Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 06:20 PM EDT

PDB ID	:	4JTD
Title	:	Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Lys27Met mutant of Charybdotoxin
Authors	:	Banerjee, A.; Lee, A.; Campbell, E.; MacKinnon, R.
Deposited on	:	2013-03-23
Resolution	:	2.54 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:

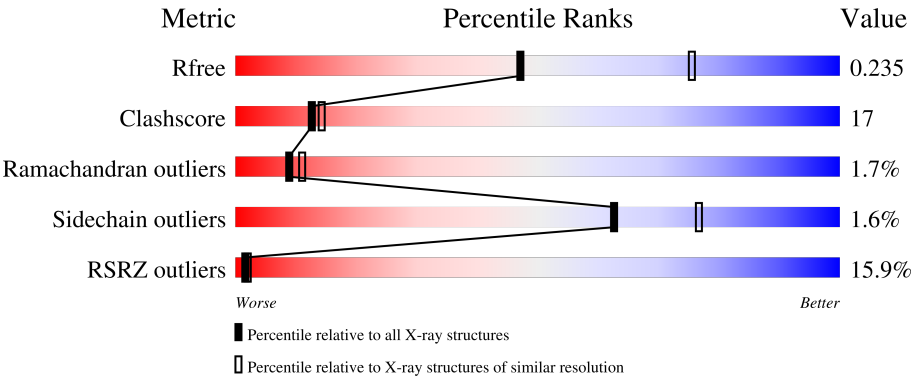
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	333	3% 76% 21%
1	G	333	2% 78% 19%
2	B	514	11% 49% 25% 25%
2	H	514	24% 38% 31% 29%
3	Y	37	89% 46% 49% 5%

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
5	K	H	504	-	-	-	X
6	PGW	B	505	-	-	-	X
6	PGW	B	508	-	-	-	X
6	PGW	B	509	-	-	-	X
6	PGW	B	510	-	-	-	X
6	PGW	B	511	-	-	-	X
6	PGW	B	513	-	-	-	X
6	PGW	B	514	-	-	-	X
6	PGW	B	516	-	-	-	X
6	PGW	B	518	-	-	-	X
6	PGW	B	519	-	-	-	X
6	PGW	B	520	-	-	-	X
6	PGW	H	505	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12082 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 Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			
1	G	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP P62483
G	35	MET	-	expression tag	UNP P62483

- Molecule 2 is a protein called Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	386	Total	C	N	O	S	0	0	0
			3088	2022	504	548	14			
2	H	363	Total	C	N	O	S	0	0	0
			2959	1950	478	518	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	expression tag	UNP P63142
B	-17	ALA	-	expression tag	UNP P63142
B	-16	HIS	-	expression tag	UNP P63142
B	-15	HIS	-	expression tag	UNP P63142
B	-14	HIS	-	expression tag	UNP P63142
B	-13	HIS	-	expression tag	UNP P63142
B	-12	HIS	-	expression tag	UNP P63142
B	-11	HIS	-	expression tag	UNP P63142
B	-10	HIS	-	expression tag	UNP P63142

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P63142
B	-8	HIS	-	expression tag	UNP P63142
B	-7	HIS	-	expression tag	UNP P63142
B	-6	GLY	-	expression tag	UNP P63142
B	-5	LEU	-	expression tag	UNP P63142
B	-4	VAL	-	expression tag	UNP P63142
B	-3	PRO	-	expression tag	UNP P63142
B	-2	ARG	-	expression tag	UNP P63142
B	-1	GLY	-	expression tag	UNP P63142
B	0	SER	-	expression tag	UNP P63142
B	31	SER	CYS	engineered mutation	UNP P63142
B	32	SER	CYS	engineered mutation	UNP P63142
B	207	GLN	ASN	engineered mutation	UNP P63142
B	431	SER	CYS	engineered mutation	UNP P63142
B	478	SER	CYS	engineered mutation	UNP P63142
H	-18	MET	-	expression tag	UNP P63142
H	-17	ALA	-	expression tag	UNP P63142
H	-16	HIS	-	expression tag	UNP P63142
H	-15	HIS	-	expression tag	UNP P63142
H	-14	HIS	-	expression tag	UNP P63142
H	-13	HIS	-	expression tag	UNP P63142
H	-12	HIS	-	expression tag	UNP P63142
H	-11	HIS	-	expression tag	UNP P63142
H	-10	HIS	-	expression tag	UNP P63142
H	-9	HIS	-	expression tag	UNP P63142
H	-8	HIS	-	expression tag	UNP P63142
H	-7	HIS	-	expression tag	UNP P63142
H	-6	GLY	-	expression tag	UNP P63142
H	-5	LEU	-	expression tag	UNP P63142
H	-4	VAL	-	expression tag	UNP P63142
H	-3	PRO	-	expression tag	UNP P63142
H	-2	ARG	-	expression tag	UNP P63142
H	-1	GLY	-	expression tag	UNP P63142
H	0	SER	-	expression tag	UNP P63142
H	31	SER	CYS	engineered mutation	UNP P63142
H	32	SER	CYS	engineered mutation	UNP P63142
H	207	GLN	ASN	engineered mutation	UNP P63142
H	431	SER	CYS	engineered mutation	UNP P63142
H	478	SER	CYS	engineered mutation	UNP P63142

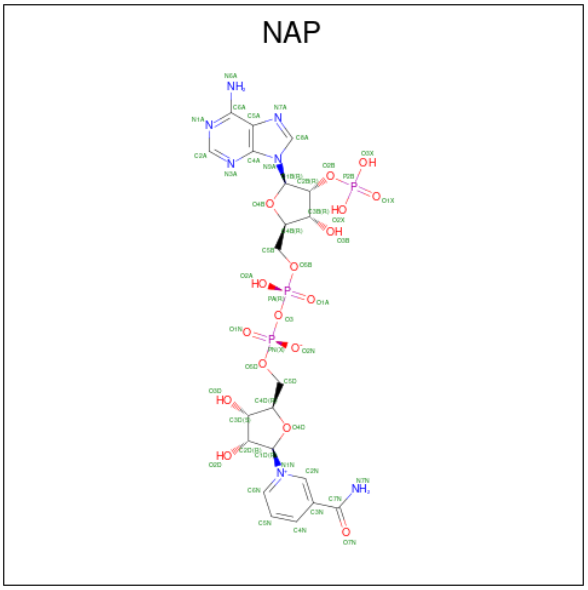
- Molecule 3 is a protein called Potassium channel toxin alpha-KTx 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	37	Total	C	N	O	S	0	0	0
			294	175	56	55	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	27	MET	LYS	engineered mutation	UNP P13487

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



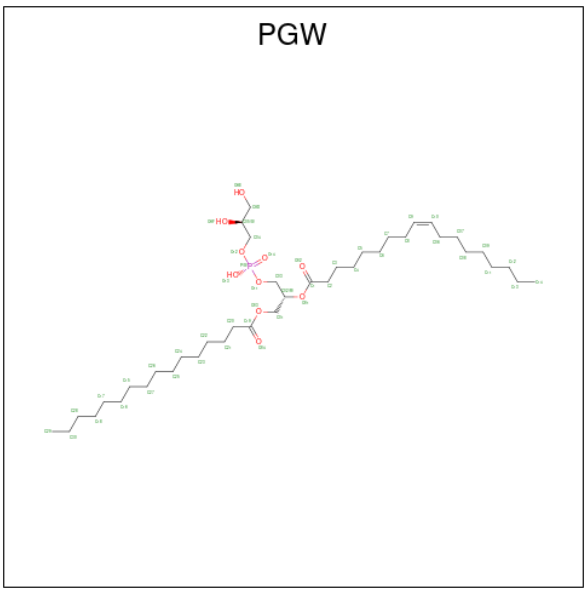
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	K	0	0
			4	4		
5	H	4	Total	K	0	0
			4	4		

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula:

$C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 22 17 5	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 7 7	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C O P 23 14 8 1	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C O P 36 25 10 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C 7 7	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C 8 8	0	0
6	H	1	Total C O 22 17 5	0	0

- Molecule 7 is water.

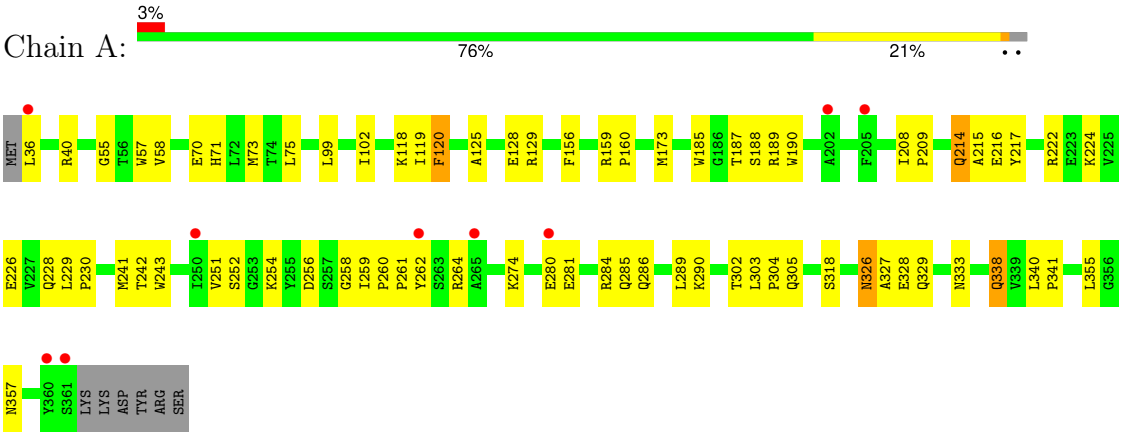
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	140	Total O 140 140	0	0
7	B	50	Total O 50 50	0	0
7	G	102	Total O 102 102	0	0
7	H	21	Total O 21 21	0	0

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.

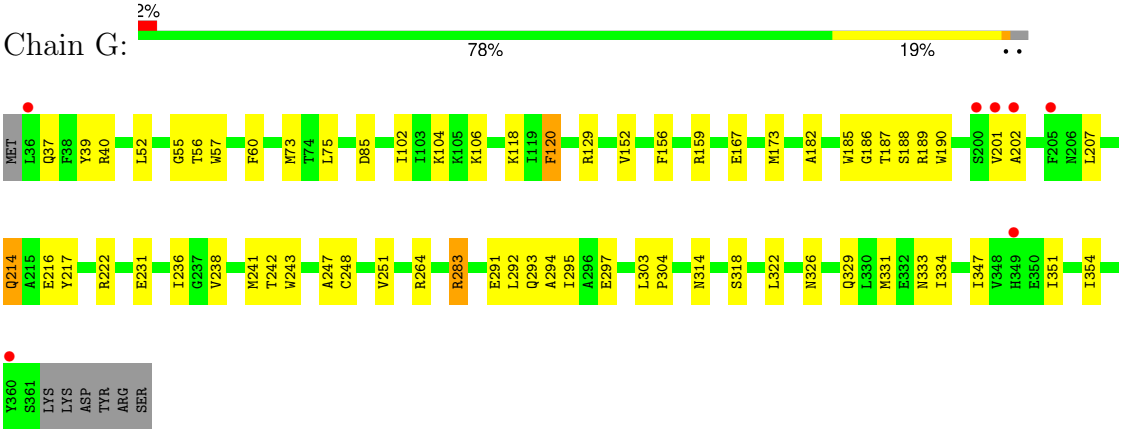
• Molecule 1: Voltage-gated potassium channel subunit beta-2

Chain A:



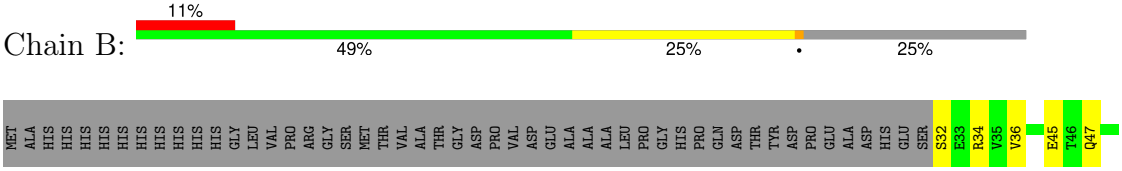
• Molecule 1: Voltage-gated potassium channel subunit beta-2

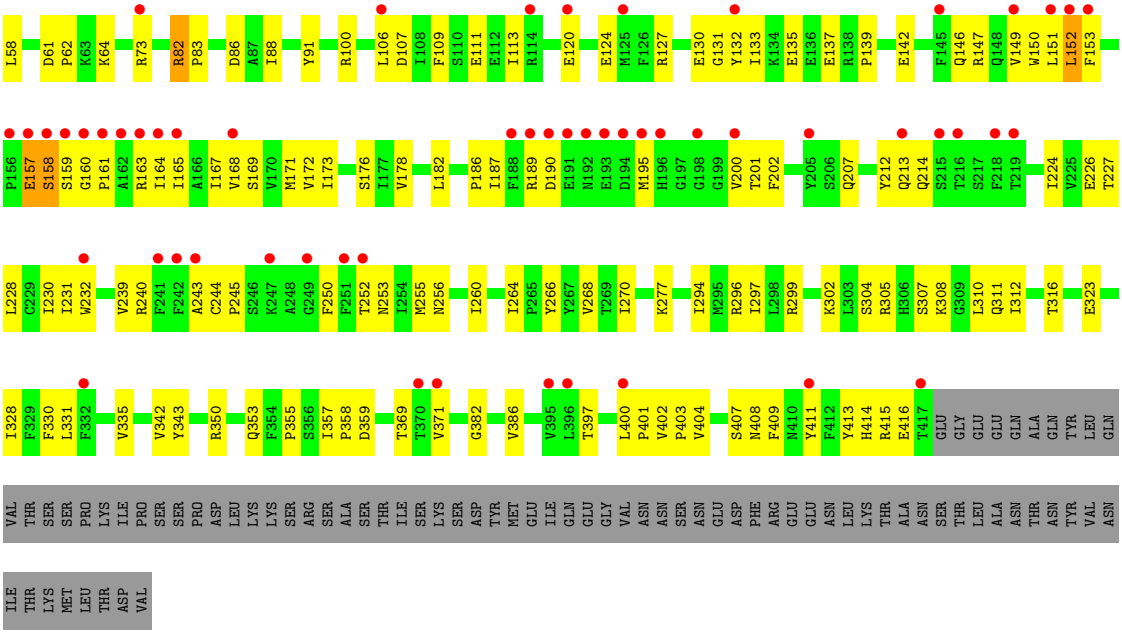
Chain G:



• Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1

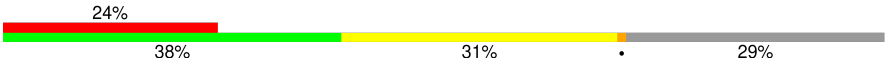
Chain B:

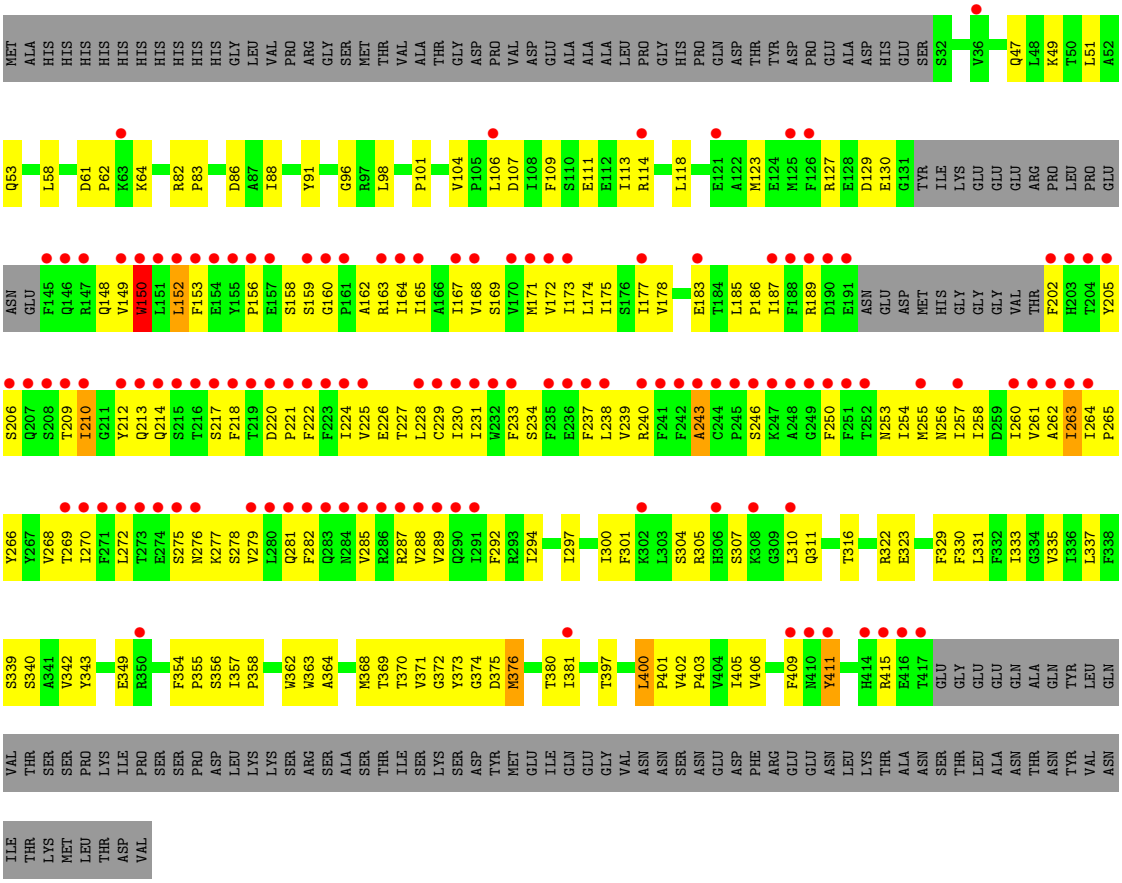




• Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1

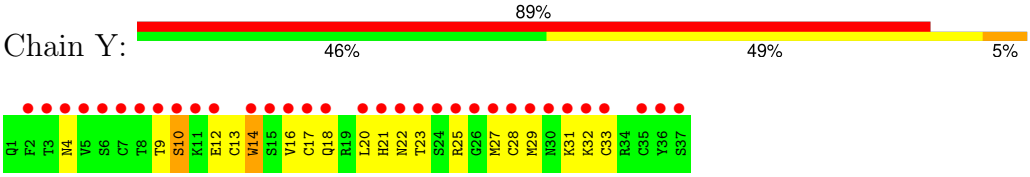
Chain H:





• Molecule 3: Potassium channel toxin alpha-KTx 1.1

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.87Å 144.87Å 284.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.54 49.71 – 2.54	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.54) 94.8 (49.71-2.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.235 0.209 , 0.235	Depositor DCC
R_{free} test set	4707 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 66.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12082	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, K, NAP, PGW

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	0.38	0/2608	0.57	0/3524
1	G	0.36	0/2608	0.56	0/3524
2	B	0.35	0/3169	0.52	0/4292
2	H	0.32	0/3036	0.49	0/4114
3	Y	0.27	0/291	0.46	0/388
All	All	0.35	0/11712	0.53	0/15842

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

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	2556	0	2582	54	0
1	G	2556	0	2582	48	0
2	B	3088	0	3034	95	0
2	H	2959	0	2956	166	0
3	Y	294	0	278	18	0
4	A	48	0	25	11	0
4	G	48	0	25	13	0
5	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	4	0	0	0	0
6	B	190	0	251	11	0
6	H	22	0	25	5	0
7	A	140	0	0	0	0
7	B	50	0	0	3	0
7	G	102	0	0	1	0
7	H	21	0	0	1	0
All	All	12082	0	11758	393	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 17.

All (393) 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)
3:Y:4:ASN:HA	3:Y:32:LYS:HD3	1.44	0.96
1:G:333:ASN:HD21	4:G:1001:NAP:H61A	1.15	0.91
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.56	0.87
1:G:55:GLY:HA3	4:G:1001:NAP:O3D	1.74	0.86
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.57	0.86
2:H:148:GLN:HE21	2:H:152:LEU:HD23	1.38	0.85
2:B:311:GLN:HG2	6:B:517:PGW:H3	1.59	0.85
2:H:210:ILE:HD13	2:H:214:GLN:HB3	1.57	0.85
1:A:55:GLY:HA3	4:A:1001:NAP:O3D	1.78	0.84
2:B:58:LEU:HD12	2:B:64:LYS:HB3	1.57	0.83
2:H:185:LEU:HD12	2:H:186:PRO:HD2	1.61	0.83
2:H:287:ARG:HB2	2:H:287:ARG:NH1	1.95	0.81
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.66	0.77
2:H:285:VAL:HG23	2:H:288:VAL:HB	1.65	0.77
2:H:213:GLN:HG2	2:H:220:ASP:HB2	1.65	0.77
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.34	0.75
2:H:358:PRO:HB3	6:H:505:PGW:H20A	1.69	0.75
1:G:40:ARG:HD2	1:G:318:SER:O	1.86	0.74
1:G:189:ARG:HH21	4:G:1001:NAP:H71N	1.35	0.72
2:H:163:ARG:HB2	2:H:163:ARG:NH1	2.04	0.72
2:H:210:ILE:HG21	2:H:214:GLN:HB2	1.73	0.69
1:A:36:LEU:HG	1:A:341:PRO:HG3	1.75	0.68
2:B:227:THR:O	2:B:231:ILE:HG12	1.93	0.68
2:H:227:THR:O	2:H:231:ILE:HG12	1.94	0.68
2:H:287:ARG:HB2	2:H:287:ARG:HH11	1.60	0.67
2:B:253:ASN:ND2	2:B:255:MET:HB2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1001:NAP:H52A	4:G:1001:NAP:H8A	1.76	0.67
2:H:107:ASP:O	2:H:111:GLU:HG3	1.94	0.67
2:B:176:SER:OG	2:B:299:ARG:HD3	1.94	0.66
4:A:1001:NAP:H8A	4:A:1001:NAP:H52A	1.77	0.66
2:H:148:GLN:NE2	2:H:152:LEU:HD23	2.08	0.66
3:Y:17:CYS:O	3:Y:21:HIS:HB2	1.97	0.65
1:A:159:ARG:HA	1:A:188:SER:O	1.97	0.65
2:B:226:GLU:O	2:B:230:ILE:HD13	1.97	0.65
2:H:264:ILE:HB	2:H:265:PRO:HD3	1.79	0.64
2:B:253:ASN:HD21	2:B:255:MET:HB2	1.63	0.64
2:H:152:LEU:HD12	2:H:153:PHE:N	2.12	0.63
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.80	0.63
2:H:240:ARG:HH22	2:H:305:ARG:HD3	1.63	0.63
2:H:363:TRP:HB2	2:H:376:MET:HE2	1.79	0.62
2:B:304:SER:HA	2:B:310:LEU:HD23	1.82	0.62
2:H:263:ILE:HD13	2:H:263:ILE:H	1.65	0.62
3:Y:13:CYS:SG	3:Y:28:CYS:HB2	2.39	0.62
1:A:189:ARG:HH21	4:A:1001:NAP:H71N	1.46	0.61
2:B:214:GLN:NE2	2:B:270:ILE:HG12	2.16	0.61
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.81	0.60
3:Y:14:TRP:HA	3:Y:14:TRP:HE3	1.66	0.60
2:B:146:GLN:HG3	2:B:243:ALA:HA	1.82	0.60
2:H:205:TYR:HE2	2:H:282:PHE:HB3	1.66	0.60
3:Y:14:TRP:HA	3:Y:14:TRP:CE3	2.35	0.60
2:H:174:LEU:O	2:H:178:VAL:HG23	2.02	0.60
2:H:381:ILE:N	2:H:381:ILE:HD12	2.16	0.60
2:H:272:LEU:HD13	2:H:289:VAL:HG22	1.84	0.60
2:H:400:LEU:O	2:H:403:PRO:HD2	2.02	0.59
1:A:258:GLY:O	1:A:260:PRO:HD3	2.03	0.59
2:H:253:ASN:HB3	2:H:256:ASN:HD22	1.68	0.59
2:B:255:MET:CE	2:B:305:ARG:HA	2.33	0.59
2:H:265:PRO:O	2:H:269:THR:HG23	2.03	0.58
2:B:330:PHE:HB3	2:B:397:THR:HG23	1.85	0.58
2:H:169:SER:O	2:H:173:ILE:HG13	2.03	0.58
2:B:328:ILE:HG23	6:B:505:PGW:C9	2.33	0.58
2:B:61:ASP:OD2	2:B:64:LYS:HG3	2.04	0.58
2:B:186:PRO:O	2:B:190:ASP:HB2	2.03	0.58
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.18	0.58
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.86	0.58
2:H:362:TRP:HB2	6:H:505:PGW:H2A	1.86	0.58
2:B:294:ILE:O	2:B:297:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ARG:HH11	2:B:305:ARG:HG3	1.68	0.57
2:H:101:PRO:HB2	2:H:104:VAL:HG23	1.86	0.57
2:H:369:THR:OG1	2:H:371:VAL:HG23	2.04	0.57
2:H:98:LEU:HD21	2:H:113:ILE:HD13	1.86	0.57
2:H:149:VAL:O	2:H:243:ALA:HB1	2.03	0.57
2:H:189:ARG:HG3	2:H:189:ARG:HH11	1.70	0.57
2:H:331:LEU:O	2:H:335:VAL:HG23	2.05	0.57
1:G:251:VAL:HG12	1:G:251:VAL:O	2.04	0.57
2:H:304:SER:HA	2:H:310:LEU:HD23	1.85	0.57
1:G:293:GLN:HE21	1:G:297:GLU:HG3	1.69	0.56
2:B:100:ARG:HG3	2:B:109:PHE:CG	2.41	0.56
2:H:276:ASN:HA	2:H:281:GLN:NE2	2.19	0.56
2:H:168:VAL:HA	2:H:171:MET:HG2	1.88	0.56
2:H:330:PHE:HB3	2:H:397:THR:HG23	1.87	0.56
2:B:323:GLU:CD	2:B:323:GLU:H	2.09	0.56
2:H:212:TYR:HB3	2:H:222:PHE:HB2	1.88	0.55
2:H:402:VAL:O	2:H:406:VAL:HG23	2.06	0.55
6:H:505:PGW:H03A	6:H:505:PGW:O02	2.07	0.55
2:H:88:ILE:O	2:H:91:TYR:HB3	2.07	0.55
2:H:158:SER:HB3	2:H:162:ALA:HB1	1.87	0.55
1:A:55:GLY:CA	4:A:1001:NAP:O3D	2.54	0.55
2:B:164:ILE:O	2:B:168:VAL:HG23	2.07	0.55
2:B:169:SER:HA	2:B:232:TRP:HE1	1.71	0.55
2:B:260:ILE:O	2:B:264:ILE:HG13	2.05	0.55
1:G:333:ASN:ND2	4:G:1001:NAP:H61A	1.94	0.55
2:B:120:GLU:O	2:B:124:GLU:HG3	2.07	0.54
2:B:142:GLU:H	2:B:147:ARG:CB	2.21	0.54
2:H:258:ILE:HG21	2:H:301:PHE:O	2.07	0.54
6:B:515:PGW:O02	6:B:515:PGW:O11	2.25	0.54
1:G:55:GLY:CA	4:G:1001:NAP:O3D	2.51	0.54
2:H:123:MET:O	2:H:127:ARG:HG3	2.07	0.54
2:H:253:ASN:O	2:H:257:ILE:HG12	2.08	0.54
2:H:187:ILE:HG22	2:H:187:ILE:O	2.06	0.54
1:A:251:VAL:O	1:A:251:VAL:HG12	2.07	0.54
2:B:107:ASP:O	2:B:111:GLU:HG3	2.08	0.54
6:B:517:PGW:H03A	6:B:517:PGW:O02	2.07	0.54
2:H:58:LEU:C	2:H:58:LEU:HD23	2.28	0.54
2:B:308:LYS:NZ	6:B:517:PGW:HAD	2.23	0.54
1:G:189:ARG:HE	4:G:1001:NAP:H72N	1.56	0.54
2:H:230:ILE:HD12	2:H:230:ILE:H	1.72	0.54
2:B:304:SER:CA	2:B:310:LEU:HD23	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ILE:O	2:B:176:SER:HB3	2.08	0.53
2:H:202:PHE:HB3	2:H:279:VAL:HG22	1.91	0.53
2:H:307:SER:O	2:H:311:GLN:HG3	2.09	0.53
2:B:73:ARG:HD3	7:B:642:HOH:O	2.09	0.53
1:G:57:TRP:HB3	4:G:1001:NAP:H3D	1.91	0.53
2:H:213:GLN:CG	2:H:220:ASP:HB2	2.36	0.53
6:H:505:PGW:O02	6:H:505:PGW:H01	2.08	0.53
3:Y:29:MET:C	3:Y:31:LYS:H	2.12	0.53
2:B:159:SER:HB2	2:B:161:PRO:HD2	1.90	0.53
3:Y:28:CYS:HB2	3:Y:33:CYS:HA	1.91	0.53
2:B:157:GLU:O	2:B:158:SER:O	2.27	0.52
6:B:505:PGW:H01	6:B:505:PGW:O02	2.09	0.52
2:H:285:VAL:CG2	2:H:288:VAL:HB	2.36	0.52
2:H:106:LEU:CD1	2:H:130:GLU:HG2	2.39	0.52
2:H:285:VAL:HG22	2:H:289:VAL:HG23	1.90	0.52
2:H:230:ILE:HD12	2:H:230:ILE:N	2.24	0.52
2:H:246:SER:O	2:H:250:PHE:HB2	2.09	0.52
1:G:37:GLN:HG3	1:G:39:TYR:O	2.10	0.52
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.44	0.52
2:H:172:VAL:HG12	2:H:233:PHE:CZ	2.44	0.52
2:H:263:ILE:HD13	2:H:263:ILE:N	2.24	0.52
2:H:268:VAL:HB	2:H:292:PHE:CE2	2.45	0.52
2:H:329:PHE:O	2:H:333:ILE:HG12	2.09	0.52
3:Y:18:GLN:HG3	3:Y:23:THR:O	2.09	0.52
2:H:287:ARG:HH11	2:H:287:ARG:CB	2.21	0.52
2:B:149:VAL:O	2:B:152:LEU:HD12	2.10	0.52
1:A:125:ALA:HB3	1:A:128:GLU:HG3	1.91	0.52
2:B:250:PHE:C	2:B:252:THR:H	2.14	0.52
2:H:411:TYR:CZ	2:H:415:ARG:HD3	2.45	0.52
2:B:316:THR:HG21	2:B:409:PHE:HB2	1.92	0.51
1:G:295:ILE:H	1:G:295:ILE:HD12	1.74	0.51
1:A:261:PRO:O	1:A:262:TYR:HB2	2.10	0.51
2:B:256:ASN:O	2:B:260:ILE:HG13	2.10	0.51
1:G:85:ASP:OD1	1:G:118:LYS:NZ	2.43	0.51
1:A:329:GLN:OE1	4:A:1001:NAP:H2B	2.10	0.51
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.46	0.51
2:B:240:ARG:NH2	2:B:305:ARG:HD3	2.26	0.51
2:H:237:PHE:CE1	2:H:260:ILE:HG12	2.46	0.51
1:G:331:MET:HE2	1:G:334:ILE:HD12	1.91	0.51
2:H:163:ARG:HB2	2:H:163:ARG:HH11	1.73	0.51
2:B:404:VAL:O	2:B:407:SER:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:511:PGW:H2A	6:B:516:PGW:H16	1.91	0.51
1:G:295:ILE:HD12	1:G:295:ILE:N	2.26	0.51
2:H:368:MET:C	2:H:370:THR:H	2.12	0.51
2:H:109:PHE:CE2	2:H:113:ILE:HD11	2.46	0.51
2:H:159:SER:O	2:H:163:ARG:HG3	2.11	0.51
1:A:36:LEU:N	1:A:36:LEU:HD12	2.26	0.51
2:H:86:ASP:HB2	7:H:616:HOH:O	2.11	0.50
2:H:217:SER:O	2:H:218:PHE:HB2	2.12	0.50
2:B:240:ARG:O	2:B:244:CYS:HB2	2.10	0.50
1:G:118:LYS:HG2	1:G:156:PHE:HB2	1.92	0.50
1:G:291:GLU:O	1:G:294:ALA:HB3	2.11	0.50
2:H:230:ILE:HG12	2:H:266:TYR:CG	2.46	0.50
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.77	0.50
1:G:236:ILE:HG13	1:G:238:VAL:HG23	1.92	0.50
2:H:224:ILE:O	2:H:228:LEU:HG	2.11	0.50
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.93	0.50
2:H:258:ILE:O	2:H:262:ALA:HB2	2.11	0.50
1:G:214:GLN:HA	1:G:241:MET:O	2.10	0.50
1:G:326:ASN:OD1	1:G:329:GLN:HG3	2.12	0.50
2:H:415:ARG:HG2	2:H:415:ARG:HH11	1.76	0.50
3:Y:25:ARG:HB2	3:Y:25:ARG:NH1	2.27	0.50
1:A:57:TRP:HB3	4:A:1001:NAP:H3D	1.93	0.49
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.27	0.49
2:B:355:PRO:HB2	2:B:359:ASP:OD2	2.12	0.49
1:G:189:ARG:NH2	4:G:1001:NAP:H71N	2.08	0.49
3:Y:20:LEU:N	3:Y:20:LEU:HD12	2.27	0.49
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.47	0.49
1:G:173:MET:HG3	1:G:185:TRP:CE3	2.48	0.49
2:H:374:GLY:C	2:H:376:MET:H	2.15	0.49
2:B:167:ILE:O	2:B:171:MET:HG2	2.13	0.49
2:B:331:LEU:O	2:B:335:VAL:HG23	2.12	0.49
2:H:264:ILE:O	2:H:268:VAL:HG23	2.12	0.49
1:G:329:GLN:OE1	4:G:1001:NAP:H2B	2.13	0.49
2:H:294:ILE:O	2:H:297:ILE:HG22	2.13	0.49
2:H:148:GLN:HE21	2:H:152:LEU:CD2	2.18	0.49
2:H:163:ARG:HH11	2:H:163:ARG:CB	2.26	0.49
2:H:322:ARG:HG3	2:H:322:ARG:HH11	1.78	0.49
2:B:168:VAL:O	2:B:172:VAL:HG23	2.12	0.49
1:G:292:LEU:HA	1:G:295:ILE:HD13	1.95	0.48
2:H:47:GLN:NE2	2:H:49:LYS:HE2	2.28	0.48
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:212:TYR:OH	2:H:226:GLU:HG2	2.13	0.48
2:H:260:ILE:O	2:H:264:ILE:HG13	2.13	0.48
2:H:159:SER:H	2:H:162:ALA:HB3	1.78	0.48
2:H:171:MET:O	2:H:175:ILE:HG13	2.13	0.48
2:H:230:ILE:HG12	2:H:266:TYR:CB	2.43	0.48
1:A:73:MET:SD	1:A:99:LEU:HD12	2.53	0.48
1:A:224:LYS:HA	1:A:228:GLN:HG3	1.96	0.48
2:B:201:THR:HG22	2:B:202:PHE:N	2.28	0.48
2:H:202:PHE:N	2:H:206:SER:HB3	2.28	0.48
2:H:255:MET:CE	2:H:305:ARG:HA	2.44	0.48
2:H:281:GLN:O	2:H:285:VAL:HG12	2.13	0.48
1:A:355:LEU:HB3	1:A:357:ASN:OD1	2.14	0.48
2:H:240:ARG:HH12	2:H:305:ARG:CZ	2.27	0.48
2:H:268:VAL:HB	2:H:292:PHE:HE2	1.79	0.48
2:B:36:VAL:HG22	2:B:45:GLU:HG2	1.96	0.47
2:B:149:VAL:C	2:B:151:LEU:H	2.18	0.47
2:H:316:THR:HG21	2:H:409:PHE:HB2	1.95	0.47
2:H:400:LEU:C	2:H:403:PRO:HD2	2.34	0.47
2:B:150:TRP:HB2	2:B:243:ALA:O	2.14	0.47
2:B:230:ILE:HG21	2:B:266:TYR:CD2	2.49	0.47
2:B:299:ARG:O	2:B:302:LYS:HB2	2.15	0.47
2:H:106:LEU:HD13	2:H:130:GLU:HG2	1.96	0.47
2:H:221:PRO:O	2:H:225:VAL:HG23	2.15	0.47
2:H:381:ILE:HD12	2:H:381:ILE:H	1.77	0.47
2:H:277:LYS:O	2:H:277:LYS:HG3	2.15	0.47
1:A:338:GLN:HE21	1:A:338:GLN:HA	1.80	0.47
1:G:247:ALA:O	1:G:248:CYS:HB2	2.15	0.47
2:H:270:ILE:N	2:H:270:ILE:HD12	2.29	0.47
2:H:339:SER:O	2:H:342:VAL:HG12	2.14	0.47
2:H:354:PHE:HE1	2:H:376:MET:HE2	1.80	0.47
2:H:212:TYR:HB3	2:H:222:PHE:CB	2.45	0.47
3:Y:17:CYS:HB2	3:Y:23:THR:O	2.15	0.47
1:A:286:GLN:NE2	1:A:289:LEU:HD12	2.30	0.47
2:B:264:ILE:O	2:B:268:VAL:HG23	2.15	0.47
2:H:285:VAL:HG22	2:H:285:VAL:O	2.14	0.47
2:B:415:ARG:HH11	2:B:415:ARG:HG2	1.80	0.47
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.97	0.46
2:H:337:LEU:C	2:H:337:LEU:HD23	2.36	0.46
1:A:216:GLU:HB2	1:A:243:TRP:CH2	2.50	0.46
1:A:326:ASN:HD22	1:A:328:GLU:H	1.62	0.46
2:B:212:TYR:CE2	2:B:226:GLU:HG2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:SER:HB3	2:H:162:ALA:CB	2.45	0.46
2:B:160:GLY:N	2:B:161:PRO:CD	2.78	0.46
2:H:212:TYR:HA	2:H:220:ASP:OD1	2.16	0.46
2:H:239:VAL:O	2:H:243:ALA:HB3	2.15	0.46
2:H:372:GLY:O	2:H:374:GLY:N	2.49	0.46
1:A:256:ASP:HB2	1:A:290:LYS:NZ	2.30	0.46
1:G:216:GLU:HB2	1:G:243:TRP:CH2	2.51	0.46
2:H:111:GLU:O	2:H:114:ARG:HB3	2.15	0.46
1:G:217:TYR:HB3	1:G:242:THR:HB	1.97	0.46
4:G:1001:NAP:H52N	4:G:1001:NAP:H6N	1.98	0.46
2:H:255:MET:HB3	2:H:305:ARG:NH2	2.30	0.46
2:H:268:VAL:HG12	2:H:268:VAL:O	2.15	0.46
2:H:305:ARG:HG3	2:H:305:ARG:HH11	1.81	0.46
2:B:305:ARG:HG3	2:B:305:ARG:NH1	2.30	0.46
1:G:167:GLU:HA	1:G:201:VAL:HG11	1.96	0.46
6:B:511:PGW:C1	6:B:516:PGW:H16	2.46	0.46
2:B:163:ARG:O	2:B:167:ILE:HG12	2.16	0.46
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.98	0.46
2:B:127:ARG:HG2	2:B:127:ARG:NH1	2.30	0.46
2:B:353:GLN:O	2:B:355:PRO:HD3	2.16	0.46
2:H:343:TYR:CE1	2:H:356:SER:HA	2.51	0.46
2:H:364:ALA:O	2:H:368:MET:HG3	2.16	0.46
2:H:254:ILE:O	2:H:258:ILE:HG13	2.16	0.46
3:Y:10:SER:C	3:Y:12:GLU:H	2.19	0.46
1:A:264:ARG:NH2	4:A:1001:NAP:H4B	2.31	0.45
2:H:276:ASN:ND2	2:H:285:VAL:HG21	2.31	0.45
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.31	0.45
2:B:106:LEU:HD13	2:B:130:GLU:HG2	1.99	0.45
2:H:82:ARG:HB2	2:H:83:PRO:HD3	1.97	0.45
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.81	0.45
2:H:229:CYS:HB3	2:H:233:PHE:HE2	1.82	0.45
2:H:189:ARG:HG3	2:H:189:ARG:NH1	2.32	0.45
1:A:217:TYR:HB3	1:A:242:THR:HB	1.99	0.45
1:A:252:SER:OG	1:A:254:LYS:HG2	2.16	0.45
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.80	0.45
2:B:307:SER:OG	2:B:310:LEU:HB2	2.16	0.45
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.51	0.45
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.52	0.45
1:G:52:LEU:HD13	1:G:322:LEU:HD11	1.98	0.45
2:H:272:LEU:CD1	2:H:289:VAL:HG22	2.45	0.45
2:H:113:ILE:HG23	2:H:118:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:16:VAL:C	3:Y:18:GLN:H	2.19	0.45
1:A:254:LYS:HE3	4:A:1001:NAP:N3A	2.31	0.44
1:A:214:GLN:HA	1:A:241:MET:O	2.16	0.44
2:H:230:ILE:H	2:H:230:ILE:CD1	2.30	0.44
2:B:328:ILE:HG13	6:B:511:PGW:C9	2.48	0.44
1:G:303:LEU:HB3	1:G:304:PRO:HD3	1.99	0.44
2:B:382:GLY:O	2:B:386:VAL:HG23	2.18	0.44
2:H:213:GLN:HA	2:H:213:GLN:NE2	2.31	0.44
2:H:234:SER:O	2:H:238:LEU:HG	2.17	0.44
2:B:32:SER:HB3	2:B:47:GLN:HE21	1.83	0.44
1:G:120:PHE:O	1:G:129:ARG:HA	2.17	0.44
2:H:177:ILE:HD13	2:H:300:ILE:CD1	2.47	0.44
2:H:213:GLN:HA	2:H:213:GLN:HE21	1.83	0.44
2:H:400:LEU:HB2	2:H:401:PRO:CD	2.39	0.44
6:B:505:PGW:O02	6:B:505:PGW:H03A	2.18	0.44
1:G:37:GLN:NE2	1:G:37:GLN:HA	2.33	0.44
2:H:343:TYR:HE1	2:H:355:PRO:O	2.01	0.44
2:B:224:ILE:O	2:B:228:LEU:HG	2.17	0.44
2:H:150:TRP:HA	2:H:150:TRP:CE3	2.53	0.44
2:H:210:ILE:HG21	2:H:214:GLN:CB	2.43	0.44
2:H:229:CYS:HB3	2:H:233:PHE:CE2	2.52	0.44
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.98	0.44
1:G:56:THR:HB	1:G:60:PHE:HB2	1.99	0.44
1:G:104:LYS:HG3	7:G:1163:HOH:O	2.18	0.44
2:H:150:TRP:HA	2:H:150:TRP:HE3	1.82	0.44
2:H:173:ILE:HG12	2:H:233:PHE:HE1	1.83	0.44
2:H:270:ILE:HG22	2:H:270:ILE:O	2.16	0.44
1:G:37:GLN:HA	1:G:37:GLN:HE21	1.83	0.43
1:G:102:ILE:O	1:G:106:LYS:HG2	2.17	0.43
2:H:91:TYR:CE2	2:H:118:LEU:HD22	2.53	0.43
2:H:162:ALA:HA	2:H:165:ILE:CD1	2.48	0.43
2:H:261:VAL:HA	2:H:264:ILE:HG13	2.00	0.43
2:H:368:MET:C	2:H:370:THR:N	2.72	0.43
1:A:188:SER:O	1:A:189:ARG:HB2	2.18	0.43
1:G:264:ARG:NH2	4:G:1001:NAP:H4B	2.33	0.43
2:H:261:VAL:HG12	2:H:261:VAL:O	2.18	0.43
1:A:229:LEU:N	1:A:230:PRO:CD	2.82	0.43
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.17	0.43
2:B:414:HIS:C	2:B:416:GLU:N	2.70	0.43
3:Y:29:MET:HG3	3:Y:31:LYS:HB3	2.00	0.43
2:H:256:ASN:O	2:H:260:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:GLU:HA	1:A:102:ILE:HD13	2.01	0.43
2:B:414:HIS:C	2:B:416:GLU:H	2.21	0.43
1:G:283:ARG:HG3	1:G:283:ARG:HH11	1.83	0.43
1:A:281:GLU:O	1:A:285:GLN:HG3	2.17	0.43
2:B:277:LYS:HG3	2:B:277:LYS:O	2.18	0.43
2:H:337:LEU:HD23	2:H:337:LEU:O	2.19	0.43
2:B:178:VAL:O	2:B:182:LEU:HG	2.19	0.43
2:B:255:MET:HE3	2:B:305:ARG:HA	2.00	0.43
1:G:156:PHE:HA	1:G:186:GLY:O	2.18	0.43
2:H:276:ASN:HD21	2:H:285:VAL:HG21	1.83	0.43
2:B:350:ARG:NH1	2:B:350:ARG:CB	2.81	0.43
2:H:152:LEU:HA	2:H:158:SER:OG	2.18	0.43
2:H:209:THR:O	2:H:209:THR:HG22	2.18	0.43
2:H:230:ILE:HG21	2:H:266:TYR:CD2	2.54	0.43
1:A:222:ARG:HB3	1:A:226:GLU:OE2	2.18	0.43
2:H:156:PRO:O	2:H:163:ARG:HA	2.19	0.43
2:H:278:SER:OG	2:H:281:GLN:HG3	2.19	0.43
2:H:358:PRO:HB3	6:H:505:PGW:C20	2.42	0.43
2:H:402:VAL:HB	2:H:403:PRO:HD3	2.01	0.43
2:B:195:MET:HE3	7:B:626:HOH:O	2.18	0.42
1:G:55:GLY:HA3	4:G:1001:NAP:HO3N	1.76	0.42
2:H:287:ARG:HB2	2:H:287:ARG:CZ	2.50	0.42
2:H:349:GLU:HG3	2:H:380:THR:CG2	2.49	0.42
1:A:119:ILE:O	1:A:120:PHE:HB2	2.19	0.42
1:G:152:VAL:O	1:G:182:ALA:HA	2.18	0.42
1:G:347:ILE:O	1:G:351:ILE:HG13	2.19	0.42
2:B:408:ASN:O	2:B:411:TYR:HB3	2.20	0.42
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.84	0.42
1:A:215:ALA:O	1:A:242:THR:HA	2.20	0.42
1:A:280:GLU:HG3	1:A:284:ARG:HH12	1.84	0.42
2:B:207:GLN:HG3	2:B:213:GLN:HB2	2.01	0.42
1:G:251:VAL:O	1:G:251:VAL:CG1	2.68	0.42
2:B:342:VAL:HG13	2:B:343:TYR:N	2.34	0.42
1:G:202:ALA:HA	1:G:207:LEU:HB2	2.02	0.42
2:H:177:ILE:HD13	2:H:300:ILE:HD12	2.02	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.55	0.42
2:H:51:LEU:C	2:H:53:GLN:H	2.23	0.42
2:H:163:ARG:O	2:H:167:ILE:HG12	2.19	0.42
1:A:187:THR:HB	1:A:190:TRP:CG	2.55	0.42
2:B:187:ILE:O	2:B:187:ILE:HG22	2.20	0.42
2:B:308:LYS:HZ1	6:B:517:PGW:HAD	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:164:ILE:HA	2:H:167:ILE:HB	2.02	0.42
2:B:312:ILE:HD13	2:B:413:TYR:HA	2.01	0.42
3:Y:10:SER:C	3:Y:12:GLU:N	2.74	0.42
1:A:120:PHE:O	1:A:129:ARG:HA	2.19	0.41
2:B:214:GLN:HE22	2:B:270:ILE:HG12	1.83	0.41
2:H:185:LEU:CD1	2:H:186:PRO:HD2	2.42	0.41
3:Y:9:THR:O	3:Y:12:GLU:N	2.43	0.41
1:A:40:ARG:HD2	1:A:318:SER:O	2.20	0.41
2:H:354:PHE:CE1	2:H:376:MET:HE2	2.55	0.41
2:H:375:ASP:O	2:H:376:MET:HB2	2.20	0.41
2:B:61:ASP:HA	2:B:62:PRO:HD3	1.91	0.41
2:B:152:LEU:HB2	2:B:165:ILE:HD12	2.03	0.41
2:B:200:VAL:HG23	2:B:200:VAL:O	2.21	0.41
2:B:350:ARG:CB	2:B:350:ARG:HH11	2.33	0.41
1:G:159:ARG:HA	1:G:188:SER:O	2.21	0.41
1:A:264:ARG:HB2	4:A:1001:NAP:O3X	2.21	0.41
1:A:326:ASN:HD22	1:A:328:GLU:N	2.18	0.41
4:A:1001:NAP:H52N	4:A:1001:NAP:H6N	2.03	0.41
2:B:369:THR:OG1	2:B:371:VAL:HG23	2.20	0.41
2:H:340:SER:HB3	2:H:357:ILE:HD13	2.02	0.41
1:A:286:GLN:NE2	1:A:286:GLN:HA	2.35	0.41
1:A:286:GLN:O	1:A:290:LYS:HG3	2.21	0.41
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.19	0.41
2:B:402:VAL:HB	2:B:403:PRO:HD3	2.03	0.41
1:G:187:THR:HB	1:G:190:TRP:CG	2.55	0.41
1:G:295:ILE:HD11	1:G:354:ILE:HD11	2.03	0.41
2:H:261:VAL:HA	2:H:264:ILE:CD1	2.51	0.41
2:H:304:SER:CA	2:H:310:LEU:HD23	2.48	0.41
3:Y:28:CYS:SG	3:Y:33:CYS:HA	2.61	0.41
2:H:61:ASP:HA	2:H:62:PRO:HD3	1.95	0.41
2:H:261:VAL:HA	2:H:264:ILE:HD12	2.02	0.41
2:H:323:GLU:HB2	2:H:405:ILE:CG1	2.51	0.41
2:B:214:GLN:NE2	7:B:634:HOH:O	2.54	0.40
2:B:88:ILE:O	2:B:91:TYR:HB3	2.21	0.40
1:A:57:TRP:CD2	1:A:58:VAL:HG23	2.55	0.40
2:H:240:ARG:HH11	2:H:240:ARG:HG3	1.86	0.40
2:H:183:GLU:C	2:H:185:LEU:H	2.25	0.40
3:Y:9:THR:O	3:Y:10:SER:C	2.60	0.40
2:H:61:ASP:OD2	2:H:64:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/333 (97%)	310 (96%)	13 (4%)	1 (0%)	41	51
1	G	324/333 (97%)	315 (97%)	8 (2%)	1 (0%)	41	51
2	B	384/514 (75%)	348 (91%)	27 (7%)	9 (2%)	6	6
2	H	357/514 (70%)	291 (82%)	55 (15%)	11 (3%)	4	3
3	Y	35/37 (95%)	17 (49%)	16 (46%)	2 (6%)	1	0
All	All	1424/1731 (82%)	1281 (90%)	119 (8%)	24 (2%)	9	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	ILE
2	B	137	GLU
2	B	158	SER
2	H	373	TYR
3	Y	22	ASN
1	A	120	PHE
2	B	135	GLU
1	G	120	PHE
2	H	243	ALA
2	B	132	TYR
2	B	245	PRO
2	H	150	TRP
2	B	157	GLU
2	H	129	ASP
2	H	275	SER
3	Y	10	SER
2	B	139	PRO
2	H	160	GLY
2	H	376	MET
2	H	411	TYR
2	H	210	ILE

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Mol	Chain	Res	Type
2	B	131	GLY
2	H	96	GLY
2	H	400	LEU

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	273/280 (98%)	269 (98%)	4 (2%)	65	77
1	G	273/280 (98%)	266 (97%)	7 (3%)	46	61
2	B	332/459 (72%)	328 (99%)	4 (1%)	71	81
2	H	324/459 (71%)	321 (99%)	3 (1%)	78	86
3	Y	35/35 (100%)	33 (94%)	2 (6%)	20	27
All	All	1237/1513 (82%)	1217 (98%)	20 (2%)	62	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	214	GLN
1	A	326	ASN
1	A	338	GLN
2	B	34	ARG
2	B	82	ARG
2	B	86	ASP
2	B	152	LEU
1	G	73	MET
1	G	75	LEU
1	G	214	GLN
1	G	222	ARG
1	G	231	GLU
1	G	283	ARG
1	G	314	ASN
2	H	150	TRP

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Mol	Chain	Res	Type
2	H	152	LEU
2	H	263	ILE
3	Y	14	TRP
3	Y	27	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	146	GLN
2	B	214	GLN
2	B	253	ASN
2	B	256	ASN
2	B	414	HIS
1	G	37	GLN
1	G	71	HIS
1	G	148	GLN
1	G	204	GLN
1	G	286	GLN
1	G	293	GLN
1	G	333	ASN
2	H	53	GLN
2	H	148	GLN
2	H	213	GLN
2	H	256	ASN
2	H	281	GLN
2	H	311	GLN
2	H	414	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PCA	Y	1	3	7,8,9	0.61	0	9,10,12	0.84	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
3	PCA	Y	1	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	516	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	518	-	6,6,50	0.37	0	5,5,56	0.45	0
4	NAP	A	1001	-	46,52,52	2.75	7 (15%)	61,80,80	2.60	16 (26%)
6	PGW	B	519	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	517	-	35,35,50	0.66	0	38,41,56	0.91	2 (5%)
6	PGW	H	505	-	21,21,50	0.61	0	23,23,56	1.32	3 (13%)
6	PGW	B	512	-	6,6,50	0.37	0	5,5,56	0.47	0
4	NAP	G	1001	-	46,52,52	2.68	7 (15%)	61,80,80	2.53	16 (26%)
6	PGW	B	520	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	506	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	511	-	8,8,50	0.35	0	7,7,56	0.54	0
6	PGW	B	513	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	505	-	21,21,50	0.61	0	23,23,56	1.25	3 (13%)
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	515	-	22,22,50	0.80	0	25,27,56	1.28	4 (16%)
6	PGW	B	514	-	7,7,50	0.36	0	6,6,56	0.52	0
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGW	B	507	-	-	0/6/6/55	-
6	PGW	B	516	-	-	0/5/5/55	-
6	PGW	B	518	-	-	0/4/4/55	-
4	NAP	A	1001	-	-	4/31/67/67	0/5/5/5
6	PGW	B	519	-	-	0/5/5/55	-
6	PGW	B	517	-	-	7/40/40/55	-
6	PGW	H	505	-	-	1/23/23/55	-
6	PGW	B	512	-	-	0/4/4/55	-
4	NAP	G	1001	-	-	3/31/67/67	0/5/5/5
6	PGW	B	520	-	-	0/5/5/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGW	B	508	-	-	0/6/6/55	-
6	PGW	B	506	-	-	0/6/6/55	-
6	PGW	B	511	-	-	0/6/6/55	-
6	PGW	B	513	-	-	0/6/6/55	-
6	PGW	B	505	-	-	1/23/23/55	-
6	PGW	B	509	-	-	0/6/6/55	-
6	PGW	B	515	-	-	8/24/24/55	-
6	PGW	B	514	-	-	0/5/5/55	-
6	PGW	B	510	-	-	0/6/6/55	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAP	PN-O3	14.23	1.74	1.59
4	G	1001	NAP	PN-O3	13.55	1.74	1.59
4	A	1001	NAP	O4B-C1B	6.08	1.48	1.40
4	G	1001	NAP	O4B-C1B	5.94	1.48	1.40
4	A	1001	NAP	PA-O3	5.18	1.65	1.59
4	G	1001	NAP	O4D-C1D	4.79	1.47	1.40
4	G	1001	NAP	PA-O3	4.57	1.64	1.59
4	A	1001	NAP	O4D-C1D	4.52	1.46	1.40
4	A	1001	NAP	C2N-C3N	3.28	1.44	1.39
4	G	1001	NAP	C2N-C3N	3.14	1.44	1.39
4	G	1001	NAP	C4N-C3N	2.91	1.43	1.39
4	G	1001	NAP	C8A-N7A	-2.66	1.29	1.34
4	A	1001	NAP	C4N-C3N	2.59	1.43	1.39
4	A	1001	NAP	O4B-C4B	2.02	1.49	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1001	NAP	O3-PA-O1A	-11.69	75.53	110.70
4	A	1001	NAP	O3-PA-O1A	-11.68	75.57	110.70
4	A	1001	NAP	O4B-C1B-N9A	7.96	119.29	108.75
4	G	1001	NAP	O4B-C1B-N9A	7.29	118.41	108.75
4	A	1001	NAP	O2A-PA-O3	-6.01	91.02	107.27
4	G	1001	NAP	O2A-PA-O3	-5.80	91.59	107.27
4	A	1001	NAP	C2B-C1B-N9A	-5.14	101.15	112.56
4	G	1001	NAP	N3A-C2A-N1A	-5.02	121.86	128.67
4	A	1001	NAP	N3A-C2A-N1A	-4.93	121.97	128.67
4	G	1001	NAP	C2B-C1B-N9A	-4.53	102.49	112.56
4	A	1001	NAP	C2B-C3B-C4B	4.00	110.60	101.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1001	NAP	C2B-C3B-C4B	3.93	110.45	101.99
4	G	1001	NAP	PN-O5D-C5D	-3.85	99.31	121.35
6	H	505	PGW	O01-C1-C2	3.77	119.63	111.48
4	A	1001	NAP	PN-O5D-C5D	-3.69	100.19	121.35
6	B	505	PGW	O01-C1-C2	3.33	118.68	111.48
4	A	1001	NAP	C4B-O4B-C1B	3.02	112.69	109.92
4	A	1001	NAP	O2B-C2B-C3B	2.97	122.34	111.68
6	B	515	PGW	C03-C02-C01	-2.89	105.05	111.78
6	B	515	PGW	O01-C1-C2	2.88	117.71	111.48
4	G	1001	NAP	C4B-O4B-C1B	2.84	112.53	109.92
4	A	1001	NAP	O4B-C4B-C5B	-2.59	101.04	109.33
6	B	505	PGW	O03-C19-C20	2.49	119.42	111.83
6	H	505	PGW	O03-C19-C20	2.48	119.40	111.83
4	G	1001	NAP	O5B-PA-O1A	2.44	118.61	108.94
6	B	515	PGW	O03-C19-C20	2.39	119.13	111.83
4	A	1001	NAP	O4D-C4D-C3D	2.39	109.90	105.15
6	B	517	PGW	O01-C1-C2	2.37	116.60	111.48
4	G	1001	NAP	O2B-C2B-C1B	2.36	118.36	110.05
4	G	1001	NAP	C5D-C4D-C3D	-2.36	106.70	115.21
4	G	1001	NAP	O4D-C4D-C3D	2.35	109.83	105.15
4	G	1001	NAP	PA-O5B-C5B	-2.28	108.28	121.35
4	A	1001	NAP	O7N-C7N-N7N	-2.26	119.34	122.62
6	B	515	PGW	O11-P-O14	2.26	112.55	106.44
6	H	505	PGW	C02-O01-C1	-2.26	112.39	117.80
4	A	1001	NAP	C5D-C4D-C3D	-2.24	107.16	115.21
6	B	517	PGW	O01-C02-C01	-2.17	100.56	108.34
4	G	1001	NAP	O7N-C7N-N7N	-2.16	119.50	122.62
4	A	1001	NAP	O5B-PA-O1A	2.15	117.45	108.94
6	B	505	PGW	C02-O01-C1	-2.14	112.68	117.80
4	A	1001	NAP	O2A-PA-O1A	2.10	122.22	112.44
4	G	1001	NAP	O4B-C4B-C5B	-2.10	102.61	109.33
4	A	1001	NAP	O2A-PA-O5B	2.03	116.75	107.57
4	G	1001	NAP	O2A-PA-O1A	2.02	121.86	112.44

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAP	C5B-O5B-PA-O1A
4	G	1001	NAP	C5B-O5B-PA-O1A
6	B	515	PGW	C02-C03-O11-P
4	A	1001	NAP	C1B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
4	G	1001	NAP	C1B-C2B-O2B-P2B
4	A	1001	NAP	C3B-C2B-O2B-P2B
6	B	517	PGW	C7-C8-C9-C10
6	B	505	PGW	C01-C02-O01-C1
6	B	515	PGW	C20-C19-O03-C01
6	B	515	PGW	O04-C19-O03-C01
6	B	517	PGW	C01-C02-O01-C1
6	H	505	PGW	C01-C02-O01-C1
6	B	515	PGW	O02-C1-O01-C02
6	B	515	PGW	O01-C1-C2-C3
6	B	517	PGW	O01-C1-C2-C3
6	B	517	PGW	O03-C19-C20-C21
6	B	515	PGW	C01-C02-O01-C1
6	B	517	PGW	C03-C02-O01-C1
4	A	1001	NAP	O4B-C4B-C5B-O5B
6	B	515	PGW	O03-C19-C20-C21
6	B	515	PGW	O02-C1-C2-C3
4	G	1001	NAP	C3B-C2B-O2B-P2B
6	B	517	PGW	O02-C1-C2-C3
6	B	517	PGW	O04-C19-C20-C21

There are no ring outliers.

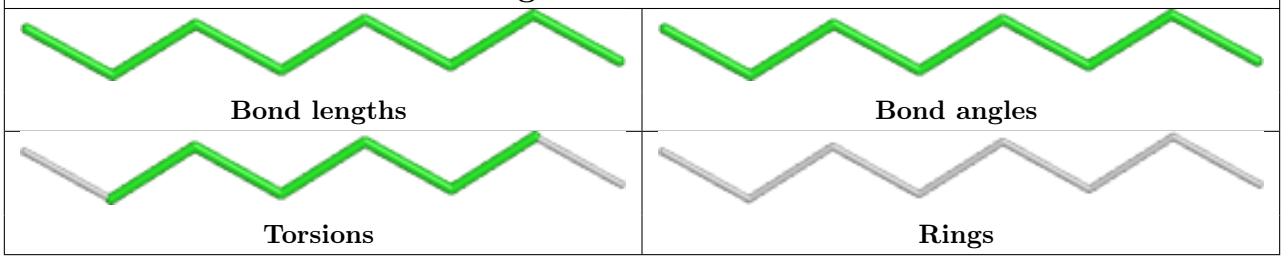
8 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	516	PGW	2	0
4	A	1001	NAP	11	0
6	B	517	PGW	4	0
6	H	505	PGW	5	0
4	G	1001	NAP	13	0
6	B	511	PGW	3	0
6	B	505	PGW	3	0
6	B	515	PGW	1	0

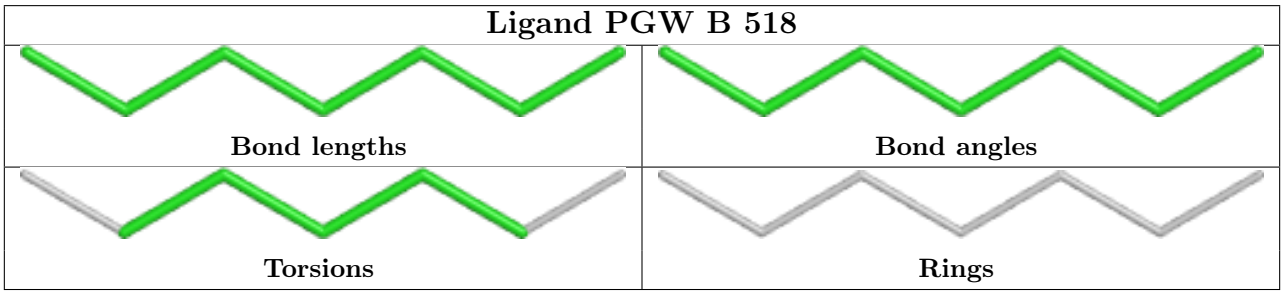
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

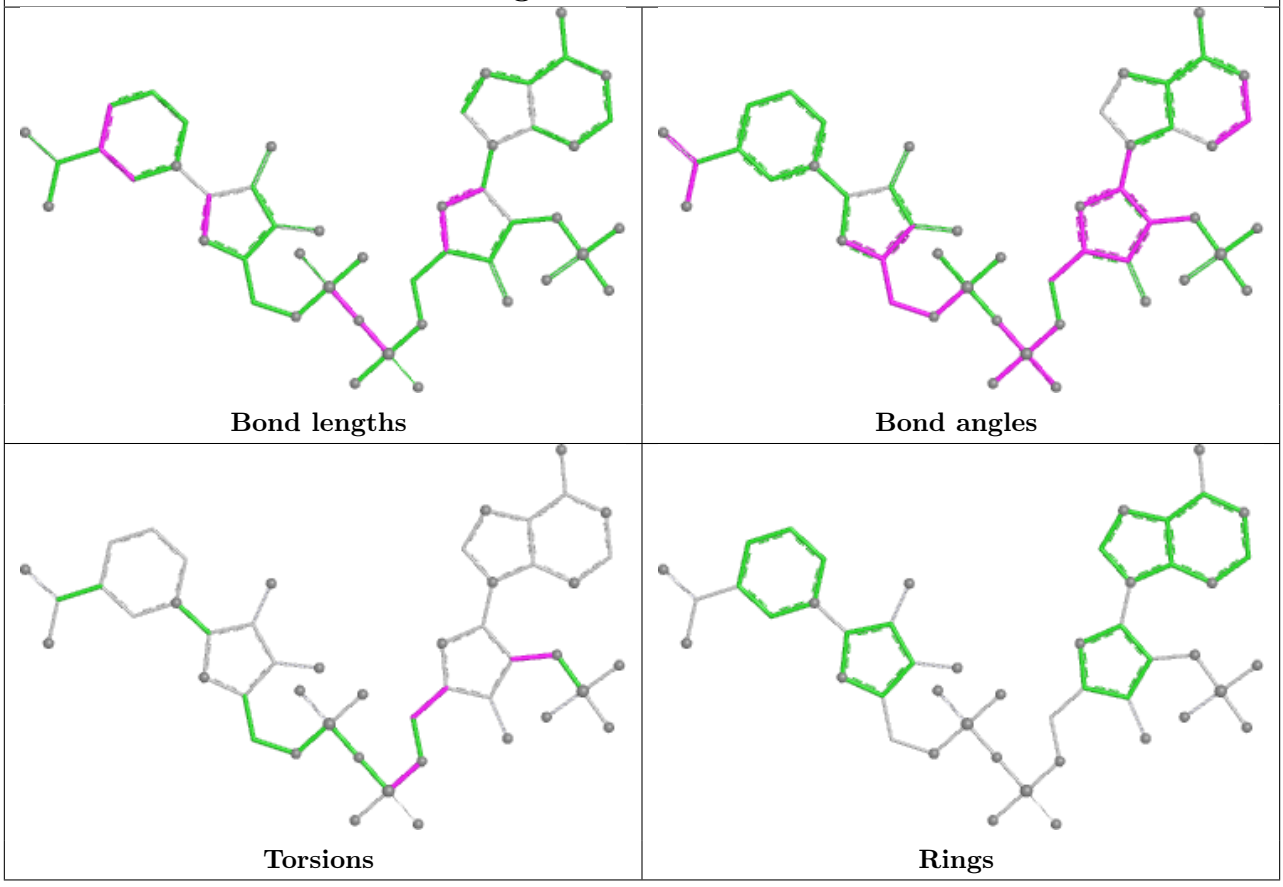
Ligand PGW B 516



Ligand PGW B 518

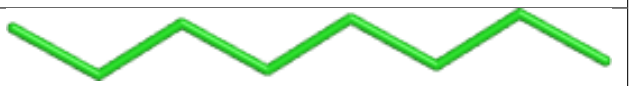


Ligand NAP A 1001

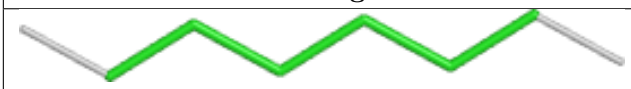


Ligand PGW B 519

Bond lengths



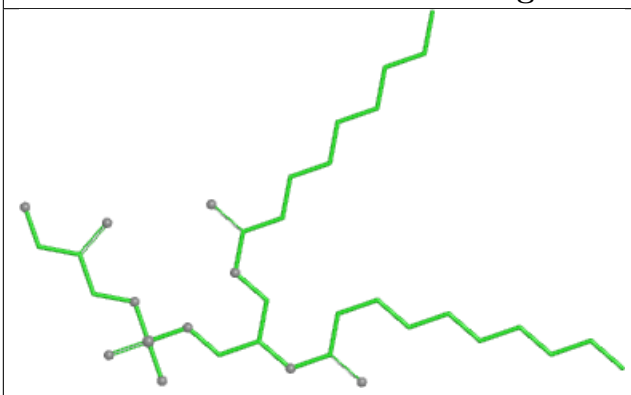
Bond angles



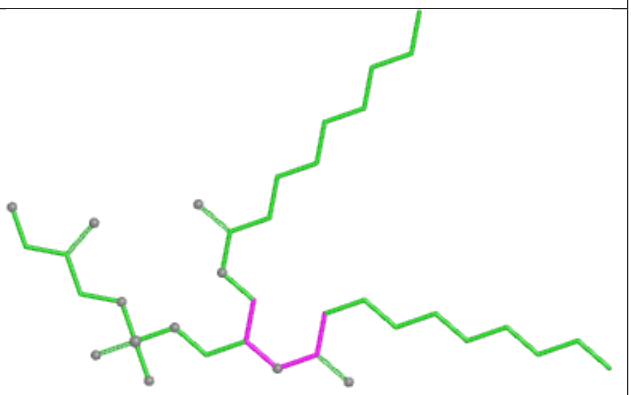
Torsions

Rings

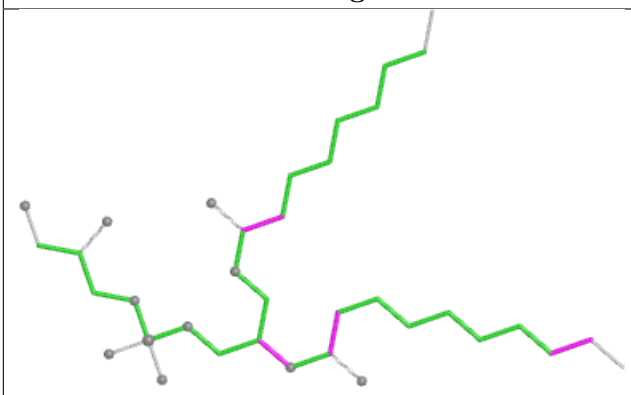
Ligand PGW B 517



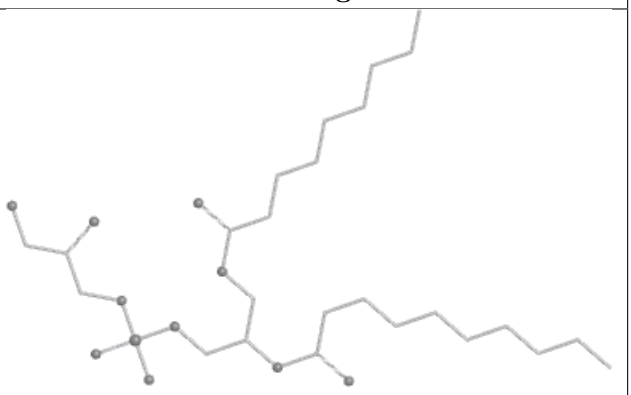
Bond lengths



Bond angles

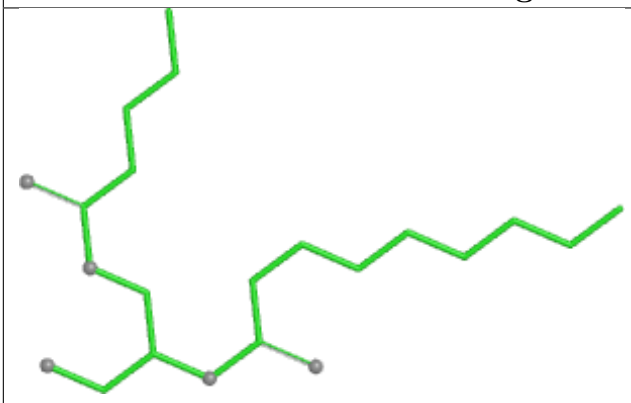


Torsions

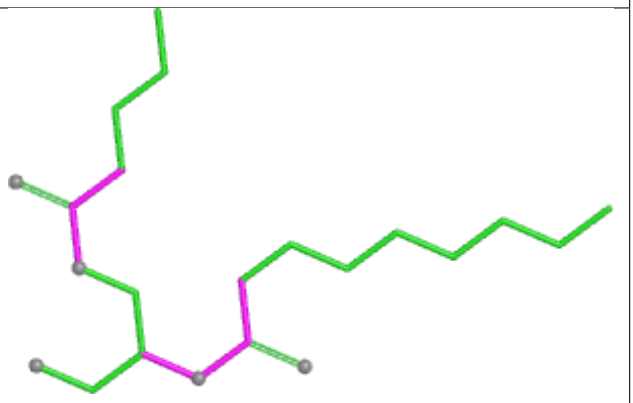


Rings

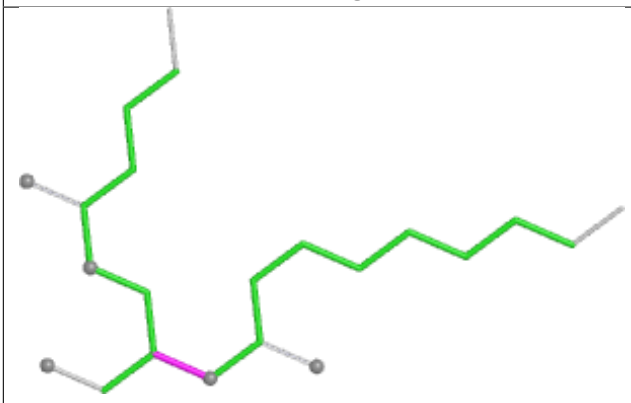
Ligand PGW H 505



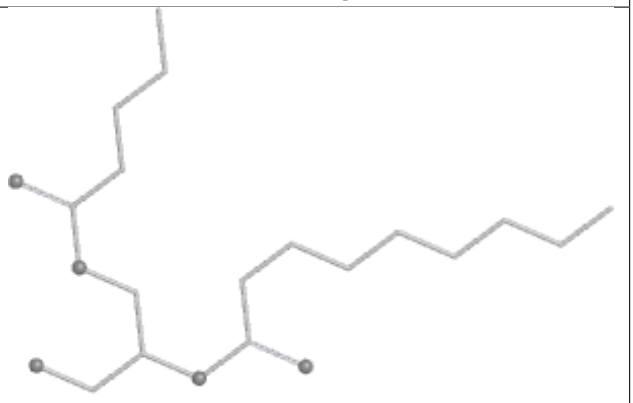
Bond lengths



Bond angles

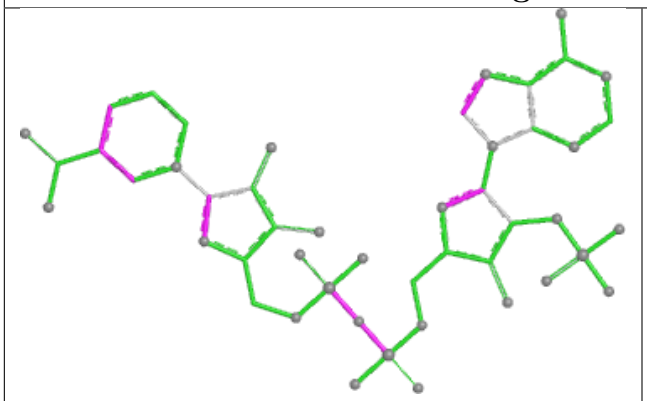


Torsions

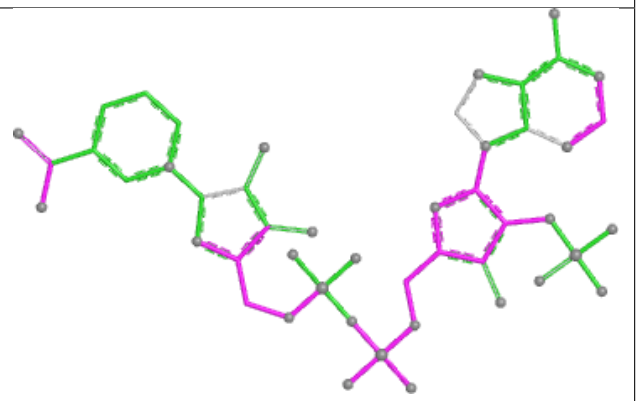


Rings

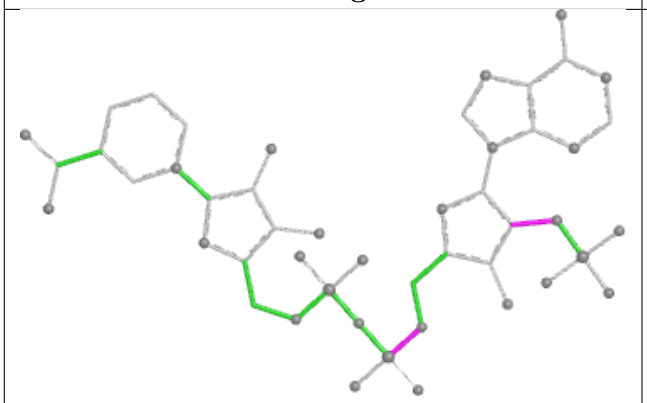
Ligand NAP G 1001



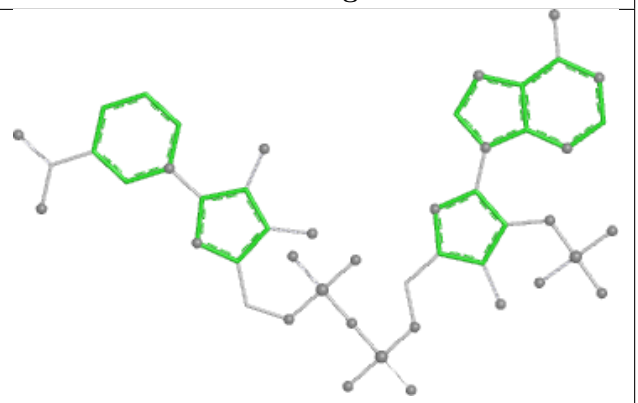
Bond lengths



Bond angles



Torsions



Rings

Ligand PGW B 520

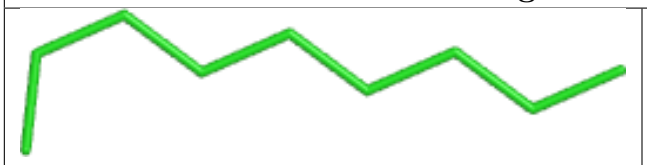
Bond lengths

Bond angles

Torsions

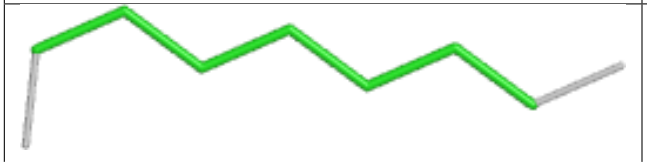
Rings

Ligand PGW B 508

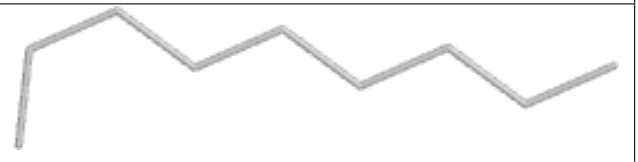


Bond lengths

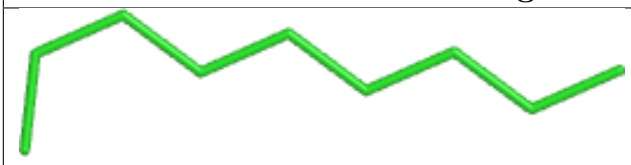
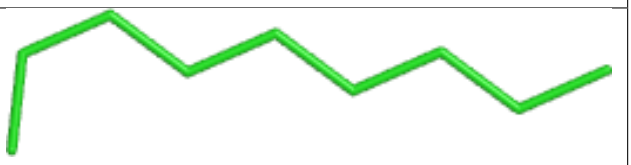
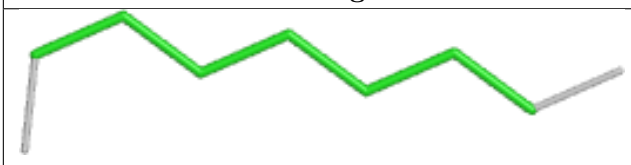
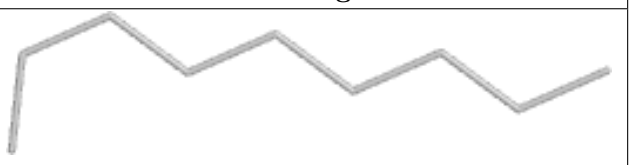
Bond angles

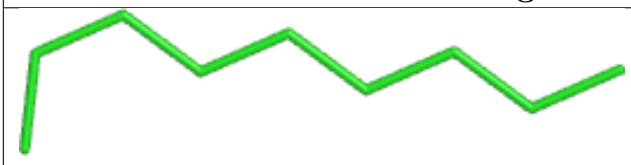
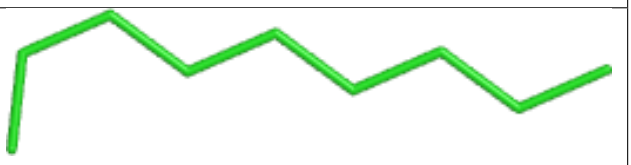
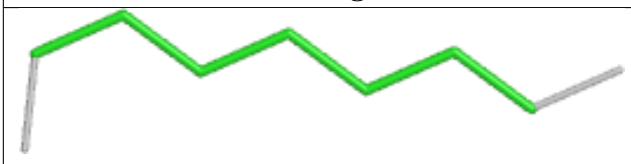
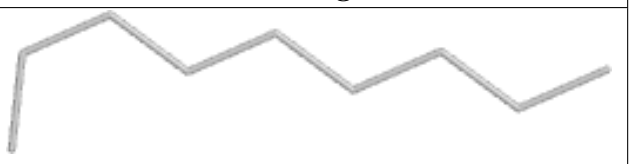


Torsions

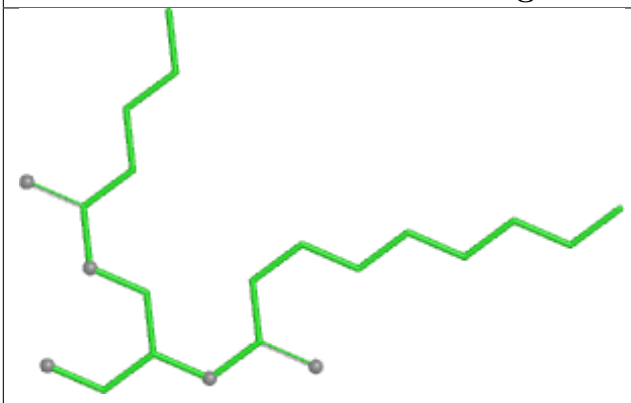


Rings

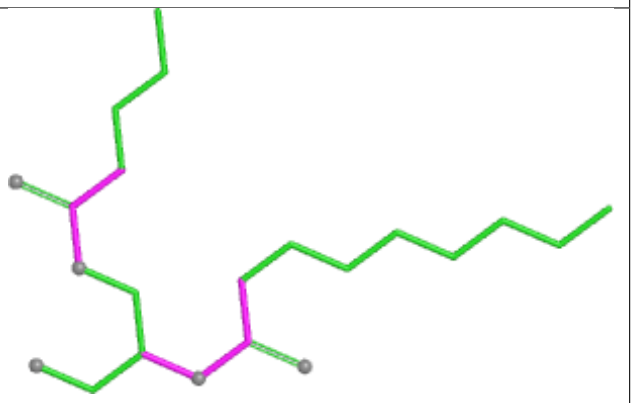
Ligand PGW B 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PGW B 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

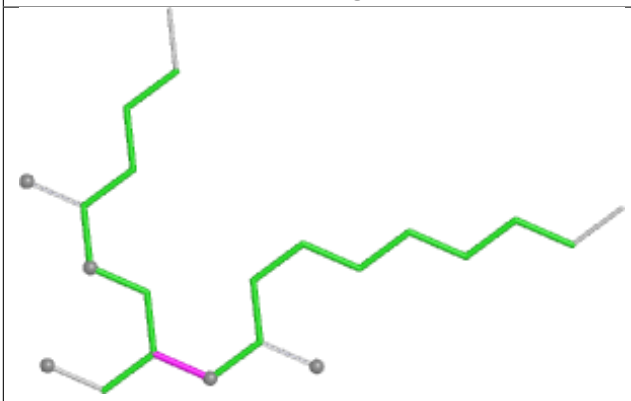
Ligand PGW B 505



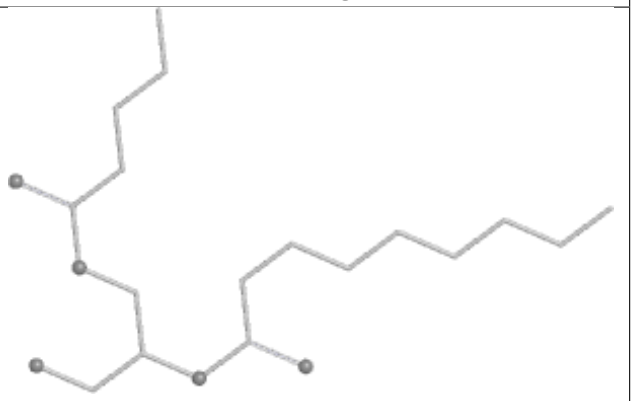
Bond lengths



Bond angles

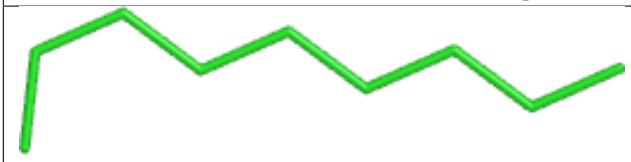


Torsions

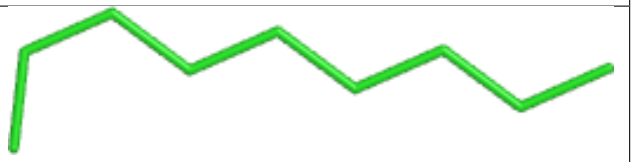


Rings

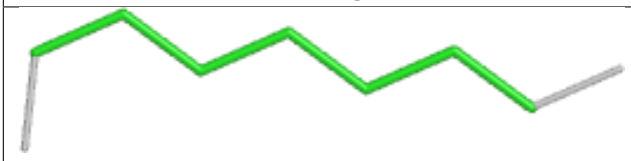
Ligand PGW B 509



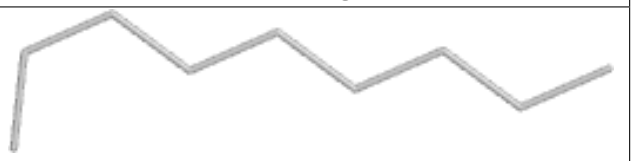
Bond lengths



Bond angles

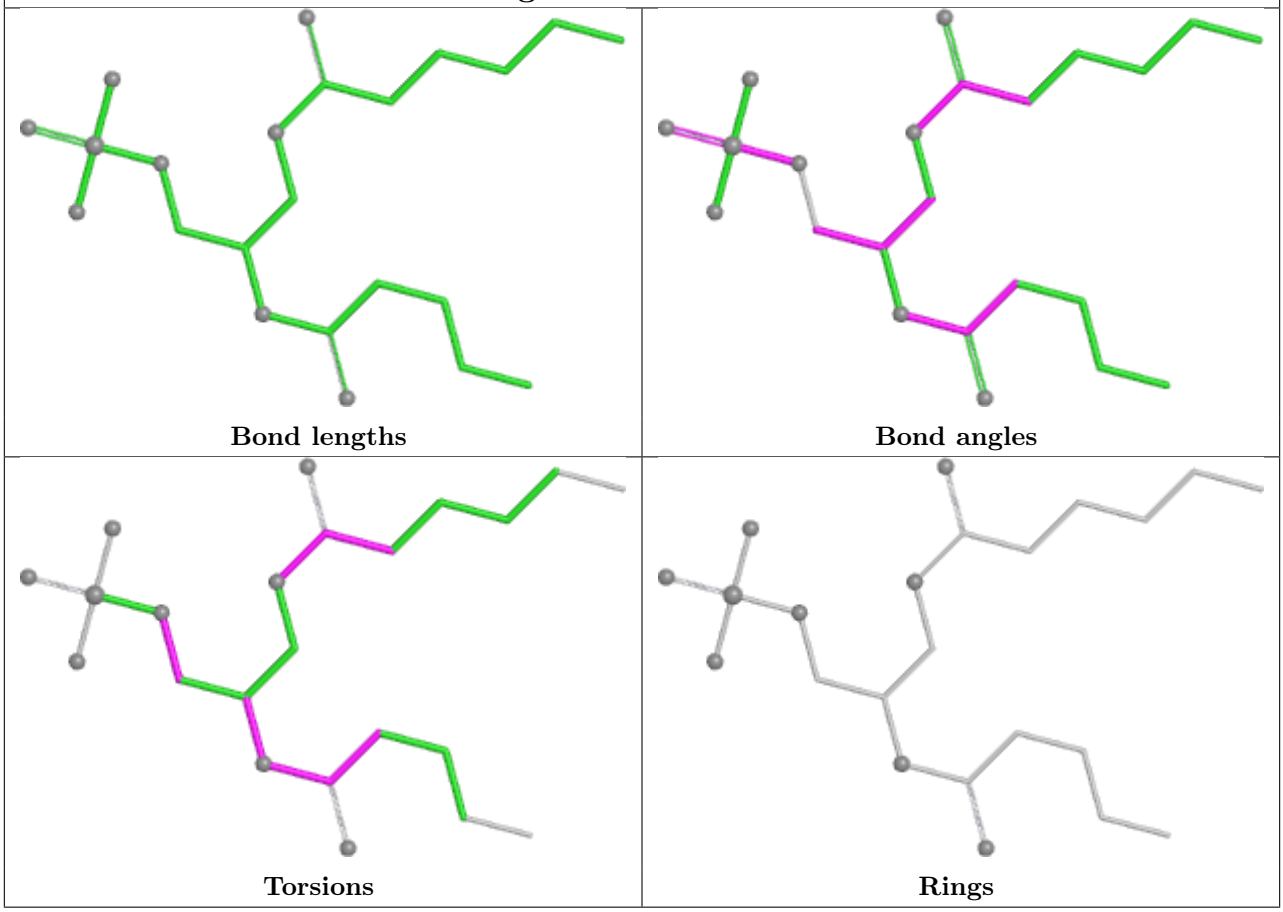


Torsions

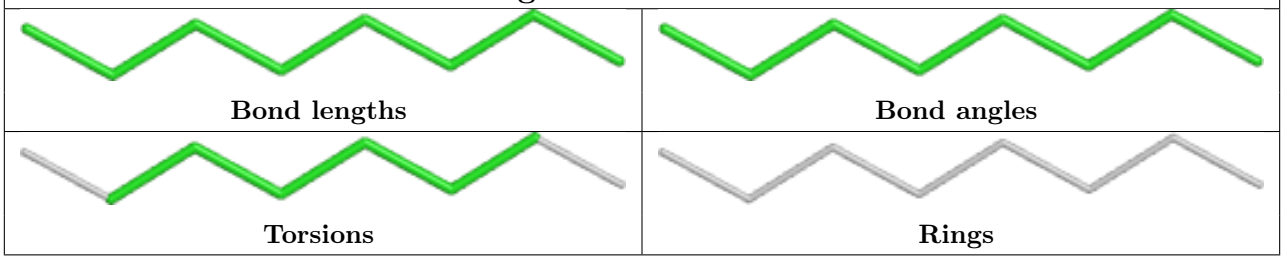


Rings

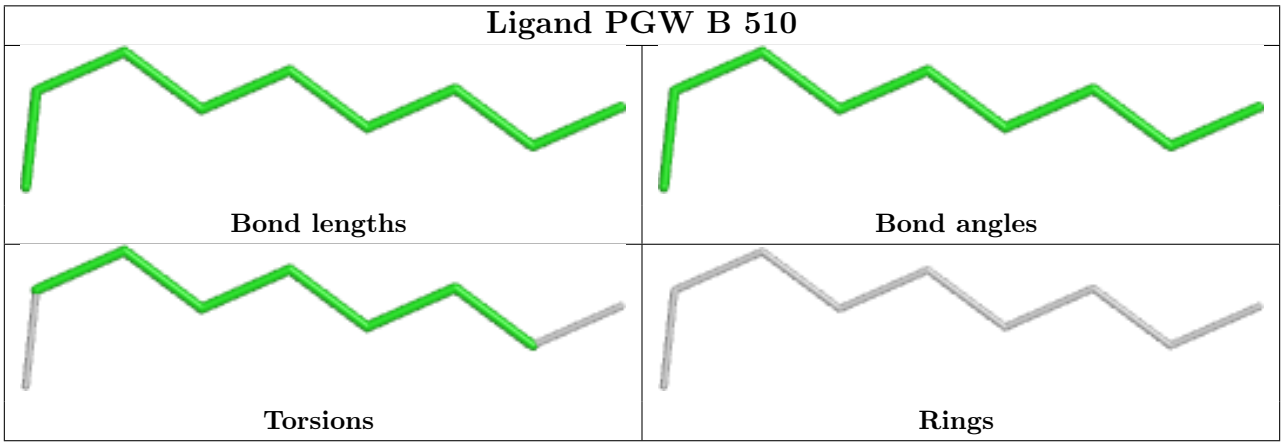
Ligand PGW B 515



Ligand PGW B 514



Ligand PGW B 510



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, 95^{th} 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	326/333 (97%)	0.21	9 (2%) 53 60	24, 41, 66, 89	0
1	G	326/333 (97%)	0.08	7 (2%) 63 70	27, 45, 77, 100	0
2	B	386/514 (75%)	0.78	55 (14%) 2 3	34, 70, 120, 128	0
2	H	363/514 (70%)	2.36	125 (34%) 0 0	44, 115, 191, 202	0
3	Y	36/37 (97%)	4.15	33 (91%) 0 0	80, 83, 88, 90	36 (100%)
All	All	1437/1731 (83%)	0.98	229 (15%) 1 2	24, 61, 175, 202	36 (2%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	272	LEU	15.6
2	H	244	CYS	14.5
2	H	280	LEU	14.0
2	H	214	GLN	13.7
2	H	215	SER	13.2
2	H	149	VAL	13.1
2	H	218	PHE	12.7
2	H	153	PHE	11.9
2	H	242	PHE	11.9
2	H	247	LYS	11.8
2	H	248	ALA	11.0
2	H	216	THR	10.6
2	H	190	ASP	10.2
2	H	161	PRO	10.2
2	H	241	PHE	10.1
2	H	282	PHE	10.1
2	H	251	PHE	9.5
2	H	245	PRO	9.3
2	H	233	PHE	8.9
3	Y	17	CYS	8.8

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Mol	Chain	Res	Type	RSRZ
2	H	150	TRP	8.8
2	H	208	SER	8.7
2	H	146	GLN	8.4
2	H	286	ARG	8.4
2	H	145	PHE	8.3
3	Y	8	THR	8.3
2	H	151	LEU	8.2
2	H	246	SER	8.2
2	H	283	GLN	8.0
2	H	250	PHE	8.0
2	H	285	VAL	7.9
2	H	224	ILE	7.9
2	H	222	PHE	7.8
2	H	217	SER	7.7
3	Y	3	THR	7.5
2	B	193	GLU	7.4
2	H	188	PHE	7.4
2	H	187	ILE	7.2
3	Y	23	THR	7.2
3	Y	5	VAL	7.2
2	H	288	VAL	7.1
2	H	203	HIS	7.0
2	H	219	THR	6.8
2	H	279	VAL	6.8
2	H	225	VAL	6.7
2	H	205	TYR	6.6
2	H	229	CYS	6.5
2	H	235	PHE	6.1
2	H	273	THR	6.1
3	Y	36	TYR	5.9
2	H	213	GLN	5.8
2	H	212	TYR	5.8
3	Y	4	ASN	5.7
2	H	249	GLY	5.7
2	H	209	THR	5.7
2	H	207	GLN	5.6
2	H	240	ARG	5.6
2	H	263	ILE	5.6
2	H	204	THR	5.6
2	H	284	ASN	5.5
2	H	164	ILE	5.5
2	H	270	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	252	THR	5.3
2	H	167	ILE	5.3
2	H	238	LEU	5.2
2	H	271	PHE	5.2
2	H	232	TRP	5.2
3	Y	21	HIS	5.1
2	H	160	GLY	5.1
2	H	415	ARG	5.0
2	H	221	PRO	5.0
3	Y	16	VAL	4.8
2	H	262	ALA	4.8
3	Y	24	SER	4.8
2	H	157	GLU	4.7
2	B	152	LEU	4.7
3	Y	30	ASN	4.7
3	Y	7	CYS	4.6
2	B	149	VAL	4.6
2	H	276	ASN	4.6
3	Y	25	ARG	4.6
3	Y	9	THR	4.6
1	A	360	TYR	4.6
2	H	202	PHE	4.6
2	H	289	VAL	4.5
2	H	172	VAL	4.5
2	H	156	PRO	4.5
2	H	236	GLU	4.5
2	H	231	ILE	4.4
3	Y	28	CYS	4.4
1	G	36	LEU	4.4
2	B	192	ASN	4.4
1	G	360	TYR	4.3
2	B	156	PRO	4.3
3	Y	6	SER	4.3
2	B	157	GLU	4.3
2	H	154	GLU	4.3
2	H	287	ARG	4.3
2	B	191	GLU	4.3
2	H	147	ARG	4.2
2	B	153	PHE	4.2
2	H	417	THR	4.1
2	B	196	HIS	4.1
2	H	189	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
2	H	168	VAL	4.0
2	H	220	ASP	4.0
2	B	161	PRO	4.0
2	H	152	LEU	4.0
3	Y	12	GLU	4.0
2	H	106	LEU	4.0
2	B	162	ALA	3.9
3	Y	15	SER	3.9
3	Y	37	SER	3.9
3	Y	14	TRP	3.9
2	H	281	GLN	3.9
2	B	190	ASP	3.8
2	H	243	ALA	3.7
2	B	219	THR	3.6
2	H	416	GLU	3.5
2	H	414	HIS	3.5
2	H	165	ILE	3.5
2	H	228	LEU	3.5
3	Y	27	MET	3.5
2	B	165	ILE	3.5
2	H	290	GLN	3.4
2	B	158	SER	3.4
2	H	260	ILE	3.4
2	H	381	ILE	3.4
2	H	155	TYR	3.4
2	H	410	ASN	3.4
2	H	163	ARG	3.3
3	Y	2	PHE	3.3
3	Y	11	LYS	3.3
3	Y	26	GLY	3.3
2	H	237	PHE	3.3
2	H	63	LYS	3.3
2	H	223	PHE	3.2
2	B	163	ARG	3.2
2	H	302	LYS	3.2
1	A	36	LEU	3.2
2	H	210	ILE	3.1
3	Y	29	MET	3.1
2	H	173	ILE	3.1
2	H	411	TYR	3.1
2	H	261	VAL	3.1
2	H	125	MET	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	121	GLU	3.1
2	H	206	SER	3.1
3	Y	18	GLN	3.1
3	Y	20	LEU	3.1
2	B	188	PHE	3.0
1	G	349	HIS	3.0
2	H	409	PHE	3.0
2	B	200	VAL	2.9
2	H	306	HIS	2.9
2	B	195	MET	2.9
2	B	198	GLY	2.9
2	B	151	LEU	2.9
2	B	132	TYR	2.9
2	B	241	PHE	2.9
2	H	308	LYS	2.9
2	H	183	GLU	2.8
1	G	202	ALA	2.8
2	B	125	MET	2.8
3	Y	33	CYS	2.7
2	H	177	ILE	2.7
2	B	215	SER	2.7
3	Y	22	ASN	2.6
2	B	159	SER	2.6
2	B	160	GLY	2.6
2	B	247	LYS	2.6
2	H	264	ILE	2.6
2	H	171	MET	2.6
2	H	114	ARG	2.6
2	B	164	ILE	2.6
2	H	291	ILE	2.6
2	H	159	SER	2.6
2	B	411	TYR	2.6
2	B	168	VAL	2.5
2	H	170	VAL	2.5
2	B	242	PHE	2.5
2	H	230	ILE	2.5
2	B	218	PHE	2.5
2	H	255	MET	2.5
2	B	114	ARG	2.4
1	A	262	TYR	2.4
2	B	205	TYR	2.4
2	B	370	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	194	ASP	2.4
2	B	120	GLU	2.4
2	B	371	VAL	2.4
2	H	36	VAL	2.4
2	B	251	PHE	2.3
2	B	396	LEU	2.3
2	H	126	PHE	2.3
2	B	252	THR	2.3
2	B	395	VAL	2.3
2	H	274	GLU	2.3
1	A	205	PHE	2.3
1	G	200	SER	2.3
1	A	280	GLU	2.3
2	H	257	ILE	2.2
2	H	350	ARG	2.2
2	B	232	TRP	2.2
2	B	145	PHE	2.2
2	B	332	PHE	2.2
2	B	106	LEU	2.2
2	B	73	ARG	2.1
2	H	310	LEU	2.1
3	Y	32	LYS	2.1
2	B	249	GLY	2.1
2	B	213	GLN	2.1
2	B	189	ARG	2.1
2	B	417	THR	2.1
1	A	250	ILE	2.1
1	G	205	PHE	2.1
2	H	275	SER	2.1
1	A	202	ALA	2.1
2	B	243	ALA	2.1
2	H	269	THR	2.1
1	G	201	VAL	2.0
2	B	400	LEU	2.0
2	H	191	GLU	2.0
3	Y	10	SER	2.0
3	Y	31	LYS	2.0
3	Y	35	CYS	2.0
1	A	265	ALA	2.0
2	B	216	THR	2.0
1	A	361	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PCA	Y	1	8/9	0.81	0.25	90,90,90,91	8

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PGW	B	513	9/51	0.25	0.53	127,129,129,129	0
6	PGW	B	509	9/51	0.32	0.90	115,115,116,116	0
6	PGW	H	505	22/51	0.33	0.73	139,145,148,148	0
6	PGW	B	505	22/51	0.36	0.81	92,107,120,121	0
6	PGW	B	520	8/51	0.38	0.41	96,100,103,104	0
6	PGW	B	507	9/51	0.54	0.35	94,97,98,99	0
6	PGW	B	517	36/51	0.56	0.33	117,135,152,152	0
6	PGW	B	518	7/51	0.57	0.40	72,74,75,75	0
6	PGW	B	519	8/51	0.59	0.73	111,114,115,115	0
6	PGW	B	506	9/51	0.61	0.31	81,84,88,88	0
6	PGW	B	516	8/51	0.63	0.55	90,94,99,99	0
6	PGW	B	510	9/51	0.72	0.98	104,106,107,107	0
6	PGW	B	514	8/51	0.72	0.52	80,82,84,85	0
6	PGW	B	515	23/51	0.73	0.36	128,136,138,138	0
6	PGW	B	511	9/51	0.74	0.41	122,123,124,124	0
5	K	H	504	1/1	0.76	0.43	55,55,55,55	1
6	PGW	B	508	9/51	0.79	0.40	96,97,98,99	0
6	PGW	B	512	7/51	0.82	0.19	76,78,79,79	0
5	K	H	503	1/1	0.93	0.18	56,56,56,56	1
5	K	H	502	1/1	0.95	0.30	55,55,55,55	1
4	NAP	G	1001	48/48	0.95	0.19	26,45,58,63	0

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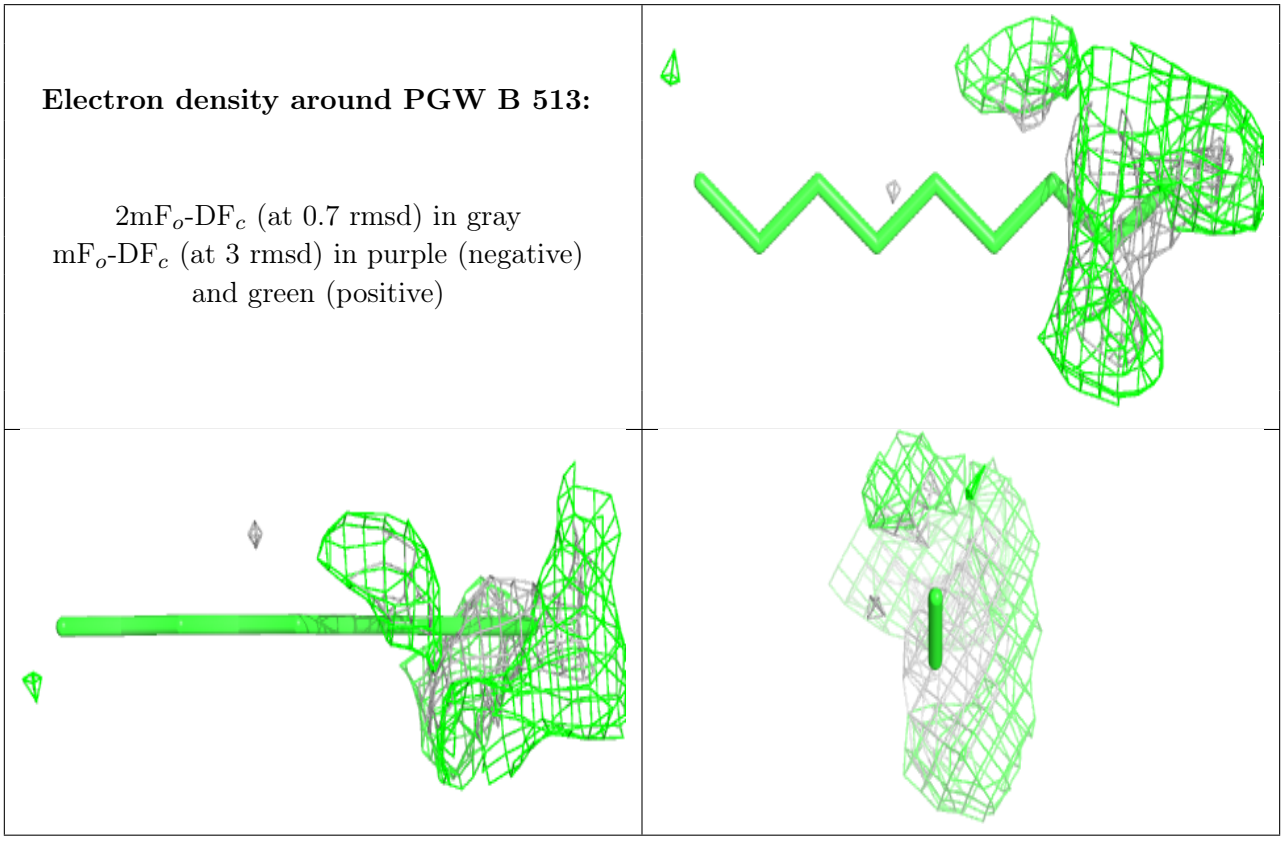
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAP	A	1001	48/48	0.96	0.19	32,42,52,55	0
5	K	B	502	1/1	0.96	0.16	39,39,39,39	1
5	K	B	503	1/1	0.97	0.19	34,34,34,34	1
5	K	B	504	1/1	0.99	0.16	39,39,39,39	1
5	K	H	501	1/1	0.99	0.41	53,53,53,53	1
5	K	B	501	1/1	1.00	0.29	42,42,42,42	1

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.

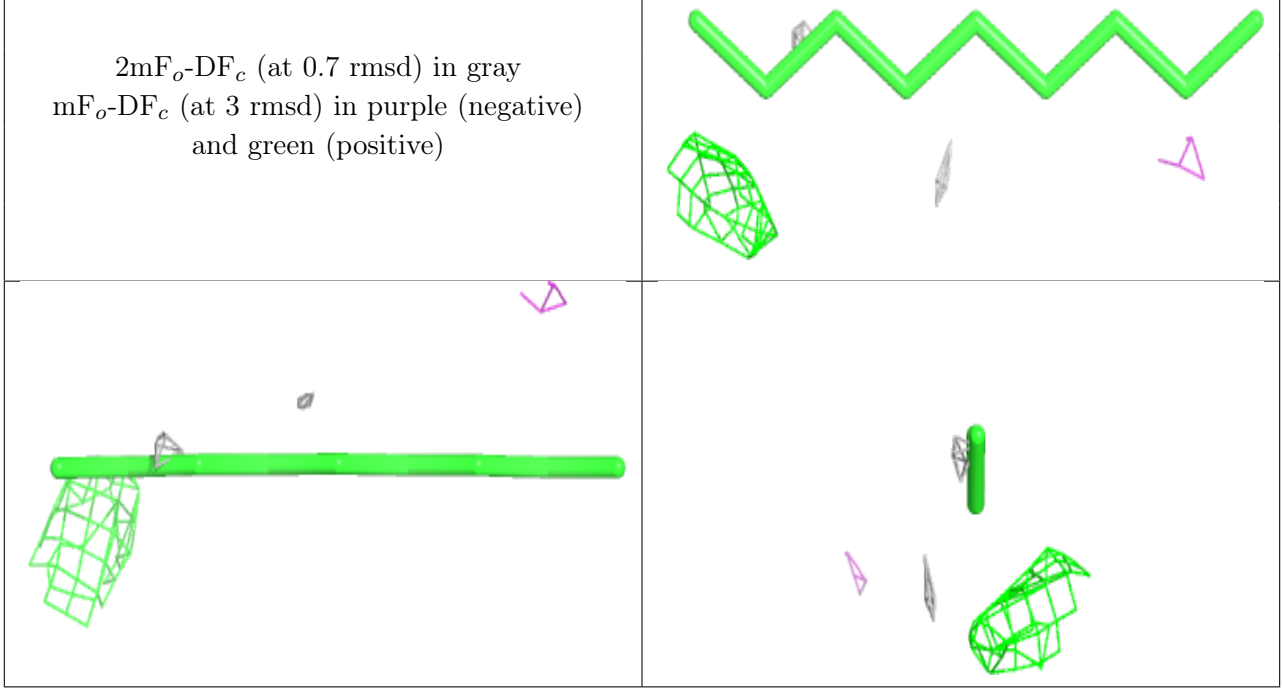
Electron density around PGW B 513:

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



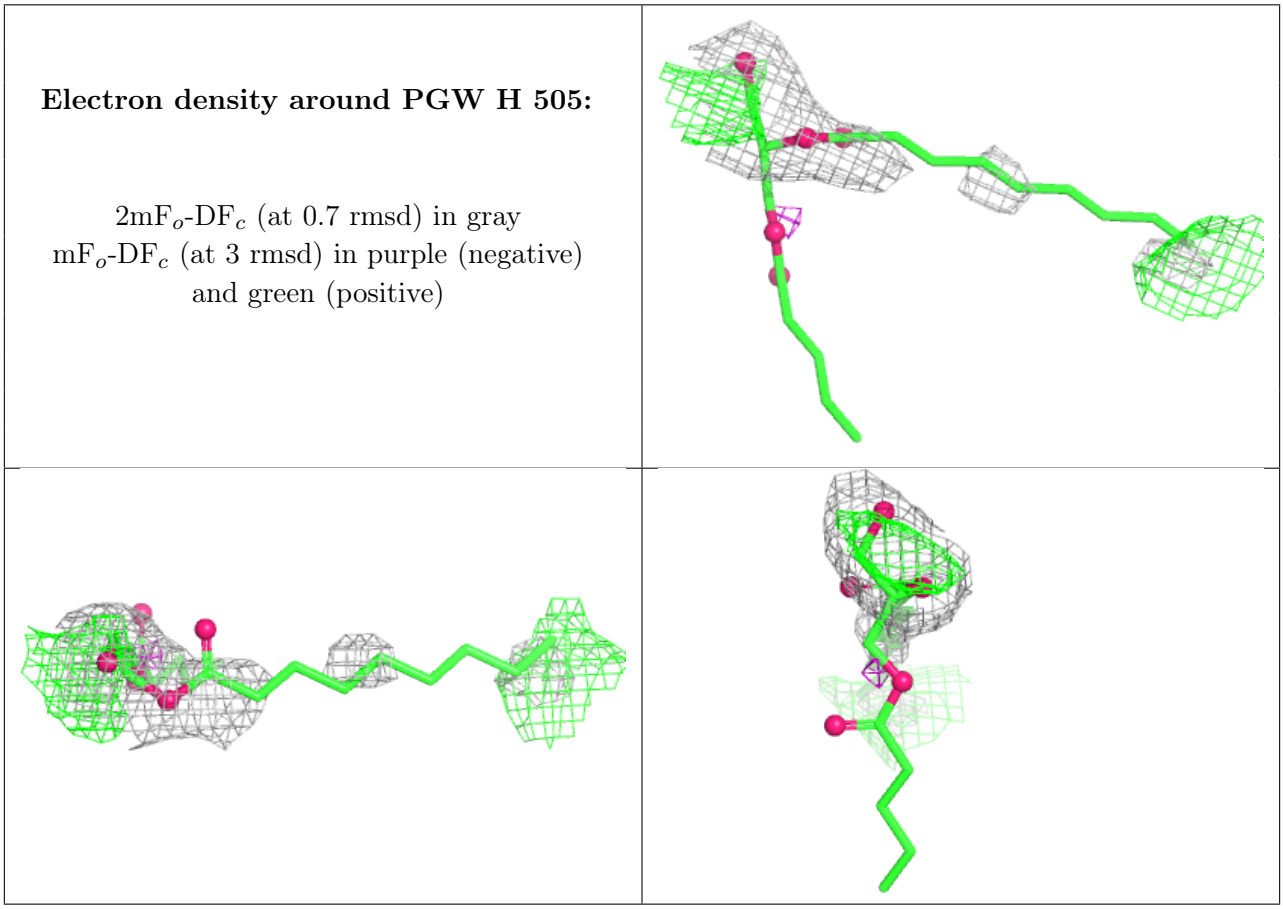
Electron density around PGW B 509:

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



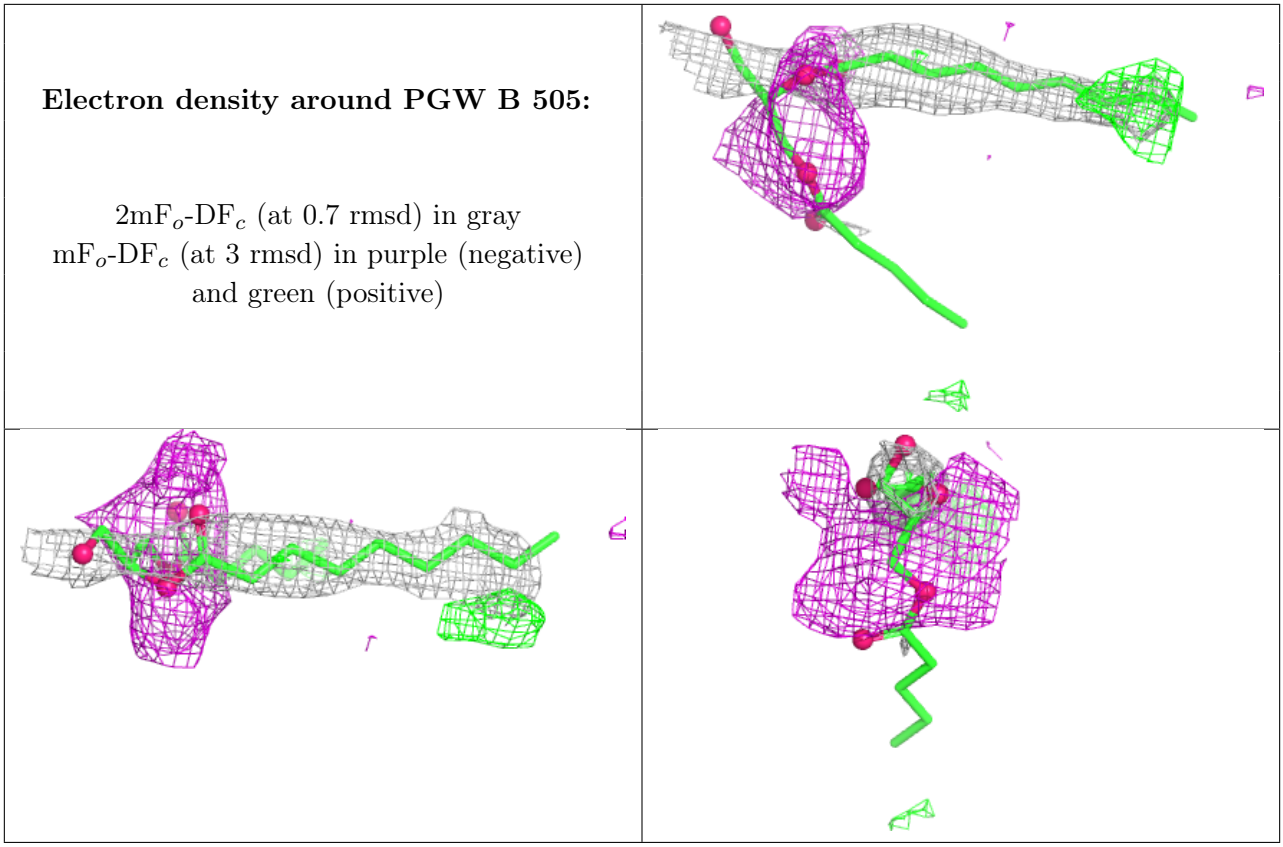
Electron density around PGW H 505:

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



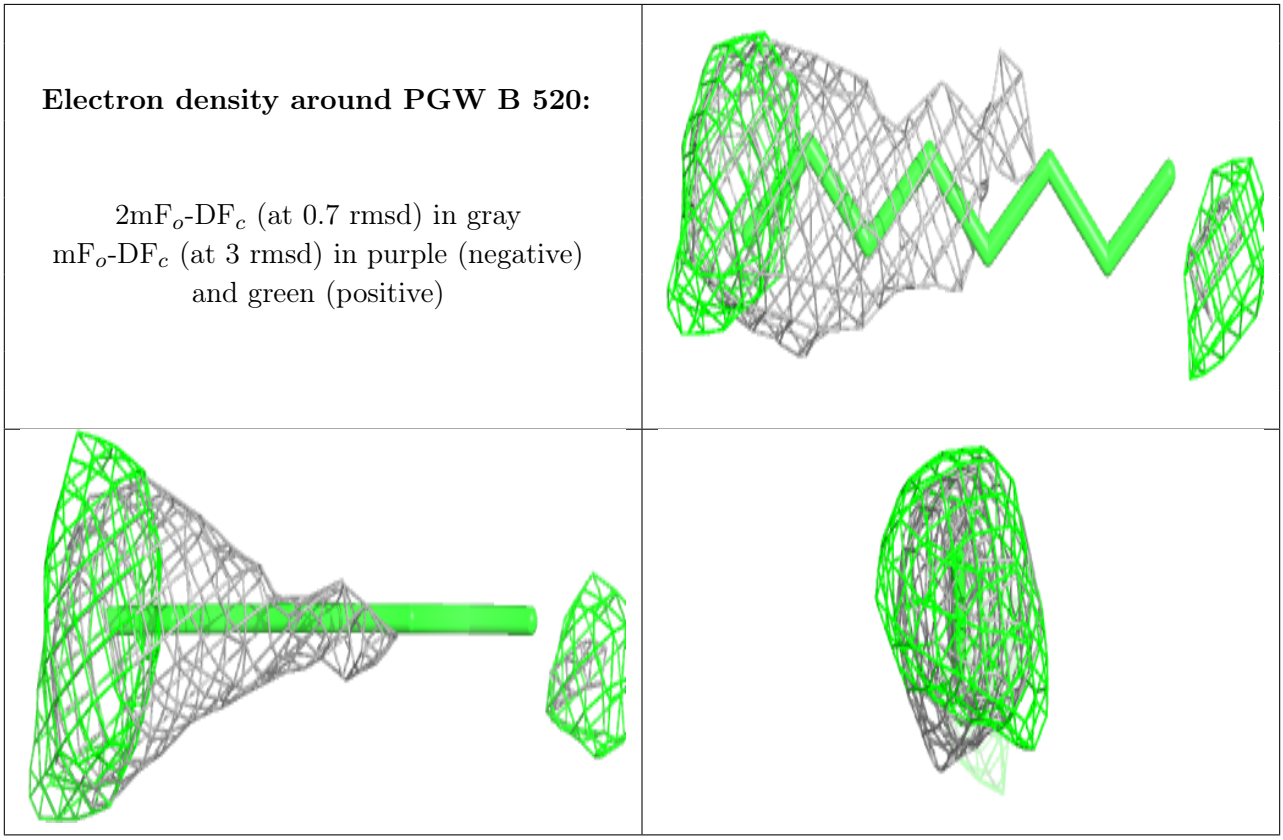
Electron density around PGW B 505:

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



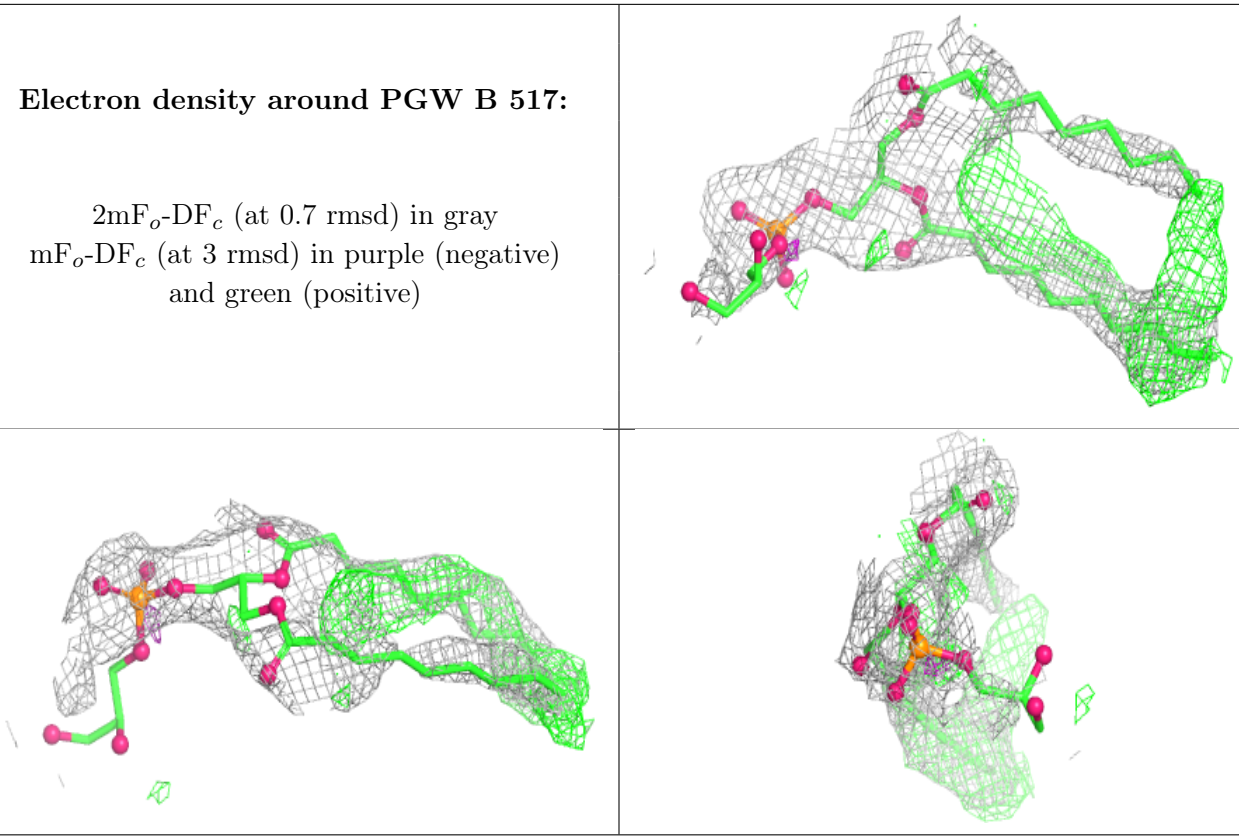
Electron density around PGW B 520:

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



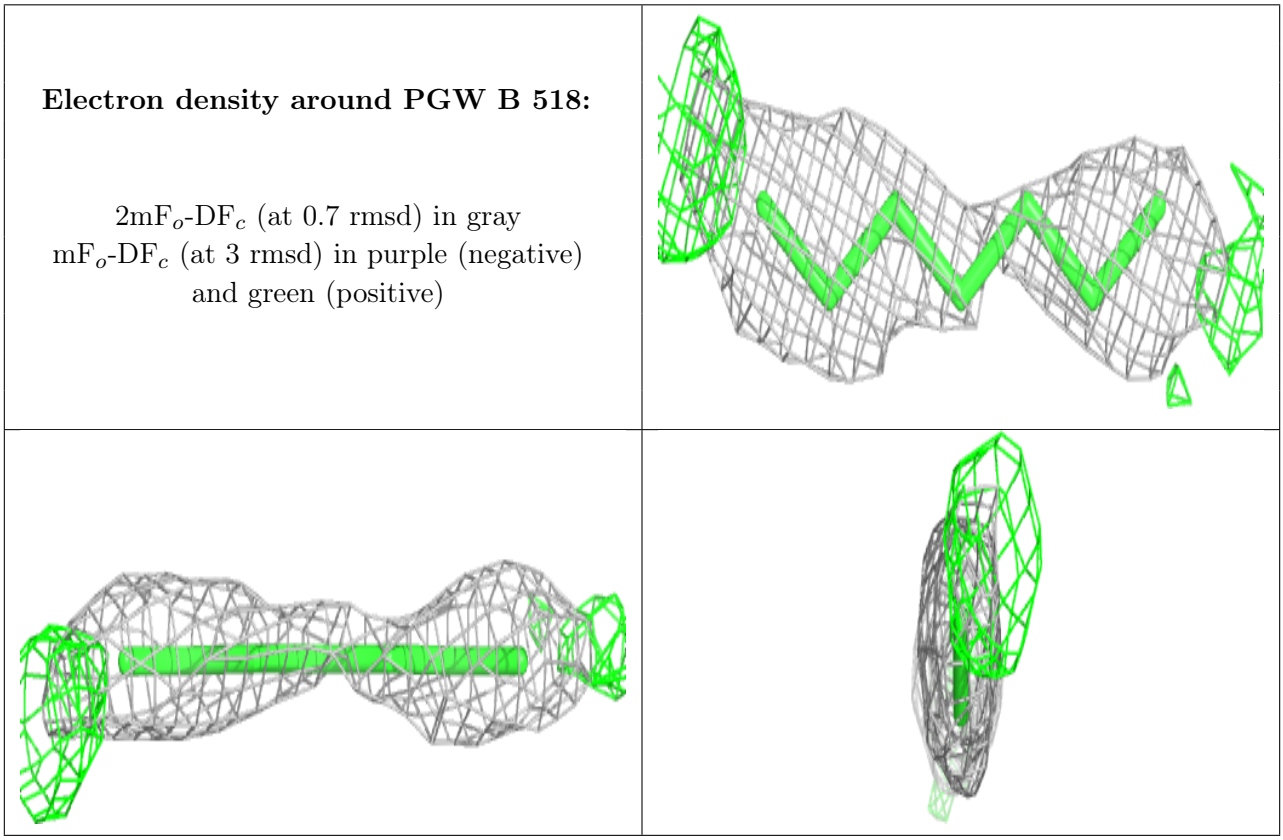
Electron density around PGW B 517:

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



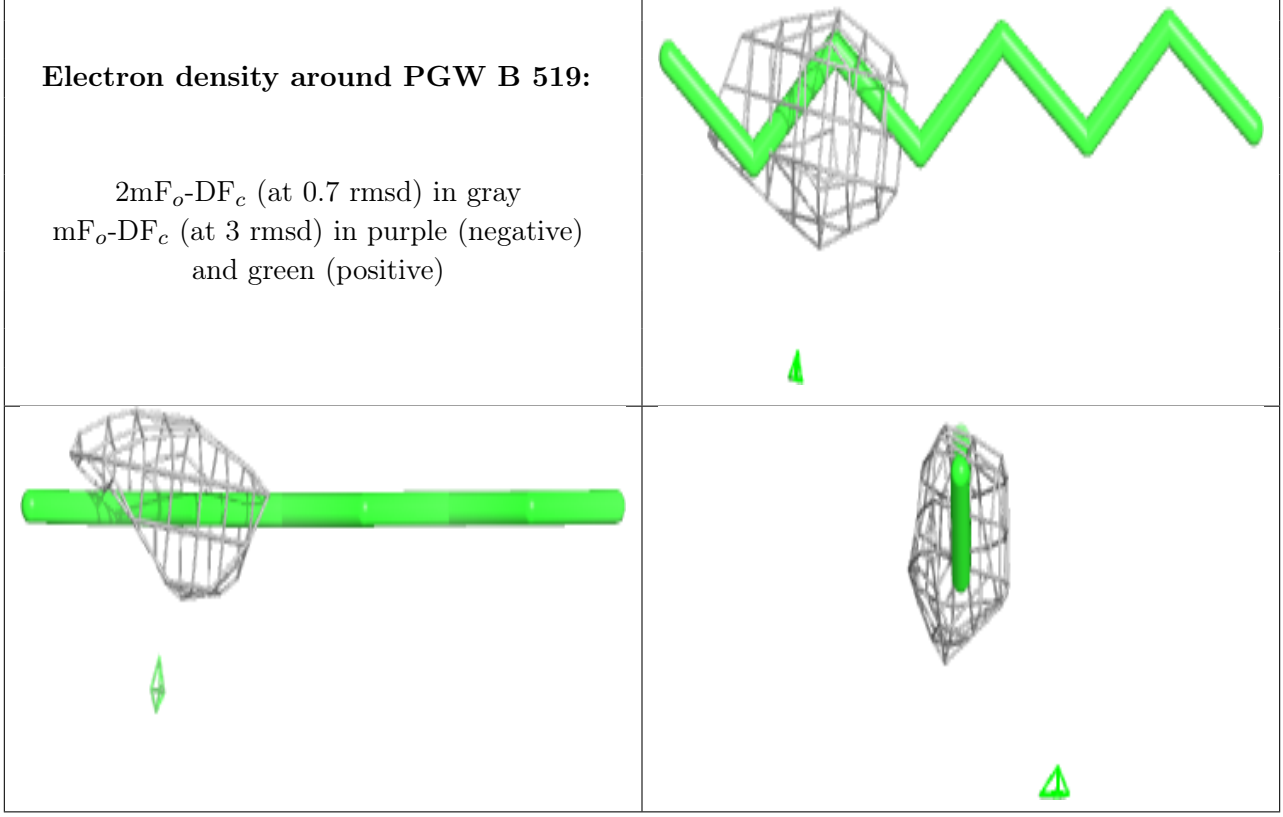
Electron density around PGW B 518:

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



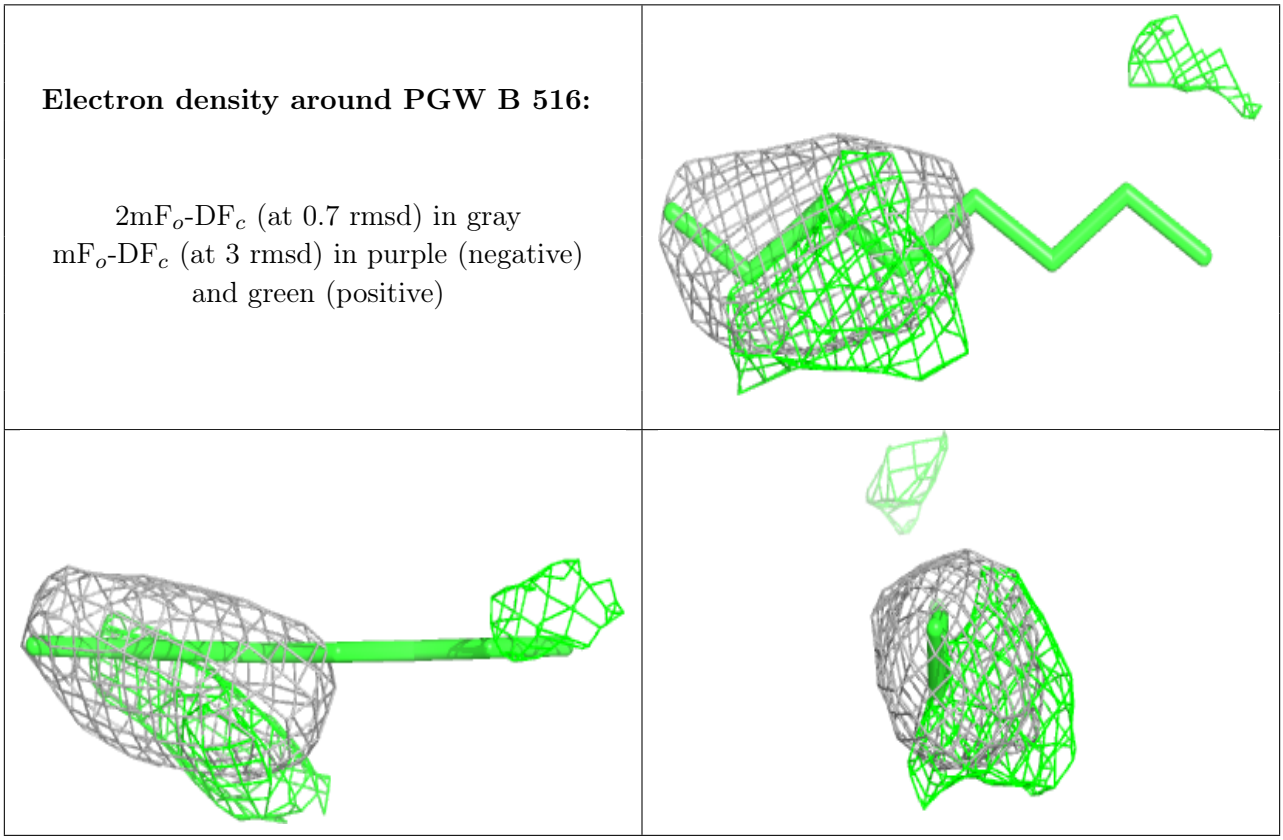
Electron density around PGW B 519:

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



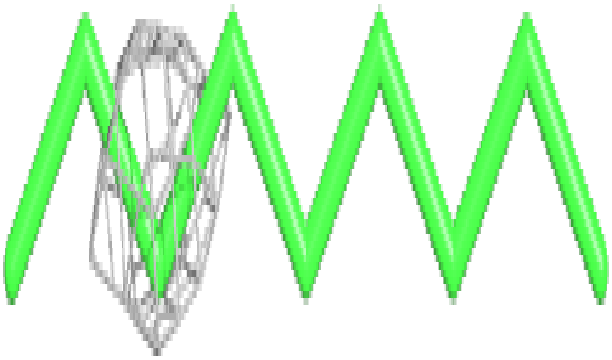
Electron density around PGW B 516:

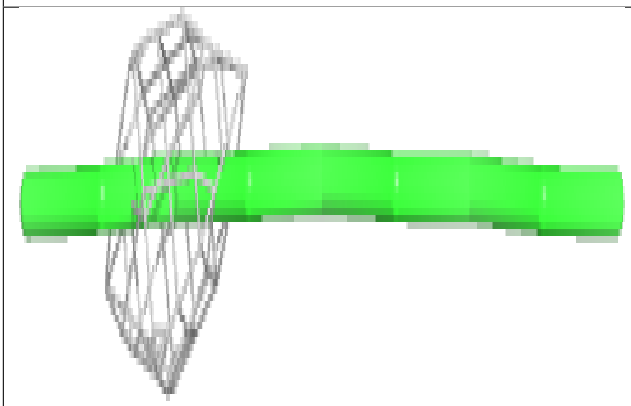
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

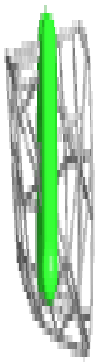


Electron density around PGW B 510:

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

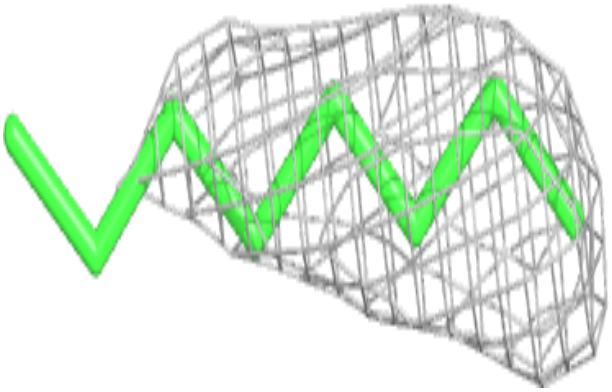


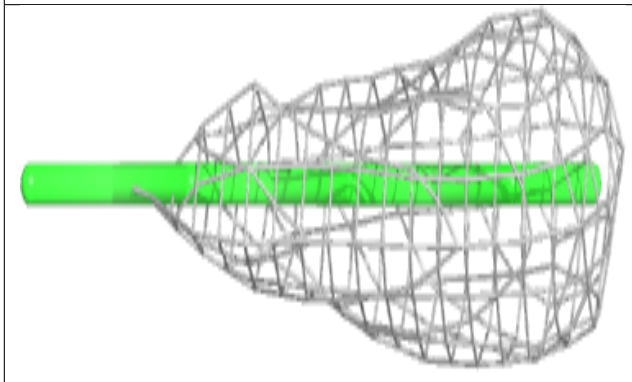


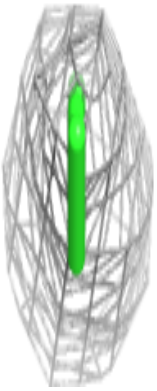


Electron density around PGW B 514:

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

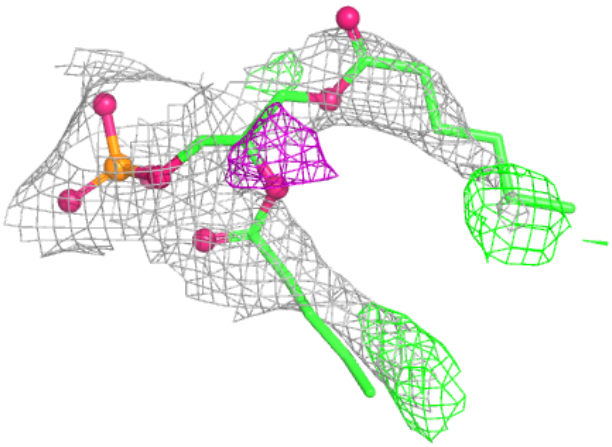


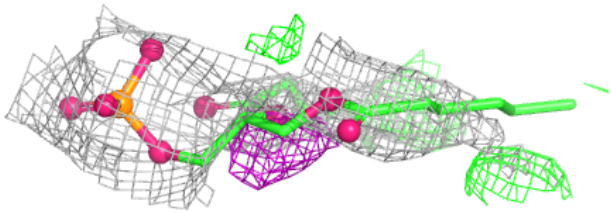


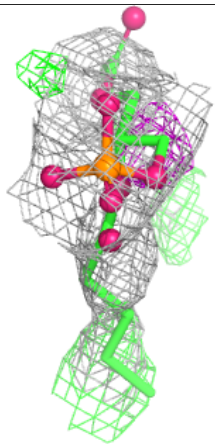


Electron density around PGW B 515:

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

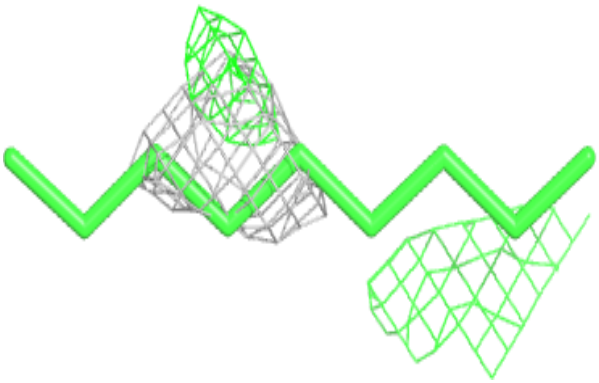


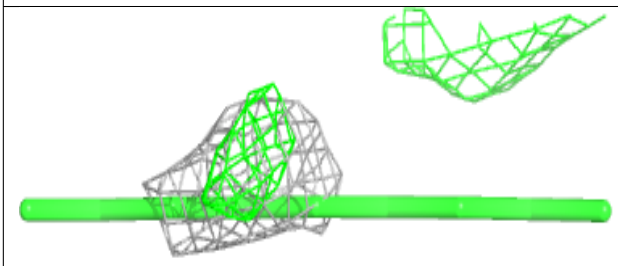


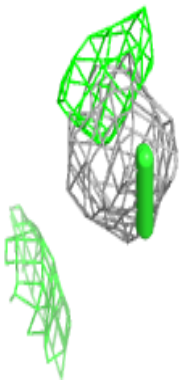


Electron density around PGW B 511:

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

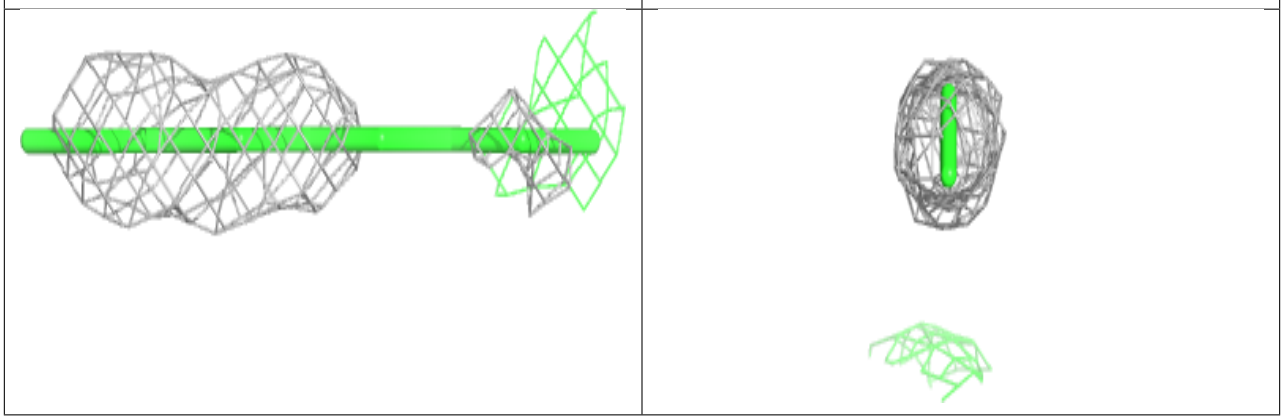






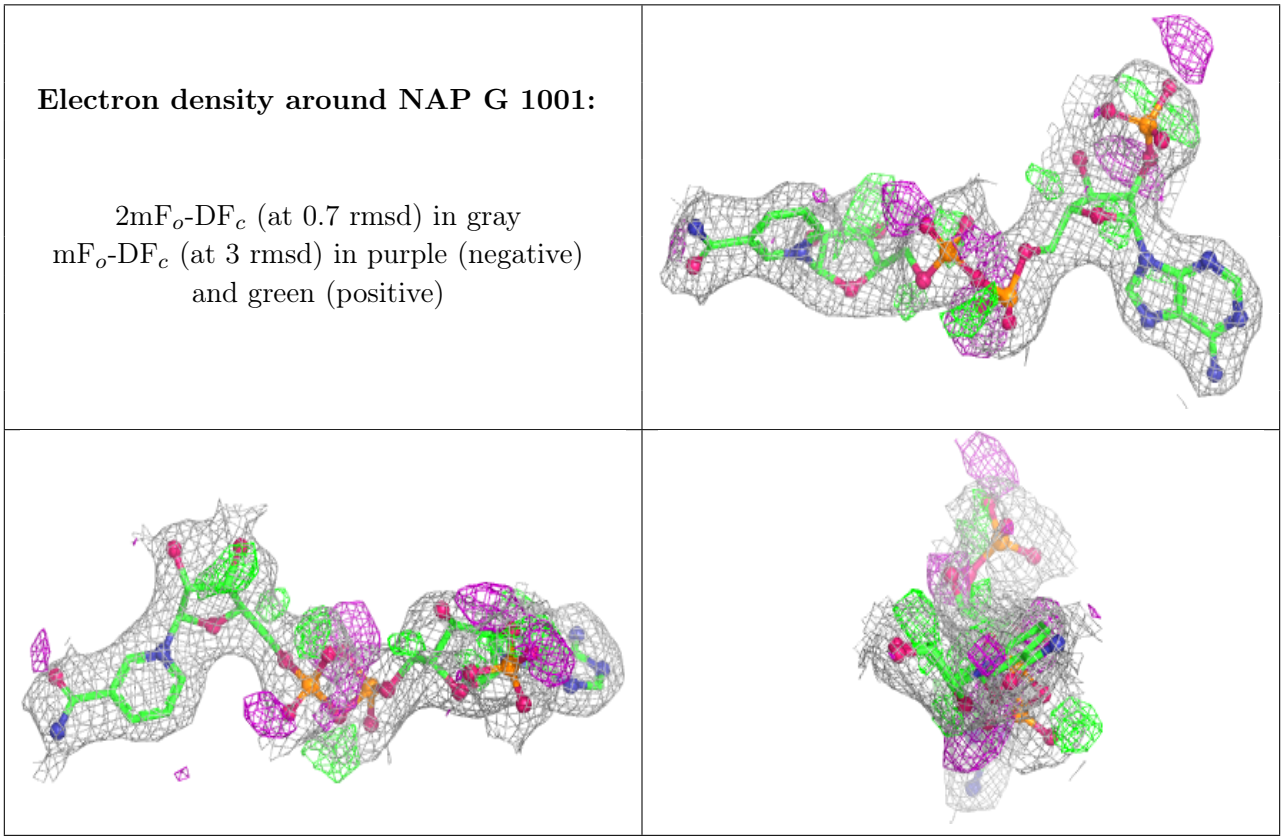
Electron density around PGW B 508:

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



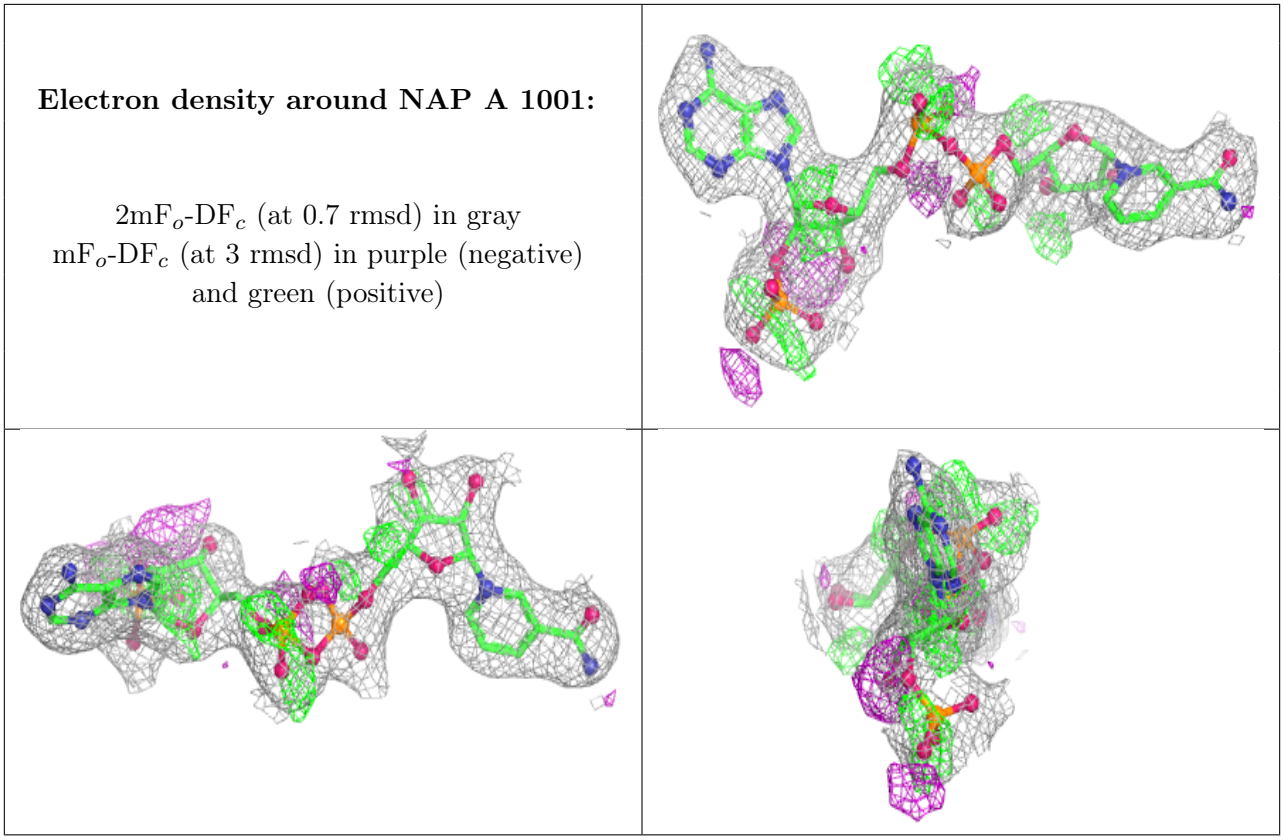
Electron density around NAP G 1001:

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



Electron density around NAP A 1001:

$2mF_o$-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.