



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:13 PM GMT

PDB ID : 4KTR
Title : Crystal structure of 2-O-alpha-glucosylglycerol phosphorylase in complex with isofagomine and glycerol
Authors : Touhara, K.K.; Nihira, T.; Kitaoka, M.; Nakai, H.; Fushinobu, S.
Deposited on : 2013-05-21
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

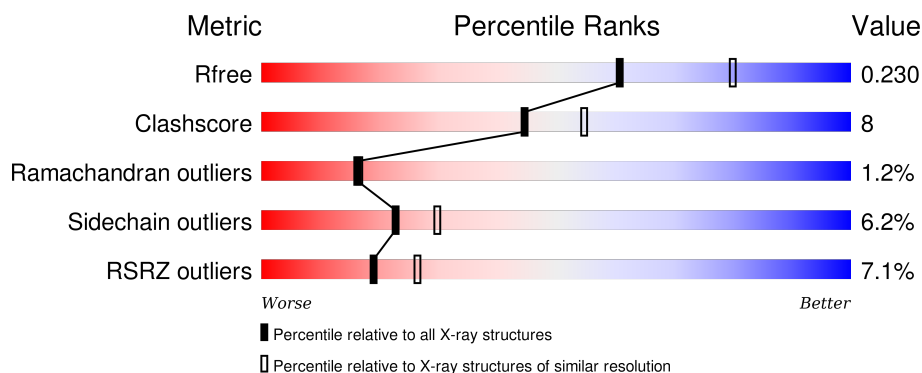
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	769	<div> <div>2%</div> <div>82%</div> <div>14%</div> <div>...</div> </div>
1	B	769	<div> <div>5%</div> <div>81%</div> <div>16%</div> <div>...</div> </div>
1	C	769	<div> <div>4%</div> <div>80%</div> <div>16%</div> <div>...</div> </div>
1	D	769	<div> <div>4%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	E	769	<div> <div>15%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	769	
1	G	769	
1	H	769	

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
10	PE4	C	805	-	-	-	X
11	PE5	H	808	-	-	-	X
2	IFM	E	801	-	-	-	X
2	IFM	F	801	-	-	-	X
2	IFM	G	801	-	-	-	X
2	IFM	H	801	-	-	-	X
3	1PE	A	802	-	-	-	X
3	1PE	C	801	-	-	-	X
3	1PE	E	802	-	-	-	X
4	GOL	A	803	-	-	-	X
4	GOL	A	811	-	-	-	X
4	GOL	B	804	-	-	X	-
4	GOL	B	805	-	-	-	X
4	GOL	B	806	-	-	-	X
4	GOL	B	807	-	-	-	X
4	GOL	D	802	-	-	-	X
4	GOL	D	804	-	-	-	X
4	GOL	D	809	-	-	X	X
4	GOL	E	804	-	-	-	X
4	GOL	G	802	-	-	-	X
4	GOL	G	804	-	-	-	X
4	GOL	H	802	-	-	-	X
4	GOL	H	804	-	-	-	X
4	GOL	H	805	-	-	-	X
4	GOL	H	807	-	-	X	-
5	P6G	E	803	-	-	-	X
6	PGE	A	812	-	-	X	X
6	PGE	F	806	-	-	-	X
6	PGE	G	805	-	-	-	X
8	PG4	B	801	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 51264 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 65 central catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	0	0
			6093	3850	1036	1185	22			
1	B	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	C	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	D	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	E	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	F	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			
1	G	762	Total	C	N	O	S	0	0	0
			6093	3850	1036	1185	22			
1	H	761	Total	C	N	O	S	0	0	0
			6085	3844	1035	1184	22			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
A	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
A	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
A	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
A	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
B	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
B	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
B	764	HIS	-	EXPRESSION TAG	UNP D6XZ22

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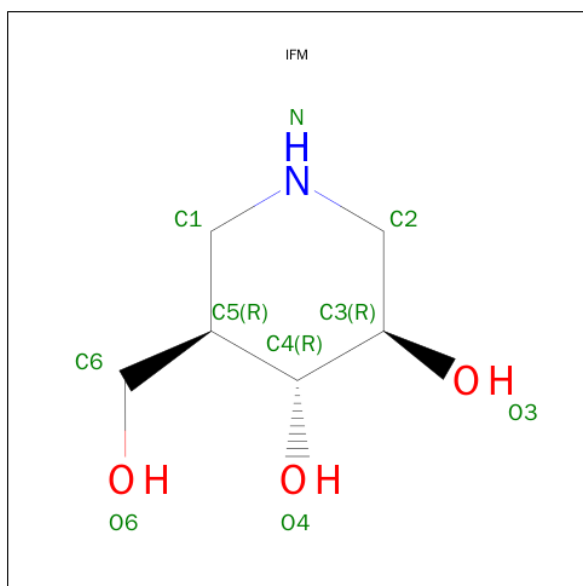
Chain	Residue	Modelled	Actual	Comment	Reference
B	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
B	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
C	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
C	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
C	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
C	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
D	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
D	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
D	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
D	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
E	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
E	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
E	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
E	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
F	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
F	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
F	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
F	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22

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Chain	Residue	Modelled	Actual	Comment	Reference
G	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
G	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
G	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
G	769	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	475	GLN	GLU	ENGINEERED MUTATION	UNP D6XZ22
H	762	LEU	-	EXPRESSION TAG	UNP D6XZ22
H	763	GLU	-	EXPRESSION TAG	UNP D6XZ22
H	764	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	765	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	766	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	767	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	768	HIS	-	EXPRESSION TAG	UNP D6XZ22
H	769	HIS	-	EXPRESSION TAG	UNP D6XZ22

- Molecule 2 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: $C_6H_{13}NO_3$).



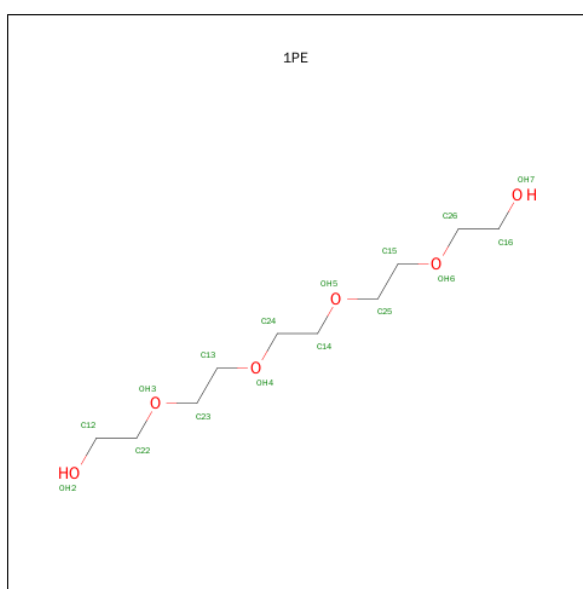
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	1	3		
2	D	1	Total	C	N	O	0	0
			10	6	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			10	6	1	3		
2	F	1	Total	C	N	O	0	0
			10	6	1	3		
2	G	1	Total	C	N	O	0	0
			10	6	1	3		
2	H	1	Total	C	N	O	0	0
			10	6	1	3		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	C	1	Total	C	O	0	0
			16	10	6		
3	E	1	Total	C	O	0	0
			16	10	6		

- 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		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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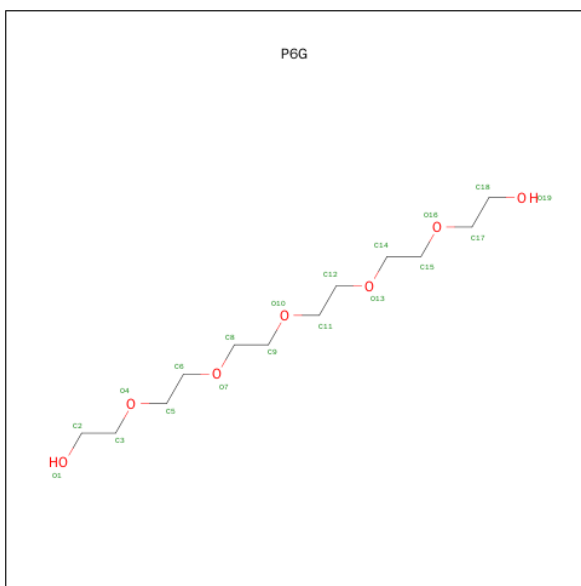
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

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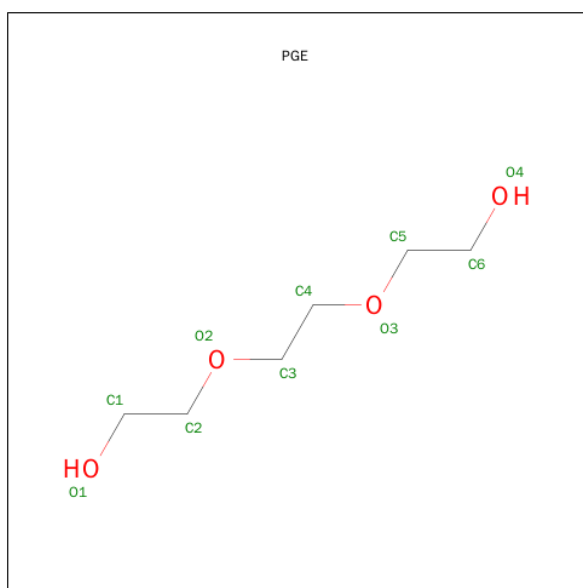
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			19	12	7		
5	E	1	Total	C	O	0	0
			19	12	7		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

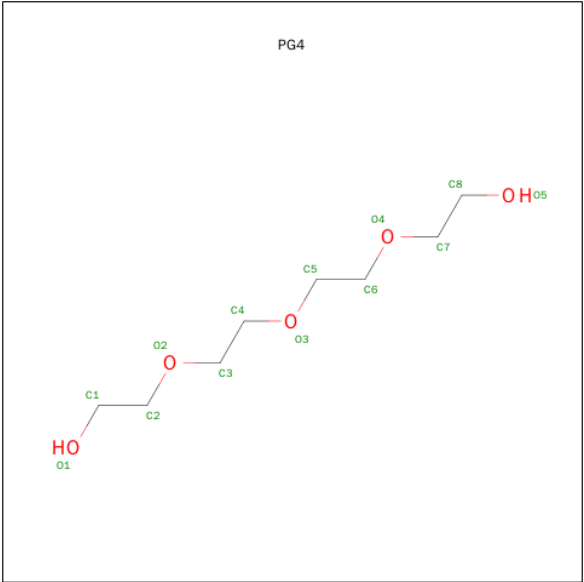


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		
6	F	1	Total	C	O	0	0
			10	6	4		
6	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

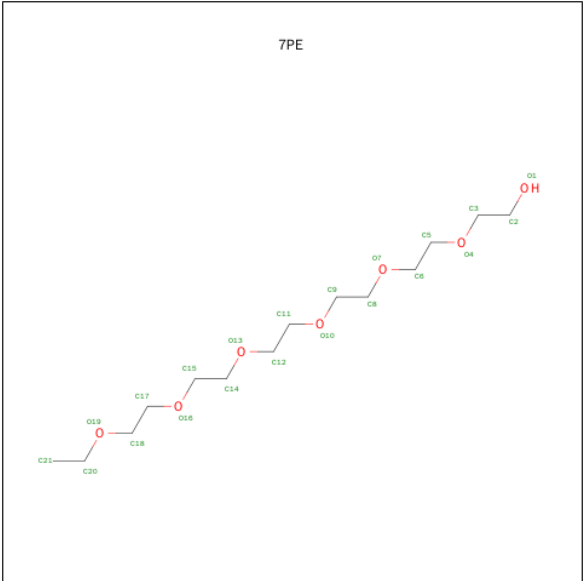
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Ca	0	0
			1	1		
7	D	2	Total	Ca	0	0
			2	2		
7	E	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		
7	A	1	Total	Ca	0	0
			1	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



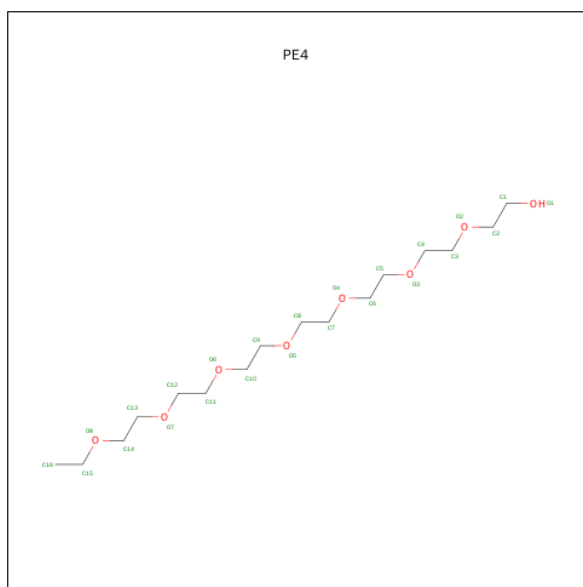
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		
8	D	1	Total	C	O	0	0
			13	8	5		
8	F	1	Total	C	O	0	0
			13	8	5		
8	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 2-(2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (three-letter code: 7PE) (formula: C₁₄H₃₀O₇).



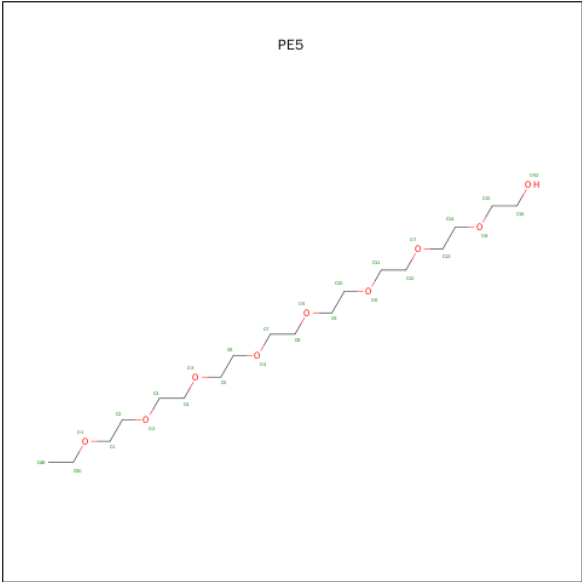
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			21	14	7		
9	D	1	Total	C	O	0	0
			21	14	7		

- Molecule 10 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			24	16	8		

- Molecule 11 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (three-letter code: PE5) (formula: C₁₈H₃₈O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total	C	O	0	0
			27	18	9		

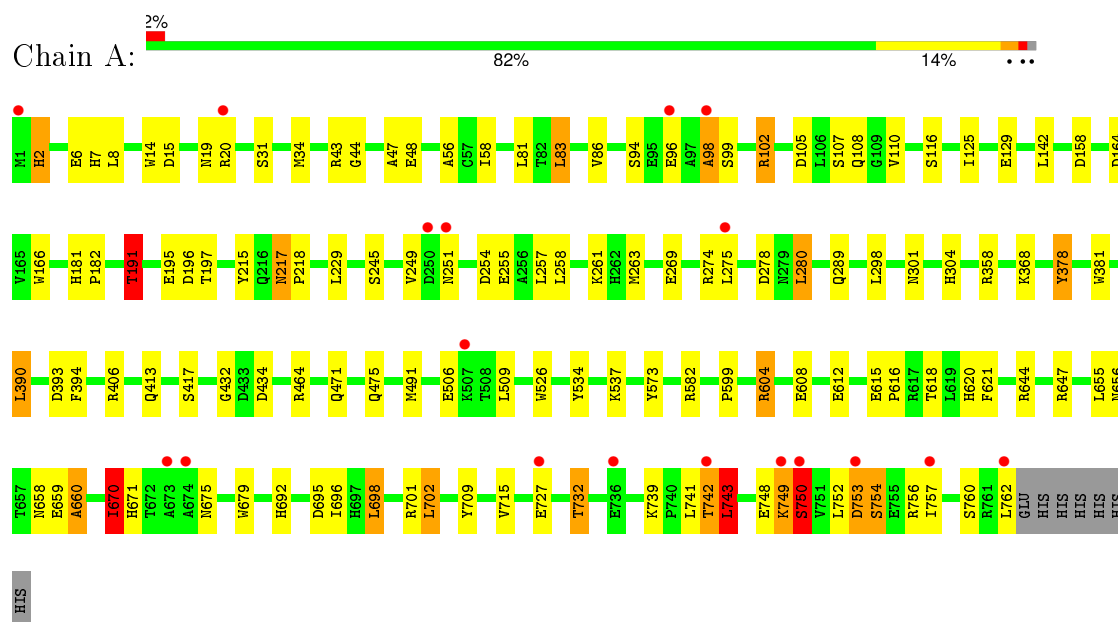
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	182	Total	O	0	0
			182	182		
12	B	303	Total	O	0	0
			303	303		
12	C	286	Total	O	0	0
			286	286		
12	D	348	Total	O	0	0
			348	348		
12	E	185	Total	O	0	0
			185	185		
12	F	247	Total	O	0	0
			247	247		
12	G	197	Total	O	0	0
			197	197		
12	H	218	Total	O	0	0
			218	218		

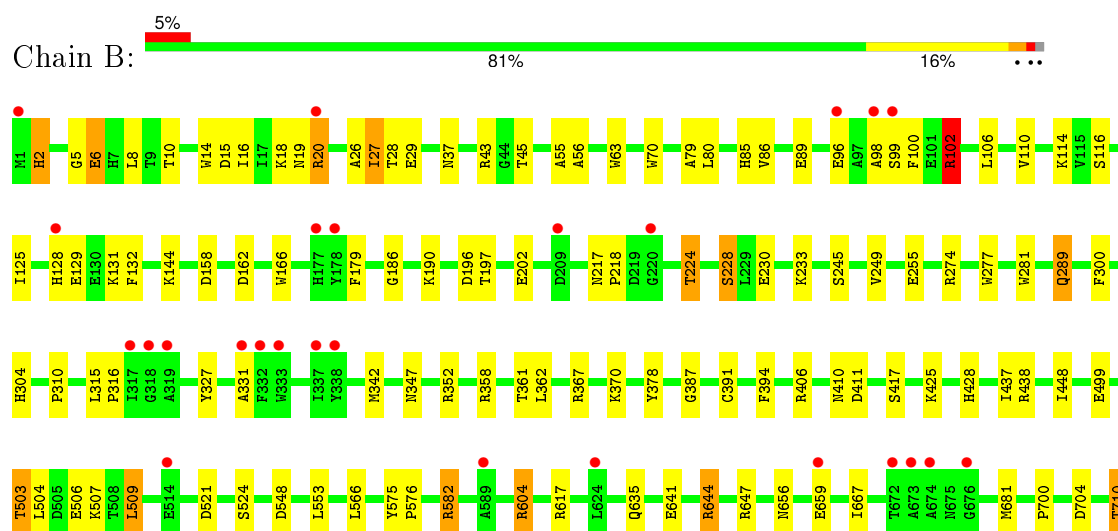
3 Residue-property plots [i](#)

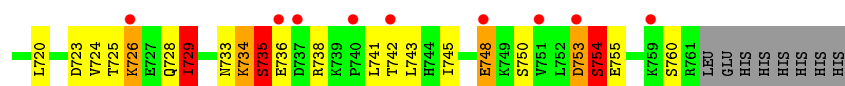
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 65 central catalytic



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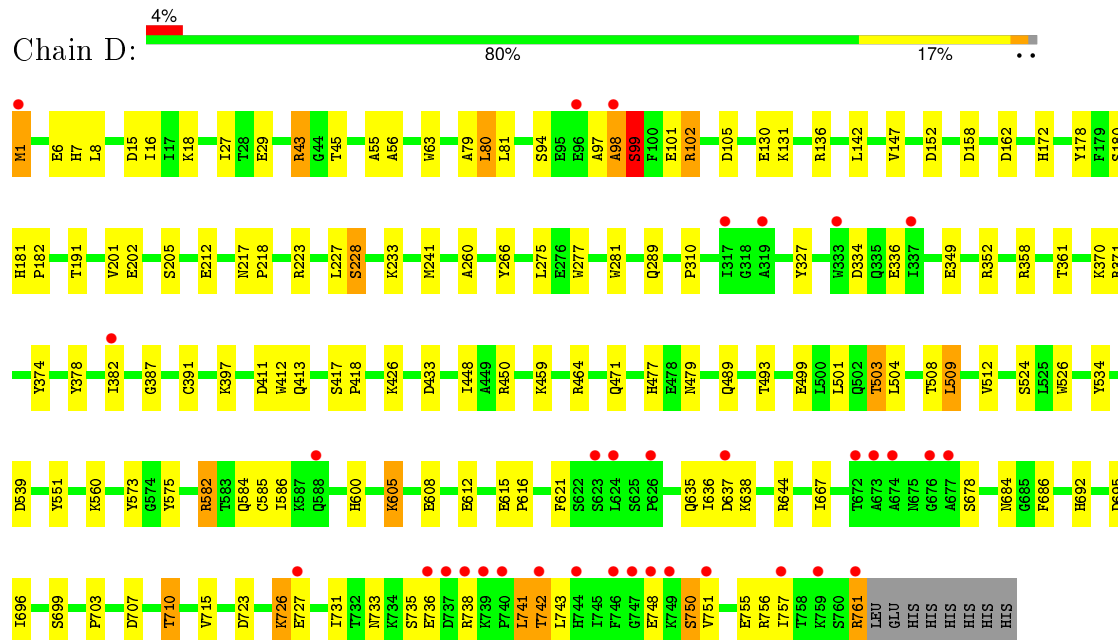




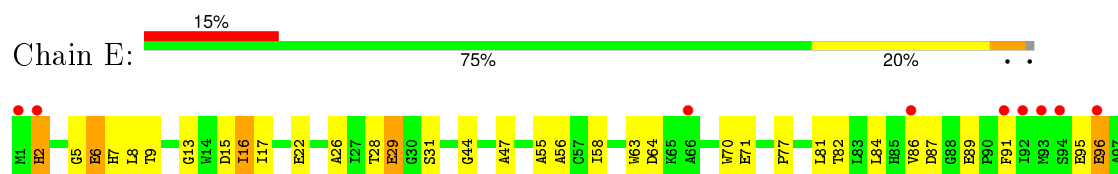
- Molecule 1: Glycoside hydrolase family 65 central catalytic

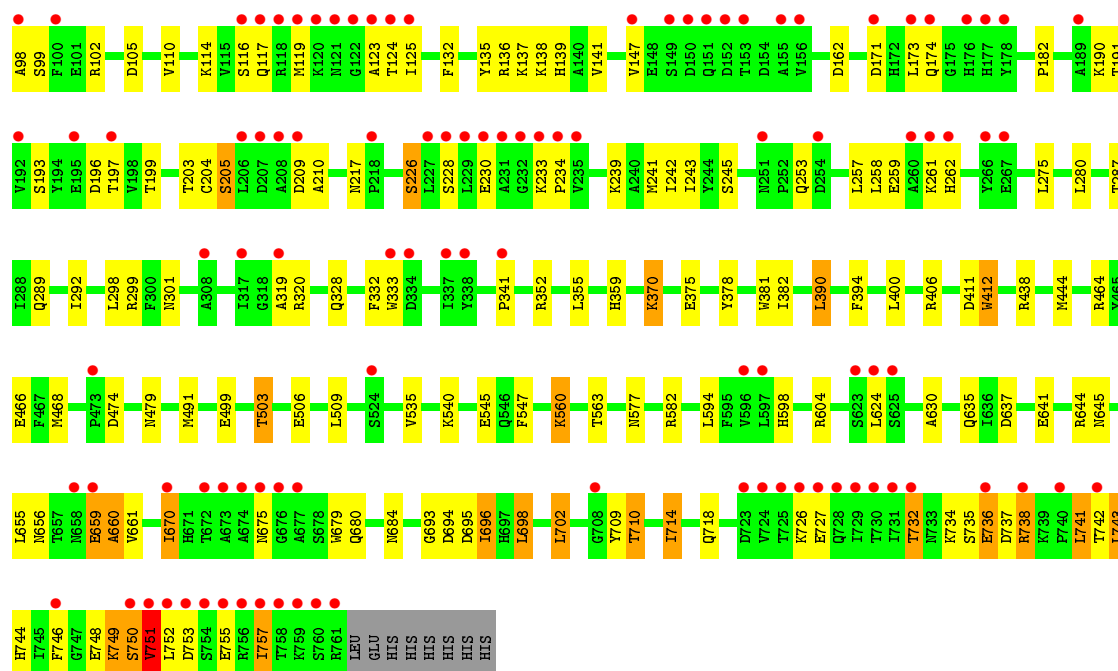


- Molecule 1: Glycoside hydrolase family 65 central catalytic

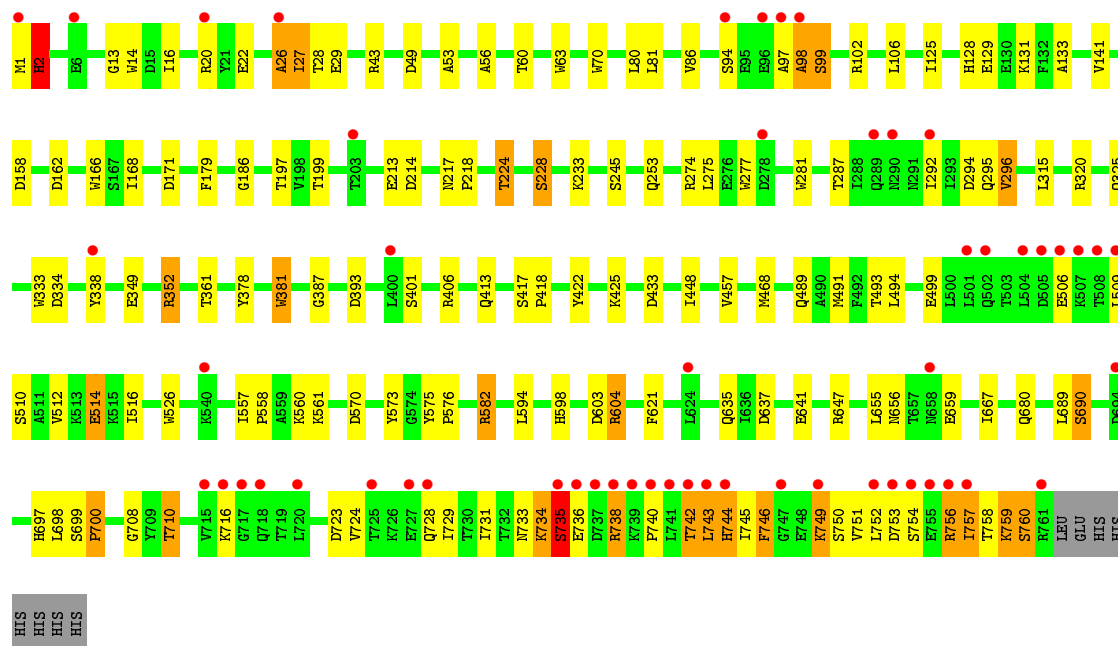
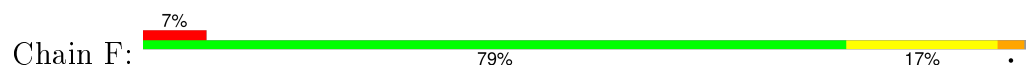


- Molecule 1: Glycoside hydrolase family 65 central catalytic

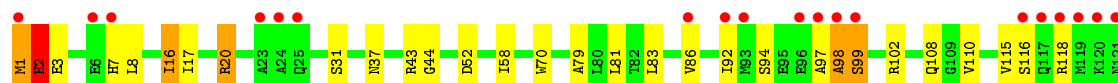
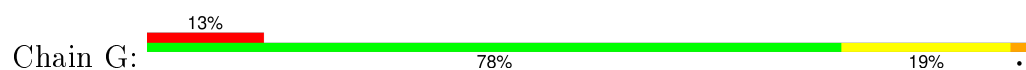


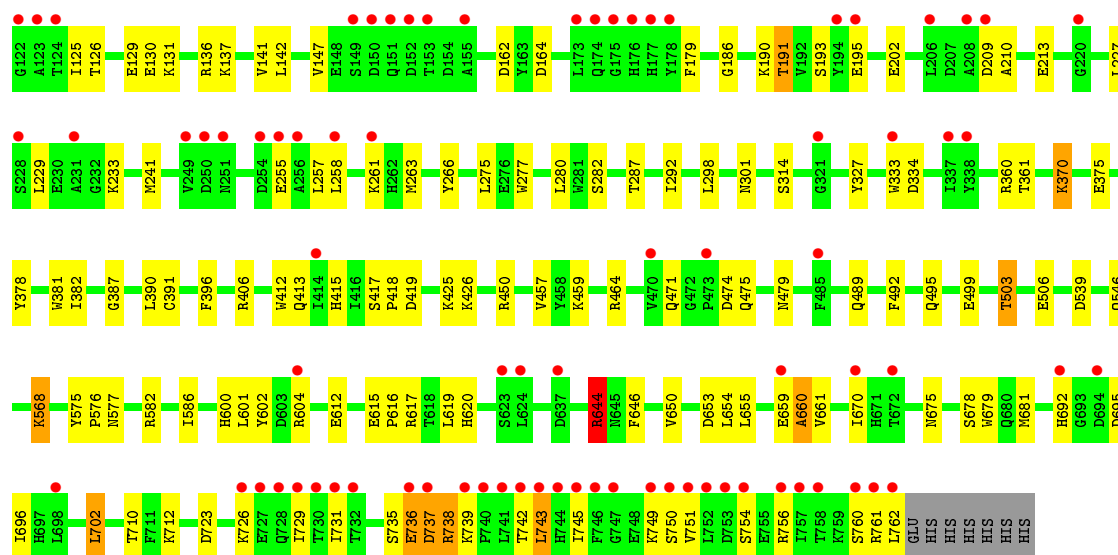


- Molecule 1: Glycoside hydrolase family 65 central catalytic

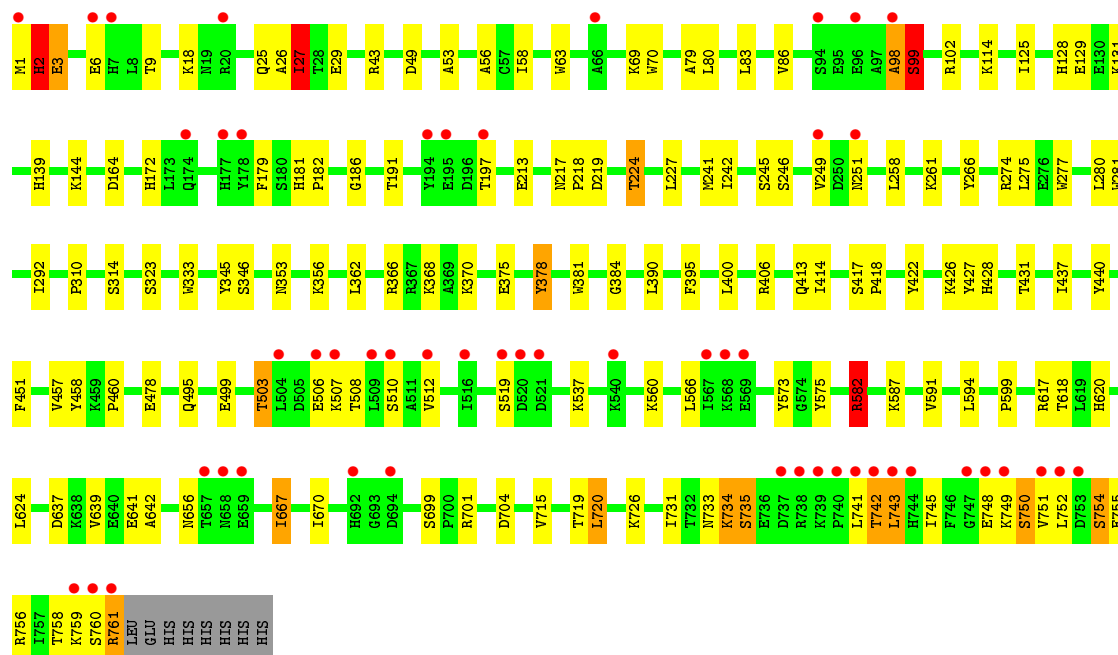
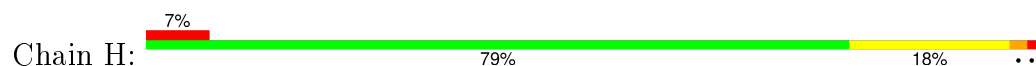


- Molecule 1: Glycoside hydrolase family 65 central catalytic





● Molecule 1: Glycoside hydrolase family 65 central catalytic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.00Å 263.21Å 138.79Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	48.99 – 2.30 48.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.99-2.30) 99.8 (48.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.167 , 0.228 0.168 , 0.230	Depositor DCC
R_{free} test set	16702 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 331431 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51264	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, PGE, PE4, PE5, CA, 1PE, PG4, P6G, IFM, 7PE

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	0.99	6/6236 (0.1%)	0.98	14/8456 (0.2%)
1	B	0.97	8/6228 (0.1%)	0.99	26/8445 (0.3%)
1	C	0.99	3/6228 (0.0%)	0.99	20/8445 (0.2%)
1	D	1.01	5/6228 (0.1%)	1.00	21/8445 (0.2%)
1	E	0.85	6/6228 (0.1%)	0.90	15/8445 (0.2%)
1	F	0.87	9/6228 (0.1%)	0.91	4/8445 (0.0%)
1	G	0.83	4/6236 (0.1%)	0.88	8/8456 (0.1%)
1	H	0.84	3/6228 (0.0%)	0.87	4/8445 (0.0%)
All	All	0.92	44/49840 (0.1%)	0.94	112/67582 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	2
1	F	0	1
1	G	0	1
All	All	0	6

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	TRP	CD2-CE2	7.43	1.50	1.41
1	B	754	SER	CB-OG	6.83	1.51	1.42
1	E	70	TRP	CD2-CE2	6.81	1.49	1.41
1	F	333	TRP	CD2-CE2	6.40	1.49	1.41
1	F	63	TRP	CD2-CE2	6.39	1.49	1.41

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ARG	NE-CZ-NH2	12.77	126.69	120.30
1	D	102	ARG	NE-CZ-NH1	-11.92	114.34	120.30
1	A	670	ILE	CG1-CB-CG2	-11.80	85.43	111.40
1	E	438	ARG	NE-CZ-NH1	-9.91	115.35	120.30
1	B	644	ARG	NE-CZ-NH1	9.13	124.86	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	HIS	Peptide
1	A	748	GLU	Peptide
1	C	1	MET	Peptide
1	C	694	ASP	Peptide
1	F	26	ALA	Peptide

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	6093	0	5855	81	0
1	B	6085	0	5844	94	0
1	C	6085	0	5844	88	0
1	D	6085	0	5844	76	0
1	E	6085	0	5844	108	0
1	F	6085	0	5844	113	0
1	G	6093	0	5855	96	0
1	H	6085	0	5844	104	0
2	A	10	0	13	4	0
2	D	10	0	12	3	0
2	E	10	0	13	0	0
2	F	10	0	13	2	0
2	G	10	0	13	3	0
2	H	10	0	13	1	0
3	A	16	0	22	0	0
3	C	16	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	16	0	22	2	0
4	A	48	0	64	12	0
4	B	36	0	47	9	0
4	C	36	0	48	2	0
4	D	54	0	72	14	0
4	E	24	0	32	1	0
4	F	18	0	24	2	0
4	G	18	0	24	4	0
4	H	30	0	40	10	0
5	A	19	0	26	3	0
5	E	19	0	26	5	0
6	A	10	0	14	7	0
6	C	10	0	14	0	0
6	F	10	0	14	2	0
6	G	10	0	14	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	2	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
8	B	13	0	18	1	0
8	D	13	0	18	1	0
8	F	13	0	18	0	0
8	H	13	0	18	1	0
9	B	21	0	30	5	0
9	D	21	0	30	3	0
10	C	24	0	34	6	0
11	H	27	0	38	12	0
12	A	182	0	0	8	0
12	B	303	0	0	8	0
12	C	286	0	0	10	0
12	D	348	0	0	11	0
12	E	185	0	0	8	0
12	F	247	0	0	13	0
12	G	197	0	0	3	0
12	H	218	0	0	7	0
All	All	51264	0	47580	765	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 8.

The worst 5 of 765 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)
2:D:801:IFM:H2C2	12:D:1243:HOH:O	1.38	1.23
2:A:801:IFM:H2C2	12:A:917:HOH:O	1.35	1.21
1:B:352:ARG:HD3	12:B:1019:HOH:O	1.45	1.17
1:A:278:ASP:HB3	12:A:1031:HOH:O	1.45	1.14
1:F:756:ARG:HH11	1:F:756:ARG:HG3	1.09	1.12

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	760/769 (99%)	721 (95%)	29 (4%)	10 (1%)	15	15
1	B	759/769 (99%)	720 (95%)	33 (4%)	6 (1%)	24	27
1	C	759/769 (99%)	728 (96%)	25 (3%)	6 (1%)	24	27
1	D	759/769 (99%)	723 (95%)	34 (4%)	2 (0%)	46	57
1	E	759/769 (99%)	696 (92%)	48 (6%)	15 (2%)	9	7
1	F	759/769 (99%)	701 (92%)	44 (6%)	14 (2%)	11	9
1	G	760/769 (99%)	718 (94%)	31 (4%)	11 (1%)	14	13
1	H	759/769 (99%)	715 (94%)	35 (5%)	9 (1%)	16	16
All	All	6074/6152 (99%)	5722 (94%)	279 (5%)	73 (1%)	16	16

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	THR
1	A	750	SER
1	A	754	SER
1	B	6	GLU
1	B	27	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/658 (99%)	616 (95%)	35 (5%)	27	36
1	B	650/658 (99%)	615 (95%)	35 (5%)	27	36
1	C	650/658 (99%)	609 (94%)	41 (6%)	22	29
1	D	650/658 (99%)	615 (95%)	35 (5%)	27	36
1	E	650/658 (99%)	598 (92%)	52 (8%)	15	18
1	F	650/658 (99%)	609 (94%)	41 (6%)	22	29
1	G	651/658 (99%)	600 (92%)	51 (8%)	16	19
1	H	650/658 (99%)	616 (95%)	34 (5%)	29	38
All	All	5202/5264 (99%)	4878 (94%)	324 (6%)	23	30

5 of 324 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2	HIS
1	E	661	VAL
1	H	274	ARG
1	E	89	GLU
1	E	261	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	289	GLN
1	E	697	HIS
1	G	429	GLN
1	C	680	GLN
1	D	429	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 74 ligands modelled in this entry, 7 are monoatomic - leaving 67 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	$\# Z > 2$
2	IFM	A	801	-	9,10,10	1.68	3 (33%)	9,13,13	3.88	3 (33%)
3	1PE	A	802	-	15,15,15	0.73	0	14,14,14	0.70	0
4	GOL	A	803	-	5,5,5	0.56	0	5,5,5	1.08	0
4	GOL	A	804	-	5,5,5	0.80	0	5,5,5	2.03	2 (40%)
4	GOL	A	805	-	5,5,5	0.24	0	5,5,5	0.63	0
5	P6G	A	806	-	18,18,18	0.60	0	17,17,17	0.82	0
4	GOL	A	807	-	5,5,5	0.53	0	5,5,5	1.06	0
4	GOL	A	808	-	5,5,5	0.45	0	5,5,5	0.67	0
4	GOL	A	809	-	5,5,5	0.48	0	5,5,5	0.45	0
4	GOL	A	810	-	5,5,5	0.53	0	5,5,5	0.88	0
4	GOL	A	811	-	5,5,5	0.49	0	5,5,5	1.19	0
6	PGE	A	812	-	9,9,9	0.56	0	8,8,8	0.43	0
8	PG4	B	801	-	12,12,12	0.57	0	11,11,11	0.45	0
9	7PE	B	802	-	20,20,20	0.62	0	19,19,19	0.98	1 (5%)
4	GOL	B	803	-	5,5,5	0.56	0	5,5,5	1.64	1 (20%)
4	GOL	B	804	-	5,5,5	0.69	0	5,5,5	1.44	1 (20%)
4	GOL	B	805	-	5,5,5	0.48	0	5,5,5	0.89	0
4	GOL	B	806	-	5,5,5	0.27	0	5,5,5	0.52	0
4	GOL	B	807	-	5,5,5	0.54	0	5,5,5	0.89	0
4	GOL	B	808	-	5,5,5	0.61	0	5,5,5	1.90	1 (20%)
3	1PE	C	801	-	15,15,15	0.66	0	14,14,14	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	802	-	5,5,5	0.49	0	5,5,5	0.39	0
4	GOL	C	803	-	5,5,5	0.27	0	5,5,5	1.21	1 (20%)
4	GOL	C	804	-	5,5,5	0.41	0	5,5,5	1.27	1 (20%)
10	PE4	C	805	-	23,23,23	0.92	0	22,22,22	1.31	2 (9%)
4	GOL	C	806	-	5,5,5	0.61	0	5,5,5	0.77	0
6	PGE	C	807	-	9,9,9	0.46	0	8,8,8	0.85	0
4	GOL	C	808	-	5,5,5	0.43	0	5,5,5	0.65	0
4	GOL	C	809	-	5,5,5	0.61	0	5,5,5	2.23	1 (20%)
2	IFM	D	801	-	9,10,10	2.28	5 (55%)	9,13,13	3.68	7 (77%)
4	GOL	D	802	-	5,5,5	0.47	0	5,5,5	0.68	0
8	PG4	D	803	-	12,12,12	0.60	0	11,11,11	0.61	0
4	GOL	D	804	-	5,5,5	0.35	0	5,5,5	0.37	0
4	GOL	D	805	-	5,5,5	0.14	0	5,5,5	0.90	0
4	GOL	D	806	-	5,5,5	0.71	0	5,5,5	1.07	0
4	GOL	D	807	-	5,5,5	0.32	0	5,5,5	0.50	0
9	7PE	D	808	-	20,20,20	0.74	0	19,19,19	1.44	3 (15%)
4	GOL	D	809	-	5,5,5	0.37	0	5,5,5	1.29	0
4	GOL	D	810	-	5,5,5	0.36	0	5,5,5	1.77	1 (20%)
4	GOL	D	811	-	5,5,5	0.36	0	5,5,5	0.29	0
4	GOL	D	812	-	5,5,5	1.34	0	5,5,5	1.87	2 (40%)
2	IFM	E	801	-	9,10,10	1.50	2 (22%)	9,13,13	3.14	4 (44%)
3	1PE	E	802	-	15,15,15	0.71	0	14,14,14	0.39	0
5	P6G	E	803	-	18,18,18	0.66	0	17,17,17	0.78	0
4	GOL	E	804	-	5,5,5	0.22	0	5,5,5	0.60	0
4	GOL	E	805	-	5,5,5	0.37	0	5,5,5	0.23	0
4	GOL	E	806	-	5,5,5	0.48	0	5,5,5	0.79	0
4	GOL	E	807	-	5,5,5	0.23	0	5,5,5	0.88	0
2	IFM	F	801	-	9,10,10	1.36	1 (11%)	9,13,13	3.25	3 (33%)
4	GOL	F	802	-	5,5,5	0.29	0	5,5,5	0.74	0
8	PG4	F	803	-	12,12,12	0.55	0	11,11,11	0.49	0
4	GOL	F	804	-	5,5,5	0.51	0	5,5,5	0.49	0
4	GOL	F	805	-	5,5,5	0.61	0	5,5,5	0.62	0
6	PGE	F	806	-	9,9,9	0.51	0	8,8,8	0.46	0
2	IFM	G	801	-	9,10,10	1.20	1 (11%)	9,13,13	3.14	5 (55%)
4	GOL	G	802	-	5,5,5	0.18	0	5,5,5	0.73	0
4	GOL	G	803	-	5,5,5	0.16	0	5,5,5	0.74	0
4	GOL	G	804	-	5,5,5	0.31	0	5,5,5	0.54	0
6	PGE	G	805	-	9,9,9	0.71	0	8,8,8	0.57	0
2	IFM	H	801	-	9,10,10	1.25	2 (22%)	9,13,13	3.92	5 (55%)
4	GOL	H	802	-	5,5,5	0.31	0	5,5,5	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PG4	H	803	-	12,12,12	0.69	0	11,11,11	0.48	0
4	GOL	H	804	-	5,5,5	0.35	0	5,5,5	0.58	0
4	GOL	H	805	-	5,5,5	0.46	0	5,5,5	0.99	0
4	GOL	H	806	-	5,5,5	0.44	0	5,5,5	1.02	0
4	GOL	H	807	-	5,5,5	0.39	0	5,5,5	0.68	0
11	PE5	H	808	-	26,26,26	0.78	0	25,25,25	0.91	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	IFM	A	801	-	-	0/2/16/16	0/1/1/1
3	1PE	A	802	-	-	0/13/13/13	0/0/0/0
4	GOL	A	803	-	-	0/4/4/4	0/0/0/0
4	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	GOL	A	805	-	-	0/4/4/4	0/0/0/0
5	P6G	A	806	-	-	0/16/16/16	0/0/0/0
4	GOL	A	807	-	-	0/4/4/4	0/0/0/0
4	GOL	A	808	-	-	0/4/4/4	0/0/0/0
4	GOL	A	809	-	-	0/4/4/4	0/0/0/0
4	GOL	A	810	-	-	0/4/4/4	0/0/0/0
4	GOL	A	811	-	-	0/4/4/4	0/0/0/0
6	PGE	A	812	-	-	0/7/7/7	0/0/0/0
8	PG4	B	801	-	-	0/10/10/10	0/0/0/0
9	7PE	B	802	-	-	0/18/18/18	0/0/0/0
4	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	GOL	B	804	-	-	0/4/4/4	0/0/0/0
4	GOL	B	805	-	-	0/4/4/4	0/0/0/0
4	GOL	B	806	-	-	0/4/4/4	0/0/0/0
4	GOL	B	807	-	-	0/4/4/4	0/0/0/0
4	GOL	B	808	-	-	0/4/4/4	0/0/0/0
3	1PE	C	801	-	-	0/13/13/13	0/0/0/0
4	GOL	C	802	-	-	0/4/4/4	0/0/0/0
4	GOL	C	803	-	-	0/4/4/4	0/0/0/0
4	GOL	C	804	-	-	0/4/4/4	0/0/0/0
10	PE4	C	805	-	-	0/21/21/21	0/0/0/0
4	GOL	C	806	-	-	0/4/4/4	0/0/0/0
6	PGE	C	807	-	-	0/7/7/7	0/0/0/0
4	GOL	C	808	-	-	0/4/4/4	0/0/0/0
4	GOL	C	809	-	-	0/4/4/4	0/0/0/0
2	IFM	D	801	-	-	0/2/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	802	-	-	0/4/4/4	0/0/0/0
8	PG4	D	803	-	-	0/10/10/10	0/0/0/0
4	GOL	D	804	-	-	0/4/4/4	0/0/0/0
4	GOL	D	805	-	-	0/4/4/4	0/0/0/0
4	GOL	D	806	-	-	0/4/4/4	0/0/0/0
4	GOL	D	807	-	-	0/4/4/4	0/0/0/0
9	7PE	D	808	-	-	0/18/18/18	0/0/0/0
4	GOL	D	809	-	-	0/4/4/4	0/0/0/0
4	GOL	D	810	-	-	0/4/4/4	0/0/0/0
4	GOL	D	811	-	-	0/4/4/4	0/0/0/0
4	GOL	D	812	-	-	0/4/4/4	0/0/0/0
2	IFM	E	801	-	-	0/2/16/16	0/1/1/1
3	1PE	E	802	-	-	0/13/13/13	0/0/0/0
5	P6G	E	803	-	-	0/16/16/16	0/0/0/0
4	GOL	E	804	-	-	0/4/4/4	0/0/0/0
4	GOL	E	805	-	-	0/4/4/4	0/0/0/0
4	GOL	E	806	-	-	0/4/4/4	0/0/0/0
4	GOL	E	807	-	-	0/4/4/4	0/0/0/0
2	IFM	F	801	-	-	0/2/16/16	1/1/1/1
4	GOL	F	802	-	-	0/4/4/4	0/0/0/0
8	PG4	F	803	-	-	0/10/10/10	0/0/0/0
4	GOL	F	804	-	-	0/4/4/4	0/0/0/0
4	GOL	F	805	-	-	0/4/4/4	0/0/0/0
6	PGE	F	806	-	-	0/7/7/7	0/0/0/0
2	IFM	G	801	-	-	0/2/16/16	0/1/1/1
4	GOL	G	802	-	-	0/4/4/4	0/0/0/0
4	GOL	G	803	-	-	0/4/4/4	0/0/0/0
4	GOL	G	804	-	-	0/4/4/4	0/0/0/0
6	PGE	G	805	-	-	0/7/7/7	0/0/0/0
2	IFM	H	801	-	-	0/2/16/16	1/1/1/1
4	GOL	H	802	-	-	0/4/4/4	0/0/0/0
8	PG4	H	803	-	-	0/10/10/10	0/0/0/0
4	GOL	H	804	-	-	0/4/4/4	0/0/0/0
4	GOL	H	805	-	-	0/4/4/4	0/0/0/0
4	GOL	H	806	-	-	0/4/4/4	0/0/0/0
4	GOL	H	807	-	-	0/4/4/4	0/0/0/0
11	PE5	H	808	-	-	0/24/24/24	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	IFM	C2-N	-3.20	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	IFM	C5-C4	-3.18	1.49	1.53
2	D	801	IFM	C5-C4	-3.07	1.49	1.53
2	D	801	IFM	O4-C4	-2.98	1.35	1.43
2	A	801	IFM	C2-N	-2.01	1.43	1.46

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	IFM	O4-C4-C5	-7.69	97.27	110.07
2	E	801	IFM	O4-C4-C5	-6.77	98.79	110.07
2	A	801	IFM	O4-C4-C5	-6.75	98.83	110.07
2	H	801	IFM	O4-C4-C5	-5.65	100.67	110.07
4	C	809	GOL	C3-C2-C1	-3.88	95.89	111.12

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	801	IFM	C1-C2-C3-C4-C5-N
2	H	801	IFM	C1-C2-C3-C4-C5-N

46 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	IFM	4	0
4	A	803	GOL	3	0
4	A	805	GOL	3	0
5	A	806	P6G	3	0
4	A	808	GOL	3	0
4	A	809	GOL	1	0
4	A	811	GOL	2	0
6	A	812	PGE	7	0
8	B	801	PG4	1	0
9	B	802	7PE	5	0
4	B	803	GOL	2	0
4	B	804	GOL	4	0
4	B	805	GOL	1	0
4	B	807	GOL	1	0
4	B	808	GOL	1	0
3	C	801	1PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	805	PE4	6	0
4	C	806	GOL	1	0
4	C	809	GOL	1	0
2	D	801	IFM	3	0
4	D	802	GOL	1	0
8	D	803	PG4	1	0
4	D	804	GOL	2	0
4	D	805	GOL	2	0
4	D	806	GOL	2	0
4	D	807	GOL	1	0
9	D	808	7PE	3	0
4	D	809	GOL	4	0
4	D	812	GOL	2	0
3	E	802	1PE	2	0
5	E	803	P6G	5	0
4	E	805	GOL	1	0
2	F	801	IFM	2	0
4	F	802	GOL	1	0
4	F	805	GOL	1	0
6	F	806	PGE	2	0
2	G	801	IFM	3	0
4	G	802	GOL	2	0
4	G	803	GOL	2	0
2	H	801	IFM	1	0
4	H	802	GOL	2	0
8	H	803	PG4	1	0
4	H	804	GOL	2	0
4	H	805	GOL	2	0
4	H	807	GOL	4	0
11	H	808	PE5	12	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, 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	762/769 (99%)	0.08	18 (2%) 62 71	30, 40, 65, 98	0
1	B	761/769 (98%)	0.27	35 (4%) 36 45	28, 40, 64, 97	0
1	C	761/769 (98%)	0.23	30 (3%) 43 52	28, 40, 64, 99	0
1	D	761/769 (98%)	0.19	34 (4%) 37 46	28, 39, 68, 97	0
1	E	761/769 (98%)	0.75	112 (14%) 3 5	35, 53, 101, 142	0
1	F	761/769 (98%)	0.39	54 (7%) 19 26	32, 49, 86, 131	0
1	G	762/769 (99%)	0.62	98 (12%) 5 7	38, 52, 83, 110	0
1	H	761/769 (98%)	0.37	52 (6%) 20 28	37, 50, 85, 115	0
All	All	6090/6152 (98%)	0.36	433 (7%) 19 26	28, 46, 80, 142	0

The worst 5 of 433 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	ALA	12.6
1	G	98	ALA	9.8
1	H	751	VAL	8.4
1	E	753	ASP	8.3
1	F	754	SER	8.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	1PE	A	802	16/16	0.87	0.22	5.08	50,62,83,101	0
4	GOL	H	802	6/6	0.94	0.24	4.91	58,73,84,85	0
4	GOL	B	805	6/6	0.74	0.24	4.86	59,73,75,75	0
3	1PE	E	802	16/16	0.84	0.23	4.58	62,75,101,104	0
4	GOL	D	802	6/6	0.96	0.34	4.45	50,58,60,62	0
2	IFM	H	801	10/10	0.89	0.25	4.23	56,70,75,82	0
4	GOL	H	805	6/6	0.95	0.20	4.00	51,52,59,60	0
4	GOL	B	806	6/6	0.91	0.23	3.91	57,64,70,77	0
4	GOL	G	802	6/6	0.93	0.38	3.82	52,64,71,76	0
2	IFM	G	801	10/10	0.83	0.38	3.78	55,79,87,98	0
4	GOL	D	804	6/6	0.95	0.19	3.40	47,54,57,62	0
4	GOL	G	804	6/6	0.91	0.21	3.40	68,68,70,72	0
6	PGE	A	812	10/10	0.90	0.22	3.00	40,51,58,60	0
4	GOL	D	809	6/6	0.95	0.16	2.93	45,54,57,60	0
11	PE5	H	808	27/27	0.85	0.22	2.86	53,72,84,96	0
4	GOL	H	804	6/6	0.95	0.17	2.86	46,52,57,61	0
3	1PE	C	801	16/16	0.88	0.16	2.66	44,61,79,82	0
4	GOL	A	811	6/6	0.97	0.14	2.65	45,50,51,51	0
4	GOL	B	807	6/6	0.86	0.22	2.57	59,65,74,82	0
2	IFM	E	801	10/10	0.86	0.35	2.55	44,59,71,73	0
10	PE4	C	805	24/24	0.94	0.26	2.47	39,48,59,68	0
2	IFM	F	801	10/10	0.90	0.28	2.42	49,56,65,72	0
6	PGE	G	805	10/10	0.82	0.22	2.41	54,66,73,78	0
4	GOL	E	804	6/6	0.93	0.20	2.37	54,59,62,63	0
8	PG4	B	801	13/13	0.93	0.18	2.32	46,57,87,88	0
5	P6G	E	803	19/19	0.88	0.30	2.15	52,67,71,73	0
6	PGE	F	806	10/10	0.92	0.24	2.14	62,65,71,74	0
4	GOL	A	803	6/6	0.91	0.28	2.02	46,60,72,75	0
5	P6G	A	806	19/19	0.93	0.21	1.93	41,49,64,70	0
4	GOL	F	802	6/6	0.94	0.25	1.88	52,58,61,65	0
6	PGE	C	807	10/10	0.93	0.15	1.52	42,51,57,59	0
4	GOL	D	810	6/6	0.98	0.22	1.50	33,37,40,41	0
8	PG4	D	803	13/13	0.87	0.17	1.45	48,65,75,77	0
2	IFM	A	801	10/10	0.93	0.22	1.39	38,51,60,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	PG4	H	803	13/13	0.86	0.18	1.35	57,68,83,88	0
8	PG4	F	803	13/13	0.92	0.16	1.26	56,62,75,77	0
4	GOL	E	805	6/6	0.88	0.18	1.26	63,77,85,87	0
4	GOL	C	804	6/6	0.96	0.24	1.21	43,46,53,57	0
4	GOL	C	803	6/6	0.98	0.13	1.12	45,48,52,59	0
4	GOL	A	804	6/6	0.95	0.18	1.04	42,43,46,52	0
4	GOL	B	804	6/6	0.95	0.20	1.03	33,35,40,47	0
4	GOL	B	808	6/6	0.96	0.28	1.02	36,43,46,48	0
4	GOL	F	804	6/6	0.95	0.20	0.98	47,48,50,53	0
4	GOL	C	802	6/6	0.96	0.16	0.96	43,57,62,73	0
4	GOL	D	812	6/6	0.94	0.23	0.96	32,38,40,45	0
9	7PE	B	802	21/21	0.94	0.21	0.95	36,45,52,55	0
4	GOL	C	806	6/6	0.66	0.24	0.91	64,77,87,89	0
4	GOL	A	808	6/6	0.87	0.19	0.72	59,61,66,85	0
4	GOL	E	806	6/6	0.95	0.17	0.63	46,47,50,54	0
4	GOL	C	809	6/6	0.95	0.20	0.55	37,42,49,52	0
4	GOL	C	808	6/6	0.98	0.14	0.54	35,38,39,42	0
4	GOL	E	807	6/6	0.96	0.20	0.48	43,53,60,60	0
4	GOL	F	805	6/6	0.83	0.15	0.38	39,62,67,70	0
4	GOL	A	810	6/6	0.98	0.14	0.30	37,37,39,40	0
9	7PE	D	808	21/21	0.94	0.17	0.21	41,48,54,59	0
4	GOL	H	807	6/6	0.70	0.17	-0.22	70,70,73,76	0
4	GOL	D	806	6/6	0.82	0.12	-0.22	56,64,67,71	0
4	GOL	A	809	6/6	0.82	0.14	-0.24	58,66,67,73	0
4	GOL	B	803	6/6	0.97	0.16	-0.26	35,41,44,46	0
2	IFM	D	801	10/10	0.95	0.21	-0.40	35,44,50,63	0
7	CA	G	806	1/1	0.94	0.11	-0.91	55,55,55,55	0
4	GOL	G	803	6/6	0.82	0.10	-1.43	65,76,86,86	0
4	GOL	A	805	6/6	0.92	0.09	-1.66	57,64,74,75	0
7	CA	B	809	1/1	1.00	0.11	-	43,43,43,43	0
7	CA	C	810	1/1	0.99	0.13	-	36,36,36,36	0
7	CA	D	814	1/1	0.97	0.16	-	45,45,45,45	0
4	GOL	A	807	6/6	0.80	0.19	-	57,59,72,79	0
7	CA	A	813	1/1	0.97	0.10	-	44,44,44,44	0
4	GOL	D	807	6/6	0.90	0.19	-	55,64,71,72	0
7	CA	D	813	1/1	0.96	0.04	-	54,54,54,54	0
7	CA	E	808	1/1	0.99	0.10	-	54,54,54,54	0
4	GOL	D	811	6/6	0.89	0.13	-	49,56,61,71	0
4	GOL	H	806	6/6	0.82	0.14	-	48,62,65,73	0
4	GOL	D	805	6/6	0.88	0.13	-	63,64,69,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.