



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 02:09 AM UTC

PDB ID : 9QC2 / pdb_00009qc2
Title : BV333 aminotransferase from Streptomyces sp. mutant W89A
Authors : De Rose, S.A.; Isupov, M.N.; Patti, S.
Deposited on : 2025-03-04
Resolution : 1.24 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

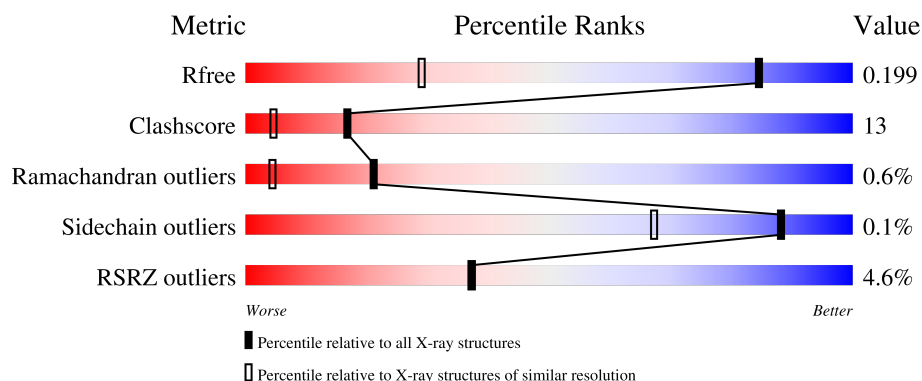
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.24 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}	180053	1630 (1.26-1.22)
Clashscore	190562	1668 (1.26-1.22)
Ramachandran outliers	187476	1635 (1.26-1.22)
Sidechain outliers	187428	1633 (1.26-1.22)
RSRZ outliers	180081	1630 (1.26-1.22)

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	461	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	B	461	<div> <div>4%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	461	<div> <div>4%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
1	D	461	<div> <div>7%</div> <div>86%</div> <div>13%</div> <div>.</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
2	PEG	A	525	-	-	X	-
2	PEG	A	526	-	-	X	-
2	PEG	B	504	-	-	X	-
2	PEG	B	515	-	-	X	-
2	PEG	B	521	-	-	X	-
2	PEG	B	529	-	-	X	-
2	PEG	C	501	-	-	X	-
3	PGE	B	519	-	-	X	-
3	PGE	C	527	-	-	X	-
3	PGE	D	505	-	-	X	-
4	EDO	A	504	-	-	X	-
4	EDO	A	517	-	-	X	-
4	EDO	A	518	-	-	X	-
4	EDO	B	510	-	-	X	-
4	EDO	B	518	-	-	X	-
4	EDO	B	532	-	-	X	-
4	EDO	B	537	-	-	X	-
4	EDO	C	508	-	-	X	-
4	EDO	C	516	-	-	X	-
4	EDO	C	519	-	-	X	-
4	EDO	C	520	-	-	X	-
4	EDO	C	526	-	-	X	-
4	EDO	D	501	-	-	X	-
4	EDO	D	517	-	-	X	-
4	EDO	D	520	-	-	X	-
4	EDO	D	528	-	-	X	-
5	GOL	B	533	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16920 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 Aspartate aminotransferase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	P	S	0	34	0
			3737	2418	612	694	1	12			
1	B	455	Total	C	N	O	P	S	0	32	0
			3725	2407	615	690	1	12			
1	C	461	Total	C	N	O	P	S	0	29	0
			3750	2420	617	700	1	12			
1	D	455	Total	C	N	O	P	S	0	30	0
			3712	2400	611	688	1	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ALA	TRP	engineered mutation	UNP A0AA46ZEV9
A	459	HIS	-	expression tag	UNP A0AA46ZEV9
A	460	HIS	-	expression tag	UNP A0AA46ZEV9
A	461	HIS	-	expression tag	UNP A0AA46ZEV9
B	89	ALA	TRP	engineered mutation	UNP A0AA46ZEV9
B	459	HIS	-	expression tag	UNP A0AA46ZEV9
B	460	HIS	-	expression tag	UNP A0AA46ZEV9
B	461	HIS	-	expression tag	UNP A0AA46ZEV9
C	89	ALA	TRP	engineered mutation	UNP A0AA46ZEV9
C	459	HIS	-	expression tag	UNP A0AA46ZEV9
C	460	HIS	-	expression tag	UNP A0AA46ZEV9
C	461	HIS	-	expression tag	UNP A0AA46ZEV9
D	89	ALA	TRP	engineered mutation	UNP A0AA46ZEV9
D	459	HIS	-	expression tag	UNP A0AA46ZEV9
D	460	HIS	-	expression tag	UNP A0AA46ZEV9
D	461	HIS	-	expression tag	UNP A0AA46ZEV9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



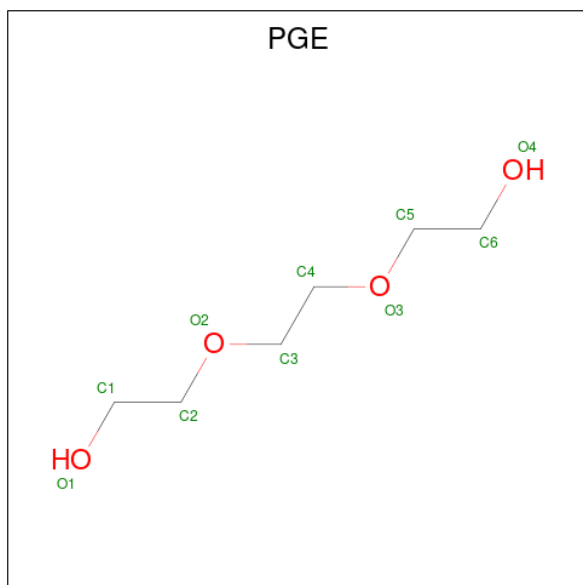
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total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

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

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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

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

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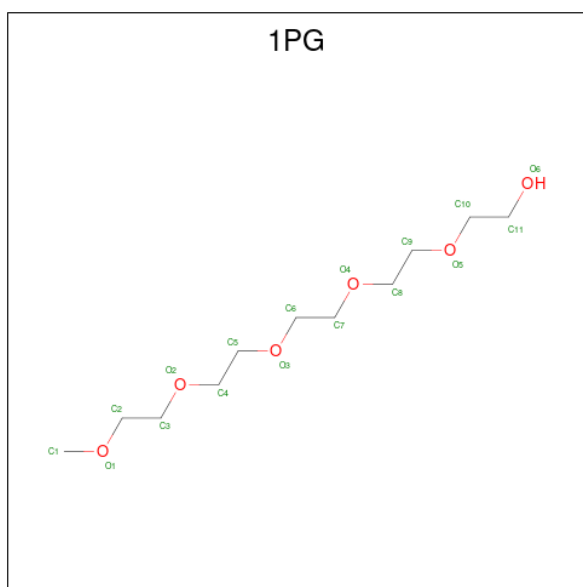
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (CCD ID: 1PG) (formula: C₁₁H₂₄O₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			17	11 6		

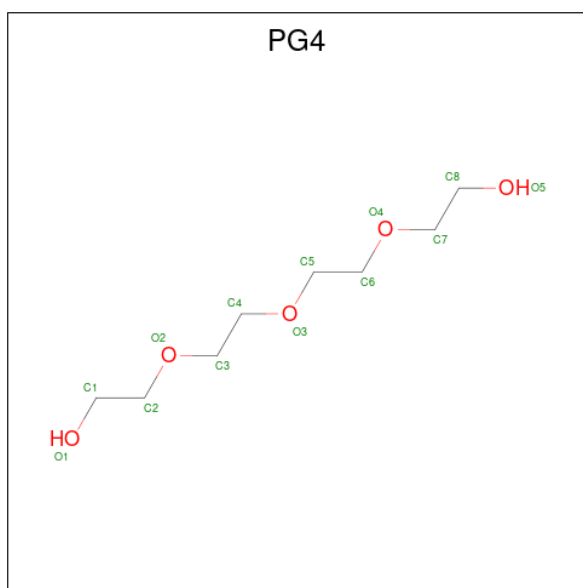
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Cl	0	0
			3	3		
7	B	2	Total	Cl	0	0
			2	2		
7	C	2	Total	Cl	0	0
			2	2		
7	D	2	Total	Cl	0	0
			2	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	Mg	0	0
			7	7		
8	B	7	Total	Mg	0	0
			7	7		
8	C	9	Total	Mg	0	0
			9	9		
8	D	4	Total	Mg	0	0
			4	4		

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: 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	C	1	Total	C	O	0	0
			13	8	5		

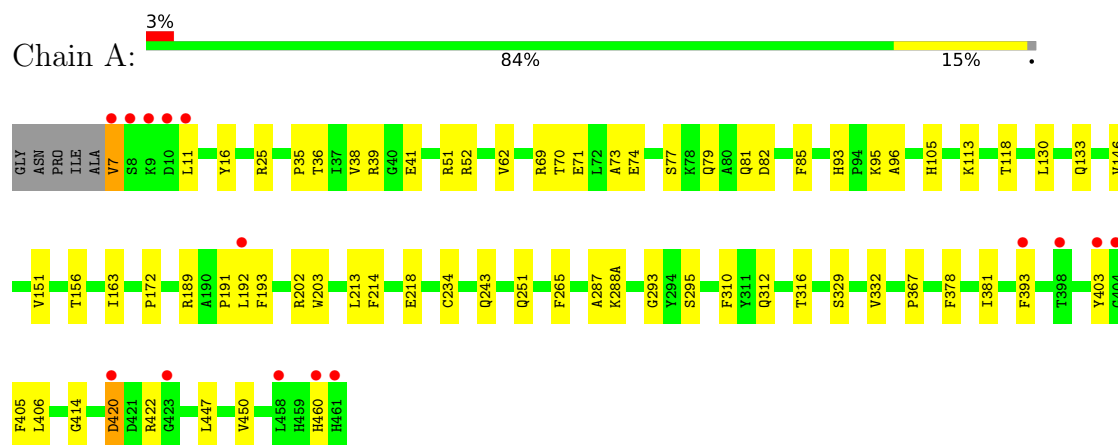
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	340	Total	O	0	0
			340	340		
10	B	365	Total	O	0	0
			365	365		
10	C	292	Total	O	0	0
			292	292		
10	D	273	Total	O	0	0
			273	273		

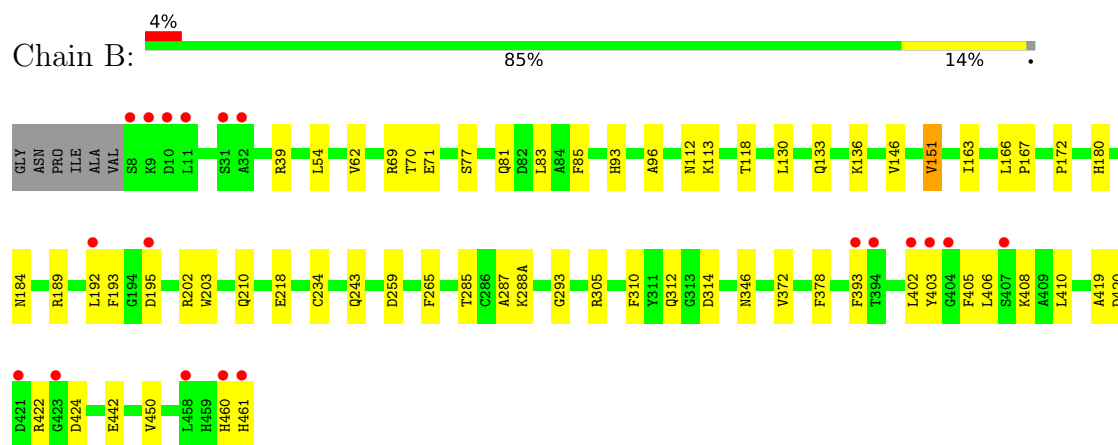
3 Residue-property plots [i](#)

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.

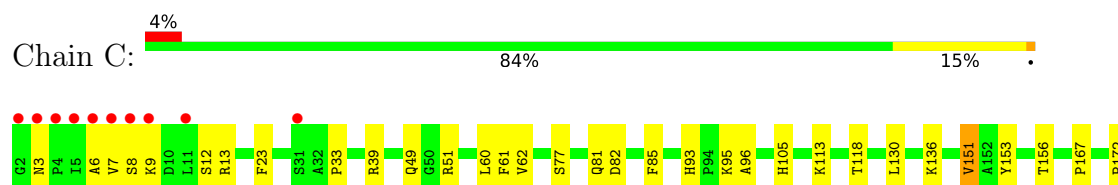
- Molecule 1: Aspartate aminotransferase family protein

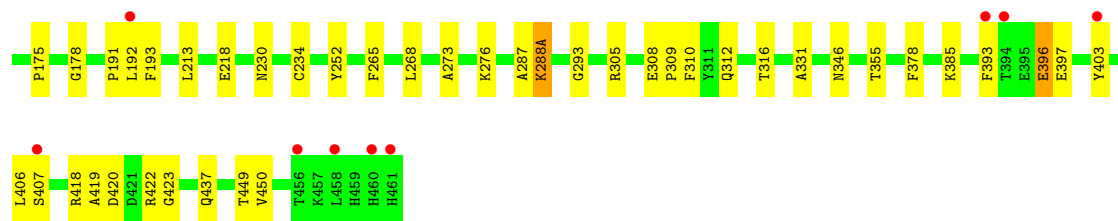


- Molecule 1: Aspartate aminotransferase family protein

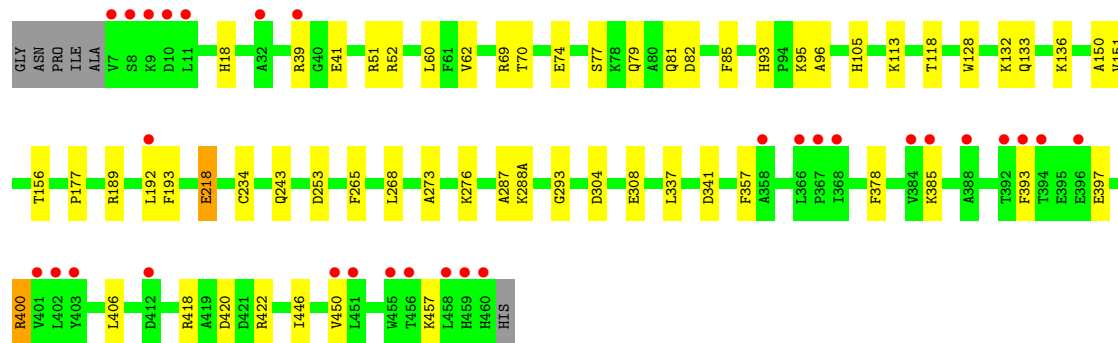
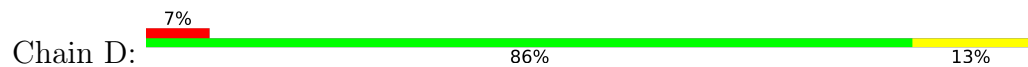


- Molecule 1: Aspartate aminotransferase family protein





• Molecule 1: Aspartate aminotransferase family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 90.24Å 99.45Å 66.94° 73.26° 69.64°	Depositor
Resolution (Å)	80.02 – 1.24 80.02 – 1.24	Depositor EDS
% Data completeness (in resolution range)	94.8 (80.02-1.24) 96.1 (80.02-1.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.171 , 0.195 0.176 , 0.199	Depositor DCC
R_{free} test set	2026 reflections (0.39%)	wwPDB-VP
Wilson B-factor (Å ²)	16.9	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	16920	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, EDO, GOL, LLP, MG, PGE, CL, 1PG, PEG

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	0.70	0/3912	1.10	8/5315 (0.2%)
1	B	0.72	0/3893	1.10	7/5288 (0.1%)
1	C	0.72	0/3902	1.09	5/5306 (0.1%)
1	D	0.71	0/3874	1.10	9/5264 (0.2%)
All	All	0.71	0/15581	1.10	29/21173 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	HIS	CB-CA-C	9.94	126.46	111.06
1	D	218[A]	GLU	CB-CG-CD	7.91	126.05	112.60
1	D	218[B]	GLU	CB-CG-CD	7.91	126.05	112.60
1	D	265	PHE	CA-CB-CG	-7.29	106.51	113.80
1	A	85	PHE	CA-CB-CG	-7.16	106.64	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	ARG	Sidechain
1	A	7	VAL	Peptide
1	B	305	ARG	Sidechain

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	3737	0	3723	77	0
1	B	3725	0	3712	90	0
1	C	3750	0	3705	95	0
1	D	3712	0	3695	89	0
2	A	49	0	69	23	0
2	B	28	0	40	28	0
2	C	35	0	50	8	0
2	D	7	0	10	0	0
3	A	10	0	14	3	0
3	B	40	0	56	9	0
3	C	20	0	28	13	0
3	D	20	0	28	8	0
4	A	88	0	131	28	0
4	B	100	0	150	33	0
4	C	92	0	138	37	0
4	D	92	0	136	67	0
5	A	18	0	24	3	0
5	B	18	0	24	8	0
5	C	18	0	24	4	0
5	D	12	0	16	2	0
6	A	17	0	24	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
8	A	7	0	0	0	0
8	B	7	0	0	0	0
8	C	9	0	0	0	0
8	D	4	0	0	0	0
9	B	13	0	18	0	0
9	C	13	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	340	0	0	16	0
10	B	365	0	0	24	0
10	C	292	0	0	19	0
10	D	273	0	0	23	0
All	All	16920	0	15833	404	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 404 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:D:243[A]:GLN:HG3	4:D:520:EDO:C2	1.39	1.47
1:A:118[B]:THR:HG21	1:B:118[B]:THR:HG21	1.19	1.15
1:D:243[A]:GLN:CG	4:D:520:EDO:H21	1.76	1.15
1:A:118[B]:THR:CG2	1:B:118[B]:THR:HG21	1.77	1.15
4:B:518:EDO:H11	3:B:519:PGE:O1	1.46	1.14

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/461 (106%)	464 (95%)	20 (4%)	3 (1%)	21	4
1	B	484/461 (105%)	463 (96%)	19 (4%)	2 (0%)	30	9
1	C	487/461 (106%)	466 (96%)	18 (4%)	3 (1%)	21	4
1	D	482/461 (105%)	463 (96%)	16 (3%)	3 (1%)	21	4
All	All	1940/1844 (105%)	1856 (96%)	73 (4%)	11 (1%)	21	4

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	VAL
1	B	151	VAL
1	C	151	VAL
1	D	151	VAL
1	A	287	ALA

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	402/371 (108%)	401 (100%)	1 (0%)	87	67
1	B	399/371 (108%)	399 (100%)	0	100	100
1	C	400/371 (108%)	399 (100%)	1 (0%)	86	66
1	D	397/371 (107%)	397 (100%)	0	100	100
All	All	1598/1484 (108%)	1596 (100%)	2 (0%)	88	67

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	C	396	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	49	GLN
1	D	428	GLN
1	D	210	GLN
1	B	459	HIS
1	C	459	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	C	288(A)	1	23,24,25	1.02	1 (4%)	25,32,34	1.14	3 (12%)
1	LLP	A	288(A)	1	23,24,25	0.93	1 (4%)	25,32,34	1.21	3 (12%)
1	LLP	B	288(A)	1	23,24,25	0.95	1 (4%)	25,32,34	1.22	3 (12%)
1	LLP	D	288(A)	1	23,24,25	0.97	1 (4%)	25,32,34	1.18	3 (12%)

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
1	LLP	C	288(A)	1	-	3/16/17/19	0/1/1/1
1	LLP	A	288(A)	1	-	3/16/17/19	0/1/1/1
1	LLP	B	288(A)	1	-	3/16/17/19	0/1/1/1
1	LLP	D	288(A)	1	-	3/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288(A)	LLP	C4'-NZ	2.74	1.36	1.27
1	A	288(A)	LLP	C4'-NZ	2.70	1.36	1.27
1	D	288(A)	LLP	C4'-NZ	2.59	1.35	1.27
1	C	288(A)	LLP	C4'-NZ	2.37	1.35	1.27

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288(A)	LLP	C3-C4-C5	-3.08	115.80	118.28
1	A	288(A)	LLP	C3-C4-C5	-2.89	115.96	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288(A)	LLP	C4-C3-C2	2.53	121.57	120.14
1	D	288(A)	LLP	C3-C4-C5	-2.45	116.31	118.28
1	B	288(A)	LLP	C4-C3-C2	2.36	121.47	120.14

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	288(A)	LLP	O-C-CA-CB
1	A	288(A)	LLP	CG-CD-CE-NZ
1	B	288(A)	LLP	O-C-CA-CB
1	B	288(A)	LLP	CG-CD-CE-NZ
1	C	288(A)	LLP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	288(A)	LLP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 169 ligands modelled in this entry, 36 are monoatomic - leaving 133 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PEG	C	522	-	6,6,6	0.16	0	5,5,5	0.11	0
4	EDO	C	504	-	3,3,3	0.09	0	2,2,2	0.16	0
4	EDO	D	515	-	3,3,3	0.03	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	C	532	-	6,6,6	0.17	0	5,5,5	0.17	0
4	EDO	A	533	-	3,3,3	0.20	0	2,2,2	0.47	0
4	EDO	C	534	-	3,3,3	0.19	0	2,2,2	0.64	0
4	EDO	B	502	-	3,3,3	0.23	0	2,2,2	0.76	0
5	GOL	A	529	-	5,5,5	0.12	0	5,5,5	0.39	0
4	EDO	B	505	-	3,3,3	0.32	0	2,2,2	0.91	0
4	EDO	D	516	-	3,3,3	0.05	0	2,2,2	0.14	0
4	EDO	B	534	-	3,3,3	0.45	0	2,2,2	0.95	0
4	EDO	B	523	-	3,3,3	0.06	0	2,2,2	0.17	0
4	EDO	D	509	-	3,3,3	0.13	0	2,2,2	0.88	0
4	EDO	B	508	-	3,3,3	0.06	0	2,2,2	0.29	0
4	EDO	C	518	-	3,3,3	0.40	0	2,2,2	0.48	0
9	PG4	C	531	8	12,12,12	0.26	0	11,11,11	0.23	0
2	PEG	B	521	-	6,6,6	0.23	0	5,5,5	0.11	0
4	EDO	A	513	-	3,3,3	0.05	0	2,2,2	0.38	0
3	PGE	D	505	-	9,9,9	0.19	0	8,8,8	0.14	0
4	EDO	B	531	-	3,3,3	0.03	0	2,2,2	0.16	0
4	EDO	D	506	-	3,3,3	0.67	0	2,2,2	0.97	0
4	EDO	A	534	8	3,3,3	0.11	0	2,2,2	0.31	0
4	EDO	D	517	-	3,3,3	0.23	0	2,2,2	0.25	0
4	EDO	A	517	-	3,3,3	0.38	0	2,2,2	0.73	0
4	EDO	C	529	-	3,3,3	0.15	0	2,2,2	0.09	0
4	EDO	C	509	-	3,3,3	0.05	0	2,2,2	0.09	0
4	EDO	A	530	-	3,3,3	0.15	0	2,2,2	0.50	0
4	EDO	B	527	-	3,3,3	0.11	0	2,2,2	0.03	0
4	EDO	C	514	-	3,3,3	0.12	0	2,2,2	0.13	0
5	GOL	A	511	-	5,5,5	0.15	0	5,5,5	0.56	0
4	EDO	D	507	-	3,3,3	0.02	0	2,2,2	0.22	0
4	EDO	A	514	-	3,3,3	0.07	0	2,2,2	0.05	0
4	EDO	D	501	-	3,3,3	0.06	0	2,2,2	0.33	0
2	PEG	A	525	-	6,6,6	0.74	0	5,5,5	0.32	0
4	EDO	A	505	-	3,3,3	0.13	0	2,2,2	0.71	0
2	PEG	B	504	-	6,6,6	0.23	0	5,5,5	0.19	0
4	EDO	D	524	-	3,3,3	0.11	0	2,2,2	0.20	0
4	EDO	A	532	-	3,3,3	0.09	0	2,2,2	0.30	0
3	PGE	A	502	-	9,9,9	0.20	0	8,8,8	0.17	0
4	EDO	B	526	-	3,3,3	0.10	0	2,2,2	0.18	0
2	PEG	A	523	-	6,6,6	0.13	0	5,5,5	0.21	0
4	EDO	B	507	-	3,3,3	0.16	0	2,2,2	0.14	0
4	EDO	C	517	-	3,3,3	0.20	0	2,2,2	0.30	0
2	PEG	A	501	-	6,6,6	0.21	0	5,5,5	0.19	0
2	PEG	A	512	-	6,6,6	0.54	0	5,5,5	0.43	0
4	EDO	D	502	-	3,3,3	0.69	0	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	516	-	3,3,3	0.27	0	2,2,2	0.68	0
4	EDO	C	507	-	3,3,3	0.31	0	2,2,2	0.77	0
4	EDO	C	526	-	3,3,3	0.19	0	2,2,2	0.41	0
4	EDO	D	526	-	3,3,3	0.11	0	2,2,2	0.23	0
4	EDO	B	535	-	3,3,3	0.14	0	2,2,2	0.40	0
4	EDO	D	528	-	3,3,3	0.38	0	2,2,2	0.28	0
2	PEG	C	523	-	6,6,6	0.12	0	5,5,5	0.08	0
4	EDO	D	520	-	3,3,3	0.39	0	2,2,2	0.51	0
4	EDO	C	512	-	3,3,3	0.11	0	2,2,2	0.38	0
4	EDO	A	520	-	3,3,3	0.23	0	2,2,2	0.42	0
5	GOL	D	503	-	5,5,5	0.12	0	5,5,5	0.66	0
4	EDO	D	510	-	3,3,3	0.13	0	2,2,2	0.29	0
4	EDO	A	516	-	3,3,3	0.24	0	2,2,2	0.36	0
4	EDO	A	510	-	3,3,3	0.07	0	2,2,2	0.48	0
4	EDO	D	519	-	3,3,3	0.12	0	2,2,2	0.35	0
4	EDO	C	528	-	3,3,3	0.08	0	2,2,2	0.16	0
4	EDO	A	531	-	3,3,3	0.27	0	2,2,2	0.41	0
3	PGE	D	514	-	9,9,9	0.49	0	8,8,8	0.39	0
9	PG4	B	503	-	12,12,12	0.21	0	11,11,11	0.17	0
4	EDO	B	512	-	3,3,3	0.20	0	2,2,2	0.28	0
5	GOL	B	511	-	5,5,5	0.24	0	5,5,5	0.72	0
4	EDO	B	518	-	3,3,3	0.37	0	2,2,2	0.67	0
3	PGE	B	509	-	9,9,9	0.17	0	8,8,8	0.09	0
3	PGE	B	519	-	9,9,9	0.24	0	8,8,8	0.26	0
2	PEG	C	501	-	6,6,6	0.13	0	5,5,5	0.08	0
4	EDO	C	519	-	3,3,3	0.10	0	2,2,2	0.20	0
4	EDO	B	525	-	3,3,3	0.22	0	2,2,2	0.25	0
3	PGE	B	506	-	9,9,9	0.27	0	8,8,8	0.20	0
4	EDO	B	537	-	3,3,3	0.21	0	2,2,2	0.60	0
5	GOL	C	505	-	5,5,5	0.08	0	5,5,5	0.33	0
3	PGE	C	527	-	9,9,9	0.20	0	8,8,8	0.33	0
4	EDO	A	506	-	3,3,3	0.31	0	2,2,2	0.83	0
4	EDO	B	514	-	3,3,3	0.18	0	2,2,2	0.17	0
5	GOL	B	533	-	5,5,5	0.07	0	5,5,5	0.69	0
2	PEG	D	508	-	6,6,6	0.12	0	5,5,5	0.06	0
4	EDO	C	524	-	3,3,3	0.16	0	2,2,2	0.33	0
2	PEG	C	502	-	6,6,6	0.20	0	5,5,5	0.15	0
4	EDO	D	521	-	3,3,3	0.16	0	2,2,2	0.31	0
4	EDO	D	527	-	3,3,3	0.08	0	2,2,2	0.29	0
4	EDO	D	522	-	3,3,3	0.25	0	2,2,2	0.15	0
4	EDO	A	524	-	3,3,3	0.32	0	2,2,2	0.68	0
6	1PG	A	521	-	16,16,16	0.32	0	15,15,15	0.21	0
4	EDO	B	532	-	3,3,3	0.13	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	523	-	3,3,3	0.23	0	2,2,2	0.56	0
4	EDO	D	504	-	3,3,3	0.08	0	2,2,2	0.17	0
4	EDO	D	525	-	3,3,3	0.05	0	2,2,2	0.08	0
4	EDO	B	536	-	3,3,3	0.16	0	2,2,2	0.52	0
4	EDO	C	521	-	3,3,3	0.07	0	2,2,2	0.27	0
5	GOL	C	513	-	5,5,5	0.14	0	5,5,5	0.39	0
4	EDO	D	513	-	3,3,3	0.08	0	2,2,2	0.15	0
2	PEG	A	526	-	6,6,6	0.48	0	5,5,5	0.55	0
4	EDO	A	509	-	3,3,3	0.15	0	2,2,2	0.29	0
4	EDO	B	501	-	3,3,3	0.20	0	2,2,2	0.13	0
4	EDO	C	533	-	3,3,3	0.41	0	2,2,2	0.53	0
4	EDO	C	510	-	3,3,3	0.11	0	2,2,2	0.28	0
4	EDO	B	524	-	3,3,3	0.10	0	2,2,2	0.27	0
4	EDO	B	513	-	3,3,3	0.09	0	2,2,2	0.14	0
4	EDO	C	525	-	3,3,3	0.28	0	2,2,2	0.63	0
3	PGE	C	530	-	9,9,9	0.25	0	8,8,8	0.08	0
4	EDO	A	507	-	3,3,3	0.06	0	2,2,2	0.15	0
2	PEG	A	515	-	6,6,6	0.13	0	5,5,5	0.18	0
4	EDO	C	506	-	3,3,3	0.10	0	2,2,2	0.13	0
5	GOL	C	503	-	5,5,5	0.14	0	5,5,5	0.57	0
4	EDO	A	503	-	3,3,3	0.63	0	2,2,2	1.12	0
4	EDO	B	528	8	3,3,3	0.15	0	2,2,2	0.26	0
4	EDO	B	520	-	3,3,3	0.11	0	2,2,2	0.35	0
4	EDO	C	511	-	3,3,3	0.14	0	2,2,2	0.16	0
4	EDO	A	528	-	3,3,3	0.08	0	2,2,2	0.07	0
4	EDO	D	512	-	3,3,3	0.14	0	2,2,2	0.23	0
4	EDO	B	510	-	3,3,3	0.08	0	2,2,2	0.32	0
4	EDO	C	508	-	3,3,3	0.12	0	2,2,2	0.17	0
4	EDO	A	522	-	3,3,3	0.06	0	2,2,2	0.24	0
4	EDO	D	518	-	3,3,3	0.13	0	2,2,2	0.70	0
5	GOL	B	522	-	5,5,5	0.14	0	5,5,5	0.44	0
4	EDO	A	518	-	3,3,3	0.42	0	2,2,2	0.79	0
5	GOL	D	511	-	5,5,5	0.11	0	5,5,5	0.37	0
5	GOL	A	519	-	5,5,5	0.13	0	5,5,5	0.52	0
4	EDO	B	530	-	3,3,3	0.03	0	2,2,2	0.69	0
4	EDO	C	520	-	3,3,3	0.06	0	2,2,2	0.37	0
2	PEG	B	515	-	6,6,6	0.21	0	5,5,5	0.28	0
3	PGE	B	517	-	9,9,9	0.21	0	8,8,8	0.13	0
4	EDO	A	508	-	3,3,3	0.09	0	2,2,2	0.39	0
4	EDO	A	504	-	3,3,3	0.15	0	2,2,2	0.71	0
4	EDO	B	516	-	3,3,3	0.08	0	2,2,2	0.11	0
2	PEG	A	527	-	6,6,6	0.23	0	5,5,5	0.12	0
2	PEG	B	529	-	6,6,6	0.51	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	515	-	3,3,3	0.06	0	2,2,2	0.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	C	522	-	-	2/4/4/4	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
2	PEG	C	532	-	-	3/4/4/4	-
4	EDO	A	533	-	-	0/1/1/1	-
4	EDO	C	534	-	-	1/1/1/1	-
4	EDO	B	502	-	-	1/1/1/1	-
5	GOL	A	529	-	-	3/4/4/4	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	D	516	-	-	1/1/1/1	-
4	EDO	B	534	-	-	1/1/1/1	-
4	EDO	B	523	-	-	1/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	B	508	-	-	1/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
9	PG4	C	531	8	-	5/10/10/10	-
2	PEG	B	521	-	-	1/4/4/4	-
4	EDO	A	513	-	-	1/1/1/1	-
3	PGE	D	505	-	-	2/7/7/7	-
4	EDO	B	531	-	-	1/1/1/1	-
4	EDO	D	506	-	-	1/1/1/1	-
4	EDO	A	534	8	-	0/1/1/1	-
4	EDO	D	517	-	-	1/1/1/1	-
4	EDO	A	517	-	-	0/1/1/1	-
4	EDO	C	529	-	-	1/1/1/1	-
4	EDO	C	509	-	-	1/1/1/1	-
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	B	527	-	-	1/1/1/1	-
4	EDO	C	514	-	-	1/1/1/1	-
5	GOL	A	511	-	-	2/4/4/4	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	A	514	-	-	1/1/1/1	-
4	EDO	D	501	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	525	-	-	3/4/4/4	-
4	EDO	A	505	-	-	0/1/1/1	-
2	PEG	B	504	-	-	3/4/4/4	-
4	EDO	D	524	-	-	1/1/1/1	-
4	EDO	A	532	-	-	1/1/1/1	-
3	PGE	A	502	-	-	7/7/7/7	-
4	EDO	B	526	-	-	0/1/1/1	-
2	PEG	A	523	-	-	3/4/4/4	-
4	EDO	B	507	-	-	1/1/1/1	-
4	EDO	C	517	-	-	0/1/1/1	-
2	PEG	A	501	-	-	4/4/4/4	-
2	PEG	A	512	-	-	1/4/4/4	-
4	EDO	D	502	-	-	1/1/1/1	-
4	EDO	C	516	-	-	1/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	C	526	-	-	1/1/1/1	-
4	EDO	D	526	-	-	1/1/1/1	-
4	EDO	B	535	-	-	1/1/1/1	-
4	EDO	D	528	-	-	1/1/1/1	-
2	PEG	C	523	-	-	3/4/4/4	-
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	C	512	-	-	0/1/1/1	-
4	EDO	A	520	-	-	1/1/1/1	-
5	GOL	D	503	-	-	0/4/4/4	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	C	528	-	-	0/1/1/1	-
4	EDO	A	531	-	-	1/1/1/1	-
3	PGE	D	514	-	-	5/7/7/7	-
9	PG4	B	503	-	-	3/10/10/10	-
4	EDO	B	512	-	-	1/1/1/1	-
5	GOL	B	511	-	-	4/4/4/4	-
4	EDO	B	518	-	-	1/1/1/1	-
3	PGE	B	509	-	-	4/7/7/7	-
3	PGE	B	519	-	-	3/7/7/7	-
2	PEG	C	501	-	-	1/4/4/4	-
4	EDO	C	519	-	-	1/1/1/1	-
4	EDO	B	525	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	B	506	-	-	7/7/7/7	-
4	EDO	B	537	-	-	1/1/1/1	-
5	GOL	C	505	-	-	2/4/4/4	-
3	PGE	C	527	-	-	4/7/7/7	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	B	514	-	-	1/1/1/1	-
5	GOL	B	533	-	-	0/4/4/4	-
2	PEG	D	508	-	-	4/4/4/4	-
4	EDO	C	524	-	-	1/1/1/1	-
2	PEG	C	502	-	-	3/4/4/4	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	D	527	-	-	0/1/1/1	-
4	EDO	D	522	-	-	1/1/1/1	-
4	EDO	A	524	-	-	0/1/1/1	-
6	1PG	A	521	-	-	8/14/14/14	-
4	EDO	B	532	-	-	0/1/1/1	-
4	EDO	D	523	-	-	1/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	D	525	-	-	0/1/1/1	-
4	EDO	B	536	-	-	0/1/1/1	-
4	EDO	C	521	-	-	1/1/1/1	-
5	GOL	C	513	-	-	2/4/4/4	-
4	EDO	D	513	-	-	1/1/1/1	-
2	PEG	A	526	-	-	3/4/4/4	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	B	501	-	-	1/1/1/1	-
4	EDO	C	533	-	-	0/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-
4	EDO	B	524	-	-	0/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	C	525	-	-	1/1/1/1	-
3	PGE	C	530	-	-	2/7/7/7	-
4	EDO	A	507	-	-	1/1/1/1	-
2	PEG	A	515	-	-	4/4/4/4	-
4	EDO	C	506	-	-	1/1/1/1	-
5	GOL	C	503	-	-	0/4/4/4	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	B	528	8	-	0/1/1/1	-
4	EDO	B	520	-	-	0/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	528	-	-	1/1/1/1	-
4	EDO	D	512	-	-	1/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
5	GOL	B	522	-	-	2/4/4/4	-
4	EDO	A	518	-	-	0/1/1/1	-
5	GOL	D	511	-	-	2/4/4/4	-
5	GOL	A	519	-	-	2/4/4/4	-
4	EDO	B	530	-	-	1/1/1/1	-
4	EDO	C	520	-	-	0/1/1/1	-
2	PEG	B	515	-	-	3/4/4/4	-
3	PGE	B	517	-	-	2/7/7/7	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
2	PEG	A	527	-	-	2/4/4/4	-
2	PEG	B	529	-	-	2/4/4/4	-
4	EDO	C	515	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 181 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	519	GOL	C1-C2-C3-O3
5	A	529	GOL	O1-C1-C2-C3
5	B	511	GOL	O1-C1-C2-C3
5	B	511	GOL	C1-C2-C3-O3
5	B	522	GOL	C1-C2-C3-O3

There are no ring outliers.

79 monomers are involved in 255 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	504	EDO	2	0
4	D	515	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	532	PEG	2	0
4	C	534	EDO	2	0
4	B	502	EDO	2	0
4	B	505	EDO	2	0
4	B	534	EDO	2	0
4	B	523	EDO	1	0
4	D	509	EDO	2	0
2	B	521	PEG	4	0
4	A	513	EDO	3	0
3	D	505	PGE	6	0
4	B	531	EDO	2	0
4	D	506	EDO	3	0
4	A	534	EDO	1	0
4	D	517	EDO	6	0
4	A	517	EDO	5	0
4	A	530	EDO	1	0
5	A	511	GOL	2	0
4	D	507	EDO	2	0
4	D	501	EDO	6	0
2	A	525	PEG	13	0
4	A	505	EDO	1	0
2	B	504	PEG	8	0
3	A	502	PGE	3	0
4	B	507	EDO	1	0
2	A	501	PEG	2	0
2	A	512	PEG	1	0
4	D	502	EDO	2	0
4	C	516	EDO	5	0
4	C	507	EDO	3	0
4	C	526	EDO	7	0
4	D	528	EDO	7	0
4	D	520	EDO	25	0
4	C	512	EDO	1	0
4	A	520	EDO	1	0
4	D	510	EDO	2	0
4	A	516	EDO	1	0
4	A	510	EDO	2	0
3	D	514	PGE	2	0
5	B	511	GOL	1	0
4	B	518	EDO	4	0
3	B	519	PGE	8	0
2	C	501	PEG	5	0

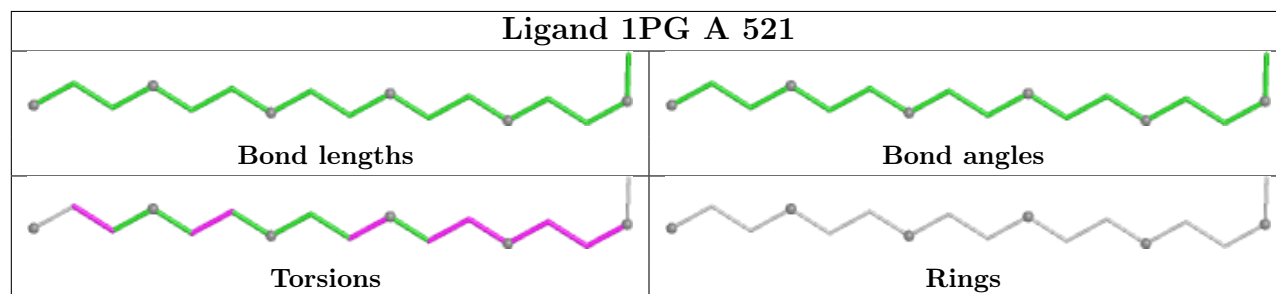
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	519	EDO	4	0
3	B	506	PGE	1	0
4	B	537	EDO	5	0
3	C	527	PGE	12	0
4	A	506	EDO	1	0
5	B	533	GOL	6	0
4	C	524	EDO	1	0
2	C	502	PEG	1	0
4	D	522	EDO	2	0
4	B	532	EDO	4	0
4	D	523	EDO	2	0
4	B	536	EDO	3	0
5	C	513	GOL	1	0
4	D	513	EDO	1	0
2	A	526	PEG	7	0
4	C	510	EDO	1	0
4	B	524	EDO	1	0
4	B	513	EDO	1	0
3	C	530	PGE	1	0
5	C	503	GOL	3	0
4	A	503	EDO	3	0
4	D	512	EDO	1	0
4	B	510	EDO	4	0
4	C	508	EDO	7	0
4	D	518	EDO	3	0
5	B	522	GOL	1	0
4	A	518	EDO	4	0
5	D	511	GOL	2	0
5	A	519	GOL	1	0
4	B	530	EDO	1	0
4	C	520	EDO	4	0
2	B	515	PEG	12	0
4	A	504	EDO	5	0
4	B	516	EDO	1	0
2	B	529	PEG	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	455/461 (98%)	-0.09	15 (3%)	49 49	7, 16, 39, 108	34 (7%)
1	B	454/461 (98%)	-0.07	19 (4%)	40 40	7, 15, 39, 120	32 (7%)
1	C	460/461 (99%)	0.09	19 (4%)	41 41	7, 17, 43, 112	29 (6%)
1	D	454/461 (98%)	0.34	30 (6%)	24 24	7, 18, 54, 137	30 (6%)
All	All	1823/1844 (98%)	0.07	83 (4%)	37 37	7, 16, 45, 137	125 (6%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	ILE	8.5
1	A	7	VAL	8.3
1	D	7	VAL	7.2
1	C	7	VAL	6.0
1	B	403	TYR	6.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
1	LLP	A	288(A)	24/25	0.98	0.05	11,12,15,17	0
1	LLP	B	288(A)	24/25	0.98	0.04	11,12,15,17	0
1	LLP	C	288(A)	24/25	0.98	0.05	11,13,17,18	0
1	LLP	D	288(A)	24/25	0.98	0.05	12,14,18,20	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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
4	EDO	C	518	4/4	0.36	0.25	78,82,85,96	0
4	EDO	B	526	4/4	0.64	0.21	57,60,72,74	0
4	EDO	C	521	4/4	0.68	0.17	60,60,60,78	0
4	EDO	D	527	4/4	0.68	0.17	70,77,80,84	0
4	EDO	B	512	4/4	0.70	0.16	58,63,64,71	0
4	EDO	C	520	4/4	0.70	0.14	44,47,53,65	0
4	EDO	C	529	4/4	0.75	0.21	59,67,72,77	0
4	EDO	D	504	4/4	0.75	0.15	52,52,60,66	0
4	EDO	D	513	4/4	0.75	0.14	62,64,65,68	0
4	EDO	D	518	4/4	0.75	0.20	32,35,36,37	4
2	PEG	A	527	7/7	0.75	0.13	53,55,71,71	0
2	PEG	A	501	7/7	0.76	0.15	51,54,62,67	0
3	PGE	B	517	10/10	0.76	0.15	58,59,69,72	0
4	EDO	C	525	4/4	0.76	0.17	53,53,63,67	0
4	EDO	A	522	4/4	0.76	0.16	56,63,72,74	0
4	EDO	A	528	4/4	0.77	0.19	63,66,67,72	0
4	EDO	A	524	4/4	0.78	0.17	52,56,60,63	0
4	EDO	A	513	4/4	0.78	0.14	54,57,60,61	0
4	EDO	D	507	4/4	0.78	0.18	43,46,59,63	0
5	GOL	A	529	6/6	0.78	0.17	44,62,66,66	0
5	GOL	C	505	6/6	0.78	0.16	60,61,62,80	0
8	MG	B	544	1/1	0.78	0.11	62,62,62,62	0
2	PEG	B	529	7/7	0.79	0.17	33,45,53,61	0
4	EDO	B	516	4/4	0.79	0.16	65,66,68,70	0
2	PEG	C	502	7/7	0.79	0.17	49,62,68,70	0
2	PEG	B	504	7/7	0.79	0.14	45,48,53,69	0
3	PGE	C	530	10/10	0.79	0.16	54,71,77,78	0
4	EDO	D	512	4/4	0.79	0.13	39,46,46,51	0
4	EDO	A	505	4/4	0.80	0.15	33,37,48,58	0
4	EDO	C	533	4/4	0.80	0.17	39,41,58,65	0
4	EDO	D	525	4/4	0.80	0.13	62,63,64,67	0
4	EDO	C	534	4/4	0.80	0.14	44,45,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	D	508	7/7	0.80	0.13	53,60,64,68	0
4	EDO	C	511	4/4	0.80	0.12	58,60,65,68	0
4	EDO	C	515	4/4	0.80	0.13	59,60,65,72	0
4	EDO	D	517	4/4	0.81	0.17	34,39,57,59	0
4	EDO	A	510	4/4	0.81	0.16	58,58,64,67	0
4	EDO	B	501	4/4	0.81	0.15	52,53,54,54	0
4	EDO	B	527	4/4	0.81	0.16	51,61,63,71	0
4	EDO	C	507	4/4	0.81	0.19	42,50,57,64	0
4	EDO	C	510	4/4	0.81	0.14	49,50,59,61	0
6	1PG	A	521	17/17	0.81	0.16	54,65,79,81	0
2	PEG	C	523	7/7	0.81	0.16	74,76,83,84	0
4	EDO	D	516	4/4	0.82	0.14	59,62,65,71	0
2	PEG	B	521	7/7	0.82	0.15	37,50,74,74	0
4	EDO	C	514	4/4	0.82	0.14	54,56,63,69	0
4	EDO	D	519	4/4	0.82	0.13	60,60,64,69	0
4	EDO	D	521	4/4	0.82	0.13	52,55,57,61	0
4	EDO	D	523	4/4	0.82	0.12	48,49,51,54	0
4	EDO	B	507	4/4	0.82	0.17	37,37,38,39	4
4	EDO	D	526	4/4	0.82	0.12	51,56,57,66	0
4	EDO	B	531	4/4	0.82	0.13	42,50,51,59	0
4	EDO	B	535	4/4	0.82	0.14	45,48,56,61	0
4	EDO	A	532	4/4	0.82	0.14	51,57,57,61	0
4	EDO	A	533	4/4	0.82	0.14	49,51,58,60	0
4	EDO	D	515	4/4	0.82	0.17	57,66,69,74	0
2	PEG	C	501	7/7	0.83	0.17	62,64,68,77	0
4	EDO	C	516	4/4	0.83	0.12	48,50,53,57	0
4	EDO	B	520	4/4	0.83	0.14	50,52,54,61	0
4	EDO	A	508	4/4	0.83	0.13	49,55,57,60	0
5	GOL	C	503	6/6	0.83	0.13	37,47,51,62	0
4	EDO	B	510	4/4	0.83	0.12	46,50,52,54	0
4	EDO	C	524	4/4	0.83	0.15	47,54,55,62	0
3	PGE	B	506	10/10	0.83	0.15	43,51,57,59	0
4	EDO	A	516	4/4	0.84	0.13	34,37,41,48	0
2	PEG	A	523	7/7	0.84	0.15	50,52,62,63	0
4	EDO	A	531	4/4	0.84	0.12	40,43,50,53	0
4	EDO	C	519	4/4	0.84	0.11	44,46,47,58	0
8	MG	A	542	1/1	0.84	0.14	64,64,64,64	0
4	EDO	C	504	4/4	0.84	0.16	59,61,66,75	0
8	MG	C	541	1/1	0.84	0.22	46,46,46,46	0
5	GOL	A	519	6/6	0.85	0.12	37,43,54,60	0
2	PEG	A	526	7/7	0.85	0.12	40,45,50,57	0
5	GOL	B	511	6/6	0.85	0.12	37,42,47,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	C	522	7/7	0.85	0.13	51,59,64,67	0
4	EDO	A	506	4/4	0.85	0.12	38,40,46,50	0
5	GOL	D	503	6/6	0.85	0.13	39,46,48,52	0
4	EDO	D	524	4/4	0.85	0.13	56,59,61,71	0
4	EDO	A	520	4/4	0.85	0.12	36,44,48,51	0
8	MG	A	544	1/1	0.85	0.09	60,60,60,60	0
4	EDO	B	534	4/4	0.85	0.13	32,39,45,51	0
3	PGE	C	527	10/10	0.85	0.15	37,48,55,62	0
4	EDO	D	528	4/4	0.86	0.15	35,37,41,62	0
5	GOL	A	511	6/6	0.86	0.11	38,39,46,46	0
4	EDO	C	509	4/4	0.86	0.13	30,30,51,56	0
3	PGE	D	514	10/10	0.86	0.16	24,44,50,59	0
4	EDO	B	532	4/4	0.86	0.12	47,48,52,52	0
5	GOL	B	522	6/6	0.86	0.12	38,46,52,55	0
4	EDO	C	526	4/4	0.86	0.12	40,47,54,57	0
3	PGE	A	502	10/10	0.86	0.14	48,57,64,67	0
4	EDO	B	524	4/4	0.86	0.13	53,55,55,60	0
4	EDO	B	536	4/4	0.86	0.12	45,46,47,64	0
4	EDO	C	517	4/4	0.86	0.13	49,50,53,63	0
3	PGE	B	519	10/10	0.86	0.12	34,44,51,53	0
4	EDO	C	506	4/4	0.86	0.14	47,53,53,53	0
8	MG	B	545	1/1	0.86	0.12	64,64,64,64	0
4	EDO	B	513	4/4	0.86	0.17	64,65,67,76	0
8	MG	C	542	1/1	0.86	0.13	56,56,56,56	0
8	MG	C	545	1/1	0.86	0.13	57,57,57,57	0
9	PG4	C	531	13/13	0.86	0.14	42,50,64,65	0
4	EDO	A	507	4/4	0.87	0.12	43,53,55,71	0
4	EDO	C	528	4/4	0.87	0.12	51,55,56,59	0
3	PGE	B	509	10/10	0.87	0.12	48,56,63,63	0
2	PEG	C	532	7/7	0.87	0.11	50,51,57,58	0
4	EDO	D	522	4/4	0.87	0.11	41,45,47,48	0
4	EDO	B	537	4/4	0.87	0.14	34,35,42,62	0
4	EDO	D	502	4/4	0.87	0.13	29,35,40,58	0
4	EDO	A	534	4/4	0.88	0.09	41,46,49,50	0
4	EDO	B	518	4/4	0.88	0.11	42,42,49,52	0
5	GOL	D	511	6/6	0.88	0.12	42,52,63,74	0
4	EDO	A	518	4/4	0.88	0.13	25,26,49,52	0
4	EDO	B	505	4/4	0.88	0.12	36,36,45,48	0
4	EDO	A	530	4/4	0.88	0.11	43,51,51,53	0
2	PEG	B	515	7/7	0.88	0.13	29,37,55,58	0
4	EDO	B	528	4/4	0.88	0.12	44,47,55,56	0
4	EDO	C	508	4/4	0.88	0.12	41,45,57,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PEG	A	512	7/7	0.88	0.10	30,36,37,41	0
5	GOL	B	533	6/6	0.88	0.11	23,37,44,57	0
2	PEG	A	515	7/7	0.88	0.12	48,51,54,58	0
4	EDO	A	503	4/4	0.89	0.09	27,35,43,49	0
4	EDO	A	517	4/4	0.89	0.12	29,29,32,47	0
4	EDO	D	506	4/4	0.89	0.12	27,32,37,49	0
5	GOL	C	513	6/6	0.89	0.12	34,44,51,62	0
4	EDO	A	514	4/4	0.89	0.12	56,56,60,62	0
4	EDO	B	514	4/4	0.89	0.13	35,38,41,55	0
4	EDO	C	512	4/4	0.89	0.10	37,42,42,45	0
8	MG	A	539	1/1	0.89	0.14	38,38,38,38	0
3	PGE	D	505	10/10	0.90	0.10	45,49,61,61	0
4	EDO	A	504	4/4	0.90	0.10	38,39,40,59	0
8	MG	C	544	1/1	0.90	0.10	65,65,65,65	0
4	EDO	A	509	4/4	0.90	0.10	45,47,49,53	0
4	EDO	B	508	4/4	0.90	0.10	48,50,52,56	0
8	MG	C	543	1/1	0.91	0.21	64,64,64,64	0
4	EDO	B	525	4/4	0.91	0.10	43,45,46,47	0
8	MG	B	543	1/1	0.91	0.29	50,50,50,50	0
4	EDO	B	530	4/4	0.91	0.09	32,34,40,55	0
8	MG	A	541	1/1	0.92	0.19	44,44,44,44	0
4	EDO	D	501	4/4	0.92	0.14	16,33,48,59	0
4	EDO	B	523	4/4	0.92	0.10	45,51,51,59	0
9	PG4	B	503	13/13	0.92	0.11	35,44,64,68	0
4	EDO	B	502	4/4	0.92	0.13	25,29,48,55	0
8	MG	C	540	1/1	0.93	0.20	52,52,52,52	0
2	PEG	A	525	7/7	0.93	0.10	26,27,35,58	0
8	MG	A	543	1/1	0.93	0.28	48,48,48,48	0
8	MG	C	538	1/1	0.93	0.12	48,48,48,48	0
8	MG	A	538	1/1	0.94	0.20	33,33,33,33	0
4	EDO	D	510	4/4	0.94	0.09	39,41,48,51	0
4	EDO	D	509	4/4	0.95	0.09	28,38,40,62	0
8	MG	A	540	1/1	0.95	0.10	33,33,33,33	0
7	CL	A	535	1/1	0.96	0.09	38,38,38,38	0
8	MG	D	531	1/1	0.96	0.14	28,28,28,28	0
7	CL	D	530	1/1	0.96	0.12	33,33,33,33	0
8	MG	B	546	1/1	0.96	0.11	32,32,32,32	0
8	MG	B	542	1/1	0.97	0.07	29,29,29,29	0
7	CL	C	536	1/1	0.97	0.14	30,30,30,30	0
4	EDO	D	520	4/4	0.97	0.07	19,24,39,41	0
8	MG	D	532	1/1	0.97	0.16	32,32,32,32	0
8	MG	D	533	1/1	0.97	0.07	40,40,40,40	0

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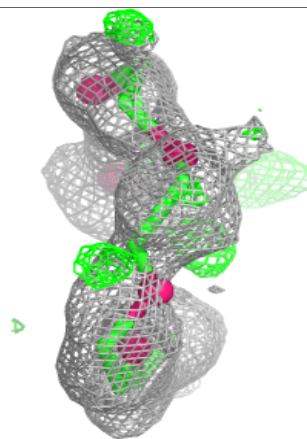
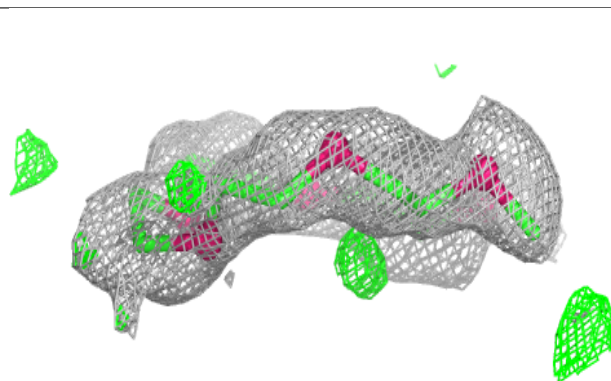
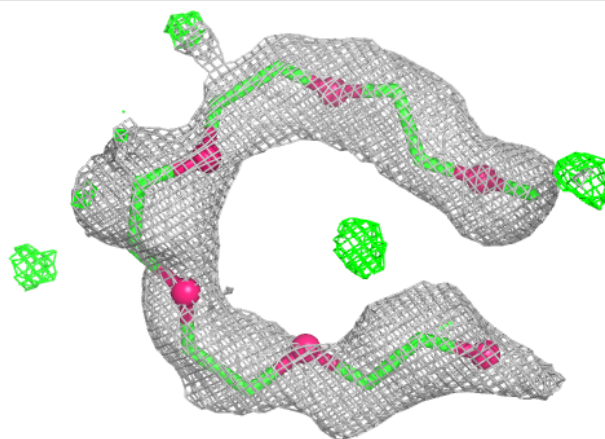
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	MG	D	534	1/1	0.97	0.09	40,40,40,40	0
7	CL	B	539	1/1	0.97	0.14	26,26,26,26	0
8	MG	B	540	1/1	0.97	0.13	27,27,27,27	0
8	MG	C	537	1/1	0.98	0.12	27,27,27,27	0
8	MG	B	541	1/1	0.98	0.13	24,24,24,24	0
7	CL	C	535	1/1	0.99	0.03	19,19,19,19	0
7	CL	A	537	1/1	0.99	0.12	28,28,28,28	0
7	CL	D	529	1/1	0.99	0.05	22,22,22,22	0
7	CL	B	538	1/1	0.99	0.03	19,19,19,19	0
7	CL	A	536	1/1	0.99	0.04	20,20,20,20	0
8	MG	C	539	1/1	0.99	0.11	29,29,29,29	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 1PG A 521:

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.