



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 6R7R / pdb_00006r7r
Title : Crystal structure of the glutamate transporter homologue GltTk in complex with D-aspartate
Authors : Arkhipova, V.; Guskov, A.; Slotboom, D.J.
Deposited on : 2019-03-29
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

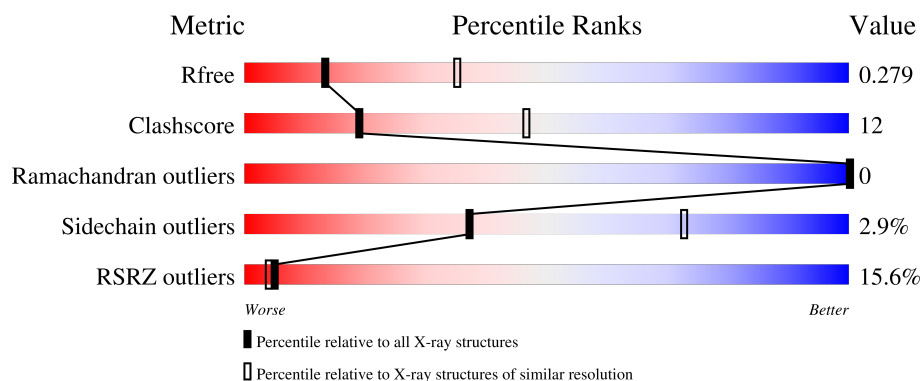
1 Overall quality at a glance

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	21% 69% 26% 5%
1	B	438	12% 67% 24% 7%
1	C	438	11% 73% 23% .

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
3	DAS	A	504	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9512 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	416	Total	C	N	O	S	0	2	0
			3109	2051	503	538	17			
1	B	406	Total	C	N	O	S	0	0	0
			3005	1980	485	524	16			
1	C	422	Total	C	N	O	S	0	0	0
			3148	2078	509	545	16			

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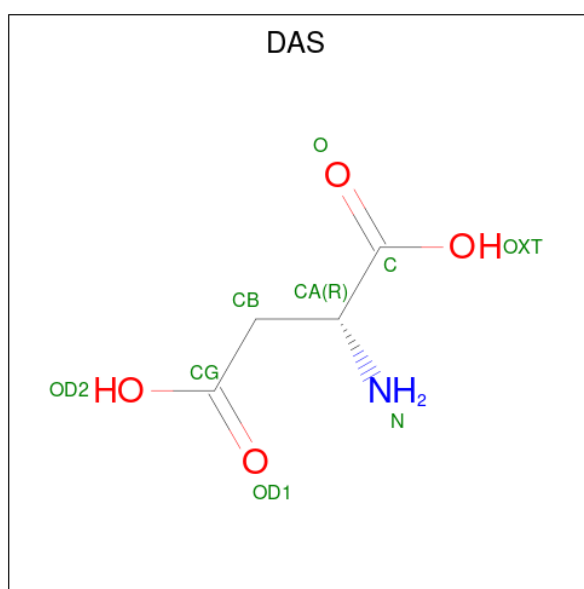
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Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	expression tag	UNP Q5JID0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

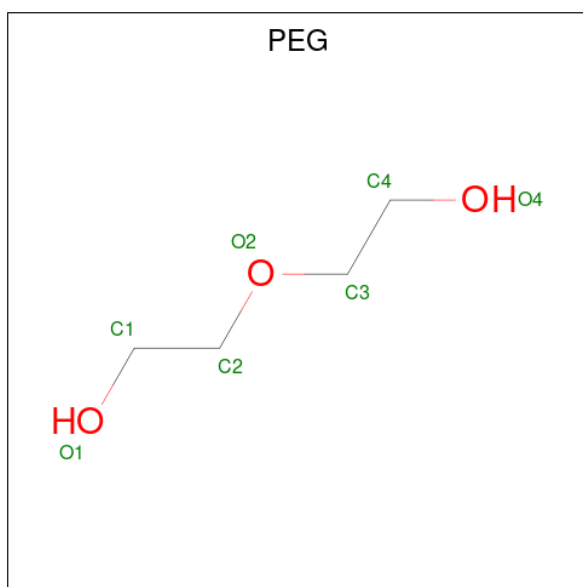
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Na	0	0
			3	3		
2	B	3	Total	Na	0	0
			3	3		
2	C	3	Total	Na	0	0
			3	3		

- Molecule 3 is D-ASPARTIC ACID (CCD ID: DAS) (formula: C₄H₇NO₄) (labeled as "Ligand of Interest" by depositor).



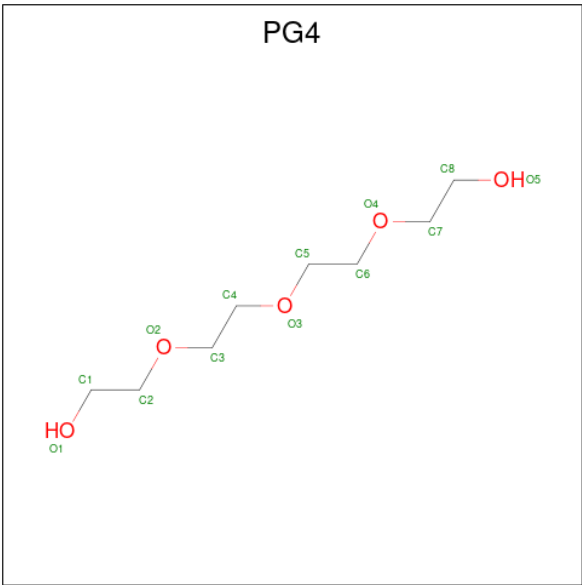
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	4	1	4		
3	B	1	Total	C	N	O	0	0
			9	4	1	4		
3	C	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



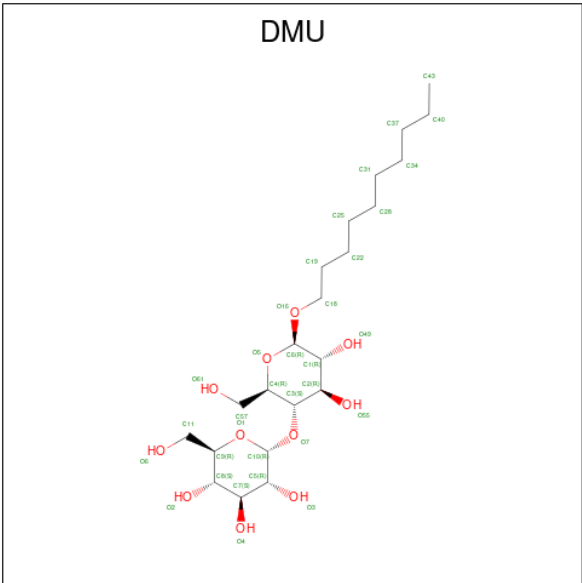
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total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

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



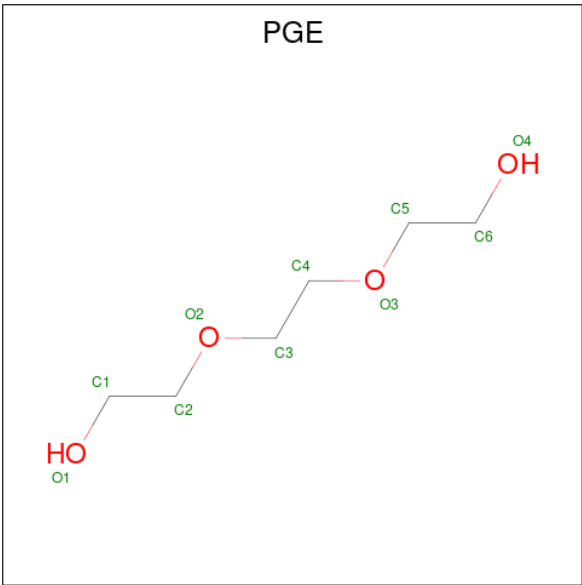
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



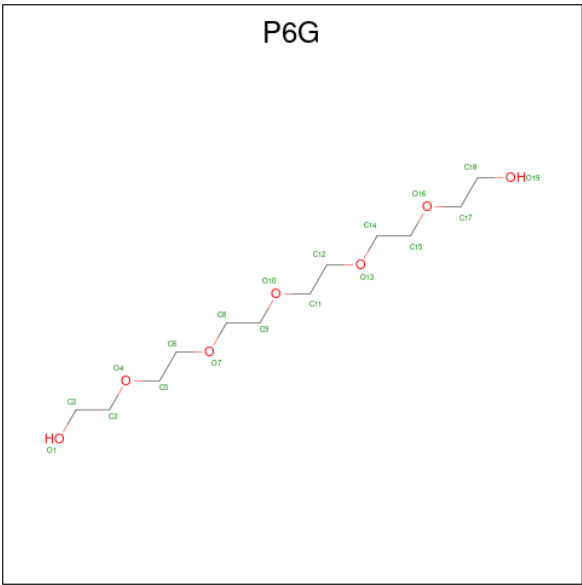
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			33	22	11		

- 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	B	1	Total	C	O	0	0
			10	6	4		
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: C₁₂H₂₆O₇).



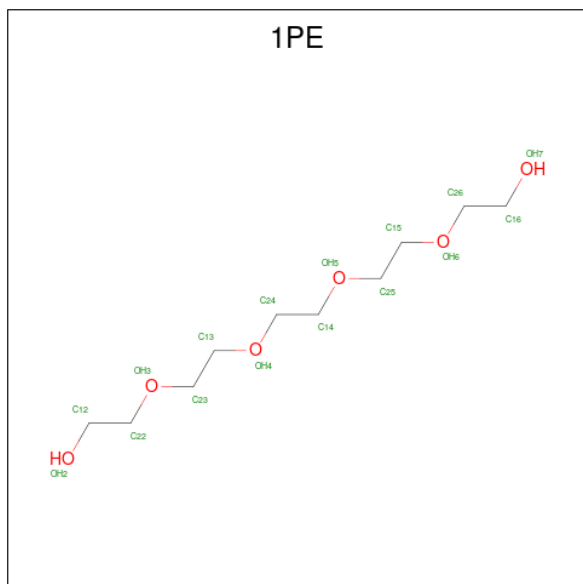
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			19	12	7		

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

- Molecule 9 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).

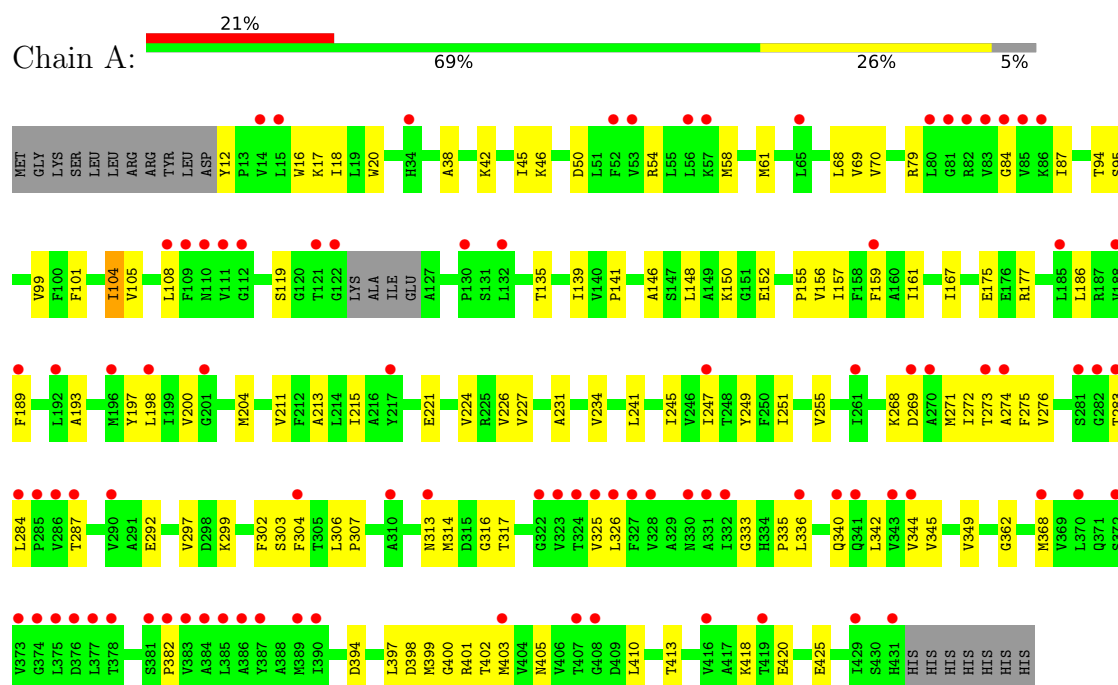


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			16	10	6		

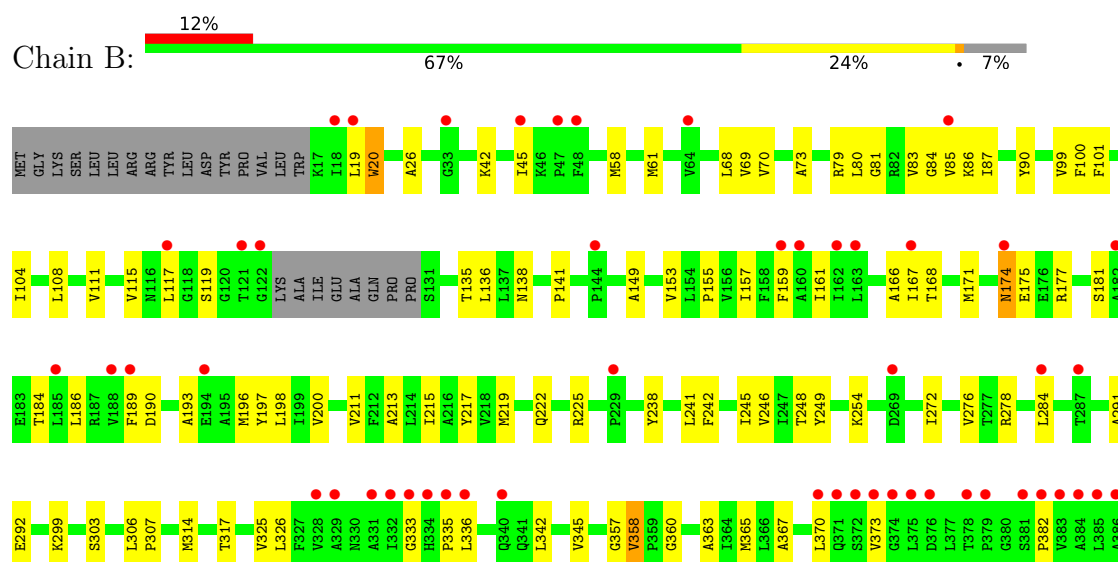
3 Residue-property plots

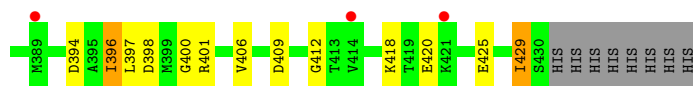
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

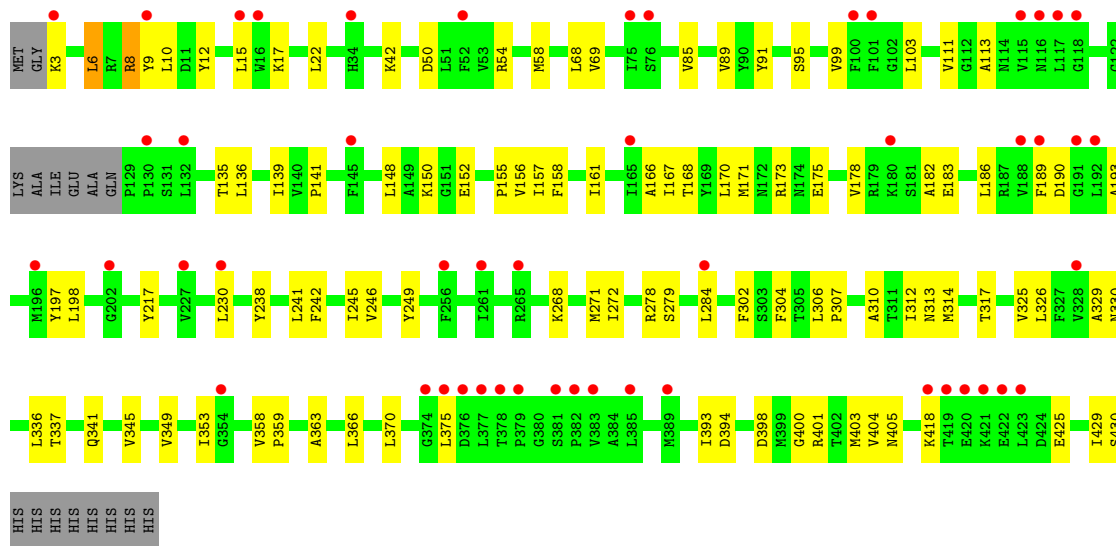
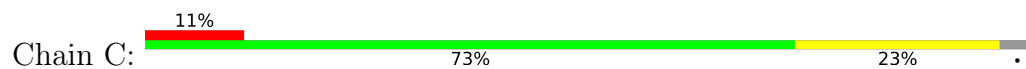


- Molecule 1: Proton/glutamate symporter, SDF family





- Molecule 1: Proton/glutamate symporter, SDF family



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.55Å 116.55Å 314.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.06 – 2.80 48.06 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.06-2.80) 99.0 (48.06-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.232 , 0.269 0.241 , 0.279	Depositor DCC
R_{free} test set	3071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	106.3	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9512	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: DMU, P6G, PG4, DAS, PGE, NA, 1PE, 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	0.39	0/3168	0.63	0/4312
1	B	0.37	0/3056	0.63	0/4155
1	C	0.34	0/3206	0.59	0/4361
All	All	0.36	0/9430	0.62	0/12828

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3109	0	3300	81	0
1	B	3005	0	3206	79	0
1	C	3148	0	3357	77	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	9	0	5	4	0
3	B	9	0	5	3	0
3	C	9	0	5	3	0
4	A	21	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	40	0	0
4	C	35	0	50	1	0
5	A	13	0	18	0	0
6	A	33	0	42	4	0
7	A	10	0	14	1	0
7	B	20	0	28	1	0
8	B	38	0	52	2	0
9	B	16	0	22	5	0
All	All	9512	0	10174	232	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 12.

All (232) 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:326:LEU:HD23	1:C:336:LEU:HD12	1.58	0.84
1:A:157:ILE:HD11	1:A:307:PRO:HB2	1.61	0.83
1:A:58:MET:HE1	1:C:158:PHE:HE1	1.48	0.77
1:C:175:GLU:OE1	1:C:175:GLU:N	2.19	0.75
1:C:68:LEU:HD21	1:C:161:ILE:HG13	1.73	0.71
1:B:159:PHE:HD1	1:C:58:MET:HE2	1.57	0.70
1:B:326:LEU:HD23	1:B:336:LEU:HD12	1.74	0.70
1:B:357:GLY:HA2	3:B:504:DAS:OXT	1.91	0.69
1:A:418:LYS:NZ	1:A:425:GLU:OE2	2.22	0.68
1:C:157:ILE:HD11	1:C:307:PRO:HB2	1.76	0.67
1:B:141:PRO:HG2	1:C:58:MET:HE3	1.75	0.67
1:C:398:ASP:HA	1:C:401:ARG:NE	2.10	0.66
1:B:177:ARG:NH1	1:C:190:ASP:OD2	2.30	0.65
1:A:99:VAL:HG11	1:A:345:VAL:HA	1.79	0.65
1:A:326:LEU:HD23	1:A:336:LEU:HD12	1.79	0.65
1:B:225:ARG:HH12	9:B:513:1PE:H161	1.62	0.65
1:A:177:ARG:NH1	1:B:190:ASP:OD2	2.31	0.64
1:B:73:ALA:HB1	1:B:168:THR:HG23	1.80	0.63
1:B:238:TYR:HE1	1:B:400:GLY:HA3	1.64	0.63
1:C:6:LEU:HD12	1:C:8:ARG:HH12	1.64	0.63
1:C:113:ALA:HA	1:C:330:ASN:HB3	1.81	0.62
1:B:238:TYR:CE1	1:B:400:GLY:HA3	2.34	0.62
3:A:504:DAS:OD2	3:A:504:DAS:N	2.32	0.62
1:C:358:VAL:HG13	1:C:359:PRO:HD2	1.82	0.61
1:C:314:MET:HB3	1:C:317:THR:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:OE1	1:A:175:GLU:N	2.30	0.61
1:B:254:LYS:NZ	8:B:509:P6G:O19	2.34	0.61
1:B:358:VAL:O	3:B:504:DAS:HA	2.01	0.61
6:A:509:DMU:O1	6:A:509:DMU:O55	2.16	0.60
1:B:157:ILE:HD11	1:B:307:PRO:HB2	1.84	0.60
1:A:247:ILE:O	1:A:251:ILE:HB	2.02	0.58
1:B:26:ALA:HA	1:B:219:MET:HG3	1.86	0.58
1:B:61:MET:HE1	1:B:153:VAL:CG2	2.33	0.58
1:C:171:MET:HE3	1:C:183:GLU:HA	1.86	0.58
1:A:211:VAL:HA	1:A:276:VAL:HG21	1.86	0.58
1:B:174:ASN:OD1	1:B:174:ASN:N	2.34	0.58
1:A:394:ASP:O	1:A:398:ASP:N	2.36	0.57
1:A:284:LEU:HD11	1:A:307:PRO:HA	1.84	0.57
1:B:101:PHE:HE2	1:B:248:THR:CG2	2.17	0.57
1:C:271:MET:O	1:C:403:MET:HG3	2.05	0.57
1:A:18:ILE:HG23	1:A:272:ILE:HD12	1.86	0.57
1:A:119:SER:HA	1:A:382:PRO:HG2	1.85	0.57
1:B:61:MET:HE1	1:B:153:VAL:HG23	1.87	0.57
1:C:238:TYR:HE1	1:C:400:GLY:HA3	1.70	0.57
1:A:101:PHE:CD1	1:A:104:ILE:HD11	2.40	0.56
1:C:370:LEU:HB3	1:C:375:LEU:HB2	1.87	0.56
1:C:418:LYS:NZ	1:C:425:GLU:OE2	2.31	0.56
1:A:150:LYS:HD2	1:A:152:GLU:OE2	2.05	0.56
1:B:90:TYR:CE2	1:B:412:GLY:HA3	2.41	0.56
1:C:238:TYR:CE1	1:C:400:GLY:HA3	2.40	0.56
1:A:61:MET:HE3	1:A:148:LEU:HD23	1.87	0.56
1:A:159:PHE:HD1	1:B:58:MET:HE2	1.70	0.55
1:C:329:ALA:HB2	1:C:375:LEU:HD11	1.88	0.55
7:B:511:PGE:H62	7:B:511:PGE:H1	1.87	0.55
1:B:314:MET:HB3	1:B:317:THR:HB	1.88	0.55
1:A:61:MET:HE1	1:A:156:VAL:HG21	1.88	0.55
1:C:95:SER:HB3	1:C:349:VAL:HG22	1.87	0.55
1:C:91:TYR:CG	1:C:313:ASN:HB2	2.41	0.55
1:B:196:MET:O	1:B:200:VAL:HG23	2.07	0.54
1:A:211:VAL:O	1:A:215:ILE:HG22	2.08	0.54
1:B:394:ASP:O	1:B:398:ASP:N	2.40	0.54
1:A:16:TRP:CD1	1:A:268:LYS:HZ2	2.26	0.54
1:A:152:GLU:O	1:A:155:PRO:HD2	2.07	0.53
1:C:161:ILE:HD11	1:C:304:PHE:CD1	2.43	0.53
1:A:68:LEU:HD21	1:A:161:ILE:HG13	1.90	0.53
1:B:278:ARG:HD2	1:B:398:ASP:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ALA:HA	1:B:370:LEU:HD12	1.90	0.53
1:C:317:THR:OG1	3:C:504:DAS:OD1	2.25	0.53
1:B:167:ILE:HG21	1:B:186:LEU:HB2	1.90	0.53
1:A:101:PHE:HD1	1:A:104:ILE:HD11	1.72	0.53
1:A:231:ALA:HB1	6:A:509:DMU:H36	1.90	0.52
1:A:269:ASP:O	1:A:273:THR:HG23	2.09	0.52
1:A:95:SER:HB3	1:A:349:VAL:HG22	1.91	0.52
1:B:222:GLN:HB2	1:B:396:ILE:HD13	1.91	0.52
1:C:325:VAL:HG12	1:C:336:LEU:HD11	1.91	0.52
1:B:357:GLY:CA	3:B:504:DAS:OXT	2.57	0.52
1:C:398:ASP:HA	1:C:401:ARG:HE	1.72	0.52
1:A:314:MET:HB3	1:A:317:THR:HB	1.91	0.52
1:A:317:THR:HA	1:A:401:ARG:HD3	1.92	0.51
1:B:19:LEU:HD13	1:B:272:ILE:HD11	1.93	0.51
1:C:284:LEU:HD11	1:C:307:PRO:HA	1.91	0.51
1:A:227:VAL:N	1:A:231:ALA:HB2	2.26	0.51
1:B:292:GLU:OE2	1:B:299:LYS:HE3	2.11	0.51
1:C:241:LEU:HB3	1:C:404:VAL:HG21	1.92	0.51
1:C:69:VAL:HG11	1:C:189:PHE:CD2	2.46	0.51
1:A:146:ALA:HB2	1:B:149:ALA:O	2.11	0.50
1:A:402:THR:HG23	3:A:504:DAS:C	2.41	0.50
1:C:15:LEU:HB2	1:C:268:LYS:HE3	1.92	0.50
1:C:152:GLU:C	1:C:155:PRO:HD2	2.36	0.50
1:C:193:ALA:O	1:C:197:TYR:HD2	1.94	0.50
1:A:161:ILE:HD11	1:A:304:PHE:CD1	2.46	0.50
1:C:279:SER:HB2	1:C:359:PRO:HD3	1.93	0.50
1:C:358:VAL:CG1	1:C:359:PRO:HD2	2.42	0.50
1:A:84:GLY:HA2	1:A:87:ILE:HG22	1.94	0.50
1:C:85:VAL:O	1:C:89:VAL:HG12	2.11	0.50
1:C:337:THR:HA	4:C:506:PEG:H41	1.93	0.49
1:B:68:LEU:HD21	1:B:161:ILE:HG13	1.94	0.49
1:C:6:LEU:HD12	1:C:8:ARG:NH1	2.25	0.49
1:C:398:ASP:OD1	3:C:504:DAS:N	2.45	0.49
1:C:141:PRO:HB3	1:C:155:PRO:HB3	1.94	0.49
1:C:242:PHE:O	1:C:246:VAL:HG22	2.11	0.49
1:B:245:ILE:HA	1:B:249:TYR:CD2	2.48	0.49
1:B:325:VAL:HG12	1:B:336:LEU:HD11	1.94	0.49
1:B:360:GLY:HA3	9:B:513:1PE:H221	1.93	0.49
1:A:226:VAL:C	1:A:231:ALA:HB2	2.38	0.48
1:A:316:GLY:C	1:A:401:ARG:HG2	2.38	0.48
1:B:397:LEU:O	1:B:401:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:TRP:HA	1:B:20:TRP:CE3	2.48	0.48
1:C:150:LYS:HD2	1:C:152:GLU:OE2	2.14	0.48
1:A:42:LYS:O	1:A:46:LYS:HB3	2.13	0.48
1:B:99:VAL:HG11	1:B:345:VAL:HA	1.96	0.48
1:C:103:LEU:HD13	1:C:341:GLN:HB3	1.95	0.48
1:C:167:ILE:HG21	1:C:186:LEU:HD13	1.94	0.48
1:C:314:MET:HG2	1:C:405:ASN:ND2	2.29	0.48
1:B:86:LYS:HZ2	1:B:420:GLU:HG2	1.79	0.48
1:B:141:PRO:HB3	1:B:155:PRO:HB3	1.94	0.48
1:A:69:VAL:HG11	1:A:189:PHE:CD2	2.49	0.47
1:B:242:PHE:CZ	1:B:246:VAL:HG21	2.49	0.47
1:C:99:VAL:HG11	1:C:345:VAL:HA	1.95	0.47
1:B:241:LEU:HD13	1:B:400:GLY:O	2.14	0.47
1:A:362:GLY:HA3	1:A:401:ARG:HH11	1.80	0.47
1:B:225:ARG:NH1	9:B:513:1PE:H161	2.29	0.47
1:C:22:LEU:HD22	1:C:272:ILE:HG23	1.96	0.47
1:C:148:LEU:HD23	1:C:156:VAL:HG21	1.97	0.47
1:A:333:GLY:C	1:A:335:PRO:HD3	2.40	0.47
1:B:84:GLY:HA2	1:B:87:ILE:HG22	1.96	0.47
1:C:166:ALA:O	1:C:170:LEU:HG	2.15	0.47
1:B:69:VAL:HG11	1:B:189:PHE:CD2	2.49	0.46
1:A:193:ALA:O	1:A:197:TYR:HD2	1.99	0.46
1:A:394:ASP:O	1:A:398:ASP:HB2	2.15	0.46
1:B:73:ALA:O	1:B:168:THR:HG21	2.15	0.46
1:C:12:TYR:HB3	1:C:17:LYS:HD3	1.95	0.46
1:B:167:ILE:HG22	1:B:171:MET:HE2	1.97	0.46
1:B:193:ALA:O	1:B:197:TYR:HD2	1.98	0.46
1:A:58:MET:HE1	1:C:158:PHE:CE1	2.39	0.46
1:A:317:THR:HA	1:A:401:ARG:CD	2.46	0.46
1:A:141:PRO:HG2	1:B:58:MET:HE3	1.98	0.46
1:B:79:ARG:O	1:B:83:VAL:N	2.33	0.46
1:C:6:LEU:HB2	1:C:8:ARG:HH12	1.81	0.46
1:A:200:VAL:O	1:A:204:MET:HG2	2.16	0.45
1:C:278:ARG:HD2	1:C:398:ASP:HB3	1.98	0.45
1:C:394:ASP:O	1:C:398:ASP:N	2.49	0.45
1:A:313:ASN:O	1:A:313:ASN:ND2	2.49	0.45
1:A:314:MET:HG2	1:A:405:ASN:ND2	2.31	0.45
1:C:9:TYR:O	1:C:10:LEU:HG	2.16	0.45
1:C:152:GLU:O	1:C:155:PRO:HD2	2.16	0.45
1:C:302:PHE:O	1:C:306:LEU:HB2	2.16	0.45
1:A:287:THR:HG22	1:A:410:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:LEU:H	1:C:230:LEU:HD22	1.82	0.45
1:C:284:LEU:HD21	1:C:310:ALA:HB2	1.99	0.45
1:A:292:GLU:OE1	1:A:299:LYS:HE3	2.17	0.45
6:A:509:DMU:H15	6:A:509:DMU:H20	1.63	0.45
1:C:173:ARG:HG3	1:C:178:VAL:HG11	1.99	0.45
1:B:363:ALA:HB2	1:B:394:ASP:OD1	2.18	0.44
1:B:418:LYS:NZ	1:B:425:GLU:OE2	2.28	0.44
1:C:42:LYS:HD2	1:C:217:TYR:HE1	1.82	0.44
1:A:152:GLU:OE2	4:A:507:PEG:H32	2.17	0.44
1:A:50:ASP:O	1:A:54:ARG:HG3	2.18	0.44
1:A:340:GLN:O	1:A:344:VAL:HG23	2.18	0.44
1:C:9:TYR:CG	1:C:10:LEU:N	2.85	0.44
1:C:358:VAL:O	3:C:504:DAS:HA	2.17	0.44
1:A:68:LEU:HD23	1:A:157:ILE:HA	1.98	0.44
1:B:42:LYS:HD2	1:B:217:TYR:HE1	1.82	0.44
1:B:166:ALA:HB1	1:C:198:LEU:HD23	2.00	0.44
1:C:268:LYS:O	1:C:272:ILE:HG12	2.18	0.44
1:A:46:LYS:HE3	1:A:50:ASP:OD2	2.18	0.43
1:A:68:LEU:HD13	1:A:303:SER:O	2.18	0.43
1:B:119:SER:HA	1:B:382:PRO:HG2	2.00	0.43
1:C:312:ILE:HB	1:C:353:ILE:HG23	2.00	0.43
1:A:152:GLU:C	1:A:155:PRO:HD2	2.43	0.43
1:B:211:VAL:HG22	1:B:276:VAL:HG21	2.00	0.43
1:A:198:LEU:HD23	1:C:166:ALA:HB1	2.00	0.43
1:C:245:ILE:HA	1:C:249:TYR:CD2	2.53	0.43
1:B:217:TYR:HE2	9:B:513:1PE:H142	1.83	0.43
1:B:365:MET:HE3	1:B:365:MET:HB3	1.85	0.43
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.83	0.43
1:B:81:GLY:O	1:B:85:VAL:HG23	2.19	0.43
1:B:68:LEU:HD13	1:B:303:SER:O	2.18	0.43
1:B:336:LEU:HD21	1:B:373:VAL:HG21	2.00	0.43
1:B:86:LYS:NZ	1:B:420:GLU:HG2	2.34	0.43
1:B:115:VAL:HG12	1:B:117:LEU:HG	2.00	0.43
1:B:333:GLY:C	1:B:335:PRO:HD3	2.43	0.43
1:C:152:GLU:HB3	1:C:155:PRO:HG2	1.99	0.43
1:A:226:VAL:HG13	1:A:231:ALA:HA	2.00	0.42
1:A:306:LEU:HD21	1:A:410:LEU:HD23	2.00	0.42
1:B:135:THR:O	1:B:138:ASN:HB2	2.20	0.42
1:B:159:PHE:CD1	1:C:58:MET:HE2	2.45	0.42
1:B:406:VAL:O	1:B:409:ASP:N	2.52	0.42
1:B:429:ILE:HD13	1:B:429:ILE:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ASN:ND2	3:A:504:DAS:OXT	2.50	0.42
1:B:100:PHE:CZ	1:B:104:ILE:HD11	2.53	0.42
1:B:222:GLN:NE2	9:B:513:1PE:H251	2.34	0.42
8:B:510:P6G:H61	8:B:510:P6G:H122	2.00	0.42
1:A:79:ARG:HH21	1:A:420:GLU:HB3	1.84	0.42
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.75	0.42
1:C:429:ILE:HG13	1:C:430:SER:H	1.83	0.42
1:A:167:ILE:HG21	1:A:186:LEU:HB2	2.01	0.42
1:C:139:ILE:O	1:C:155:PRO:HA	2.20	0.42
1:A:317:THR:OG1	3:A:504:DAS:OD1	2.37	0.42
7:A:510:PGE:H1	7:A:510:PGE:H3	1.71	0.42
1:C:230:LEU:HB3	1:C:393:ILE:HD13	2.02	0.42
1:A:12:TYR:HB3	1:A:17:LYS:HD3	2.02	0.42
1:B:181:SER:O	1:B:184:THR:HB	2.20	0.42
1:A:38:ALA:HB1	1:A:221:GLU:OE2	2.20	0.42
1:A:403:MET:HE2	1:A:403:MET:HB3	1.96	0.41
6:A:509:DMU:H9	6:A:509:DMU:H29	2.02	0.41
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.66	0.41
1:C:50:ASP:O	1:C:54:ARG:HG3	2.20	0.41
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.73	0.41
1:A:245:ILE:HA	1:A:249:TYR:CD2	2.55	0.41
1:B:211:VAL:HA	1:B:276:VAL:HG21	2.03	0.41
1:A:42:LYS:HA	1:A:46:LYS:HB2	2.02	0.41
1:A:45:ILE:O	1:A:213:ALA:HB1	2.21	0.41
1:A:297:VAL:HG21	1:A:413:THR:HG22	2.02	0.41
1:A:362:GLY:HA3	1:A:401:ARG:NH1	2.36	0.41
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.72	0.41
1:A:274:ALA:HA	1:A:283:THR:HG21	2.03	0.41
1:A:275:PHE:CZ	1:A:399:MET:HE3	2.55	0.41
1:C:403:MET:HE2	1:C:403:MET:HB3	1.89	0.41
1:A:241:LEU:HD13	1:A:400:GLY:O	2.21	0.40
1:A:139:ILE:O	1:A:155:PRO:HA	2.21	0.40
1:A:152:GLU:OE1	4:A:507:PEG:H32	2.21	0.40
1:B:291:ALA:HB2	1:B:306:LEU:HD11	2.03	0.40
1:C:136:LEU:HD23	1:C:136:LEU:HA	1.65	0.40
1:A:234:VAL:HA	1:A:397:LEU:HD21	2.02	0.40
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.83	0.40
1:A:268:LYS:HA	1:A:271:MET:HE2	2.03	0.40
1:A:302:PHE:O	1:A:306:LEU:HB2	2.21	0.40
1:B:45:ILE:O	1:B:213:ALA:HB1	2.22	0.40
1:B:211:VAL:O	1:B:215:ILE:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:HB2	1:C:182:ALA:HB2	2.04	0.40
1:C:363:ALA:O	1:C:366:LEU:HB3	2.21	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	414/438 (94%)	393 (95%)	21 (5%)	0	100	100
1	B	402/438 (92%)	385 (96%)	17 (4%)	0	100	100
1	C	418/438 (95%)	397 (95%)	21 (5%)	0	100	100
All	All	1234/1314 (94%)	1175 (95%)	59 (5%)	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	327/345 (95%)	314 (96%)	13 (4%)	28	63
1	B	316/345 (92%)	306 (97%)	10 (3%)	34	70
1	C	332/345 (96%)	326 (98%)	6 (2%)	51	82
All	All	975/1035 (94%)	946 (97%)	29 (3%)	37	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TRP
1	A	70	VAL
1	A	94	THR
1	A	104	ILE
1	A	105	VAL
1	A	108	LEU
1	A	135	THR
1	A	224	VAL
1	A	255	VAL
1	A	325	VAL
1	A	342	LEU
1	A	368[A]	MET
1	A	368[B]	MET
1	B	20	TRP
1	B	70	VAL
1	B	108	LEU
1	B	111	VAL
1	B	174	ASN
1	B	175	GLU
1	B	342	LEU
1	B	358	VAL
1	B	396	ILE
1	B	429	ILE
1	C	3	LYS
1	C	6	LEU
1	C	8	ARG
1	C	111	VAL
1	C	135	THR
1	C	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	C	116	ASN

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 32 ligands modelled in this entry, 9 are monoatomic - leaving 23 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	$\# Z > 2$
4	PEG	C	509	-	6,6,6	0.59	0	5,5,5	0.54	0
3	DAS	A	504	-	7,8,8	1.03	0	6,10,10	1.65	1 (16%)
8	P6G	B	509	-	18,18,18	0.56	0	17,17,17	0.28	0
4	PEG	B	506	-	6,6,6	0.51	0	5,5,5	0.33	0
4	PEG	B	505	-	6,6,6	0.52	0	5,5,5	0.40	0
3	DAS	C	504	-	7,8,8	1.01	0	6,10,10	1.46	1 (16%)
4	PEG	C	507	-	6,6,6	0.53	0	5,5,5	0.39	0
5	PG4	A	508	-	12,12,12	0.57	0	11,11,11	0.42	0
4	PEG	C	508	-	6,6,6	0.54	0	5,5,5	0.48	0
4	PEG	A	505	-	6,6,6	0.54	0	5,5,5	0.32	0
6	DMU	A	509	-	34,34,34	1.61	7 (20%)	45,45,45	1.32	6 (13%)
4	PEG	A	507	-	6,6,6	0.55	0	5,5,5	0.68	0
7	PGE	B	511	-	9,9,9	0.55	0	8,8,8	0.78	0
8	P6G	B	510	-	18,18,18	0.59	0	17,17,17	0.42	0
4	PEG	B	507	-	6,6,6	0.58	0	5,5,5	0.69	0
4	PEG	C	506	-	6,6,6	0.49	0	5,5,5	0.34	0
4	PEG	B	508	-	6,6,6	0.55	0	5,5,5	0.37	0
4	PEG	A	506	-	6,6,6	0.54	0	5,5,5	0.27	0
3	DAS	B	504	-	7,8,8	1.08	0	6,10,10	0.90	0
7	PGE	B	512	-	9,9,9	0.41	0	8,8,8	0.25	0
7	PGE	A	510	-	9,9,9	0.51	0	8,8,8	0.47	0
9	1PE	B	513	-	15,15,15	0.55	0	14,14,14	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PEG	C	505	-	6,6,6	0.56	0	5,5,5	0.54	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	PEG	C	509	-	-	2/4/4/4	-
3	DAS	A	504	-	-	4/8/8/8	-
8	P6G	B	509	-	-	9/16/16/16	-
4	PEG	B	506	-	-	1/4/4/4	-
4	PEG	B	505	-	-	3/4/4/4	-
3	DAS	C	504	-	-	5/8/8/8	-
4	PEG	C	507	-	-	2/4/4/4	-
5	PG4	A	508	-	-	4/10/10/10	-
4	PEG	C	508	-	-	3/4/4/4	-
4	PEG	A	505	-	-	2/4/4/4	-
6	DMU	A	509	-	-	13/19/59/59	0/2/2/2
4	PEG	A	507	-	-	3/4/4/4	-
7	PGE	B	511	-	-	2/7/7/7	-
8	P6G	B	510	-	-	8/16/16/16	-
4	PEG	B	507	-	-	1/4/4/4	-
4	PEG	C	506	-	-	1/4/4/4	-
4	PEG	B	508	-	-	1/4/4/4	-
4	PEG	A	506	-	-	3/4/4/4	-
3	DAS	B	504	-	-	4/8/8/8	-
7	PGE	B	512	-	-	4/7/7/7	-
7	PGE	A	510	-	-	3/7/7/7	-
9	1PE	B	513	-	-	8/13/13/13	-
4	PEG	C	505	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	DMU	O1-C9	4.48	1.55	1.44
6	A	509	DMU	C11-C9	-3.26	1.40	1.51
6	A	509	DMU	O5-C6	2.99	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	DMU	O5-C4	2.56	1.50	1.44
6	A	509	DMU	C8-C9	2.32	1.58	1.53
6	A	509	DMU	O4-C7	2.31	1.48	1.43
6	A	509	DMU	O1-C10	2.31	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	504	DAS	OXT-C-O	-3.64	115.81	124.08
6	A	509	DMU	O5-C4-C3	3.43	116.81	109.72
6	A	509	DMU	C6-O5-C4	3.04	119.66	113.72
6	A	509	DMU	O7-C3-C2	2.98	114.80	107.23
3	C	504	DAS	OXT-C-O	-2.85	117.60	124.08
6	A	509	DMU	O7-C10-C5	2.65	114.62	108.09
6	A	509	DMU	O7-C3-C4	-2.33	103.36	109.48
6	A	509	DMU	O5-C6-C1	2.05	114.59	110.37

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	DAS	O-C-CA-N
3	A	504	DAS	N-CA-CB-CG
3	A	504	DAS	C-CA-CB-CG
3	B	504	DAS	N-CA-CB-CG
3	B	504	DAS	C-CA-CB-CG
3	C	504	DAS	N-CA-CB-CG
6	A	509	DMU	O1-C10-O7-C3
6	A	509	DMU	O5-C4-C57-O61
7	A	510	PGE	C1-C2-O2-C3
8	B	509	P6G	O13-C14-C15-O16
9	B	513	1PE	OH5-C14-C24-OH4
3	C	504	DAS	OXT-C-CA-N
8	B	510	P6G	O7-C8-C9-O10
4	B	505	PEG	O2-C3-C4-O4
7	B	512	PGE	O2-C3-C4-O3
8	B	509	P6G	C9-C8-O7-C6
3	A	504	DAS	OXT-C-CA-N
8	B	509	P6G	O4-C5-C6-O7
4	A	506	PEG	O2-C3-C4-O4
4	A	507	PEG	O1-C1-C2-O2
8	B	509	P6G	O16-C17-C18-O19

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Mol	Chain	Res	Type	Atoms
4	B	505	PEG	O1-C1-C2-O2
4	B	506	PEG	O2-C3-C4-O4
4	C	505	PEG	O1-C1-C2-O2
4	C	509	PEG	O1-C1-C2-O2
7	B	512	PGE	O3-C5-C6-O4
8	B	510	P6G	O1-C2-C3-O4
9	B	513	1PE	OH2-C12-C22-OH3
8	B	509	P6G	C18-C17-O16-C15
9	B	513	1PE	OH6-C15-C25-OH5
6	A	509	DMU	C5-C10-O7-C3
4	A	507	PEG	O2-C3-C4-O4
4	C	507	PEG	O1-C1-C2-O2
4	C	507	PEG	C4-C3-O2-C2
5	A	508	PG4	O4-C7-C8-O5
3	C	504	DAS	C-CA-CB-CG
6	A	509	DMU	C22-C25-C28-C31
6	A	509	DMU	O16-C18-C19-C22
8	B	510	P6G	O13-C14-C15-O16
5	A	508	PG4	O3-C5-C6-O4
6	A	509	DMU	C18-C19-C22-C25
6	A	509	DMU	C25-C28-C31-C34
4	B	508	PEG	O2-C3-C4-O4
6	A	509	DMU	C4-C3-O7-C10
6	A	509	DMU	C28-C31-C34-C37
6	A	509	DMU	C2-C3-O7-C10
4	B	507	PEG	O2-C3-C4-O4
4	C	508	PEG	O2-C3-C4-O4
8	B	510	P6G	C9-C8-O7-C6
4	C	506	PEG	C1-C2-O2-C3
9	B	513	1PE	C12-C22-OH3-C23
4	C	508	PEG	C1-C2-O2-C3
7	B	511	PGE	C1-C2-O2-C3
7	B	511	PGE	C4-C3-O2-C2
8	B	510	P6G	C6-C5-O4-C3
4	A	505	PEG	O1-C1-C2-O2
4	A	505	PEG	O2-C3-C4-O4
4	C	505	PEG	O2-C3-C4-O4
4	C	508	PEG	O1-C1-C2-O2
7	B	512	PGE	O1-C1-C2-O2
9	B	513	1PE	C23-C13-OH4-C24
4	B	505	PEG	C1-C2-O2-C3
5	A	508	PG4	C3-C4-O3-C5

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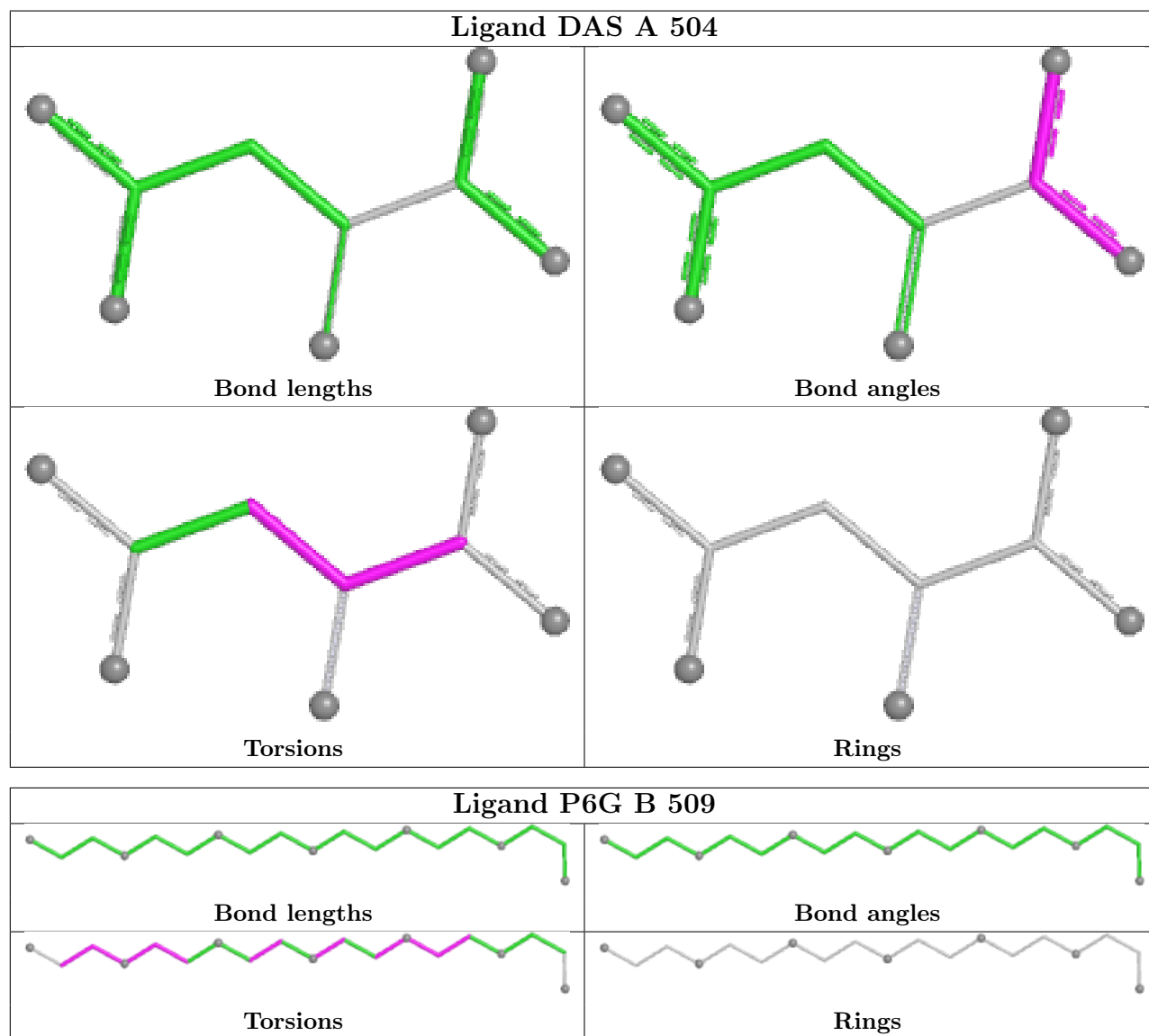
Mol	Chain	Res	Type	Atoms
9	B	513	1PE	C13-C23-OH3-C22
6	A	509	DMU	C19-C18-O16-C6
8	B	509	P6G	C14-C15-O16-C17
8	B	509	P6G	O10-C11-C12-O13
9	B	513	1PE	C15-C25-OH5-C14
7	A	510	PGE	C3-C4-O3-C5
7	B	512	PGE	C3-C4-O3-C5
5	A	508	PG4	C5-C6-O4-C7
8	B	510	P6G	C8-C9-O10-C11
6	A	509	DMU	C3-C4-C57-O61
9	B	513	1PE	C25-C15-OH6-C26
4	A	506	PEG	C1-C2-O2-C3
8	B	510	P6G	C2-C3-O4-C5
4	A	507	PEG	C1-C2-O2-C3
3	B	504	DAS	CA-CB-CG-OD1
3	B	504	DAS	OXT-C-CA-N
8	B	510	P6G	O10-C11-C12-O13
4	A	506	PEG	O1-C1-C2-O2
8	B	509	P6G	C5-C6-O7-C8
3	C	504	DAS	CA-CB-CG-OD1
6	A	509	DMU	O6-C11-C9-O1
7	A	510	PGE	O3-C5-C6-O4
4	C	509	PEG	C1-C2-O2-C3
3	C	504	DAS	O-C-CA-N
8	B	509	P6G	C8-C9-O10-C11

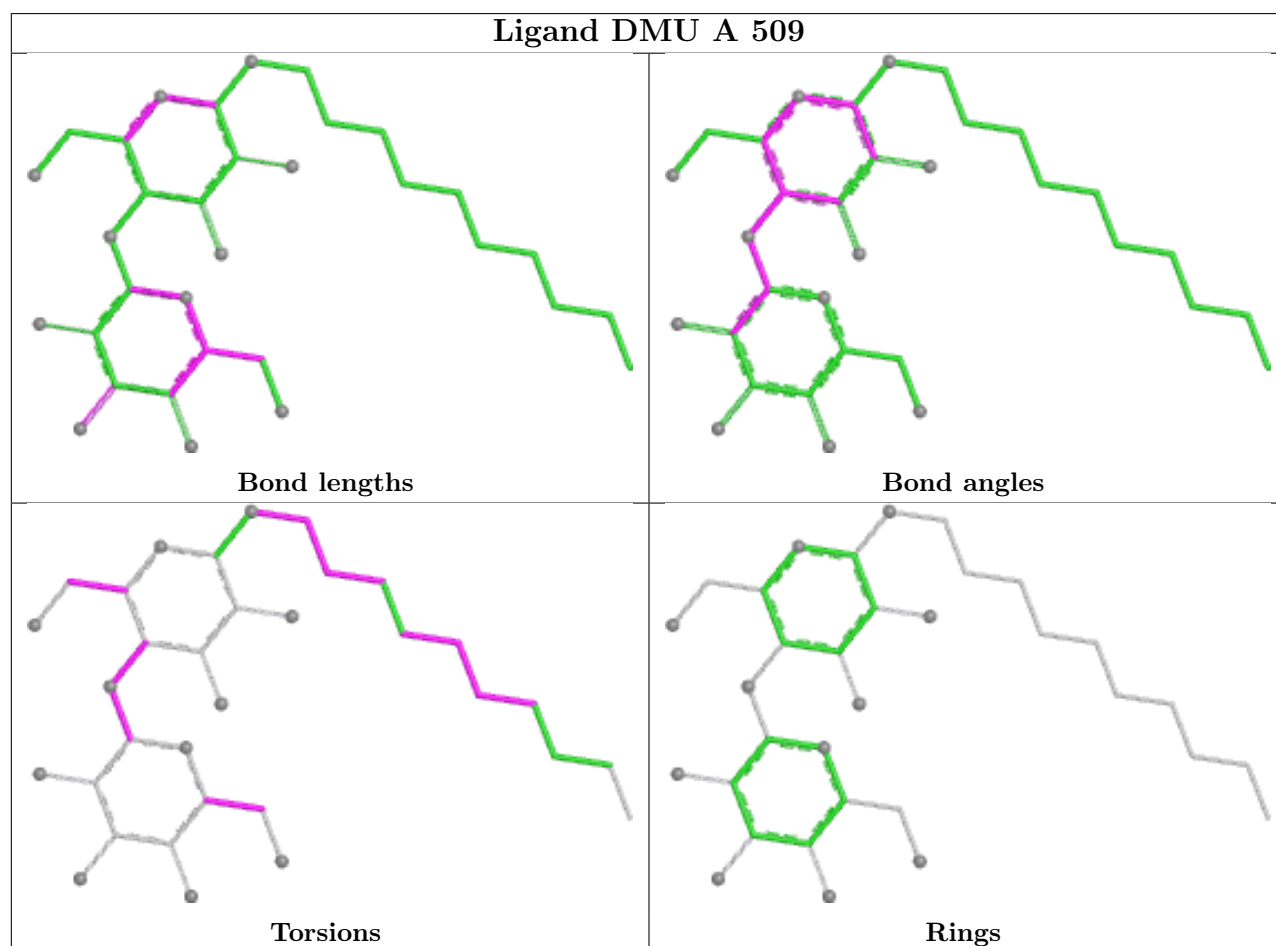
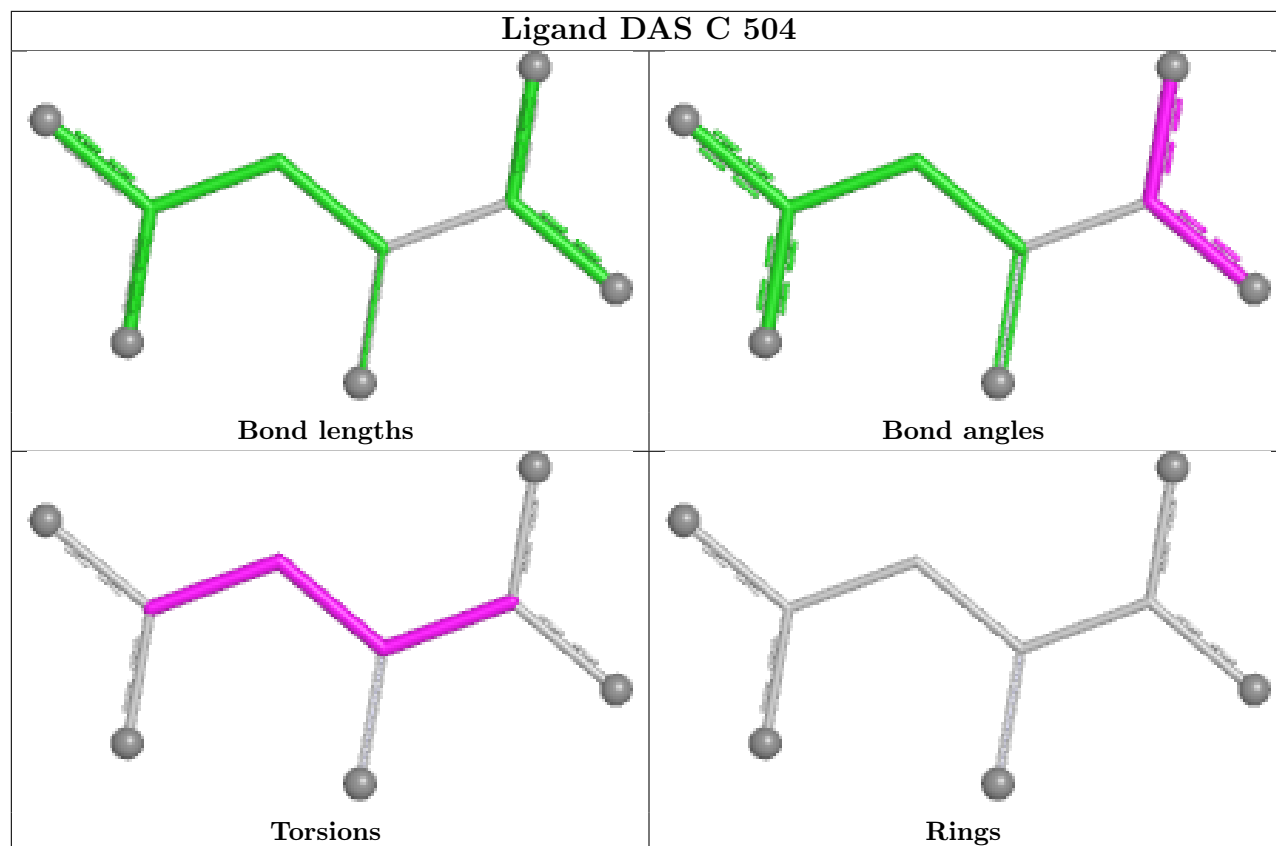
There are no ring outliers.

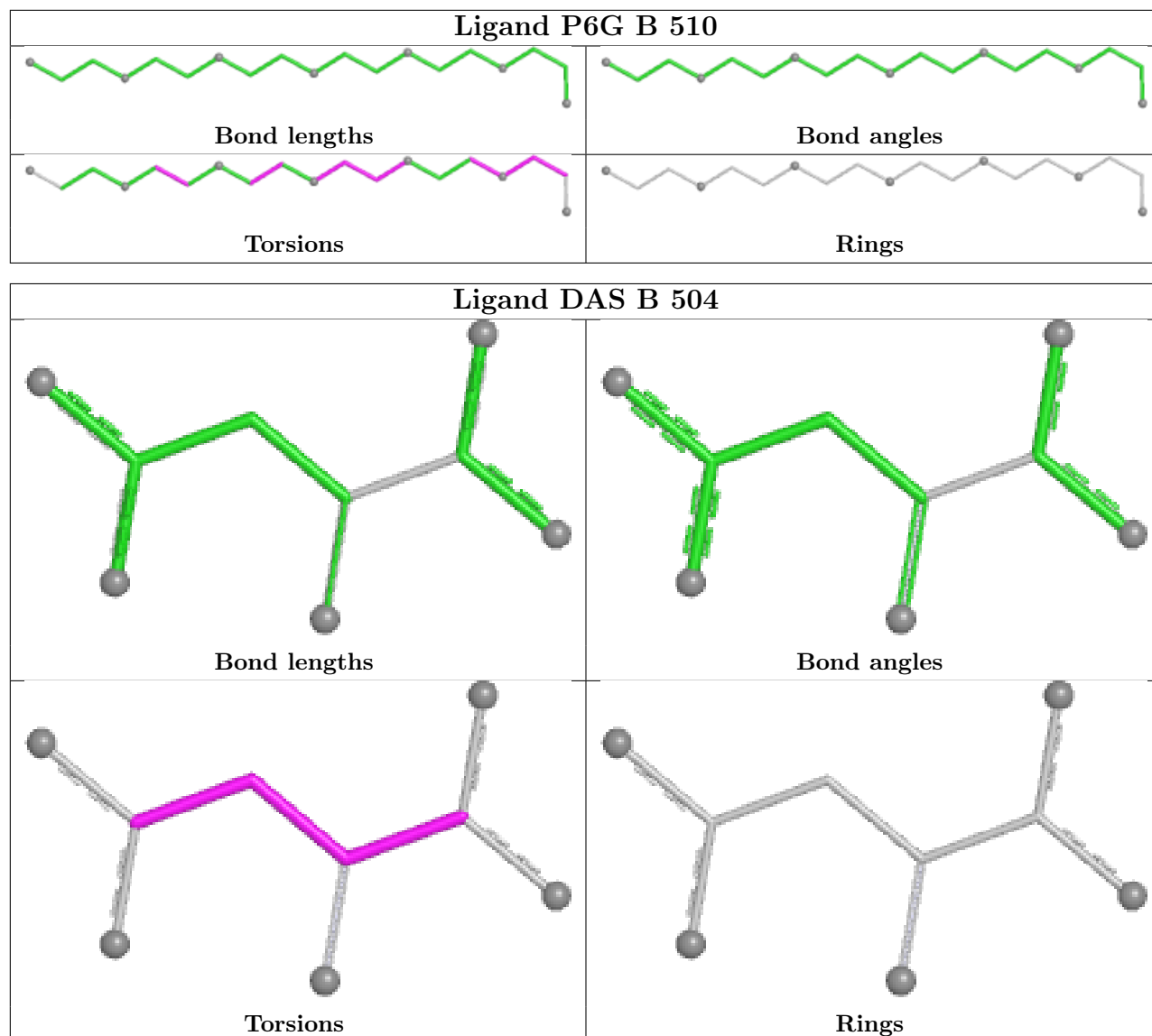
11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	DAS	4	0
8	B	509	P6G	1	0
3	C	504	DAS	3	0
6	A	509	DMU	4	0
4	A	507	PEG	2	0
7	B	511	PGE	1	0
8	B	510	P6G	1	0
4	C	506	PEG	1	0
3	B	504	DAS	3	0
7	A	510	PGE	1	0
9	B	513	1PE	5	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	416/438 (94%)	1.01	90 (21%) 2 2	54, 115, 169, 258	2 (0%)
1	B	406/438 (92%)	0.61	54 (13%) 7 5	84, 123, 166, 249	0
1	C	422/438 (96%)	0.51	50 (11%) 9 7	78, 132, 193, 278	0
All	All	1244/1314 (94%)	0.71	194 (15%) 5 4	54, 123, 177, 278	2 (0%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	375	LEU	10.1
1	A	326	LEU	8.5
1	A	84	GLY	7.8
1	A	15	LEU	7.5
1	A	324	THR	7.4
1	C	382	PRO	6.9
1	A	375	LEU	6.8
1	B	371	GLN	6.8
1	A	111	VAL	6.7
1	B	385	LEU	6.5
1	A	327	PHE	6.4
1	B	374	GLY	6.4
1	A	325	VAL	6.2
1	A	14	VAL	6.1
1	B	373	VAL	6.0
1	A	287	THR	6.0
1	C	376	ASP	6.0
1	A	386	ALA	6.0
1	A	385	LEU	6.0
1	C	375	LEU	5.9
1	A	383	VAL	5.8
1	A	387	TYR	5.8
1	A	384	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	5.8
1	A	376	ASP	5.7
1	A	328	VAL	5.7
1	B	383	VAL	5.5
1	C	227	VAL	5.5
1	C	118	GLY	5.4
1	C	188	VAL	5.4
1	B	159	PHE	5.3
1	A	85	VAL	5.2
1	A	189	PHE	5.2
1	B	332	ILE	5.2
1	A	269	ASP	5.1
1	B	188	VAL	5.1
1	C	421	LYS	5.0
1	B	382	PRO	5.0
1	B	376	ASP	5.0
1	A	389	MET	5.0
1	A	373	VAL	5.0
1	A	374	GLY	5.0
1	C	15	LEU	4.9
1	B	19	LEU	4.8
1	B	185	LEU	4.8
1	C	385	LEU	4.8
1	C	383	VAL	4.7
1	A	273	THR	4.7
1	B	189	PHE	4.7
1	C	117	LEU	4.6
1	A	370	LEU	4.6
1	B	328	VAL	4.6
1	A	284	LEU	4.5
1	C	100	PHE	4.5
1	C	378	THR	4.4
1	B	333	GLY	4.4
1	C	116	ASN	4.3
1	A	81	GLY	4.2
1	C	423	LEU	4.2
1	B	48	PHE	4.1
1	B	386	ALA	4.1
1	A	332	ILE	4.1
1	B	329	ALA	4.1
1	C	3	LYS	4.0
1	B	287	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	163	LEU	4.0
1	A	283	THR	3.9
1	A	340	GLN	3.9
1	A	192	LEU	3.9
1	A	86	LYS	3.8
1	B	340	GLN	3.8
1	A	82	ARG	3.7
1	A	270	ALA	3.7
1	C	115	VAL	3.7
1	A	109	PHE	3.7
1	C	191	GLY	3.7
1	B	144	PRO	3.6
1	B	160	ALA	3.5
1	A	336	LEU	3.5
1	A	431	HIS	3.5
1	A	372	SER	3.5
1	A	313	ASN	3.5
1	C	34	HIS	3.5
1	C	189	PHE	3.4
1	A	381	SER	3.4
1	C	422	GLU	3.4
1	A	368[A]	MET	3.4
1	B	335	PRO	3.4
1	A	408	GLY	3.3
1	A	285	PRO	3.3
1	C	192	LEU	3.3
1	A	382	PRO	3.3
1	A	34[A]	HIS	3.3
1	C	379	PRO	3.3
1	B	45	ILE	3.3
1	C	420	GLU	3.2
1	B	18	ILE	3.2
1	B	370	LEU	3.2
1	A	159	PHE	3.2
1	A	416	VAL	3.2
1	A	281	SER	3.2
1	A	83	VAL	3.1
1	B	384	ALA	3.1
1	A	130	PRO	3.1
1	B	269	ASP	3.1
1	A	331	ALA	3.0
1	C	381	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	377	LEU	3.0
1	C	202	GLY	2.9
1	B	47	PRO	2.9
1	A	378	THR	2.9
1	C	196	MET	2.9
1	A	323	VAL	2.9
1	B	334	HIS	2.9
1	C	284	LEU	2.9
1	A	286	VAL	2.8
1	B	85	VAL	2.8
1	C	354	GLY	2.8
1	A	390	ILE	2.8
1	A	112	GLY	2.8
1	A	341	GLN	2.8
1	A	419	THR	2.8
1	C	256	PHE	2.7
1	B	162	ILE	2.7
1	B	174	ASN	2.7
1	A	122	GLY	2.7
1	C	9	TYR	2.7
1	B	33	GLY	2.7
1	A	403	MET	2.6
1	A	185	LEU	2.6
1	A	290	VAL	2.6
1	A	57	LYS	2.6
1	B	421	LYS	2.6
1	C	76	SER	2.6
1	A	304	PHE	2.6
1	A	201	GLY	2.5
1	B	336	LEU	2.5
1	C	130	PRO	2.5
1	B	372	SER	2.5
1	A	132	LEU	2.5
1	C	377	LEU	2.5
1	B	167	ILE	2.5
1	A	274	ALA	2.5
1	A	429	ILE	2.5
1	C	75	ILE	2.5
1	A	330	ASN	2.5
1	C	230	LEU	2.4
1	B	117	LEU	2.4
1	A	282	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	328	VAL	2.4
1	A	52	PHE	2.4
1	B	122	GLY	2.3
1	C	101	PHE	2.3
1	C	261	ILE	2.3
1	B	381	SER	2.3
1	A	198	LEU	2.3
1	A	56	LEU	2.3
1	A	344	VAL	2.3
1	A	196	MET	2.2
1	A	53	VAL	2.2
1	A	108	LEU	2.2
1	B	194	GLU	2.2
1	C	180	LYS	2.2
1	C	374	GLY	2.2
1	A	121	THR	2.2
1	C	16	TRP	2.2
1	A	110	ASN	2.2
1	B	64	VAL	2.2
1	A	322	GLY	2.2
1	C	132	LEU	2.2
1	C	265	ARG	2.1
1	B	121	THR	2.1
1	A	310	ALA	2.1
1	B	182	ALA	2.1
1	A	261	ILE	2.1
1	B	414	VAL	2.1
1	C	145	PHE	2.1
1	A	217	TYR	2.1
1	C	389	MET	2.1
1	A	65	LEU	2.1
1	A	80	LEU	2.1
1	A	407	THR	2.1
1	A	247	ILE	2.1
1	B	331	ALA	2.1
1	C	165	ILE	2.1
1	B	389	MET	2.0
1	B	284	LEU	2.0
1	C	52	PHE	2.0
1	C	419	THR	2.0
1	C	418	LYS	2.0
1	B	229	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	379	PRO	2.0
1	B	378	THR	2.0
1	A	343	VAL	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.

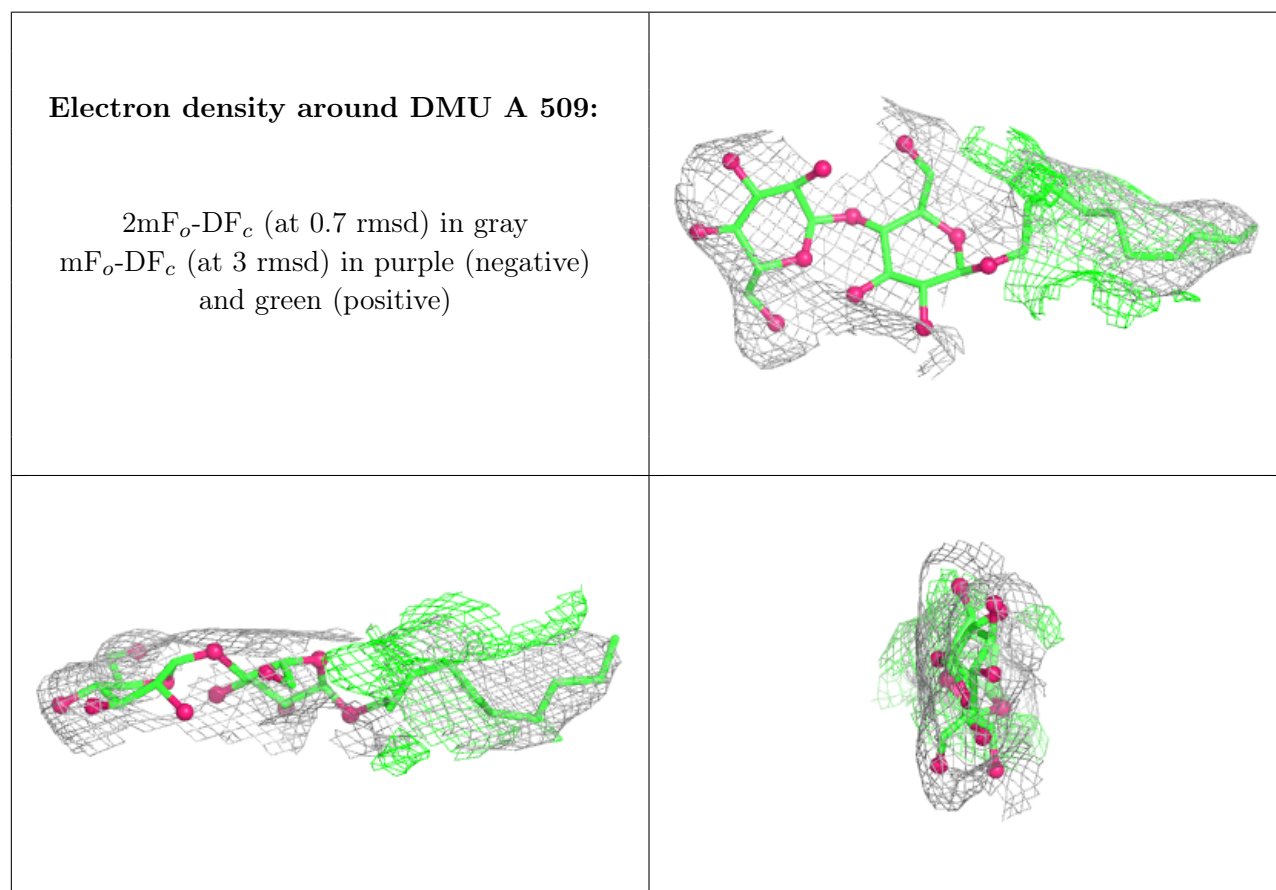
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PEG	C	509	7/7	0.62	0.16	125,149,163,166	0
7	PGE	B	512	10/10	0.64	0.14	109,151,160,160	0
6	DMU	A	509	33/33	0.66	0.21	123,181,192,193	0
4	PEG	B	505	7/7	0.66	0.24	135,144,149,154	0
4	PEG	B	506	7/7	0.72	0.20	141,149,154,156	0
8	P6G	B	509	19/19	0.75	0.12	152,176,191,192	0
4	PEG	C	506	7/7	0.78	0.12	134,141,144,146	0
4	PEG	B	507	7/7	0.79	0.17	114,128,141,147	0
8	P6G	B	510	19/19	0.79	0.22	96,156,170,172	0
4	PEG	A	505	7/7	0.81	0.15	134,145,154,155	0
4	PEG	C	508	7/7	0.82	0.20	134,144,153,158	0
5	PG4	A	508	13/13	0.83	0.18	136,146,158,162	0
4	PEG	A	506	7/7	0.85	0.25	128,143,159,161	0
4	PEG	B	508	7/7	0.85	0.16	125,140,143,145	0
3	DAS	B	504	9/9	0.86	0.10	100,111,114,116	0
4	PEG	C	505	7/7	0.89	0.21	99,102,119,129	0
2	NA	A	503	1/1	0.90	0.17	120,120,120,120	0
4	PEG	A	507	7/7	0.90	0.12	106,127,145,147	0
7	PGE	A	510	10/10	0.90	0.16	98,119,134,135	0
9	1PE	B	513	16/16	0.91	0.16	106,153,158,161	0

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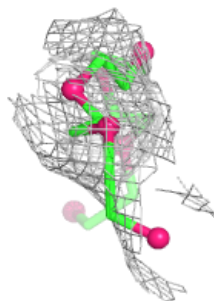
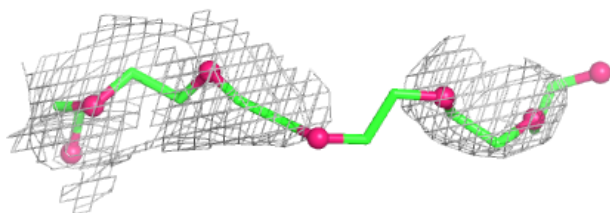
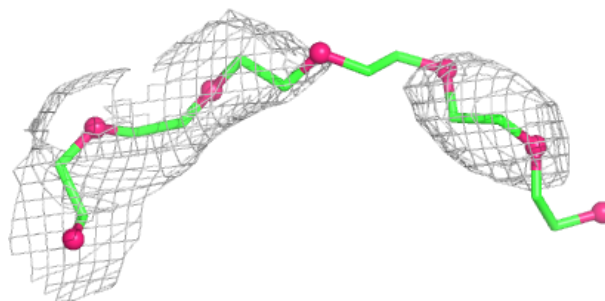
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PGE	B	511	10/10	0.92	0.31	125,150,171,172	0
4	PEG	C	507	7/7	0.93	0.17	124,140,152,155	0
3	DAS	C	504	9/9	0.94	0.07	101,116,127,129	0
3	DAS	A	504	9/9	0.94	0.06	101,112,123,129	0
2	NA	B	502	1/1	0.94	0.08	98,98,98,98	0
2	NA	B	503	1/1	0.95	0.07	142,142,142,142	0
2	NA	A	501	1/1	0.95	0.12	103,103,103,103	0
2	NA	C	503	1/1	0.96	0.06	109,109,109,109	0
2	NA	C	501	1/1	0.97	0.09	111,111,111,111	0
2	NA	C	502	1/1	0.97	0.06	102,102,102,102	0
2	NA	A	502	1/1	0.98	0.06	96,96,96,96	0
2	NA	B	501	1/1	0.98	0.06	169,169,169,169	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.

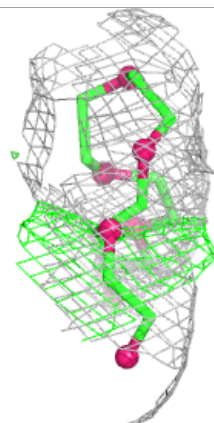
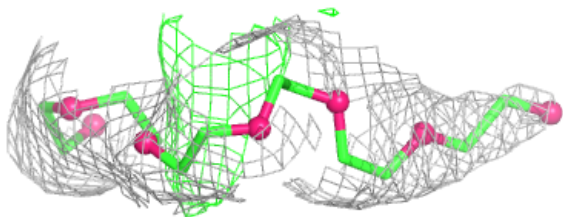
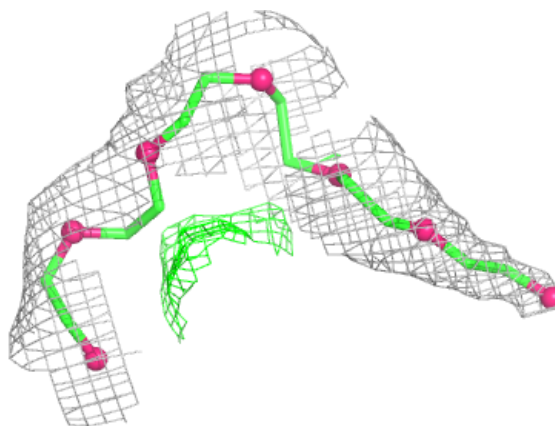


Electron density around P6G B 509:

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

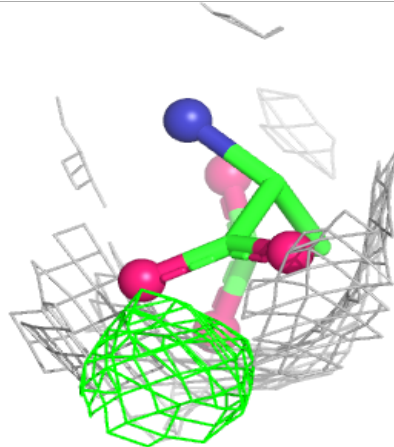
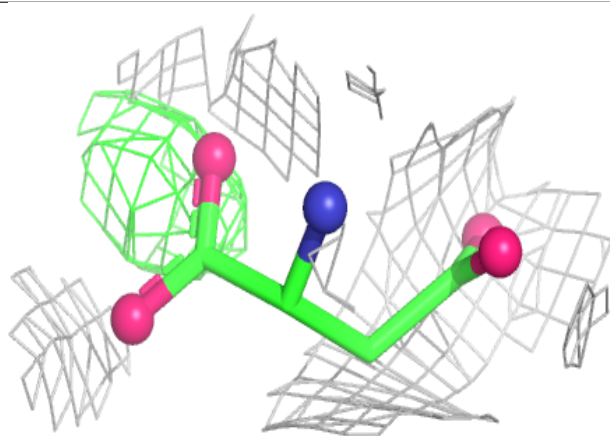
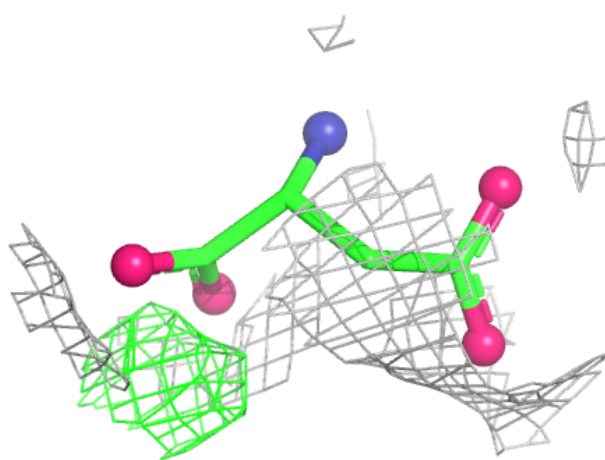
**Electron density around P6G B 510:**

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



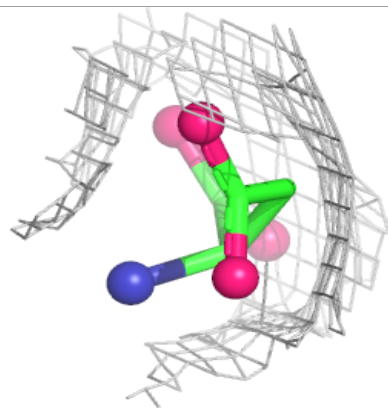
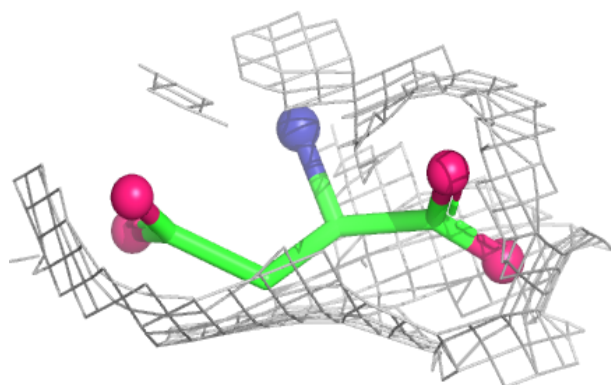
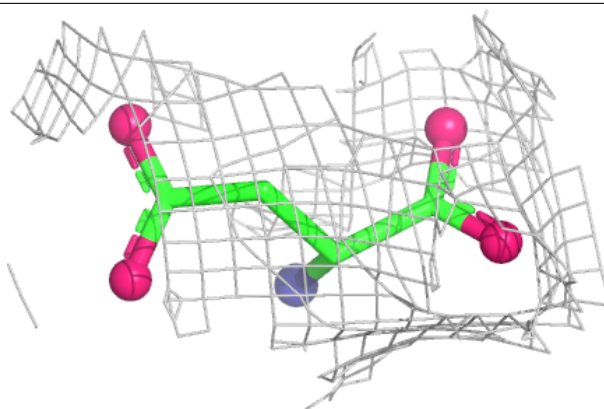
Electron density around DAS B 504:

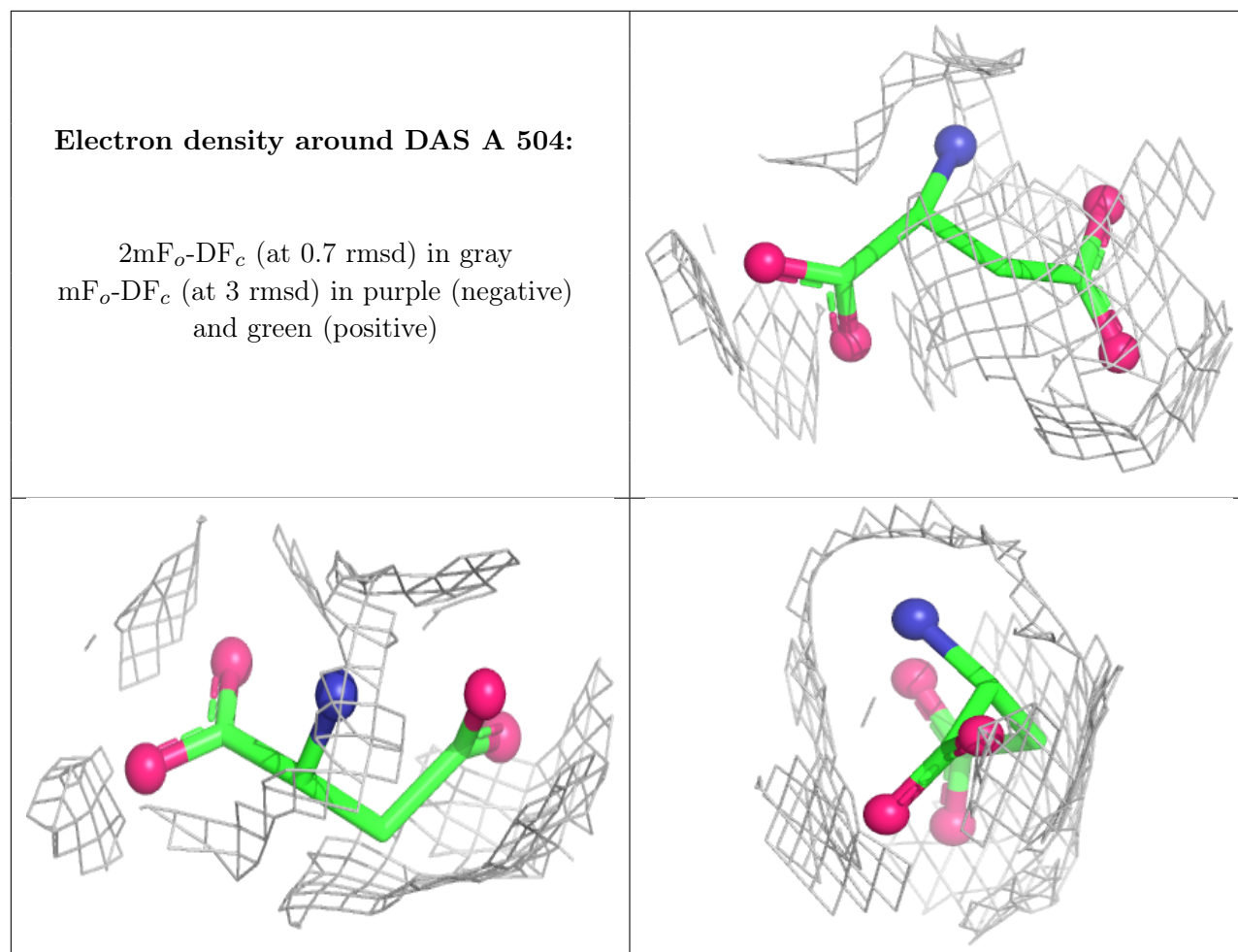
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DAS C 504:

$2mF_o-DF_c$ (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.