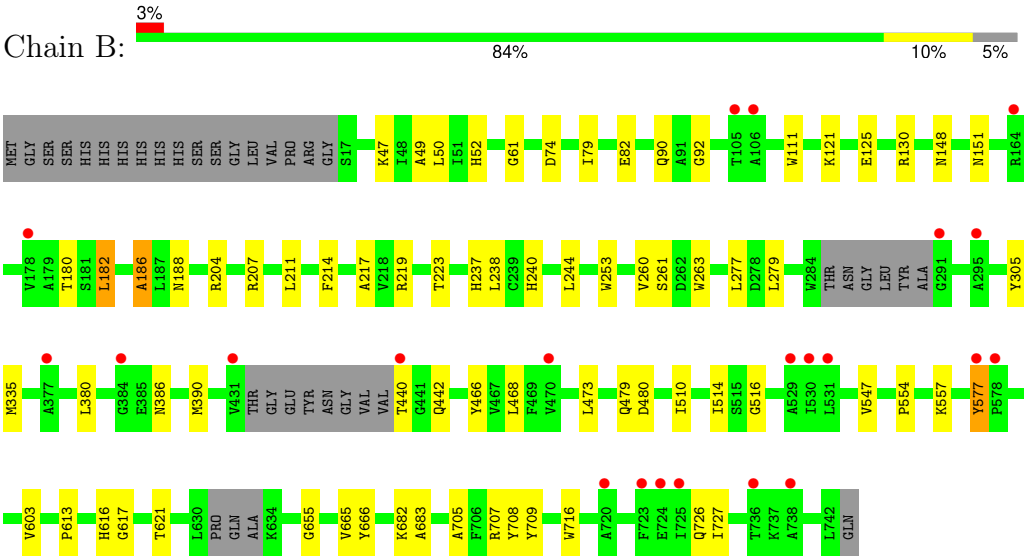
• Molecule 1: Glycoside hydrolase family 3

Chain A:



• Molecule 1: Glycoside hydrolase family 3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	135.61Å 132.87Å 99.22Å 90.00° 116.27° 90.00°	Depositor
Resolution (Å)	47.22 – 2.60 47.22 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (47.22-2.60) 96.5 (47.22-2.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.222 , 0.266 0.222 , 0.266	Depositor DCC
R_{free} test set	3985 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	51.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 5.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11327	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PEG, PO4, PGE

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	0.24	0/5671	0.49	0/7700
1	B	0.23	0/5696	0.50	0/7731
All	All	0.23	0/11367	0.49	0/15431

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	5549	0	5432	39	0
1	B	5574	0	5468	43	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	7	0	10	0	0
5	B	10	0	14	0	0
6	A	87	0	0	1	0
6	B	68	0	0	1	0
All	All	11327	0	10940	82	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 4.

All (82) 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:331:TYR:HA	1:B:335:MET:HB2	1.71	0.72
1:A:547:VAL:HG13	1:A:554:PRO:HG3	1.75	0.69
1:B:547:VAL:HG13	1:B:554:PRO:HG3	1.76	0.68
1:B:79:ILE:HG21	1:B:130:ARG:HG3	1.78	0.64
1:A:260:VAL:HG23	1:A:279:LEU:HB3	1.84	0.60
1:B:613:PRO:HD2	1:B:616:HIS:HB2	1.85	0.59
1:B:170:ILE:HA	1:B:180:THR:HG21	1.83	0.58
1:A:79:ILE:HG21	1:A:130:ARG:HG3	1.86	0.57
1:B:82:GLU:OE1	1:B:130:ARG:NH2	2.37	0.57
1:A:386:ASN:HB3	1:A:514:ILE:HD12	1.87	0.56
1:B:621:THR:HG23	1:B:655:GLY:HA3	1.86	0.56
1:B:90:GLN:HG2	1:B:92:GLY:H	1.71	0.55
1:B:682:LYS:HE2	1:B:705:ALA:HA	1.87	0.55
1:A:36:ASP:OD1	1:A:324:ARG:NH1	2.40	0.55
1:A:82:GLU:OE1	1:A:130:ARG:NH2	2.40	0.54
1:A:467:VAL:HB	1:A:509:THR:HA	1.90	0.54
1:A:141:ASN:ND2	3:A:802:PO4:O1	2.42	0.53
1:B:557:LYS:HD3	1:B:617:GLY:HA3	1.90	0.53
1:A:676:ARG:HH11	1:A:708:TYR:HB3	1.75	0.52
1:B:238:LEU:HD11	1:B:244:LEU:HD12	1.91	0.52
1:A:605:ARG:O	1:A:607:ARG:NH1	2.43	0.52
1:A:136:LEU:HD13	2:A:801:GOL:H11	1.91	0.51
1:A:628:LEU:HD23	1:A:738:ALA:HB3	1.91	0.51
1:B:386:ASN:HB3	1:B:514:ILE:HD12	1.91	0.51
1:A:234:ARG:NH1	6:A:903:HOH:O	2.44	0.51
1:B:390:MET:SD	1:B:440:THR:OG1	2.68	0.50
1:A:473:LEU:HB3	1:A:479:GLN:HB3	1.94	0.49
1:A:707:ARG:HD2	1:A:716:TRP:HB3	1.95	0.49
1:B:582:ARG:HB2	1:B:585:SER:HB3	1.95	0.49
1:A:242:GLN:HB3	1:A:275:HIS:CD2	2.48	0.48
1:B:170:ILE:HD13	1:B:223:THR:HB	1.94	0.48
1:B:600:TYR:HA	1:B:603:VAL:HG22	1.94	0.48
1:B:260:VAL:HG22	1:B:279:LEU:HB3	1.94	0.48
1:B:182:LEU:HD13	1:B:214:PHE:HD1	1.78	0.48
1:A:49:ALA:HA	1:A:52:HIS:CE1	2.49	0.48
1:B:207:ARG:HD2	1:B:211:LEU:HD12	1.96	0.47
1:A:600:TYR:HA	1:A:603:VAL:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TRP:NE1	1:B:557:LYS:HB2	2.30	0.46
1:B:468:LEU:HD23	1:B:510:ILE:HB	1.97	0.46
1:B:47:LYS:HB3	1:B:323:VAL:HG21	1.96	0.46
1:A:136:LEU:HA	1:A:181:SER:HB3	1.98	0.46
1:B:121:LYS:NZ	1:B:125:GLU:OE2	2.47	0.46
1:A:331:TYR:HA	1:A:335:MET:HB3	1.98	0.46
1:B:480:ASP:OD2	1:B:516:GLY:N	2.48	0.46
1:A:238:LEU:HA	1:A:241:ASN:HB2	1.98	0.45
1:A:584:ASP:OD1	1:A:585:SER:N	2.49	0.45
1:A:385:GLU:OE1	1:A:429:GLY:N	2.37	0.45
1:B:665:VAL:HB	1:B:683:ALA:HB3	1.99	0.45
1:B:148:ASN:HB3	1:B:151:ASN:ND2	2.33	0.44
1:B:49:ALA:HA	1:B:52:HIS:CE1	2.53	0.44
1:B:707:ARG:HD2	1:B:716:TRP:HB3	1.98	0.44
1:B:186:ALA:CB	1:B:238:LEU:HG	2.48	0.44
1:A:84:LEU:HB2	1:A:87:GLU:HB2	2.00	0.44
1:A:148:ASN:HB3	1:A:151:ASN:ND2	2.33	0.44
1:B:207:ARG:HG3	1:B:709:TYR:CZ	2.53	0.43
1:B:188:ASN:ND2	6:B:904:HOH:O	2.40	0.43
1:B:380:LEU:HD22	1:B:466:TYR:HB2	1.99	0.43
1:B:666:TYR:HB2	1:B:726:GLN:HB2	2.00	0.43
1:B:182:LEU:HD11	1:B:217:ALA:HB3	2.00	0.43
1:B:50:LEU:HD12	1:B:61:GLY:HA2	2.01	0.43
1:A:111:TRP:NE1	1:A:557:LYS:HB2	2.34	0.43
1:A:372:PRO:HG3	1:A:620:TYR:CD2	2.54	0.43
1:B:237:HIS:HB2	1:B:240:HIS:CE1	2.54	0.43
1:A:170:ILE:HD13	1:A:223:THR:HB	2.01	0.43
1:A:685:ARG:NH2	1:A:698:THR:O	2.52	0.43
1:B:219:ARG:HH11	1:B:253:TRP:HA	1.83	0.43
1:A:186:ALA:CB	1:A:238:LEU:HG	2.49	0.42
1:B:204:ARG:HH12	1:B:708:TYR:HD2	1.67	0.42
1:B:390:MET:HG3	1:B:442:GLN:NE2	2.34	0.42
1:B:261:SER:HB3	1:B:277:LEU:HD11	2.01	0.42
1:B:473:LEU:HB3	1:B:479:GLN:HB3	2.01	0.42
1:A:628:LEU:HD13	1:A:727:ILE:HD12	2.02	0.41
1:B:167:VAL:HB	1:B:168:PRO:HD3	2.02	0.41
1:A:116:SER:HB2	1:A:165:MET:HE3	2.02	0.41
1:A:256:ASP:OD2	1:A:332:ARG:NH2	2.41	0.41
1:B:665:VAL:HG22	1:B:727:ILE:HG12	2.02	0.41
1:A:164:ARG:NH2	1:A:220:GLU:OE1	2.39	0.41
1:A:581:LYS:HE2	1:A:586:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:LEU:HB2	1:A:540:ALA:HA	2.03	0.41
1:A:676:ARG:NH1	1:A:708:TYR:HB3	2.35	0.41
1:A:468:LEU:HD23	1:A:510:ILE:HB	2.01	0.41
1:A:354:ARG:CZ	1:A:542:HIS:HB3	2.51	0.41

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	698/745 (94%)	658 (94%)	37 (5%)	3 (0%)	30	52
1	B	702/745 (94%)	659 (94%)	39 (6%)	4 (1%)	22	43
All	All	1400/1490 (94%)	1317 (94%)	76 (5%)	7 (0%)	25	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	TRP
1	A	182	LEU
1	A	185	PHE
1	A	186	ALA
1	B	182	LEU
1	B	186	ALA
1	B	577	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	572/601 (95%)	569 (100%)	3 (0%)	86 95
1	B	574/601 (96%)	571 (100%)	3 (0%)	86 95
All	All	1146/1202 (95%)	1140 (100%)	6 (0%)	86 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	422	ARG
1	A	584	ASP
1	B	74	ASP
1	B	305	TYR
1	B	577	TYR

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)

8 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	$\#\|Z\| > 2$
5	PGE	B	801	-	9,9,9	0.32	0	8,8,8	0.35	0
3	PO4	B	803	-	4,4,4	0.94	0	6,6,6	0.44	0
3	PO4	B	804	-	4,4,4	0.96	0	6,6,6	0.47	0
4	PEG	A	804	-	6,6,6	0.13	0	5,5,5	0.08	0
2	GOL	B	802	-	5,5,5	0.93	0	5,5,5	1.09	0
3	PO4	A	802	-	4,4,4	0.99	0	6,6,6	0.46	0
2	GOL	A	801	-	5,5,5	0.91	0	5,5,5	1.08	0
3	PO4	A	803	-	4,4,4	0.96	0	6,6,6	0.47	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
5	PGE	B	801	-	-	5/7/7/7	-
2	GOL	B	802	-	-	0/4/4/4	-
4	PEG	A	804	-	-	0/4/4/4	-
2	GOL	A	801	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	PGE	O1-C1-C2-O2
5	B	801	PGE	O2-C3-C4-O3
5	B	801	PGE	C4-C3-O2-C2
5	B	801	PGE	C6-C5-O3-C4
5	B	801	PGE	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PO4	1	0
2	A	801	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

6.1 Protein, DNA and RNA chains

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	A	704/745 (94%)	0.21	9 (1%) 74 70	32, 49, 69, 100	2 (0%)
1	B	709/745 (95%)	0.39	22 (3%) 51 46	26, 54, 81, 103	1 (0%)
All	All	1413/1490 (94%)	0.30	31 (2%) 62 57	26, 52, 77, 103	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	THR	3.9
1	B	384	GLY	3.8
1	B	440	THR	3.7
1	B	530	ILE	3.6
1	B	431	VAL	3.3
1	A	431	VAL	3.0
1	A	75	GLY	3.0
1	B	578	PRO	2.9
1	B	531	LEU	2.8
1	B	105	THR	2.7
1	B	738	ALA	2.7
1	A	186	ALA	2.7
1	B	106	ALA	2.6
1	A	578	PRO	2.6
1	B	725	ILE	2.6
1	B	470	VAL	2.5
1	B	724	GLU	2.5
1	A	631	PRO	2.3
1	B	377	ALA	2.3
1	B	164[A]	ARG	2.2
1	B	291	GLY	2.2
1	A	743	GLN	2.2
1	B	295	ALA	2.2
1	A	430[A]	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	TRP	2.1
1	B	736	THR	2.1
1	B	577	TYR	2.1
1	B	723	PHE	2.0
1	B	529	ALA	2.0
1	B	178	VAL	2.0
1	B	720	ALA	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	B-factors(Å^2)	Q<0.9
4	PEG	A	804	7/7	0.72	0.21	42,48,59,59	0
2	GOL	B	802	6/6	0.80	0.14	68,72,75,80	0
5	PGE	B	801	10/10	0.83	0.19	41,46,55,60	0
3	PO4	B	803	5/5	0.87	0.25	53,53,68,85	0
3	PO4	A	802	5/5	0.89	0.19	53,53,65,75	0
2	GOL	A	801	6/6	0.89	0.14	49,57,58,65	0
3	PO4	B	804	5/5	0.91	0.21	58,59,80,86	0
3	PO4	A	803	5/5	0.92	0.21	46,50,60,67	0

6.5 Other polymers (i)

There are no such residues in this entry.