



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 22, 2021 – 12:10 AM EDT

PDB ID : 7K9T
Title : Co-crystal structure of alpha glucosidase with compound 5
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-09-29
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.23.1
buster-report : 1.1.7 (2018)
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) : 2.23.1

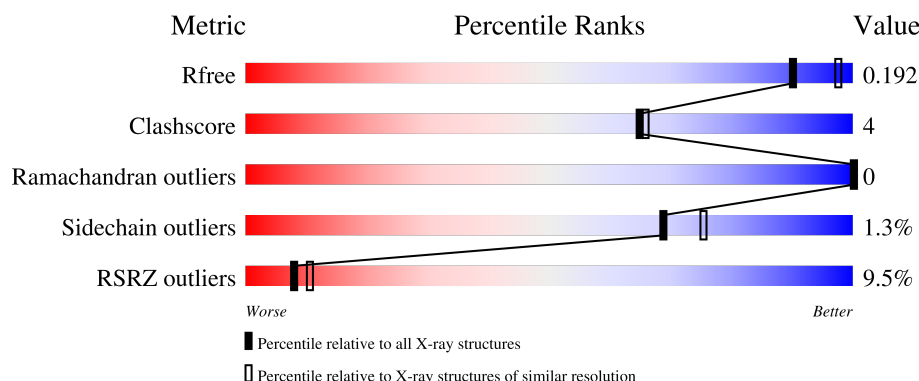
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	977	<div> <div>4%</div> <div>79%</div> <div>7%</div> <div>13%</div> </div>
1	C	977	<div> <div>9%</div> <div>80%</div> <div>7%</div> <div>12%</div> </div>
2	B	547	<div> <div>4%</div> <div>14%</div> <div>85%</div> </div>
2	D	547	<div> <div>5%</div> <div>15%</div> <div>84%</div> </div>

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
5	PEG	A	1008	-	-	-	X
5	PEG	C	1019	-	-	-	X
6	EDO	C	1012	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16450 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 Alpha glucosidase 2 alpha neutral subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	850	Total	C	N	O	S	0	5	0
			6862	4397	1179	1256	30			
1	C	857	Total	C	N	O	S	0	8	0
			6947	4451	1201	1265	30			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A1A4T2
A	3	GLY	-	expression tag	UNP A1A4T2
A	4	ILE	-	expression tag	UNP A1A4T2
A	5	LEU	-	expression tag	UNP A1A4T2
A	6	PRO	-	expression tag	UNP A1A4T2
A	7	SER	-	expression tag	UNP A1A4T2
A	8	PRO	-	expression tag	UNP A1A4T2
A	9	GLY	-	expression tag	UNP A1A4T2
A	10	MET	-	expression tag	UNP A1A4T2
A	11	PRO	-	expression tag	UNP A1A4T2
A	12	ALA	-	expression tag	UNP A1A4T2
A	13	LEU	-	expression tag	UNP A1A4T2
A	14	LEU	-	expression tag	UNP A1A4T2
A	15	SER	-	expression tag	UNP A1A4T2
A	16	LEU	-	expression tag	UNP A1A4T2
A	17	VAL	-	expression tag	UNP A1A4T2
A	18	SER	-	expression tag	UNP A1A4T2
A	19	LEU	-	expression tag	UNP A1A4T2
A	20	LEU	-	expression tag	UNP A1A4T2
A	21	SER	-	expression tag	UNP A1A4T2
A	22	VAL	-	expression tag	UNP A1A4T2
A	23	LEU	-	expression tag	UNP A1A4T2
A	24	LEU	-	expression tag	UNP A1A4T2
A	25	MET	-	expression tag	UNP A1A4T2
A	26	GLY	-	expression tag	UNP A1A4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	CYS	-	expression tag	UNP A1A4T2
A	28	VAL	-	expression tag	UNP A1A4T2
A	29	ALA	-	expression tag	UNP A1A4T2
A	30	GLU	-	expression tag	UNP A1A4T2
A	31	THR	-	expression tag	UNP A1A4T2
A	32	GLY	-	expression tag	UNP A1A4T2
A	97	ASP	ASN	engineered mutation	UNP A1A4T2
A	967	SER	-	expression tag	UNP A1A4T2
A	968	ALA	-	expression tag	UNP A1A4T2
A	969	TRP	-	expression tag	UNP A1A4T2
A	970	SER	-	expression tag	UNP A1A4T2
A	971	HIS	-	expression tag	UNP A1A4T2
A	972	PRO	-	expression tag	UNP A1A4T2
A	973	GLN	-	expression tag	UNP A1A4T2
A	974	PHE	-	expression tag	UNP A1A4T2
A	975	GLU	-	expression tag	UNP A1A4T2
A	976	LYS	-	expression tag	UNP A1A4T2
A	977	LEU	-	expression tag	UNP A1A4T2
A	978	GLU	-	expression tag	UNP A1A4T2
C	2	MET	-	initiating methionine	UNP A1A4T2
C	3	GLY	-	expression tag	UNP A1A4T2
C	4	ILE	-	expression tag	UNP A1A4T2
C	5	LEU	-	expression tag	UNP A1A4T2
C	6	PRO	-	expression tag	UNP A1A4T2
C	7	SER	-	expression tag	UNP A1A4T2
C	8	PRO	-	expression tag	UNP A1A4T2
C	9	GLY	-	expression tag	UNP A1A4T2
C	10	MET	-	expression tag	UNP A1A4T2
C	11	PRO	-	expression tag	UNP A1A4T2
C	12	ALA	-	expression tag	UNP A1A4T2
C	13	LEU	-	expression tag	UNP A1A4T2
C	14	LEU	-	expression tag	UNP A1A4T2
C	15	SER	-	expression tag	UNP A1A4T2
C	16	LEU	-	expression tag	UNP A1A4T2
C	17	VAL	-	expression tag	UNP A1A4T2
C	18	SER	-	expression tag	UNP A1A4T2
C	19	LEU	-	expression tag	UNP A1A4T2
C	20	LEU	-	expression tag	UNP A1A4T2
C	21	SER	-	expression tag	UNP A1A4T2
C	22	VAL	-	expression tag	UNP A1A4T2
C	23	LEU	-	expression tag	UNP A1A4T2
C	24	LEU	-	expression tag	UNP A1A4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MET	-	expression tag	UNP A1A4T2
C	26	GLY	-	expression tag	UNP A1A4T2
C	27	CYS	-	expression tag	UNP A1A4T2
C	28	VAL	-	expression tag	UNP A1A4T2
C	29	ALA	-	expression tag	UNP A1A4T2
C	30	GLU	-	expression tag	UNP A1A4T2
C	31	THR	-	expression tag	UNP A1A4T2
C	32	GLY	-	expression tag	UNP A1A4T2
C	97	ASP	ASN	engineered mutation	UNP A1A4T2
C	967	SER	-	expression tag	UNP A1A4T2
C	968	ALA	-	expression tag	UNP A1A4T2
C	969	TRP	-	expression tag	UNP A1A4T2
C	970	SER	-	expression tag	UNP A1A4T2
C	971	HIS	-	expression tag	UNP A1A4T2
C	972	PRO	-	expression tag	UNP A1A4T2
C	973	GLN	-	expression tag	UNP A1A4T2
C	974	PHE	-	expression tag	UNP A1A4T2
C	975	GLU	-	expression tag	UNP A1A4T2
C	976	LYS	-	expression tag	UNP A1A4T2
C	977	LEU	-	expression tag	UNP A1A4T2
C	978	GLU	-	expression tag	UNP A1A4T2

- Molecule 2 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	83	Total	C	N	O	S	0	0	0
			600	356	99	135	10			
2	D	87	Total	C	N	O	S	0	0	0
			639	382	103	144	10			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression tag	UNP O08795
B	-9	GLY	-	expression tag	UNP O08795
B	-8	MET	-	expression tag	UNP O08795

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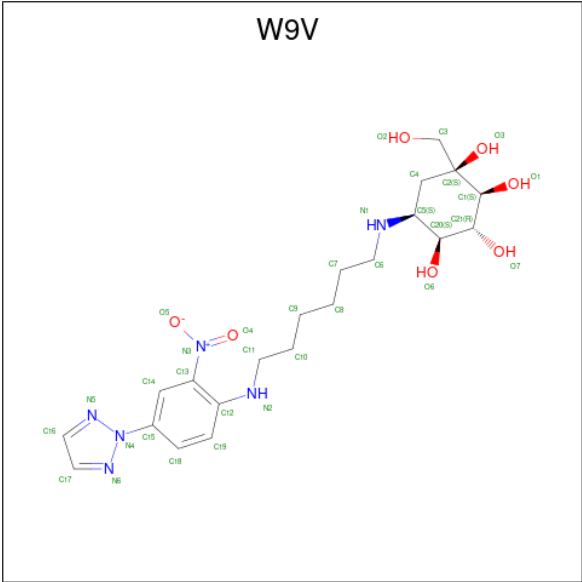
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	PRO	-	expression tag	UNP O08795
B	-6	ALA	-	expression tag	UNP O08795
B	-5	LEU	-	expression tag	UNP O08795
B	-4	LEU	-	expression tag	UNP O08795
B	-3	SER	-	expression tag	UNP O08795
B	-2	LEU	-	expression tag	UNP O08795
B	-1	VAL	-	expression tag	UNP O08795
B	0	SER	-	expression tag	UNP O08795
B	1	LEU	-	expression tag	UNP O08795
B	2	LEU	-	expression tag	UNP O08795
B	3	SER	-	expression tag	UNP O08795
B	4	VAL	-	expression tag	UNP O08795
B	5	LEU	-	expression tag	UNP O08795
B	6	LEU	-	expression tag	UNP O08795
B	7	MET	-	expression tag	UNP O08795
B	8	GLY	-	expression tag	UNP O08795
B	9	CYS	-	expression tag	UNP O08795
B	10	VAL	-	expression tag	UNP O08795
B	11	ALA	-	expression tag	UNP O08795
B	12	GLU	-	expression tag	UNP O08795
B	13	THR	-	expression tag	UNP O08795
B	14	GLY	-	expression tag	UNP O08795
B	518	SER	-	expression tag	UNP O08795
B	519	ALA	-	expression tag	UNP O08795
B	520	TRP	-	expression tag	UNP O08795
B	521	LEU	-	expression tag	UNP O08795
B	522	GLU	-	expression tag	UNP O08795
B	523	THR	-	expression tag	UNP O08795
B	524	LYS	-	expression tag	UNP O08795
B	525	HIS	-	expression tag	UNP O08795
B	526	HIS	-	expression tag	UNP O08795
B	527	HIS	-	expression tag	UNP O08795
B	528	HIS	-	expression tag	UNP O08795
B	529	HIS	-	expression tag	UNP O08795
B	530	HIS	-	expression tag	UNP O08795
D	-16	MET	-	initiating methionine	UNP O08795
D	-15	GLY	-	expression tag	UNP O08795
D	-14	ILE	-	expression tag	UNP O08795
D	-13	LEU	-	expression tag	UNP O08795
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795

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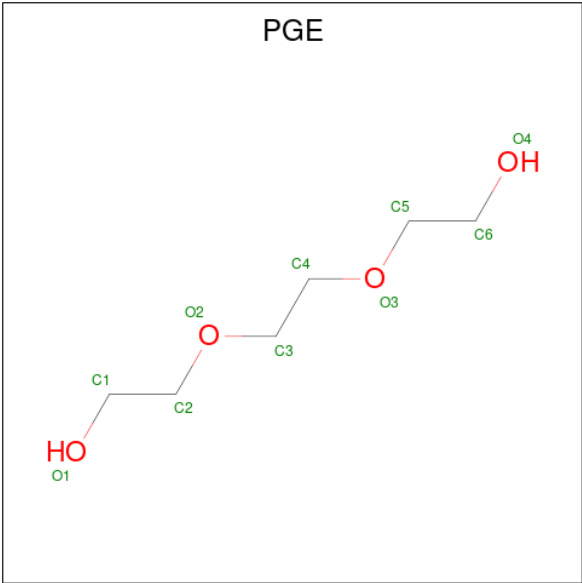
Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	GLY	-	expression tag	UNP O08795
D	-8	MET	-	expression tag	UNP O08795
D	-7	PRO	-	expression tag	UNP O08795
D	-6	ALA	-	expression tag	UNP O08795
D	-5	LEU	-	expression tag	UNP O08795
D	-4	LEU	-	expression tag	UNP O08795
D	-3	SER	-	expression tag	UNP O08795
D	-2	LEU	-	expression tag	UNP O08795
D	-1	VAL	-	expression tag	UNP O08795
D	0	SER	-	expression tag	UNP O08795
D	1	LEU	-	expression tag	UNP O08795
D	2	LEU	-	expression tag	UNP O08795
D	3	SER	-	expression tag	UNP O08795
D	4	VAL	-	expression tag	UNP O08795
D	5	LEU	-	expression tag	UNP O08795
D	6	LEU	-	expression tag	UNP O08795
D	7	MET	-	expression tag	UNP O08795
D	8	GLY	-	expression tag	UNP O08795
D	9	CYS	-	expression tag	UNP O08795
D	10	VAL	-	expression tag	UNP O08795
D	11	ALA	-	expression tag	UNP O08795
D	12	GLU	-	expression tag	UNP O08795
D	13	THR	-	expression tag	UNP O08795
D	14	GLY	-	expression tag	UNP O08795
D	518	SER	-	expression tag	UNP O08795
D	519	ALA	-	expression tag	UNP O08795
D	520	TRP	-	expression tag	UNP O08795
D	521	LEU	-	expression tag	UNP O08795
D	522	GLU	-	expression tag	UNP O08795
D	523	THR	-	expression tag	UNP O08795
D	524	LYS	-	expression tag	UNP O08795
D	525	HIS	-	expression tag	UNP O08795
D	526	HIS	-	expression tag	UNP O08795
D	527	HIS	-	expression tag	UNP O08795
D	528	HIS	-	expression tag	UNP O08795
D	529	HIS	-	expression tag	UNP O08795
D	530	HIS	-	expression tag	UNP O08795

- Molecule 3 is (1S,2S,3R,4S,5S)-1-(hydroxymethyl)-5-[[[(5Z)-6-[[2-nitro-4-(2H-1,2,3-triazol-2-yl)phenyl]amino}hex-5-en-1-yl]amino}cyclohexane-1,2,3,4-tetrol (three-letter code: W9V) (formula: C₂₁H₃₂N₆O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	21	6	7		
3	C	1	Total	C	N	O	0	0
			34	21	6	7		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



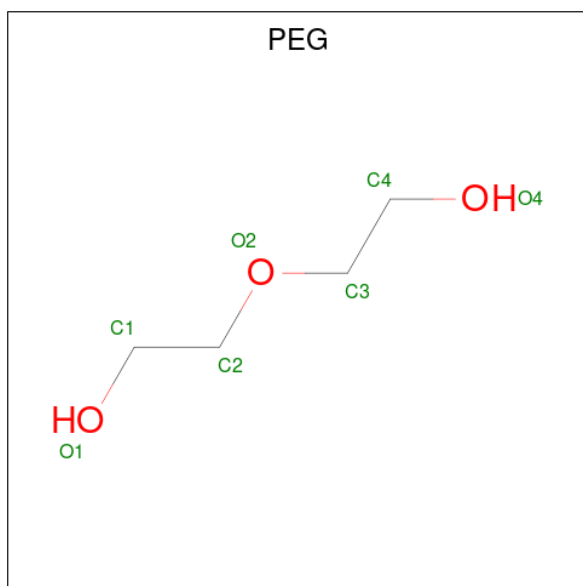
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		

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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



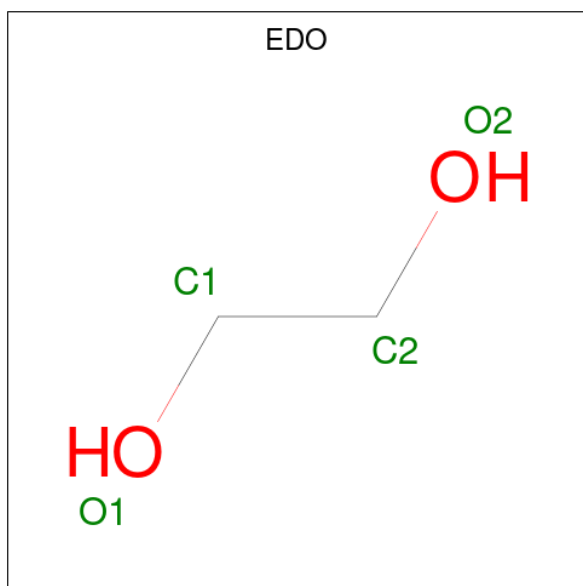
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0

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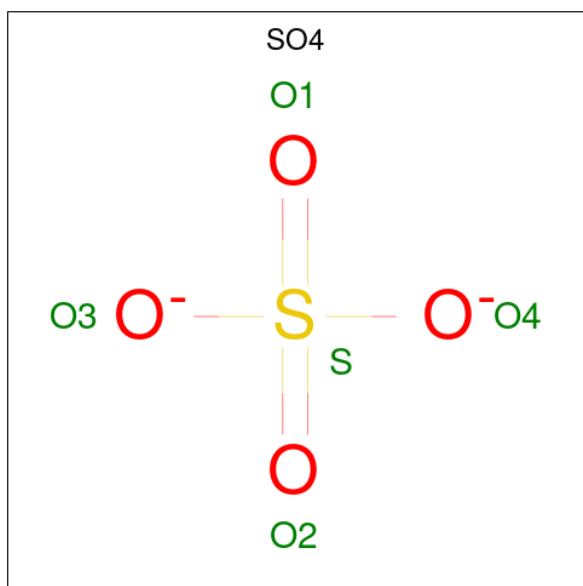
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	C	1	Total 4	C 2	O 2	0	0
6	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

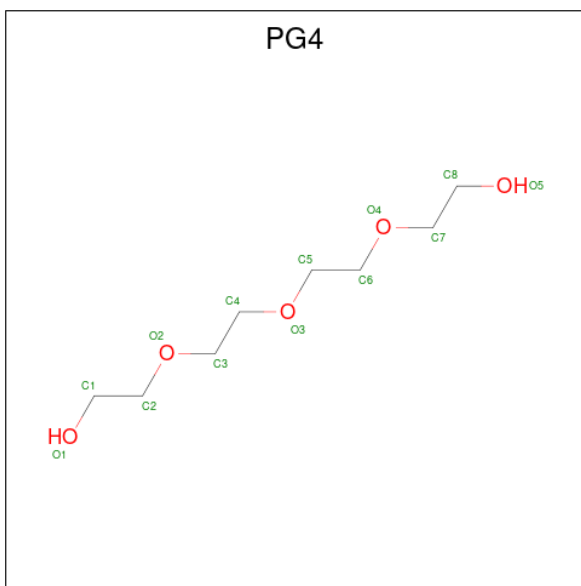


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

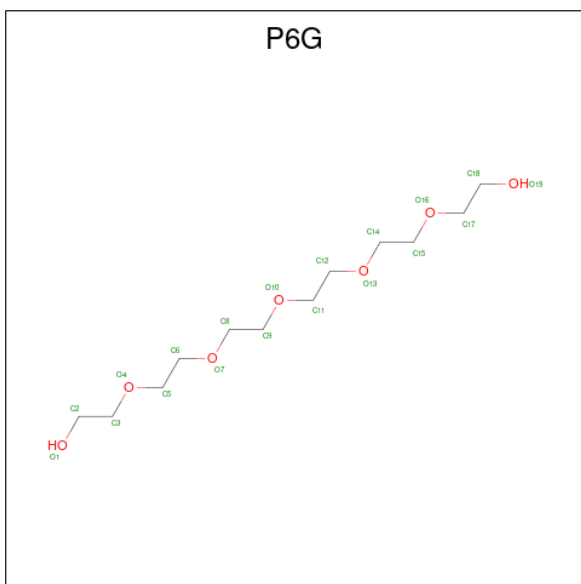
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		
8	D	2	Total	Ca	0	0
			2	2		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 10 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			19	12	7		

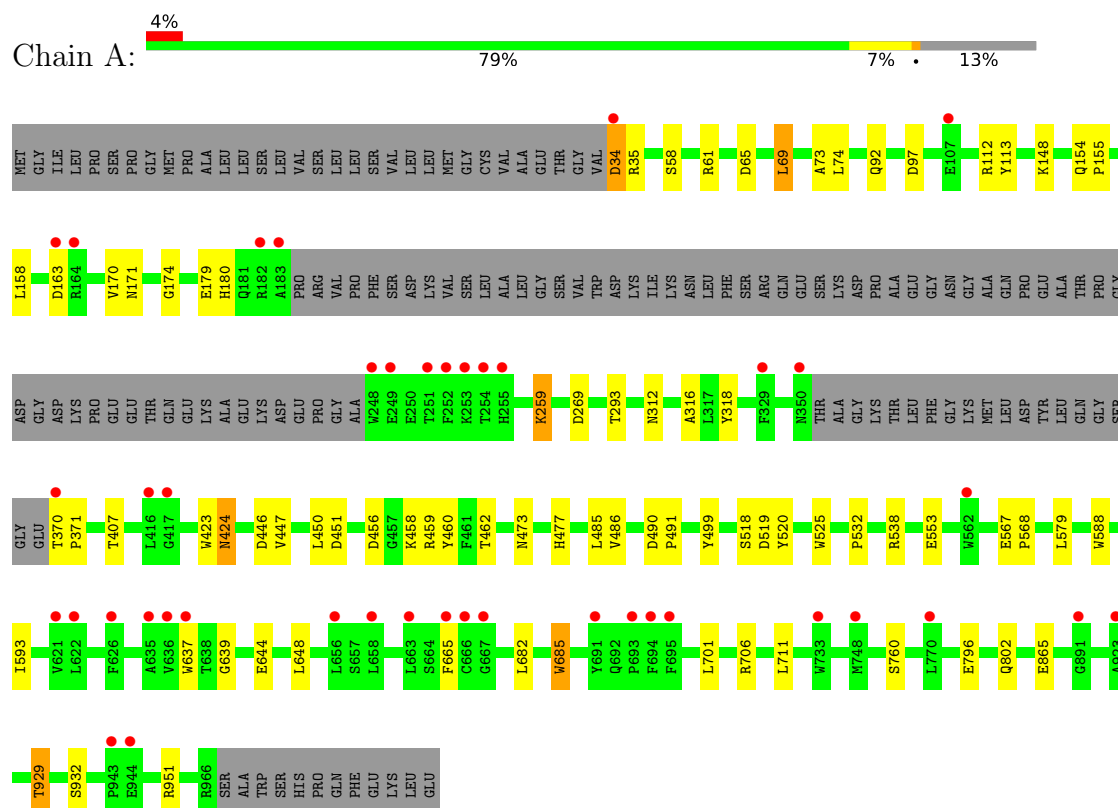
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	504	Total 504	O 504	0	0
11	B	34	Total 34	O 34	0	0
11	C	411	Total 411	O 411	0	0
11	D	32	Total 32	O 32	0	0

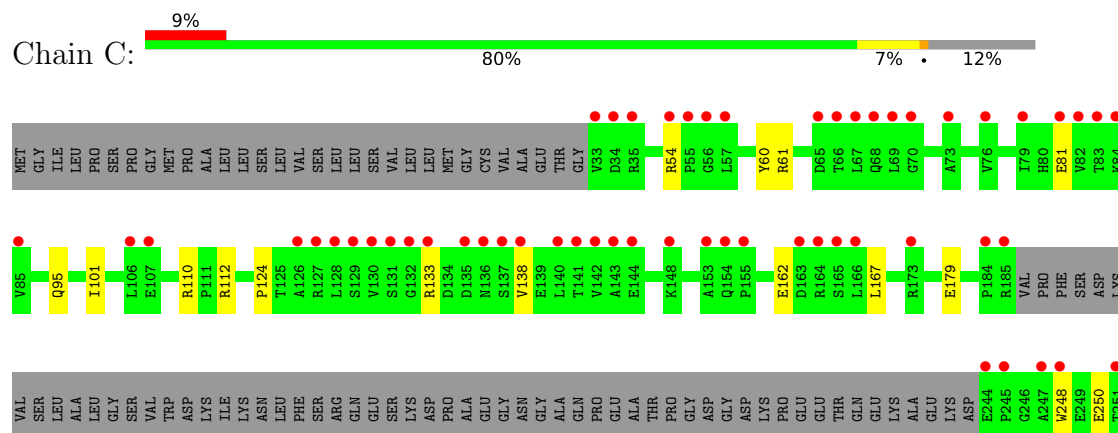
3 Residue-property plots

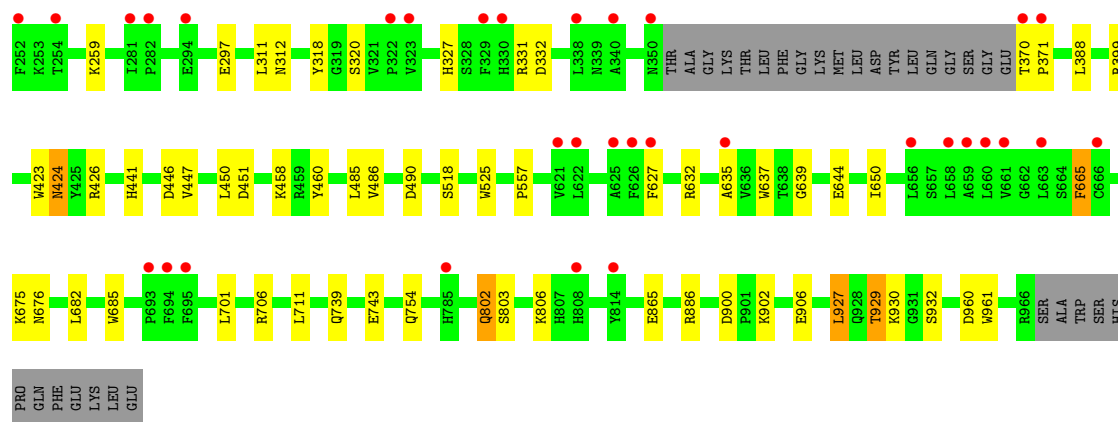
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha glucosidase 2 alpha neutral subunit

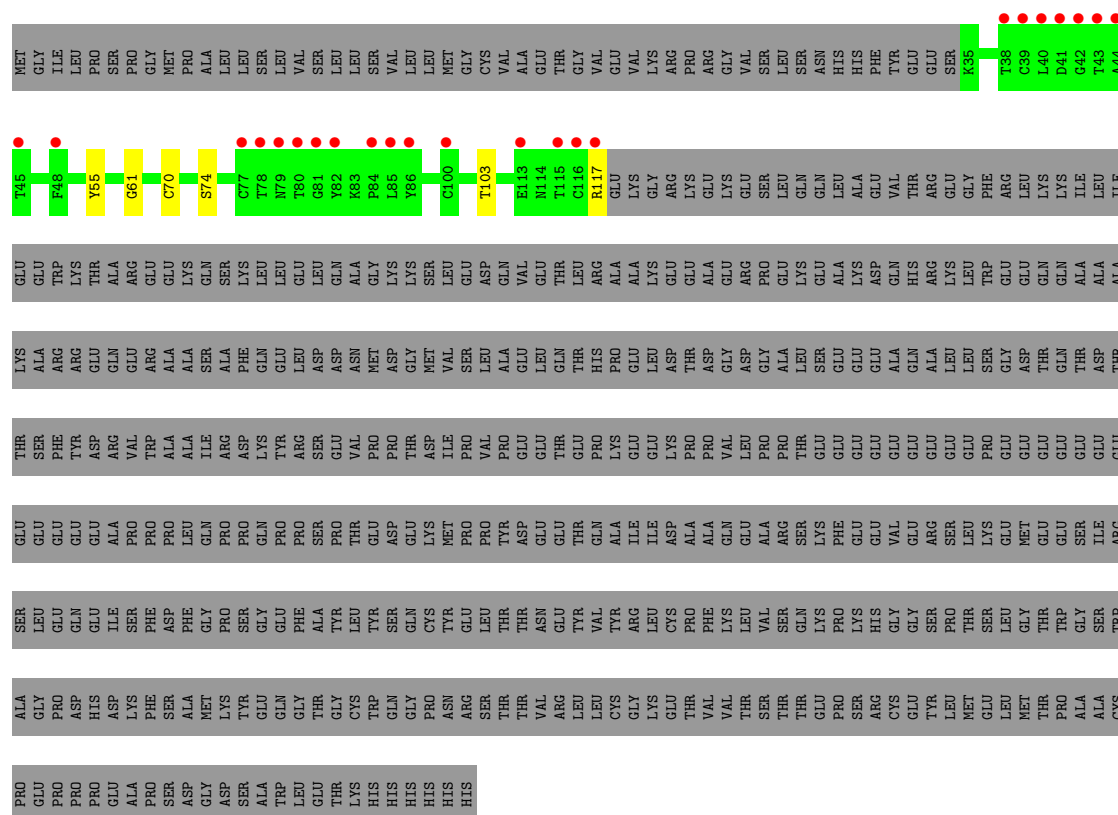


- Molecule 1: Alpha glucosidase 2 alpha neutral subunit

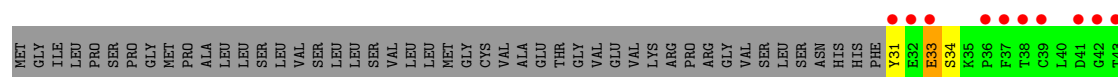


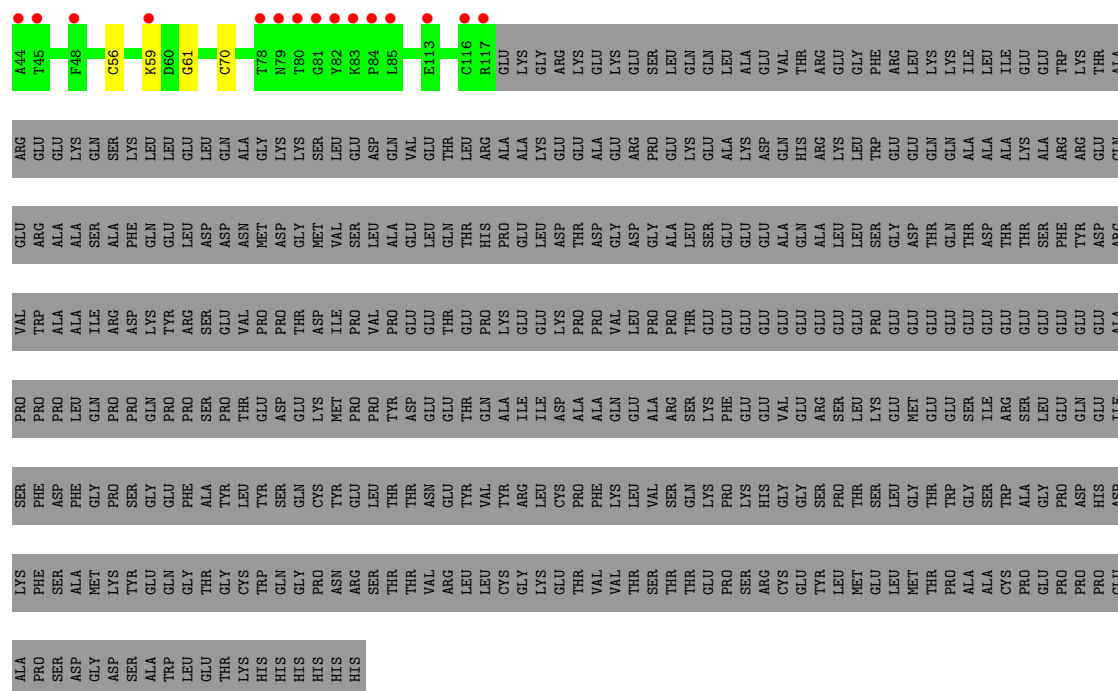


- Molecule 2: Glucosidase 2 subunit beta



- Molecule 2: Glucosidase 2 subunit beta





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	102.87Å 102.87Å 240.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.35 – 2.10 42.35 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.35-2.10) 94.3 (42.35-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.171 , 0.192 0.171 , 0.192	Depositor DCC
R_{free} test set	2002 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.034 for h,-h-k,-l 0.020 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16450	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PGE, PEG, SO4, W9V, P6G, CA, PG4

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	0.28	0/7086	0.50	1/9649 (0.0%)
1	C	0.28	0/7182	0.49	0/9775
2	B	0.27	0/611	0.55	0/835
2	D	0.28	0/652	0.57	0/891
All	All	0.28	0/15531	0.50	1/21150 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6862	0	6590	54	0
1	C	6947	0	6714	58	0
2	B	600	0	504	5	0
2	D	639	0	533	5	0
3	A	34	0	0	0	0
3	C	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	60	0	84	7	0
4	B	10	0	14	1	0
4	C	20	0	28	2	0
5	A	42	0	60	3	2
5	C	42	0	60	2	2
6	A	48	0	71	5	0
6	C	44	0	60	10	0
6	D	8	0	12	0	0
7	A	20	0	0	0	0
7	C	10	0	0	0	0
8	B	2	0	0	0	0
8	D	2	0	0	0	0
9	B	13	0	18	1	0
9	D	13	0	18	2	0
10	C	19	0	26	0	0
11	A	504	0	0	16	0
11	B	34	0	0	2	0
11	C	411	0	0	17	0
11	D	32	0	0	1	0
All	All	16450	0	14792	125	2

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 (125) 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:A:553:GLU:OE2	11:A:1101:HOH:O	1.89	0.89
1:C:886:ARG:NH2	11:C:1102:HOH:O	2.08	0.87
1:A:644:GLU:OE1	11:A:1102:HOH:O	1.95	0.81
1:A:180:HIS:O	11:A:1103:HOH:O	2.01	0.79
1:A:588:TRP:HE1	4:A:1013:PGE:H22	1.49	0.75
1:C:676:ASN:H	4:C:1018:PGE:H52	1.49	0.75
1:C:802:GLN:OE1	11:C:1101:HOH:O	2.07	0.73
1:C:960:ASP:HB3	5:C:1008:PEG:H41	1.69	0.73
2:B:103:THR:OG1	11:B:701:HOH:O	2.08	0.72
1:A:865:GLU:H	6:A:1005:EDO:H21	1.53	0.72
6:C:1021:EDO:H22	11:C:1408:HOH:O	1.89	0.72
1:A:459:ARG:HD3	4:A:1024:PGE:H22	1.71	0.71
1:A:65:ASP:H	6:A:1011:EDO:H21	1.56	0.71
1:C:399:ARG:NH2	1:C:743:GLU:OE2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:518:SER:HB2	6:C:1003:EDO:H22	1.74	0.69
4:A:1025:PGE:O4	11:A:1104:HOH:O	2.10	0.69
1:A:796:GLU:OE1	11:A:1105:HOH:O	2.11	0.68
1:C:61:ARG:NH1	1:C:81:GLU:OE1	2.27	0.68
1:C:95:GLN:O	11:C:1103:HOH:O	2.12	0.68
1:A:499:TYR:HA	4:A:1024:PGE:H2	1.76	0.67
1:A:932:SER:OG	11:A:1106:HOH:O	2.12	0.66
1:C:644:GLU:OE1	11:C:1104:HOH:O	2.14	0.66
1:A:682:LEU:HD23	1:A:711:LEU:HD11	1.80	0.64
2:B:117:ARG:N	11:B:703:HOH:O	2.31	0.63
1:A:112:ARG:NH2	1:A:179:GLU:O	2.32	0.63
1:C:112:ARG:NH2	1:C:179:GLU:O	2.32	0.62
1:C:250:GLU:OE1	1:C:259:LYS:NZ	2.32	0.62
1:C:739:GLN:HG2	6:C:1002:EDO:H21	1.81	0.62
1:C:248:TRP:O	1:C:259:LYS:HE2	2.00	0.61
1:C:54:ARG:O	11:C:1105:HOH:O	2.16	0.61
1:A:407:THR:H	6:A:1019:EDO:H22	1.66	0.60
1:C:60:TYR:OH	11:C:1106:HOH:O	2.17	0.60
2:D:31:TYR:OH	11:D:2101:HOH:O	2.17	0.58
1:A:148:LYS:NZ	1:A:163:ASP:O	2.27	0.58
1:C:312:ASN:ND2	11:C:1116:HOH:O	2.35	0.58
1:A:423:TRP:O	1:A:701:LEU:HA	2.04	0.57
1:C:682:LEU:HD23	1:C:711:LEU:HD11	1.87	0.56
1:C:259:LYS:HD2	11:C:1412:HOH:O	2.05	0.56
1:C:754:GLN:HB3	11:C:1216:HOH:O	2.05	0.56
1:A:865:GLU:OE1	6:A:1004:EDO:O2	2.24	0.55
1:C:327:HIS:ND1	1:C:332:ASP:OD1	2.32	0.55
1:A:34:ASP:OD1	1:A:34:ASP:N	2.40	0.55
1:C:557:PRO:HD3	6:C:1007:EDO:H22	1.89	0.54
1:C:110:ARG:NH2	11:C:1121:HOH:O	2.38	0.54
1:C:423:TRP:O	1:C:701:LEU:HA	2.06	0.54
1:A:520:TYR:HE2	1:A:579:LEU:HD12	1.72	0.54
1:C:743:GLU:OE1	6:C:1002:EDO:O1	2.24	0.54
1:C:865:GLU:H	6:C:1016:EDO:H21	1.72	0.54
1:C:930:LYS:HD3	1:C:960:ASP:HB2	1.90	0.53
1:C:929:THR:HG23	1:C:932:SER:HB2	1.90	0.53
1:A:477[A]:HIS:NE2	11:A:1113:HOH:O	2.34	0.53
1:C:297:GLU:O	11:C:1107:HOH:O	2.19	0.53
1:A:462:THR:HG21	4:A:1024:PGE:H4	1.90	0.52
1:C:632:ARG:HG2	6:C:1021:EDO:H21	1.90	0.52
1:A:929:THR:HG23	1:A:932:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HG	1:A:485:LEU:HD21	1.93	0.50
1:A:370:THR:N	1:A:371:PRO:HD2	2.27	0.50
1:C:424:ASN:OD1	1:C:451:ASP:HB3	2.12	0.50
1:C:450:LEU:HG	1:C:485:LEU:HD21	1.94	0.49
1:C:370:THR:N	1:C:371:PRO:HD2	2.27	0.49
1:C:95:GLN:HG3	1:C:124:PRO:HB2	1.95	0.49
1:C:311:LEU:HD22	1:C:650:ILE:HD13	1.95	0.49
1:C:675:LYS:HA	4:C:1018:PGE:H4	1.95	0.48
1:A:760:SER:HB2	5:A:1014:PEG:H31	1.96	0.48
1:A:424:ASN:OD1	1:A:451:ASP:HB3	2.13	0.48
1:A:473:ASN:HB2	11:A:1152:HOH:O	2.14	0.48
1:C:886:ARG:HD3	11:C:1169:HOH:O	2.15	0.47
1:A:293:THR:HG22	6:A:1023:EDO:H21	1.96	0.47
1:A:519:ASP:H	5:A:1016:PEG:H11	1.80	0.47
1:A:460:TYR:CE2	1:A:490:ASP:HB2	2.50	0.47
1:A:538:ARG:NH2	11:A:1127:HOH:O	2.48	0.47
1:C:318:TYR:CE2	1:C:639:GLY:HA3	2.49	0.46
4:A:1021:PGE:H5	4:A:1021:PGE:H3	1.59	0.46
11:A:1265:HOH:O	9:B:603:PG4:H41	2.15	0.46
1:A:802:GLN:HG3	11:A:1459:HOH:O	2.14	0.46
1:C:906:GLU:H	1:C:906:GLU:CD	2.18	0.46
1:C:739:GLN:HG2	6:C:1002:EDO:C2	2.44	0.46
1:C:447:VAL:HG11	1:C:486:VAL:HG23	1.97	0.46
1:A:456:ASP:OD2	4:A:1024:PGE:H42	2.15	0.46
1:C:162:GLU:OE1	1:C:331:ARG:NH1	2.41	0.46
1:C:458:LYS:HG2	1:C:525:TRP:HB3	1.99	0.45
2:B:61:GLY:HA2	2:B:70:CYS:SG	2.57	0.45
1:A:318:TYR:CE2	1:A:639:GLY:HA3	2.52	0.44
1:A:447:VAL:HG11	1:A:486:VAL:HG23	1.99	0.44
1:A:73:ALA:HB2	1:A:92:GLN:HG2	1.99	0.44
1:A:171:ASN:HA	1:A:269:ASP:OD1	2.17	0.44
1:A:951:ARG:HG3	2:B:55:TYR:CE1	2.53	0.44
1:C:441:HIS:HD2	11:C:1151:HOH:O	2.00	0.44
1:A:158:LEU:HB2	1:A:170:VAL:HB	2.00	0.44
1:C:101:ILE:HD12	1:C:388:LEU:HD21	1.99	0.44
1:C:803:SER:OG	6:C:1017:EDO:H21	2.18	0.44
1:C:927:LEU:HD23	11:C:1319:HOH:O	2.18	0.44
1:C:960:ASP:CB	5:C:1008:PEG:H41	2.46	0.43
2:D:61:GLY:HA2	2:D:70:CYS:SG	2.58	0.43
1:C:900:ASP:OD2	1:C:902:LYS:HE2	2.17	0.43
1:A:312:ASN:HB2	11:A:1551:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:O	11:C:1108:HOH:O	2.21	0.43
1:A:113:TYR:CZ	1:A:593:ILE:HG22	2.54	0.43
1:A:458:LYS:HG2	1:A:525:TRP:HB3	2.01	0.43
1:A:69:LEU:HD21	1:A:74:LEU:HD12	2.00	0.43
1:C:929:THR:HB	1:C:961:TRP:HB3	2.00	0.43
2:D:33:GLU:HG2	2:D:34:SER:N	2.34	0.42
1:C:133:ARG:HG3	1:C:138:VAL:HG22	2.01	0.42
1:A:518:SER:HB2	5:A:1016:PEG:H11	2.02	0.42
1:C:426:ARG:NH2	11:C:1139:HOH:O	2.49	0.42
1:A:316:ALA:HB1	11:A:1325:HOH:O	2.19	0.42
1:A:491:PRO:O	1:A:532:PRO:HD2	2.19	0.42
1:C:460:TYR:CE2	1:C:490:ASP:HB2	2.55	0.42
1:A:61:ARG:HD3	11:A:1123:HOH:O	2.20	0.41
1:A:154:GLN:HA	1:A:155:PRO:HA	1.96	0.41
1:C:320:SER:O	1:C:627:PHE:HA	2.20	0.41
1:C:635:ALA:HB2	1:C:665:PHE:CD2	2.55	0.41
1:C:900:ASP:OD1	1:C:902:LYS:HG2	2.21	0.41
1:A:259:LYS:HD2	11:A:1425:HOH:O	2.20	0.41
1:A:567:GLU:N	1:A:568:PRO:HA	2.35	0.41
1:A:34:ASP:N	11:A:1120:HOH:O	2.52	0.41
1:A:259:LYS:HE3	1:A:259:LYS:HB2	1.70	0.41
1:C:806:LYS:HE2	1:C:806:LYS:HB3	1.87	0.41
2:D:56:CYS:SG	9:D:2004:PG4:H31	2.60	0.41
1:C:632:ARG:CG	6:C:1021:EDO:H21	2.51	0.41
1:A:485:LEU:HD23	1:A:486:VAL:N	2.36	0.40
2:B:74:SER:HB3	4:B:604:PGE:H32	2.03	0.40
1:A:648:LEU:HD13	1:A:685:TRP:CG	2.57	0.40
1:A:58:SER:HB2	1:A:174:GLY:HA2	2.04	0.40
2:D:59:LYS:NZ	9:D:2004:PG4:H21	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1008:PEG:C3	5:C:1019:PEG:C2[3_665]	1.50	0.70
5:A:1008:PEG:O2	5:C:1019:PEG:C2[3_665]	1.70	0.50

5.3 Torsion angles

5.3.1 Protein backbone

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	849/977 (87%)	824 (97%)	25 (3%)	0	100	100
1	C	859/977 (88%)	831 (97%)	28 (3%)	0	100	100
2	B	81/547 (15%)	79 (98%)	2 (2%)	0	100	100
2	D	85/547 (16%)	79 (93%)	6 (7%)	0	100	100
All	All	1874/3048 (62%)	1813 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	743/846 (88%)	732 (98%)	11 (2%)	65	71
1	C	755/846 (89%)	746 (99%)	9 (1%)	71	77
2	B	69/478 (14%)	69 (100%)	0	100	100
2	D	73/478 (15%)	72 (99%)	1 (1%)	67	73
All	All	1640/2648 (62%)	1619 (99%)	21 (1%)	69	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	35	ARG

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	259	LYS
1	A	424	ASN
1	A	446	ASP
1	A	637	TRP
1	A	665	PHE
1	A	685	TRP
1	A	706	ARG
1	A	929	THR
1	C	424	ASN
1	C	446	ASP
1	C	637	TRP
1	C	665	PHE
1	C	685	TRP
1	C	706	ARG
1	C	802	GLN
1	C	927	LEU
1	C	929	THR
2	D	33	GLU

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 4 are monoatomic - leaving 57 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	$\# Z > 2$
3	W9V	A	1001	-	35,36,36	2.04	2 (5%)	40,50,50	3.50	14 (35%)
6	EDO	A	1005	-	3,3,3	0.51	0	2,2,2	0.36	0
5	PEG	A	1016	-	6,6,6	0.48	0	5,5,5	0.24	0
6	EDO	A	1022	-	3,3,3	0.43	0	2,2,2	0.50	0
5	PEG	A	1003	-	6,6,6	0.48	0	5,5,5	0.26	0
7	SO4	C	1023	-	4,4,4	0.12	0	6,6,6	0.12	0
9	PG4	D	2004	-	12,12,12	0.51	0	11,11,11	0.70	0
6	EDO	A	1023	-	3,3,3	0.48	0	2,2,2	0.38	0
6	EDO	C	1003	-	3,3,3	0.44	0	2,2,2	0.38	0
7	SO4	C	1022	-	4,4,4	0.13	0	6,6,6	0.15	0
6	EDO	C	1006	-	3,3,3	0.42	0	2,2,2	0.36	0
5	PEG	C	1008	-	6,6,6	0.51	0	5,5,5	0.69	0
6	EDO	A	1010	-	3,3,3	0.51	0	2,2,2	0.16	0
5	PEG	A	1014	-	6,6,6	0.48	0	5,5,5	0.35	0
7	SO4	A	1028	-	4,4,4	0.13	0	6,6,6	0.07	0
6	EDO	A	1017	-	3,3,3	0.47	0	2,2,2	0.40	0
5	PEG	A	1008	-	6,6,6	0.65	0	5,5,5	1.52	1 (20%)
4	PGE	B	604	-	9,9,9	0.31	0	8,8,8	0.34	0
6	EDO	A	1011	-	3,3,3	0.44	0	2,2,2	0.45	0
5	PEG	C	1011	-	6,6,6	0.48	0	5,5,5	0.30	0
10	P6G	C	1020	-	18,18,18	0.54	0	17,17,17	0.33	0
6	EDO	C	1013	-	3,3,3	0.47	0	2,2,2	0.36	0
3	W9V	C	1001	-	35,36,36	2.08	3 (8%)	40,50,50	3.56	14 (35%)
6	EDO	C	1015	-	3,3,3	0.49	0	2,2,2	0.30	0
6	EDO	D	2005	-	3,3,3	0.43	0	2,2,2	0.49	0
4	PGE	A	1013	-	9,9,9	0.30	0	8,8,8	0.31	0
6	EDO	A	1006	-	3,3,3	0.45	0	2,2,2	0.41	0
5	PEG	A	1007	-	6,6,6	0.52	0	5,5,5	0.39	0
4	PGE	A	1002	-	9,9,9	0.29	0	8,8,8	0.38	0
4	PGE	A	1024	-	9,9,9	0.32	0	8,8,8	0.38	0
5	PEG	A	1015	-	6,6,6	0.49	0	5,5,5	0.29	0
6	EDO	C	1012	-	3,3,3	0.52	0	2,2,2	0.35	0
6	EDO	A	1018	-	3,3,3	0.51	0	2,2,2	0.24	0
6	EDO	C	1010	-	3,3,3	0.49	0	2,2,2	0.27	0
7	SO4	A	1026	-	4,4,4	0.12	0	6,6,6	0.12	0
6	EDO	C	1017	-	3,3,3	0.44	0	2,2,2	0.35	0
6	EDO	C	1002	-	3,3,3	0.42	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	SO4	A	1029	-	4,4,4	0.14	0	6,6,6	0.14	0
6	EDO	A	1012	-	3,3,3	0.45	0	2,2,2	0.44	0
5	PEG	C	1019	-	6,6,6	0.55	0	5,5,5	0.58	0
9	PG4	B	603	-	12,12,12	0.53	0	11,11,11	0.34	0
4	PGE	C	1018	-	9,9,9	0.35	0	8,8,8	0.24	0
5	PEG	C	1014	-	6,6,6	0.50	0	5,5,5	0.33	0
7	SO4	A	1027	-	4,4,4	0.14	0	6,6,6	0.07	0
6	EDO	C	1021	-	3,3,3	0.48	0	2,2,2	0.35	0
4	PGE	A	1025	-	9,9,9	0.30	0	8,8,8	0.37	0
5	PEG	C	1004	-	6,6,6	0.49	0	5,5,5	0.27	0
6	EDO	A	1004	-	3,3,3	0.42	0	2,2,2	0.47	0
6	EDO	D	2001	-	3,3,3	0.61	0	2,2,2	0.61	0
6	EDO	A	1009	-	3,3,3	0.41	0	2,2,2	0.61	0
4	PGE	A	1021	-	9,9,9	0.33	0	8,8,8	0.26	0
4	PGE	A	1020	-	9,9,9	0.31	0	8,8,8	0.33	0
4	PGE	C	1005	-	9,9,9	0.33	0	8,8,8	0.31	0
6	EDO	C	1007	-	3,3,3	0.48	0	2,2,2	0.29	0
6	EDO	A	1019	-	3,3,3	0.45	0	2,2,2	0.44	0
6	EDO	C	1016	-	3,3,3	0.46	0	2,2,2	0.42	0
5	PEG	C	1009	-	6,6,6	0.49	0	5,5,5	0.28	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
3	W9V	A	1001	-	-	8/20/45/45	0/3/3/3
6	EDO	A	1005	-	-	0/1/1/1	-
5	PEG	A	1016	-	-	2/4/4/4	-
6	EDO	A	1022	-	-	1/1/1/1	-
5	PEG	A	1003	-	-	3/4/4/4	-
9	PG4	D	2004	-	-	7/10/10/10	-
6	EDO	A	1023	-	-	0/1/1/1	-
6	EDO	C	1003	-	-	1/1/1/1	-
6	EDO	C	1006	-	-	1/1/1/1	-
5	PEG	C	1008	-	-	1/4/4/4	-
6	EDO	A	1010	-	-	1/1/1/1	-
5	PEG	A	1014	-	-	2/4/4/4	-
6	EDO	A	1017	-	-	1/1/1/1	-
5	PEG	A	1008	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	B	604	-	-	4/7/7/7	-
6	EDO	A	1011	-	-	0/1/1/1	-
5	PEG	C	1011	-	-	2/4/4/4	-
10	P6G	C	1020	-	-	9/16/16/16	-
6	EDO	C	1013	-	-	1/1/1/1	-
3	W9V	C	1001	-	-	10/20/45/45	0/3/3/3
6	EDO	C	1015	-	-	1/1/1/1	-
6	EDO	D	2005	-	-	0/1/1/1	-
4	PGE	A	1013	-	-	3/7/7/7	-
6	EDO	A	1006	-	-	1/1/1/1	-
5	PEG	A	1007	-	-	2/4/4/4	-
4	PGE	A	1002	-	-	6/7/7/7	-
4	PGE	A	1024	-	-	5/7/7/7	-
5	PEG	A	1015	-	-	1/4/4/4	-
6	EDO	C	1012	-	-	0/1/1/1	-
6	EDO	A	1018	-	-	1/1/1/1	-
6	EDO	C	1010	-	-	1/1/1/1	-
6	EDO	C	1017	-	-	1/1/1/1	-
6	EDO	C	1002	-	-	0/1/1/1	-
6	EDO	A	1012	-	-	0/1/1/1	-
5	PEG	C	1019	-	-	4/4/4/4	-
9	PG4	B	603	-	-	6/10/10/10	-
4	PGE	C	1018	-	-	4/7/7/7	-
5	PEG	C	1014	-	-	0/4/4/4	-
6	EDO	C	1021	-	-	1/1/1/1	-
4	PGE	A	1025	-	-	5/7/7/7	-
5	PEG	C	1004	-	-	3/4/4/4	-
6	EDO	A	1004	-	-	0/1/1/1	-
6	EDO	D	2001	-	-	0/1/1/1	-
6	EDO	A	1009	-	-	0/1/1/1	-
4	PGE	A	1021	-	-	3/7/7/7	-
4	PGE	A	1020	-	-	3/7/7/7	-
4	PGE	C	1005	-	-	3/7/7/7	-
6	EDO	C	1007	-	-	0/1/1/1	-
6	EDO	A	1019	-	-	1/1/1/1	-
6	EDO	C	1016	-	-	0/1/1/1	-
5	PEG	C	1009	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	W9V	O4-N3	10.80	1.41	1.22
3	A	1001	W9V	O4-N3	10.66	1.40	1.22
3	A	1001	W9V	C12-N2	3.73	1.47	1.37
3	C	1001	W9V	C12-N2	3.73	1.47	1.37
3	C	1001	W9V	O3-C2	-2.01	1.41	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	W9V	O3-C2-C3	-16.01	87.62	108.38
3	A	1001	W9V	O3-C2-C3	-15.10	88.79	108.38
3	C	1001	W9V	O3-C2-C4	-11.59	84.09	108.36
3	A	1001	W9V	O3-C2-C4	-10.51	86.35	108.36
3	C	1001	W9V	C4-C2-C3	4.80	117.11	110.17
3	A	1001	W9V	C4-C2-C3	4.69	116.96	110.17
3	A	1001	W9V	C11-N2-C12	-4.21	113.26	123.39
3	A	1001	W9V	C10-C11-N2	3.71	121.47	111.49
3	A	1001	W9V	C18-C15-N4	3.46	123.00	118.33
3	A	1001	W9V	C19-C12-N2	-3.43	115.95	121.80
3	A	1001	W9V	O2-C3-C2	-3.24	101.21	112.50
3	A	1001	W9V	C15-N4-N5	3.04	126.26	123.45
3	C	1001	W9V	O2-C3-C2	-2.92	102.34	112.50
5	A	1008	PEG	O2-C3-C4	2.87	122.66	110.07
3	C	1001	W9V	C18-C15-N4	2.76	122.05	118.33
3	C	1001	W9V	C6-N1-C5	-2.72	110.35	114.20
3	C	1001	W9V	C2-C1-C21	2.44	117.02	111.68
3	C	1001	W9V	C19-C12-N2	-2.34	117.82	121.80
3	C	1001	W9V	C10-C11-N2	2.31	117.69	111.49
3	A	1001	W9V	C3-C2-C1	2.21	117.62	111.63
3	C	1001	W9V	O1-C1-C2	2.21	116.41	110.65
3	A	1001	W9V	C2-C1-C21	2.19	116.49	111.68
3	A	1001	W9V	C14-C13-C12	-2.17	119.56	121.53
3	A	1001	W9V	C6-N1-C5	-2.13	111.19	114.20
3	C	1001	W9V	C15-N4-N6	2.13	125.42	123.45
3	C	1001	W9V	C3-C2-C1	2.08	117.25	111.63
3	C	1001	W9V	C11-N2-C12	-2.03	118.50	123.39
3	A	1001	W9V	O1-C1-C2	2.02	115.91	110.65
3	C	1001	W9V	C18-C15-C14	-2.01	119.36	121.74

There are no chirality outliers.

All (110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	W9V	C4-C2-C3-O2
3	A	1001	W9V	C1-C2-C3-O2
3	C	1001	W9V	C4-C2-C3-O2
3	C	1001	W9V	C1-C2-C3-O2
9	D	2004	PG4	C5-C6-O4-C7
10	C	1020	P6G	C2-C3-O4-C5
4	B	604	PGE	O3-C5-C6-O4
4	A	1020	PGE	O2-C3-C4-O3
10	C	1020	P6G	C15-C14-O13-C12
10	C	1020	P6G	O13-C14-C15-O16
4	A	1013	PGE	O2-C3-C4-O3
4	A	1021	PGE	C3-C4-O3-C5
4	A	1024	PGE	O2-C3-C4-O3
9	B	603	PG4	C5-C6-O4-C7
5	A	1003	PEG	O2-C3-C4-O4
3	A	1001	W9V	C9-C10-C11-N2
3	C	1001	W9V	C9-C10-C11-N2
5	C	1011	PEG	C4-C3-O2-C2
9	D	2004	PG4	C4-C3-O2-C2
4	A	1002	PGE	O2-C3-C4-O3
9	B	603	PG4	C4-C3-O2-C2
5	C	1004	PEG	O2-C3-C4-O4
6	A	1010	EDO	O1-C1-C2-O2
6	C	1010	EDO	O1-C1-C2-O2
6	C	1013	EDO	O1-C1-C2-O2
3	A	1001	W9V	C14-C13-N3-O4
4	A	1021	PGE	O2-C3-C4-O3
4	A	1025	PGE	O3-C5-C6-O4
4	B	604	PGE	O1-C1-C2-O2
9	D	2004	PG4	O2-C3-C4-O3
4	C	1005	PGE	O1-C1-C2-O2
9	B	603	PG4	O2-C3-C4-O3
10	C	1020	P6G	O10-C11-C12-O13
4	A	1024	PGE	C1-C2-O2-C3
5	A	1007	PEG	O2-C3-C4-O4
6	A	1018	EDO	O1-C1-C2-O2
6	C	1003	EDO	O1-C1-C2-O2
6	C	1015	EDO	O1-C1-C2-O2
6	C	1017	EDO	O1-C1-C2-O2
3	C	1001	W9V	C6-C7-C8-C9
3	A	1001	W9V	C6-C7-C8-C9
4	A	1002	PGE	O1-C1-C2-O2
4	A	1024	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
5	A	1014	PEG	O1-C1-C2-O2
5	A	1016	PEG	O2-C3-C4-O4
5	C	1019	PEG	O2-C3-C4-O4
4	A	1013	PGE	O3-C5-C6-O4
3	C	1001	W9V	N1-C6-C7-C8
4	A	1020	PGE	O1-C1-C2-O2
5	C	1019	PEG	O1-C1-C2-O2
4	C	1018	PGE	C3-C4-O3-C5
10	C	1020	P6G	C14-C15-O16-C17
3	C	1001	W9V	C14-C13-N3-O4
10	C	1020	P6G	O16-C17-C18-O19
4	A	1024	PGE	C4-C3-O2-C2
10	C	1020	P6G	C8-C9-O10-C11
5	A	1003	PEG	C4-C3-O2-C2
4	B	604	PGE	C1-C2-O2-C3
4	A	1025	PGE	C4-C3-O2-C2
5	A	1014	PEG	C1-C2-O2-C3
4	A	1024	PGE	C6-C5-O3-C4
3	A	1001	W9V	N1-C6-C7-C8
4	A	1013	PGE	C3-C4-O3-C5
4	A	1002	PGE	C1-C2-O2-C3
4	C	1018	PGE	O3-C5-C6-O4
5	C	1004	PEG	O1-C1-C2-O2
5	C	1019	PEG	C4-C3-O2-C2
5	A	1003	PEG	C1-C2-O2-C3
5	A	1007	PEG	O1-C1-C2-O2
5	A	1016	PEG	O1-C1-C2-O2
6	A	1022	EDO	O1-C1-C2-O2
6	C	1021	EDO	O1-C1-C2-O2
4	A	1002	PGE	C3-C4-O3-C5
9	B	603	PG4	O4-C7-C8-O5
5	C	1009	PEG	C1-C2-O2-C3
4	A	1025	PGE	C1-C2-O2-C3
9	D	2004	PG4	O4-C7-C8-O5
5	C	1019	PEG	C1-C2-O2-C3
4	C	1005	PGE	C3-C4-O3-C5
4	C	1018	PGE	C4-C3-O2-C2
4	A	1021	PGE	O3-C5-C6-O4
6	A	1019	EDO	O1-C1-C2-O2
10	C	1020	P6G	C12-C11-O10-C9
9	D	2004	PG4	C1-C2-O2-C3
5	C	1004	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	A	1001	W9V	C12-C13-N3-O4
5	C	1008	PEG	C1-C2-O2-C3
4	A	1002	PGE	C4-C3-O2-C2
4	A	1025	PGE	C3-C4-O3-C5
5	C	1011	PEG	O1-C1-C2-O2
5	A	1015	PEG	C1-C2-O2-C3
4	C	1018	PGE	O2-C3-C4-O3
3	A	1001	W9V	C18-C15-N4-N6
3	C	1001	W9V	C14-C15-N4-N5
3	C	1001	W9V	C14-C15-N4-N6
3	C	1001	W9V	C18-C15-N4-N6
3	C	1001	W9V	C13-C12-N2-C11
9	B	603	PG4	C3-C4-O3-C5
9	D	2004	PG4	C8-C7-O4-C6
10	C	1020	P6G	C9-C8-O7-C6
4	A	1020	PGE	O3-C5-C6-O4
9	B	603	PG4	O3-C5-C6-O4
9	D	2004	PG4	O3-C5-C6-O4
6	A	1006	EDO	O1-C1-C2-O2
6	A	1017	EDO	O1-C1-C2-O2
6	C	1006	EDO	O1-C1-C2-O2
4	B	604	PGE	C6-C5-O3-C4
4	A	1025	PGE	O2-C3-C4-O3
4	C	1005	PGE	O2-C3-C4-O3
4	A	1002	PGE	O3-C5-C6-O4

There are no ring outliers.

24 monomers are involved in 35 short contacts:

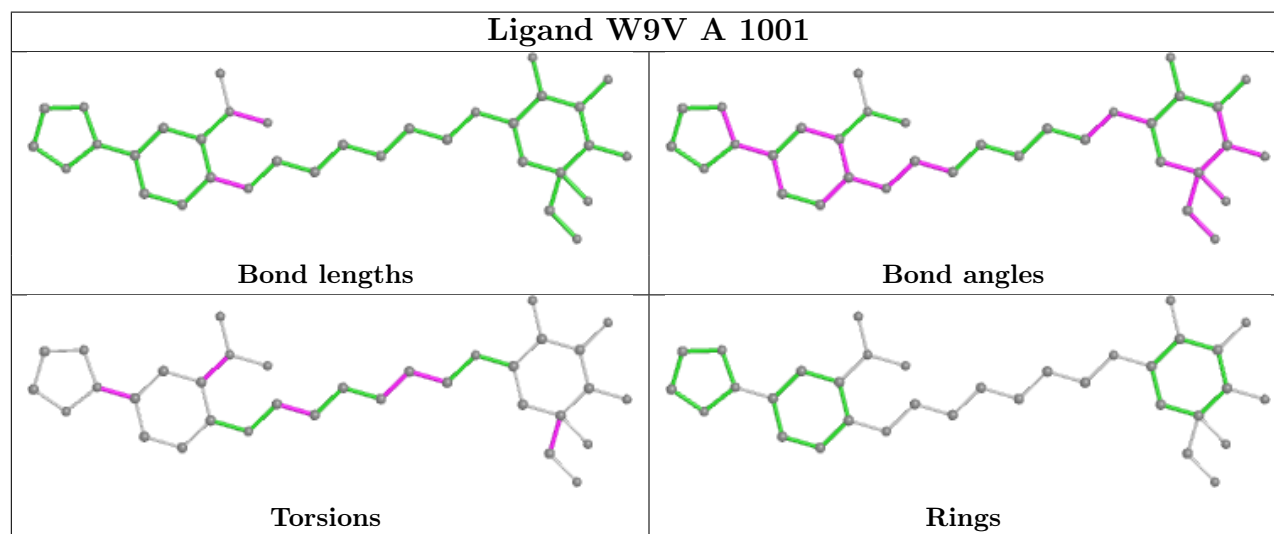
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1005	EDO	1	0
5	A	1016	PEG	2	0
9	D	2004	PG4	2	0
6	A	1023	EDO	1	0
6	C	1003	EDO	1	0
5	C	1008	PEG	2	0
5	A	1014	PEG	1	0
5	A	1008	PEG	0	2
4	B	604	PGE	1	0
6	A	1011	EDO	1	0
4	A	1013	PGE	1	0
4	A	1024	PGE	4	0

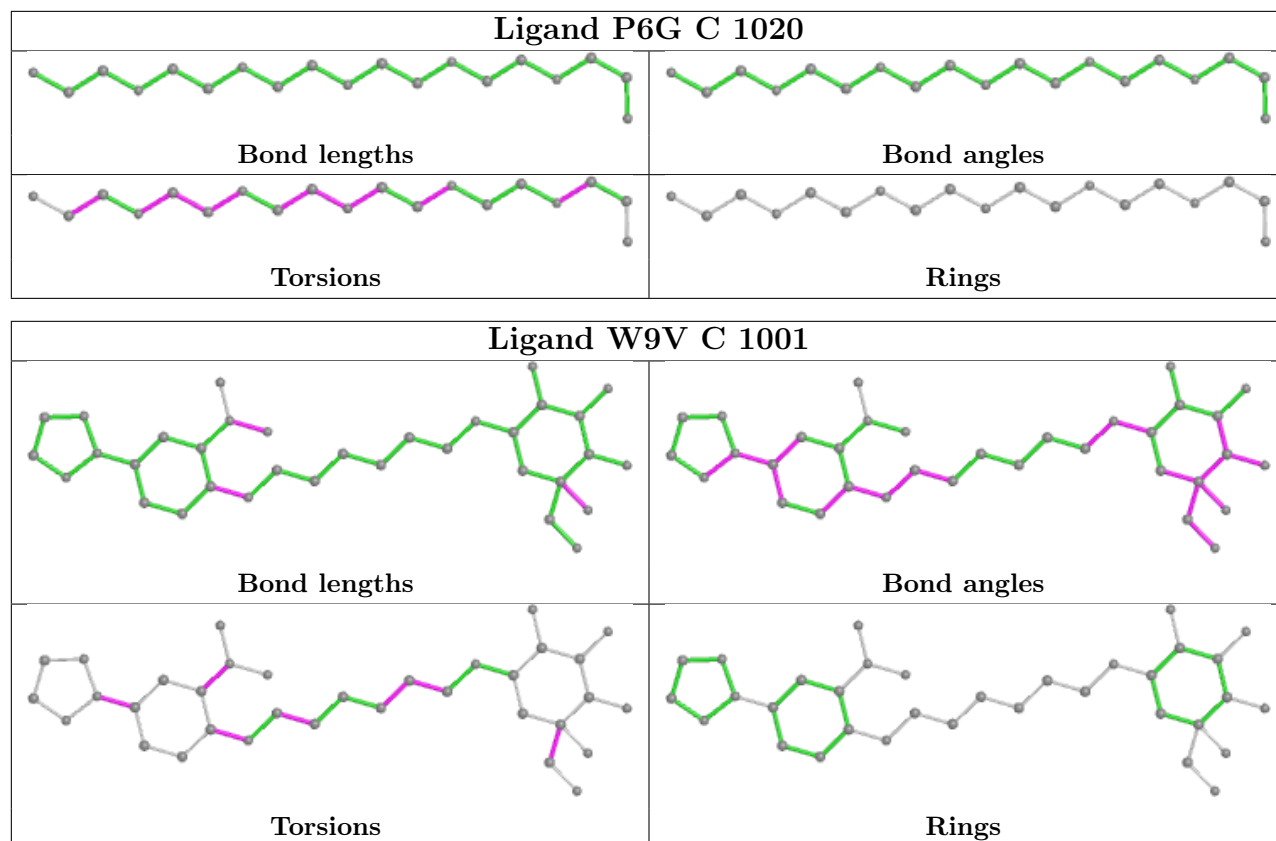
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1017	EDO	1	0
6	C	1002	EDO	3	0
5	C	1019	PEG	0	2
9	B	603	PG4	1	0
4	C	1018	PGE	2	0
6	C	1021	EDO	3	0
4	A	1025	PGE	1	0
6	A	1004	EDO	1	0
4	A	1021	PGE	1	0
6	C	1007	EDO	1	0
6	A	1019	EDO	1	0
6	C	1016	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	850/977 (87%)	0.06	42 (4%) 29 35	23, 35, 61, 102	0
1	C	857/977 (87%)	0.34	89 (10%) 6 8	24, 40, 78, 104	0
2	B	83/547 (15%)	0.89	23 (27%) 0 0	31, 49, 88, 102	0
2	D	87/547 (15%)	1.30	25 (28%) 0 0	31, 53, 100, 119	0
All	All	1877/3048 (61%)	0.28	179 (9%) 8 10	23, 38, 78, 119	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	31	TYR	9.8
2	D	43	THR	9.3
2	D	81	GLY	7.9
2	B	43	THR	7.9
1	A	248	TRP	7.4
2	D	32	GLU	7.4
1	C	57	LEU	7.0
2	D	80	THR	6.8
1	C	185	ARG	6.7
2	D	82	TYR	6.7
1	C	370	THR	6.3
2	D	44	ALA	6.2
2	D	117	ARG	6.1
1	C	34	ASP	5.8
1	C	244	GLU	5.7
2	D	48	PHE	5.5
2	B	48	PHE	5.2
1	C	69	LEU	5.1
1	C	33	VAL	5.0
2	D	84	PRO	5.0
2	B	41	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLU	4.9
1	C	245	PRO	4.8
1	A	251	THR	4.7
1	C	164	ARG	4.7
1	C	329	PHE	4.6
1	C	136	ASN	4.6
1	A	254	THR	4.5
1	A	183	ALA	4.5
1	A	255	HIS	4.3
1	C	165	SER	4.3
2	B	44	ALA	4.2
2	B	82	TYR	4.1
1	A	252	PHE	4.1
2	B	117	ARG	4.1
1	A	370	THR	4.0
2	D	41	ASP	4.0
2	D	116	CYS	4.0
1	A	164	ARG	3.9
1	C	163	ASP	3.8
1	C	127	ARG	3.7
1	C	184	PRO	3.7
2	B	39	CYS	3.6
2	D	39	CYS	3.6
1	C	141	THR	3.6
2	B	84	PRO	3.6
1	C	128	LEU	3.5
1	C	67	LEU	3.5
1	A	34	ASP	3.5
1	C	663	LEU	3.5
1	C	627	PHE	3.5
2	D	33	GLU	3.5
1	C	126	ALA	3.4
1	C	132	GLY	3.4
1	C	85	VAL	3.4
2	D	37	PHE	3.3
1	A	658	LEU	3.3
1	C	65	ASP	3.3
2	B	40	LEU	3.3
2	D	38	THR	3.3
1	C	81	GLU	3.3
1	C	144	GLU	3.3
2	B	80	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	658	LEU	3.2
1	C	135	ASP	3.2
2	B	116	CYS	3.2
1	C	131	SER	3.2
1	C	83	THR	3.1
2	D	78	THR	3.1
2	D	45	THR	3.1
1	C	661	VAL	3.1
1	A	891	GLY	3.1
2	B	81	GLY	3.0
1	A	253	LYS	3.0
1	C	330	HIS	3.0
1	C	350	ASN	3.0
1	C	371	PRO	3.0
1	A	622	LEU	3.0
1	A	665	PHE	2.9
1	C	54	ARG	2.9
1	A	663	LEU	2.9
1	C	137	SER	2.9
1	C	808	HIS	2.9
1	C	35	ARG	2.9
2	B	86	TYR	2.9
1	C	73	ALA	2.8
1	C	153	ALA	2.8
1	C	626	PHE	2.8
1	C	55	PRO	2.8
1	C	133	ARG	2.8
1	C	129	SER	2.8
2	B	113	GLU	2.8
2	D	85	LEU	2.8
1	C	70	GLY	2.7
1	C	66	THR	2.7
1	C	622	LEU	2.7
1	C	130	VAL	2.7
1	A	416	LEU	2.7
1	C	82	VAL	2.7
1	C	323	VAL	2.6
1	C	247	ALA	2.6
1	C	142	VAL	2.6
2	B	78	THR	2.6
1	C	79	ILE	2.6
2	D	36	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	143	ALA	2.6
1	C	140	LEU	2.6
1	C	84	LYS	2.5
1	C	693	PRO	2.5
1	A	163	ASP	2.5
1	C	635	ALA	2.5
1	C	254	THR	2.4
1	C	666	CYS	2.4
1	C	248	TRP	2.4
2	B	38	THR	2.4
1	C	656	LEU	2.4
2	D	83	LYS	2.4
1	A	350	ASN	2.4
1	C	625	ALA	2.4
1	C	694	PHE	2.4
1	A	943	PRO	2.4
2	B	42	GLY	2.4
1	A	329	PHE	2.3
1	C	338	LEU	2.3
2	B	79	ASN	2.3
1	C	785	HIS	2.3
2	B	115	THR	2.3
1	C	252	PHE	2.3
1	A	636	VAL	2.3
1	A	626	PHE	2.3
1	A	944	GLU	2.3
1	C	251	THR	2.3
2	B	45	THR	2.3
1	C	660	LEU	2.3
1	A	923	ALA	2.3
1	A	666	CYS	2.3
2	D	42	GLY	2.3
1	A	656	LEU	2.3
1	C	138	VAL	2.3
1	A	107	GLU	2.3
1	A	694	PHE	2.2
1	A	667	GLY	2.2
1	C	814	TYR	2.2
1	A	621	VAL	2.2
1	A	733	TRP	2.2
1	C	76	VAL	2.2
1	A	562	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	635	ALA	2.2
1	C	340	ALA	2.2
1	A	417	GLY	2.2
1	A	693	PRO	2.2
1	C	322	PRO	2.2
1	C	155	PRO	2.2
1	C	173	ARG	2.2
1	C	281	ILE	2.1
1	C	148	LYS	2.1
1	C	282	PRO	2.1
1	C	106	LEU	2.1
2	B	85	LEU	2.1
1	C	695	PHE	2.1
1	C	56	GLY	2.1
2	B	77	CYS	2.1
1	C	154	GLN	2.1
1	C	107	GLU	2.1
1	C	621	VAL	2.1
2	D	79	ASN	2.1
2	D	59	LYS	2.1
1	A	637	TRP	2.1
1	C	68	GLN	2.1
2	D	113	GLU	2.1
2	B	100	CYS	2.1
1	C	166	LEU	2.1
1	A	182	ARG	2.1
1	A	695	PHE	2.1
1	A	691	TYR	2.1
1	C	294	GLU	2.0
1	A	748	MET	2.0
1	A	770	LEU	2.0
1	C	659	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	C	1019	7/7	0.60	0.43	74,83,103,109	0
6	EDO	C	1015	4/4	0.60	0.30	46,62,63,70	0
6	EDO	A	1017	4/4	0.62	0.29	61,67,77,87	0
6	EDO	C	1012	4/4	0.65	0.70	89,94,101,104	0
6	EDO	A	1018	4/4	0.65	0.16	58,59,60,61	0
6	EDO	A	1010	4/4	0.67	0.36	53,59,66,66	0
5	PEG	A	1007	7/7	0.74	0.19	59,69,82,92	0
10	P6G	C	1020	19/19	0.74	0.25	48,76,89,89	0
6	EDO	A	1011	4/4	0.76	0.28	59,70,70,84	0
5	PEG	A	1003	7/7	0.77	0.19	43,62,69,83	0
5	PEG	A	1008	7/7	0.77	0.64	59,62,80,83	7
9	PG4	D	2004	13/13	0.78	0.18	54,68,79,82	0
4	PGE	A	1021	10/10	0.79	0.24	51,64,72,80	0
4	PGE	C	1018	10/10	0.82	0.24	37,53,73,79	0
9	PG4	B	603	13/13	0.82	0.18	54,69,70,74	0
5	PEG	C	1009	7/7	0.83	0.20	49,61,72,85	0
6	EDO	C	1010	4/4	0.84	0.18	49,51,52,53	0
5	PEG	C	1014	7/7	0.84	0.28	53,67,79,83	0
4	PGE	C	1005	10/10	0.84	0.17	40,57,66,73	0
6	EDO	C	1003	4/4	0.85	0.17	55,61,65,71	0
4	PGE	A	1020	10/10	0.85	0.29	55,65,83,92	0
7	SO4	A	1027	5/5	0.85	0.26	80,89,94,119	0
4	PGE	B	604	10/10	0.86	0.34	56,68,82,88	0
5	PEG	A	1016	7/7	0.86	0.27	49,57,72,74	0
5	PEG	C	1008	7/7	0.86	0.23	53,56,76,77	0
4	PGE	A	1024	10/10	0.87	0.32	38,57,70,73	0
6	EDO	C	1021	4/4	0.87	0.31	62,73,80,82	0
6	EDO	C	1013	4/4	0.87	0.25	51,51,56,68	0
3	W9V	A	1001	34/34	0.88	0.21	23,62,102,113	0
5	PEG	A	1015	7/7	0.89	0.23	49,64,75,83	0
7	SO4	A	1028	5/5	0.89	0.30	77,95,101,132	0
4	PGE	A	1002	10/10	0.89	0.15	51,62,75,75	0
6	EDO	C	1007	4/4	0.89	0.14	52,52,66,72	0
3	W9V	C	1001	34/34	0.89	0.18	24,51,97,107	0
4	PGE	A	1025	10/10	0.90	0.29	55,61,70,80	0
7	SO4	C	1022	5/5	0.90	0.23	72,77,86,93	0
6	EDO	A	1009	4/4	0.90	0.18	55,57,64,68	0

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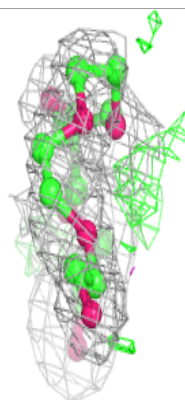
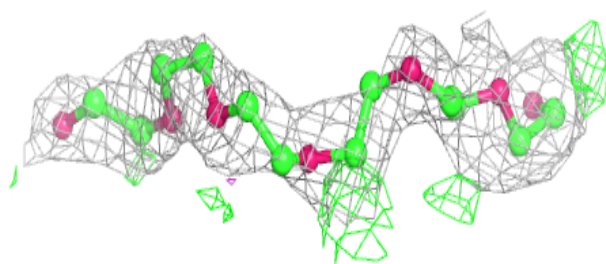
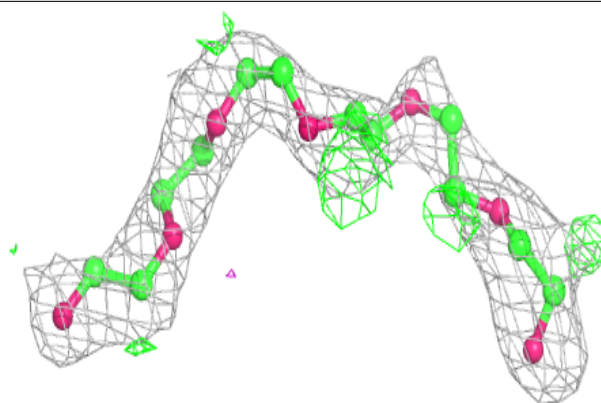
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PGE	A	1013	10/10	0.90	0.20	57,65,71,71	0
6	EDO	C	1002	4/4	0.90	0.20	49,52,55,75	0
6	EDO	A	1019	4/4	0.91	0.16	44,56,56,69	0
7	SO4	A	1029	5/5	0.91	0.50	70,81,106,126	0
6	EDO	C	1017	4/4	0.91	0.39	59,60,66,76	0
7	SO4	A	1026	5/5	0.92	0.18	59,67,79,103	0
7	SO4	C	1023	5/5	0.92	0.22	61,65,87,95	0
5	PEG	C	1004	7/7	0.92	0.30	51,63,75,80	0
6	EDO	C	1016	4/4	0.92	0.18	38,41,47,51	0
6	EDO	D	2001	4/4	0.92	0.10	42,54,55,64	0
6	EDO	A	1004	4/4	0.93	0.18	54,55,55,60	0
5	PEG	A	1014	7/7	0.93	0.21	58,62,76,80	0
5	PEG	C	1011	7/7	0.93	0.17	45,56,67,90	0
6	EDO	A	1022	4/4	0.94	0.17	46,56,60,63	0
6	EDO	A	1005	4/4	0.95	0.11	38,38,39,50	0
6	EDO	A	1012	4/4	0.95	0.10	35,36,39,43	0
6	EDO	D	2005	4/4	0.96	0.16	46,52,54,58	0
6	EDO	A	1023	4/4	0.96	0.09	42,46,46,57	0
6	EDO	C	1006	4/4	0.97	0.11	47,51,60,66	0
6	EDO	A	1006	4/4	0.97	0.20	50,50,55,66	0
8	CA	D	2002	1/1	0.98	0.07	40,40,40,40	0
8	CA	B	601	1/1	0.98	0.07	39,39,39,39	0
8	CA	D	2003	1/1	0.99	0.06	33,33,33,33	0
8	CA	B	602	1/1	0.99	0.07	34,34,34,34	0

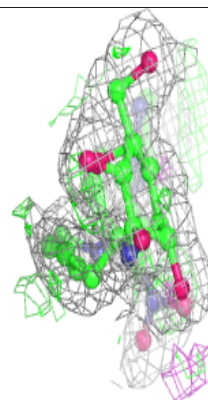
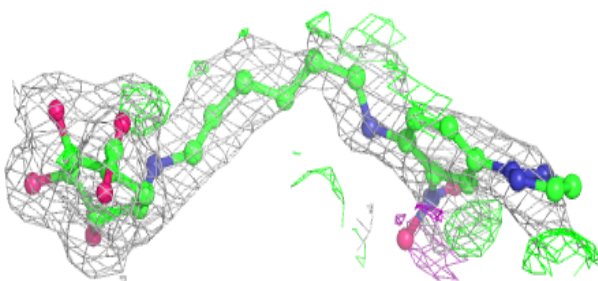
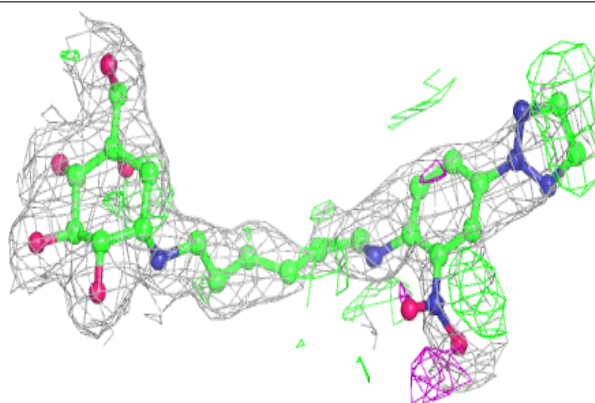
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P6G C 1020:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

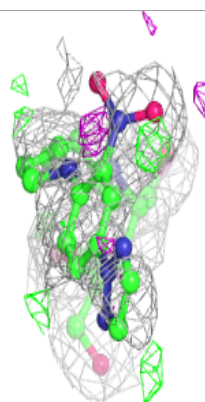
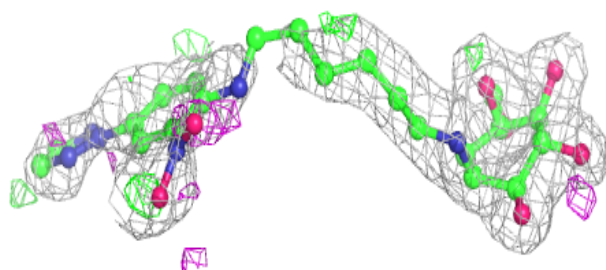
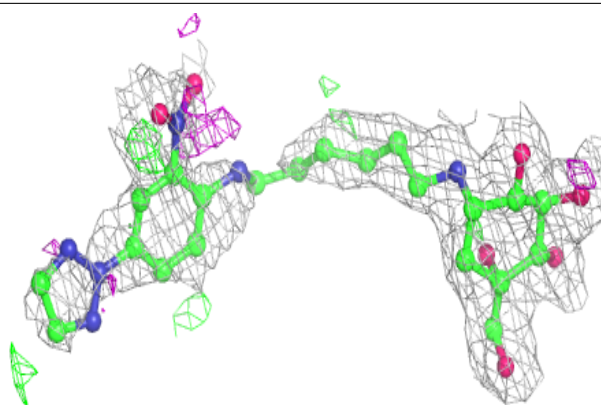
**Electron density around W9V A 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around W9V C 1001:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.