



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:27 PM UTC

PDB ID : 5E9S / pdb_00005e9s
Title : Crystal structure of substrate-bound glutamate transporter homologue GltTk
Authors : Guskov, A.; Slotboom, D.J.
Deposited on : 2015-10-15
Resolution : 2.80 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 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

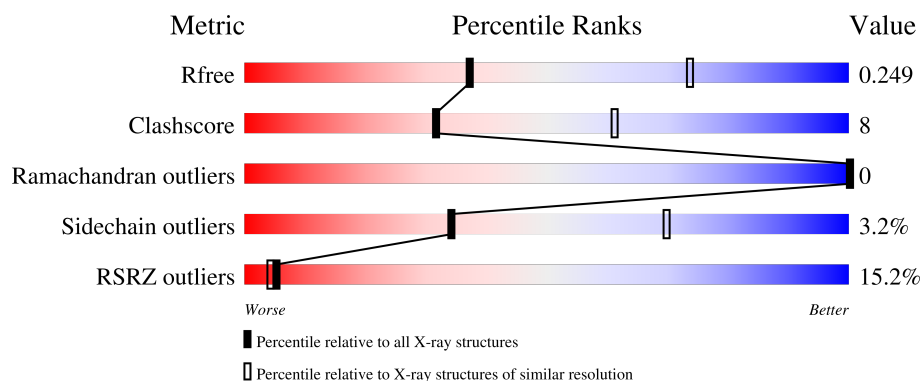
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	438	19% 74% 23% ..
1	B	438	12% 78% 19% ..
1	C	438	14% 77% 20% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10213 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	427	Total	C	N	O	S	0	1	0
			3196	2108	518	553	17			
1	B	427	Total	C	N	O	S	0	0	0
			3188	2103	517	552	16			
1	C	426	Total	C	N	O	S	0	1	0
			3186	2102	515	552	17			

There are 24 discrepancies between the modelled and reference sequences:

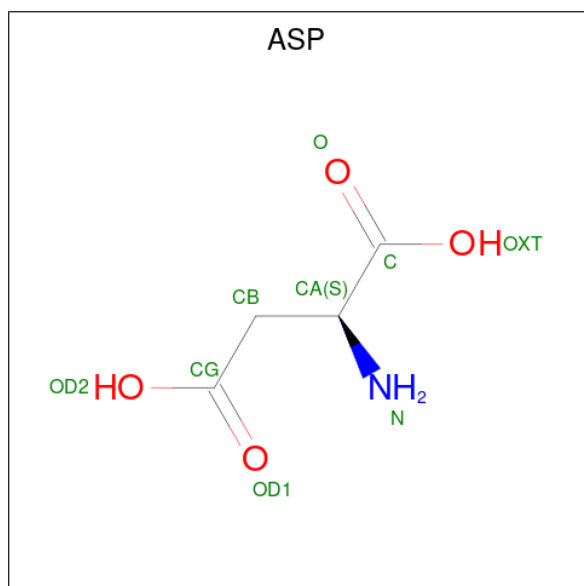
Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q5JID0
A	432	HIS	-	expression tag	UNP Q5JID0
A	433	HIS	-	expression tag	UNP Q5JID0
A	434	HIS	-	expression tag	UNP Q5JID0
A	435	HIS	-	expression tag	UNP Q5JID0
A	436	HIS	-	expression tag	UNP Q5JID0
A	437	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).

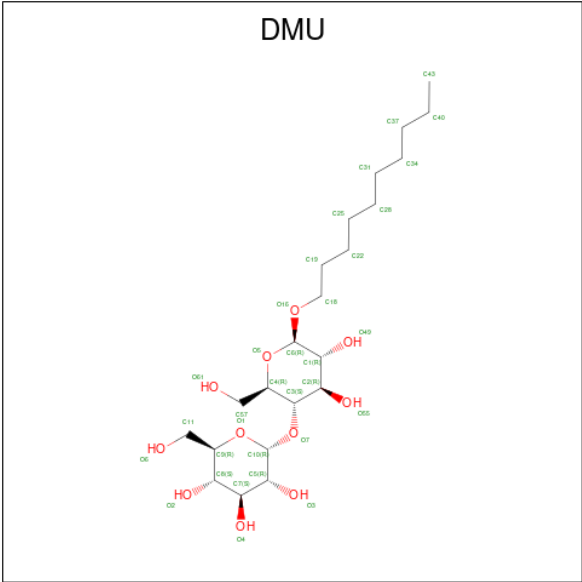


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

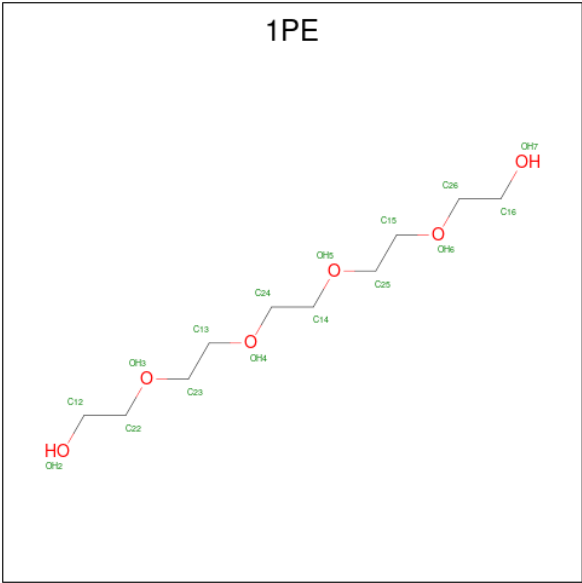
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Na	0	0
			3	3		
3	B	3	Total	Na	0	0
			3	3		
3	C	3	Total	Na	0	0
			3	3		

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			33	22	11		
4	B	1	Total	C	O	0	0
			33	22	11		
4	C	1	Total	C	O	0	0
			33	22	11		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



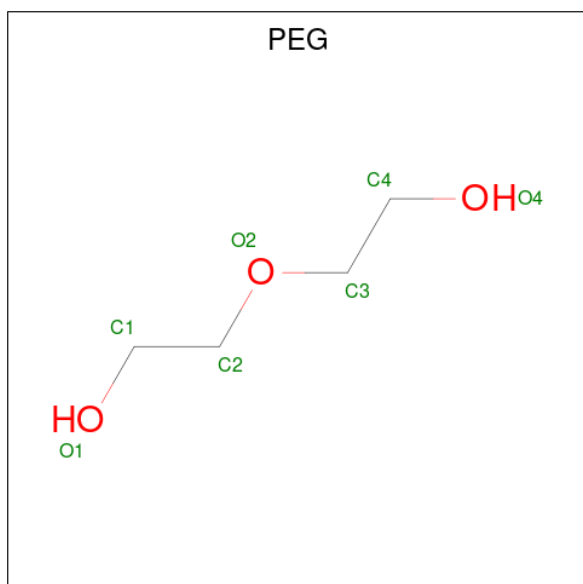
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		
5	C	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

Continued on next page...

Continued from previous page...

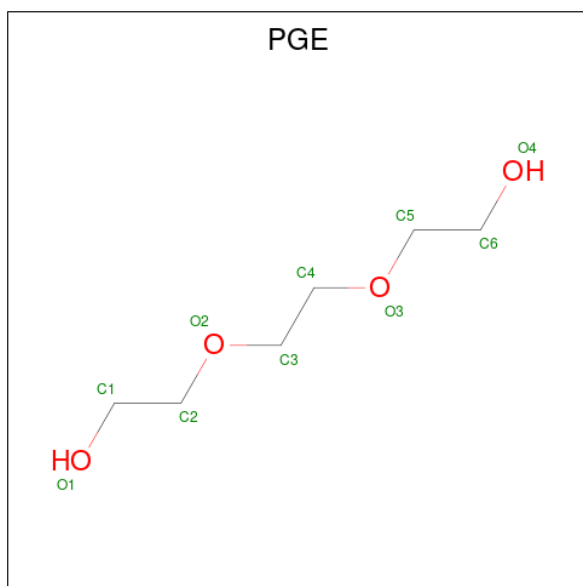
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



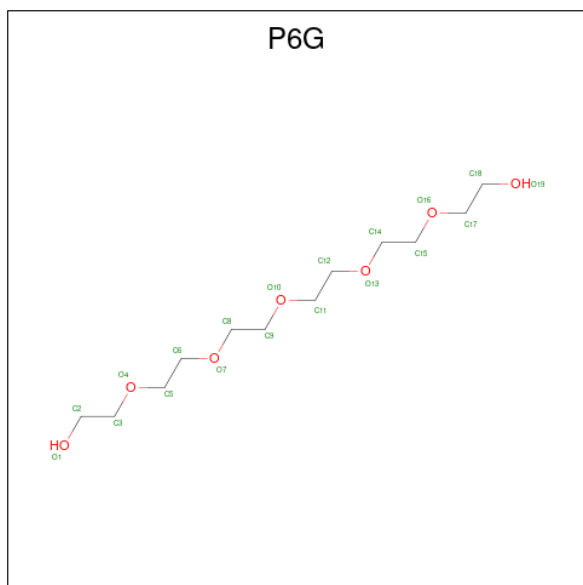
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		
7	A	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

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

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).

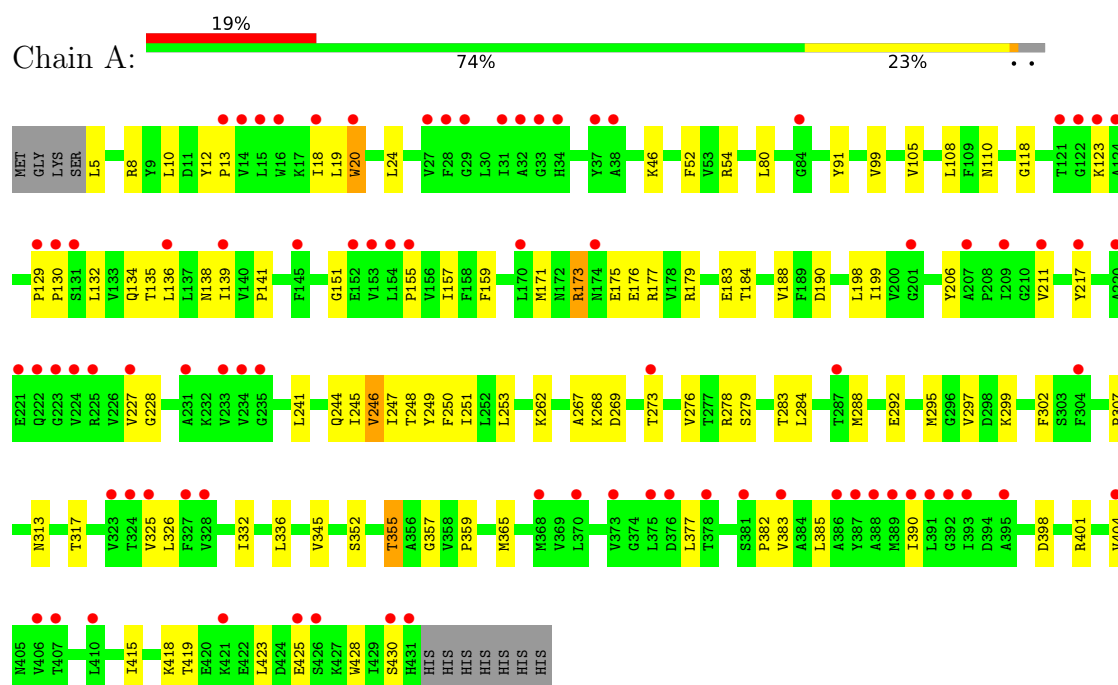


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			19	12	7		
8	B	1	Total	C	O	0	0
			19	12	7		
8	B	1	Total	C	O	0	0
			19	12	7		
8	C	1	Total	C	O	0	0
			19	12	7		
8	C	1	Total	C	O	0	0
			19	12	7		

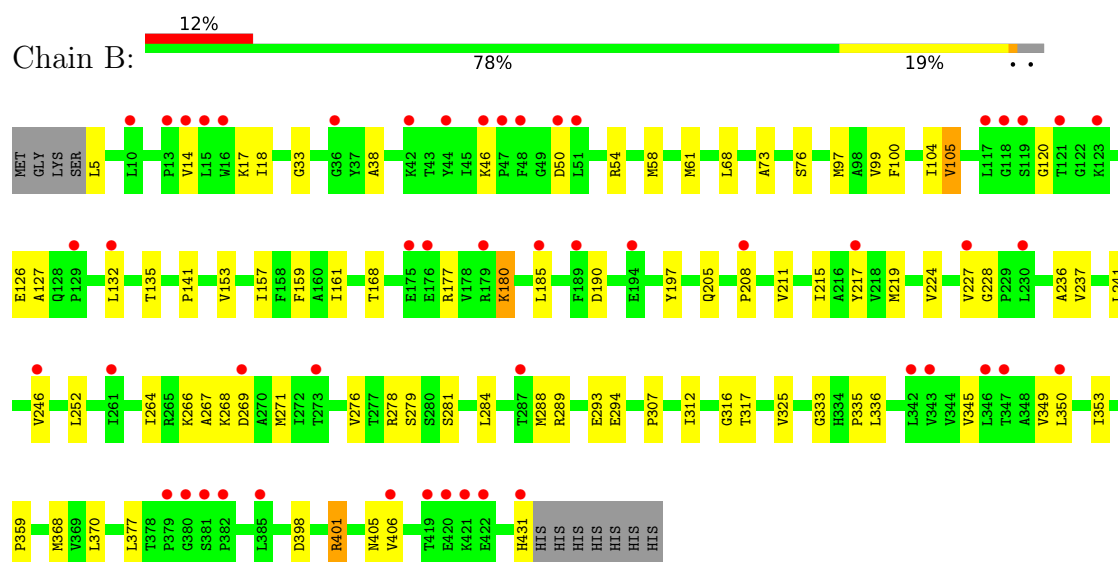
3 Residue-property plots

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

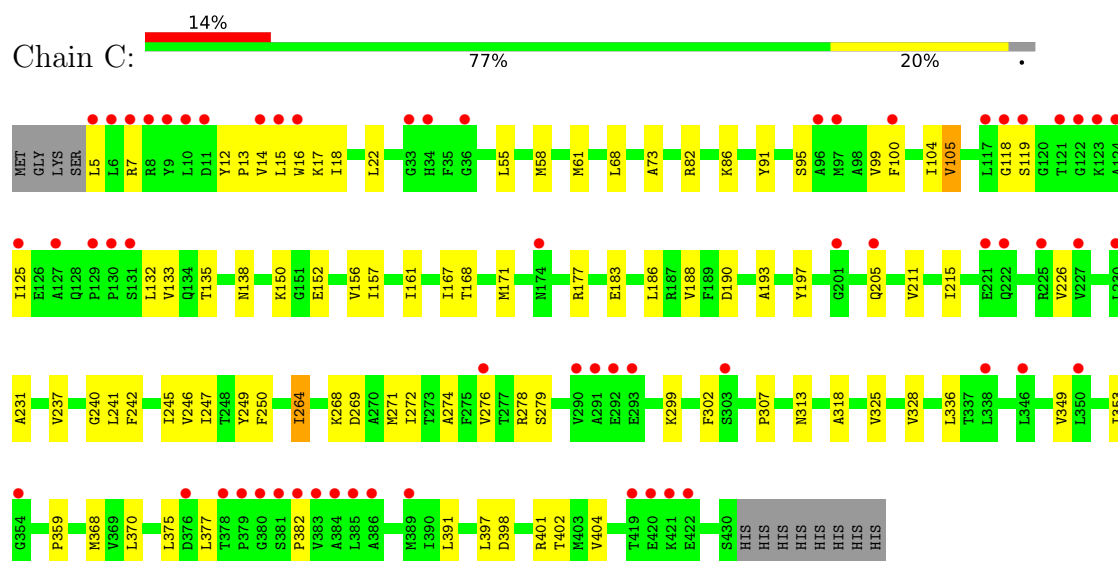
- Molecule 1: Proton/glutamate symporter, SDF family



- 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	117.52Å 117.52Å 310.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.36 – 2.80 48.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.36-2.80) 97.4 (48.36-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.213 , 0.242 0.221 , 0.249	Depositor DCC
R_{free} test set	2009 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10213	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: PGE, P6G, 1PE, DMU, PEG, NA

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	0.40	0/3256	0.64	0/4431
1	B	0.39	1/3248 (0.0%)	0.60	0/4421
1	C	0.35	0/3245	0.61	0/4416
All	All	0.38	1/9749 (0.0%)	0.62	0/13268

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	GLY	N-CA	-5.56	1.40	1.44

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	118	GLY	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3196	0	3402	68	0
1	B	3188	0	3394	50	0
1	C	3186	0	3395	56	0
2	A	9	0	3	2	0
2	B	9	0	3	3	0
2	C	9	0	3	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	33	0	42	0	0
4	B	33	0	42	1	0
4	C	33	0	42	2	0
5	A	32	0	44	2	0
5	B	48	0	66	4	0
5	C	32	0	44	0	0
6	A	70	0	100	1	0
6	B	98	0	140	3	0
6	C	63	0	90	5	0
7	A	40	0	56	2	0
7	B	10	0	14	0	0
7	C	20	0	28	0	0
8	A	19	0	26	0	0
8	B	38	0	52	2	0
8	C	38	0	52	1	0
All	All	10213	0	11038	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LEU:HD22	1:A:288:MET:HE2	1.58	0.85
5:B:508:1PE:H241	6:B:522:PEG:H22	1.63	0.81
1:A:357:GLY:H	7:A:520:PGE:H12	1.47	0.79
1:A:110:ASN:HB2	5:A:507:1PE:H251	1.65	0.78
1:A:177:ARG:NH1	1:B:190:ASP:OD2	2.20	0.74
1:A:159:PHE:HD1	1:B:58:MET:HE2	1.56	0.70
1:C:241:LEU:HB3	1:C:404:VAL:HG21	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HD11	1:B:307:PRO:HB2	1.73	0.69
1:C:12:TYR:HD1	1:C:17:LYS:HD3	1.57	0.69
1:C:157:ILE:HD11	1:C:307:PRO:HB2	1.74	0.69
1:A:246:VAL:HG12	1:A:247:ILE:HD12	1.74	0.69
1:A:157:ILE:HD11	1:A:307:PRO:HB2	1.76	0.68
1:C:15:LEU:HB3	1:C:16:TRP:HD1	1.58	0.68
1:B:14:VAL:HG13	1:B:17:LYS:HE2	1.77	0.66
1:C:119:SER:HA	1:C:382:PRO:HG2	1.78	0.65
1:A:190:ASP:OD2	1:C:177:ARG:NH1	2.30	0.65
1:B:99:VAL:HG11	1:B:345:VAL:HA	1.79	0.64
1:A:355:THR:HG22	1:A:365:MET:HG3	1.79	0.64
1:B:159:PHE:HD1	1:C:58:MET:HE2	1.62	0.63
1:A:262:LYS:HE2	1:A:428:TRP:O	2.00	0.62
1:A:5:LEU:HD23	1:A:8:ARG:HD3	1.80	0.61
1:C:246:VAL:HG23	1:C:247:ILE:HD12	1.82	0.61
5:B:507:1PE:H221	6:B:509:PEG:H32	1.82	0.60
1:C:264:ILE:HG13	1:C:271:MET:HE1	1.83	0.60
1:C:274:ALA:HB1	1:C:402:THR:HG22	1.83	0.59
1:C:325:VAL:HG12	1:C:336:LEU:HD11	1.82	0.59
1:C:55:LEU:O	1:C:58:MET:HG2	2.03	0.58
1:C:167:ILE:HG21	1:C:186:LEU:HD13	1.86	0.58
1:A:279:SER:HB2	1:A:359:PRO:HD3	1.85	0.57
1:B:17:LYS:HE3	1:B:208:PRO:HG2	1.85	0.57
1:C:171:MET:HE3	1:C:183:GLU:HG2	1.86	0.57
1:C:246:VAL:O	1:C:250:PHE:HB2	2.05	0.57
1:C:237:VAL:O	1:C:241:LEU:HG	2.05	0.56
1:B:177:ARG:NH1	1:C:190:ASP:OD2	2.38	0.56
1:A:418:LYS:NZ	1:A:425:GLU:OE2	2.40	0.55
1:B:325:VAL:HG22	1:B:370:LEU:HD12	1.89	0.55
1:A:325:VAL:HG12	1:A:336:LEU:HD11	1.87	0.55
1:C:12:TYR:CD1	1:C:17:LYS:HD3	2.39	0.55
1:B:205:GLN:NE2	4:B:505:DMU:O49	2.36	0.55
1:B:278:ARG:HD2	1:B:398:ASP:HB3	1.89	0.55
1:A:20:TRP:HA	1:A:20:TRP:CE3	2.41	0.54
1:A:269:ASP:O	1:A:273:THR:HG23	2.08	0.54
1:A:262:LYS:NZ	1:A:430:SER:OG	2.38	0.54
1:C:325:VAL:HG22	1:C:370:LEU:HD12	1.90	0.54
1:B:73:ALA:O	1:B:168:THR:HG21	2.09	0.53
1:A:20:TRP:HA	1:A:20:TRP:HE3	1.73	0.53
1:B:266:LYS:HB3	1:B:294:GLU:HB3	1.91	0.52
1:C:278:ARG:HD2	1:C:398:ASP:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG11	1:A:345:VAL:HA	1.92	0.51
1:A:141:PRO:HG2	1:B:58:MET:HE3	1.92	0.51
1:A:401:ARG:NH1	2:A:501:ASP:OD1	2.43	0.51
1:C:99:VAL:HG22	1:C:318:ALA:HB1	1.93	0.51
1:A:12:TYR:CG	1:A:13:PRO:HD2	2.46	0.51
1:A:52:PHE:HB2	1:A:206:TYR:CE2	2.45	0.51
1:B:126:GLU:HB2	1:B:127:ALA:HA	1.94	0.50
1:A:278:ARG:HD2	1:A:398:ASP:HB3	1.93	0.50
1:C:226:VAL:HG13	1:C:231:ALA:HA	1.93	0.50
1:B:267:ALA:O	1:B:271:MET:HG3	2.12	0.50
1:A:184:THR:O	1:A:188:VAL:HG23	2.12	0.49
1:A:54:ARG:NH2	1:C:138:ASN:HA	2.28	0.49
1:A:295:MET:HB2	1:A:297:VAL:HG23	1.94	0.49
1:A:211:VAL:HG22	1:A:276:VAL:HG21	1.94	0.49
1:B:215:ILE:HD11	1:B:219:MET:HE2	1.94	0.48
1:B:325:VAL:HG12	1:B:336:LEU:HD11	1.94	0.48
1:A:132:LEU:O	1:A:135:THR:HB	2.14	0.48
2:B:501:ASP:N	2:B:501:ASP:OD1	2.42	0.48
1:A:245:ILE:HA	1:A:249:TYR:CD2	2.49	0.48
1:B:317:THR:OG1	2:B:501:ASP:OXT	2.30	0.48
1:A:108:LEU:HA	5:A:507:1PE:H242	1.95	0.48
1:A:199:ILE:HG23	6:C:510:PEG:H11	1.96	0.47
1:B:279:SER:HB2	1:B:359:PRO:HD3	1.95	0.47
1:A:423:LEU:HD11	1:A:428:TRP:HE1	1.79	0.47
1:A:246:VAL:O	1:A:250:PHE:HB2	2.15	0.47
1:C:73:ALA:O	1:C:168:THR:OG1	2.32	0.47
6:C:508:PEG:H22	6:C:509:PEG:H21	1.95	0.47
1:A:139:ILE:O	1:A:155:PRO:HA	2.15	0.47
1:A:317:THR:OG1	2:A:501:ASP:OD2	2.29	0.47
1:B:316:GLY:C	1:B:401:ARG:HG3	2.40	0.47
1:C:105:VAL:HG21	1:C:240:GLY:HA2	1.97	0.47
1:C:132:LEU:O	1:C:135:THR:N	2.47	0.47
1:C:242:PHE:O	1:C:246:VAL:HG22	2.14	0.47
1:C:22:LEU:HD22	1:C:272:ILE:HG12	1.95	0.47
1:C:150:LYS:HD3	1:C:152:GLU:OE2	2.14	0.47
1:C:91:TYR:CG	1:C:313:ASN:HB2	2.50	0.46
1:C:302:PHE:C	1:C:302:PHE:CD1	2.94	0.46
1:A:151:GLY:HA3	7:A:521:PGE:H4	1.98	0.46
1:B:281:SER:O	1:B:284:LEU:HB2	2.15	0.46
1:A:118:GLY:O	1:A:382:PRO:HG2	2.15	0.46
1:A:227:VAL:HG13	1:A:228:GLY:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LEU:O	1:B:135:THR:HB	2.16	0.45
1:B:353:ILE:HG21	5:B:506:1PE:H252	1.97	0.45
1:C:68:LEU:HD21	1:C:161:ILE:HG13	1.98	0.45
1:A:173:ARG:NH2	1:A:175:GLU:OE1	2.50	0.45
1:A:171:MET:HE2	1:A:183:GLU:HA	1.99	0.45
1:C:5:LEU:HG	1:C:7:ARG:H	1.81	0.45
1:A:176:GLU:HG3	1:A:179:ARG:NH2	2.32	0.45
1:A:267:ALA:HB2	1:A:295:MET:HE1	1.99	0.44
1:A:268:LYS:HG3	1:A:269:ASP:N	2.32	0.44
1:B:405:ASN:ND2	2:B:501:ASP:HB2	2.32	0.44
1:A:46:LYS:HD2	1:A:217:TYR:CG	2.53	0.44
1:C:349:VAL:O	1:C:353:ILE:HG13	2.17	0.44
8:C:520:P6G:H141	8:C:520:P6G:H92	2.00	0.44
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.53	0.44
1:B:141:PRO:HG2	1:C:58:MET:HE3	1.99	0.44
1:B:197:TYR:OH	1:B:288:MET:HE2	2.17	0.44
1:B:211:VAL:O	1:B:215:ILE:HG22	2.18	0.44
5:B:508:1PE:H131	6:B:522:PEG:H32	1.98	0.44
1:A:123:LYS:HE3	1:A:123:LYS:HB3	1.71	0.44
1:A:273:THR:OG1	1:A:283:THR:HG23	2.16	0.44
1:A:332:ILE:HD13	1:A:383:VAL:HG22	1.99	0.44
1:C:193:ALA:O	1:C:197:TYR:HD2	2.00	0.44
1:A:198:LEU:HD22	6:C:510:PEG:H41	2.00	0.44
1:C:245:ILE:HA	1:C:249:TYR:CD2	2.53	0.44
1:C:211:VAL:HG22	1:C:276:VAL:HG21	1.99	0.44
1:B:237:VAL:O	1:B:241:LEU:HG	2.18	0.43
1:C:186:LEU:HD23	6:C:512:PEG:H32	2.00	0.43
1:C:272:ILE:O	1:C:276:VAL:HG22	2.18	0.43
1:C:268:LYS:HG3	1:C:269:ASP:N	2.33	0.43
1:C:61:MET:CE	1:C:156:VAL:HG21	2.48	0.43
1:C:99:VAL:CG2	1:C:318:ALA:HB1	2.49	0.43
1:C:279:SER:HB2	1:C:359:PRO:HD3	2.00	0.43
1:A:129:PRO:HB2	1:A:130:PRO:C	2.43	0.43
1:B:61:MET:HE1	1:B:153:VAL:HG22	2.01	0.43
1:B:33:GLY:HA2	1:B:38:ALA:HB2	1.99	0.43
1:B:276:VAL:O	1:B:278:ARG:NH1	2.52	0.43
1:B:312:ILE:HG21	8:B:524:P6G:H182	2.01	0.43
1:A:317:THR:HG21	1:A:355:THR:HG21	2.01	0.43
1:A:141:PRO:O	1:B:58:MET:HB3	2.18	0.43
1:A:80:LEU:HA	1:A:80:LEU:HD12	1.72	0.42
1:C:328:VAL:HG12	1:C:375:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LEU:O	1:C:401:ARG:HG2	2.19	0.42
1:A:247:ILE:HG23	1:A:251:ILE:HD12	2.01	0.42
8:B:525:P6G:H21	8:B:525:P6G:H52	1.84	0.42
1:A:134:GLN:HG3	1:A:138:ASN:HD21	1.84	0.42
1:A:91:TYR:CG	1:A:313:ASN:HB2	2.55	0.42
1:B:289:ARG:NE	1:B:293:GLU:OE1	2.52	0.42
6:C:515:PEG:H11	6:C:515:PEG:H32	1.78	0.42
1:B:97:MET:HE2	1:B:97:MET:HB2	1.86	0.41
1:C:12:TYR:CG	1:C:13:PRO:HD2	2.55	0.41
4:C:505:DMU:H35	4:C:505:DMU:H30	2.01	0.41
1:A:352:SER:HA	1:A:355:THR:HG23	2.01	0.41
1:A:326:LEU:HD23	1:A:336:LEU:HD12	2.02	0.41
1:B:105:VAL:HG11	1:B:236:ALA:O	2.20	0.41
1:B:100:PHE:CE2	1:B:104:ILE:HD11	2.55	0.41
1:B:180:LYS:O	1:B:180:LYS:HD2	2.20	0.41
1:A:292:GLU:HB2	1:A:302:PHE:CZ	2.55	0.41
1:A:244:GLN:O	1:A:248:THR:HB	2.20	0.41
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.83	0.41
1:B:268:LYS:HG3	1:B:269:ASP:N	2.35	0.41
1:C:377:LEU:HA	1:C:377:LEU:HD23	1.67	0.41
1:B:333:GLY:C	1:B:335:PRO:HD3	2.46	0.41
1:A:136:LEU:O	1:A:139:ILE:HB	2.21	0.41
6:A:511:PEG:H12	6:A:511:PEG:H31	1.88	0.41
1:B:50:ASP:O	1:B:54:ARG:HG3	2.20	0.41
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.96	0.41
1:B:349:VAL:O	1:B:353:ILE:HG13	2.20	0.41
1:C:95:SER:O	1:C:99:VAL:HG23	2.20	0.41
1:A:241:LEU:HB3	1:A:404:VAL:HG21	2.03	0.41
1:A:415:ILE:O	1:A:419:THR:HG23	2.21	0.41
1:B:46:LYS:HD2	1:B:217:TYR:CD2	2.55	0.41
1:B:227:VAL:HG13	1:B:228:GLY:N	2.36	0.41
1:A:20:TRP:O	1:A:24:LEU:HG	2.21	0.40
1:C:205:GLN:HB3	4:C:505:DMU:H13	2.03	0.40
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.92	0.40
1:B:68:LEU:HD21	1:B:161:ILE:HG13	2.02	0.40
1:B:141:PRO:O	1:C:58:MET:HB3	2.21	0.40
1:B:185:LEU:HD13	1:C:188:VAL:HG13	2.03	0.40
1:C:299:LYS:HG3	1:C:302:PHE:CZ	2.56	0.40
1:A:299:LYS:HE2	1:A:299:LYS:HB2	1.89	0.40
1:A:390:ILE:HD13	1:A:390:ILE:HA	1.83	0.40
1:C:82:ARG:HG2	1:C:86:LYS:HE3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PHE:CE2	1:C:104:ILE:HD11	2.56	0.40
1:C:132:LEU:O	1:C:133:VAL:C	2.65	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	425/438 (97%)	415 (98%)	10 (2%)	0	100	100
1	C	425/438 (97%)	413 (97%)	12 (3%)	0	100	100
All	All	1276/1314 (97%)	1246 (98%)	30 (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%)	327 (97%)	9 (3%)	39	74
1	B	335/345 (97%)	322 (96%)	13 (4%)	28	64
1	C	335/345 (97%)	326 (97%)	9 (3%)	39	74
All	All	1006/1035 (97%)	975 (97%)	31 (3%)	34	70

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	18	ILE
1	A	19	LEU
1	A	20	TRP
1	A	105	VAL
1	A	173	ARG
1	A	246	VAL
1	A	355	THR
1	A	385	LEU
1	B	5	LEU
1	B	18	ILE
1	B	76	SER
1	B	105	VAL
1	B	180	LYS
1	B	224	VAL
1	B	246	VAL
1	B	264	ILE
1	B	368	MET
1	B	377	LEU
1	B	401	ARG
1	B	406	VAL
1	B	431	HIS
1	C	14	VAL
1	C	18	ILE
1	C	105	VAL
1	C	125	ILE
1	C	215	ILE
1	C	264	ILE
1	C	368[A]	MET
1	C	368[B]	MET
1	C	391	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 9 are monoatomic - leaving 58 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	$\# Z > 2$
6	PEG	C	513	-	6,6,6	0.51	0	5,5,5	0.35	0
6	PEG	A	514	-	6,6,6	0.52	0	5,5,5	0.25	0
7	PGE	A	518	-	9,9,9	0.36	0	8,8,8	0.34	0
6	PEG	B	521	-	6,6,6	0.50	0	5,5,5	0.30	0
2	ASP	B	501	-	7,8,8	1.14	0	6,10,10	1.54	1 (16%)
8	P6G	C	520	-	18,18,18	0.55	0	17,17,17	0.50	0
6	PEG	C	510	-	6,6,6	0.49	0	5,5,5	0.38	0
6	PEG	B	517	-	6,6,6	0.51	0	5,5,5	0.24	0
5	1PE	A	507	-	15,15,15	0.55	0	14,14,14	0.42	0
5	1PE	B	506	-	15,15,15	0.57	0	14,14,14	0.49	0
6	PEG	B	512	-	6,6,6	0.55	0	5,5,5	0.32	0
6	PEG	B	522	-	6,6,6	0.52	0	5,5,5	0.28	0
7	PGE	A	520	-	9,9,9	0.46	0	8,8,8	0.34	0
6	PEG	A	508	-	6,6,6	0.49	0	5,5,5	0.32	0
6	PEG	B	520	-	6,6,6	0.54	0	5,5,5	0.41	0
8	P6G	A	522	-	18,18,18	0.61	0	17,17,17	0.47	0
8	P6G	C	519	-	18,18,18	0.61	0	17,17,17	0.55	0
6	PEG	C	514	-	6,6,6	0.52	0	5,5,5	0.38	0
6	PEG	B	518	-	6,6,6	0.50	0	5,5,5	0.38	0
5	1PE	B	507	-	15,15,15	0.56	0	14,14,14	0.33	0
5	1PE	C	506	-	15,15,15	0.53	0	14,14,14	0.57	0
5	1PE	C	507	-	15,15,15	0.55	0	14,14,14	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	B	519	-	6,6,6	0.50	0	5,5,5	0.29	0
7	PGE	C	518	-	9,9,9	0.31	0	8,8,8	0.58	0
6	PEG	B	513	-	6,6,6	0.52	0	5,5,5	0.37	0
6	PEG	C	508	-	6,6,6	0.52	0	5,5,5	0.43	0
6	PEG	B	514	-	6,6,6	0.50	0	5,5,5	0.31	0
5	1PE	A	506	-	15,15,15	0.55	0	14,14,14	0.36	0
7	PGE	C	517	-	9,9,9	0.35	0	8,8,8	0.26	0
6	PEG	B	511	-	6,6,6	0.49	0	5,5,5	0.31	0
6	PEG	A	515	-	6,6,6	0.52	0	5,5,5	0.26	0
2	ASP	A	501	-	7,8,8	1.13	1 (14%)	6,10,10	1.18	0
6	PEG	A	517	-	6,6,6	0.57	0	5,5,5	0.79	0
6	PEG	A	512	-	6,6,6	0.48	0	5,5,5	0.38	0
4	DMU	B	505	-	34,34,34	1.60	8 (23%)	45,45,45	1.07	5 (11%)
6	PEG	A	516	-	6,6,6	0.54	0	5,5,5	0.30	0
6	PEG	C	512	-	6,6,6	0.52	0	5,5,5	0.34	0
6	PEG	C	509	-	6,6,6	0.54	0	5,5,5	0.34	0
4	DMU	A	505	-	34,34,34	1.68	9 (26%)	45,45,45	1.33	7 (15%)
6	PEG	B	515	-	6,6,6	0.50	0	5,5,5	0.41	0
7	PGE	A	519	-	9,9,9	0.38	0	8,8,8	0.33	0
8	P6G	B	525	-	18,18,18	0.57	0	17,17,17	0.49	0
6	PEG	B	509	-	6,6,6	0.54	0	5,5,5	0.31	0
2	ASP	C	501	-	7,8,8	1.08	0	6,10,10	1.22	1 (16%)
6	PEG	A	510	-	6,6,6	0.50	0	5,5,5	0.32	0
6	PEG	B	510	-	6,6,6	0.53	0	5,5,5	0.28	0
6	PEG	B	516	-	6,6,6	0.55	0	5,5,5	0.27	0
6	PEG	C	511	-	6,6,6	0.53	0	5,5,5	0.38	0
6	PEG	A	513	-	6,6,6	0.52	0	5,5,5	0.35	0
8	P6G	B	524	-	18,18,18	0.56	0	17,17,17	0.47	0
6	PEG	C	516	-	6,6,6	0.46	0	5,5,5	0.30	0
4	DMU	C	505	-	34,34,34	1.59	8 (23%)	45,45,45	1.07	3 (6%)
5	1PE	B	508	-	15,15,15	0.55	0	14,14,14	0.24	0
6	PEG	A	511	-	6,6,6	0.53	0	5,5,5	0.47	0
6	PEG	C	515	-	6,6,6	0.51	0	5,5,5	0.27	0
7	PGE	B	523	-	9,9,9	0.43	0	8,8,8	0.27	0
7	PGE	A	521	-	9,9,9	0.37	0	8,8,8	0.40	0
6	PEG	A	509	-	6,6,6	0.50	0	5,5,5	0.29	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
6	PEG	C	513	-	-	0/4/4/4	-
6	PEG	A	514	-	-	2/4/4/4	-
7	PGE	A	518	-	-	6/7/7/7	-
6	PEG	B	521	-	-	2/4/4/4	-
2	ASP	B	501	-	-	4/8/8/8	-
8	P6G	C	520	-	-	11/16/16/16	-
6	PEG	C	510	-	-	3/4/4/4	-
6	PEG	B	517	-	-	3/4/4/4	-
5	1PE	A	507	-	-	9/13/13/13	-
5	1PE	B	506	-	-	9/13/13/13	-
6	PEG	B	512	-	-	1/4/4/4	-
6	PEG	B	522	-	-	1/4/4/4	-
7	PGE	A	520	-	-	3/7/7/7	-
6	PEG	A	508	-	-	2/4/4/4	-
6	PEG	B	520	-	-	2/4/4/4	-
8	P6G	A	522	-	-	9/16/16/16	-
8	P6G	C	519	-	-	9/16/16/16	-
6	PEG	C	514	-	-	2/4/4/4	-
6	PEG	B	518	-	-	1/4/4/4	-
5	1PE	B	507	-	-	7/13/13/13	-
5	1PE	C	506	-	-	4/13/13/13	-
5	1PE	C	507	-	-	7/13/13/13	-
6	PEG	B	519	-	-	2/4/4/4	-
7	PGE	C	518	-	-	3/7/7/7	-
6	PEG	B	513	-	-	2/4/4/4	-
6	PEG	C	508	-	-	1/4/4/4	-
6	PEG	B	514	-	-	2/4/4/4	-
5	1PE	A	506	-	-	7/13/13/13	-
7	PGE	C	517	-	-	2/7/7/7	-
6	PEG	B	511	-	-	1/4/4/4	-
6	PEG	A	515	-	-	2/4/4/4	-
2	ASP	A	501	-	-	2/8/8/8	-
6	PEG	A	517	-	-	2/4/4/4	-
6	PEG	A	512	-	-	3/4/4/4	-
4	DMU	B	505	-	-	10/19/59/59	0/2/2/2
6	PEG	A	516	-	-	3/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	C	512	-	-	3/4/4/4	-
6	PEG	C	509	-	-	1/4/4/4	-
4	DMU	A	505	-	-	7/19/59/59	0/2/2/2
6	PEG	B	515	-	-	2/4/4/4	-
7	PGE	A	519	-	-	4/7/7/7	-
8	P6G	B	525	-	-	10/16/16/16	-
6	PEG	B	509	-	-	0/4/4/4	-
2	ASP	C	501	-	-	4/8/8/8	-
6	PEG	A	510	-	-	2/4/4/4	-
6	PEG	B	510	-	-	2/4/4/4	-
6	PEG	B	516	-	-	4/4/4/4	-
6	PEG	C	511	-	-	3/4/4/4	-
6	PEG	A	513	-	-	1/4/4/4	-
8	P6G	B	524	-	-	6/16/16/16	-
6	PEG	C	516	-	-	1/4/4/4	-
4	DMU	C	505	-	-	10/19/59/59	0/2/2/2
5	1PE	B	508	-	-	6/13/13/13	-
6	PEG	A	511	-	-	3/4/4/4	-
6	PEG	C	515	-	-	4/4/4/4	-
7	PGE	B	523	-	-	4/7/7/7	-
7	PGE	A	521	-	-	2/7/7/7	-
6	PEG	A	509	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	DMU	O1-C9	4.70	1.55	1.44
4	B	505	DMU	O1-C9	4.62	1.55	1.44
4	C	505	DMU	O1-C9	4.59	1.55	1.44
4	C	505	DMU	C11-C9	-3.32	1.40	1.51
4	B	505	DMU	C11-C9	-3.14	1.41	1.51
4	A	505	DMU	C11-C9	-3.13	1.41	1.51
4	A	505	DMU	O5-C6	2.99	1.49	1.41
4	A	505	DMU	O5-C4	2.79	1.51	1.44
4	B	505	DMU	O5-C6	2.63	1.48	1.41
4	B	505	DMU	C8-C9	2.56	1.58	1.53
4	B	505	DMU	O4-C7	2.53	1.49	1.43
4	A	505	DMU	O4-C7	2.46	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	505	DMU	O4-C7	2.37	1.48	1.43
4	C	505	DMU	C8-C9	2.35	1.58	1.53
4	B	505	DMU	O5-C4	2.35	1.50	1.44
4	A	505	DMU	O1-C10	2.34	1.47	1.41
4	C	505	DMU	O5-C6	2.31	1.47	1.41
4	A	505	DMU	C8-C9	2.30	1.57	1.53
4	C	505	DMU	C7-C5	-2.28	1.46	1.52
4	C	505	DMU	O5-C4	2.26	1.49	1.44
2	A	501	ASP	OXT-C	-2.25	1.23	1.30
4	B	505	DMU	O3-C5	2.15	1.48	1.43
4	A	505	DMU	C7-C5	-2.08	1.46	1.52
4	C	505	DMU	O1-C10	2.08	1.47	1.41
4	B	505	DMU	C7-C5	-2.07	1.47	1.52
4	A	505	DMU	O3-C5	2.02	1.48	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	505	DMU	O5-C4-C3	3.88	117.73	109.72
4	A	505	DMU	C18-O16-C6	3.28	119.29	113.68
4	C	505	DMU	O5-C4-C3	3.21	116.37	109.72
2	B	501	ASP	OXT-C-O	-3.08	117.10	124.08
4	B	505	DMU	O5-C4-C3	2.99	115.91	109.72
4	B	505	DMU	C7-C8-C9	2.80	115.30	110.23
4	A	505	DMU	O55-C2-C1	-2.78	103.82	110.38
4	A	505	DMU	C57-C4-C3	-2.38	106.69	113.38
4	A	505	DMU	C2-C3-C4	2.35	116.14	110.93
4	A	505	DMU	C7-C8-C9	2.32	114.43	110.23
4	A	505	DMU	C6-O5-C4	2.30	118.21	113.72
4	B	505	DMU	C10-O7-C3	-2.23	112.69	117.98
2	C	501	ASP	OXT-C-O	-2.18	119.14	124.08
4	B	505	DMU	C18-O16-C6	2.17	117.38	113.68
4	C	505	DMU	C10-O7-C3	-2.14	112.92	117.98
4	C	505	DMU	C1-C2-C3	2.09	114.43	109.68
4	B	505	DMU	C57-C4-C3	-2.09	107.52	113.38

There are no chirality outliers.

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	DMU	O5-C6-O16-C18
4	B	505	DMU	O5-C6-O16-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	505	DMU	O5-C6-O16-C18
4	A	505	DMU	C2-C3-O7-C10
4	B	505	DMU	O6-C11-C9-O1
6	C	515	PEG	O2-C3-C4-O4
7	A	519	PGE	O3-C5-C6-O4
6	B	512	PEG	C1-C2-O2-C3
8	A	522	P6G	C2-C3-O4-C5
6	B	513	PEG	C4-C3-O2-C2
4	B	505	DMU	O6-C11-C9-C8
5	B	507	1PE	OH4-C13-C23-OH3
7	A	518	PGE	O2-C3-C4-O3
8	B	525	P6G	C2-C3-O4-C5
5	A	507	1PE	OH4-C13-C23-OH3
8	B	524	P6G	O7-C8-C9-O10
8	B	525	P6G	O4-C5-C6-O7
4	B	505	DMU	O5-C4-C57-O61
4	C	505	DMU	O6-C11-C9-O1
4	C	505	DMU	O6-C11-C9-C8
8	C	519	P6G	O7-C8-C9-O10
4	B	505	DMU	C3-C4-C57-O61
6	B	513	PEG	O2-C3-C4-O4
7	A	518	PGE	O1-C1-C2-O2
5	B	506	1PE	OH4-C13-C23-OH3
8	C	520	P6G	O4-C5-C6-O7
4	C	505	DMU	O16-C18-C19-C22
5	B	508	1PE	OH4-C13-C23-OH3
5	B	508	1PE	OH6-C15-C25-OH5
5	A	506	1PE	OH7-C16-C26-OH6
5	B	507	1PE	OH7-C16-C26-OH6
5	B	508	1PE	OH7-C16-C26-OH6
5	C	506	1PE	OH2-C12-C22-OH3
6	A	512	PEG	O1-C1-C2-O2
6	C	510	PEG	O2-C3-C4-O4
6	C	511	PEG	O1-C1-C2-O2
7	A	519	PGE	O1-C1-C2-O2
7	A	521	PGE	O1-C1-C2-O2
4	A	505	DMU	C3-C4-C57-O61
8	C	520	P6G	O7-C8-C9-O10
8	A	522	P6G	O7-C8-C9-O10
8	B	524	P6G	O13-C14-C15-O16
8	B	525	P6G	O10-C11-C12-O13
6	A	508	PEG	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	509	PEG	O2-C3-C4-O4
6	B	510	PEG	O2-C3-C4-O4
8	C	520	P6G	O16-C17-C18-O19
7	B	523	PGE	O2-C3-C4-O3
5	A	506	1PE	OH4-C13-C23-OH3
6	A	517	PEG	C1-C2-O2-C3
4	B	505	DMU	C1-C6-O16-C18
4	C	505	DMU	C1-C6-O16-C18
2	B	501	ASP	OXT-C-CA-N
5	C	507	1PE	OH7-C16-C26-OH6
6	A	516	PEG	O2-C3-C4-O4
6	B	521	PEG	O1-C1-C2-O2
6	C	512	PEG	O1-C1-C2-O2
7	A	520	PGE	O3-C5-C6-O4
4	C	505	DMU	C18-C19-C22-C25
2	B	501	ASP	OXT-C-CA-CB
8	C	519	P6G	O10-C11-C12-O13
5	A	506	1PE	OH2-C12-C22-OH3
6	A	510	PEG	O1-C1-C2-O2
6	A	514	PEG	O2-C3-C4-O4
6	B	514	PEG	O1-C1-C2-O2
7	C	518	PGE	O1-C1-C2-O2
8	B	524	P6G	O1-C2-C3-O4
8	B	525	P6G	O1-C2-C3-O4
6	C	515	PEG	C1-C2-O2-C3
4	A	505	DMU	C31-C34-C37-C40
5	A	507	1PE	OH5-C14-C24-OH4
6	A	516	PEG	O1-C1-C2-O2
6	B	516	PEG	O1-C1-C2-O2
8	A	522	P6G	O1-C2-C3-O4
8	B	524	P6G	O16-C17-C18-O19
8	B	525	P6G	O13-C14-C15-O16
4	B	505	DMU	C31-C34-C37-C40
5	A	506	1PE	OH6-C15-C25-OH5
4	A	505	DMU	O6-C11-C9-O1
7	C	518	PGE	O2-C3-C4-O3
8	C	519	P6G	O13-C14-C15-O16
6	B	515	PEG	O2-C3-C4-O4
6	B	516	PEG	O2-C3-C4-O4
6	B	522	PEG	O1-C1-C2-O2
7	B	523	PGE	O3-C5-C6-O4
6	A	517	PEG	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	510	PEG	O1-C1-C2-O2
6	C	512	PEG	O2-C3-C4-O4
7	C	517	PGE	O3-C5-C6-O4
4	B	505	DMU	O16-C18-C19-C22
5	C	506	1PE	OH5-C14-C24-OH4
5	B	506	1PE	OH5-C14-C24-OH4
5	C	507	1PE	OH2-C12-C22-OH3
6	B	517	PEG	O2-C3-C4-O4
8	B	525	P6G	O16-C17-C18-O19
8	A	522	P6G	O10-C11-C12-O13
7	A	519	PGE	C4-C3-O2-C2
4	C	505	DMU	C22-C25-C28-C31
2	B	501	ASP	O-C-CA-CB
5	A	506	1PE	OH5-C14-C24-OH4
8	C	520	P6G	C12-C11-O10-C9
4	B	505	DMU	C34-C37-C40-C43
5	B	507	1PE	OH6-C15-C25-OH5
5	A	507	1PE	OH2-C12-C22-OH3
2	B	501	ASP	O-C-CA-N
6	B	514	PEG	C4-C3-O2-C2
8	C	519	P6G	C2-C3-O4-C5
7	A	521	PGE	O2-C3-C4-O3
4	B	505	DMU	C28-C31-C34-C37
7	A	518	PGE	C1-C2-O2-C3
5	A	507	1PE	C24-C14-OH5-C25
8	C	520	P6G	C11-C12-O13-C14
5	A	507	1PE	C15-C25-OH5-C14
5	B	508	1PE	C15-C25-OH5-C14
8	A	522	P6G	C15-C14-O13-C12
5	A	506	1PE	C13-C23-OH3-C22
5	C	506	1PE	C12-C22-OH3-C23
6	C	512	PEG	C1-C2-O2-C3
6	A	508	PEG	C1-C2-O2-C3
6	A	511	PEG	C1-C2-O2-C3
5	A	507	1PE	C12-C22-OH3-C23
7	B	523	PGE	C6-C5-O3-C4
7	C	517	PGE	C3-C4-O3-C5
5	B	506	1PE	C25-C15-OH6-C26
6	A	514	PEG	C4-C3-O2-C2
5	B	506	1PE	C24-C14-OH5-C25
6	C	515	PEG	C4-C3-O2-C2
8	C	520	P6G	C5-C6-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	507	1PE	C14-C24-OH4-C13
6	A	512	PEG	C4-C3-O2-C2
8	B	525	P6G	C8-C9-O10-C11
6	A	512	PEG	O2-C3-C4-O4
6	B	518	PEG	O2-C3-C4-O4
6	C	514	PEG	O2-C3-C4-O4
6	C	511	PEG	C4-C3-O2-C2
4	A	505	DMU	O5-C4-C57-O61
6	C	511	PEG	C1-C2-O2-C3
5	B	507	1PE	C23-C13-OH4-C24
8	B	524	P6G	C9-C8-O7-C6
2	C	501	ASP	N-CA-CB-CG
6	B	521	PEG	C1-C2-O2-C3
7	B	523	PGE	C4-C3-O2-C2
8	A	522	P6G	C11-C12-O13-C14
8	B	525	P6G	C18-C17-O16-C15
8	C	519	P6G	O4-C5-C6-O7
6	C	516	PEG	O1-C1-C2-O2
8	C	520	P6G	C14-C15-O16-C17
6	A	510	PEG	C1-C2-O2-C3
6	A	516	PEG	C1-C2-O2-C3
6	C	515	PEG	O1-C1-C2-O2
8	C	520	P6G	O13-C14-C15-O16
2	A	501	ASP	CA-CB-CG-OD1
5	A	507	1PE	C25-C15-OH6-C26
8	C	520	P6G	C18-C17-O16-C15
5	C	507	1PE	C14-C24-OH4-C13
6	B	517	PEG	C1-C2-O2-C3
5	A	506	1PE	C12-C22-OH3-C23
5	C	506	1PE	C14-C24-OH4-C13
4	C	505	DMU	O1-C10-O7-C3
5	B	506	1PE	C23-C13-OH4-C24
7	C	518	PGE	C1-C2-O2-C3
4	C	505	DMU	C25-C28-C31-C34
7	A	518	PGE	O3-C5-C6-O4
6	C	510	PEG	C4-C3-O2-C2
6	B	515	PEG	C4-C3-O2-C2
5	B	506	1PE	C12-C22-OH3-C23
2	A	501	ASP	CA-CB-CG-OD2
8	C	520	P6G	C2-C3-O4-C5
8	C	520	P6G	C6-C5-O4-C3
7	A	518	PGE	C3-C4-O3-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	519	PEG	C4-C3-O2-C2
6	B	516	PEG	C1-C2-O2-C3
5	B	506	1PE	C13-C23-OH3-C22
4	A	505	DMU	C18-C19-C22-C25
6	A	511	PEG	C4-C3-O2-C2
5	B	506	1PE	OH7-C16-C26-OH6
8	A	522	P6G	O16-C17-C18-O19
7	A	520	PGE	O2-C3-C4-O3
6	A	513	PEG	C1-C2-O2-C3
7	A	520	PGE	C1-C2-O2-C3
8	C	519	P6G	C8-C9-O10-C11
5	B	506	1PE	C14-C24-OH4-C13
6	C	508	PEG	C4-C3-O2-C2
6	C	510	PEG	C1-C2-O2-C3
5	C	507	1PE	OH4-C13-C23-OH3
6	B	519	PEG	O1-C1-C2-O2
5	C	507	1PE	C15-C25-OH5-C14
6	A	509	PEG	C4-C3-O2-C2
5	B	508	1PE	C25-C15-OH6-C26
5	B	507	1PE	C16-C26-OH6-C15
2	C	501	ASP	CA-CB-CG-OD1
8	C	519	P6G	C9-C8-O7-C6
6	B	517	PEG	O1-C1-C2-O2
8	B	524	P6G	C11-C12-O13-C14
4	C	505	DMU	C5-C10-O7-C3
7	A	518	PGE	C6-C5-O3-C4
5	B	508	1PE	C16-C26-OH6-C15
2	C	501	ASP	C-CA-CB-CG
6	B	511	PEG	C4-C3-O2-C2
5	A	507	1PE	C14-C24-OH4-C13
6	C	509	PEG	O1-C1-C2-O2
8	B	525	P6G	C5-C6-O7-C8
2	C	501	ASP	CA-CB-CG-OD2
6	B	520	PEG	C1-C2-O2-C3
6	A	515	PEG	O1-C1-C2-O2
5	B	507	1PE	C24-C14-OH5-C25
5	C	507	1PE	C13-C23-OH3-C22
5	A	507	1PE	OH6-C15-C25-OH5
6	A	511	PEG	O1-C1-C2-O2
8	C	519	P6G	O1-C2-C3-O4
8	A	522	P6G	O13-C14-C15-O16
8	B	525	P6G	O7-C8-C9-O10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	B	516	PEG	C4-C3-O2-C2
8	A	522	P6G	C5-C6-O7-C8
6	B	520	PEG	O1-C1-C2-O2
8	C	519	P6G	O16-C17-C18-O19
5	C	507	1PE	C25-C15-OH6-C26
7	A	519	PGE	O2-C3-C4-O3
6	A	515	PEG	O2-C3-C4-O4
6	C	514	PEG	C1-C2-O2-C3

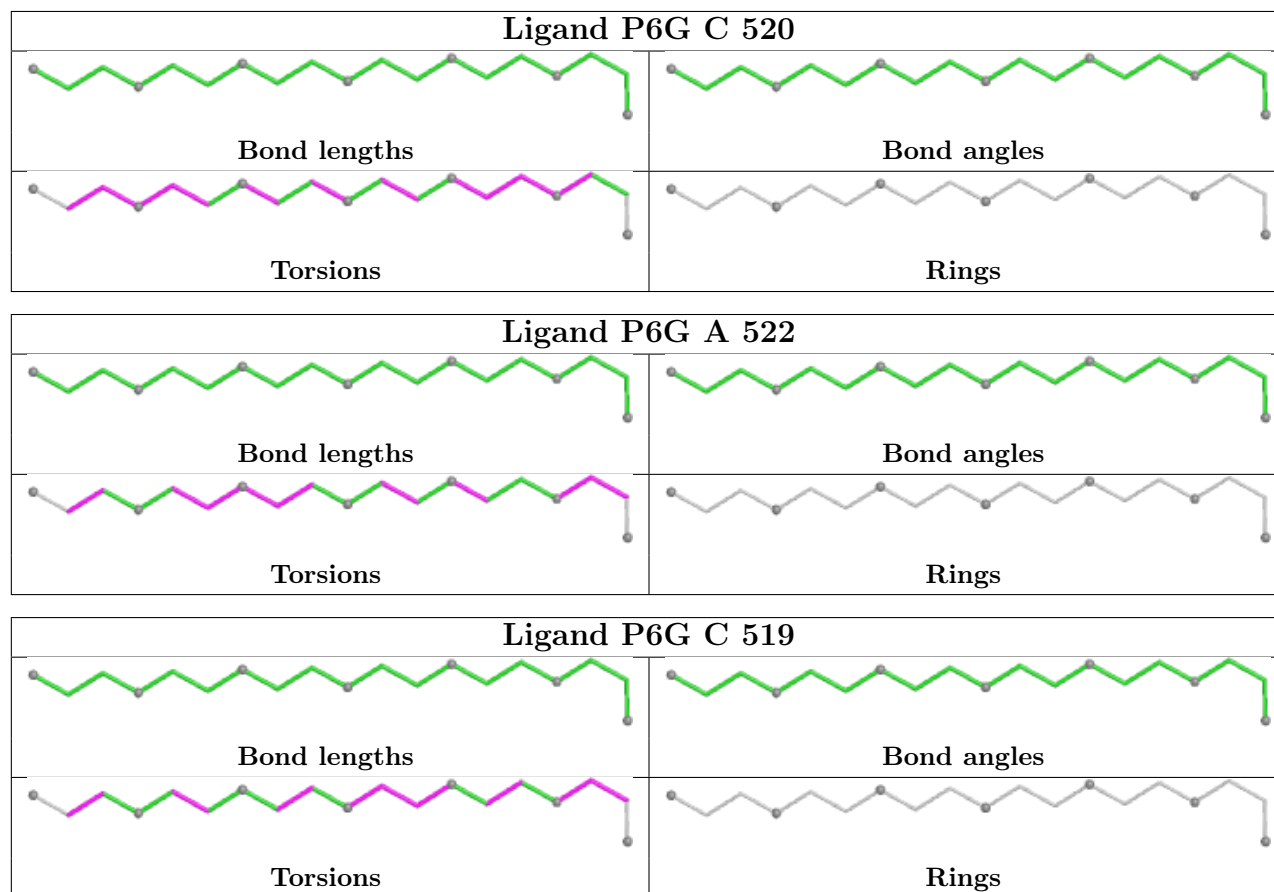
There are no ring outliers.

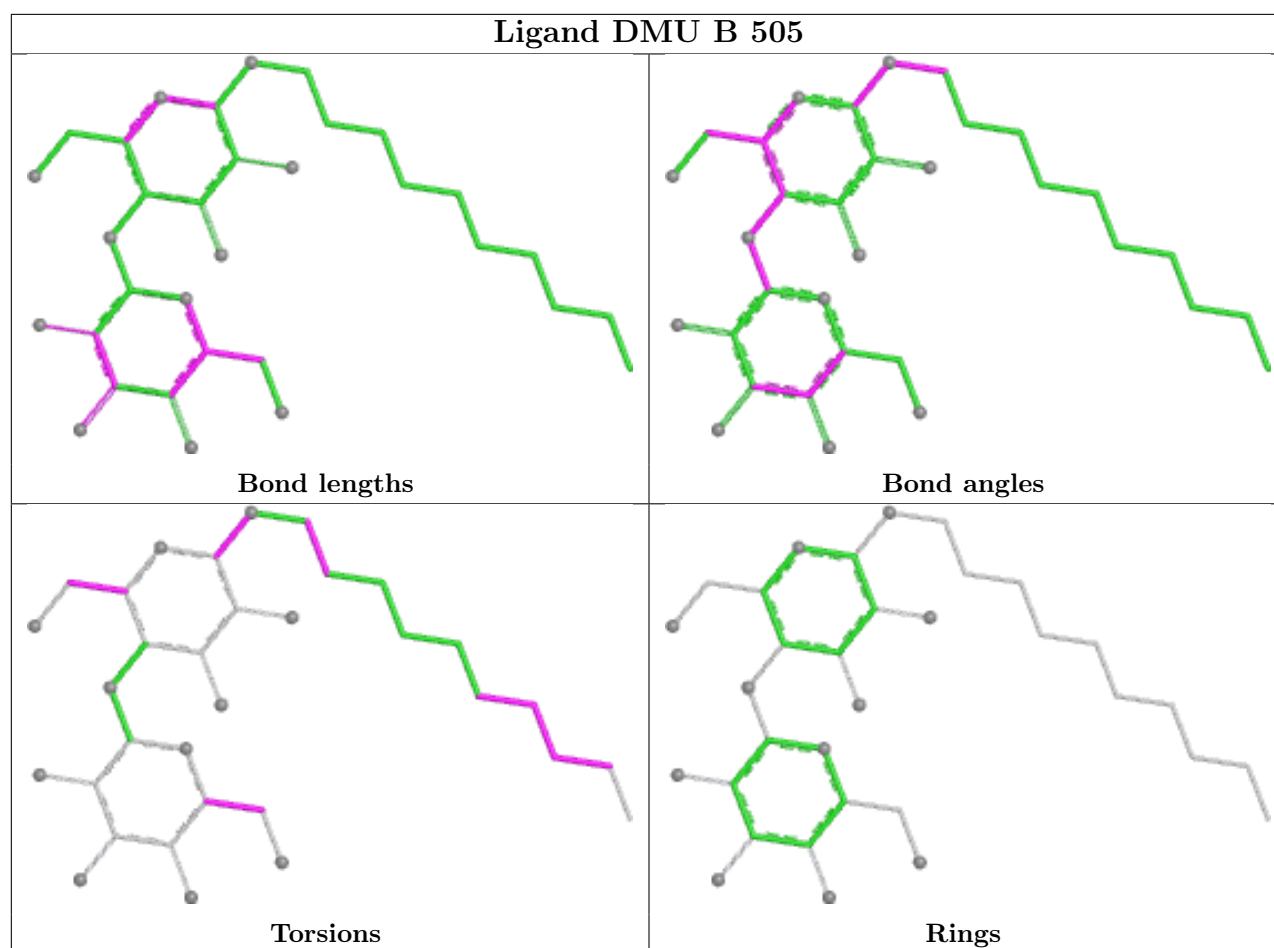
21 monomers are involved in 25 short contacts:

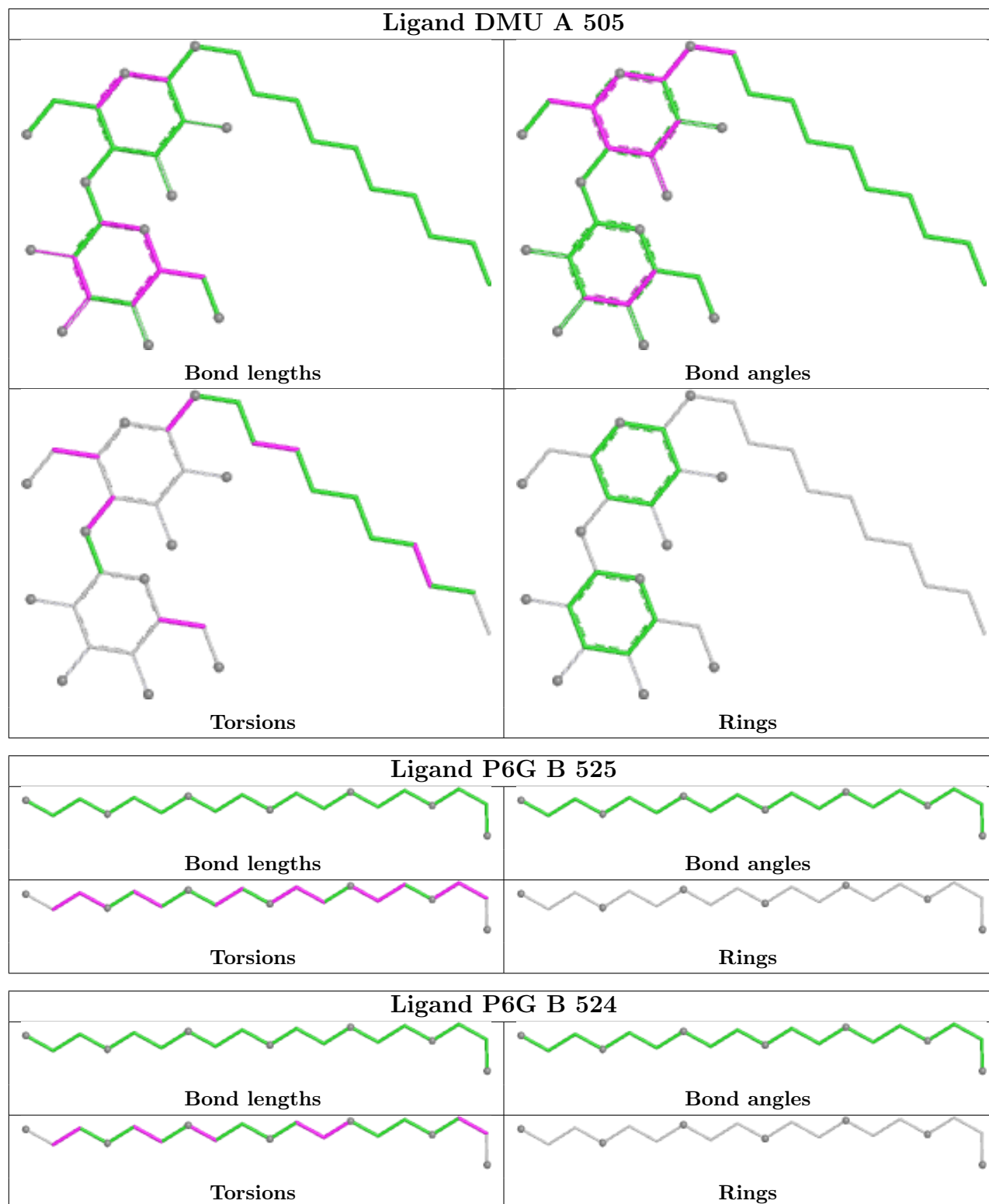
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ASP	3	0
8	C	520	P6G	1	0
6	C	510	PEG	2	0
5	A	507	1PE	2	0
5	B	506	1PE	1	0
6	B	522	PEG	2	0
7	A	520	PGE	1	0
5	B	507	1PE	1	0
6	C	508	PEG	1	0
2	A	501	ASP	2	0
4	B	505	DMU	1	0
6	C	512	PEG	1	0
6	C	509	PEG	1	0
8	B	525	P6G	1	0
6	B	509	PEG	1	0
8	B	524	P6G	1	0
4	C	505	DMU	2	0
5	B	508	1PE	2	0
6	A	511	PEG	1	0
6	C	515	PEG	1	0
7	A	521	PGE	1	0

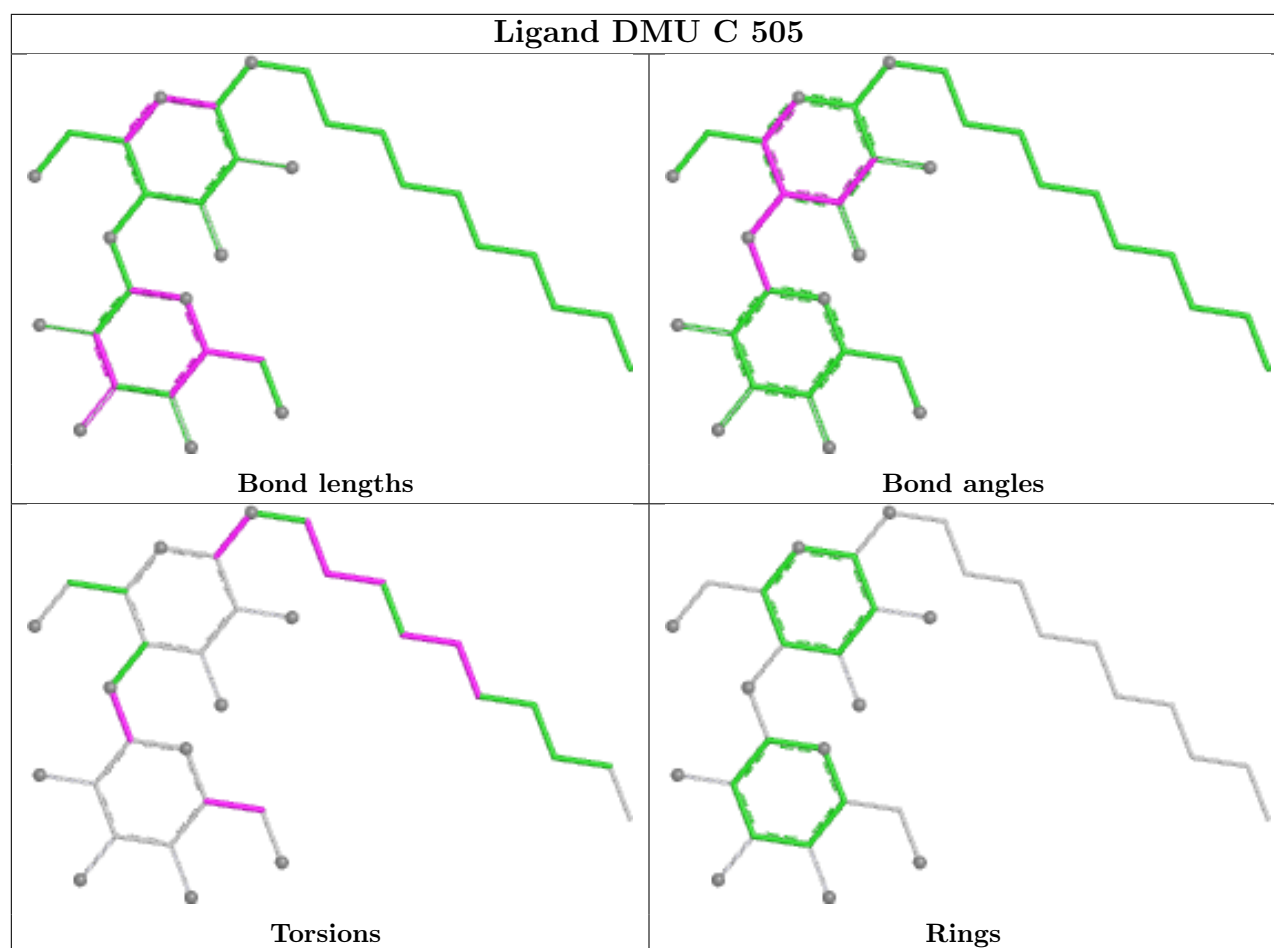
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	427/438 (97%)	0.84	82 (19%) 3 2	42, 84, 153, 243	1 (0%)
1	B	427/438 (97%)	0.46	51 (11%) 9 7	58, 90, 159, 234	0
1	C	426/438 (97%)	0.67	61 (14%) 6 5	44, 94, 146, 212	1 (0%)
All	All	1280/1314 (97%)	0.66	194 (15%) 5 4	42, 89, 154, 243	2 (0%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	384	ALA	9.8
1	C	10	LEU	8.9
1	B	421	LYS	8.1
1	B	16	TRP	8.1
1	C	381	SER	8.0
1	A	221	GLU	7.5
1	C	385	LEU	7.5
1	B	176	GLU	7.5
1	A	31	ILE	7.2
1	C	382	PRO	6.7
1	C	378	THR	6.7
1	C	123	LYS	6.4
1	C	225	ARG	6.3
1	C	6	LEU	6.3
1	A	390	ILE	6.2
1	C	97	MET	6.1
1	C	205	GLN	6.1
1	C	11	ASP	6.0
1	C	380	GLY	6.0
1	A	121	THR	5.9
1	A	130	PRO	5.9
1	C	383	VAL	5.7
1	A	28	PHE	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	8	ARG	5.6
1	A	375	LEU	5.6
1	A	383	VAL	5.5
1	B	175	GLU	5.5
1	A	324	THR	5.3
1	C	9	TYR	5.3
1	C	379	PRO	5.2
1	A	387	TYR	5.1
1	A	368[A]	MET	5.1
1	B	380	GLY	5.1
1	A	386	ALA	5.1
1	A	14	VAL	5.0
1	C	130	PRO	4.8
1	C	119	SER	4.8
1	A	328	VAL	4.8
1	B	15	LEU	4.8
1	C	118	GLY	4.7
1	B	10	LEU	4.6
1	C	36	GLY	4.6
1	C	354	GLY	4.5
1	B	117	LEU	4.5
1	A	325	VAL	4.4
1	A	421	LYS	4.3
1	C	100	PHE	4.3
1	A	154	LEU	4.3
1	A	235	GLY	4.3
1	A	393	ILE	4.2
1	C	389	MET	4.2
1	C	117	LEU	4.1
1	B	287	THR	4.1
1	C	96	ALA	4.0
1	A	388	ALA	4.0
1	B	346	LEU	4.0
1	B	381	SER	4.0
1	B	382	PRO	3.9
1	C	129	PRO	3.9
1	A	389	MET	3.9
1	A	38	ALA	3.8
1	A	29	GLY	3.8
1	B	14	VAL	3.8
1	C	7	ARG	3.7
1	A	391	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	174	ASN	3.7
1	B	431	HIS	3.7
1	C	421	LYS	3.7
1	C	122	GLY	3.7
1	A	430	SER	3.6
1	A	217	TYR	3.6
1	B	132	LEU	3.6
1	A	129	PRO	3.6
1	C	5	LEU	3.6
1	B	46	LYS	3.5
1	A	392	GLY	3.5
1	B	42	LYS	3.5
1	A	370	LEU	3.4
1	A	139	ILE	3.3
1	A	273	THR	3.3
1	B	44	TYR	3.3
1	C	422	GLU	3.3
1	A	225	ARG	3.3
1	C	290	VAL	3.3
1	B	385	LEU	3.3
1	A	327	PHE	3.1
1	B	121	THR	3.1
1	C	33	GLY	3.1
1	A	152	GLU	3.1
1	A	378	THR	3.1
1	C	14	VAL	3.1
1	C	376	ASP	3.1
1	C	125	ILE	3.0
1	C	16	TRP	3.0
1	A	425	GLU	3.0
1	B	419	THR	3.0
1	C	386	ALA	3.0
1	A	407	THR	3.0
1	A	233	VAL	3.0
1	A	34	HIS	3.0
1	C	303	SER	2.9
1	A	211	VAL	2.9
1	A	234	VAL	2.9
1	B	123	LYS	2.9
1	B	230	LEU	2.9
1	B	342	LEU	2.9
1	B	420	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	406	VAL	2.9
1	C	350	LEU	2.9
1	C	230	LEU	2.8
1	A	27	VAL	2.8
1	B	50	ASP	2.8
1	C	222	GLN	2.7
1	C	221	GLU	2.7
1	A	153	VAL	2.7
1	A	323	VAL	2.7
1	A	222	GLN	2.7
1	A	170	LEU	2.7
1	A	15	LEU	2.7
1	A	18	ILE	2.7
1	C	15	LEU	2.7
1	A	223	GLY	2.7
1	A	224	VAL	2.7
1	A	426	SER	2.7
1	A	84	GLY	2.6
1	A	207	ALA	2.6
1	C	124	ALA	2.6
1	B	273	THR	2.6
1	B	189	PHE	2.6
1	A	33	GLY	2.6
1	B	350	LEU	2.6
1	C	121	THR	2.6
1	A	376	ASP	2.6
1	A	20	TRP	2.6
1	B	422	GLU	2.6
1	B	48	PHE	2.6
1	B	227	VAL	2.5
1	B	246	VAL	2.5
1	A	231	ALA	2.5
1	C	293	GLU	2.5
1	A	220	ALA	2.5
1	B	406	VAL	2.5
1	A	37	TYR	2.5
1	C	34	HIS	2.5
1	B	269	ASP	2.5
1	A	410	LEU	2.5
1	A	122	GLY	2.5
1	B	179	ARG	2.5
1	A	155	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	127	ALA	2.4
1	A	431	HIS	2.4
1	C	338	LEU	2.4
1	B	379	PRO	2.4
1	C	276	VAL	2.4
1	C	227	VAL	2.4
1	B	261	ILE	2.4
1	A	227	VAL	2.4
1	A	124	ALA	2.4
1	A	13	PRO	2.4
1	A	123	LYS	2.3
1	A	373	VAL	2.3
1	A	32	ALA	2.3
1	A	395	ALA	2.3
1	C	292	GLU	2.3
1	B	129	PRO	2.3
1	A	209	ILE	2.2
1	A	287	THR	2.2
1	A	136	LEU	2.2
1	B	343	VAL	2.2
1	B	119	SER	2.2
1	A	304	PHE	2.2
1	B	194	GLU	2.2
1	C	420	GLU	2.2
1	B	208	PRO	2.2
1	B	347	THR	2.2
1	B	118	GLY	2.2
1	C	346	LEU	2.2
1	B	47	PRO	2.2
1	A	381	SER	2.2
1	C	131	SER	2.2
1	C	291	ALA	2.2
1	A	174	ASN	2.1
1	A	201	GLY	2.1
1	B	217	TYR	2.1
1	A	404	VAL	2.1
1	B	36	GLY	2.1
1	C	201	GLY	2.1
1	B	13	PRO	2.1
1	B	51	LEU	2.1
1	C	419	THR	2.1
1	A	131	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	185	LEU	2.0
1	A	145	PHE	2.0
1	A	16	TRP	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 oligosaccharides 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(Å ²)	Q<0.9
6	PEG	C	515	7/7	0.49	0.16	121,121,123,123	0
5	1PE	C	507	16/16	0.62	0.17	127,143,149,151	0
6	PEG	B	519	7/7	0.64	0.11	132,133,142,142	0
8	P6G	C	520	19/19	0.65	0.21	111,120,138,139	0
5	1PE	B	507	16/16	0.68	0.31	80,121,137,138	0
8	P6G	B	525	19/19	0.69	0.28	95,125,130,131	0
5	1PE	B	506	16/16	0.70	0.30	94,113,121,125	0
6	PEG	B	520	7/7	0.70	0.27	120,125,133,138	0
6	PEG	B	522	7/7	0.70	0.16	120,125,133,134	0
5	1PE	A	507	16/16	0.73	0.20	111,124,133,133	0
6	PEG	A	511	7/7	0.73	0.16	111,116,121,121	0
6	PEG	B	521	7/7	0.74	0.26	124,124,128,129	0
5	1PE	C	506	16/16	0.78	0.34	91,137,155,156	0
7	PGE	B	523	10/10	0.78	0.16	108,130,138,139	0
8	P6G	A	522	19/19	0.78	0.28	99,124,135,137	0
6	PEG	B	512	7/7	0.78	0.14	100,106,116,117	0
5	1PE	A	506	16/16	0.78	0.23	107,117,124,125	0
4	DMU	A	505	33/33	0.79	0.21	108,156,169,172	0
8	P6G	C	519	19/19	0.81	0.29	83,109,120,122	0
6	PEG	A	517	7/7	0.81	0.25	112,123,133,133	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	P6G	B	524	19/19	0.82	0.21	78,96,112,114	0
7	PGE	A	518	10/10	0.82	0.20	78,94,102,104	0
6	PEG	A	514	7/7	0.82	0.16	119,128,132,132	0
6	PEG	A	509	7/7	0.82	0.19	87,88,95,95	0
4	DMU	C	505	33/33	0.83	0.18	81,140,149,151	0
6	PEG	A	515	7/7	0.83	0.20	128,133,136,138	0
6	PEG	B	514	7/7	0.83	0.15	104,110,117,118	0
6	PEG	A	513	7/7	0.84	0.22	125,130,134,137	0
4	DMU	B	505	33/33	0.84	0.17	93,142,154,161	0
6	PEG	C	511	7/7	0.84	0.17	115,118,120,120	0
6	PEG	C	512	7/7	0.84	0.16	106,115,124,124	0
7	PGE	A	519	10/10	0.85	0.21	81,87,108,113	0
6	PEG	B	517	7/7	0.86	0.19	110,113,118,119	0
5	1PE	B	508	16/16	0.86	0.13	121,139,151,151	0
7	PGE	A	520	10/10	0.86	0.24	97,102,114,117	0
7	PGE	C	518	10/10	0.87	0.23	124,133,135,137	0
7	PGE	A	521	10/10	0.87	0.24	125,136,140,141	0
6	PEG	B	515	7/7	0.87	0.11	109,110,118,120	0
6	PEG	C	514	7/7	0.89	0.22	122,124,129,130	0
6	PEG	C	516	7/7	0.90	0.27	130,134,140,144	0
6	PEG	B	510	7/7	0.90	0.16	95,98,100,102	0
6	PEG	B	511	7/7	0.90	0.27	109,122,129,132	0
6	PEG	A	512	7/7	0.91	0.22	96,112,119,119	0
6	PEG	B	518	7/7	0.91	0.22	103,114,121,125	0
6	PEG	A	510	7/7	0.91	0.17	105,106,110,113	0
6	PEG	C	508	7/7	0.91	0.11	93,96,97,97	0
6	PEG	A	508	7/7	0.92	0.16	87,89,92,93	0
7	PGE	C	517	10/10	0.92	0.21	124,132,137,137	0
6	PEG	C	513	7/7	0.93	0.19	113,118,124,125	0
6	PEG	C	509	7/7	0.93	0.13	92,105,108,108	0
6	PEG	B	516	7/7	0.93	0.18	105,118,124,124	0
6	PEG	A	516	7/7	0.93	0.23	105,108,133,140	0
3	NA	A	502	1/1	0.94	0.13	63,63,63,63	0
6	PEG	B	509	7/7	0.94	0.14	98,101,106,108	0
3	NA	C	503	1/1	0.95	0.17	66,66,66,66	0
2	ASP	B	501	9/9	0.95	0.10	63,73,87,104	0
6	PEG	C	510	7/7	0.95	0.16	102,109,111,115	0
3	NA	C	502	1/1	0.96	0.14	75,75,75,75	0
2	ASP	A	501	9/9	0.96	0.08	63,70,79,87	0
6	PEG	B	513	7/7	0.96	0.17	98,105,121,123	0
3	NA	B	503	1/1	0.97	0.06	61,61,61,61	0
2	ASP	C	501	9/9	0.97	0.06	71,76,81,86	0

Continued on next page...

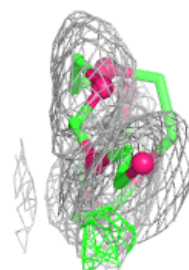
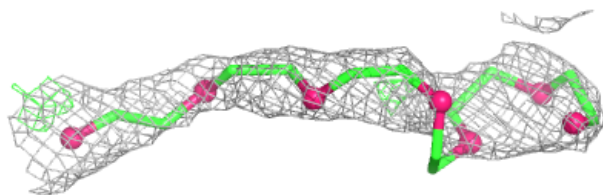
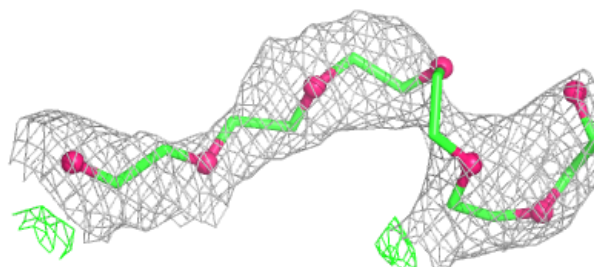
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	504	1/1	0.98	0.06	112,112,112,112	0
3	NA	B	502	1/1	0.98	0.09	68,68,68,68	0
3	NA	A	503	1/1	0.99	0.02	65,65,65,65	0
3	NA	C	504	1/1	0.99	0.03	85,85,85,85	0
3	NA	A	504	1/1	0.99	0.05	86,86,86,86	0

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

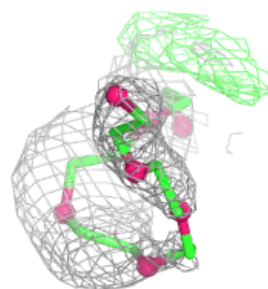
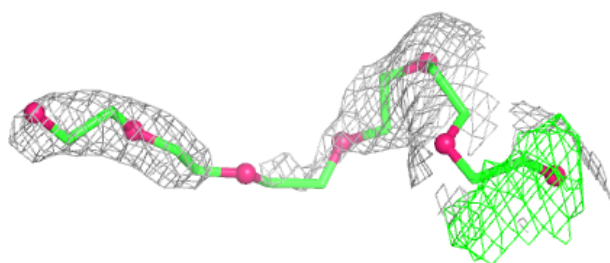
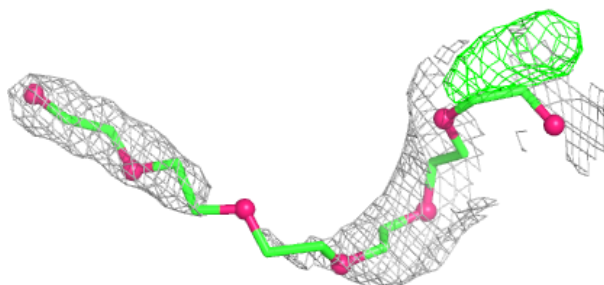
Electron density around P6G C 520:

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

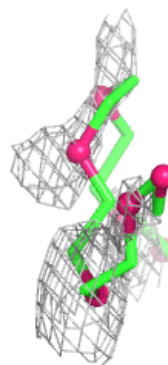
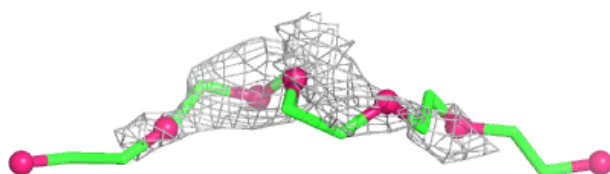
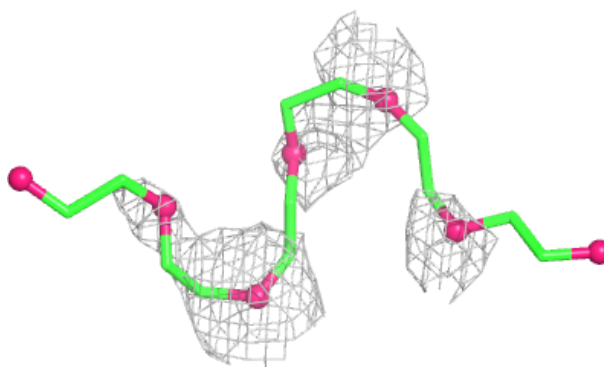


Electron density around P6G B 525:

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

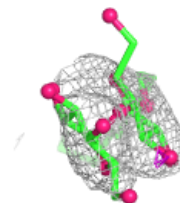
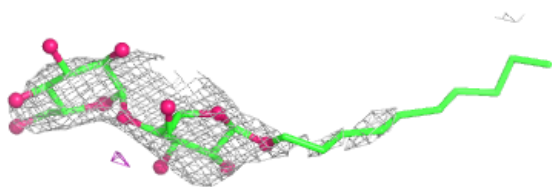
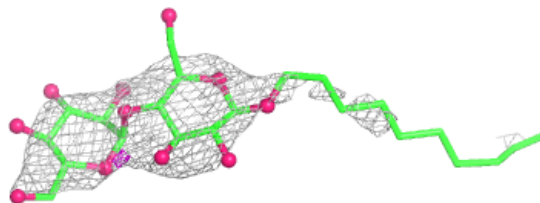
**Electron density around P6G A 522:**

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

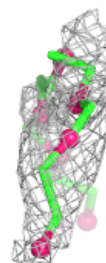
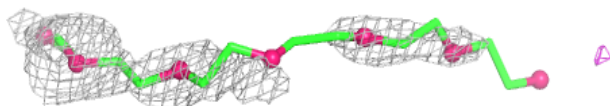
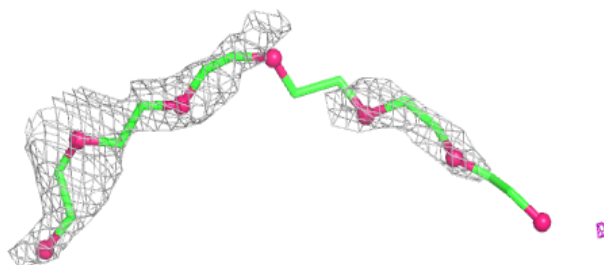


Electron density around DMU A 505:

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

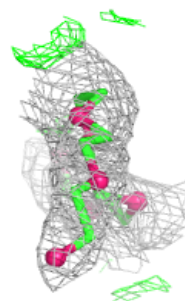
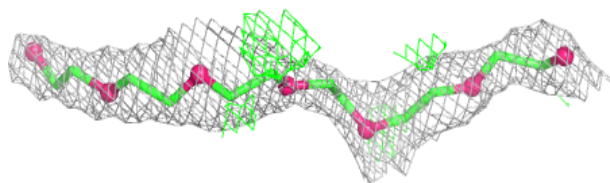
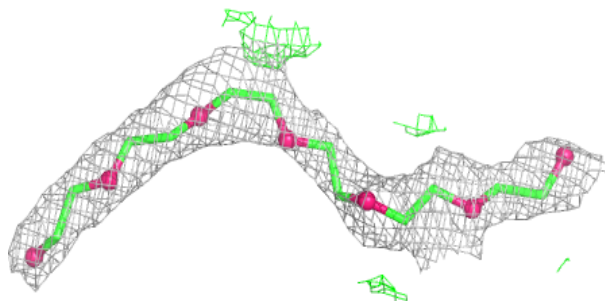
**Electron density around P6G C 519:**

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

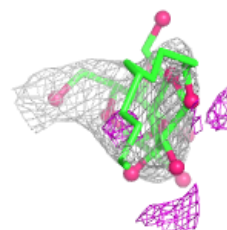
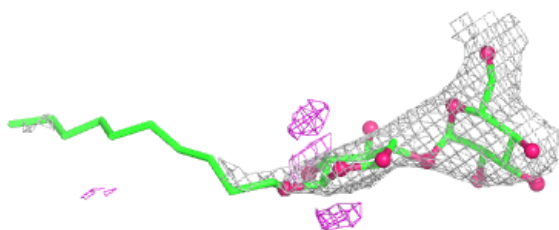
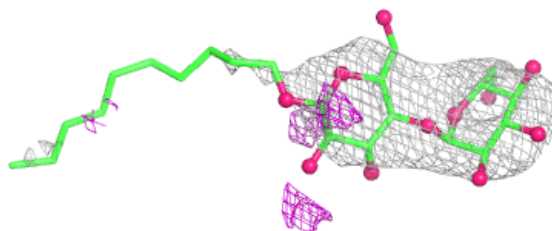


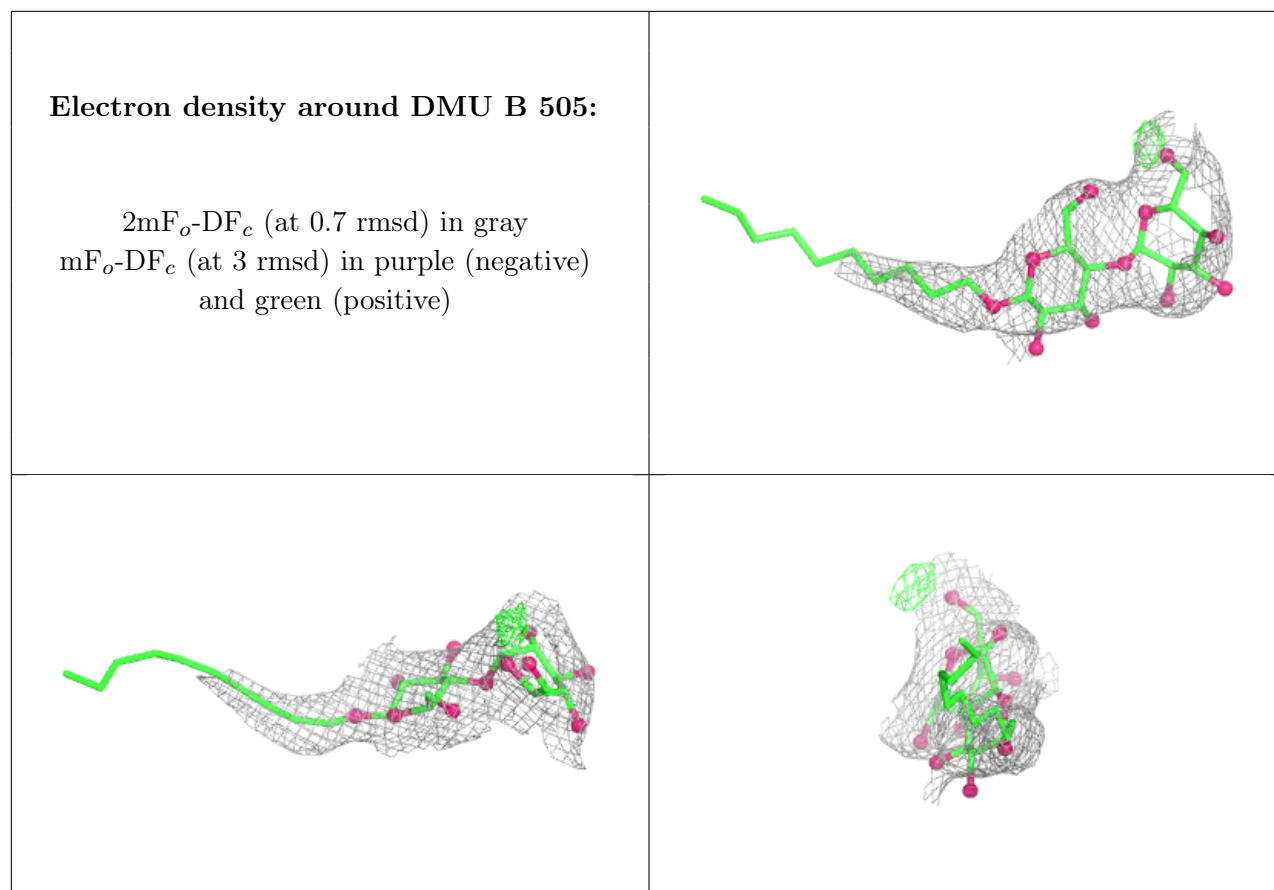
Electron density around P6G B 524:

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

**Electron density around DMU C 505:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.