



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 03:11 PM BST

PDB ID : 5DWY
Title : Crystal structure of a substrate-free glutamate transporter homologue GltTk
Authors : Guskov, A.; Slotboom, D.J.
Deposited on : 2015-09-23
Resolution : 2.70 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 : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

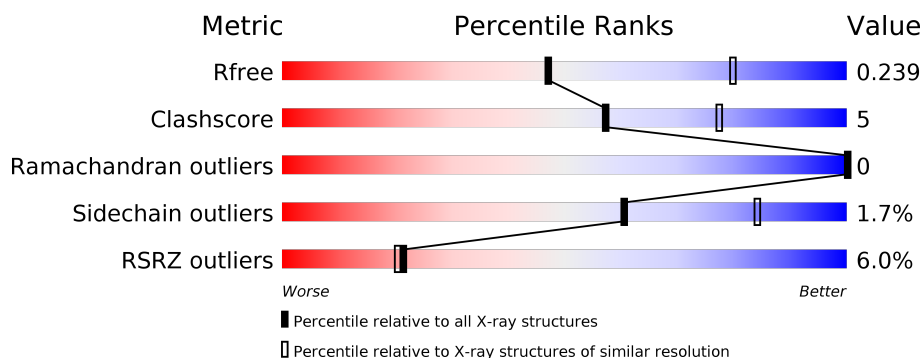
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	438	<div> <div>7%</div> <div>83%</div> <div>14%</div> <div>•</div> </div>
1	B	438	<div> <div>6%</div> <div>87%</div> <div>10%</div> <div>••</div> </div>
1	C	438	<div> <div>5%</div> <div>84%</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	PGE	A	504	-	-	-	X
2	PGE	B	502	-	-	-	X
2	PGE	C	501	-	-	-	X
3	PEG	A	508	-	-	-	X
3	PEG	A	514	-	-	-	X
3	PEG	B	507	-	-	-	X
3	PEG	B	508	-	-	-	X
3	PEG	C	505	-	-	-	X
3	PEG	C	510	-	-	-	X
3	PEG	C	511[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10016 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 Proton/glutamate symporter, SDF family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3197	2108	519	553	17			
1	B	428	Total	C	N	O	S	0	2	0
			3212	2117	522	556	17			
1	C	427	Total	C	N	O	S	0	4	0
			3229	2126	530	556	17			

There are 24 discrepancies between the modelled and reference sequences:

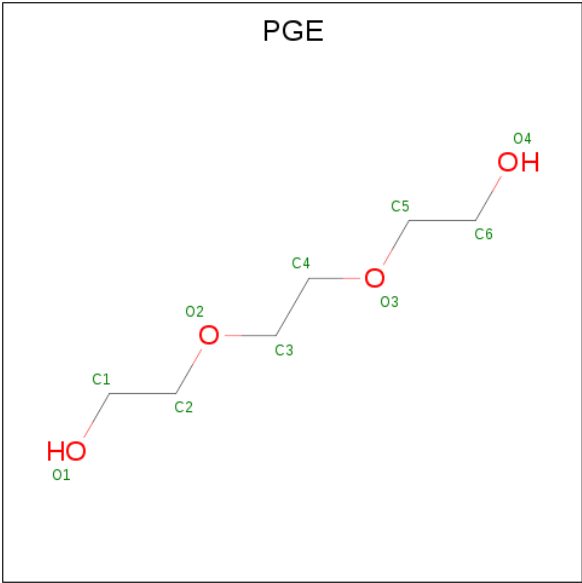
Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q5JID0
A	432	HIS	-	expression tag	UNP Q5JID0
A	433	HIS	-	expression tag	UNP Q5JID0
A	434	HIS	-	expression tag	UNP Q5JID0
A	435	HIS	-	expression tag	UNP Q5JID0
A	436	HIS	-	expression tag	UNP Q5JID0
A	437	HIS	-	expression tag	UNP Q5JID0
A	438	HIS	-	expression tag	UNP Q5JID0
B	431	HIS	-	expression tag	UNP Q5JID0
B	432	HIS	-	expression tag	UNP Q5JID0
B	433	HIS	-	expression tag	UNP Q5JID0
B	434	HIS	-	expression tag	UNP Q5JID0
B	435	HIS	-	expression tag	UNP Q5JID0
B	436	HIS	-	expression tag	UNP Q5JID0
B	437	HIS	-	expression tag	UNP Q5JID0
B	438	HIS	-	expression tag	UNP Q5JID0
C	431	HIS	-	expression tag	UNP Q5JID0
C	432	HIS	-	expression tag	UNP Q5JID0
C	433	HIS	-	expression tag	UNP Q5JID0
C	434	HIS	-	expression tag	UNP Q5JID0
C	435	HIS	-	expression tag	UNP Q5JID0
C	436	HIS	-	expression tag	UNP Q5JID0
C	437	HIS	-	expression tag	UNP Q5JID0

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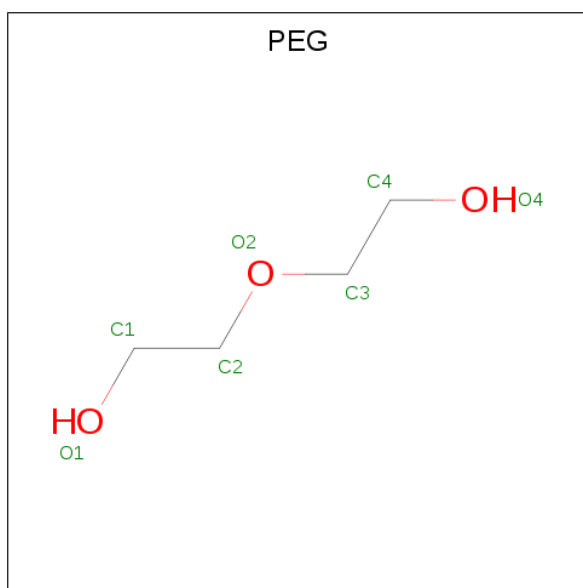
Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	expression tag	UNP Q5JID0

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



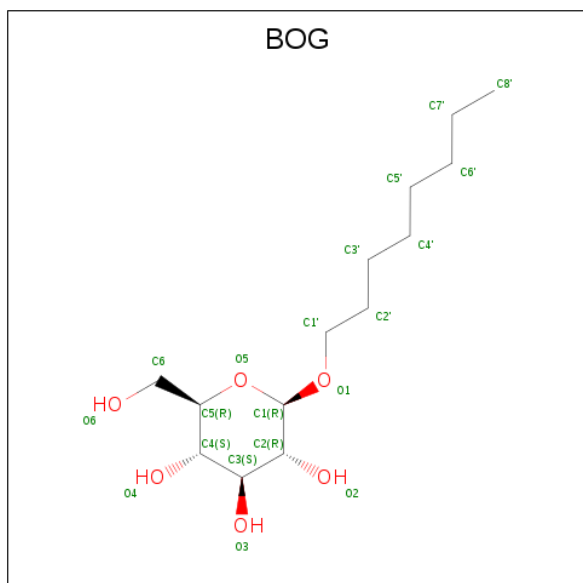
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	1
			14	8	6		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			20	14	6		

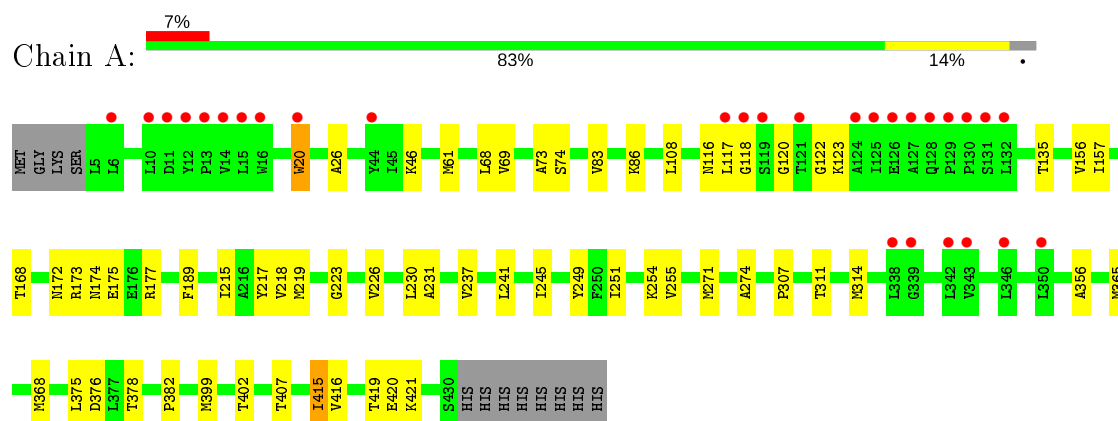
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	16	Total	O	0	0
			16	16		
5	C	23	Total	O	0	0
			23	23		

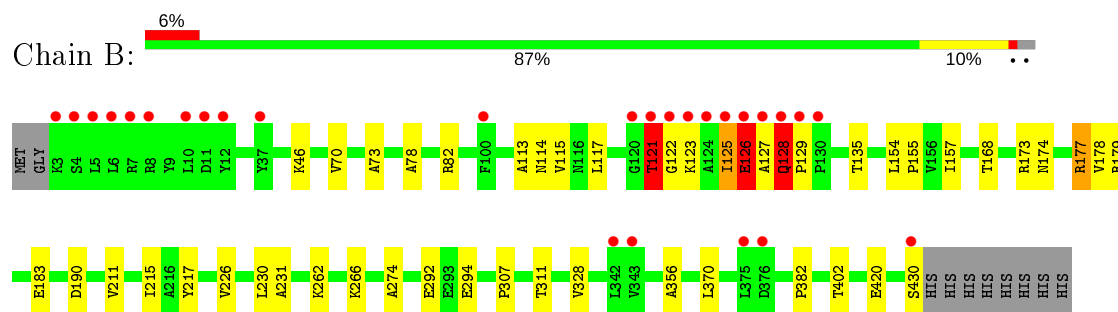
3 Residue-property plots [i](#)

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.

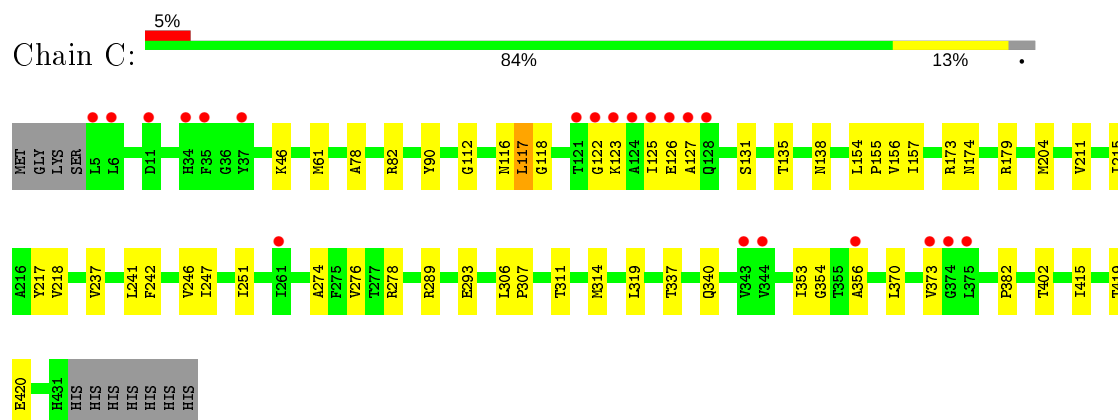
- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.01Å 116.01Å 308.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.77 – 2.70 47.76 – 2.57	Depositor EDS
% Data completeness (in resolution range)	78.8 (47.77-2.70) 68.8 (47.76-2.57)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.198 , 0.237 0.200 , 0.239	Depositor DCC
R_{free} test set	2675 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10016	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: PEG, PGE, BOG

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	0.41	0/3256	0.62	0/4430
1	B	0.40	0/3271	0.65	2/4449 (0.0%)
1	C	0.41	0/3289	0.62	1/4473 (0.0%)
All	All	0.41	0/9816	0.63	3/13352 (0.0%)

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	B	0	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	GLY	N-CA-C	5.30	126.36	113.10
1	B	126	GLU	N-CA-C	5.23	125.11	111.00
1	B	121	THR	N-CA-C	-5.12	97.19	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	113	ALA	Peptide
1	B	125	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	B	128	GLN	Peptide
1	C	117	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3197	0	3408	39	0
1	B	3212	0	3426	27	0
1	C	3229	0	3439	36	0
2	A	60	0	84	1	0
2	B	20	0	28	2	0
2	C	30	0	42	1	0
3	A	56	0	80	3	0
3	B	49	0	70	1	0
3	C	63	0	90	7	0
4	A	20	0	28	2	0
4	B	20	0	28	1	0
5	A	21	0	0	1	0
5	B	16	0	0	0	0
5	C	23	0	0	1	0
All	All	10016	0	10723	102	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 5.

All (102) 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:C:354:GLY:HA3	3:C:511[A]:PEG:H41	1.60	0.81
1:B:155:PRO:HD3	2:B:501:PGE:H2	1.68	0.74
1:A:157:ILE:HD11	1:A:307:PRO:HB2	1.72	0.72
1:C:157:ILE:HD11	1:C:307:PRO:HB2	1.74	0.69
1:B:121:THR:HG22	1:B:122:GLY:HA3	1.76	0.67
1:B:114:ASN:OD1	1:B:115:VAL:N	2.29	0.66
1:B:82:ARG:NH1	1:B:420:GLU:OE2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:GLU:OE2	5:C:601:HOH:O	2.16	0.62
1:A:254:LYS:HE2	3:A:510:PEG:H42	1.82	0.61
1:C:125:ILE:HG22	1:C:127:ALA:HB2	1.81	0.61
1:A:420:GLU:O	1:A:421:LYS:HG2	1.99	0.61
1:C:241:LEU:HD23	1:C:319:LEU:HD13	1.83	0.61
1:B:73:ALA:O	1:B:168:THR:HG21	2.02	0.60
1:B:157:ILE:HD11	1:B:307:PRO:HB2	1.84	0.60
3:B:508:PEG:H32	3:C:510:PEG:H11	1.84	0.60
1:C:61:MET:HE1	1:C:156:VAL:HG21	1.83	0.59
1:A:73:ALA:O	1:A:168:THR:HG21	2.04	0.58
1:C:122:GLY:HA2	1:C:123:LYS:HB2	1.85	0.58
1:A:20:TRP:HA	1:A:20:TRP:CE3	2.39	0.58
1:C:117:LEU:HD23	1:C:118:GLY:HA2	1.85	0.57
1:A:177:ARG:NH1	1:B:190:ASP:OD2	2.37	0.57
1:C:311:THR:HA	1:C:356:ALA:HA	1.88	0.56
1:C:126:GLU:HB2	1:C:127:ALA:HA	1.87	0.56
1:B:274:ALA:HB1	1:B:402:THR:HG22	1.88	0.55
1:C:135:THR:HG23	3:C:511[A]:PEG:H22	1.88	0.55
1:B:174:ASN:O	1:B:179:ARG:NH1	2.40	0.54
1:C:237:VAL:O	1:C:241:LEU:HG	2.07	0.54
1:B:135:THR:HG23	2:B:501:PGE:H5	1.91	0.53
1:B:177:ARG:HG3	1:B:178:VAL:N	2.22	0.52
1:A:20:TRP:HA	1:A:20:TRP:HE3	1.74	0.52
1:A:117:LEU:HD23	1:A:118:GLY:N	2.24	0.52
1:C:61:MET:CE	1:C:156:VAL:HG21	2.40	0.51
1:A:274:ALA:HB1	1:A:402:THR:HG22	1.92	0.50
1:C:276:VAL:O	1:C:278[B]:ARG:NH2	2.43	0.50
1:C:138:ASN:HB2	3:C:511[A]:PEG:H21	1.93	0.50
1:A:123:LYS:NZ	5:A:601:HOH:O	2.44	0.50
1:B:262:LYS:NZ	1:B:430:SER:HB3	2.26	0.50
1:C:46:LYS:HD2	1:C:217:TYR:CD2	2.47	0.49
1:C:306:LEU:HB2	1:C:307:PRO:HD3	1.96	0.48
1:B:78:ALA:HA	4:B:510:BOG:H1'1	1.96	0.47
1:B:266:LYS:HB3	1:B:294:GLU:HB3	1.97	0.46
1:A:26:ALA:HA	1:A:219:MET:HG3	1.97	0.46
1:C:138:ASN:HD22	3:C:511[A]:PEG:H12	1.79	0.46
1:A:135:THR:HG23	2:A:506:PGE:H12	1.97	0.46
1:A:226:VAL:HG23	1:A:231:ALA:HA	1.98	0.46
1:B:125:ILE:HG23	1:B:126:GLU:O	2.15	0.46
1:A:120:GLY:HA3	1:A:375:LEU:HD23	1.98	0.46
1:B:311:THR:HA	1:B:356:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HD2	1:B:217:TYR:CD2	2.51	0.45
1:A:223:GLY:O	1:A:226:VAL:HG12	2.16	0.45
1:A:311:THR:HA	1:A:356:ALA:HA	1.99	0.45
1:C:211:VAL:O	1:C:215:ILE:HG22	2.17	0.45
1:A:251:ILE:O	1:A:255:VAL:HG23	2.17	0.44
1:C:117:LEU:O	1:C:382:PRO:HG2	2.16	0.44
1:A:86:LYS:HE2	4:A:515:BOG:H1	1.98	0.44
1:C:415:ILE:O	1:C:419:THR:HG23	2.18	0.44
1:C:82:ARG:NH1	1:C:420:GLU:OE2	2.46	0.44
1:A:83:VAL:HG13	1:A:416:VAL:HG11	2.00	0.43
1:B:117:LEU:O	1:B:382:PRO:HG2	2.18	0.43
1:C:218:VAL:HG21	1:C:278[B]:ARG:NH2	2.32	0.43
1:C:90:TYR:HA	3:C:509:PEG:H42	1.99	0.43
1:C:242:PHE:O	1:C:246:VAL:HG22	2.19	0.43
1:C:337:THR:HG23	1:C:340:GLN:H	1.83	0.43
1:A:245:ILE:HA	1:A:249:TYR:CD2	2.53	0.43
1:A:172:ASN:O	3:A:513:PEG:H22	2.17	0.43
1:B:328:VAL:HG21	1:B:370:LEU:HD21	2.01	0.43
1:A:117:LEU:O	1:A:382:PRO:HG2	2.18	0.43
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.76	0.43
1:B:262:LYS:HZ1	1:B:430:SER:HB3	1.83	0.43
1:A:46:LYS:HD2	1:A:217:TYR:CD2	2.54	0.43
1:A:376:ASP:OD1	1:A:378:THR:HG23	2.19	0.43
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.87	0.42
1:C:289[A]:ARG:HG2	1:C:293:GLU:HG2	2.01	0.42
1:A:86:LYS:HE2	4:A:515:BOG:H2'2	2.00	0.42
1:B:126:GLU:HB3	1:B:127:ALA:H	1.45	0.42
1:C:78:ALA:HA	2:C:501:PGE:H42	2.01	0.42
1:B:70:VAL:HG21	1:B:190:ASP:HA	2.02	0.42
1:C:204:MET:HE2	1:C:204:MET:HA	2.01	0.42
1:A:173:ARG:HH21	1:A:175:GLU:CD	2.23	0.42
1:A:173:ARG:NH2	1:A:175:GLU:OE1	2.44	0.42
1:C:370:LEU:O	1:C:373:VAL:HG12	2.19	0.42
1:C:155:PRO:HD3	3:C:511[B]:PEG:H12	2.02	0.42
1:C:154:LEU:HD12	1:C:154:LEU:HA	1.93	0.42
1:A:237:VAL:O	1:A:241:LEU:HG	2.20	0.41
1:A:218:VAL:HB	1:A:399:MET:HE1	2.02	0.41
1:A:230:LEU:HA	1:A:230:LEU:HD23	1.78	0.41
1:A:271:MET:HG2	1:A:407:THR:OG1	2.20	0.41
1:A:68:LEU:HD23	1:A:157:ILE:HA	2.02	0.41
1:B:226:VAL:HG13	1:B:231:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MET:CE	1:A:156:VAL:HG21	2.50	0.41
1:C:174:ASN:O	1:C:179:ARG:NH1	2.54	0.41
1:A:365:MET:HA	1:A:368:MET:HE3	2.02	0.41
1:A:69:VAL:HG11	1:A:189:PHE:CD2	2.56	0.41
1:A:174:ASN:OD1	3:A:513:PEG:O1	2.38	0.40
1:A:415:ILE:O	1:A:419:THR:HG23	2.21	0.40
1:B:128:GLN:HB3	1:B:129:PRO:HA	2.03	0.40
1:A:215:ILE:HA	1:A:215:ILE:HD12	1.89	0.40
1:C:274:ALA:HB1	1:C:402:THR:HG22	2.03	0.40
1:A:122:GLY:O	1:A:123:LYS:HD3	2.21	0.40
1:C:247:ILE:O	1:C:251:ILE:HG12	2.22	0.40
1:C:314[A]:MET:CE	1:C:353:ILE:HA	2.51	0.40
1:B:211:VAL:O	1:B:215:ILE:HG22	2.22	0.40

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	426/438 (97%)	418 (98%)	8 (2%)	0	100	100
1	B	428/438 (98%)	417 (97%)	11 (3%)	0	100	100
1	C	429/438 (98%)	417 (97%)	12 (3%)	0	100	100
All	All	1283/1314 (98%)	1252 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/345 (97%)	329 (98%)	7 (2%)	53	80
1	B	338/345 (98%)	330 (98%)	8 (2%)	49	77
1	C	339/345 (98%)	335 (99%)	4 (1%)	71	88
All	All	1013/1035 (98%)	994 (98%)	19 (2%)	60	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TRP
1	A	74	SER
1	A	108	LEU
1	A	116	ASN
1	A	314[A]	MET
1	A	314[B]	MET
1	A	415	ILE
1	B	121	THR
1	B	123	LYS
1	B	126	GLU
1	B	128	GLN
1	B	173	ARG
1	B	177	ARG
1	B	183	GLU
1	B	292	GLU
1	C	116	ASN
1	C	131	SER
1	C	173[A]	ARG
1	C	173[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BOG	A	515	-	20,20,20	1.24	2 (10%)	25,25,25	1.14	2 (8%)
3	PEG	A	509	-	6,6,6	0.48	0	5,5,5	0.24	0
3	PEG	B	504	-	6,6,6	0.49	0	5,5,5	0.25	0
4	BOG	B	510	-	20,20,20	1.11	2 (10%)	25,25,25	1.05	0
3	PEG	A	511	-	6,6,6	0.51	0	5,5,5	0.26	0
2	PGE	A	505	-	9,9,9	0.28	0	8,8,8	0.32	0
3	PEG	A	508	-	6,6,6	0.51	0	5,5,5	0.41	0
3	PEG	C	507	-	6,6,6	0.49	0	5,5,5	0.33	0
2	PGE	C	501	-	9,9,9	0.35	0	8,8,8	0.31	0
3	PEG	A	510	-	6,6,6	0.48	0	5,5,5	0.28	0
3	PEG	C	511[A]	-	6,6,6	0.49	0	5,5,5	0.62	0
3	PEG	A	513	-	6,6,6	0.48	0	5,5,5	0.33	0
3	PEG	B	509	-	6,6,6	0.46	0	5,5,5	0.34	0
2	PGE	B	502	-	9,9,9	0.34	0	8,8,8	0.31	0
3	PEG	C	505	-	6,6,6	0.49	0	5,5,5	0.24	0
3	PEG	B	506	-	6,6,6	0.48	0	5,5,5	0.34	0
3	PEG	A	514	-	6,6,6	0.51	0	5,5,5	0.26	0
2	PGE	A	501	-	9,9,9	0.30	0	8,8,8	0.24	0
3	PEG	B	505	-	6,6,6	0.49	0	5,5,5	0.30	0
2	PGE	C	502	-	9,9,9	0.36	0	8,8,8	0.35	0
3	PEG	C	509	-	6,6,6	0.48	0	5,5,5	0.25	0
3	PEG	B	508	-	6,6,6	0.49	0	5,5,5	0.31	0
3	PEG	C	508	-	6,6,6	0.48	0	5,5,5	0.32	0
3	PEG	A	512	-	6,6,6	0.47	0	5,5,5	0.30	0
3	PEG	B	507	-	6,6,6	0.48	0	5,5,5	0.25	0
3	PEG	B	503	-	6,6,6	0.49	0	5,5,5	0.23	0
2	PGE	B	501	-	9,9,9	0.50	0	8,8,8	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	C	510	-	6,6,6	0.49	0	5,5,5	0.28	0
2	PGE	A	504	-	9,9,9	0.29	0	8,8,8	0.36	0
2	PGE	A	502	-	9,9,9	0.32	0	8,8,8	0.26	0
3	PEG	A	507	-	6,6,6	0.49	0	5,5,5	0.40	0
3	PEG	C	504	-	6,6,6	0.47	0	5,5,5	0.33	0
2	PGE	C	503	-	9,9,9	0.47	0	8,8,8	0.30	0
2	PGE	A	503	-	9,9,9	0.33	0	8,8,8	0.47	0
3	PEG	C	511[B]	-	6,6,6	0.49	0	5,5,5	0.45	0
2	PGE	A	506	-	9,9,9	0.40	0	8,8,8	0.30	0
3	PEG	C	506	-	6,6,6	0.47	0	5,5,5	0.44	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
4	BOG	A	515	-	-	8/11/31/31	0/1/1/1
3	PEG	A	509	-	-	2/4/4/4	-
3	PEG	B	504	-	-	3/4/4/4	-
4	BOG	B	510	-	-	4/11/31/31	0/1/1/1
3	PEG	A	511	-	-	3/4/4/4	-
2	PGE	A	505	-	-	3/7/7/7	-
3	PEG	A	508	-	-	2/4/4/4	-
3	PEG	C	507	-	-	3/4/4/4	-
2	PGE	C	501	-	-	1/7/7/7	-
3	PEG	A	510	-	-	2/4/4/4	-
3	PEG	C	511[A]	-	-	3/4/4/4	-
3	PEG	A	513	-	-	2/4/4/4	-
3	PEG	B	509	-	-	3/4/4/4	-
2	PGE	B	502	-	-	3/7/7/7	-
3	PEG	C	505	-	-	2/4/4/4	-
3	PEG	B	506	-	-	4/4/4/4	-
3	PEG	A	514	-	-	0/4/4/4	-
2	PGE	A	501	-	-	3/7/7/7	-
3	PEG	B	505	-	-	0/4/4/4	-
2	PGE	C	502	-	-	3/7/7/7	-
3	PEG	C	509	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	508	-	-	2/4/4/4	-
3	PEG	C	508	-	-	2/4/4/4	-
3	PEG	A	512	-	-	0/4/4/4	-
3	PEG	B	507	-	-	1/4/4/4	-
3	PEG	B	503	-	-	2/4/4/4	-
2	PGE	B	501	-	-	5/7/7/7	-
3	PEG	C	510	-	-	2/4/4/4	-
2	PGE	A	504	-	-	1/7/7/7	-
2	PGE	A	502	-	-	4/7/7/7	-
3	PEG	A	507	-	-	3/4/4/4	-
3	PEG	C	504	-	-	1/4/4/4	-
2	PGE	C	503	-	-	3/7/7/7	-
2	PGE	A	503	-	-	3/7/7/7	-
3	PEG	C	511[B]	-	-	4/4/4/4	-
2	PGE	A	506	-	-	3/7/7/7	-
3	PEG	C	506	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	515	BOG	O5-C1	3.83	1.51	1.41
4	B	510	BOG	O5-C1	3.45	1.50	1.41
4	A	515	BOG	O5-C5	2.30	1.49	1.44
4	B	510	BOG	O1-C1	-2.04	1.36	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	515	BOG	O5-C5-C4	2.85	114.88	109.69
4	A	515	BOG	C6-C5-C4	-2.23	107.78	113.00

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	515	BOG	C2-C1-O1-C1'
4	A	515	BOG	O5-C1-O1-C1'
3	A	511	PEG	C4-C3-O2-C2
4	A	515	BOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	503	PGE	O2-C3-C4-O3
3	A	509	PEG	O2-C3-C4-O4
2	C	501	PGE	O2-C3-C4-O3
2	A	505	PGE	O2-C3-C4-O3
2	B	502	PGE	O2-C3-C4-O3
2	C	503	PGE	O2-C3-C4-O3
3	C	511[A]	PEG	C4-C3-O2-C2
3	B	506	PEG	O2-C3-C4-O4
3	B	508	PEG	O2-C3-C4-O4
2	B	501	PGE	O3-C5-C6-O4
3	B	507	PEG	O2-C3-C4-O4
3	A	507	PEG	O1-C1-C2-O2
4	A	515	BOG	C4-C5-C6-O6
2	A	501	PGE	O2-C3-C4-O3
3	B	504	PEG	O2-C3-C4-O4
3	A	510	PEG	O1-C1-C2-O2
3	C	511[A]	PEG	O1-C1-C2-O2
3	A	513	PEG	O2-C3-C4-O4
3	B	509	PEG	O1-C1-C2-O2
2	B	502	PGE	O1-C1-C2-O2
3	C	504	PEG	O2-C3-C4-O4
3	C	511[B]	PEG	O1-C1-C2-O2
2	A	506	PGE	C1-C2-O2-C3
4	B	510	BOG	C2'-C1'-O1-C1
3	B	506	PEG	O1-C1-C2-O2
3	C	509	PEG	O2-C3-C4-O4
2	A	506	PGE	O3-C5-C6-O4
4	A	515	BOG	C3'-C4'-C5'-C6'
4	B	510	BOG	C4'-C5'-C6'-C7'
3	A	511	PEG	O1-C1-C2-O2
3	A	511	PEG	O2-C3-C4-O4
3	B	508	PEG	O1-C1-C2-O2
3	C	508	PEG	O2-C3-C4-O4
2	B	501	PGE	O1-C1-C2-O2
2	A	502	PGE	O1-C1-C2-O2
2	A	503	PGE	O1-C1-C2-O2
4	B	510	BOG	O5-C5-C6-O6
2	C	502	PGE	O1-C1-C2-O2
3	C	507	PEG	O1-C1-C2-O2
3	A	510	PEG	O2-C3-C4-O4
2	B	501	PGE	C4-C3-O2-C2
2	B	502	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
3	C	511[B]	PEG	C1-C2-O2-C3
2	A	505	PGE	C1-C2-O2-C3
3	B	509	PEG	C4-C3-O2-C2
2	B	501	PGE	C6-C5-O3-C4
3	B	504	PEG	C4-C3-O2-C2
3	B	506	PEG	C1-C2-O2-C3
3	C	511[A]	PEG	C1-C2-O2-C3
3	C	510	PEG	C4-C3-O2-C2
3	A	509	PEG	C4-C3-O2-C2
3	B	504	PEG	O1-C1-C2-O2
3	A	513	PEG	C4-C3-O2-C2
2	C	503	PGE	C3-C4-O3-C5
3	C	505	PEG	C1-C2-O2-C3
4	A	515	BOG	C2'-C1'-O1-C1
3	C	511[B]	PEG	C4-C3-O2-C2
3	B	503	PEG	C4-C3-O2-C2
4	A	515	BOG	C2'-C3'-C4'-C5'
2	A	502	PGE	C4-C3-O2-C2
2	A	504	PGE	O2-C3-C4-O3
2	A	502	PGE	O2-C3-C4-O3
2	C	502	PGE	O2-C3-C4-O3
3	A	508	PEG	C4-C3-O2-C2
3	A	508	PEG	O2-C3-C4-O4
3	C	511[B]	PEG	O2-C3-C4-O4
3	C	507	PEG	C4-C3-O2-C2
3	B	503	PEG	C1-C2-O2-C3
2	B	501	PGE	C1-C2-O2-C3
3	C	507	PEG	C1-C2-O2-C3
2	A	506	PGE	O1-C1-C2-O2
3	C	506	PEG	C1-C2-O2-C3
2	A	502	PGE	C1-C2-O2-C3
2	A	505	PGE	O1-C1-C2-O2
3	A	507	PEG	C4-C3-O2-C2
2	C	502	PGE	C6-C5-O3-C4
3	C	505	PEG	O1-C1-C2-O2
3	A	507	PEG	C1-C2-O2-C3
2	A	501	PGE	C6-C5-O3-C4
2	C	503	PGE	C6-C5-O3-C4
3	C	508	PEG	O1-C1-C2-O2
4	B	510	BOG	C3'-C4'-C5'-C6'
3	C	509	PEG	C4-C3-O2-C2
3	B	509	PEG	C1-C2-O2-C3

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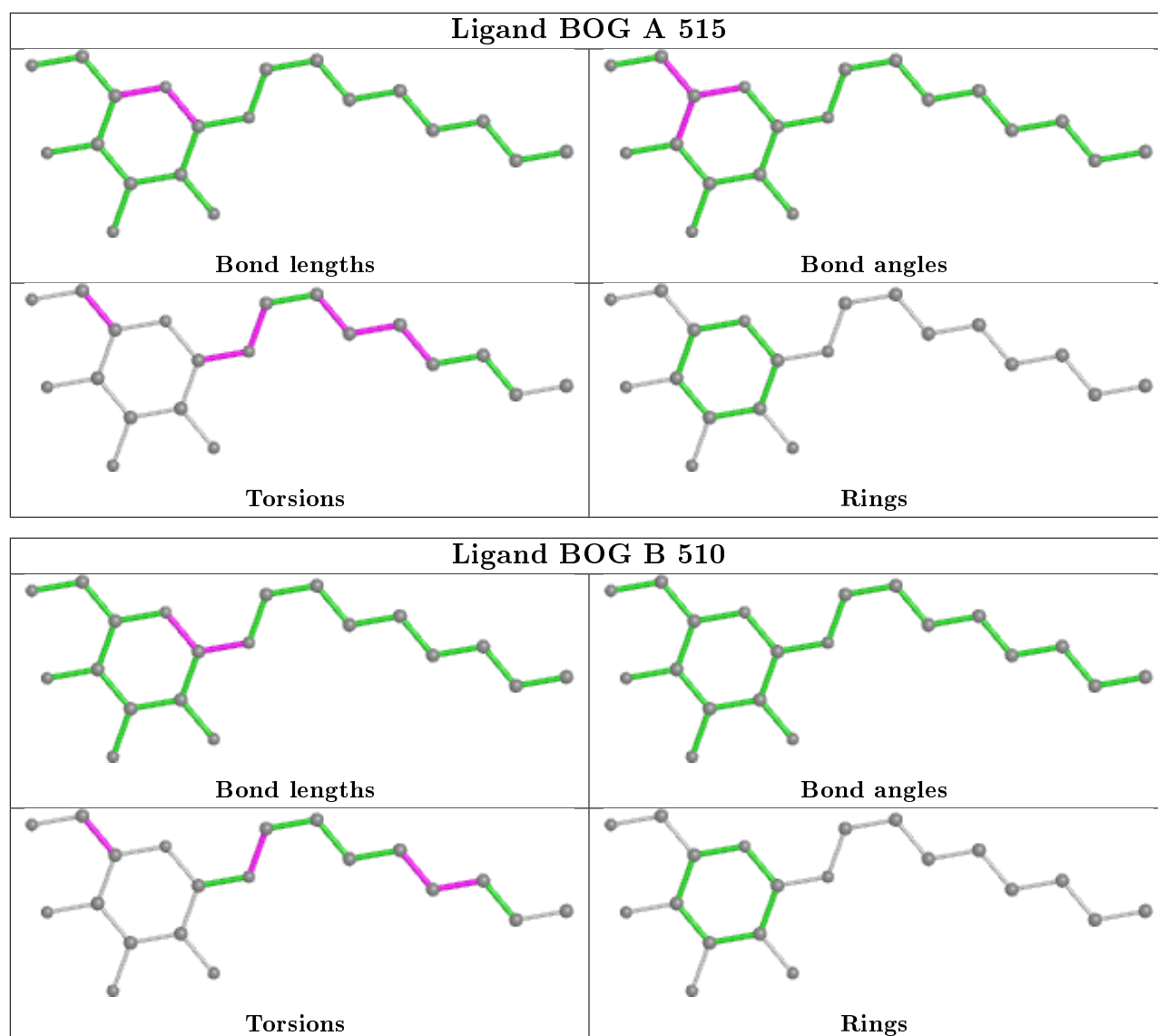
Mol	Chain	Res	Type	Atoms
3	B	506	PEG	C4-C3-O2-C2
2	A	503	PGE	C6-C5-O3-C4
2	A	501	PGE	C4-C3-O2-C2
4	A	515	BOG	C1'-C2'-C3'-C4'
3	C	510	PEG	C1-C2-O2-C3

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	515	BOG	2	0
4	B	510	BOG	1	0
2	C	501	PGE	1	0
3	A	510	PEG	1	0
3	C	511[A]	PEG	4	0
3	A	513	PEG	2	0
3	C	509	PEG	1	0
3	B	508	PEG	1	0
2	B	501	PGE	2	0
3	C	510	PEG	1	0
3	C	511[B]	PEG	1	0
2	A	506	PGE	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	426/438 (97%)	-0.18	29 (6%)	17 15	44, 73, 142, 219	0
1	B	428/438 (97%)	-0.15	27 (6%)	20 19	40, 74, 125, 210	0
1	C	427/438 (97%)	-0.12	21 (4%)	29 28	42, 66, 134, 207	0
All	All	1281/1314 (97%)	-0.15	77 (6%)	21 20	40, 71, 134, 219	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LYS	9.8
1	A	15	LEU	9.0
1	C	124	ALA	8.5
1	A	16	TRP	8.5
1	C	127	ALA	6.9
1	C	123	LYS	6.9
1	C	126	GLU	6.1
1	C	122	GLY	6.0
1	B	121	THR	5.9
1	B	127	ALA	5.8
1	C	125	ILE	5.8
1	B	129	PRO	5.7
1	A	342	LEU	5.6
1	C	121	THR	5.4
1	A	11	ASP	5.4
1	B	125	ILE	5.4
1	B	124	ALA	5.3
1	B	120	GLY	5.2
1	A	129	PRO	5.1
1	A	130	PRO	5.0
1	A	127	ALA	5.0
1	B	4	SER	4.9
1	B	122	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	128	GLN	4.7
1	A	126	GLU	4.6
1	A	10	LEU	4.5
1	A	12	TYR	4.4
1	B	5	LEU	4.3
1	C	6	LEU	4.3
1	A	124	ALA	4.2
1	B	11	ASP	4.2
1	B	375	LEU	4.2
1	B	130	PRO	4.0
1	A	13	PRO	4.0
1	C	35	PHE	3.7
1	A	20	TRP	3.6
1	B	37	TYR	3.6
1	B	343	VAL	3.5
1	A	14	VAL	3.4
1	B	376	ASP	3.4
1	A	128	GLN	3.3
1	B	8	ARG	3.3
1	C	128	GLN	3.3
1	A	125	ILE	3.3
1	B	126	GLU	3.2
1	A	343	VAL	3.1
1	B	430	SER	3.1
1	B	6	LEU	3.1
1	B	7	ARG	3.1
1	A	132	LEU	3.0
1	C	373	VAL	2.9
1	A	121	THR	2.8
1	A	44	TYR	2.8
1	B	10	LEU	2.7
1	C	37	TYR	2.7
1	C	375	LEU	2.7
1	C	343	VAL	2.7
1	B	12	TYR	2.6
1	A	346	LEU	2.5
1	C	344	VAL	2.5
1	C	261	ILE	2.5
1	C	356	ALA	2.5
1	B	100	PHE	2.5
1	A	117	LEU	2.4
1	A	338	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	11	ASP	2.3
1	A	6	LEU	2.3
1	B	342	LEU	2.2
1	A	131	SER	2.2
1	C	5	LEU	2.2
1	A	350	LEU	2.2
1	B	123	LYS	2.2
1	A	339	GLY	2.2
1	A	118	GLY	2.1
1	A	119	SER	2.1
1	C	374	GLY	2.1
1	C	34	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	A	514	7/7	0.29	0.75	107,125,136,137	0
2	PGE	A	506	10/10	0.57	0.27	106,121,136,137	0
2	PGE	B	501	10/10	0.61	0.27	102,106,111,114	0
2	PGE	B	502	10/10	0.61	0.47	104,113,127,128	0
3	PEG	B	506	7/7	0.62	0.30	137,141,153,155	0
2	PGE	A	502	10/10	0.63	0.34	129,148,156,157	0
3	PEG	A	510	7/7	0.63	0.23	132,136,143,146	0
3	PEG	B	503	7/7	0.64	0.38	131,135,136,136	0
3	PEG	C	507	7/7	0.66	0.29	118,128,134,135	0
3	PEG	C	511[B]	7/7	0.67	0.33	47,68,81,82	7
3	PEG	C	511[A]	7/7	0.67	0.33	38,65,82,83	7

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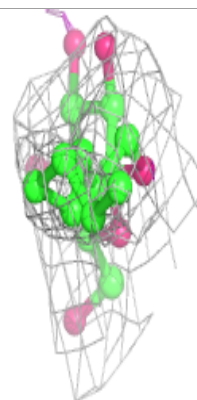
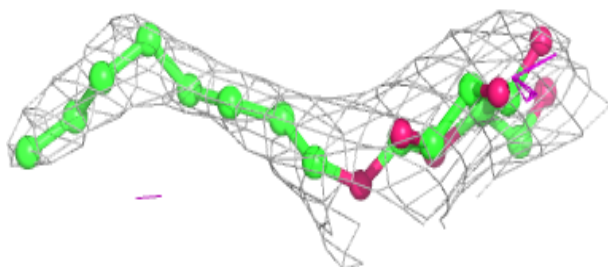
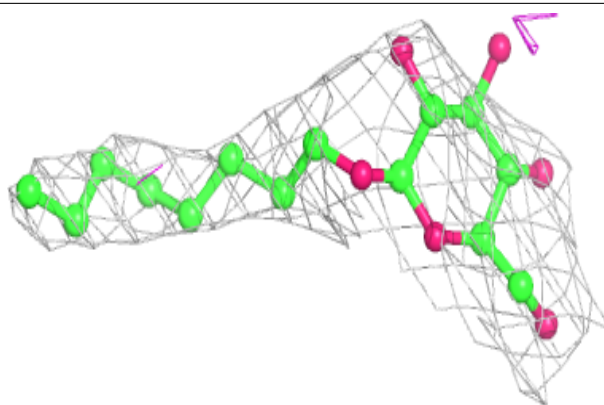
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PGE	C	502	10/10	0.73	0.27	96,102,110,113	0
3	PEG	C	505	7/7	0.73	1.07	118,119,122,123	0
3	PEG	A	507	7/7	0.75	0.33	96,109,118,118	0
3	PEG	C	510	7/7	0.75	0.50	96,103,111,115	0
3	PEG	A	508	7/7	0.75	0.49	116,123,129,131	0
2	PGE	A	505	10/10	0.76	0.28	93,107,121,121	0
2	PGE	C	501	10/10	0.76	0.54	93,112,134,135	0
3	PEG	B	507	7/7	0.77	0.77	127,133,137,138	0
3	PEG	B	508	7/7	0.78	0.57	76,91,106,109	0
3	PEG	B	504	7/7	0.78	0.20	133,136,141,142	0
4	BOG	A	515	20/20	0.78	0.25	69,124,140,146	0
2	PGE	A	504	10/10	0.79	0.43	108,112,119,120	0
3	PEG	A	511	7/7	0.80	0.15	83,89,92,97	0
3	PEG	B	505	7/7	0.81	0.76	101,104,110,111	0
2	PGE	A	503	10/10	0.82	0.18	94,112,130,130	0
3	PEG	A	512	7/7	0.82	1.06	111,122,141,146	0
2	PGE	C	503	10/10	0.82	0.24	72,94,100,101	0
3	PEG	A	513	7/7	0.83	0.20	109,110,112,113	0
4	BOG	B	510	20/20	0.83	0.33	118,157,169,169	0
3	PEG	B	509	7/7	0.85	0.45	92,94,97,103	0
3	PEG	A	509	7/7	0.86	0.20	115,123,130,130	0
2	PGE	A	501	10/10	0.87	0.25	112,124,132,134	0
3	PEG	C	506	7/7	0.87	0.21	93,97,108,109	0
3	PEG	C	504	7/7	0.88	0.42	90,91,94,98	0
3	PEG	C	508	7/7	0.88	0.57	101,108,117,119	0
3	PEG	C	509	7/7	0.91	0.65	97,99,102,102	0

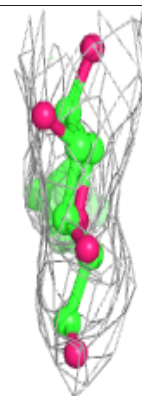
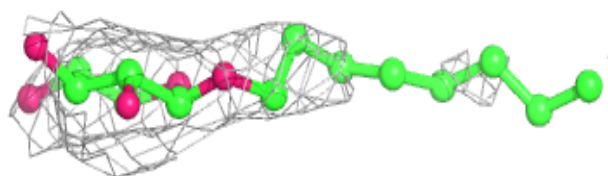
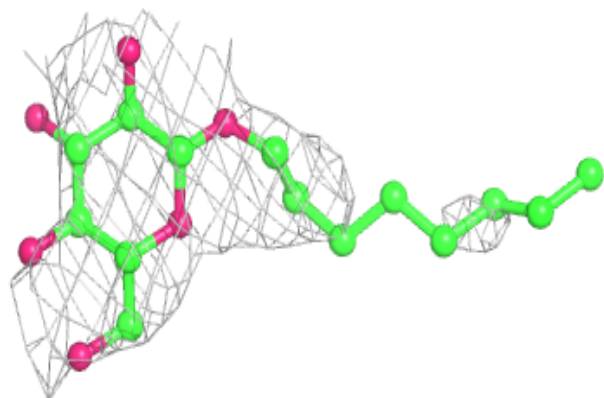
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BOG A 515:

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

**Electron density around BOG B 510:**

$2mF_o-DF_c$ (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.