



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 12:43 PM EDT

PDB ID : 7KBR
Title : Co-crystal structure of alpha glucosidase with compound 10
Authors : Karade, S.S.; Mariuzza, R.A.
Deposited on : 2020-10-02
Resolution : 2.09 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 : 2.23.2
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) : 2.23.2

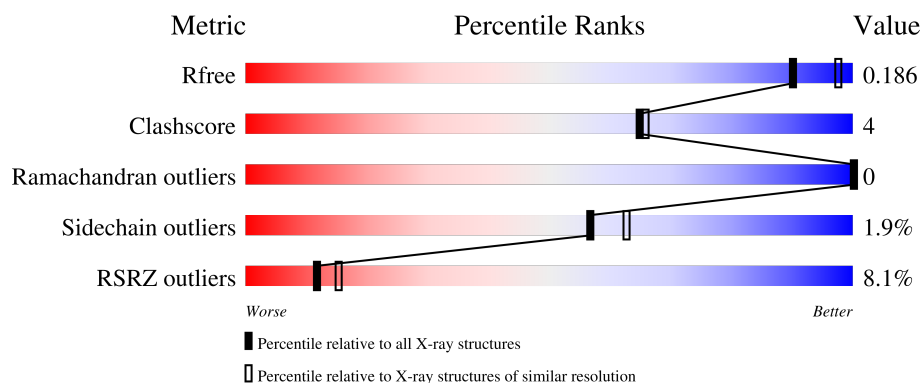
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	G	183	<div> <div>3%</div> <div>74%</div> <div>8%</div> <div>17%</div> </div>
1	I	183	<div> <div>21%</div> <div>70%</div> <div>13%</div> <div>17%</div> </div>
2	H	107	<div> <div>6%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
2	J	107	<div> <div>14%</div> <div>89%</div> <div>11%</div> </div>
3	A	609	<div> <div>4%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	609	
4	B	134	
4	D	134	

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	EDO	A	1101	-	-	-	X
5	EDO	C	1105	-	-	-	X
6	PEG	C	1104	-	-	X	-
6	PEG	C	1115	-	-	-	X
7	SO4	C	1122	-	-	X	-
7	SO4	G	1304	-	-	-	X
8	PGE	A	1106	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 16766 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 Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	151	Total	C	N	O	S	0	1	0
			1205	756	223	222	4			
1	I	152	Total	C	N	O	S	0	0	0
			1180	745	211	220	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2	MET	-	initiating methionine	UNP Q8BHN3
G	3	GLY	-	expression tag	UNP Q8BHN3
G	4	ILE	-	expression tag	UNP Q8BHN3
G	5	LEU	-	expression tag	UNP Q8BHN3
G	6	PRO	-	expression tag	UNP Q8BHN3
G	7	SER	-	expression tag	UNP Q8BHN3
G	8	PRO	-	expression tag	UNP Q8BHN3
G	9	GLY	-	expression tag	UNP Q8BHN3
G	10	MET	-	expression tag	UNP Q8BHN3
G	11	PRO	-	expression tag	UNP Q8BHN3
G	12	ALA	-	expression tag	UNP Q8BHN3
G	13	LEU	-	expression tag	UNP Q8BHN3
G	14	LEU	-	expression tag	UNP Q8BHN3
G	15	SER	-	expression tag	UNP Q8BHN3
G	16	LEU	-	expression tag	UNP Q8BHN3
G	17	VAL	-	expression tag	UNP Q8BHN3
G	18	SER	-	expression tag	UNP Q8BHN3
G	19	LEU	-	expression tag	UNP Q8BHN3
G	20	LEU	-	expression tag	UNP Q8BHN3
G	21	SER	-	expression tag	UNP Q8BHN3
G	22	VAL	-	expression tag	UNP Q8BHN3
G	23	LEU	-	expression tag	UNP Q8BHN3
G	24	LEU	-	expression tag	UNP Q8BHN3
G	25	MET	-	expression tag	UNP Q8BHN3
G	26	GLY	-	expression tag	UNP Q8BHN3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	27	CYS	-	expression tag	UNP Q8BHN3
G	28	VAL	-	expression tag	UNP Q8BHN3
G	29	ALA	-	expression tag	UNP Q8BHN3
G	30	GLU	-	expression tag	UNP Q8BHN3
G	31	THR	-	expression tag	UNP Q8BHN3
G	32	GLY	-	expression tag	UNP Q8BHN3
G	97	ASP	ASN	engineered mutation	UNP Q8BHN3
I	2	MET	-	initiating methionine	UNP Q8BHN3
I	3	GLY	-	expression tag	UNP Q8BHN3
I	4	ILE	-	expression tag	UNP Q8BHN3
I	5	LEU	-	expression tag	UNP Q8BHN3
I	6	PRO	-	expression tag	UNP Q8BHN3
I	7	SER	-	expression tag	UNP Q8BHN3
I	8	PRO	-	expression tag	UNP Q8BHN3
I	9	GLY	-	expression tag	UNP Q8BHN3
I	10	MET	-	expression tag	UNP Q8BHN3
I	11	PRO	-	expression tag	UNP Q8BHN3
I	12	ALA	-	expression tag	UNP Q8BHN3
I	13	LEU	-	expression tag	UNP Q8BHN3
I	14	LEU	-	expression tag	UNP Q8BHN3
I	15	SER	-	expression tag	UNP Q8BHN3
I	16	LEU	-	expression tag	UNP Q8BHN3
I	17	VAL	-	expression tag	UNP Q8BHN3
I	18	SER	-	expression tag	UNP Q8BHN3
I	19	LEU	-	expression tag	UNP Q8BHN3
I	20	LEU	-	expression tag	UNP Q8BHN3
I	21	SER	-	expression tag	UNP Q8BHN3
I	22	VAL	-	expression tag	UNP Q8BHN3
I	23	LEU	-	expression tag	UNP Q8BHN3
I	24	LEU	-	expression tag	UNP Q8BHN3
I	25	MET	-	expression tag	UNP Q8BHN3
I	26	GLY	-	expression tag	UNP Q8BHN3
I	27	CYS	-	expression tag	UNP Q8BHN3
I	28	VAL	-	expression tag	UNP Q8BHN3
I	29	ALA	-	expression tag	UNP Q8BHN3
I	30	GLU	-	expression tag	UNP Q8BHN3
I	31	THR	-	expression tag	UNP Q8BHN3
I	32	GLY	-	expression tag	UNP Q8BHN3
I	97	ASP	ASN	engineered mutation	UNP Q8BHN3

- Molecule 2 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	105	Total	C	N	O	S	0	1	0
			841	542	138	159	2			
2	J	107	Total	C	N	O	S	0	0	0
			853	550	138	163	2			

- Molecule 3 is a protein called Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	597	Total	C	N	O	S	0	9	0
			4886	3139	838	886	23			
3	C	597	Total	C	N	O	S	0	12	0
			4898	3150	841	883	24			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	967	SER	-	expression tag	UNP Q8BHN3
A	968	ALA	-	expression tag	UNP Q8BHN3
A	969	TRP	-	expression tag	UNP Q8BHN3
A	970	SER	-	expression tag	UNP Q8BHN3
A	971	HIS	-	expression tag	UNP Q8BHN3
A	972	PRO	-	expression tag	UNP Q8BHN3
A	973	GLN	-	expression tag	UNP Q8BHN3
A	974	PHE	-	expression tag	UNP Q8BHN3
A	975	GLU	-	expression tag	UNP Q8BHN3
A	976	LYS	-	expression tag	UNP Q8BHN3
A	977	LEU	-	expression tag	UNP Q8BHN3
A	978	GLU	-	expression tag	UNP Q8BHN3
C	967	SER	-	expression tag	UNP Q8BHN3
C	968	ALA	-	expression tag	UNP Q8BHN3
C	969	TRP	-	expression tag	UNP Q8BHN3
C	970	SER	-	expression tag	UNP Q8BHN3
C	971	HIS	-	expression tag	UNP Q8BHN3
C	972	PRO	-	expression tag	UNP Q8BHN3
C	973	GLN	-	expression tag	UNP Q8BHN3
C	974	PHE	-	expression tag	UNP Q8BHN3
C	975	GLU	-	expression tag	UNP Q8BHN3
C	976	LYS	-	expression tag	UNP Q8BHN3
C	977	LEU	-	expression tag	UNP Q8BHN3
C	978	GLU	-	expression tag	UNP Q8BHN3

- Molecule 4 is a protein called Glucosidase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	83	Total	C	N	O	S	0	0	0
			597	353	98	136	10			
4	D	84	Total	C	N	O	S	0	0	0
			602	359	96	137	10			

There are 62 discrepancies between the modelled and reference sequences:

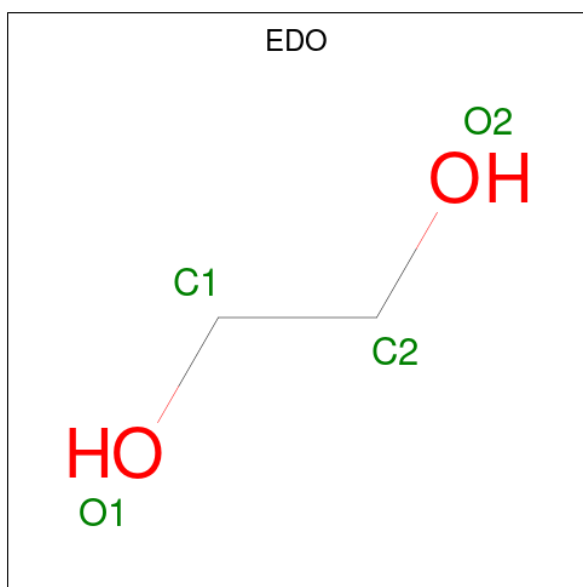
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP O08795
B	-15	GLY	-	expression tag	UNP O08795
B	-14	ILE	-	expression tag	UNP O08795
B	-13	LEU	-	expression tag	UNP O08795
B	-12	PRO	-	expression tag	UNP O08795
B	-11	SER	-	expression tag	UNP O08795
B	-10	PRO	-	expression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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	PRO	-	expression tag	UNP O08795
D	-11	SER	-	expression tag	UNP O08795
D	-10	PRO	-	expression tag	UNP O08795
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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



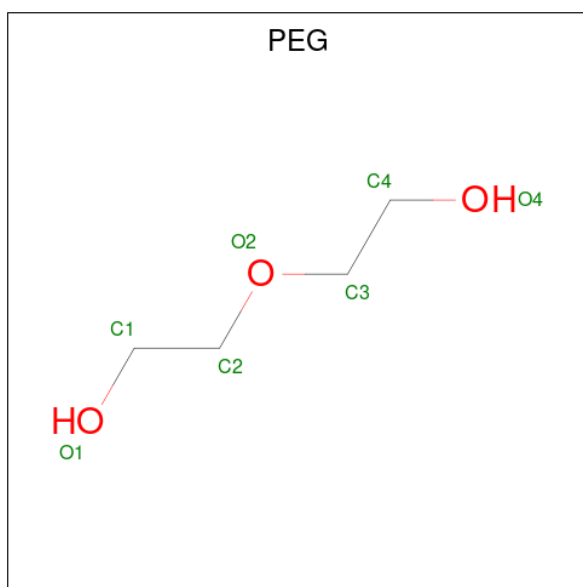
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

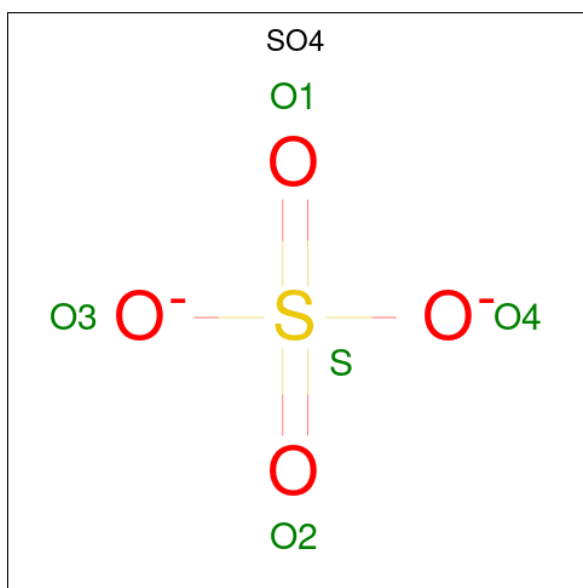
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	I	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	J	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



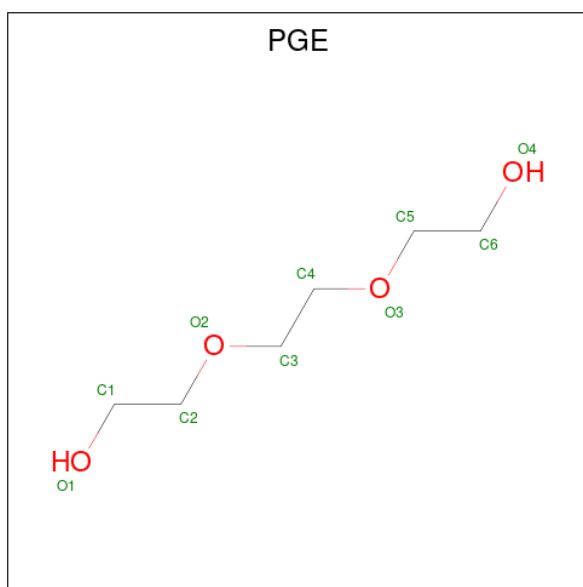
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total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

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



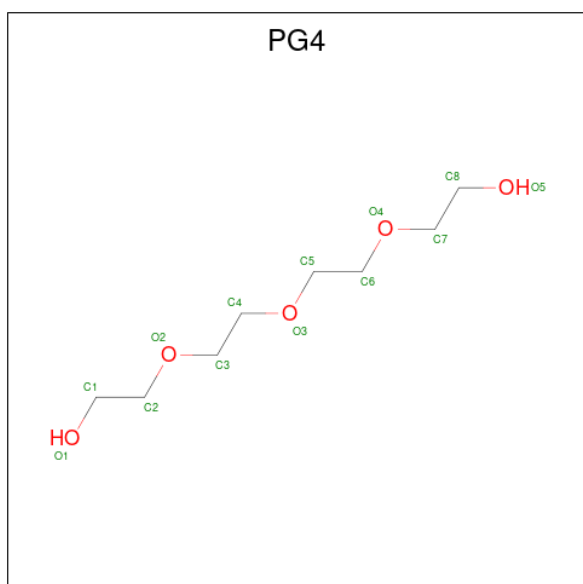
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



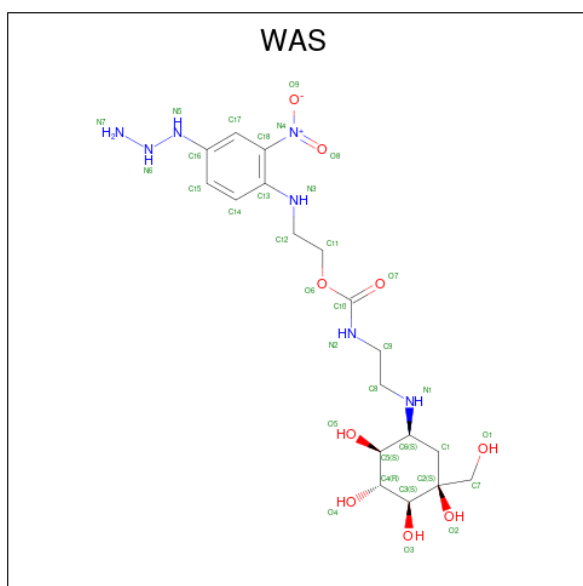
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	B	1	Total	C	O	0	0
			10	6	4		

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



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

- Molecule 10 is 2-{[2-nitro-4-(triazan-1-yl)phenyl]amino}ethyl (2-{[(1S,2S,3R,4S,5S)-2,3,4,5-tetrahydroxy-5-(hydroxymethyl)cyclohexyl]amino}ethyl)carbamate (three-letter code: WAS) (formula: C₁₈H₃₁N₇O₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			34	18	7	9		
10	C	1	Total	C	N	O	0	0
			34	18	7	9		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

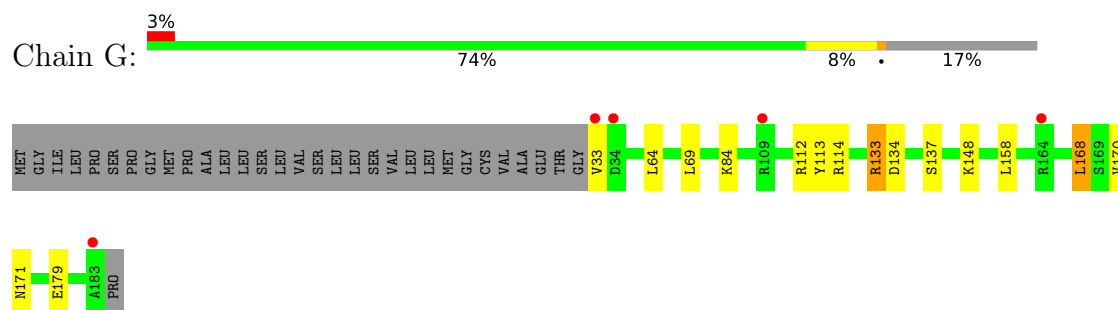
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	G	116	Total 116	O 116	0	0
12	H	69	Total 69	O 69	0	0
12	A	481	Total 481	O 481	0	0
12	B	42	Total 42	O 42	0	0
12	I	64	Total 64	O 64	0	0
12	J	57	Total 57	O 57	0	0
12	C	411	Total 411	O 411	0	0
12	D	41	Total 41	O 41	0	0

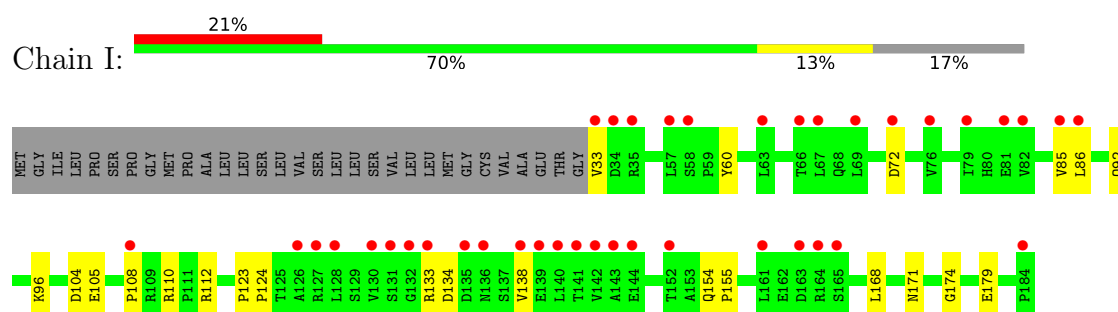
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

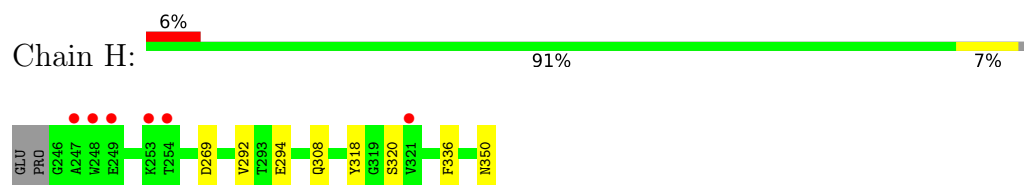
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1



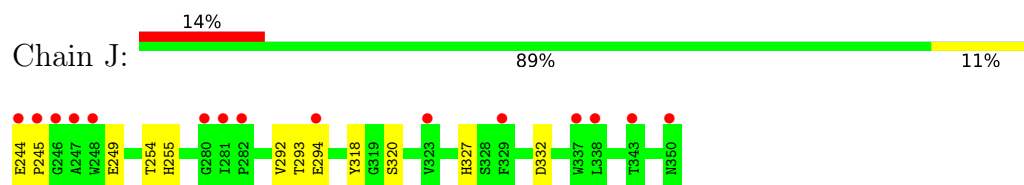
- Molecule 1: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #1



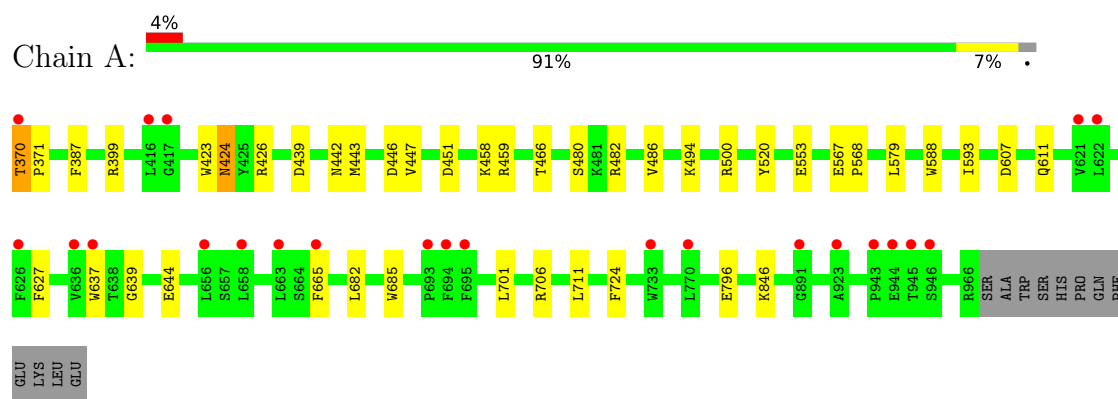
- Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2



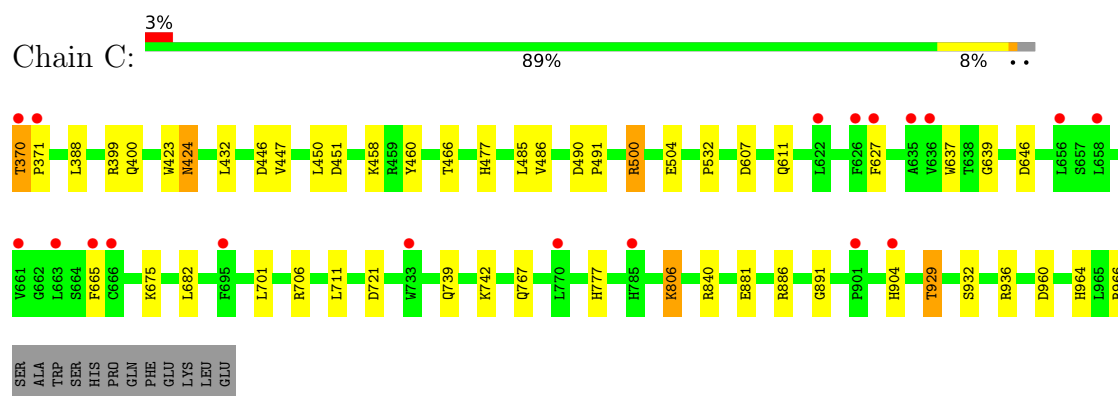
- Molecule 2: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #2



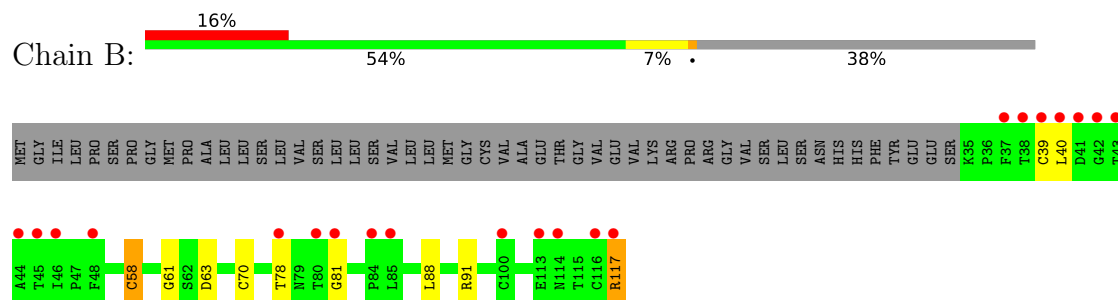
- Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3



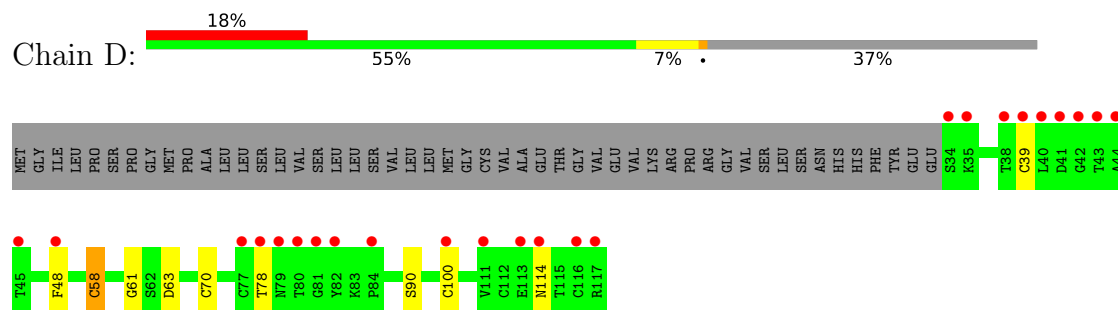
• Molecule 3: Neutral alpha-glucosidase AB Trypsin-cleaved Fragment #3



• Molecule 4: Glucosidase 2 subunit beta



• Molecule 4: 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	102.81Å 102.81Å 240.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.33 – 2.09 42.33 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.33-2.09) 93.4 (42.33-2.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.163 , 0.186 0.164 , 0.186	Depositor DCC
R_{free} test set	2025 reflections (1.21%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	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 0.035 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16766	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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, WAS, CA, PEG, SO4, PG4, PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.31	0/1224	0.56	1/1659 (0.1%)
1	I	0.28	0/1200	0.50	0/1632
2	H	0.36	0/869	0.56	0/1187
2	J	0.32	0/882	0.54	0/1205
3	A	0.37	0/5063	0.55	0/6897
3	C	0.35	0/5082	0.54	0/6922
4	B	0.37	0/608	0.60	0/831
4	D	0.45	0/614	0.61	0/842
All	All	0.35	0/15542	0.55	1/21175 (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	G	168	LEU	CA-CB-CG	5.17	127.18	115.30

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	G	1205	0	1237	10	0
1	I	1180	0	1197	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	841	0	784	7	0
2	J	853	0	796	10	0
3	A	4886	0	4643	31	0
3	C	4898	0	4662	39	0
4	B	597	0	493	9	0
4	D	602	0	491	4	0
5	A	44	0	64	4	0
5	B	8	0	12	0	0
5	C	44	0	66	5	0
5	D	4	0	6	0	0
5	G	8	0	12	1	0
5	H	4	0	6	0	0
5	I	4	0	6	0	0
5	J	8	0	12	1	0
6	A	42	0	60	1	0
6	C	49	0	68	8	0
6	G	7	0	8	2	0
7	A	15	0	0	0	0
7	B	5	0	0	0	0
7	C	10	0	0	3	0
7	G	5	0	0	0	0
7	H	5	0	0	0	0
8	A	40	0	56	11	0
8	B	10	0	14	1	0
9	A	13	0	18	0	0
9	C	13	0	18	0	0
9	D	13	0	18	0	0
10	A	34	0	0	0	0
10	C	34	0	0	1	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
12	A	481	0	0	7	0
12	B	42	0	0	2	0
12	C	411	0	0	5	2
12	D	41	0	0	1	0
12	G	116	0	0	2	3
12	H	69	0	0	2	0
12	I	64	0	0	8	1
12	J	57	0	0	4	0
All	All	16766	0	14747	123	3

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 (123) 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)
3:C:399:ARG:NH1	12:C:1201:HOH:O	1.92	1.02
1:I:33:VAL:N	12:I:1401:HOH:O	1.97	0.97
3:A:553:GLU:OE2	12:A:1201:HOH:O	1.83	0.95
3:A:796:GLU:OE1	12:A:1202:HOH:O	1.86	0.94
3:A:399:ARG:NH1	12:A:1203:HOH:O	2.03	0.90
3:C:886:ARG:NH1	12:C:1202:HOH:O	1.97	0.90
3:C:964[A]:HIS:HD2	3:C:966:ARG:HE	1.25	0.85
3:C:960:ASP:HB3	6:C:1115:PEG:H22	1.62	0.80
3:C:675:LYS:H	6:C:1104:PEG:H42	1.46	0.80
1:I:60:TYR:OH	12:I:1402:HOH:O	2.01	0.78
3:A:607[B]:ASP:OD2	3:A:611:GLN:NE2	2.17	0.78
2:H:350:ASN:ND2	12:H:1301:HOH:O	2.22	0.72
3:C:607[B]:ASP:OD2	3:C:611:GLN:NE2	2.22	0.72
4:B:81:GLY:N	12:B:301:HOH:O	2.15	0.68
8:A:1106:PGE:H5	4:B:91:ARG:HH21	1.59	0.67
3:C:891:GLY:O	12:C:1204:HOH:O	2.14	0.65
1:I:133:ARG:NH1	1:I:134:ASP:O	2.30	0.65
3:A:846:LYS:HB2	5:A:1105:EDO:H11	1.78	0.64
2:J:249:GLU:OE2	12:J:1501:HOH:O	2.14	0.63
3:A:644:GLU:OE2	12:A:1204:HOH:O	2.15	0.63
1:I:104:ASP:OD2	12:I:1405:HOH:O	2.16	0.61
1:I:110:ARG:NH2	12:I:1409:HOH:O	2.30	0.60
1:G:134:ASP:HA	6:G:1303:PEG:H31	1.82	0.60
6:C:1101:PEG:H11	12:D:313:HOH:O	2.01	0.60
1:I:112:ARG:NH2	1:I:179:GLU:O	2.36	0.58
3:C:423:TRP:O	3:C:701:LEU:HA	2.03	0.58
4:B:88:LEU:HD23	8:B:203:PGE:H2	1.85	0.58
3:C:682:LEU:HD23	3:C:711:LEU:HD11	1.85	0.58
2:J:293:THR:HG22	5:J:1401:EDO:H12	1.86	0.57
3:C:739:GLN:HG2	5:C:1116:EDO:H12	1.87	0.57
1:G:33:VAL:N	12:G:1406:HOH:O	2.38	0.57
5:A:1118:EDO:O2	12:A:1206:HOH:O	2.18	0.57
6:C:1101:PEG:H41	4:D:90:SER:OG	2.05	0.57
3:A:426:ARG:NH1	12:A:1205:HOH:O	2.17	0.56
4:B:117:ARG:NH1	12:B:302:HOH:O	2.29	0.56
1:I:85:VAL:HA	12:I:1403:HOH:O	2.04	0.56
3:C:742:LYS:NZ	12:C:1208:HOH:O	2.35	0.56
3:C:929:THR:HG23	3:C:932:SER:HB2	1.88	0.56
3:A:399:ARG:NE	12:A:1207:HOH:O	2.37	0.55
3:C:840:ARG:HA	6:C:1101:PEG:H12	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:675:LYS:N	6:C:1104:PEG:H42	2.20	0.55
3:A:682:LEU:HD23	3:A:711:LEU:HD11	1.89	0.55
1:G:148:LYS:NZ	12:G:1401:HOH:O	2.12	0.54
3:A:439:ASP:HA	8:A:1106:PGE:H62	1.90	0.54
1:I:133:ARG:HD2	1:I:138:VAL:HG22	1.90	0.54
1:G:133[B]:ARG:HG2	1:G:134:ASP:N	2.23	0.53
1:I:168:LEU:HD11	3:C:388:LEU:HD13	1.91	0.53
4:D:58:CYS:HB2	4:D:63:ASP:OD1	2.08	0.52
3:A:480:SER:HA	6:A:1112:PEG:H22	1.90	0.52
1:I:86:LEU:N	12:I:1403:HOH:O	2.06	0.52
2:J:292:VAL:HG12	2:J:294:GLU:H	1.75	0.52
1:G:112:ARG:NH2	1:G:179:GLU:O	2.43	0.52
3:C:739:GLN:HG2	5:C:1116:EDO:C1	2.40	0.51
3:C:491:PRO:O	3:C:532:PRO:HD2	2.11	0.51
3:A:466:THR:HB	3:C:458:LYS:HE2	1.92	0.51
3:C:675:LYS:HA	6:C:1104:PEG:H12	1.92	0.51
1:I:96:LYS:HB3	5:C:1117:EDO:H12	1.92	0.51
4:B:58:CYS:HB2	4:B:63:ASP:OD1	2.10	0.50
3:A:459:ARG:NH1	3:A:494:LYS:HE2	2.27	0.50
3:C:936:ARG:NH1	7:C:1122:SO4:O3	2.44	0.50
3:C:806:LYS:NZ	7:C:1121:SO4:O4	2.42	0.50
3:C:964[A]:HIS:CD2	3:C:966:ARG:HE	2.17	0.50
2:H:318:TYR:CE2	3:A:639:GLY:HA3	2.47	0.50
2:J:249:GLU:CG	12:J:1501:HOH:O	2.60	0.49
3:A:423:TRP:O	3:A:701:LEU:HA	2.12	0.49
8:A:1106:PGE:H5	4:B:91:ARG:NH2	2.27	0.49
3:C:400:GLN:HE21	5:C:1117:EDO:H11	1.78	0.49
3:C:450:LEU:HG	3:C:485:LEU:HD21	1.96	0.48
1:I:171:ASN:N	12:I:1414:HOH:O	2.46	0.47
6:C:1104:PEG:H22	6:C:1104:PEG:H41	1.62	0.47
3:C:721[A]:ASP:OD1	12:C:1205:HOH:O	2.20	0.47
3:C:500:ARG:NE	3:C:504[A]:GLU:OE2	2.43	0.47
3:C:370:THR:N	3:C:371:PRO:HD2	2.29	0.47
3:A:588:TRP:HE1	8:A:1111:PGE:H2	1.80	0.46
3:A:370:THR:N	3:A:371:PRO:HD2	2.31	0.46
3:A:442:ASN:ND2	8:A:1106:PGE:O3	2.49	0.46
2:H:320:SER:O	3:A:627:PHE:HA	2.16	0.46
2:J:255:HIS:HE1	12:J:1552:HOH:O	1.98	0.45
3:C:432:LEU:HD22	3:C:477[B]:HIS:ND1	2.32	0.45
1:G:114:ARG:H	8:A:1111:PGE:H5	1.80	0.45
3:A:424:ASN:OD1	3:A:451:ASP:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:TYR:CZ	3:A:593:ILE:HG22	2.52	0.45
1:I:105:GLU:HB2	1:I:108:PRO:HB3	1.99	0.45
4:B:61:GLY:HA2	4:B:70:CYS:SG	2.57	0.44
3:C:424:ASN:OD1	3:C:451:ASP:HB3	2.17	0.43
6:G:1303:PEG:H31	6:G:1303:PEG:H11	1.76	0.43
3:A:846:LYS:HB2	5:A:1105:EDO:C1	2.46	0.43
8:A:1106:PGE:C5	4:B:91:ARG:HH21	2.28	0.43
3:A:520:TYR:HE2	3:A:579:LEU:HD12	1.83	0.43
3:A:724:PHE:CZ	8:A:1106:PGE:H3	2.54	0.43
4:D:100:CYS:O	4:D:114:ASN:HA	2.19	0.43
3:A:458:LYS:HE2	3:C:466:THR:HB	2.00	0.42
2:J:327:HIS:ND1	2:J:332:ASP:OD1	2.36	0.42
1:G:64:LEU:N	5:G:1301:EDO:H11	2.34	0.42
1:G:171:ASN:HA	2:H:269:ASP:OD1	2.19	0.42
3:C:721[B]:ASP:OD1	5:C:1119:EDO:O1	2.29	0.42
3:A:447:VAL:HG11	3:A:486:VAL:HG23	2.02	0.42
8:A:1103:PGE:H42	8:A:1103:PGE:H6	1.75	0.42
2:J:320:SER:O	3:C:627:PHE:HA	2.19	0.42
2:J:244:GLU:HB3	2:J:245:PRO:HD3	2.00	0.42
3:C:447:VAL:HG11	3:C:486:VAL:HG23	2.00	0.42
3:A:567:GLU:N	3:A:568:PRO:HA	2.34	0.42
1:I:174:GLY:O	12:I:1407:HOH:O	2.22	0.42
2:H:292:VAL:HG12	2:H:294:GLU:H	1.85	0.42
3:C:936:ARG:HG2	7:C:1122:SO4:O1	2.20	0.42
2:H:308:GLN:NE2	12:H:1305:HOH:O	2.52	0.41
3:A:588:TRP:NE1	8:A:1111:PGE:H2	2.35	0.41
3:A:443:MET:N	8:A:1106:PGE:H6	2.35	0.41
2:J:318:TYR:CE2	3:C:639:GLY:HA3	2.56	0.41
1:G:158:LEU:HB2	1:G:170:VAL:HB	2.02	0.41
3:C:881:GLU:HA	3:C:904:HIS:O	2.21	0.41
3:C:460:TYR:CE2	3:C:490:ASP:HB2	2.55	0.41
1:I:154:GLN:HA	1:I:155:PRO:HA	1.96	0.41
2:J:249:GLU:HG3	12:J:1501:HOH:O	2.20	0.41
2:H:336:PHE:HB3	3:A:387:PHE:HB2	2.03	0.41
1:I:72:ASP:O	1:I:92:GLN:HG2	2.21	0.41
4:B:40:LEU:HD23	4:B:40:LEU:HA	1.85	0.40
1:I:123:PRO:HA	1:I:124:PRO:HD3	1.96	0.40
3:C:767:GLN:HG2	3:C:777:HIS:HB2	2.02	0.40
10:C:1120:WAS:C12	10:C:1120:WAS:O9	2.69	0.40
4:D:61:GLY:HA2	4:D:70:CYS:SG	2.61	0.40
3:A:482:ARG:HH12	5:A:1113:EDO:H21	1.86	0.40

All (3) 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)
12:G:1487:HOH:O	12:C:1518:HOH:O[2_564]	1.83	0.37
12:G:1487:HOH:O	12:C:1582:HOH:O[2_564]	1.91	0.29
12:G:1488:HOH:O	12:I:1425:HOH:O[2_664]	1.94	0.26

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	G	150/183 (82%)	147 (98%)	3 (2%)	0	100	100
1	I	150/183 (82%)	146 (97%)	4 (3%)	0	100	100
2	H	104/107 (97%)	97 (93%)	7 (7%)	0	100	100
2	J	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
3	A	604/609 (99%)	587 (97%)	17 (3%)	0	100	100
3	C	607/609 (100%)	591 (97%)	16 (3%)	0	100	100
4	B	81/134 (60%)	79 (98%)	2 (2%)	0	100	100
4	D	82/134 (61%)	80 (98%)	2 (2%)	0	100	100
All	All	1883/2066 (91%)	1825 (97%)	58 (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	G	135/162 (83%)	129 (96%)	6 (4%)	28	28
1	I	131/162 (81%)	131 (100%)	0	100	100
2	H	90/92 (98%)	90 (100%)	0	100	100
2	J	92/92 (100%)	91 (99%)	1 (1%)	73	79
3	A	525/529 (99%)	517 (98%)	8 (2%)	65	71
3	C	526/529 (99%)	517 (98%)	9 (2%)	60	67
4	B	68/116 (59%)	64 (94%)	4 (6%)	19	17
4	D	68/116 (59%)	64 (94%)	4 (6%)	19	17
All	All	1635/1798 (91%)	1603 (98%)	32 (2%)	57	60

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	69	LEU
1	G	84	LYS
1	G	133[A]	ARG
1	G	133[B]	ARG
1	G	137	SER
1	G	168	LEU
3	A	370	THR
3	A	424	ASN
3	A	446	ASP
3	A	500	ARG
3	A	637	TRP
3	A	665	PHE
3	A	685	TRP
3	A	706	ARG
4	B	39	CYS
4	B	58	CYS
4	B	78	THR
4	B	117	ARG
2	J	254	THR
3	C	370	THR
3	C	424	ASN
3	C	446	ASP
3	C	500	ARG
3	C	637	TRP
3	C	665	PHE
3	C	706	ARG
3	C	806	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	929	THR
4	D	39	CYS
4	D	48	PHE
4	D	58	CYS
4	D	78	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	508	HIS
3	C	611	GLN
3	C	808	HIS

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 67 ligands modelled in this entry, 4 are monoatomic - leaving 63 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	$\# Z > 2$
7	SO4	A	1125	-	4,4,4	0.13	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	1101	3	3,3,3	0.68	0	2,2,2	0.14	0
6	PEG	A	1112	-	6,6,6	0.51	0	5,5,5	0.47	0
8	PGE	A	1103	-	9,9,9	0.32	0	8,8,8	0.24	0
5	EDO	D	201	-	3,3,3	0.45	0	2,2,2	0.46	0
5	EDO	A	1119	-	3,3,3	0.49	0	2,2,2	0.24	0
7	SO4	C	1121	-	4,4,4	0.15	0	6,6,6	0.17	0
5	EDO	J	1402	-	3,3,3	0.45	0	2,2,2	0.48	0
5	EDO	A	1118	-	3,3,3	0.50	0	2,2,2	0.28	0
6	PEG	C	1115	-	6,6,6	0.47	0	5,5,5	0.31	0
6	PEG	A	1120	-	6,6,6	0.49	0	5,5,5	0.31	0
8	PGE	A	1123	-	9,9,9	0.35	0	8,8,8	0.23	0
5	EDO	C	1108	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	C	1106	-	3,3,3	0.51	0	2,2,2	0.32	0
7	SO4	B	206	-	4,4,4	0.15	0	6,6,6	0.05	0
6	PEG	A	1116	-	6,6,6	0.48	0	5,5,5	0.26	0
8	PGE	A	1106	-	9,9,9	0.32	0	8,8,8	0.49	0
6	PEG	A	1114	-	6,6,6	0.47	0	5,5,5	0.25	0
5	EDO	A	1115	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	B	202	-	3,3,3	0.46	0	2,2,2	0.35	0
6	PEG	C	1101	3	6,6,6	0.47	0	5,5,5	1.05	1 (20%)
6	PEG	C	1110	-	6,6,6	0.47	0	5,5,5	0.24	0
5	EDO	C	1112	-	3,3,3	0.45	0	2,2,2	0.37	0
7	SO4	A	1126	-	4,4,4	0.15	0	6,6,6	0.08	0
9	PG4	C	1103	-	12,12,12	0.55	0	11,11,11	0.33	0
5	EDO	C	1109	-	3,3,3	0.49	0	2,2,2	0.39	0
5	EDO	C	1117	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	A	1105	-	3,3,3	0.44	0	2,2,2	0.44	0
5	EDO	A	1122	-	3,3,3	0.48	0	2,2,2	0.24	0
5	EDO	C	1107	-	3,3,3	0.49	0	2,2,2	0.26	0
5	EDO	C	1116	-	3,3,3	0.40	0	2,2,2	0.17	0
8	PGE	A	1111	-	9,9,9	0.32	0	8,8,8	0.29	0
9	PG4	A	1107	-	12,12,12	0.52	0	11,11,11	0.24	0
10	WAS	C	1120	-	34,35,35	2.62	6 (17%)	39,48,48	1.98	9 (23%)
7	SO4	G	1304	-	4,4,4	0.15	0	6,6,6	0.05	0
6	PEG	C	1114	-	6,6,6	0.47	0	5,5,5	0.40	0
10	WAS	A	1121	-	34,35,35	2.67	8 (23%)	39,48,48	1.53	7 (17%)
5	EDO	C	1102	-	3,3,3	0.44	0	2,2,2	0.41	0
6	PEG	A	1117	-	6,6,6	0.50	0	5,5,5	0.27	0
5	EDO	A	1110	-	3,3,3	0.42	0	2,2,2	0.37	0
5	EDO	C	1119	-	3,3,3	0.38	0	2,2,2	0.50	0
7	SO4	H	1202	-	4,4,4	0.17	0	6,6,6	0.15	0
5	EDO	C	1105	-	3,3,3	0.47	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	C	1118	-	6,6,6	0.49	0	5,5,5	0.27	0
7	SO4	A	1124	-	4,4,4	0.14	0	6,6,6	0.20	0
5	EDO	A	1104	-	3,3,3	0.50	0	2,2,2	0.28	0
5	EDO	I	1301	-	3,3,3	0.46	0	2,2,2	0.27	0
6	PEG	C	1104	-	6,6,6	0.51	0	5,5,5	0.32	0
5	EDO	G	1302	-	3,3,3	0.47	0	2,2,2	0.34	0
5	EDO	B	201	-	3,3,3	0.47	0	2,2,2	0.39	0
8	PGE	B	203	-	9,9,9	0.30	0	8,8,8	0.32	0
5	EDO	A	1102	-	3,3,3	0.53	0	2,2,2	0.21	0
7	SO4	C	1122	-	4,4,4	0.15	0	6,6,6	0.15	0
5	EDO	G	1301	-	3,3,3	0.43	0	2,2,2	0.36	0
5	EDO	J	1401	-	3,3,3	0.45	0	2,2,2	0.31	0
5	EDO	A	1113	-	3,3,3	0.49	0	2,2,2	0.31	0
5	EDO	A	1109	-	3,3,3	0.53	0	2,2,2	0.20	0
6	PEG	A	1108	-	6,6,6	0.48	0	5,5,5	0.25	0
9	PG4	D	202	-	12,12,12	0.54	0	11,11,11	0.46	0
5	EDO	H	1201	-	3,3,3	0.49	0	2,2,2	0.28	0
6	PEG	C	1111	-	6,6,6	0.47	0	5,5,5	0.22	0
5	EDO	C	1113	-	3,3,3	0.52	0	2,2,2	0.44	0
6	PEG	G	1303	1	6,6,6	0.50	0	5,5,5	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1101	3	-	1/1/1/1	-
6	PEG	A	1112	-	-	3/4/4/4	-
8	PGE	A	1103	-	-	5/7/7/7	-
5	EDO	D	201	-	-	0/1/1/1	-
5	EDO	A	1119	-	-	0/1/1/1	-
8	PGE	A	1123	-	-	3/7/7/7	-
5	EDO	J	1402	-	-	0/1/1/1	-
5	EDO	A	1118	-	-	0/1/1/1	-
6	PEG	C	1115	-	-	0/4/4/4	-
6	PEG	A	1120	-	-	1/4/4/4	-
5	EDO	C	1108	-	-	1/1/1/1	-
5	EDO	C	1106	-	-	0/1/1/1	-
6	PEG	A	1116	-	-	1/4/4/4	-
8	PGE	A	1106	-	-	3/7/7/7	-
6	PEG	A	1114	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1115	-	-	0/1/1/1	-
5	EDO	B	202	-	-	0/1/1/1	-
6	PEG	C	1101	3	-	4/4/4/4	-
6	PEG	C	1110	-	-	2/4/4/4	-
5	EDO	C	1112	-	-	0/1/1/1	-
9	PG4	C	1103	-	-	7/10/10/10	-
5	EDO	C	1109	-	-	0/1/1/1	-
5	EDO	C	1117	-	-	0/1/1/1	-
5	EDO	A	1105	-	-	0/1/1/1	-
5	EDO	A	1122	-	-	0/1/1/1	-
5	EDO	C	1107	-	-	1/1/1/1	-
5	EDO	C	1116	-	-	0/1/1/1	-
8	PGE	A	1111	-	-	6/7/7/7	-
9	PG4	A	1107	-	-	4/10/10/10	-
10	WAS	C	1120	-	-	8/21/47/47	0/2/2/2
6	PEG	C	1114	-	-	2/4/4/4	-
10	WAS	A	1121	-	-	8/21/47/47	0/2/2/2
5	EDO	C	1102	-	-	1/1/1/1	-
6	PEG	A	1117	-	-	1/4/4/4	-
5	EDO	A	1110	-	-	0/1/1/1	-
5	EDO	C	1119	-	-	1/1/1/1	-
5	EDO	C	1105	-	-	0/1/1/1	-
6	PEG	C	1118	-	-	3/4/4/4	-
5	EDO	A	1104	-	-	1/1/1/1	-
5	EDO	I	1301	-	-	0/1/1/1	-
6	PEG	C	1104	-	-	2/4/4/4	-
5	EDO	G	1302	-	-	0/1/1/1	-
5	EDO	B	201	-	-	0/1/1/1	-
8	PGE	B	203	-	-	4/7/7/7	-
5	EDO	A	1102	-	-	0/1/1/1	-
5	EDO	G	1301	-	-	1/1/1/1	-
5	EDO	J	1401	-	-	0/1/1/1	-
5	EDO	A	1113	-	-	0/1/1/1	-
5	EDO	A	1109	-	-	1/1/1/1	-
6	PEG	A	1108	-	-	1/4/4/4	-
9	PG4	D	202	-	-	5/10/10/10	-
5	EDO	H	1201	-	-	1/1/1/1	-
6	PEG	C	1111	-	-	1/4/4/4	-
5	EDO	C	1113	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	G	1303	1	-	3/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1121	WAS	O8-N4	11.12	1.41	1.22
10	C	1120	WAS	O8-N4	11.05	1.41	1.22
10	A	1121	WAS	C10-N2	6.77	1.49	1.34
10	C	1120	WAS	C10-N2	6.55	1.48	1.34
10	C	1120	WAS	C13-N3	4.74	1.50	1.37
10	A	1121	WAS	C13-N3	4.23	1.49	1.37
10	A	1121	WAS	O6-C10	3.69	1.42	1.35
10	C	1120	WAS	O6-C10	3.50	1.41	1.35
10	A	1121	WAS	C16-N5	3.18	1.49	1.40
10	C	1120	WAS	C16-N5	3.04	1.49	1.40
10	A	1121	WAS	N5-N6	2.61	1.44	1.41
10	A	1121	WAS	O2-C2	-2.45	1.40	1.44
10	A	1121	WAS	C7-C2	2.23	1.56	1.52
10	C	1120	WAS	N5-N6	2.19	1.43	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1120	WAS	C14-C13-N3	-5.80	111.92	121.80
10	A	1121	WAS	O6-C10-N2	5.45	119.10	110.61
10	C	1120	WAS	O6-C10-N2	5.08	118.52	110.61
10	C	1120	WAS	C17-C18-C13	-3.99	117.92	121.53
10	C	1120	WAS	C16-C17-C18	3.48	122.03	119.63
10	C	1120	WAS	C18-C13-N3	3.17	128.91	123.33
10	A	1121	WAS	O6-C10-O7	-2.78	118.91	124.25
10	C	1120	WAS	C8-N1-C6	-2.57	110.56	114.20
10	C	1120	WAS	C12-N3-C13	2.53	129.47	123.39
10	C	1120	WAS	O6-C10-O7	-2.48	119.50	124.25
10	A	1121	WAS	C17-C18-C13	-2.41	119.34	121.53
10	A	1121	WAS	C12-N3-C13	-2.16	118.19	123.39
10	A	1121	WAS	C9-C8-N1	-2.16	107.54	111.06
10	C	1120	WAS	C16-N5-N6	2.12	120.40	116.91
10	A	1121	WAS	C11-C12-N3	-2.10	106.25	111.17
6	C	1101	PEG	O2-C3-C4	-2.09	100.89	110.07
10	A	1121	WAS	C16-N5-N6	2.07	120.33	116.91

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1121	WAS	C18-C13-N3-C12
10	A	1121	WAS	N2-C10-O6-C11
10	A	1121	WAS	O7-C10-O6-C11
10	A	1121	WAS	C15-C16-N5-N6
10	A	1121	WAS	C17-C16-N5-N6
10	C	1120	WAS	C14-C13-N3-C12
10	C	1120	WAS	C18-C13-N3-C12
10	C	1120	WAS	C15-C16-N5-N6
10	C	1120	WAS	C17-C16-N5-N6
6	G	1303	PEG	C1-C2-O2-C3
6	C	1118	PEG	O2-C3-C4-O4
10	A	1121	WAS	O6-C11-C12-N3
10	A	1121	WAS	C14-C13-N3-C12
6	C	1104	PEG	C4-C3-O2-C2
9	C	1103	PG4	O3-C5-C6-O4
10	C	1120	WAS	O6-C11-C12-N3
8	A	1103	PGE	O2-C3-C4-O3
6	G	1303	PEG	O1-C1-C2-O2
6	G	1303	PEG	O2-C3-C4-O4
6	C	1118	PEG	O1-C1-C2-O2
8	B	203	PGE	O1-C1-C2-O2
9	A	1107	PG4	O1-C1-C2-O2
9	C	1103	PG4	O1-C1-C2-O2
8	A	1111	PGE	O1-C1-C2-O2
8	A	1106	PGE	O2-C3-C4-O3
6	A	1112	PEG	O1-C1-C2-O2
6	C	1101	PEG	O2-C3-C4-O4
6	C	1114	PEG	O2-C3-C4-O4
8	A	1106	PGE	O3-C5-C6-O4
8	A	1103	PGE	C1-C2-O2-C3
8	A	1103	PGE	C6-C5-O3-C4
6	A	1114	PEG	O2-C3-C4-O4
9	C	1103	PG4	O4-C7-C8-O5
5	A	1101	EDO	O1-C1-C2-O2
5	A	1104	EDO	O1-C1-C2-O2
5	C	1107	EDO	O1-C1-C2-O2
6	A	1112	PEG	O2-C3-C4-O4
6	C	1110	PEG	O1-C1-C2-O2
9	D	202	PG4	O4-C7-C8-O5
6	A	1108	PEG	O2-C3-C4-O4
6	C	1114	PEG	O1-C1-C2-O2
9	D	202	PG4	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	G	1301	EDO	O1-C1-C2-O2
6	A	1117	PEG	C4-C3-O2-C2
6	A	1120	PEG	C4-C3-O2-C2
8	A	1106	PGE	O1-C1-C2-O2
8	A	1103	PGE	C3-C4-O3-C5
8	A	1111	PGE	C1-C2-O2-C3
6	A	1116	PEG	C1-C2-O2-C3
6	A	1114	PEG	C1-C2-O2-C3
9	C	1103	PG4	C3-C4-O3-C5
6	C	1118	PEG	C1-C2-O2-C3
8	A	1111	PGE	C4-C3-O2-C2
9	C	1103	PG4	C1-C2-O2-C3
8	A	1103	PGE	O3-C5-C6-O4
9	A	1107	PG4	C5-C6-O4-C7
8	A	1123	PGE	C6-C5-O3-C4
8	B	203	PGE	C6-C5-O3-C4
6	A	1112	PEG	C4-C3-O2-C2
10	C	1120	WAS	N2-C10-O6-C11
9	C	1103	PG4	O2-C3-C4-O3
8	B	203	PGE	O2-C3-C4-O3
9	A	1107	PG4	O4-C7-C8-O5
10	C	1120	WAS	O7-C10-O6-C11
8	B	203	PGE	C4-C3-O2-C2
9	D	202	PG4	C4-C3-O2-C2
6	C	1110	PEG	C4-C3-O2-C2
5	A	1109	EDO	O1-C1-C2-O2
5	C	1108	EDO	O1-C1-C2-O2
9	A	1107	PG4	C3-C4-O3-C5
8	A	1111	PGE	O2-C3-C4-O3
6	A	1114	PEG	O1-C1-C2-O2
6	C	1101	PEG	O1-C1-C2-O2
6	C	1101	PEG	C4-C3-O2-C2
6	C	1104	PEG	C1-C2-O2-C3
10	C	1120	WAS	C11-C12-N3-C13
8	A	1111	PGE	O3-C5-C6-O4
5	C	1102	EDO	O1-C1-C2-O2
5	C	1119	EDO	O1-C1-C2-O2
6	C	1101	PEG	C1-C2-O2-C3
6	C	1111	PEG	C4-C3-O2-C2
8	A	1111	PGE	C6-C5-O3-C4
5	H	1201	EDO	O1-C1-C2-O2
10	A	1121	WAS	C12-C11-O6-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	D	202	PG4	O2-C3-C4-O3
8	A	1123	PGE	O1-C1-C2-O2
9	C	1103	PG4	C5-C6-O4-C7
8	A	1123	PGE	O3-C5-C6-O4
9	D	202	PG4	O1-C1-C2-O2

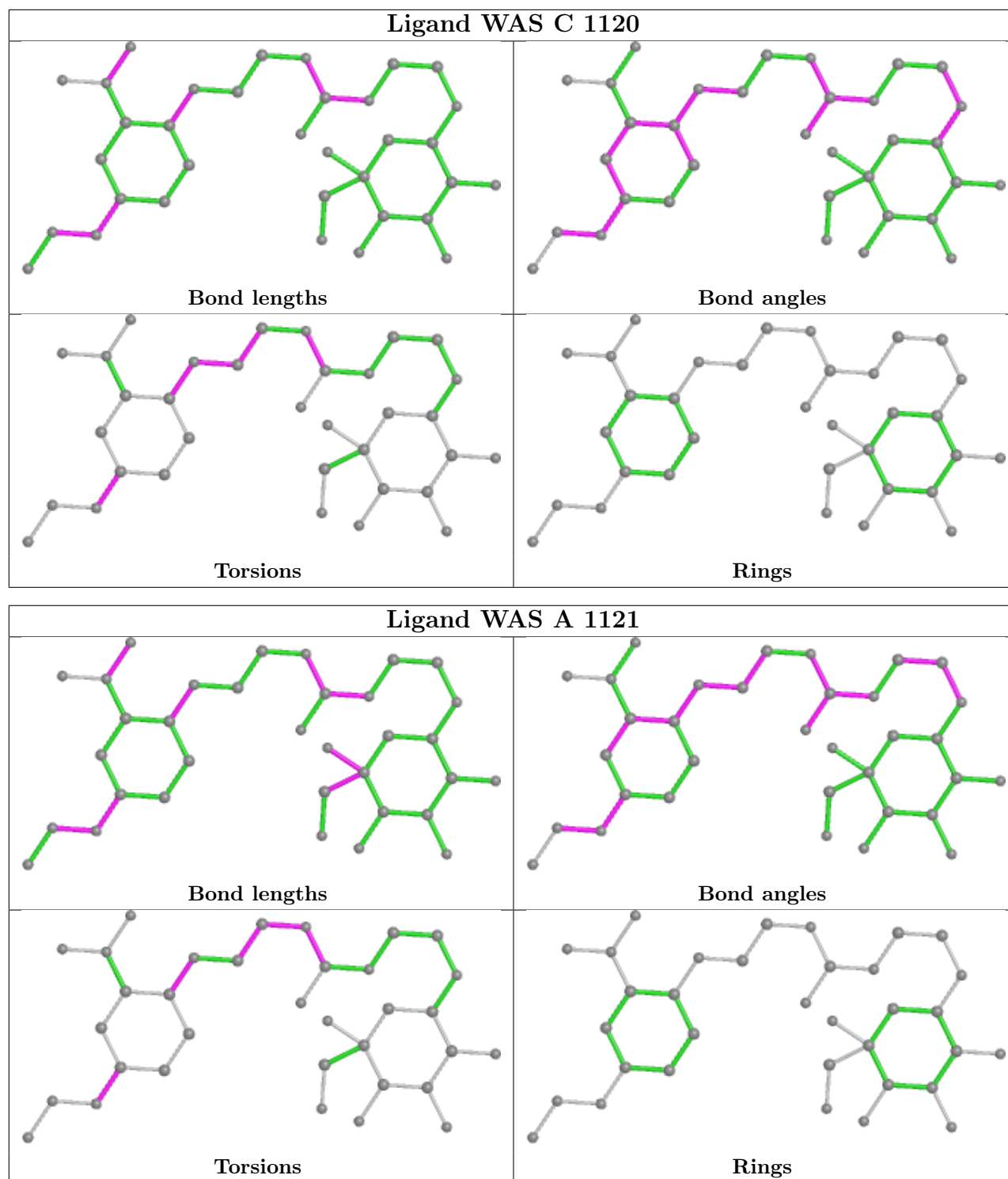
There are no ring outliers.

20 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1112	PEG	1	0
8	A	1103	PGE	1	0
7	C	1121	SO4	1	0
5	A	1118	EDO	1	0
6	C	1115	PEG	1	0
8	A	1106	PGE	7	0
6	C	1101	PEG	3	0
5	C	1117	EDO	2	0
5	A	1105	EDO	2	0
5	C	1116	EDO	2	0
8	A	1111	PGE	3	0
10	C	1120	WAS	1	0
5	C	1119	EDO	1	0
6	C	1104	PEG	4	0
8	B	203	PGE	1	0
7	C	1122	SO4	2	0
5	G	1301	EDO	1	0
5	J	1401	EDO	1	0
5	A	1113	EDO	1	0
6	G	1303	PEG	2	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 ⓘ

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	G	151/183 (82%)	-0.04	5 (3%) 46 53	23, 39, 64, 84	0
1	I	152/183 (83%)	1.06	39 (25%) 0 0	32, 60, 81, 92	0
2	H	105/107 (98%)	0.24	6 (5%) 23 29	22, 29, 62, 79	0
2	J	107/107 (100%)	0.48	15 (14%) 2 3	26, 40, 67, 94	0
3	A	597/609 (98%)	0.01	23 (3%) 39 45	19, 27, 47, 78	0
3	C	597/609 (98%)	-0.07	19 (3%) 47 54	19, 30, 48, 94	0
4	B	83/134 (61%)	0.90	21 (25%) 0 0	26, 43, 79, 94	0
4	D	84/134 (62%)	0.98	24 (28%) 0 0	25, 45, 80, 105	0
All	All	1876/2066 (90%)	0.19	152 (8%) 12 15	19, 32, 69, 105	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	81	GLY	9.1
4	D	82	TYR	7.2
4	B	39	CYS	7.1
4	B	42	GLY	7.0
4	D	43	THR	6.7
3	C	370	THR	6.1
4	B	117	ARG	5.7
4	D	80	THR	5.6
1	I	69	LEU	5.2
1	I	57	LEU	4.9
1	G	34	ASP	4.8
4	B	41	ASP	4.8
4	D	44	ALA	4.7
4	D	78	THR	4.6
4	B	38	THR	4.4
4	D	42	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	44	ALA	4.2
1	I	163	ASP	4.2
3	C	371	PRO	4.1
4	B	43	THR	4.0
1	I	127	ARG	4.0
1	I	165	SER	3.9
1	G	33	VAL	3.9
4	B	80	THR	3.9
2	J	244	GLU	3.7
3	A	416	LEU	3.7
2	H	247	ALA	3.7
1	I	67	LEU	3.7
1	I	34	ASP	3.6
1	I	142	VAL	3.6
3	C	627	PHE	3.5
1	I	143	ALA	3.5
4	B	40	LEU	3.4
1	I	66	THR	3.3
4	B	116	CYS	3.3
4	D	84	PRO	3.3
1	I	82	VAL	3.3
4	D	117	ARG	3.3
2	J	329	PHE	3.2
1	I	79	ILE	3.2
1	I	126	ALA	3.2
2	H	254	THR	3.2
4	D	41	ASP	3.2
2	J	246	GLY	3.1
4	D	34	SER	3.1
4	D	39	CYS	3.1
3	A	622	LEU	3.1
3	A	944	GLU	3.1
4	B	100	CYS	3.1
4	D	116	CYS	3.1
3	A	370	THR	3.1
1	I	76	VAL	3.1
2	H	253	LYS	3.1
3	A	658	LEU	3.1
1	I	144	GLU	3.0
3	A	945	THR	3.0
4	B	84	PRO	3.0
1	I	58	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	132	GLY	2.9
1	I	130	VAL	2.9
4	D	48	PHE	2.9
4	D	100	CYS	2.9
3	C	661	VAL	2.9
4	D	114	ASN	2.9
1	G	183	ALA	2.9
2	J	247	ALA	2.9
4	B	48	PHE	2.8
4	B	45	THR	2.8
2	J	350	ASN	2.8
1	I	138	VAL	2.7
1	I	184	PRO	2.7
1	I	141	THR	2.7
1	I	85	VAL	2.7
4	D	40	LEU	2.7
2	H	248	TRP	2.6
1	I	86	LEU	2.6
2	J	248	TRP	2.6
3	C	635	ALA	2.6
4	B	78	THR	2.6
3	A	637	TRP	2.6
3	C	626	PHE	2.6
4	B	37	PHE	2.6
3	A	695	PHE	2.5
2	J	323	VAL	2.5
1	G	164	ARG	2.5
1	I	161	LEU	2.5
3	C	656	LEU	2.5
3	C	636	VAL	2.5
4	D	77	CYS	2.5
4	D	111	VAL	2.5
3	A	694	PHE	2.5
3	A	621	VAL	2.4
3	C	904	HIS	2.4
4	B	46	ILE	2.4
4	D	45	THR	2.4
2	H	249	GLU	2.4
3	C	622	LEU	2.4
2	J	280	GLY	2.4
2	J	245	PRO	2.4
1	I	81	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	A	665	PHE	2.4
4	D	35	LYS	2.4
3	C	733	TRP	2.3
3	C	785	HIS	2.3
1	I	139	GLU	2.3
4	D	79	ASN	2.3
1	I	164	ARG	2.3
3	A	626	PHE	2.3
3	A	770	LEU	2.3
1	G	109	ARG	2.3
1	I	135	ASP	2.3
2	J	281	ILE	2.3
2	J	338	LEU	2.3
2	H	321	VAL	2.3
4	D	38	THR	2.2
1	I	33	VAL	2.2
3	A	636	VAL	2.2
3	C	658	LEU	2.2
4	B	85	LEU	2.2
1	I	136	ASN	2.2
1	I	108	PRO	2.2
1	I	140	LEU	2.2
1	I	72	ASP	2.2
4	B	114	ASN	2.2
1	I	131	SER	2.2
3	A	693	PRO	2.2
3	A	663	LEU	2.1
3	C	666	CYS	2.1
4	D	113	GLU	2.1
1	I	35	ARG	2.1
3	A	417	GLY	2.1
1	I	152	THR	2.1
2	J	282	PRO	2.1
3	A	943	PRO	2.1
1	I	133	ARG	2.1
4	B	113	GLU	2.1
3	A	733	TRP	2.1
1	I	128	LEU	2.1
2	J	343	THR	2.1
2	J	294	GLU	2.1
3	A	891	GLY	2.1
4	B	81	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	695	PHE	2.1
1	I	63	LEU	2.0
3	C	665	PHE	2.0
2	J	337	TRP	2.0
3	C	770	LEU	2.0
3	A	946	SER	2.0
3	C	901	PRO	2.0
3	A	656	LEU	2.0
3	A	923	ALA	2.0
3	C	663	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
5	EDO	A	1101	4/4	0.67	0.52	53,66,75,81	0
5	EDO	A	1109	4/4	0.68	0.18	49,60,63,66	0
5	EDO	I	1301	4/4	0.71	0.35	69,76,78,84	0
7	SO4	G	1304	5/5	0.71	0.45	84,99,114,134	0
9	PG4	C	1103	13/13	0.71	0.23	50,65,77,86	0
6	PEG	C	1115	7/7	0.74	0.40	44,50,68,79	0
6	PEG	A	1112	7/7	0.75	0.24	46,51,67,72	0
9	PG4	D	202	13/13	0.75	0.20	46,55,69,70	0
5	EDO	C	1105	4/4	0.77	0.42	54,60,60,60	0
5	EDO	C	1107	4/4	0.78	0.25	47,50,57,64	0
9	PG4	A	1107	13/13	0.78	0.27	50,61,76,77	0
6	PEG	G	1303	7/7	0.80	0.26	62,66,69,70	0
6	PEG	A	1114	7/7	0.80	0.25	46,59,68,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PGE	B	203	10/10	0.80	0.33	54,58,74,79	0
5	EDO	G	1301	4/4	0.81	0.30	52,57,59,64	0
6	PEG	C	1101	7/7	0.81	0.29	32,44,57,65	0
6	PEG	A	1116	7/7	0.82	0.13	49,58,66,67	0
6	PEG	C	1114	7/7	0.82	0.19	48,53,70,72	0
7	SO4	H	1202	5/5	0.83	0.30	62,72,79,105	0
5	EDO	C	1106	4/4	0.84	0.24	54,54,55,60	0
8	PGE	A	1103	10/10	0.84	0.17	49,64,67,69	0
5	EDO	A	1113	4/4	0.84	0.25	48,53,54,65	0
5	EDO	C	1109	4/4	0.85	0.15	45,47,57,61	0
5	EDO	C	1102	4/4	0.85	0.45	47,55,58,62	0
6	PEG	C	1110	7/7	0.85	0.15	36,51,56,59	0
5	EDO	C	1112	4/4	0.86	0.13	49,52,57,63	0
6	PEG	A	1117	7/7	0.86	0.21	57,64,65,74	0
5	EDO	A	1115	4/4	0.86	0.23	41,49,51,53	0
8	PGE	A	1123	10/10	0.86	0.23	49,61,66,67	0
6	PEG	A	1108	7/7	0.87	0.27	48,50,60,64	0
7	SO4	A	1126	5/5	0.87	0.39	72,86,102,113	0
7	SO4	C	1122	5/5	0.87	0.50	72,88,104,118	0
6	PEG	C	1111	7/7	0.88	0.12	39,64,74,76	0
6	PEG	C	1118	7/7	0.88	0.13	54,56,69,74	0
5	EDO	A	1122	4/4	0.89	0.17	48,51,52,59	0
5	EDO	A	1118	4/4	0.89	0.12	47,50,60,61	0
8	PGE	A	1106	10/10	0.90	0.32	31,44,53,60	0
6	PEG	A	1120	7/7	0.90	0.25	45,58,62,63	0
5	EDO	A	1104	4/4	0.90	0.18	49,56,62,69	0
10	WAS	A	1121	34/34	0.91	0.16	22,40,67,71	0
7	SO4	C	1121	5/5	0.92	0.30	71,76,83,91	0
5	EDO	H	1201	4/4	0.92	0.09	34,36,38,50	0
7	SO4	A	1125	5/5	0.92	0.19	60,68,79,88	0
5	EDO	A	1105	4/4	0.92	0.16	32,35,47,57	0
7	SO4	B	206	5/5	0.92	0.46	81,83,113,131	0
5	EDO	C	1116	4/4	0.93	0.15	45,46,53,63	0
5	EDO	C	1117	4/4	0.93	0.16	49,53,54,61	0
7	SO4	A	1124	5/5	0.93	0.10	53,61,71,90	0
5	EDO	C	1113	4/4	0.93	0.24	39,45,46,54	0
5	EDO	A	1102	4/4	0.94	0.14	32,35,40,44	0
5	EDO	A	1119	4/4	0.94	0.16	36,38,43,53	0
6	PEG	C	1104	7/7	0.94	0.27	36,43,54,69	0
5	EDO	J	1402	4/4	0.94	0.16	44,52,52,61	0
10	WAS	C	1120	34/34	0.94	0.15	21,41,70,76	0
8	PGE	A	1111	10/10	0.95	0.20	49,58,65,69	0

Continued on next page...

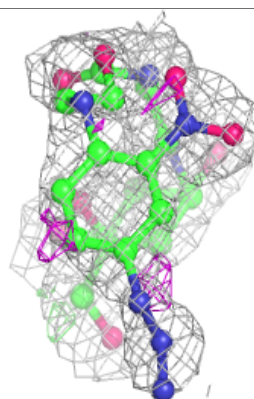
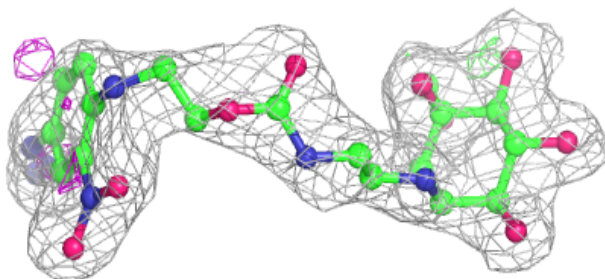
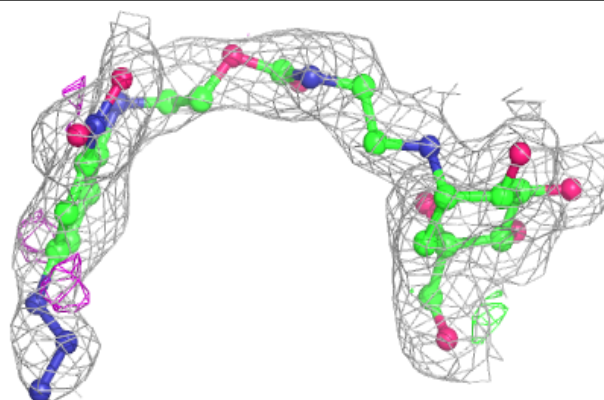
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	EDO	B	202	4/4	0.95	0.10	50,53,57,60	0
5	EDO	A	1110	4/4	0.95	0.14	40,42,47,63	0
5	EDO	B	201	4/4	0.95	0.19	40,46,47,54	0
5	EDO	D	201	4/4	0.96	0.14	45,47,52,55	0
5	EDO	C	1108	4/4	0.96	0.14	33,35,45,52	0
5	EDO	J	1401	4/4	0.96	0.09	42,42,47,56	0
5	EDO	C	1119	4/4	0.97	0.10	38,40,50,55	0
5	EDO	G	1302	4/4	0.97	0.08	30,31,32,39	0
11	CA	D	204	1/1	0.97	0.05	34,34,34,34	0
11	CA	B	205	1/1	0.98	0.05	35,35,35,35	0
11	CA	D	203	1/1	0.99	0.05	28,28,28,28	0
11	CA	B	204	1/1	0.99	0.08	27,27,27,27	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.

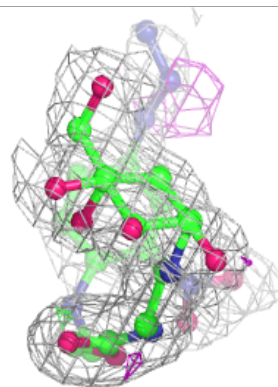
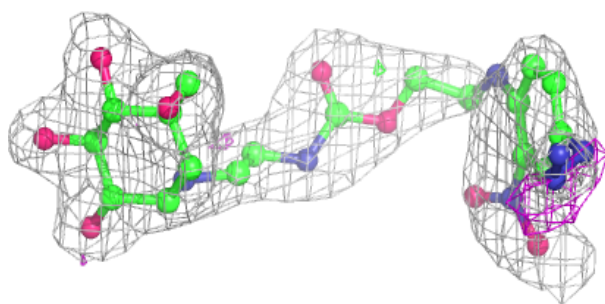
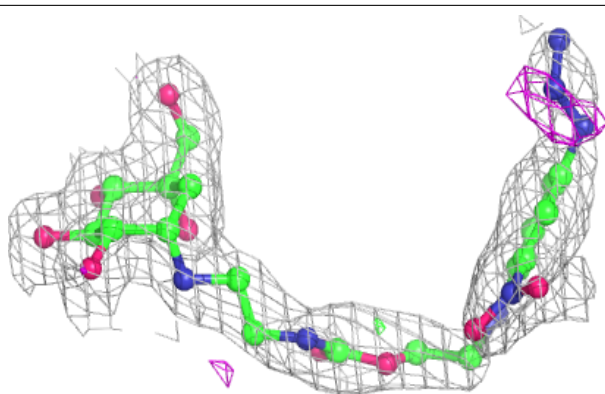
Electron density around WAS A 1121:

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 WAS C 1120:

$2mF_o-DF_c$ (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.