



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:13 am BST

PDB ID : 6R7R
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

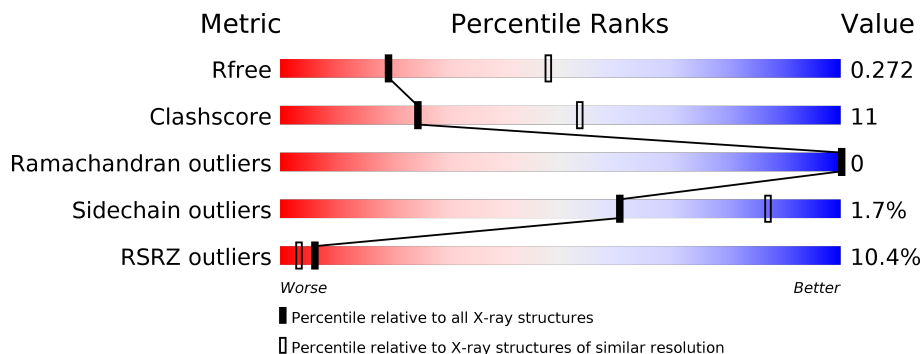
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	438	 10% 72% 23% • 5%
1	B	438	 8% 70% 22% • 7%
1	C	438	 11% 74% 22% • •

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	-
4	PEG	B	505	-	-	-	X
4	PEG	C	505	-	-	-	X
7	PGE	B	511	-	-	-	X
8	P6G	B	509	-	-	-	X

2 Entry composition i

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
			Total	C	N	O	S			
1	A	416	Total 3109	C 2051	N 503	O 538	S 17	0	2	0
1	B	406	Total 3005	C 1980	N 485	O 524	S 16	0	0	0
1	C	422	Total 3148	C 2078	N 509	O 545	S 16	0	0	0

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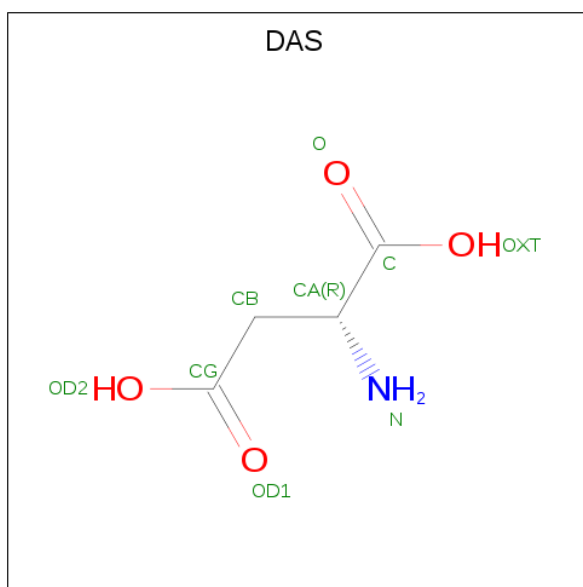
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Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	expression tag	UNP Q5JID0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is D-ASPARTIC ACID (three-letter code: DAS) (formula: C₄H₇NO₄) (labeled as "Ligand of Interest" by author).



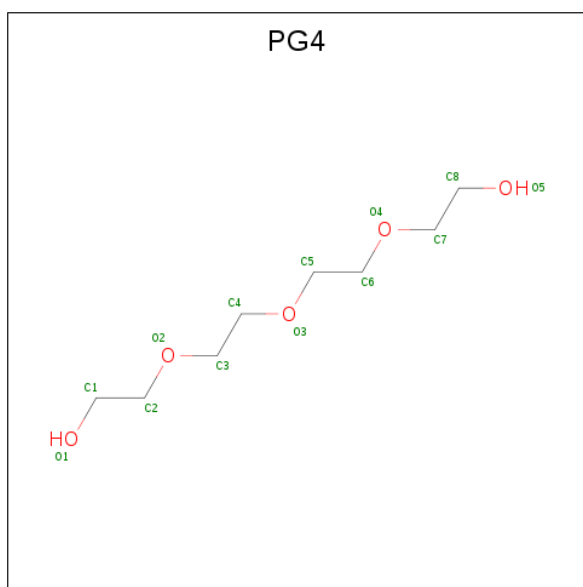
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 4 1 4	0	0
3	B	1	Total C N O 9 4 1 4	0	0
3	C	1	Total C N O 9 4 1 4	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



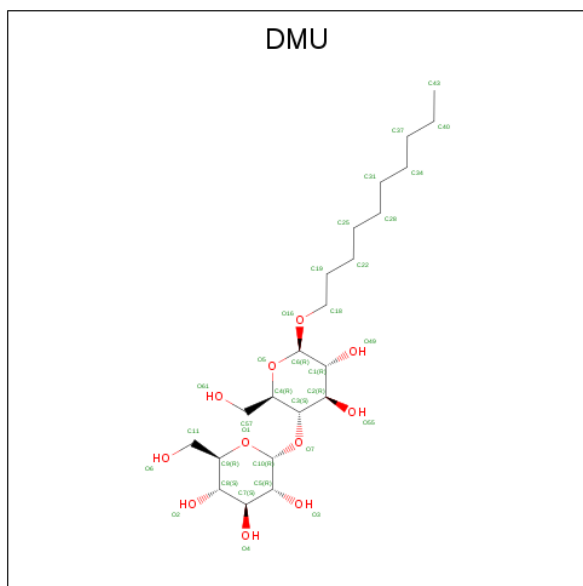
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



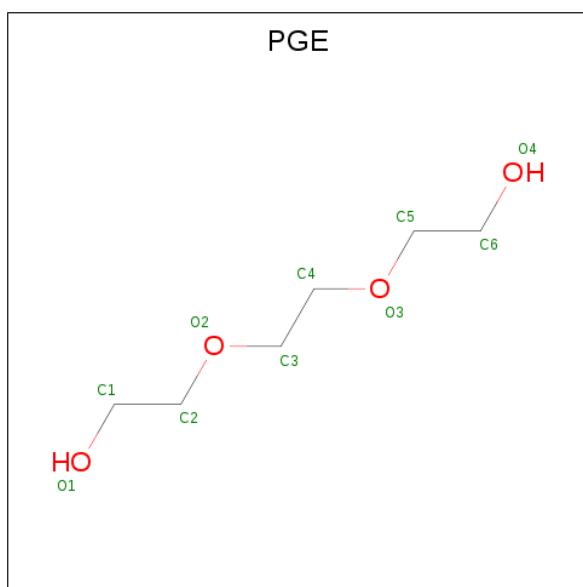
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

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



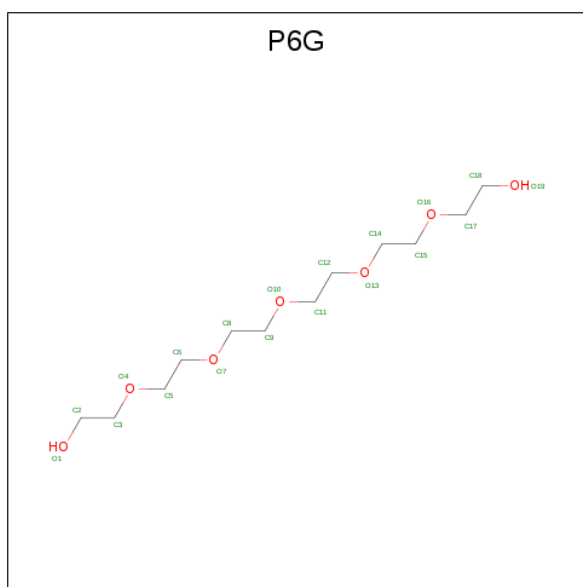
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			33	22	11		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: 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 (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



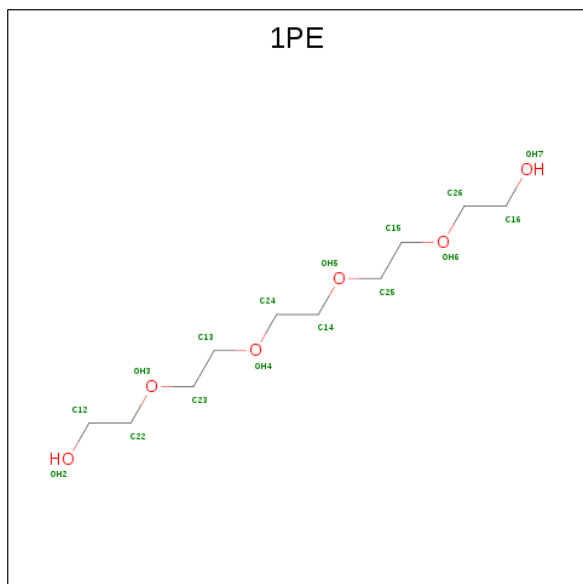
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			19	12	7		

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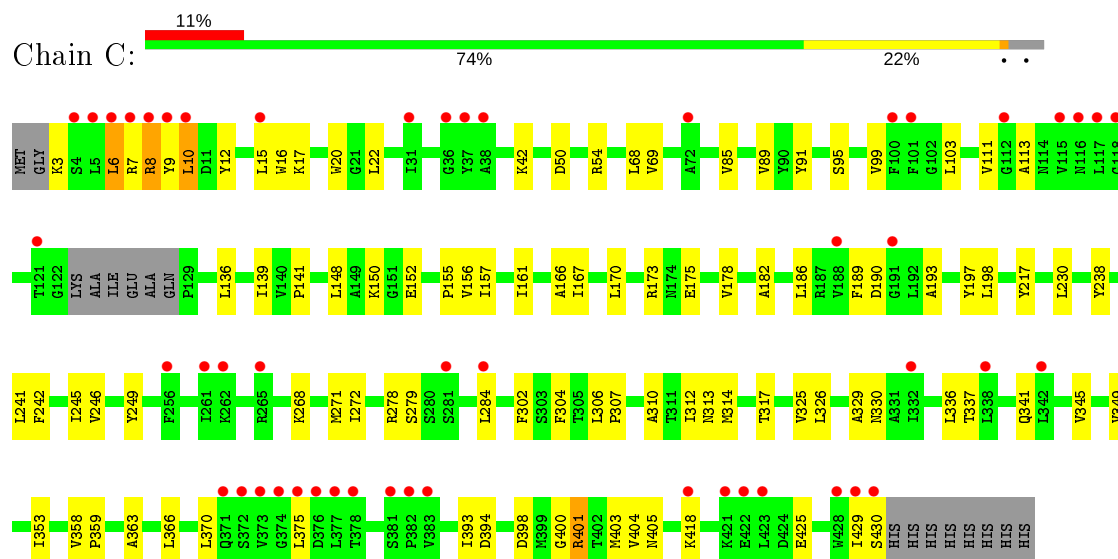
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 1: Proton/glutamate symporter, SDF family



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	116.55Å 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)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.232 , 0.269 0.234 , 0.272	Depositor DCC
R_{free} test set	3071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	106.3	Xtrriage
Anisotropy	0.314	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtrriage
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

Xtrriage'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: PGE, NA, 1PE, PG4, DMU, P6G, DAS, 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	0.45	0/3168	0.65	2/4312 (0.0%)
1	B	0.42	0/3056	0.66	0/4155
1	C	0.37	0/3206	0.62	2/4361 (0.0%)
All	All	0.42	0/9430	0.64	4/12828 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	401	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	401	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	10	LEU	CA-CB-CG	5.94	128.96	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3109	0	3300	74	0
1	B	3005	0	3206	70	0
1	C	3148	0	3357	70	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	3	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	215	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 11.

All (215) 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:C:175:GLU:N	1:C:175:GLU:OE1	2.19	0.75
1:C:68:LEU:HD21	1:C:161:ILE:HG13	1.73	0.71
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:DAS:N	3:A:504:DAS:OD2	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
1:A:175:GLU:N	1:A:175:GLU:OE1	2.30	0.61
1:B:358:VAL:O	3:B:504:DAS:HA	2.01	0.61
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: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:B:254:LYS:NZ	8:B:509:P6G:O19	2.34	0.57
1:A:119:SER:HA	1:A:382:PRO:HG2	1.85	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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:402:THR:HG23	3:A:504:DAS:C	2.41	0.50
1:A:146:ALA:HB2	1:B:149:ALA:O	2.11	0.50
1:C:193:ALA:O	1:C:197:TYR:HD2	1.94	0.50
1:C:15:LEU:HB2	1:C:268:LYS:HE3	1.92	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:398:ASP:OD1	3:C:504:DAS:N	2.45	0.49
1:C:6:LEU:HD12	1:C:8:ARG:NH1	2.25	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:B:397:LEU:O	1:B:401:ARG:HB2	2.13	0.48
1:B:20:TRP:CE3	1:B:20:TRP:HA	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:167:ILE:HG21	1:C:186:LEU:HD13	1.94	0.48
1:C:103:LEU:HD13	1:C:341:GLN:HB3	1.95	0.48
1:C:314:MET:HG2	1:C:405:ASN:ND2	2.29	0.48
1:A:74:SER:OG	1:A:74:SER:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:61:MET:HE3	1:A:156:VAL:HG21	1.96	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:193:ALA:O	1:B:197:TYR:HD2	1.98	0.46
1:A:317:THR:HA	1:A:401:ARG:CD	2.46	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
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:C:152:GLU:C	1:C:155:PRO:HD2	2.36	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:275:PHE:CZ	1:A:399:MET:HE3	2.51	0.44
1:A:152:GLU:OE2	4:A:507:PEG:H32	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLN:O	1:A:344:VAL:HG23	2.18	0.44
1:A:50:ASP:O	1:A:54:ARG:HG3	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:226:VAL:C	1:A:231:ALA:HB2	2.38	0.44
1:A:316:GLY:C	1:A:401:ARG:HG2	2.38	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: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:A:55:LEU:HD23	1:A:58:MET:HE1	1.99	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:336:LEU:HD21	1:B:373:VAL:HG21	2.00	0.43
1:B:68:LEU:HD13	1:B:303:SER:O	2.18	0.43
1:B:115:VAL:HG12	1:B:117:LEU:HG	2.00	0.43
1:B:86:LYS:NZ	1:B:420:GLU:HG2	2.34	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: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
1:B:86:LYS:HZ1	1:B:419:THR:HG22	1.83	0.42
1:B:86:LYS:HZ2	1:B:420:GLU:HG2	1.85	0.42
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:H122	8:B:510:P6G:H61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:GLY:C	1:A:335:PRO:HD3	2.40	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
6:A:509:DMU:H9	6:A:509:DMU:H29	2.02	0.41
1:B:284:LEU:HA	1:B:284:LEU:HD23	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:297:VAL:HG21	1:A:413:THR:HG22	2.02	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:362:GLY:HA3	1:A:401:ARG:NH1	2.36	0.41
1:A:410:LEU:HA	1:A:410:LEU:HD23	1.72	0.41
1:A:274:ALA:HA	1:A:283:THR:HG21	2.03	0.41
1:A:241:LEU:HD13	1:A:400:GLY:O	2.21	0.40
1:A:152:GLU:OE1	4:A:507:PEG:H32	2.21	0.40
1:A:139:ILE:O	1:A:155:PRO:HA	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:302:PHE:O	1:A:306:LEU:HB2	2.21	0.40
1:B:211:VAL:O	1:B:215:ILE:HG22	2.22	0.40
1:B:45:ILE:O	1:B:213:ALA:HB1	2.22	0.40
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%)	320 (98%)	7 (2%)	53	84
1	B	316/345 (92%)	312 (99%)	4 (1%)	69	91
1	C	332/345 (96%)	325 (98%)	7 (2%)	53	84
All	All	975/1035 (94%)	957 (98%)	18 (2%)	60	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	20	TRP
1	A	74	SER
1	A	94	THR
1	A	135	THR
1	A	368[A]	MET
1	A	368[B]	MET
1	B	20	TRP
1	B	111	VAL
1	B	181	SER
1	B	358	VAL

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Mol	Chain	Res	Type
1	C	3	LYS
1	C	6	LEU
1	C	7	ARG
1	C	8	ARG
1	C	16	TRP
1	C	20	TRP
1	C	111	VAL

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
5	PG4	A	508	-	12,12,12	0.56	0	11,11,11	0.42	0
9	1PE	B	513	-	15,15,15	0.54	0	14,14,14	0.36	0
4	PEG	A	507	-	6,6,6	0.54	0	5,5,5	0.69	0
7	PGE	B	512	-	9,9,9	0.41	0	8,8,8	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DAS	B	504	-	2,8,8	0.71	0	1,10,10	0.65	0
7	PGE	A	510	-	9,9,9	0.50	0	8,8,8	0.47	0
4	PEG	B	507	-	6,6,6	0.57	0	5,5,5	0.70	0
3	DAS	C	504	-	2,8,8	0.28	0	1,10,10	0.03	0
4	PEG	C	507	-	6,6,6	0.52	0	5,5,5	0.40	0
6	DMU	A	509	-	34,34,34	1.62	8 (23%)	45,45,45	1.29	6 (13%)
4	PEG	B	508	-	6,6,6	0.53	0	5,5,5	0.37	0
4	PEG	C	506	-	6,6,6	0.48	0	5,5,5	0.34	0
4	PEG	C	508	-	6,6,6	0.53	0	5,5,5	0.49	0
8	P6G	B	510	-	18,18,18	0.58	0	17,17,17	0.42	0
7	PGE	B	511	-	9,9,9	0.54	0	8,8,8	0.78	0
4	PEG	C	505	-	6,6,6	0.54	0	5,5,5	0.55	0
8	P6G	B	509	-	18,18,18	0.55	0	17,17,17	0.29	0
4	PEG	C	509	-	6,6,6	0.58	0	5,5,5	0.55	0
4	PEG	A	505	-	6,6,6	0.53	0	5,5,5	0.32	0
4	PEG	A	506	-	6,6,6	0.52	0	5,5,5	0.28	0
4	PEG	B	506	-	6,6,6	0.49	0	5,5,5	0.34	0
3	DAS	A	504	-	2,8,8	0.19	0	1,10,10	1.06	0
4	PEG	B	505	-	6,6,6	0.51	0	5,5,5	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	A	508	-	-	4/10/10/10	-
9	1PE	B	513	-	-	8/13/13/13	-
4	PEG	A	507	-	-	3/4/4/4	-
7	PGE	B	512	-	-	4/7/7/7	-
3	DAS	B	504	-	-	2/2/8/8	-
7	PGE	A	510	-	-	4/7/7/7	-
4	PEG	B	507	-	-	1/4/4/4	-
3	DAS	C	504	-	-	2/2/8/8	-
4	PEG	C	507	-	-	2/4/4/4	-
6	DMU	A	509	-	-	13/19/59/59	0/2/2/2
4	PEG	B	508	-	-	1/4/4/4	-
4	PEG	C	506	-	-	1/4/4/4	-
4	PEG	C	508	-	-	3/4/4/4	-
8	P6G	B	510	-	-	8/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PGE	B	511	-	-	2/7/7/7	-
4	PEG	C	505	-	-	2/4/4/4	-
8	P6G	B	509	-	-	9/16/16/16	-
4	PEG	C	509	-	-	2/4/4/4	-
4	PEG	A	505	-	-	2/4/4/4	-
4	PEG	A	506	-	-	3/4/4/4	-
4	PEG	B	506	-	-	1/4/4/4	-
3	DAS	A	504	-	-	2/2/8/8	-
4	PEG	B	505	-	-	3/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	509	DMU	O1-C9	4.53	1.55	1.44
6	A	509	DMU	C11-C9	-3.27	1.40	1.51
6	A	509	DMU	O5-C6	3.02	1.49	1.41
6	A	509	DMU	O5-C4	2.59	1.50	1.44
6	A	509	DMU	O4-C7	2.42	1.48	1.43
6	A	509	DMU	C8-C9	2.34	1.58	1.53
6	A	509	DMU	O1-C10	2.33	1.47	1.41
6	A	509	DMU	O3-C5	2.03	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	509	DMU	O5-C4-C3	3.35	116.81	109.75
6	A	509	DMU	C6-O5-C4	3.04	119.66	113.69
6	A	509	DMU	O7-C3-C2	2.83	114.80	107.28
6	A	509	DMU	O7-C10-C5	2.52	114.62	108.10
6	A	509	DMU	O7-C3-C4	-2.22	103.36	109.45
6	A	509	DMU	O5-C6-C1	2.00	114.59	110.35

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	DAS	N-CA-CB-CG
3	B	504	DAS	C-CA-CB-CG
3	C	504	DAS	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
3	A	504	DAS	N-CA-CB-CG
3	A	504	DAS	C-CA-CB-CG
6	A	509	DMU	O1-C10-O7-C3
4	B	505	PEG	O2-C3-C4-O4
7	A	510	PGE	C1-C2-O2-C3
6	A	509	DMU	O5-C4-C57-O61
9	B	513	1PE	OH5-C14-C24-OH4
8	B	509	P6G	O13-C14-C15-O16
8	B	510	P6G	O7-C8-C9-O10
7	B	512	PGE	O2-C3-C4-O3
8	B	509	P6G	C9-C8-O7-C6
8	B	509	P6G	O4-C5-C6-O7
7	B	512	PGE	O3-C5-C6-O4
4	A	507	PEG	O1-C1-C2-O2
4	C	505	PEG	O1-C1-C2-O2
8	B	509	P6G	O16-C17-C18-O19
4	C	509	PEG	O1-C1-C2-O2
8	B	510	P6G	O1-C2-C3-O4
4	A	506	PEG	O2-C3-C4-O4
4	B	506	PEG	O2-C3-C4-O4
6	A	509	DMU	C5-C10-O7-C3
8	B	509	P6G	C18-C17-O16-C15
9	B	513	1PE	OH6-C15-C25-OH5
9	B	513	1PE	OH2-C12-C22-OH3
4	C	507	PEG	O1-C1-C2-O2
4	B	505	PEG	O1-C1-C2-O2
4	C	507	PEG	C4-C3-O2-C2
4	A	507	PEG	O2-C3-C4-O4
6	A	509	DMU	C22-C25-C28-C31
6	A	509	DMU	C19-C18-O16-C6
5	A	508	PG4	O4-C7-C8-O5
6	A	509	DMU	C25-C28-C31-C34
6	A	509	DMU	O16-C18-C19-C22
5	A	508	PG4	O3-C5-C6-O4
8	B	510	P6G	O13-C14-C15-O16
6	A	509	DMU	C18-C19-C22-C25
4	B	508	PEG	O2-C3-C4-O4
6	A	509	DMU	C28-C31-C34-C37
4	C	508	PEG	O2-C3-C4-O4
6	A	509	DMU	C4-C3-O7-C10
4	B	507	PEG	O2-C3-C4-O4
6	A	509	DMU	C2-C3-O7-C10

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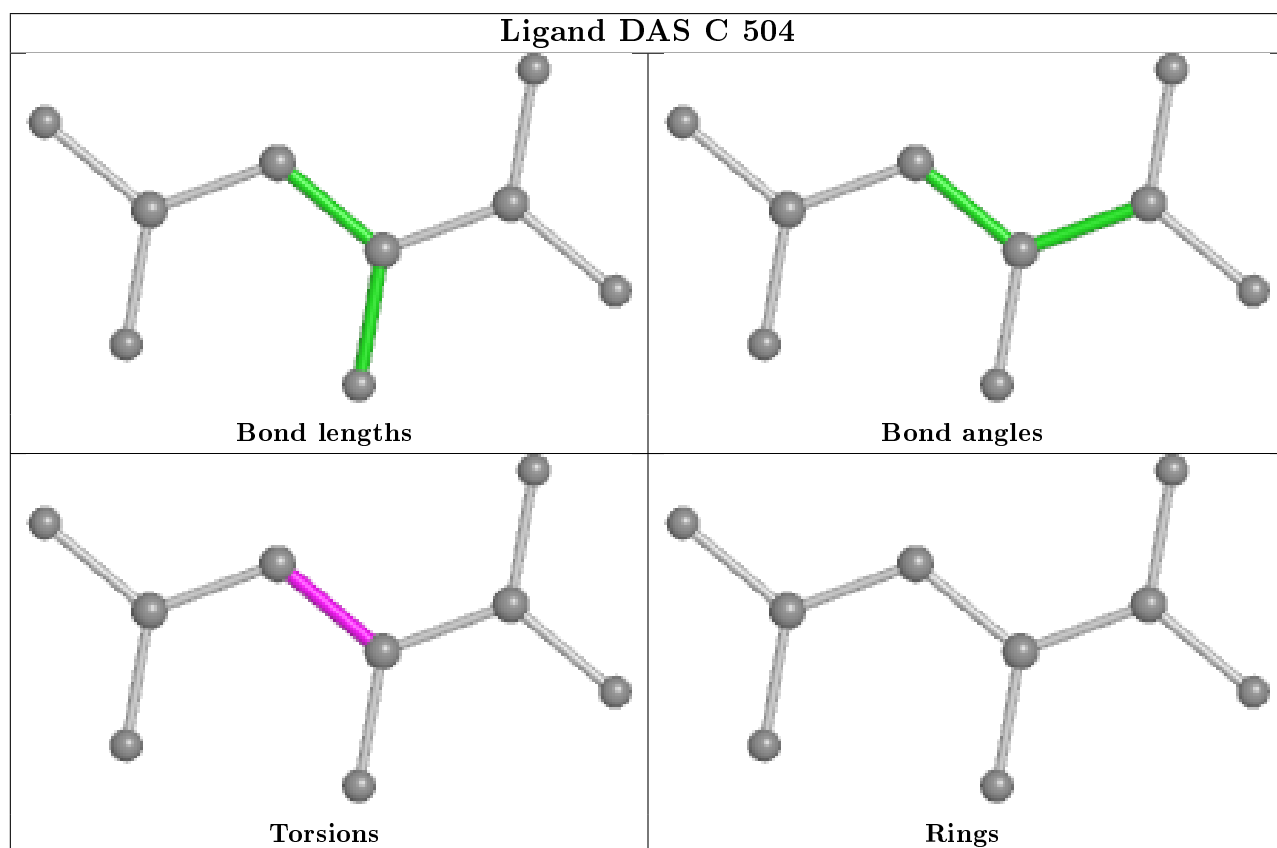
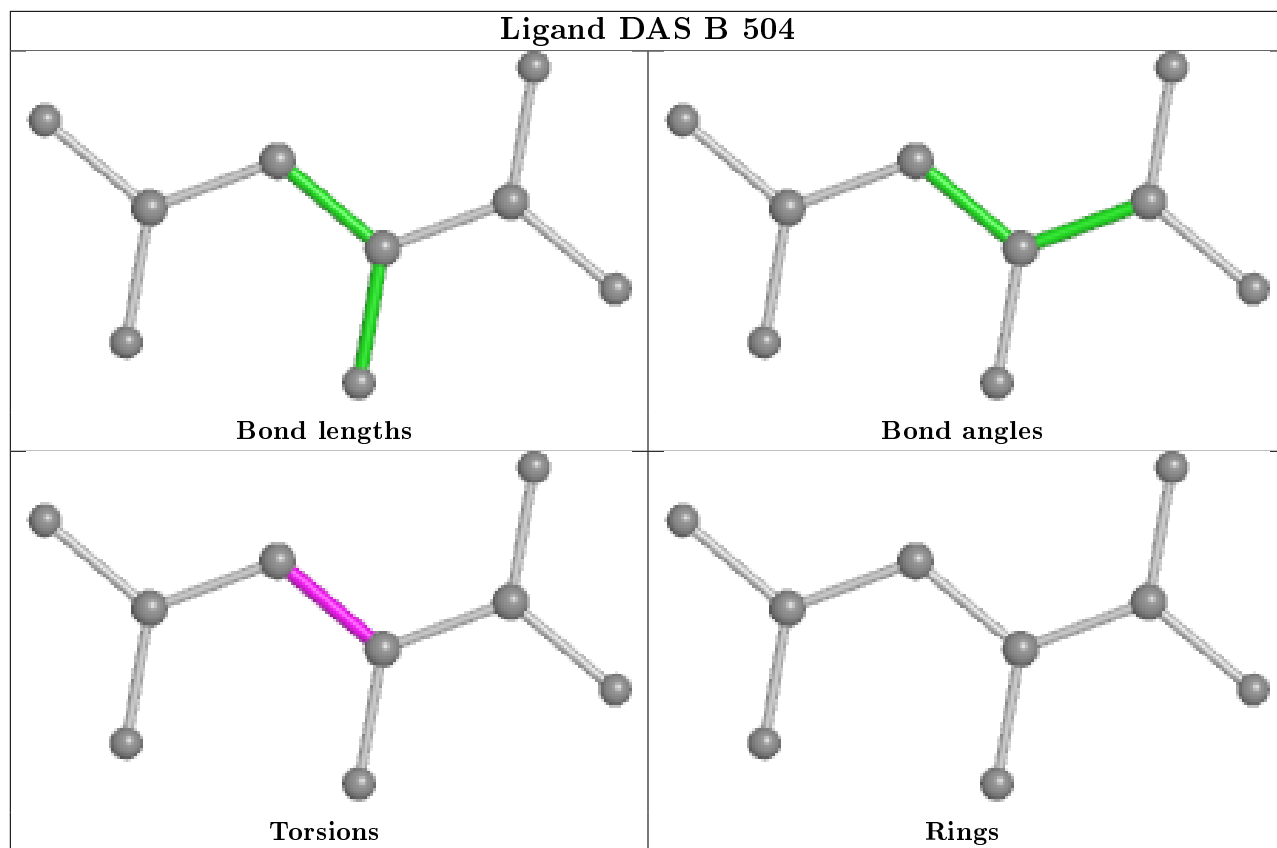
Mol	Chain	Res	Type	Atoms
7	B	511	PGE	C4-C3-O2-C2
7	B	512	PGE	O1-C1-C2-O2
4	C	508	PEG	O1-C1-C2-O2
4	A	505	PEG	O2-C3-C4-O4
4	C	505	PEG	O2-C3-C4-O4
4	C	506	PEG	C1-C2-O2-C3
4	C	508	PEG	C1-C2-O2-C3
8	B	510	P6G	C9-C8-O7-C6
7	B	511	PGE	C1-C2-O2-C3
9	B	513	1PE	C12-C22-OH3-C23
8	B	510	P6G	C6-C5-O4-C3
9	B	513	1PE	C23-C13-OH4-C24
4	A	505	PEG	O1-C1-C2-O2
4	B	505	PEG	C1-C2-O2-C3
5	A	508	PG4	C3-C4-O3-C5
8	B	509	P6G	O10-C11-C12-O13
8	B	509	P6G	C14-C15-O16-C17
9	B	513	1PE	C13-C23-OH3-C22
3	C	504	DAS	C-CA-CB-CG
9	B	513	1PE	C15-C25-OH5-C14
7	A	510	PGE	C3-C4-O3-C5
7	B	512	PGE	C3-C4-O3-C5
9	B	513	1PE	C25-C15-OH6-C26
5	A	508	PG4	C5-C6-O4-C7
8	B	510	P6G	C8-C9-O10-C11
6	A	509	DMU	C3-C4-C57-O61
8	B	510	P6G	C2-C3-O4-C5
4	A	507	PEG	C1-C2-O2-C3
4	A	506	PEG	C1-C2-O2-C3
8	B	510	P6G	O10-C11-C12-O13
4	A	506	PEG	O1-C1-C2-O2
8	B	509	P6G	C5-C6-O7-C8
6	A	509	DMU	O6-C11-C9-O1
8	B	509	P6G	O7-C8-C9-O10
7	A	510	PGE	O2-C3-C4-O3
4	C	509	PEG	C1-C2-O2-C3
7	A	510	PGE	O3-C5-C6-O4

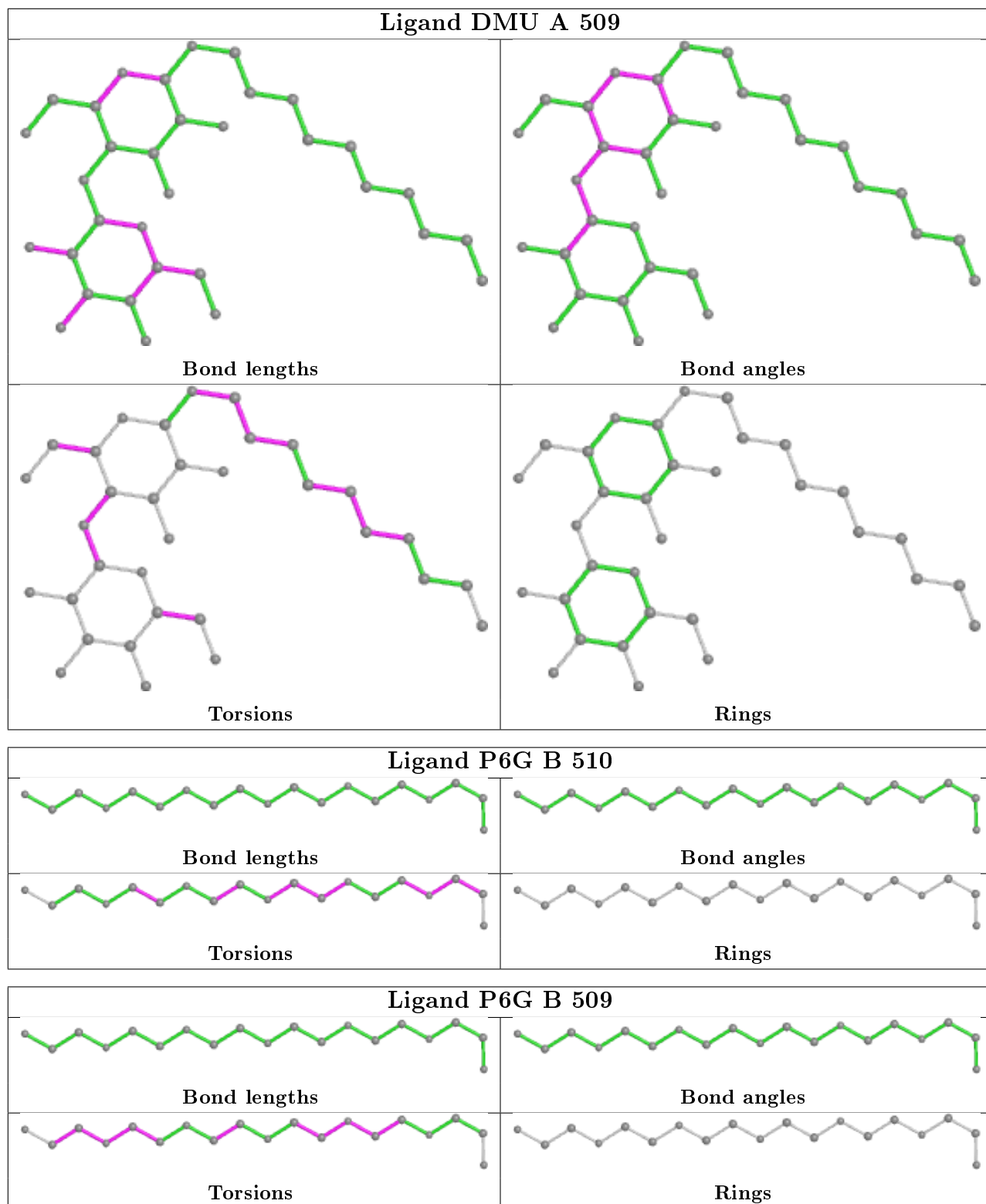
There are no ring outliers.

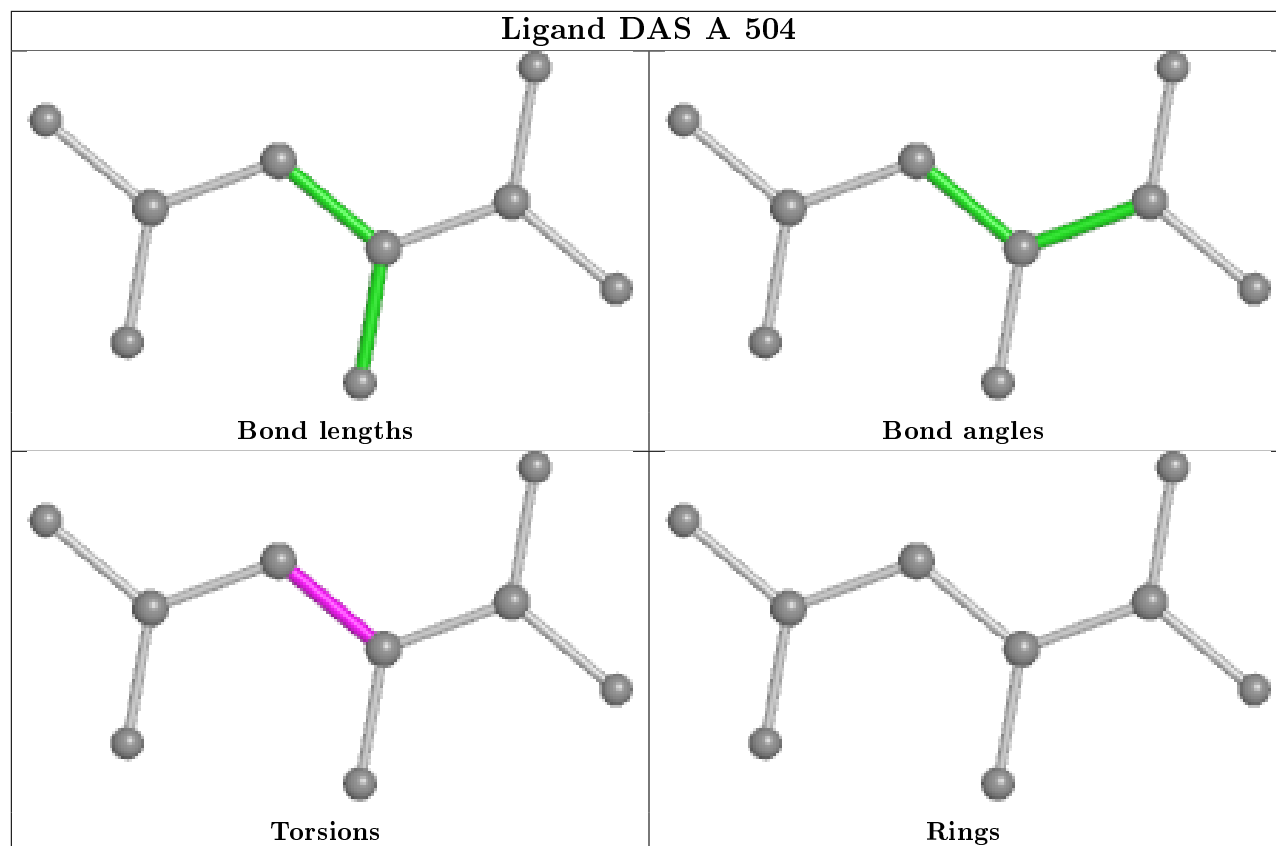
11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	513	1PE	5	0
4	A	507	PEG	2	0
3	B	504	DAS	3	0
7	A	510	PGE	1	0
3	C	504	DAS	3	0
6	A	509	DMU	3	0
4	C	506	PEG	1	0
8	B	510	P6G	1	0
7	B	511	PGE	1	0
8	B	509	P6G	1	0
3	A	504	DAS	4	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.33	43 (10%) 6 3	83, 115, 169, 258	0
1	B	406/438 (92%)	0.23	36 (8%) 9 5	84, 123, 166, 249	0
1	C	422/438 (96%)	0.38	50 (11%) 4 2	78, 132, 193, 278	0
All	All	1244/1314 (94%)	0.31	129 (10%) 6 3	78, 123, 177, 278	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	375	LEU	7.4
1	C	375	LEU	7.1
1	C	15	LEU	6.1
1	A	375	LEU	5.7
1	C	376	ASP	5.6
1	C	382	PRO	5.3
1	C	118	GLY	5.1
1	A	376	ASP	5.1
1	A	111	VAL	5.0
1	B	373	VAL	5.0
1	A	372	SER	5.0
1	C	423	LEU	5.0
1	A	373	VAL	4.8
1	C	116	ASN	4.8
1	C	9	TYR	4.7
1	A	326	LEU	4.6
1	C	421	LYS	4.6
1	C	428	TRP	4.6
1	C	112	GLY	4.5
1	B	371	GLN	4.5
1	A	374	GLY	4.5
1	B	131	SER	4.4
1	A	338	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	115	VAL	4.3
1	A	340	GLN	4.3
1	C	37	TYR	4.1
1	C	342	LEU	4.0
1	C	6	LEU	3.9
1	C	265	ARG	3.8
1	B	374	GLY	3.8
1	C	377	LEU	3.8
1	A	387	TYR	3.7
1	A	339	GLY	3.5
1	B	421	LYS	3.5
1	C	256	PHE	3.5
1	C	5	LEU	3.4
1	C	429	ILE	3.4
1	B	332	ILE	3.3
1	B	376	ASP	3.3
1	B	338	LEU	3.3
1	A	386	ALA	3.3
1	B	334	HIS	3.3
1	B	377	LEU	3.3
1	A	325	VAL	3.2
1	C	4	SER	3.2
1	B	340	GLN	3.2
1	B	429	ILE	3.2
1	C	383	VAL	3.2
1	C	371	GLN	3.1
1	C	117	LEU	3.1
1	A	377	LEU	3.1
1	A	324	THR	3.1
1	A	343	VAL	3.0
1	C	422	GLU	3.0
1	B	383	VAL	3.0
1	A	176	GLU	2.9
1	A	370	LEU	2.9
1	C	338	LEU	2.9
1	A	127	ALA	2.9
1	B	251	ILE	2.9
1	B	176	GLU	2.9
1	A	109	PHE	2.9
1	A	84	GLY	2.9
1	B	370	LEU	2.8
1	A	371	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	428	TRP	2.8
1	C	378	THR	2.8
1	C	373	VAL	2.8
1	A	189	PHE	2.8
1	C	430	SER	2.8
1	B	328	VAL	2.8
1	C	418	LYS	2.8
1	C	281	SER	2.7
1	B	333	GLY	2.7
1	B	329	ALA	2.7
1	C	8	ARG	2.7
1	B	430	SER	2.6
1	A	281	SER	2.6
1	A	342	LEU	2.6
1	B	336	LEU	2.6
1	B	111	VAL	2.6
1	B	247	ILE	2.6
1	C	38	ALA	2.6
1	A	188	VAL	2.5
1	A	341	GLN	2.5
1	A	287	THR	2.5
1	A	273	THR	2.5
1	C	72	ALA	2.5
1	C	374	GLY	2.5
1	C	121	THR	2.5
1	B	343	VAL	2.4
1	C	36	GLY	2.4
1	A	284	LEU	2.4
1	C	284	LEU	2.4
1	B	335	PRO	2.4
1	A	327	PHE	2.4
1	C	7	ARG	2.4
1	A	385	LEU	2.3
1	A	82	ARG	2.3
1	A	108	LEU	2.3
1	A	283	THR	2.3
1	A	25	GLY	2.2
1	C	10	LEU	2.2
1	B	45	ILE	2.2
1	C	100	PHE	2.2
1	A	86	LYS	2.2
1	B	372	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	383	VAL	2.2
1	C	31	ILE	2.2
1	B	269	ASP	2.2
1	B	385	LEU	2.1
1	A	384	ALA	2.1
1	B	185	LEU	2.1
1	B	20	TRP	2.1
1	C	381	SER	2.1
1	C	188	VAL	2.1
1	C	261	ILE	2.1
1	A	337	THR	2.1
1	C	101	PHE	2.1
1	C	191	GLY	2.1
1	A	336	LEU	2.1
1	A	112	GLY	2.1
1	B	337	THR	2.1
1	B	273	THR	2.1
1	C	262	LYS	2.1
1	A	369	VAL	2.1
1	C	332	ILE	2.0
1	C	372	SER	2.0
1	B	368	MET	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 carbohydrates 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
7	PGE	B	511	10/10	0.55	0.65	125,150,171,172	0

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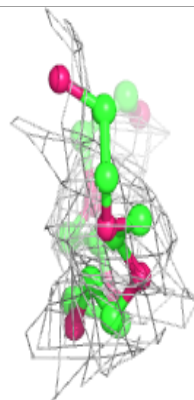
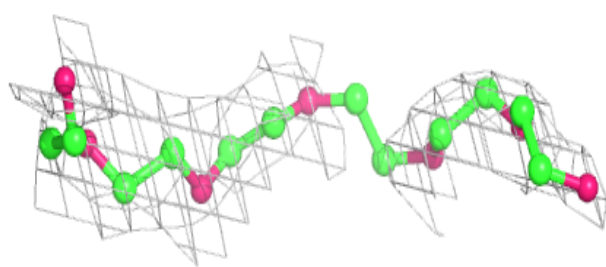
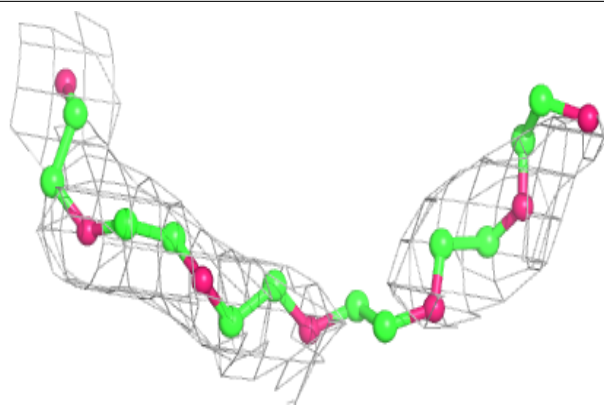
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	P6G	B	509	19/19	0.60	0.46	152,176,191,192	0
4	PEG	B	506	7/7	0.63	0.28	141,149,154,156	0
7	PGE	B	512	10/10	0.64	0.17	109,151,160,160	0
4	PEG	C	509	7/7	0.66	0.24	125,149,163,166	0
4	PEG	A	505	7/7	0.67	0.20	134,145,154,155	0
8	P6G	B	510	19/19	0.69	0.26	96,156,170,172	0
4	PEG	B	508	7/7	0.69	0.26	125,140,143,145	0
4	PEG	B	507	7/7	0.70	0.27	114,128,141,147	0
4	PEG	A	506	7/7	0.71	0.24	128,143,159,161	0
4	PEG	B	505	7/7	0.71	0.40	135,144,149,154	0
5	PG4	A	508	13/13	0.73	0.26	136,146,158,162	0
4	PEG	C	505	7/7	0.75	0.41	99,102,119,129	0
6	DMU	A	509	33/33	0.76	0.17	123,181,192,193	0
9	1PE	B	513	16/16	0.79	0.29	106,153,158,161	0
4	PEG	C	508	7/7	0.79	0.22	134,144,153,158	0
2	NA	A	503	1/1	0.80	0.20	120,120,120,120	0
4	PEG	A	507	7/7	0.81	0.21	106,127,145,147	0
4	PEG	C	507	7/7	0.81	0.24	124,140,152,155	0
7	PGE	A	510	10/10	0.82	0.17	98,119,134,135	0
4	PEG	C	506	7/7	0.84	0.10	134,141,144,146	0
2	NA	A	502	1/1	0.87	0.16	96,96,96,96	0
3	DAS	B	504	9/9	0.88	0.24	100,111,114,116	0
3	DAS	C	504	9/9	0.93	0.19	101,116,127,129	0
2	NA	C	503	1/1	0.93	0.11	109,109,109,109	0
2	NA	B	503	1/1	0.94	0.10	142,142,142,142	0
2	NA	C	502	1/1	0.94	0.05	102,102,102,102	0
3	DAS	A	504	9/9	0.95	0.18	101,112,123,129	0
2	NA	B	501	1/1	0.95	0.09	169,169,169,169	0
2	NA	B	502	1/1	0.96	0.23	98,98,98,98	0
2	NA	A	501	1/1	0.98	0.24	103,103,103,103	0
2	NA	C	501	1/1	0.98	0.28	111,111,111,111	0

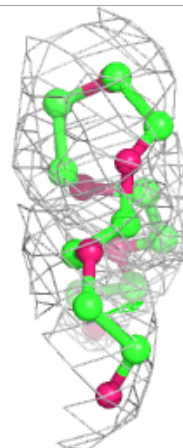
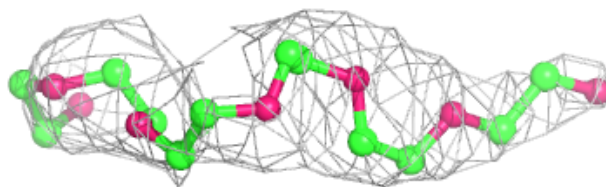
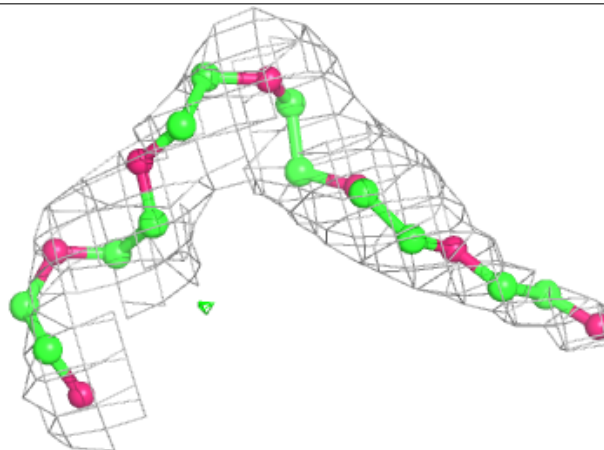
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

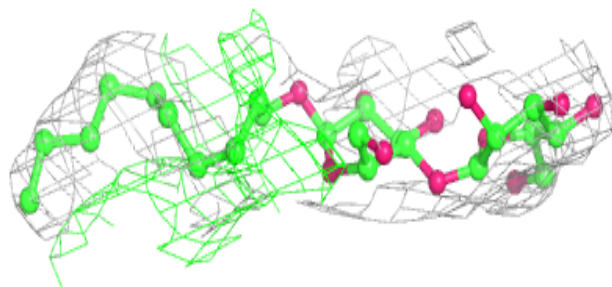
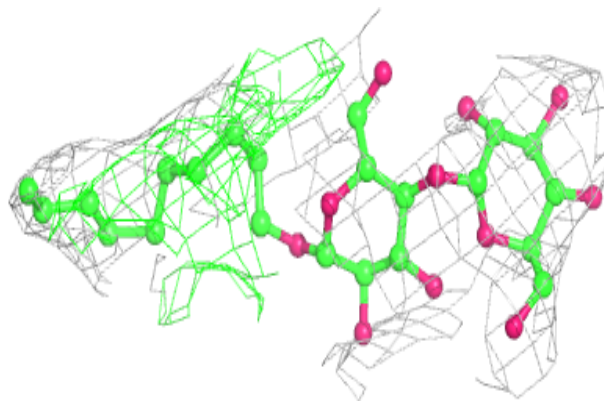
**Electron density around P6G B 510:**

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

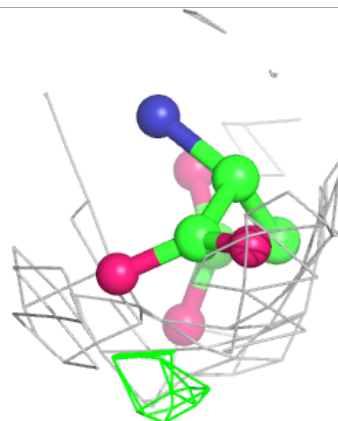
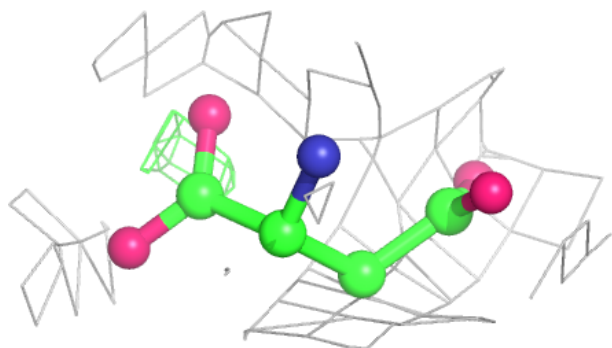
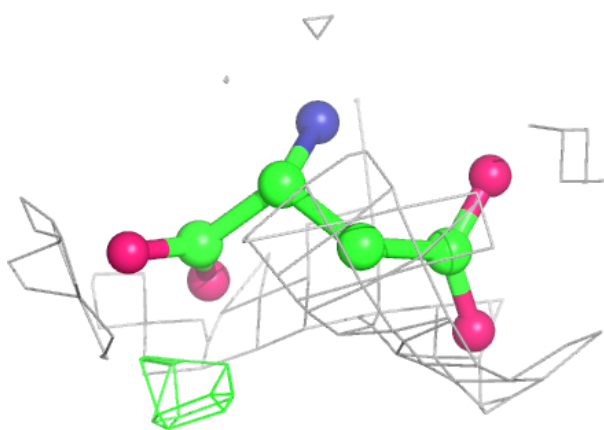


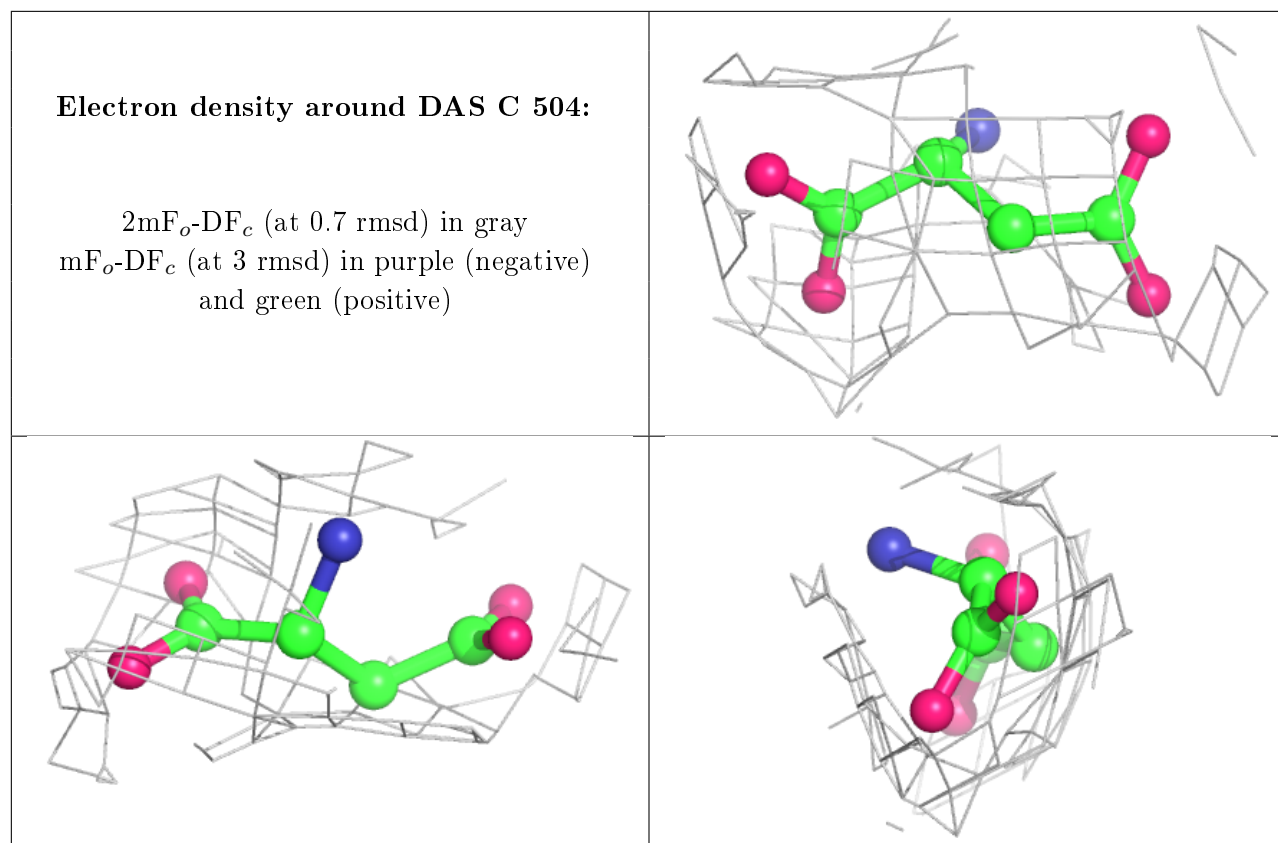
Electron density around DMU A 509:

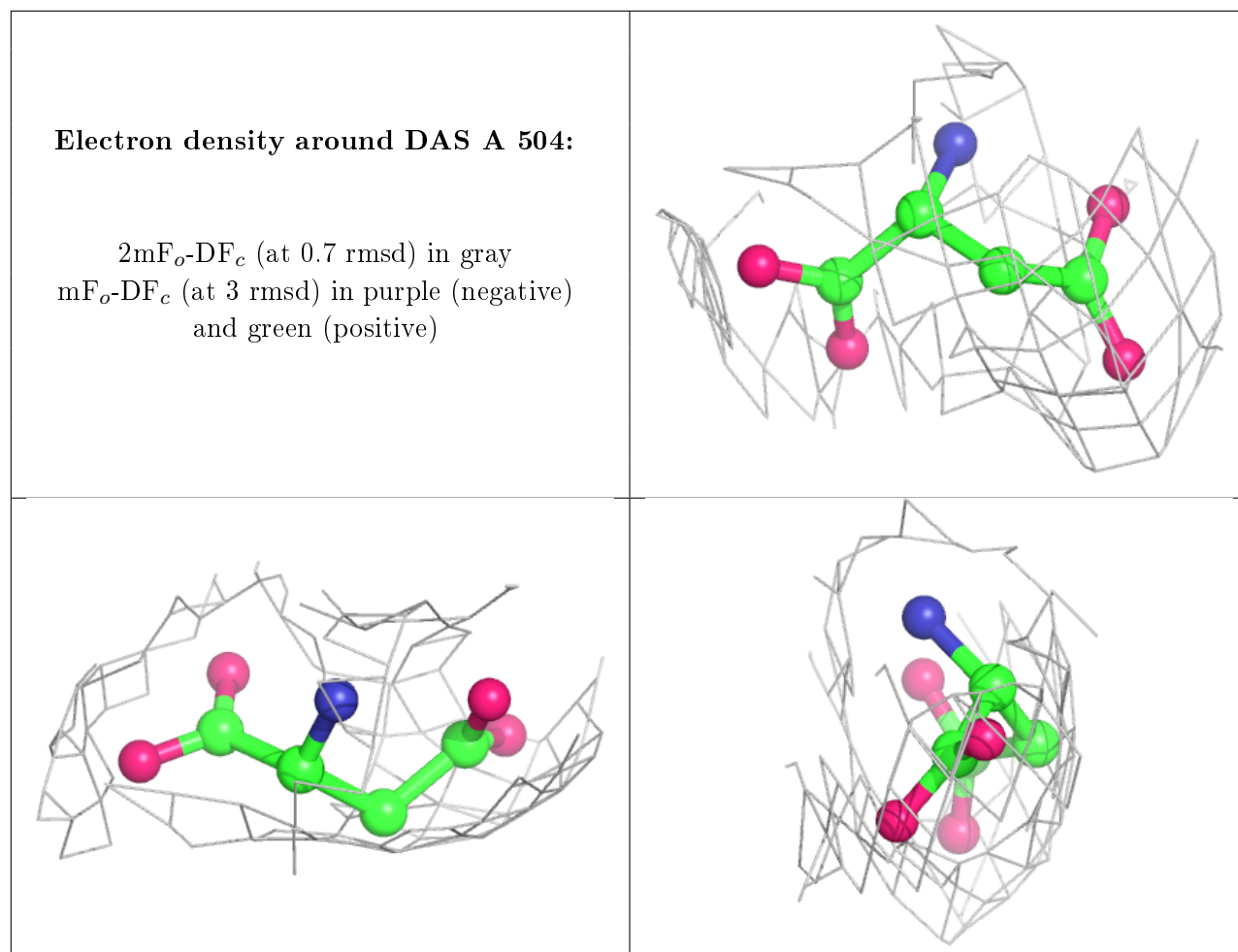
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 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)







6.5 Other polymers [i](#)

There are no such residues in this entry.