



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:20 AM UTC

PDB ID : 8OXX / pdb_00008oxx
Title : Transglutaminase 3 in complex with inhibitor Z-don and DH patient-derived Fab DH63-B02
Authors : Heggelund, J.E.; Sollid, L.M.
Deposited on : 2023-05-02
Resolution : 2.50 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

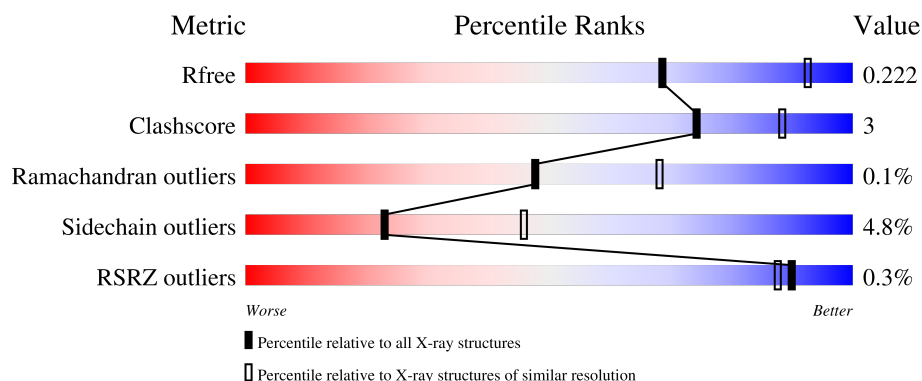
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	460	 83% 16% .
2	B	223	 92% 7%
3	C	216	 92% 8%

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 14186 atoms, of which 6753 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 Protein-glutamine gamma-glutamyltransferase E 27 kDa non-catalytic chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	460	Total	C	H	N	O	S	98	1	0
			7068	2263	3471	634	687	13			

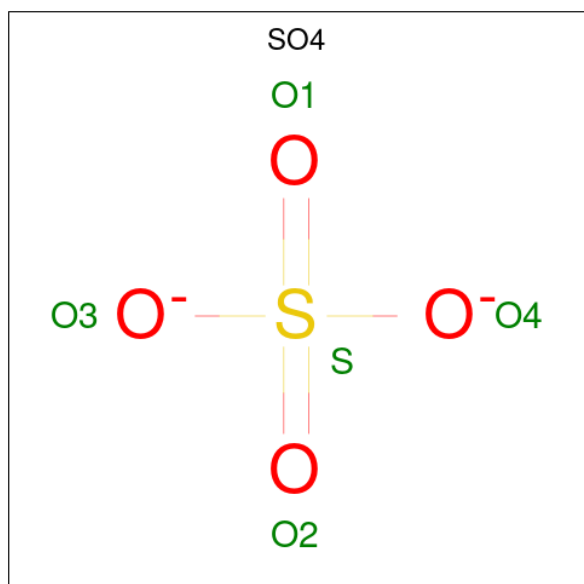
- Molecule 2 is a protein called Antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	223	Total	C	H	N	O	S	71	0	0
			3323	1054	1642	288	332	7			

- Molecule 3 is a protein called Antibody fab fragment light chain.

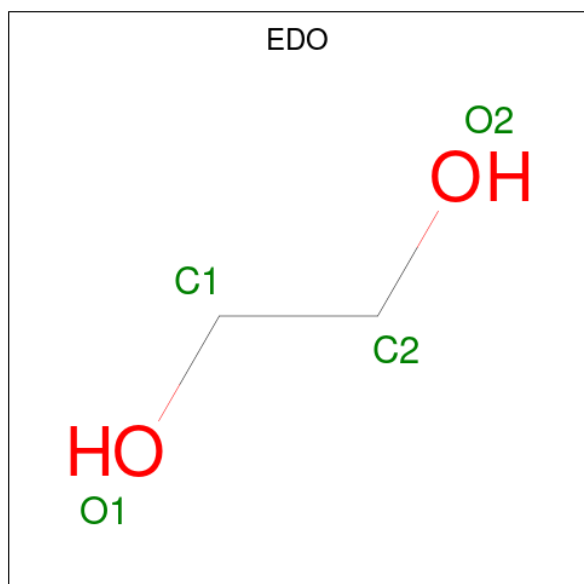
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	216	Total	C	H	N	O	S	74	0	0
			3185	1007	1559	272	341	6			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

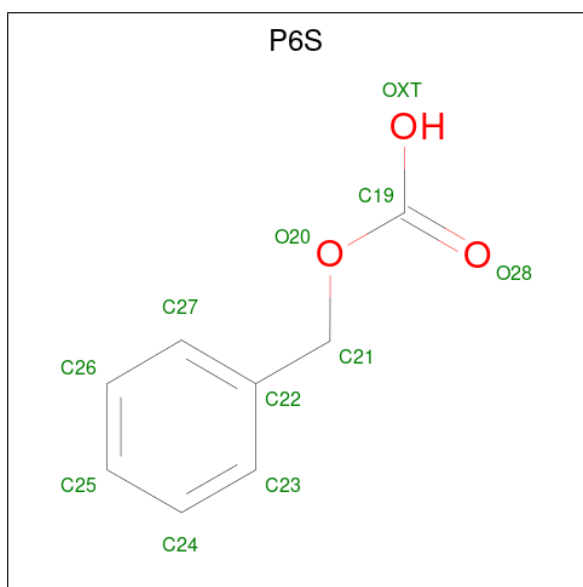


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	1	0
			10	2	6	2		
5	A	1	Total	C	H	O	1	0
			10	2	6	2		
5	B	1	Total	C	H	O	1	0
			10	2	6	2		
5	B	1	Total	C	H	O	1	0
			10	2	6	2		
5	C	1	Total	C	H	O	1	0
			10	2	6	2		
5	C	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

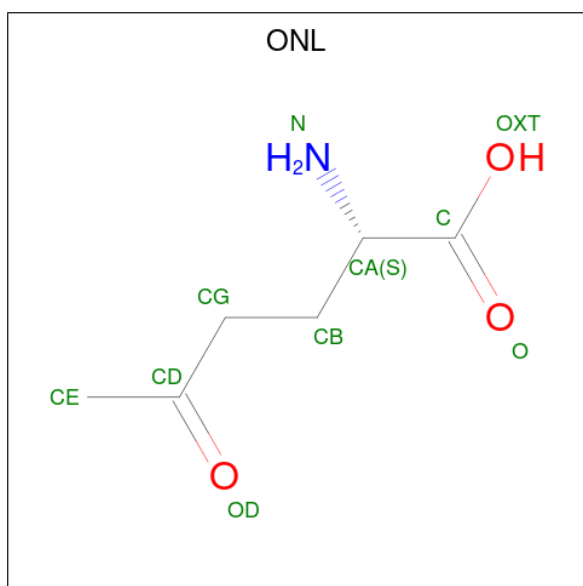
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		

- Molecule 7 is benzyl hydrogen carbonate (CCD ID: P6S) (formula: $C_8H_8O_3$) (labeled as "Ligand of Interest" by depositor).



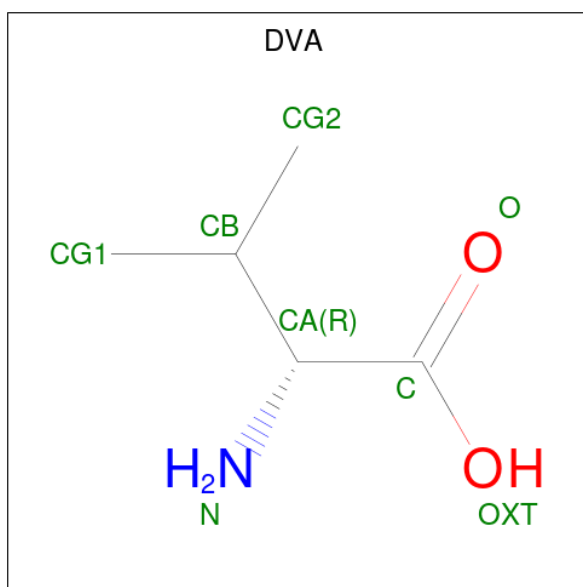
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			17	8	7	2		

- Molecule 8 is 5-OXO-L-NORLEUCINE (CCD ID: ONL) (formula: $C_6H_{11}NO_3$) (labeled as "Ligand of Interest" by depositor).



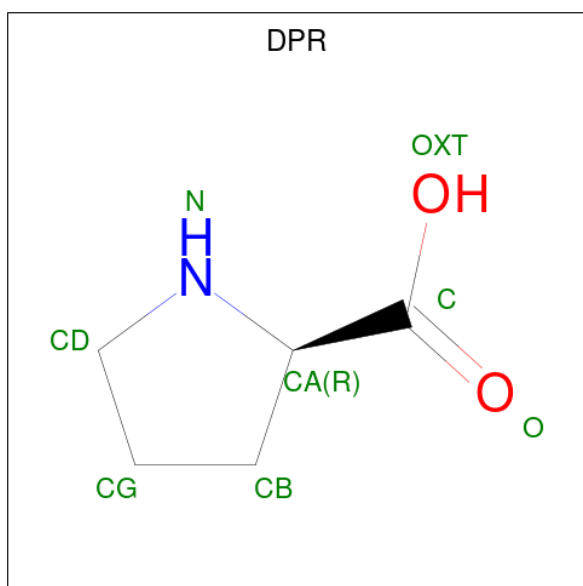
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			17	6	8	1	2		

- Molecule 9 is D-VALINE (CCD ID: DVA) (formula: $C_5H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



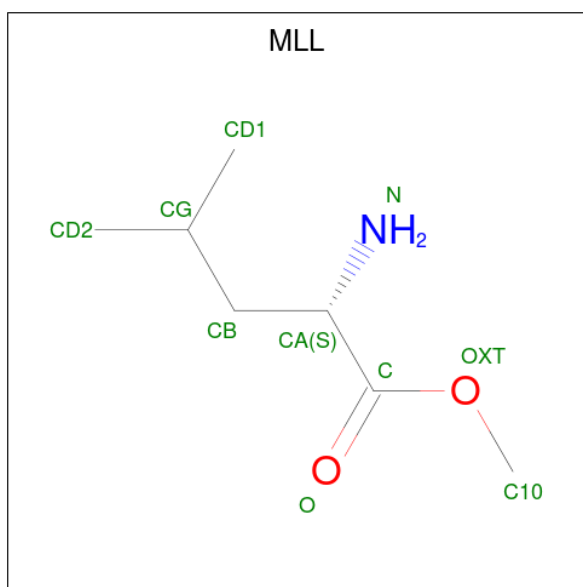
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	H	N	O	0	0
			16	5	9	1	1		

- Molecule 10 is D-PROLINE (CCD ID: DPR) (formula: C₅H₉NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			14	5	7	1	1		

- Molecule 11 is METHYL L-LEUCINATE (CCD ID: MLL) (formula: C₇H₁₅NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	0	0
			24	7	14	1	2		

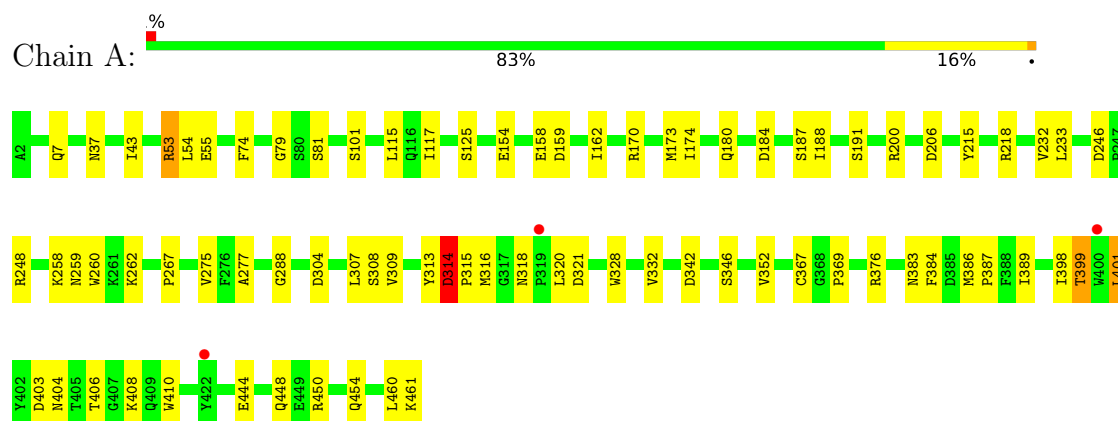
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	225	Total	O	0	1
			226	226		
12	B	124	Total	O	0	0
			124	124		
12	C	104	Total	O	0	0
			104	104		

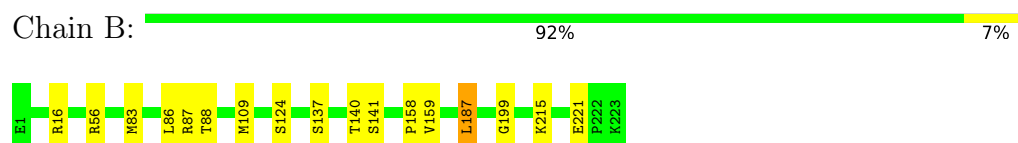
3 Residue-property plots [i](#)

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

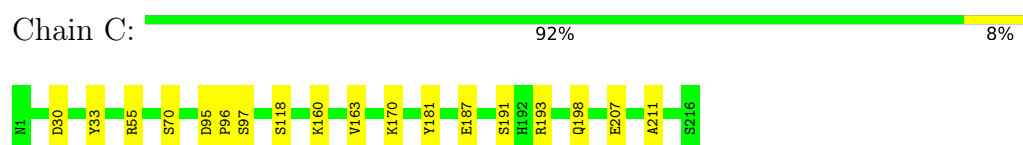
- Molecule 1: Protein-glutamine gamma-glutamyltransferase E 27 kDa non-catalytic chain



- Molecule 2: Antibody fab fragment heavy chain



- Molecule 3: Antibody fab fragment light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.27Å 65.00Å 90.91Å 90.00° 96.85° 90.00°	Depositor
Resolution (Å)	52.80 – 2.50 52.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.3 (52.80-2.50) 91.1 (52.80-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0411, REFMAC 5.8.0411	Depositor
R, R_{free}	0.154 , 0.222 0.154 , 0.222	Depositor DCC
R_{free} test set	1532 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14186	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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: MLL, SO4, CA, P6S, DPR, ONL, DVA, EDO

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	0.69	1/3683 (0.0%)	1.16	8/4995 (0.2%)
2	B	0.68	0/1721	1.06	2/2342 (0.1%)
3	C	0.68	0/1665	1.08	1/2273 (0.0%)
All	All	0.68	1/7069 (0.0%)	1.12	11/9610 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
2	B	0	2
3	C	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	SER	CA-CB	-5.81	1.44	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	88	THR	CA-CB-OG1	-6.57	99.75	109.60
1	A	314	ASP	CA-CB-CG	5.93	118.53	112.60
2	B	221	GLU	CB-CG-CD	5.84	122.53	112.60
1	A	288	GLY	CA-C-N	-5.51	116.56	122.85
1	A	288	GLY	C-N-CA	-5.51	116.56	122.85
1	A	246	ASP	O-C-N	-5.40	116.95	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ASN	N-CA-C	-5.35	105.62	111.82
1	A	74	PHE	CB-CA-C	5.30	116.54	109.65
1	A	403	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	267	PRO	N-CA-C	5.22	119.42	111.11
3	C	55	ARG	CB-CA-C	5.10	115.49	109.47

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	ARG	Sidechain
1	A	200	ARG	Sidechain
1	A	218	ARG	Sidechain
1	A	248	ARG	Sidechain
1	A	376	ARG	Sidechain
1	A	53	ARG	Sidechain
1	A	79	GLY	Peptide
2	B	56	ARG	Sidechain
2	B	87	ARG	Sidechain
3	C	193	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3597	3471	3462	30	1
2	B	1681	1642	1640	5	0
3	C	1626	1559	1556	7	0
4	A	5	0	0	0	0
5	A	8	12	12	0	0
5	B	8	12	12	0	0
5	C	8	12	12	0	0
6	A	3	0	0	0	0
7	A	10	7	0	0	0
8	A	9	8	6	1	0
9	A	7	9	8	1	0
10	A	7	7	7	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	10	14	10	0	0
12	A	226	0	0	1	0
12	B	124	0	0	1	0
12	C	104	0	0	1	0
All	All	7433	6753	6725	42	1

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 3.

All (42) 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:313:TYR:CE1	1:A:399:THR:HG22	2.34	0.62
3:C:95:ASP:HB2	3:C:96:PRO:CD	2.34	0.57
1:A:328:TRP:HZ3	10:A:510:DPR:HD3	1.73	0.54
1:A:206:ASP:OD1	1:A:215:TYR:OH	2.21	0.54
1:A:315:PRO:O	1:A:316:MET:HB2	2.08	0.53
1:A:188:ILE:O	1:A:191:SER:HB2	2.09	0.53
1:A:54:LEU:HD22	1:A:117:ILE:HG12	1.93	0.51
2:B:187:LEU:HD12	2:B:187:LEU:C	2.35	0.50
2:B:199:GLY:HA2	12:B:496:HOH:O	2.11	0.50
1:A:315:PRO:HB3	1:A:401:LEU:HD23	1.94	0.49
1:A:307:LEU:HG	1:A:460:LEU:HD11	1.95	0.49
1:A:232:VAL:HA	1:A:260:TRP:CD1	2.48	0.49
3:C:187:GLU:O	3:C:191:SER:HB3	2.12	0.48
1:A:154:GLU:O	1:A:158:GLU:HB3	2.13	0.48
1:A:401:LEU:N	1:A:410:TRP:O	2.46	0.48
1:A:386:MET:N	1:A:387:PRO:CD	2.77	0.48
1:A:277:ALA:CB	1:A:332:VAL:HG12	2.44	0.47
1:A:313:TYR:CD1	1:A:399:THR:HG22	2.49	0.47
8:A:508:ONL:C	9:A:509:DVA:HG23	2.45	0.46
1:A:233:LEU:HD11	1:A:275:VAL:HG12	1.98	0.46
1:A:55:GLU:O	1:A:115:LEU:HD12	2.15	0.46
1:A:262:LYS:HD2	3:C:33:TYR:CD1	2.52	0.45
3:C:163:VAL:HA	3:C:181:TYR:O	2.16	0.45
2:B:140:THR:O	2:B:140:THR:HG22	2.17	0.44
12:A:623:HOH:O	3:C:30:ASP:HA	2.16	0.44
1:A:7:GLN:HB2	1:A:43:ILE:O	2.18	0.44
3:C:211:ALA:HB1	12:C:439:HOH:O	2.18	0.44
1:A:314:ASP:CG	1:A:320:LEU:HD11	2.43	0.43
3:C:198:GLN:NE2	3:C:207:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:TYR:HD1	1:A:399:THR:O	2.02	0.43
1:A:159:ASP:HA	1:A:180:GLN:OE1	2.19	0.42
1:A:461:LYS:OXT	1:A:461:LYS:CD	2.67	0.42
1:A:444:GLU:HA	1:A:444:GLU:OE1	2.19	0.42
1:A:367:CYS:SG	1:A:389:ILE:HD11	2.59	0.42
1:A:352:VAL:O	1:A:369:PRO:HA	2.19	0.42
1:A:383:ASN:HA	1:A:384:PHE:HA	1.88	0.42
1:A:342:ASP:OD1	1:A:342:ASP:N	2.53	0.41
2:B:140:THR:O	2:B:141:SER:C	2.64	0.41
1:A:314:ASP:OD1	1:A:320:LEU:HD11	2.21	0.41
1:A:313:TYR:O	1:A:401:LEU:HA	2.21	0.40
2:B:83:MET:HB3	2:B:86:LEU:HD21	2.03	0.40
1:A:386:MET:N	1:A:387:PRO:HD2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:NE2	1:A:454:GLN:OE1[1_455]	2.11	0.09

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	459/460 (100%)	431 (94%)	27 (6%)	1 (0%)	43	63
2	B	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
3	C	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
All	All	894/899 (99%)	847 (95%)	46 (5%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/387 (100%)	364 (94%)	24 (6%)	16	34
2	B	189/189 (100%)	181 (96%)	8 (4%)	26	52
3	C	189/189 (100%)	184 (97%)	5 (3%)	40	68
All	All	766/765 (100%)	729 (95%)	37 (5%)	23	46

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	53	ARG
1	A	81	SER
1	A	101	SER
1	A	125	SER
1	A	162	ILE
1	A	173	MET
1	A	174	ILE
1	A	184	ASP
1	A	258	LYS
1	A	308	SER
1	A	309	VAL
1	A	314	ASP
1	A	318	ASN
1	A	321	ASP
1	A	346	SER
1	A	398	ILE
1	A	399	THR
1	A	401	LEU
1	A	404	ASN
1	A	406	THR
1	A	408	LYS

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	450	ARG
2	B	16	ARG
2	B	109	MET
2	B	124	SER
2	B	137	SER
2	B	158	PRO
2	B	159	VAL
2	B	187	LEU
2	B	215	LYS
3	C	70	SER
3	C	97	SER
3	C	118	SER
3	C	160	LYS
3	C	170	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	92	ASN
1	A	149	HIS
1	A	169	ASN
2	B	3	GLN
2	B	39	GLN
2	B	77	ASN
2	B	208	ASN
3	C	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	$\# Z > 2$
8	ONL	A	508	1,9,7	7,8,9	0.76	0	4,9,11	1.68	1 (25%)
5	EDO	B	302	-	3,3,3	0.31	0	2,2,2	0.39	0
5	EDO	C	301	-	3,3,3	0.29	0	2,2,2	0.32	0
5	EDO	B	301	-	3,3,3	0.13	0	2,2,2	0.31	0
4	SO4	A	501	-	4,4,4	0.27	0	6,6,6	0.32	0
5	EDO	C	302	-	3,3,3	0.30	0	2,2,2	0.38	0
5	EDO	A	503	-	3,3,3	0.37	0	2,2,2	0.35	0
11	MLL	A	511	10	8,9,9	0.33	0	9,11,11	1.68	1 (11%)
10	DPR	A	510	11,9	6,7,8	0.87	0	7,8,10	1.96	3 (42%)
9	DVA	A	509	8,10	4,6,7	0.40	0	6,7,9	2.88	2 (33%)
5	EDO	A	502	-	3,3,3	0.25	0	2,2,2	0.45	0
7	P6S	A	507	8	9,10,11	0.50	0	10,11,13	1.04	1 (10%)

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
8	ONL	A	508	1,9,7	-	3/6/7/9	-
5	EDO	B	302	-	-	1/1/1/1	-
5	EDO	C	301	-	-	1/1/1/1	-
5	EDO	B	301	-	-	1/1/1/1	-
5	EDO	C	302	-	-	1/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
11	MLL	A	511	10	-	7/10/10/10	-
10	DPR	A	510	11,9	-	0/0/9/11	0/1/1/1
9	DVA	A	509	8,10	-	2/5/6/8	-
5	EDO	A	502	-	-	1/1/1/1	-
7	P6S	A	507	8	-	0/4/4/5	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	509	DVA	CB-CA-C	6.56	121.82	112.87
11	A	511	MLL	C10-OXT-C	4.73	126.64	115.92
10	A	510	DPR	O-C-CA	-3.35	116.16	124.77
7	A	507	P6S	O20-C21-C22	3.01	116.71	109.41
9	A	509	DVA	O-C-CA	-2.44	118.49	124.77
8	A	508	ONL	OD-CD-CG	2.38	128.26	121.47
10	A	510	DPR	CG-CD-N	-2.38	99.04	105.72
10	A	510	DPR	CB-CA-N	-2.36	98.12	104.72

There are no chirality outliers.

All (17) torsion outliers are listed below:

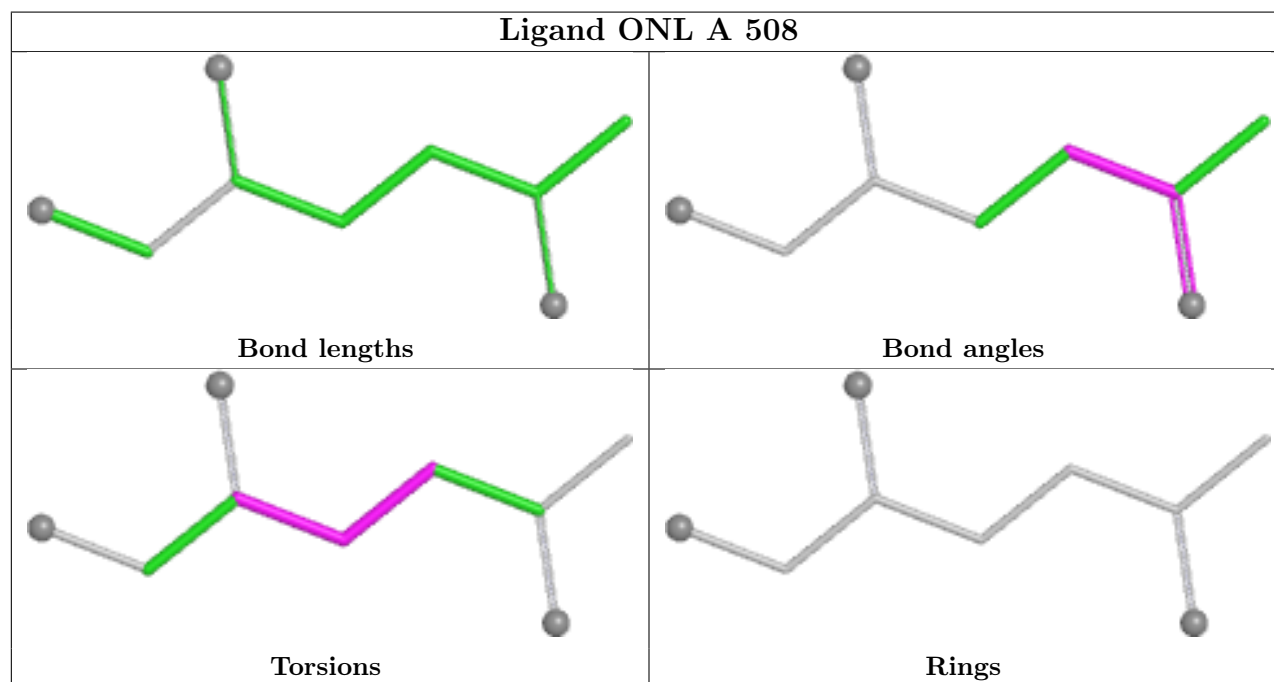
Mol	Chain	Res	Type	Atoms
8	A	508	ONL	N-CA-CB-CG
8	A	508	ONL	C-CA-CB-CG
9	A	509	DVA	N-CA-CB-CG2
11	A	511	MLL	O-C-OXT-C10
11	A	511	MLL	CA-C-OXT-C10
5	B	301	EDO	O1-C1-C2-O2
5	B	302	EDO	O1-C1-C2-O2
5	A	502	EDO	O1-C1-C2-O2
9	A	509	DVA	O-C-CA-CB
5	C	301	EDO	O1-C1-C2-O2
11	A	511	MLL	OXT-C-CA-CB
5	C	302	EDO	O1-C1-C2-O2
11	A	511	MLL	O-C-CA-CB
11	A	511	MLL	O-C-CA-N
11	A	511	MLL	CA-CB-CG-CD2
8	A	508	ONL	CA-CB-CG-CD
11	A	511	MLL	OXT-C-CA-N

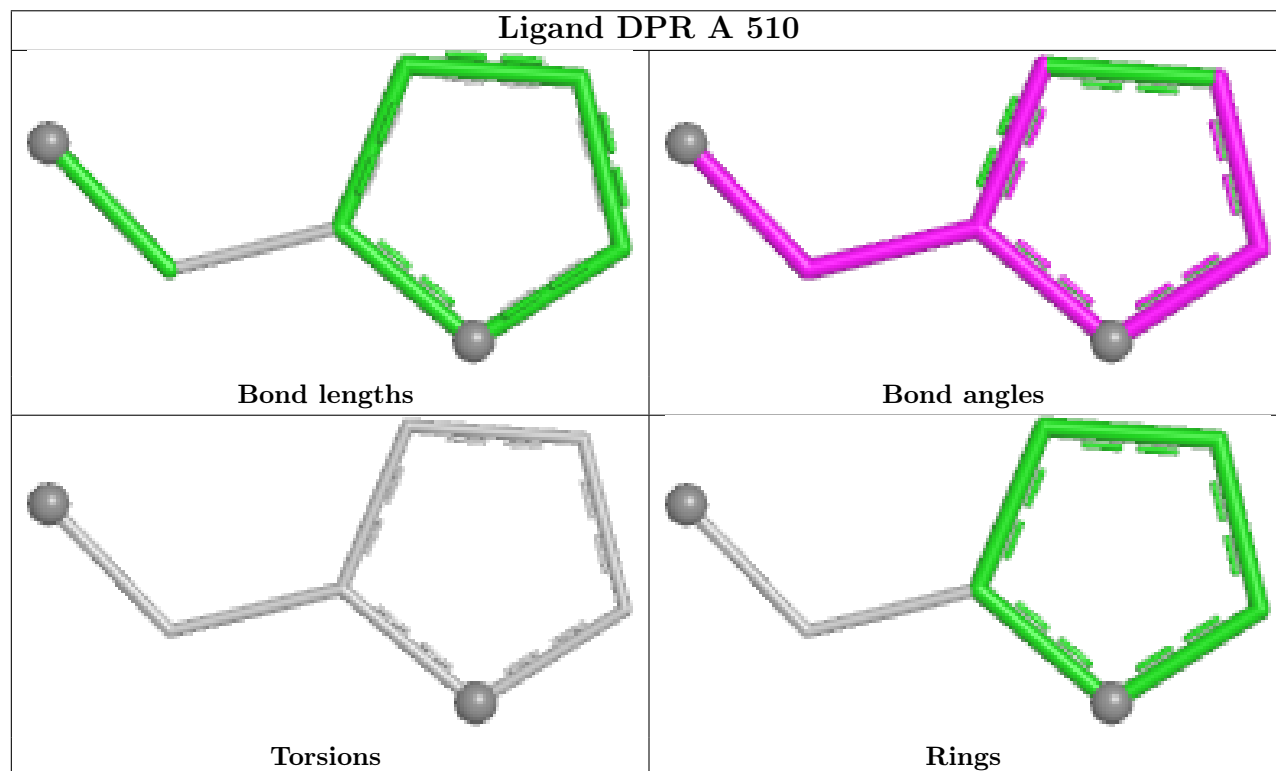
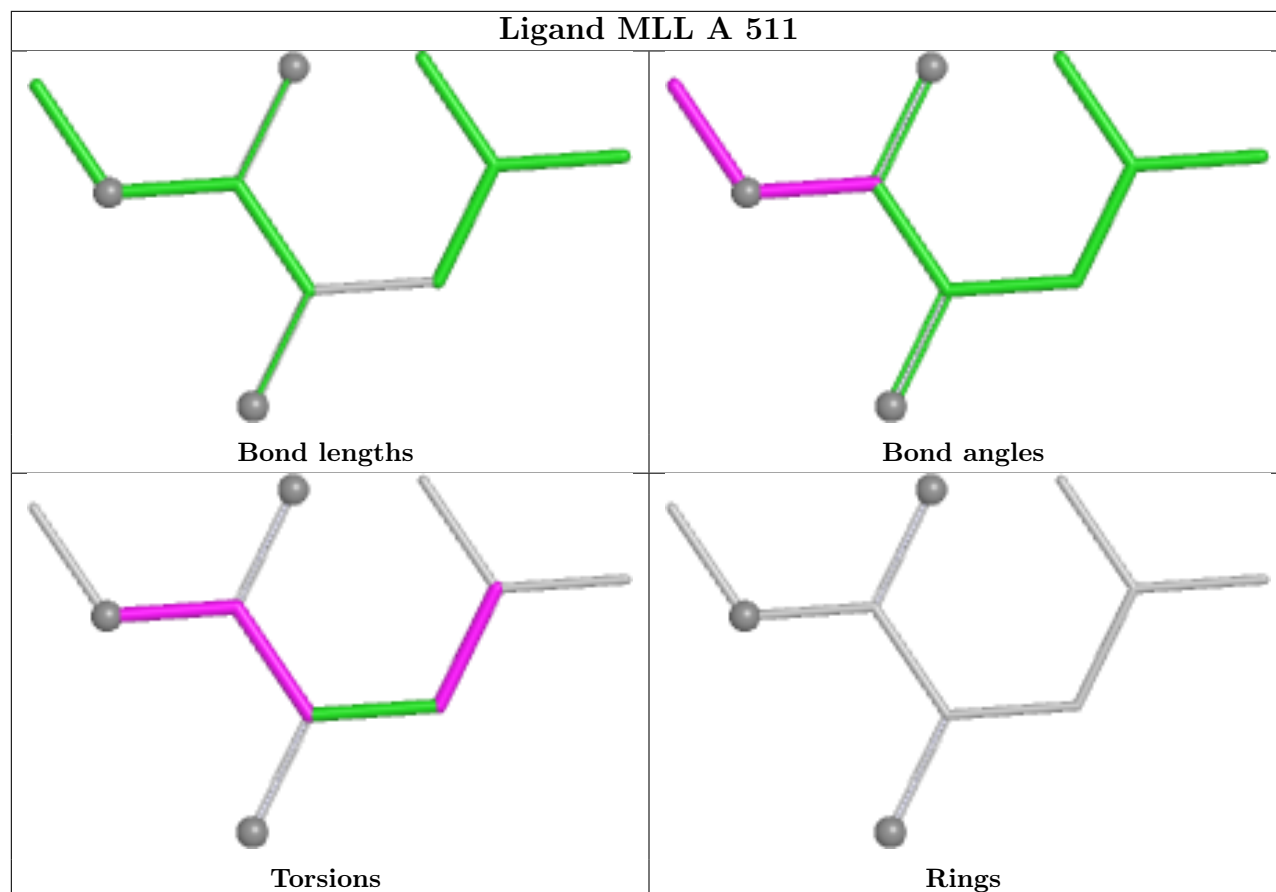
There are no ring outliers.

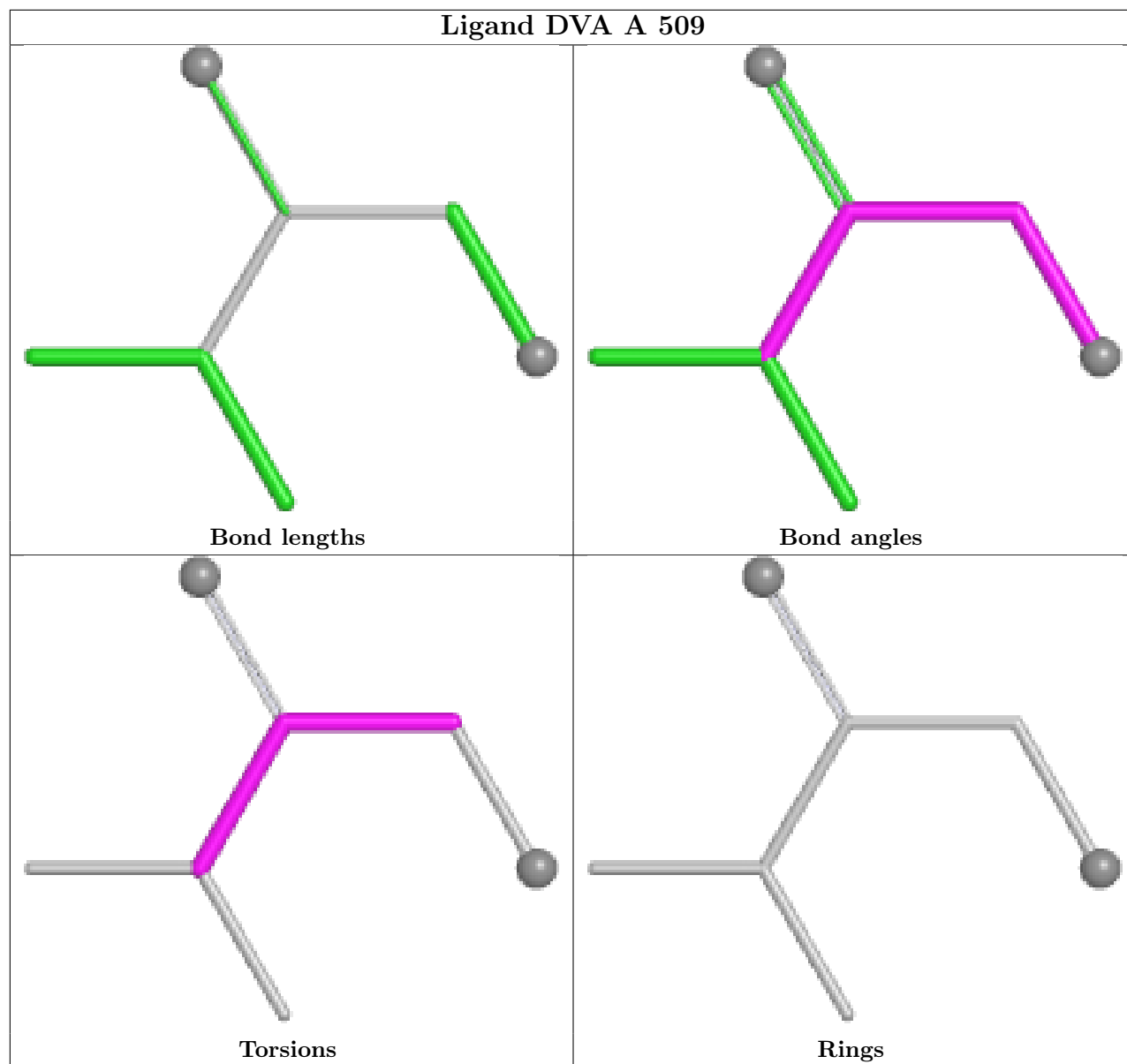
3 monomers are involved in 2 short contacts:

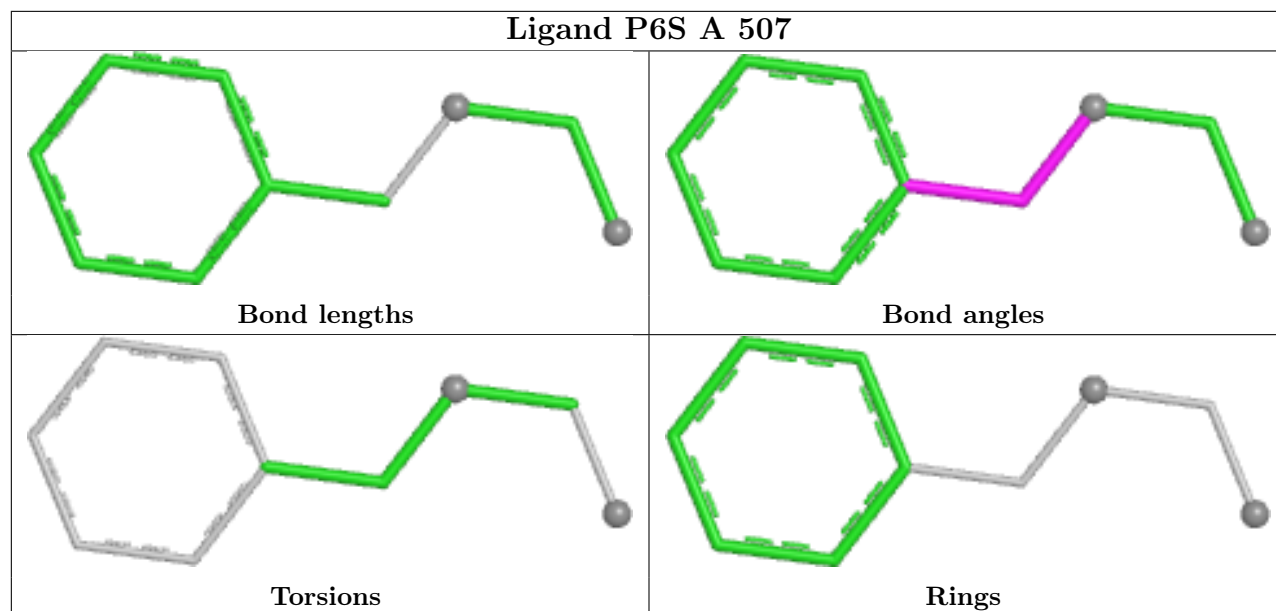
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	508	ONL	1	0
10	A	510	DPR	1	0
9	A	509	DVA	1	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/460 (100%)	-0.56	3 (0%) 84 81	11, 40, 101, 154	1 (0%)
2	B	223/223 (100%)	-0.50	0 100 100	28, 40, 68, 131	0
3	C	216/216 (100%)	-0.61	0 100 100	26, 40, 65, 113	0
All	All	899/899 (100%)	-0.56	3 (0%) 90 87	11, 40, 87, 154	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	PRO	2.3
1	A	422	TYR	2.2
1	A	400	TRP	2.1

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.

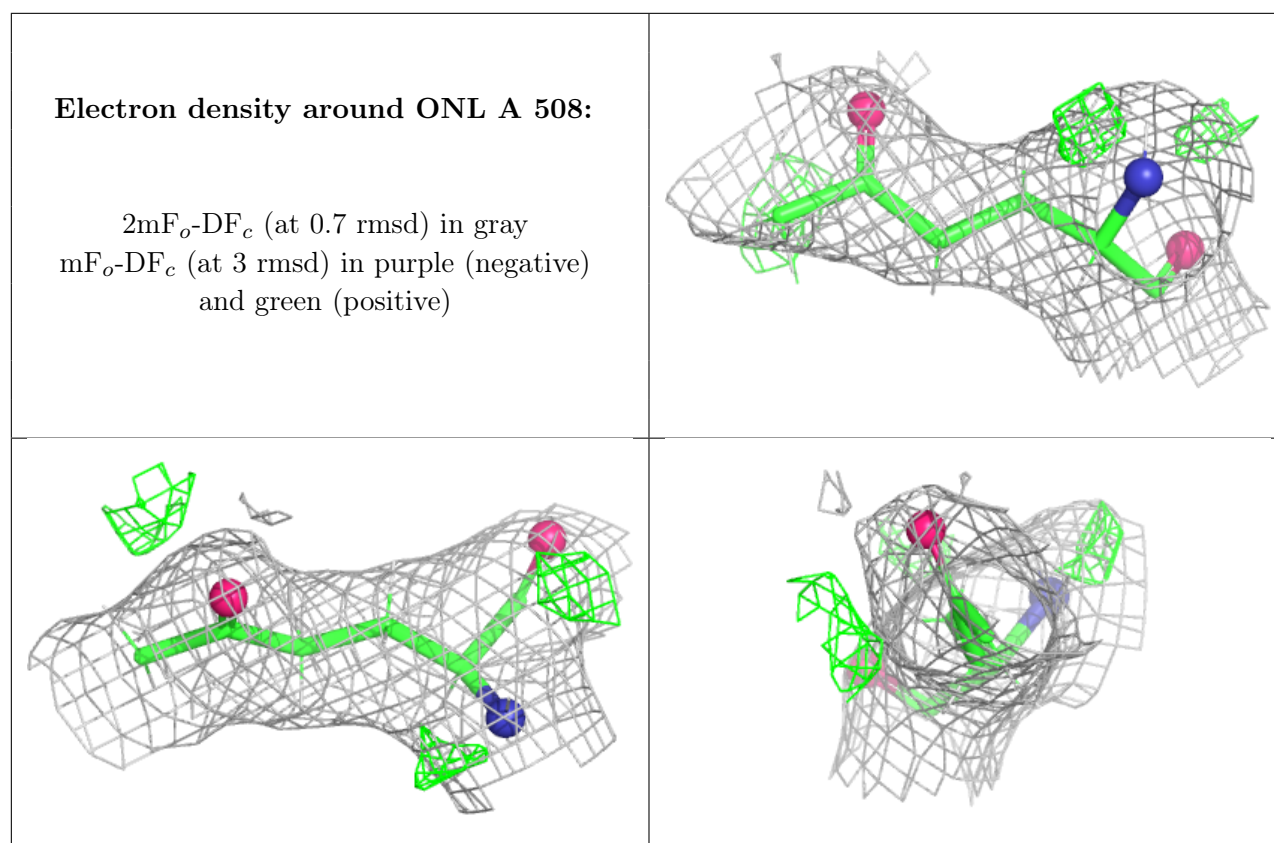
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	C	301	4/4	0.82	0.19	62,71,74,75	1

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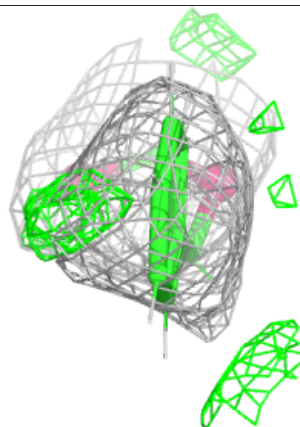
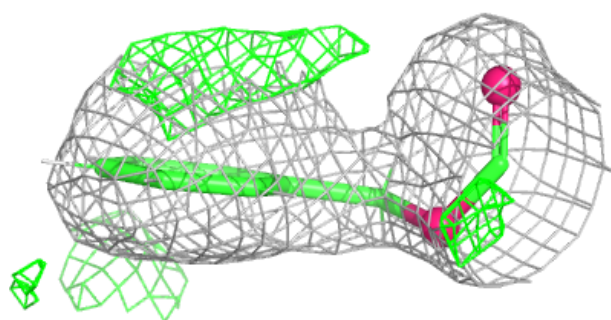
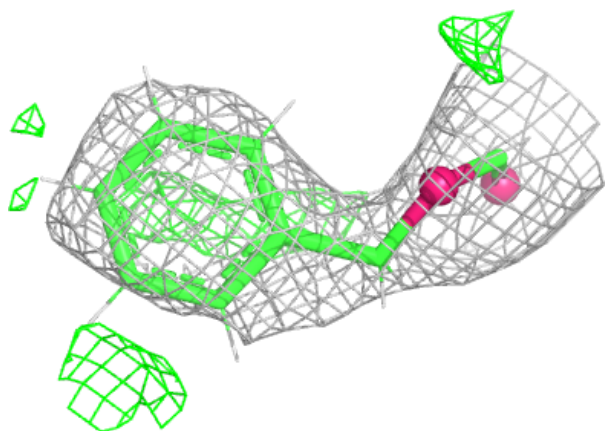
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	503	4/4	0.85	0.14	60,74,82,84	1
5	EDO	B	302	4/4	0.88	0.15	63,72,74,76	1
5	EDO	C	302	4/4	0.89	0.18	71,88,94,97	1
8	ONL	A	508	9/10	0.89	0.09	45,47,57,61	0
7	P6S	A	507	10/11	0.91	0.12	49,68,73,73	0
11	MLL	A	511	10/10	0.91	0.10	61,70,76,80	0
10	DPR	A	510	7/8	0.92	0.11	53,57,64,66	0
5	EDO	B	301	4/4	0.92	0.11	43,55,63,64	1
5	EDO	A	502	4/4	0.93	0.11	56,60,64,64	1
9	DVA	A	509	7/8	0.93	0.12	55,69,77,79	0
6	CA	A	506	1/1	0.98	0.04	55,55,55,55	0
4	SO4	A	501	5/5	0.98	0.09	47,59,64,73	0
6	CA	A	504	1/1	0.99	0.02	28,28,28,28	0
6	CA	A	505	1/1	0.99	0.03	51,51,51,51	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.

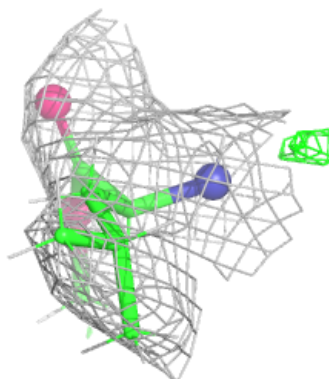
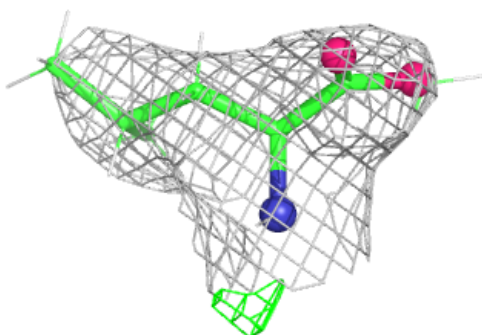
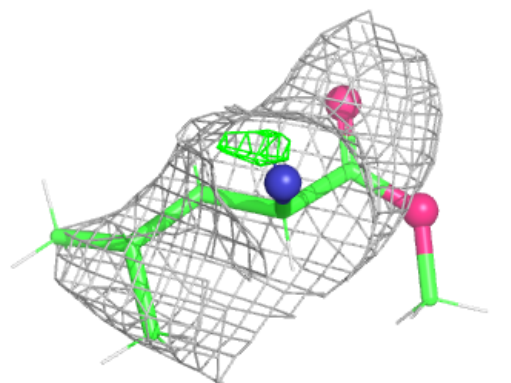


Electron density around P6S A 507:

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

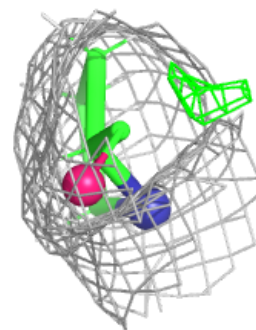
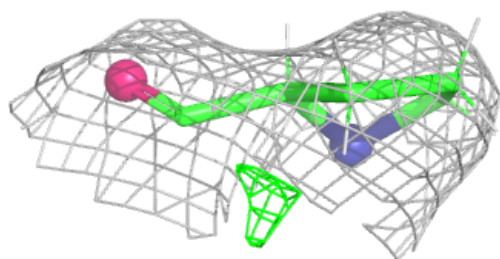
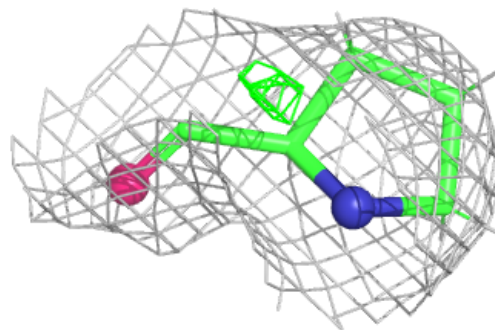
**Electron density around MLL A 511:**

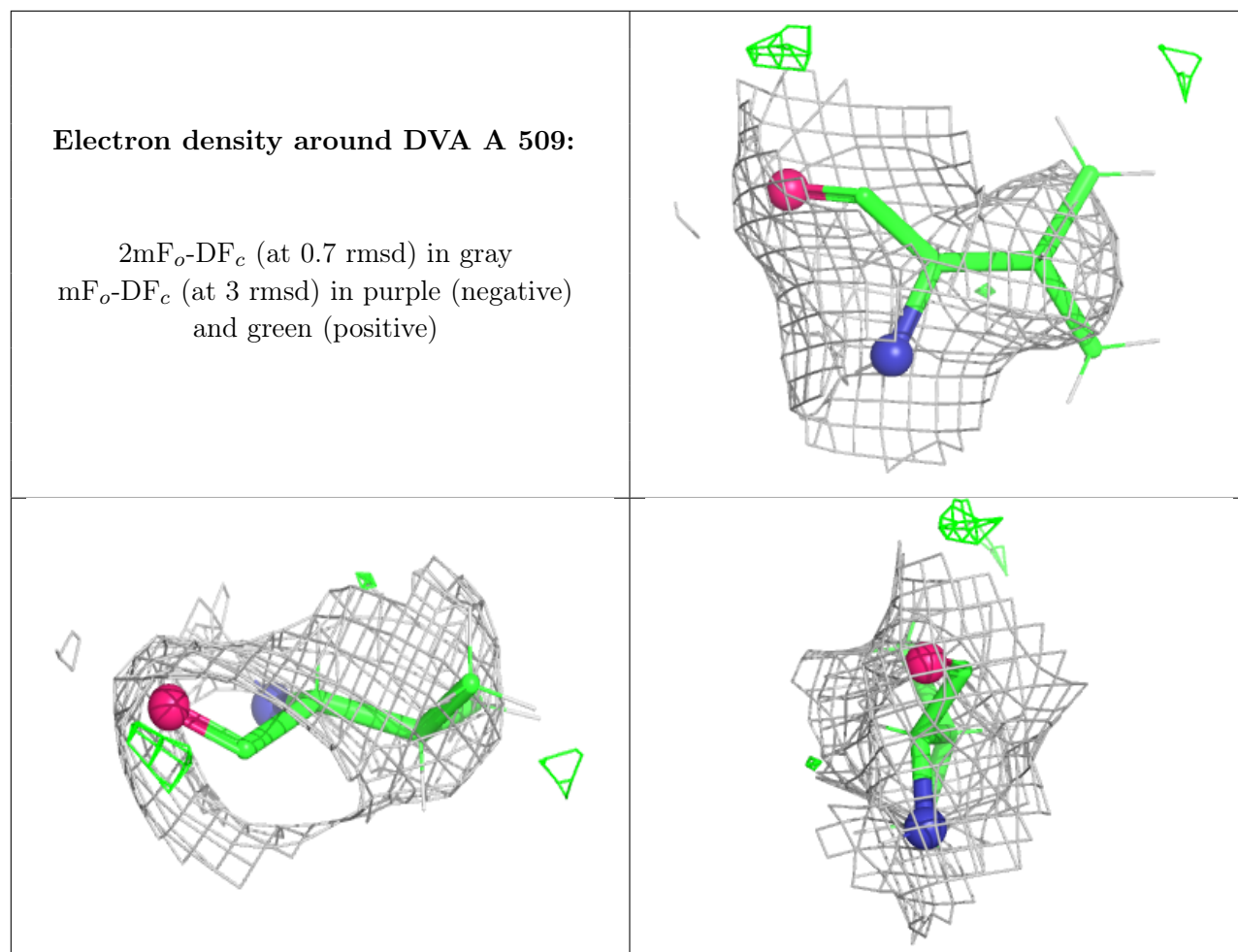
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DPR A 510:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.