Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 06:05 PM EDT

PDB ID	:	4JTC
Title	:	Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Charybdotoxin in Cs+
Authors	:	Banerjee, A.; Lee, A.; Campbell, E.; MacKinnon, R.
Deposited on	:	2013-03-23
Resolution	:	2.56 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:

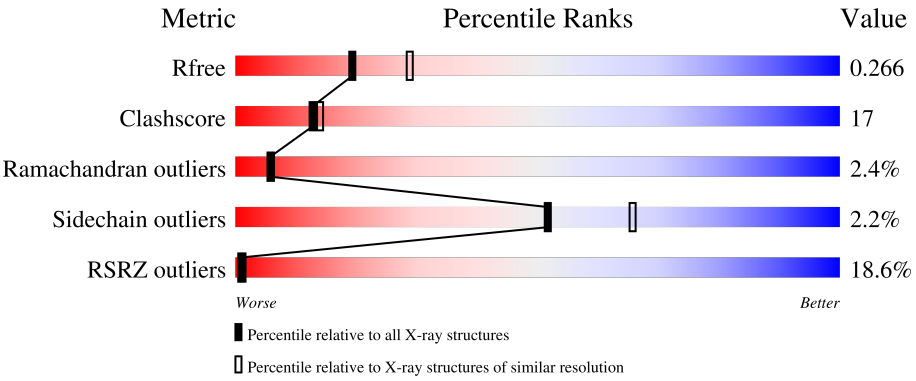
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	2% 79% 17%
1	G	333	2% 78% 19%
2	B	514	12% 48% 25% 25%
2	H	514	31% 37% 31% 29%
3	Y	37	97% 59% 38%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PCA	Y	1	-	-	-	X
6	PGW	B	504	-	-	-	X
6	PGW	B	506	-	-	-	X
6	PGW	B	507	-	-	-	X
6	PGW	B	508	-	-	-	X
6	PGW	B	510	-	-	-	X
6	PGW	B	512	-	-	-	X
6	PGW	B	513	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	517	-	-	-	X
6	PGW	B	518	-	-	-	X
6	PGW	H	504	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11770 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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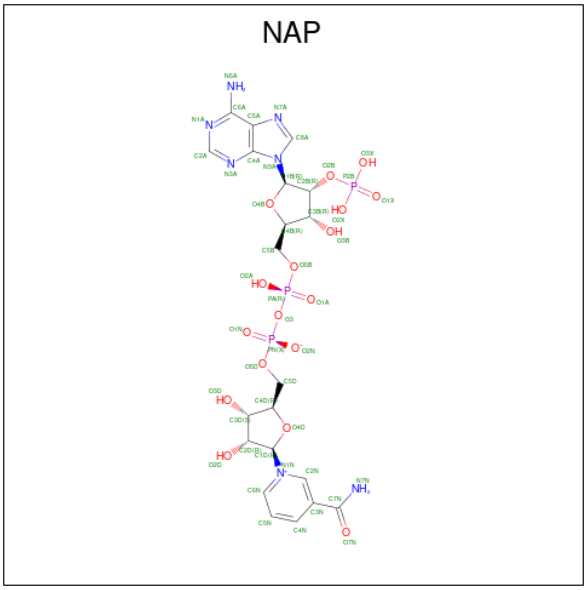
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P63142
B	-8	HIS	-	expression tag	UNP P63142
B	-7	HIS	-	expression tag	UNP P63142
B	-6	GLY	-	expression tag	UNP P63142
B	-5	LEU	-	expression tag	UNP P63142
B	-4	VAL	-	expression tag	UNP P63142
B	-3	PRO	-	expression tag	UNP P63142
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
			295	176	57	55	7			

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

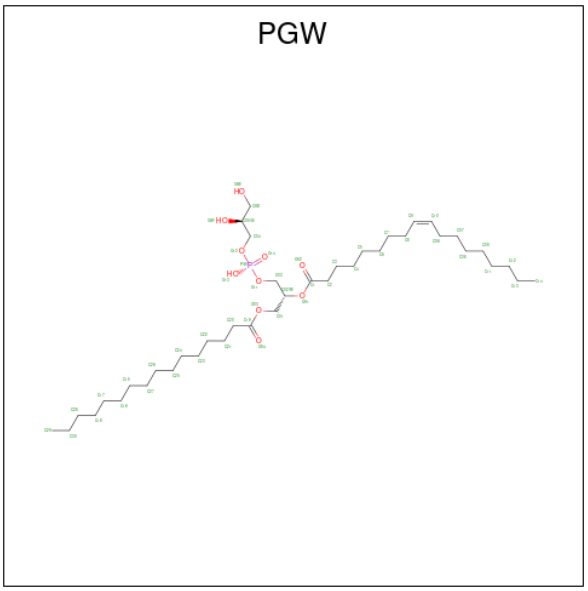


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	4	Total	Cs	0	0
			4	4		
5	H	4	Total	Cs	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
6	B	1	Total C 7 7	0	0

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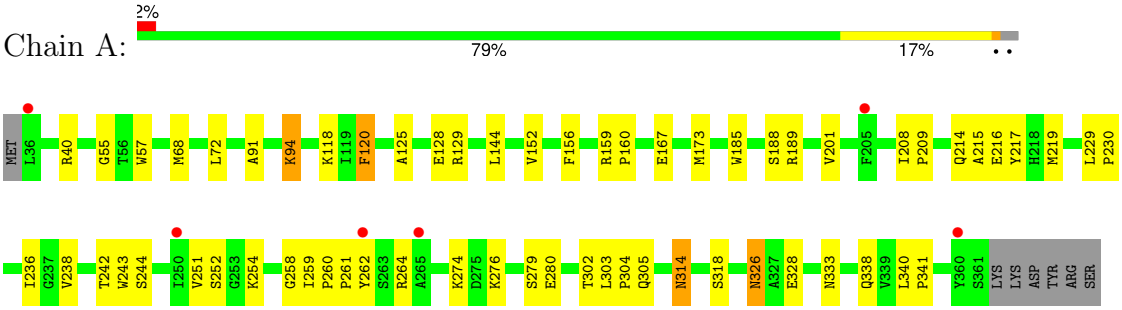
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C 8 8	0	0
6	B	1	Total C 8 8	0	0
6	H	1	Total C O 22 17 5	0	0

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.

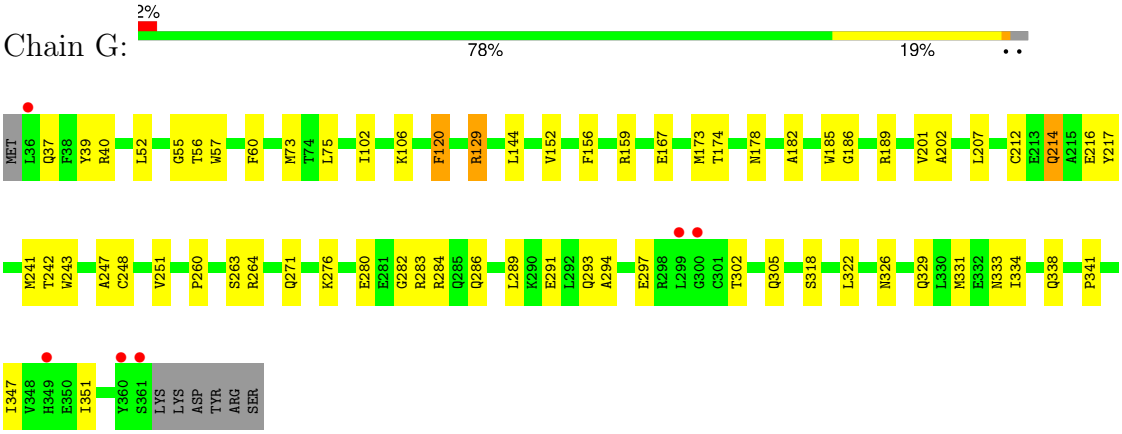
• Molecule 1: Voltage-gated potassium channel subunit beta-2

Chain A:



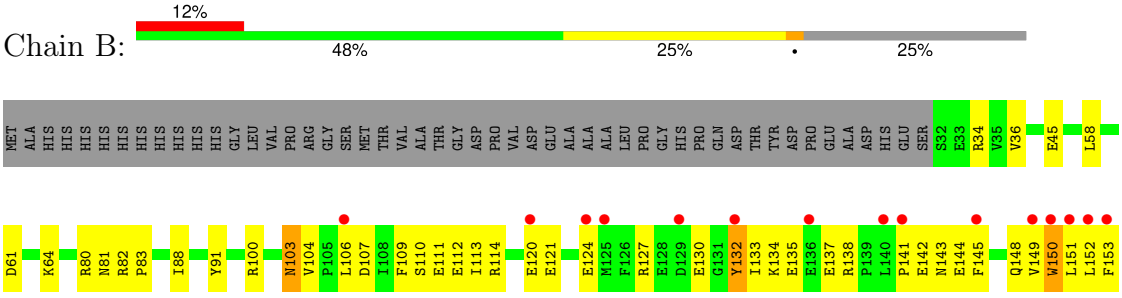
• Molecule 1: Voltage-gated potassium channel subunit beta-2

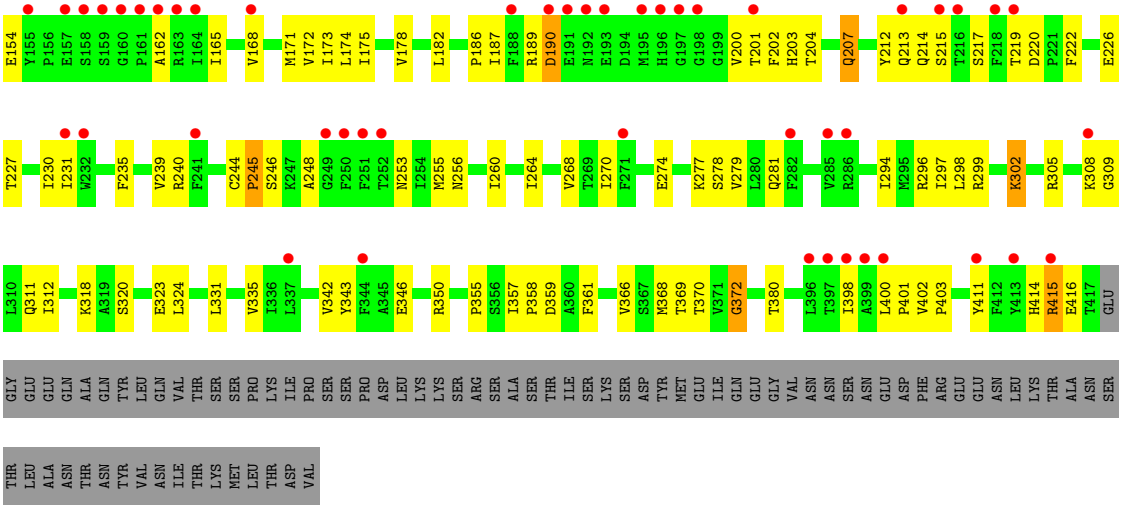
Chain G:



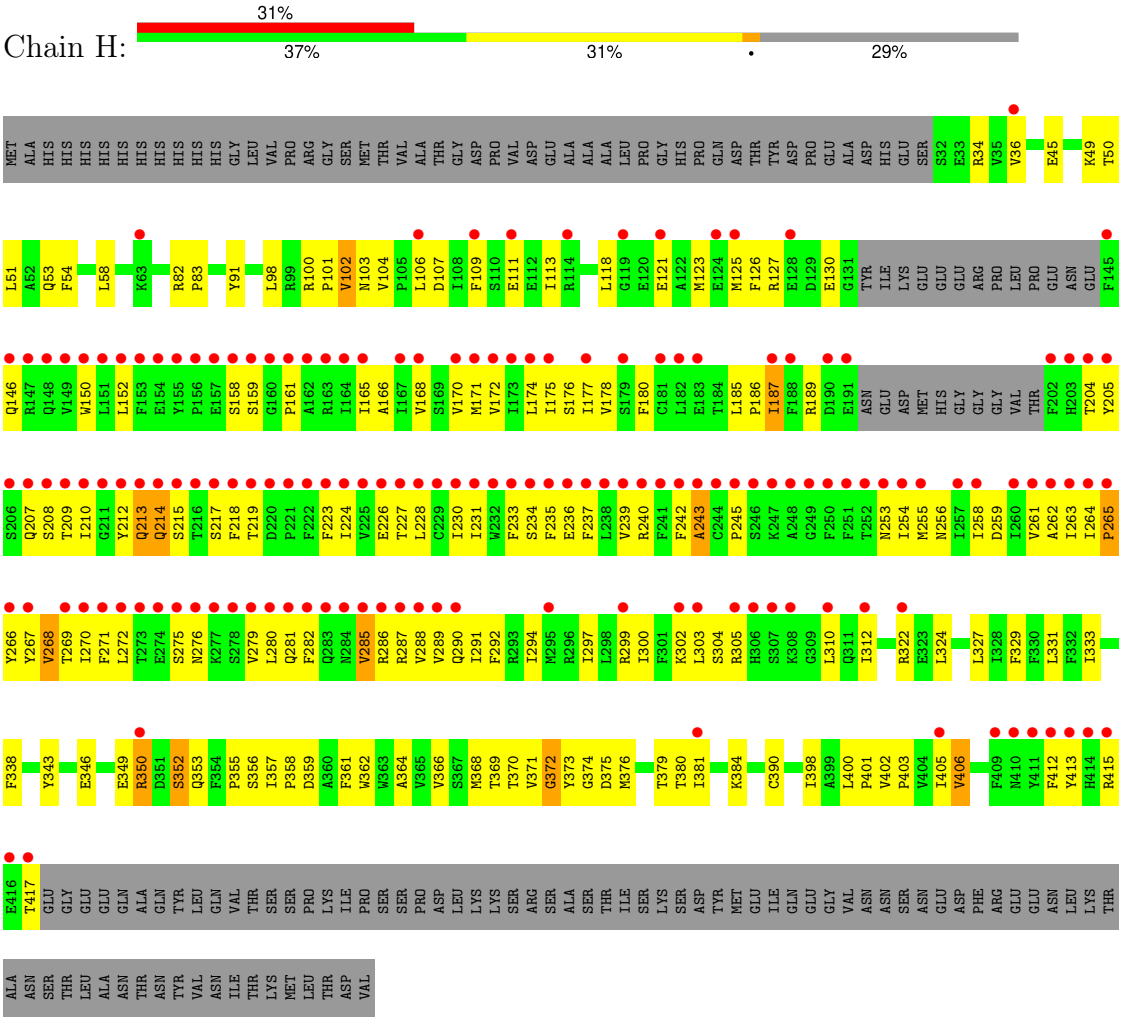
• Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1

Chain B:



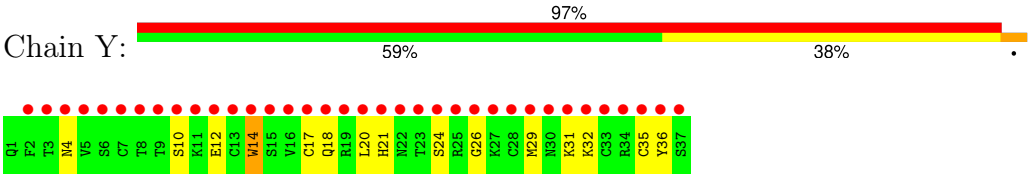


• Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



• Molecule 3: Potassium channel toxin alpha-KTx 1.1

Chain Y:


97%
59%
38%
Q1
F2
T3
N4
V5
S6
C7
T8
T9
S10
K11
E12
C13
W14
S15
V16
C17
Q18
R19
L20
H21
N22
T23
S24
R25
G26
K27
C28
M29
H30
K31
K32
C33
R34
C35
Y36
S37

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	145.43Å 145.43Å 285.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 49.93 – 2.56	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.00-2.56) 92.1 (49.93-2.56)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.262 0.238 , 0.266	Depositor DCC
R_{free} test set	4652 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 58.4	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	0.91	EDS
Total number of atoms	11770	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, PGW, CS, NAP

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	0.42	0/2608	0.61	0/3524
1	G	0.39	0/2608	0.60	0/3524
2	B	0.37	0/3169	0.55	0/4292
2	H	0.33	0/3036	0.50	0/4114
3	Y	0.26	0/292	0.46	0/389
All	All	0.38	0/11713	0.56	0/15843

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	44	0
1	G	2556	0	2582	46	0
2	B	3088	0	3034	118	0
2	H	2959	0	2956	161	0
3	Y	295	0	282	10	0
4	A	48	0	25	11	0
4	G	48	0	25	12	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	18	0
6	H	22	0	25	7	0
All	All	11770	0	11762	391	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 (391) 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)
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.43	1.00
1:G:55:GLY:HA3	4:G:1001:NAP:O3D	1.68	0.93
2:H:213:GLN:HE21	2:H:215:SER:HB3	1.31	0.91
2:H:146:GLN:HB3	2:H:243:ALA:HA	1.51	0.90
1:A:55:GLY:HA3	4:A:1001:NAP:O3D	1.73	0.89
1:A:314:ASN:H	1:A:314:ASN:ND2	1.69	0.88
2:H:350:ARG:HH11	2:H:350:ARG:HB3	1.40	0.87
1:G:333:ASN:HD21	4:G:1001:NAP:H61A	1.22	0.87
2:H:358:PRO:HB3	6:H:504:PGW:H20A	1.61	0.83
1:G:40:ARG:HD2	1:G:318:SER:O	1.77	0.82
1:A:314:ASN:H	1:A:314:ASN:HD22	1.26	0.81
3:Y:4:ASN:HA	3:Y:32:LYS:HD3	1.62	0.81
2:H:185:LEU:HD12	2:H:186:PRO:HD2	1.63	0.80
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.31	0.78
1:G:189:ARG:HH21	4:G:1001:NAP:H71N	1.32	0.78
2:H:358:PRO:HB3	6:H:504:PGW:C20	2.14	0.78
2:H:349:GLU:HB2	2:H:352:SER:HB2	1.66	0.76
2:B:311:GLN:HG2	6:B:516:PGW:H3	1.67	0.75
3:Y:26:GLY:HA3	3:Y:35:CYS:HA	1.69	0.74
2:H:213:GLN:HE21	2:H:215:SER:CB	2.01	0.73
1:G:293:GLN:O	1:G:297:GLU:HG3	1.89	0.72
2:H:412:PHE:HD1	2:H:415:ARG:HH21	1.34	0.72
2:B:400:LEU:O	2:B:403:PRO:HD2	1.88	0.72
2:B:227:THR:O	2:B:231:ILE:HG12	1.88	0.72
1:G:129:ARG:HB3	1:G:129:ARG:HH11	1.53	0.72
2:H:113:ILE:HG23	2:H:118:LEU:HD12	1.72	0.71
2:B:253:ASN:ND2	2:B:255:MET:HB2	2.04	0.71
2:H:177:ILE:HD11	2:H:300:ILE:HA	1.71	0.71
2:H:270:ILE:HD12	2:H:270:ILE:H	1.55	0.71
2:H:366:VAL:HG12	2:H:372:GLY:HA2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ASN:H	2:B:103:ASN:HD22	1.39	0.70
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.72	0.70
2:H:375:ASP:O	2:H:376:MET:HG3	1.92	0.70
2:B:120:GLU:O	2:B:124:GLU:HG3	1.92	0.69
1:A:258:GLY:O	1:A:260:PRO:HD3	1.92	0.69
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.72	0.69
2:H:364:ALA:O	2:H:368:MET:HG3	1.93	0.67
2:B:100:ARG:NH1	2:B:106:LEU:HB2	2.10	0.67
2:B:226:GLU:O	2:B:230:ILE:HD13	1.94	0.67
2:H:109:PHE:CE2	2:H:113:ILE:HD11	2.28	0.66
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.11	0.66
1:A:314:ASN:HD22	1:A:314:ASN:N	1.92	0.65
2:H:230:ILE:HG12	2:H:266:TYR:HB2	1.78	0.65
4:G:1001:NAP:H52A	4:G:1001:NAP:H8A	1.77	0.65
1:G:338:GLN:O	1:G:341:PRO:HD2	1.96	0.65
2:H:350:ARG:HH11	2:H:350:ARG:CB	2.09	0.65
4:A:1001:NAP:H8A	4:A:1001:NAP:H52A	1.79	0.65
2:B:61:ASP:HB3	2:B:64:LYS:HB2	1.79	0.65
2:B:366:VAL:HG12	2:B:372:GLY:HA2	1.80	0.64
2:B:416:GLU:HA	6:B:516:PGW:HADA	1.78	0.64
2:H:276:ASN:HB3	2:H:282:PHE:HB2	1.80	0.63
2:H:276:ASN:OD1	2:H:281:GLN:HG2	1.99	0.63
2:B:253:ASN:HD21	2:B:255:MET:HB2	1.63	0.62
2:H:213:GLN:NE2	2:H:215:SER:HB3	2.09	0.62
2:H:402:VAL:O	2:H:406:VAL:HG23	1.99	0.62
2:H:207:GLN:HE21	2:H:213:GLN:HA	1.64	0.62
2:B:58:LEU:HD12	2:B:64:LYS:HB3	1.80	0.62
2:H:270:ILE:HD12	2:H:270:ILE:N	2.15	0.62
2:H:305:ARG:HH11	2:H:305:ARG:HG2	1.65	0.62
2:H:210:ILE:HD11	2:H:214:GLN:N	2.15	0.62
2:B:400:LEU:CB	2:B:401:PRO:HD3	2.25	0.61
2:H:331:LEU:HD11	2:H:398:ILE:HG12	1.82	0.61
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.15	0.61
2:H:212:TYR:O	2:H:213:GLN:HB2	2.01	0.61
2:H:362:TRP:HB2	6:H:504:PGW:H2A	1.82	0.61
2:H:302:LYS:HA	2:H:302:LYS:HE2	1.82	0.61
2:H:230:ILE:HD12	2:H:230:ILE:N	2.16	0.61
2:B:187:ILE:HG21	6:B:512:PGW:H2A	1.82	0.61
2:H:294:ILE:O	2:H:297:ILE:HG22	2.01	0.61
2:B:100:ARG:HH11	2:B:106:LEU:HB2	1.65	0.60
2:H:381:ILE:HD12	2:H:381:ILE:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:O	2:B:335:VAL:HG23	2.01	0.60
1:A:91:ALA:O	1:A:94:LYS:HB2	2.01	0.60
2:B:255:MET:CE	2:B:305:ARG:HA	2.32	0.59
1:G:302:THR:OG1	1:G:305:GLN:HG3	2.02	0.59
2:B:186:PRO:O	2:B:190:ASP:HB2	2.02	0.59
2:H:36:VAL:HG22	2:H:45:GLU:HG3	1.83	0.59
2:B:323:GLU:CD	2:B:323:GLU:H	2.06	0.59
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.83	0.59
2:B:414:HIS:C	2:B:416:GLU:H	2.04	0.58
2:H:398:ILE:HG22	2:H:398:ILE:O	2.03	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:HE3	1.68	0.58
1:G:55:GLY:HA3	4:G:1001:NAP:HO3N	1.69	0.58
2:H:264:ILE:HB	2:H:265:PRO:HD3	1.86	0.58
2:H:381:ILE:HD12	2:H:381:ILE:N	2.18	0.58
6:B:516:PGW:O02	6:B:516:PGW:H03A	2.04	0.58
2:H:161:PRO:O	2:H:165:ILE:HG13	2.04	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:CE3	2.38	0.58
2:B:171:MET:O	2:B:175:ILE:HG13	2.03	0.58
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.39	0.57
2:H:402:VAL:HB	2:H:403:PRO:HD3	1.86	0.57
2:H:207:GLN:NE2	2:H:213:GLN:HG3	2.18	0.57
2:H:231:ILE:O	2:H:235:PHE:HB2	2.04	0.57
2:B:142:GLU:O	2:B:144:GLU:N	2.34	0.57
2:H:415:ARG:HG2	2:H:415:ARG:HH11	1.69	0.57
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.86	0.57
2:B:149:VAL:C	2:B:151:LEU:H	2.07	0.57
2:B:201:THR:HB	2:B:204:THR:OG1	2.05	0.57
2:B:222:PHE:CE1	6:B:513:PGW:H15A	2.39	0.57
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.40	0.56
2:B:213:GLN:HE22	2:B:219:THR:HB	1.70	0.56
1:G:280:GLU:HG2	1:G:284:ARG:NH1	2.19	0.56
1:A:251:VAL:O	1:A:251:VAL:HG12	2.05	0.56
2:B:152:LEU:N	2:B:152:LEU:HD12	2.21	0.56
1:A:125:ALA:HB3	1:A:128:GLU:HG3	1.85	0.56
2:H:152:LEU:HD22	2:H:161:PRO:HG2	1.87	0.56
2:H:400:LEU:O	2:H:403:PRO:HD2	2.06	0.56
2:B:152:LEU:HA	2:B:162:ALA:HB1	1.87	0.56
2:H:346:GLU:HG2	2:H:380:THR:CG2	2.35	0.56
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.40	0.56
2:H:58:LEU:C	2:H:58:LEU:HD23	2.25	0.55
2:B:278:SER:OG	2:B:281:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:LEU:HB2	2:B:401:PRO:CD	2.27	0.55
1:G:214:GLN:HA	1:G:241:MET:O	2.06	0.55
2:H:91:TYR:CE2	2:H:118:LEU:HD22	2.42	0.55
2:H:101:PRO:HB2	2:H:104:VAL:HG23	1.89	0.55
2:H:82:ARG:HB2	2:H:83:PRO:HD3	1.87	0.55
1:A:159:ARG:HA	1:A:188:SER:O	2.06	0.55
2:H:180:PHE:CE2	2:H:297:ILE:HD13	2.42	0.55
2:H:355:PRO:HB2	2:H:359:ASP:OD2	2.07	0.55
2:B:277:LYS:HG3	2:B:277:LYS:O	2.07	0.55
2:B:103:ASN:HD22	2:B:103:ASN:N	2.05	0.54
1:G:286:GLN:HA	1:G:289:LEU:HD12	1.88	0.54
6:B:514:PGW:O11	6:B:514:PGW:O02	2.26	0.54
1:G:144:LEU:HD21	1:G:152:VAL:HG13	1.89	0.54
2:H:121:GLU:O	2:H:125:MET:HB2	2.08	0.54
2:H:327:LEU:O	2:H:331:LEU:HD13	2.08	0.54
2:H:230:ILE:HG12	2:H:266:TYR:CB	2.38	0.54
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.89	0.54
2:H:152:LEU:O	2:H:165:ILE:HD12	2.08	0.54
2:H:285:VAL:HG22	2:H:285:VAL:O	2.08	0.54
2:H:107:ASP:O	2:H:111:GLU:HG3	2.07	0.54
1:G:216:GLU:HB2	1:G:243:TRP:CH2	2.43	0.54
1:G:264:ARG:NH2	4:G:1001:NAP:H4B	2.22	0.54
1:A:276:LYS:O	1:A:279:SER:HB3	2.08	0.54
2:H:253:ASN:HB3	2:H:256:ASN:OD1	2.08	0.54
2:B:255:MET:HE1	2:B:305:ARG:HA	1.88	0.53
2:B:355:PRO:HB2	2:B:359:ASP:OD2	2.08	0.53
1:G:251:VAL:HG12	1:G:251:VAL:O	2.08	0.53
2:H:236:GLU:HA	2:H:239:VAL:CG2	2.38	0.53
2:H:324:LEU:HD13	2:H:405:ILE:HD13	1.91	0.53
2:B:201:THR:HG22	2:B:202:PHE:N	2.23	0.53
1:G:280:GLU:HG2	1:G:284:ARG:HH12	1.73	0.53
2:B:127:ARG:HG2	2:B:132:TYR:HB2	1.90	0.53
2:B:294:ILE:O	2:B:297:ILE:HG22	2.09	0.53
2:B:36:VAL:HG22	2:B:45:GLU:HG2	1.92	0.52
2:B:88:ILE:O	2:B:91:TYR:HB3	2.10	0.52
2:H:224:ILE:O	2:H:228:LEU:HG	2.09	0.52
2:H:287:ARG:HG2	2:H:290:GLN:OE1	2.10	0.52
2:H:303:LEU:O	2:H:310:LEU:HD23	2.10	0.52
2:H:361:PHE:HB3	6:H:504:PGW:H4	1.91	0.52
1:G:247:ALA:O	1:G:248:CYS:HB2	2.10	0.52
1:G:120:PHE:O	1:G:129:ARG:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:ILE:HG21	2:H:269:THR:HG23	1.91	0.52
2:B:110:SER:O	2:B:114:ARG:HG3	2.10	0.51
2:H:230:ILE:HD12	2:H:230:ILE:H	1.73	0.51
2:B:153:PHE:CE1	2:B:165:ILE:HD13	2.45	0.51
1:G:291:GLU:O	1:G:294:ALA:HB3	2.10	0.51
2:H:268:VAL:HG12	2:H:268:VAL:O	2.10	0.51
6:H:504:PGW:H01	6:H:504:PGW:O02	2.09	0.51
3:Y:29:MET:C	3:Y:31:LYS:H	2.13	0.51
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.10	0.51
2:B:178:VAL:O	2:B:182:LEU:HG	2.10	0.51
1:G:37:GLN:NE2	1:G:37:GLN:HA	2.25	0.51
1:G:331:MET:HE2	1:G:334:ILE:HD12	1.93	0.51
2:H:279:VAL:HG12	2:H:279:VAL:O	2.11	0.51
2:H:381:ILE:H	2:H:381:ILE:CD1	2.24	0.51
6:B:510:PGW:H2	6:B:515:PGW:H16	1.93	0.51
2:H:168:VAL:O	2:H:172:VAL:HG23	2.11	0.51
2:H:210:ILE:HD12	2:H:212:TYR:CE1	2.46	0.50
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.94	0.50
2:B:203:HIS:HE1	2:B:277:LYS:NZ	2.09	0.50
2:B:414:HIS:O	2:B:416:GLU:N	2.39	0.50
1:G:217:TYR:HB3	1:G:242:THR:HB	1.93	0.50
2:B:107:ASP:O	2:B:111:GLU:HG3	2.12	0.50
2:H:205:TYR:CE2	2:H:279:VAL:HG13	2.47	0.50
1:A:216:GLU:HB2	1:A:243:TRP:CH2	2.45	0.50
6:B:504:PGW:H01	6:B:504:PGW:O02	2.12	0.50
1:G:189:ARG:NH2	4:G:1001:NAP:H71N	2.04	0.50
2:H:213:GLN:HG2	2:H:215:SER:HB3	1.94	0.50
2:H:368:MET:C	2:H:370:THR:H	2.15	0.50
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.76	0.50
2:H:152:LEU:HD22	2:H:161:PRO:CG	2.42	0.50
2:H:353:GLN:O	2:H:355:PRO:HD3	2.10	0.50
2:H:150:TRP:HB2	2:H:243:ALA:HB1	1.93	0.49
1:A:144:LEU:HD21	1:A:152:VAL:HG13	1.93	0.49
1:A:217:TYR:HB3	1:A:242:THR:HB	1.95	0.49
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.94	0.49
2:H:322:ARG:HG3	2:H:322:ARG:HH11	1.77	0.49
1:A:120:PHE:O	1:A:129:ARG:HA	2.13	0.49
6:B:510:PGW:C2	6:B:515:PGW:H16	2.42	0.49
1:G:55:GLY:CA	4:G:1001:NAP:O3D	2.50	0.49
1:A:55:GLY:CA	4:A:1001:NAP:O3D	2.52	0.49
2:B:152:LEU:HA	2:B:162:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:106:LEU:HD11	2:H:130:GLU:HG2	1.92	0.49
2:H:176:SER:HB2	2:H:299:ARG:NH1	2.27	0.49
2:H:177:ILE:O	2:H:180:PHE:HB3	2.12	0.49
3:Y:20:LEU:N	3:Y:20:LEU:HD12	2.28	0.49
2:B:145:PHE:O	2:B:148:GLN:HB3	2.13	0.49
2:H:146:GLN:HG3	2:H:242:PHE:O	2.12	0.49
2:H:212:TYR:CE2	2:H:226:GLU:HG2	2.46	0.49
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.93	0.49
2:B:299:ARG:O	2:B:302:LYS:HB2	2.12	0.49
2:B:320:SER:O	2:B:324:LEU:HB2	2.12	0.49
2:B:369:THR:HA	2:B:398:ILE:HD11	1.94	0.49
2:B:150:TRP:CE2	2:B:154:GLU:HG2	2.48	0.49
2:B:361:PHE:HB2	6:B:504:PGW:H2	1.94	0.49
1:A:57:TRP:HB3	4:A:1001:NAP:H3D	1.93	0.49
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.48	0.49
6:H:504:PGW:O02	6:H:504:PGW:H03A	2.12	0.49
2:H:187:ILE:HG22	2:H:187:ILE:O	2.13	0.48
2:H:267:TYR:C	2:H:269:THR:H	2.16	0.48
2:H:224:ILE:HD12	2:H:224:ILE:N	2.27	0.48
1:A:326:ASN:HD22	1:A:328:GLU:H	1.61	0.48
2:H:127:ARG:HH11	2:H:127:ARG:HG2	1.78	0.48
2:B:246:SER:C	2:B:248:ALA:H	2.17	0.48
2:B:260:ILE:O	2:B:264:ILE:HG13	2.14	0.48
2:H:287:ARG:HH11	2:H:287:ARG:HB3	1.79	0.48
2:B:318:LYS:HD2	6:B:516:PGW:H22	1.95	0.48
6:B:510:PGW:C1	6:B:515:PGW:H16	2.43	0.48
1:G:52:LEU:HD13	1:G:322:LEU:HD11	1.95	0.48
1:G:333:ASN:ND2	4:G:1001:NAP:H61A	2.01	0.48
2:H:171:MET:HB3	2:H:175:ILE:HD12	1.96	0.48
2:B:235:PHE:O	2:B:239:VAL:HG23	2.13	0.48
2:H:123:MET:O	2:H:127:ARG:HG3	2.13	0.48
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.48	0.48
1:G:156:PHE:HA	1:G:186:GLY:O	2.13	0.48
2:H:234:SER:HA	2:H:237:PHE:HB2	1.96	0.48
2:H:152:LEU:HA	2:H:158:SER:OG	2.14	0.48
2:H:210:ILE:HD11	2:H:213:GLN:C	2.35	0.48
3:Y:17:CYS:O	3:Y:21:HIS:HB2	2.14	0.48
2:H:204:THR:HG23	2:H:208:SER:OG	2.13	0.47
2:H:253:ASN:HD21	2:H:255:MET:HE3	1.78	0.47
2:B:127:ARG:CG	2:B:132:TYR:HB2	2.43	0.47
1:A:229:LEU:N	1:A:230:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ARG:NH2	2:B:305:ARG:HD3	2.29	0.47
2:H:231:ILE:O	2:H:231:ILE:HG22	2.13	0.47
2:H:280:LEU:HD12	2:H:280:LEU:N	2.30	0.47
2:H:358:PRO:HB3	6:H:504:PGW:H20	1.94	0.47
2:H:374:GLY:C	2:H:376:MET:H	2.18	0.47
2:B:309:GLY:HA2	2:B:312:ILE:HD12	1.94	0.47
2:H:180:PHE:HE2	2:H:297:ILE:HD13	1.77	0.47
2:B:311:GLN:HA	6:B:516:PGW:H5	1.96	0.47
4:A:1001:NAP:H52N	4:A:1001:NAP:H6N	1.97	0.47
2:B:368:MET:C	2:B:370:THR:H	2.18	0.47
1:G:329:GLN:OE1	4:G:1001:NAP:H2B	2.14	0.47
2:H:127:ARG:HG2	2:H:127:ARG:NH1	2.30	0.47
2:H:327:LEU:HD11	2:H:398:ILE:HG23	1.97	0.47
2:B:264:ILE:O	2:B:268:VAL:HG23	2.15	0.47
2:B:366:VAL:CG1	2:B:372:GLY:HA2	2.44	0.47
2:B:174:LEU:O	2:B:178:VAL:HG23	2.15	0.46
2:H:175:ILE:HG22	2:H:175:ILE:O	2.14	0.46
2:H:366:VAL:O	2:H:372:GLY:N	2.45	0.46
2:H:369:THR:OG1	2:H:371:VAL:HG23	2.15	0.46
2:B:240:ARG:HH21	2:B:305:ARG:HD3	1.81	0.46
2:B:414:HIS:C	2:B:416:GLU:N	2.69	0.46
1:A:215:ALA:O	1:A:242:THR:HA	2.15	0.46
2:B:173:ILE:HD13	2:B:302:LYS:HB3	1.98	0.46
2:B:200:VAL:HG23	2:B:200:VAL:O	2.15	0.46
2:B:350:ARG:NH1	2:B:350:ARG:CB	2.79	0.46
1:G:37:GLN:HA	1:G:37:GLN:HE21	1.80	0.46
2:B:80:ARG:NH1	2:B:112:GLU:OE1	2.48	0.46
1:G:167:GLU:HA	1:G:201:VAL:HG11	1.97	0.46
2:H:53:GLN:HB3	2:H:54:PHE:CD1	2.51	0.46
1:A:188:SER:O	1:A:189:ARG:HB2	2.16	0.46
2:B:202:PHE:HB2	2:B:279:VAL:HG22	1.98	0.46
2:B:320:SER:HA	2:B:323:GLU:OE2	2.16	0.46
1:G:37:GLN:HG3	1:G:39:TYR:O	2.16	0.46
2:H:240:ARG:HH12	2:H:305:ARG:CD	2.29	0.46
2:H:312:ILE:HD13	2:H:413:TYR:HA	1.98	0.46
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.31	0.46
2:H:98:LEU:HD21	2:H:113:ILE:HD13	1.97	0.46
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.52	0.45
1:A:254:LYS:HE3	4:A:1001:NAP:N3A	2.32	0.45
2:B:207:GLN:O	2:B:207:GLN:HG2	2.17	0.45
2:B:212:TYR:CE2	2:B:226:GLU:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:MET:HG3	1:G:185:TRP:CE3	2.52	0.45
2:H:262:ALA:HB1	2:H:302:LYS:HD2	1.98	0.45
2:H:286:ARG:HH11	2:H:286:ARG:HG2	1.81	0.45
2:H:291:ILE:HG22	2:H:291:ILE:O	2.16	0.45
1:A:189:ARG:HH21	4:A:1001:NAP:H71N	1.64	0.45
2:B:168:VAL:O	2:B:172:VAL:HG23	2.17	0.45
1:A:252:SER:OG	1:A:254:LYS:HG2	2.16	0.45
1:G:260:PRO:HG2	1:G:263:SER:HB3	1.98	0.45
2:H:204:THR:HG22	2:H:204:THR:O	2.17	0.45
2:H:415:ARG:C	2:H:417:THR:H	2.20	0.45
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.82	0.45
1:G:251:VAL:O	1:G:251:VAL:CG1	2.65	0.45
2:H:276:ASN:HD21	2:H:285:VAL:HG11	1.81	0.45
2:H:230:ILE:HG23	2:H:263:ILE:HG22	1.99	0.45
2:H:288:VAL:HG12	2:H:288:VAL:O	2.17	0.45
2:H:302:LYS:C	2:H:304:SER:H	2.20	0.45
3:Y:26:GLY:HA2	3:Y:36:TYR:HD1	1.82	0.45
2:B:149:VAL:O	2:B:151:LEU:N	2.50	0.44
2:H:219:THR:HG22	2:H:219:THR:O	2.16	0.44
2:H:270:ILE:H	2:H:270:ILE:CD1	2.27	0.44
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.98	0.44
2:H:305:ARG:HG2	2:H:305:ARG:NH1	2.30	0.44
2:H:346:GLU:HG2	2:H:380:THR:HG23	2.00	0.44
2:B:270:ILE:O	2:B:274:GLU:HG2	2.17	0.44
2:B:350:ARG:CB	2:B:350:ARG:HH11	2.29	0.44
1:G:57:TRP:HB3	4:G:1001:NAP:H3D	1.99	0.44
2:H:276:ASN:ND2	2:H:285:VAL:HG11	2.33	0.44
1:A:40:ARG:HD2	1:A:318:SER:O	2.17	0.44
1:G:189:ARG:NE	4:G:1001:NAP:N7N	2.66	0.44
2:H:285:VAL:HG23	2:H:288:VAL:HG21	1.99	0.44
2:H:227:THR:HG23	2:H:231:ILE:HG13	1.99	0.44
2:B:357:ILE:HB	2:B:358:PRO:HD3	2.00	0.44
2:B:411:TYR:CE1	2:B:415:ARG:HD3	2.53	0.44
1:G:56:THR:HB	1:G:60:PHE:HB2	1.98	0.44
2:H:106:LEU:CD1	2:H:130:GLU:HG2	2.48	0.44
2:H:287:ARG:HB3	2:H:287:ARG:NH1	2.32	0.44
1:G:202:ALA:HA	1:G:207:LEU:HB2	1.99	0.44
2:H:102:VAL:HG23	2:H:102:VAL:O	2.17	0.44
2:H:258:ILE:HG22	2:H:258:ILE:O	2.18	0.44
2:H:343:TYR:HE1	2:H:355:PRO:O	2.01	0.44
3:Y:10:SER:C	3:Y:12:GLU:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:NH2	4:A:1001:NAP:H4B	2.33	0.43
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.16	0.43
2:H:152:LEU:HB3	2:H:159:SER:OG	2.17	0.43
2:H:174:LEU:O	2:H:178:VAL:HG23	2.18	0.43
2:H:343:TYR:CE1	2:H:356:SER:HA	2.53	0.43
2:B:297:ILE:C	2:B:299:ARG:H	2.20	0.43
1:G:152:VAL:O	1:G:182:ALA:HA	2.18	0.43
2:H:368:MET:C	2:H:370:THR:N	2.71	0.43
2:B:214:GLN:O	2:B:215:SER:HB2	2.18	0.43
2:H:189:ARG:HG3	2:H:189:ARG:HH11	1.84	0.43
2:H:259:ASP:CG	2:H:305:ARG:HH21	2.21	0.43
2:H:322:ARG:HG3	2:H:322:ARG:NH1	2.33	0.43
1:A:125:ALA:HB3	1:A:128:GLU:CG	2.48	0.43
2:B:81:ASN:OD1	2:B:83:PRO:HD2	2.19	0.43
2:B:152:LEU:HB3	2:B:165:ILE:HD12	2.01	0.43
2:B:106:LEU:CD1	2:B:130:GLU:HG2	2.49	0.43
2:B:149:VAL:HA	2:B:152:LEU:HD13	2.00	0.43
2:H:172:VAL:HG12	2:H:233:PHE:CZ	2.54	0.43
2:B:215:SER:C	2:B:217:SER:H	2.22	0.42
2:B:308:LYS:O	2:B:312:ILE:HG13	2.19	0.42
2:H:271:PHE:O	2:H:271:PHE:CG	2.72	0.42
2:B:415:ARG:O	6:B:516:PGW:HADA	2.19	0.42
2:H:212:TYR:OH	2:H:269:THR:HG21	2.19	0.42
2:H:230:ILE:H	2:H:230:ILE:CD1	2.32	0.42
2:H:329:PHE:O	2:H:333:ILE:HG12	2.19	0.42
2:B:149:VAL:C	2:B:151:LEU:N	2.73	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.54	0.42
2:H:379:THR:HA	2:H:384:LYS:HE3	2.01	0.42
1:A:244:SER:HA	4:A:1001:NAP:O3	2.19	0.42
2:B:246:SER:C	2:B:248:ALA:N	2.73	0.42
2:H:261:VAL:HA	2:H:264:ILE:CD1	2.50	0.42
2:H:338:PHE:CE2	2:H:390:CYS:HA	2.55	0.42
2:B:100:ARG:HG3	2:B:109:PHE:CG	2.55	0.42
2:B:106:LEU:HD13	2:B:130:GLU:HG2	2.01	0.42
2:B:80:ARG:NH1	2:B:112:GLU:OE2	2.52	0.42
2:B:350:ARG:HB3	2:B:350:ARG:CZ	2.50	0.42
6:B:504:PGW:O02	6:B:504:PGW:H03A	2.20	0.42
1:G:347:ILE:O	1:G:351:ILE:HG13	2.20	0.42
2:H:230:ILE:HG21	2:H:266:TYR:HB3	2.02	0.42
1:G:276:LYS:O	1:G:282:GLY:HA3	2.19	0.41
2:H:100:ARG:HB2	2:H:126:PHE:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:GLN:CG	6:B:516:PGW:H3	2.43	0.41
2:B:318:LYS:CD	6:B:516:PGW:H22	2.50	0.41
2:H:312:ILE:CD1	2:H:413:TYR:HD1	2.32	0.41
2:H:254:ILE:C	2:H:256:ASN:H	2.23	0.41
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.83	0.41
2:H:49:LYS:HG3	2:H:50:THR:N	2.36	0.41
2:H:166:ALA:O	2:H:170:VAL:HG23	2.20	0.41
2:H:272:LEU:CD2	2:H:289:VAL:HG22	2.50	0.41
2:B:109:PHE:O	2:B:113:ILE:HG13	2.21	0.41
2:B:342:VAL:CG1	2:B:343:TYR:N	2.84	0.41
2:H:236:GLU:HA	2:H:239:VAL:HG23	2.02	0.41
1:A:333:ASN:ND2	4:A:1001:NAP:H61A	2.09	0.41
1:A:261:PRO:O	1:A:262:TYR:HB2	2.20	0.41
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.51	0.41
2:H:171:MET:HE2	2:H:174:LEU:HD12	2.03	0.41
2:H:264:ILE:O	2:H:268:VAL:HG23	2.21	0.41
2:B:83:PRO:HB2	2:B:104:VAL:HG22	2.03	0.41
2:B:150:TRP:O	2:B:150:TRP:CG	2.73	0.41
2:B:346:GLU:OE2	2:B:380:THR:HG23	2.21	0.41
1:G:174:THR:HG22	1:G:178:ASN:ND2	2.36	0.41
1:A:236:ILE:HG13	1:A:238:VAL:HG23	2.02	0.40
2:B:368:MET:C	2:B:370:THR:N	2.73	0.40
2:H:400:LEU:C	2:H:403:PRO:HD2	2.40	0.40
1:A:167:GLU:HA	1:A:201:VAL:HG11	2.03	0.40
2:B:187:ILE:HG21	6:B:512:PGW:C2	2.49	0.40
2:H:261:VAL:HA	2:H:264:ILE:HD12	2.02	0.40
1:G:102:ILE:O	1:G:106:LYS:HG2	2.22	0.40
1:G:326:ASN:OD1	1:G:329:GLN:HG3	2.21	0.40
2:H:51:LEU:C	2:H:53:GLN:H	2.25	0.40
1:A:68:MET:O	1:A:72:LEU:HG	2.20	0.40
2:B:244:CYS:HA	2:B:245:PRO:HD3	1.90	0.40
3:Y:26:GLY:HA2	3:Y:36:TYR:CD1	2.56	0.40
2:H:172:VAL:O	2:H:176:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/333 (97%)	308 (95%)	14 (4%)	2 (1%)	25	33
1	G	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	41	50
2	B	384/514 (75%)	344 (90%)	27 (7%)	13 (3%)	3	2
2	H	357/514 (70%)	280 (78%)	60 (17%)	17 (5%)	2	1
3	Y	35/37 (95%)	17 (49%)	17 (49%)	1 (3%)	4	4
All	All	1424/1731 (82%)	1262 (89%)	128 (9%)	34 (2%)	6	6

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	132	TYR
2	B	133	ILE
2	B	134	LYS
2	B	135	GLU
2	B	137	GLU
2	H	275	SER
2	H	285	VAL
1	A	120	PHE
2	B	150	TRP
2	B	372	GLY
1	G	120	PHE
2	H	102	VAL
2	H	213	GLN
2	H	243	ALA
2	H	245	PRO
2	H	268	VAL
2	H	372	GLY
2	H	103	ASN
2	H	217	SER
1	A	219	MET
2	B	138	ARG

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Mol	Chain	Res	Type
2	B	141	PRO
2	B	143	ASN
2	B	298	LEU
2	B	415	ARG
2	H	218	PHE
2	H	373	TYR
3	Y	24	SER
2	B	245	PRO
2	H	209	THR
2	H	352	SER
2	H	187	ILE
2	H	265	PRO
2	H	406	VAL

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%)	267 (98%)	6 (2%)	52	66
1	G	273/280 (98%)	266 (97%)	7 (3%)	46	59
2	B	332/459 (72%)	325 (98%)	7 (2%)	53	67
2	H	324/459 (71%)	319 (98%)	5 (2%)	65	77
3	Y	35/35 (100%)	33 (94%)	2 (6%)	20	27
All	All	1237/1513 (82%)	1210 (98%)	27 (2%)	52	66

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	LYS
1	A	214	GLN
1	A	280	GLU
1	A	314	ASN
1	A	326	ASN
1	A	338	GLN

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Mol	Chain	Res	Type
2	B	34	ARG
2	B	82	ARG
2	B	103	ASN
2	B	121	GLU
2	B	190	ASP
2	B	207	GLN
2	B	302	LYS
1	G	73	MET
1	G	75	LEU
1	G	129	ARG
1	G	212	CYS
1	G	214	GLN
1	G	271	GLN
1	G	283	ARG
2	H	34	ARG
2	H	214	GLN
2	H	223	PHE
2	H	292	PHE
2	H	350	ARG
3	Y	14	TRP
3	Y	18	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	204	GLN
1	A	286	GLN
1	A	314	ASN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	53	GLN
2	B	103	ASN
2	B	203	HIS
2	B	207	GLN
2	B	213	GLN
2	B	253	ASN
2	B	256	ASN
1	G	37	GLN
1	G	148	GLN
1	G	178	ASN

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Mol	Chain	Res	Type
1	G	333	ASN
2	H	53	GLN
2	H	207	GLN
2	H	213	GLN
2	H	284	ASN
3	Y	18	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	0.62	0	9,10,12	0.99	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	508	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	517	-	6,6,50	0.37	0	5,5,56	0.43	0
6	PGW	B	513	-	7,7,50	0.37	0	6,6,56	0.51	0
6	PGW	B	504	-	21,21,50	0.61	0	23,23,56	1.24	3 (13%)
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.53	0
4	NAP	G	1001	-	46,52,52	2.70	9 (19%)	61,80,80	2.58	16 (26%)
4	NAP	A	1001	-	46,52,52	3.01	8 (17%)	61,80,80	2.57	16 (26%)
6	PGW	B	511	-	6,6,50	0.37	0	5,5,56	0.47	0
6	PGW	B	506	-	8,8,50	0.36	0	7,7,56	0.50	0
6	PGW	B	516	-	35,35,50	0.66	0	38,41,56	0.91	2 (5%)
6	PGW	B	505	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	514	-	22,22,50	0.80	0	25,27,56	1.26	4 (16%)
6	PGW	B	515	-	7,7,50	0.36	0	6,6,56	0.50	0
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.55	0
6	PGW	B	519	-	7,7,50	0.36	0	6,6,56	0.50	0
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	512	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	H	504	-	21,21,50	0.61	0	23,23,56	1.29	3 (13%)
6	PGW	B	518	-	7,7,50	0.36	0	6,6,56	0.51	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	508	-	-	0/6/6/55	-
6	PGW	B	517	-	-	0/4/4/55	-
6	PGW	B	513	-	-	0/5/5/55	-
6	PGW	B	504	-	-	1/23/23/55	-
6	PGW	B	509	-	-	0/6/6/55	-
4	NAP	G	1001	-	-	4/31/67/67	0/5/5/5
4	NAP	A	1001	-	-	4/31/67/67	0/5/5/5
6	PGW	B	511	-	-	0/4/4/55	-
6	PGW	B	506	-	-	0/6/6/55	-
6	PGW	B	516	-	-	9/40/40/55	-
6	PGW	B	505	-	-	0/6/6/55	-
6	PGW	B	514	-	-	9/24/24/55	-
6	PGW	B	515	-	-	0/5/5/55	-
6	PGW	B	507	-	-	0/6/6/55	-
6	PGW	B	519	-	-	0/5/5/55	-
6	PGW	B	510	-	-	0/6/6/55	-
6	PGW	B	512	-	-	0/6/6/55	-
6	PGW	H	504	-	-	1/23/23/55	-
6	PGW	B	518	-	-	0/5/5/55	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAP	PN-O3	15.70	1.76	1.59
4	G	1001	NAP	PN-O3	13.80	1.74	1.59
4	A	1001	NAP	PA-O3	6.45	1.66	1.59
4	A	1001	NAP	O4B-C1B	6.40	1.49	1.40
4	G	1001	NAP	O4B-C1B	6.35	1.49	1.40
4	A	1001	NAP	O4D-C1D	4.96	1.47	1.40
4	G	1001	NAP	PA-O3	4.73	1.64	1.59
4	G	1001	NAP	O4D-C1D	4.11	1.46	1.40
4	A	1001	NAP	C2N-C3N	3.36	1.44	1.39
4	G	1001	NAP	C2N-C3N	2.65	1.43	1.39
4	G	1001	NAP	C4N-C3N	2.55	1.43	1.39
4	G	1001	NAP	C8A-N7A	-2.44	1.30	1.34
4	G	1001	NAP	P2B-O2B	2.33	1.63	1.59
4	G	1001	NAP	O3D-C3D	-2.21	1.37	1.43
4	A	1001	NAP	C4N-C3N	2.15	1.42	1.39
4	A	1001	NAP	C8A-N7A	-2.11	1.30	1.34
4	A	1001	NAP	C3N-C7N	-2.02	1.47	1.50

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	-11.38	76.46	110.70
4	A	1001	NAP	O3-PA-O1A	-10.93	77.84	110.70
4	A	1001	NAP	O4B-C1B-N9A	8.00	119.35	108.75
4	G	1001	NAP	O4B-C1B-N9A	7.86	119.17	108.75
4	A	1001	NAP	O2A-PA-O3	-6.58	89.48	107.27
4	G	1001	NAP	O2A-PA-O3	-6.24	90.39	107.27
4	A	1001	NAP	C2B-C1B-N9A	-5.26	100.87	112.56
4	G	1001	NAP	N3A-C2A-N1A	-5.04	121.83	128.67
4	A	1001	NAP	N3A-C2A-N1A	-4.84	122.10	128.67
4	G	1001	NAP	C2B-C1B-N9A	-4.48	102.61	112.56
4	A	1001	NAP	C2B-C3B-C4B	3.88	110.34	101.99
4	G	1001	NAP	C2B-C3B-C4B	3.86	110.28	101.99
4	A	1001	NAP	O2B-C2B-C3B	3.78	125.22	111.68
4	G	1001	NAP	C4B-O4B-C1B	3.71	113.33	109.92
6	H	504	PGW	O01-C1-C2	3.55	119.17	111.48
4	G	1001	NAP	PN-O5D-C5D	-3.55	101.00	121.35
4	A	1001	NAP	PN-O5D-C5D	-3.37	102.06	121.35
6	B	504	PGW	O01-C1-C2	3.34	118.70	111.48
4	G	1001	NAP	O2B-C2B-C3B	3.30	123.51	111.68
4	A	1001	NAP	C4B-O4B-C1B	3.26	112.91	109.92
4	A	1001	NAP	O4B-C4B-C5B	-2.96	99.86	109.33
4	G	1001	NAP	O4B-C4B-C5B	-2.94	99.92	109.33
6	B	514	PGW	O01-C1-C2	2.78	117.50	111.48
6	B	514	PGW	C03-C02-C01	-2.71	105.47	111.78
6	H	504	PGW	O03-C19-C20	2.55	119.61	111.83
6	B	516	PGW	O01-C1-C2	2.46	116.81	111.48
6	B	504	PGW	O03-C19-C20	2.46	119.33	111.83
6	B	514	PGW	O03-C19-C20	2.45	119.31	111.83
6	B	514	PGW	O11-P-O14	2.32	112.72	106.44
4	G	1001	NAP	C5D-C4D-C3D	-2.26	107.08	115.21
4	A	1001	NAP	O2A-PA-O5B	2.26	117.80	107.57
4	G	1001	NAP	O5B-PA-O1A	2.23	117.76	108.94
4	A	1001	NAP	O7N-C7N-N7N	-2.21	119.43	122.62
4	A	1001	NAP	C5D-C4D-C3D	-2.20	107.30	115.21
4	A	1001	NAP	O5B-PA-O1A	2.12	117.33	108.94
4	G	1001	NAP	O7N-C7N-N7N	-2.11	119.56	122.62
4	G	1001	NAP	O2A-PA-O5B	2.11	117.12	107.57
6	H	504	PGW	C02-O01-C1	-2.10	112.76	117.80
6	B	516	PGW	O01-C02-C01	-2.10	100.81	108.34
6	B	504	PGW	C02-O01-C1	-2.06	112.87	117.80
4	A	1001	NAP	O4D-C4D-C3D	2.05	109.22	105.15
4	G	1001	NAP	O2A-PA-O1A	2.04	121.92	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1001	NAP	O4D-C4D-C3D	2.02	109.16	105.15
4	A	1001	NAP	C4A-C5A-N7A	-2.01	107.21	109.34

There are no chirality outliers.

All (28) 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	514	PGW	C02-C03-O11-P
4	G	1001	NAP	C1B-C2B-O2B-P2B
4	A	1001	NAP	C1B-C2B-O2B-P2B
4	A	1001	NAP	C3B-C2B-O2B-P2B
4	G	1001	NAP	C3B-C2B-O2B-P2B
6	B	514	PGW	C2-C1-O01-C02
6	B	516	PGW	C7-C8-C9-C10
6	B	514	PGW	O02-C1-O01-C02
6	B	514	PGW	C20-C19-O03-C01
6	B	514	PGW	O04-C19-O03-C01
6	B	504	PGW	C01-C02-O01-C1
6	B	516	PGW	C01-C02-O01-C1
6	H	504	PGW	C01-C02-O01-C1
6	B	516	PGW	O02-C1-O01-C02
6	B	514	PGW	O01-C1-C2-C3
6	B	516	PGW	C2-C1-O01-C02
6	B	516	PGW	O01-C1-C2-C3
6	B	516	PGW	O03-C19-C20-C21
6	B	514	PGW	C01-C02-O01-C1
6	B	516	PGW	C03-C02-O01-C1
4	A	1001	NAP	O4B-C4B-C5B-O5B
4	G	1001	NAP	O4B-C4B-C5B-O5B
6	B	514	PGW	O03-C19-C20-C21
6	B	514	PGW	O02-C1-C2-C3
6	B	516	PGW	O04-C19-C20-C21
6	B	516	PGW	O02-C1-C2-C3

There are no ring outliers.

10 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	513	PGW	1	0

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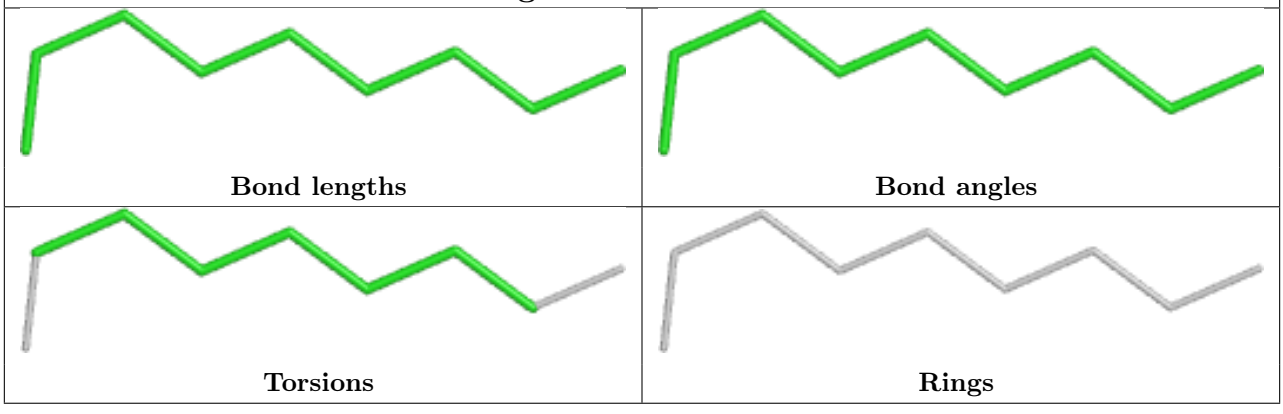
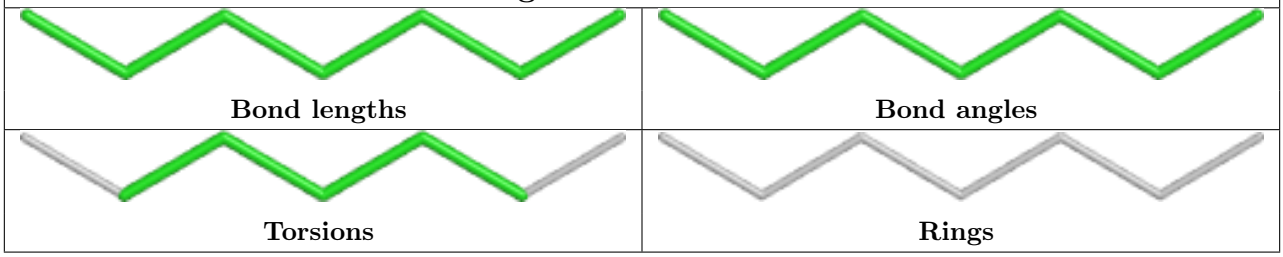
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	504	PGW	3	0
4	G	1001	NAP	12	0
4	A	1001	NAP	11	0
6	B	516	PGW	8	0
6	B	514	PGW	1	0
6	B	515	PGW	3	0
6	B	510	PGW	3	0
6	B	512	PGW	2	0
6	H	504	PGW	7	0

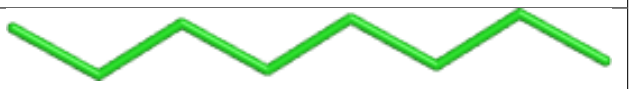
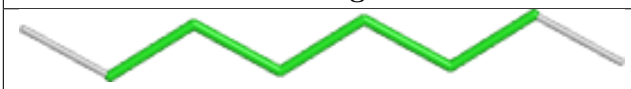
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

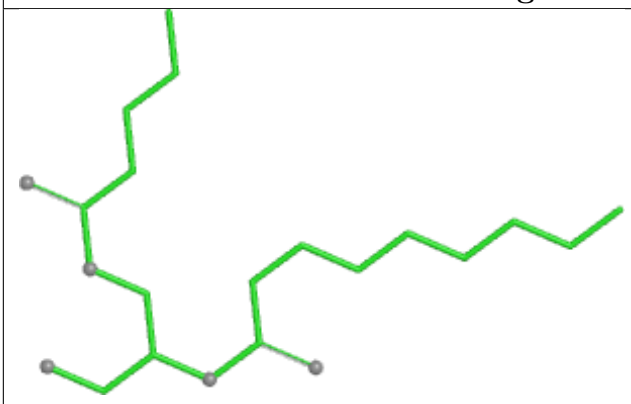
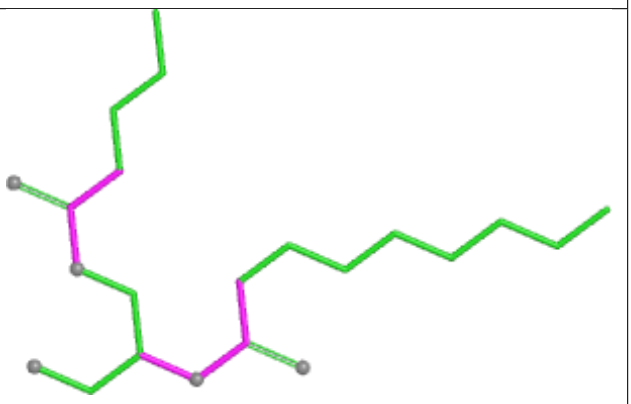
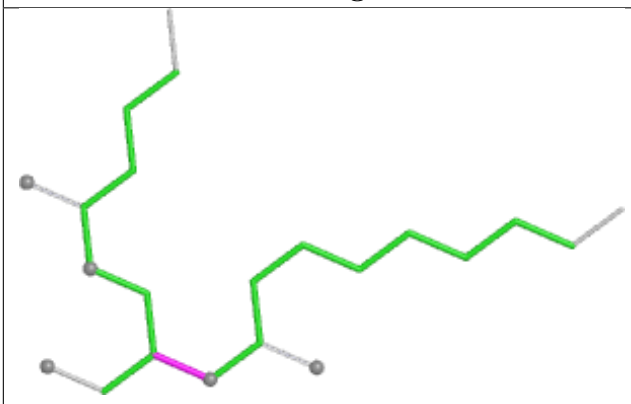
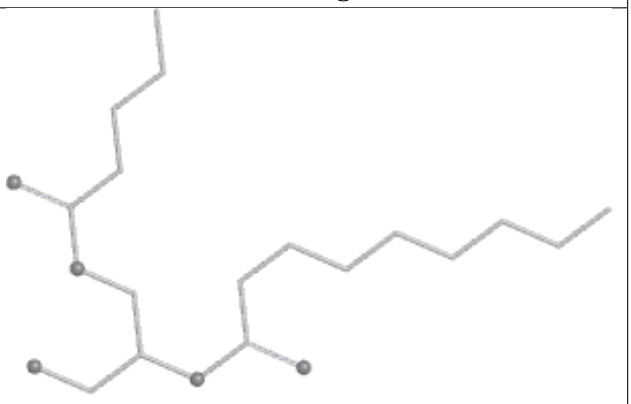
Ligand PGW B 508



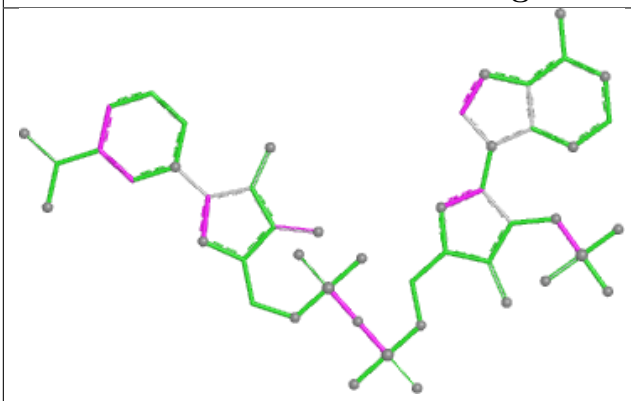
Ligand PGW B 517



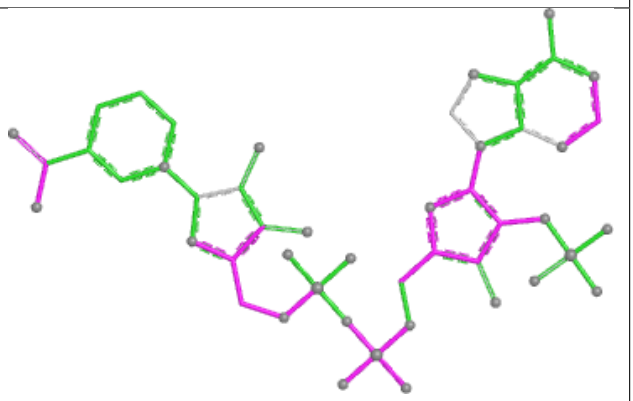
Ligand PGW B 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGW B 504	
 Bond lengths	 Bond angles
 Torsions	 Rings

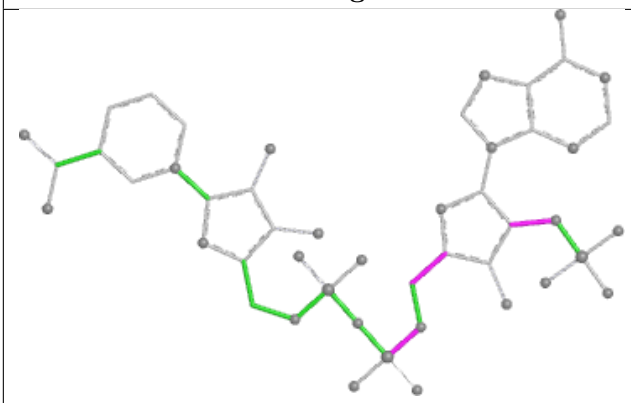
Ligand NAP G 1001



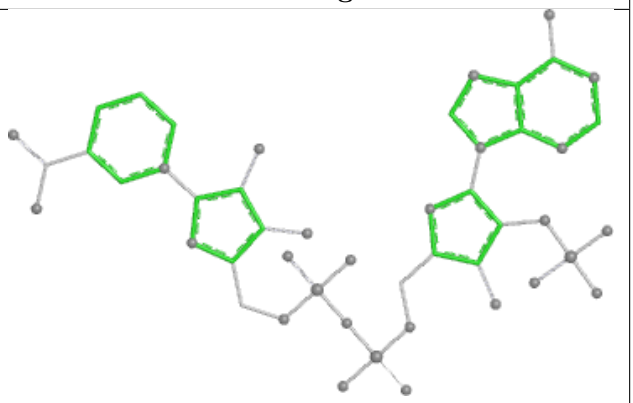
Bond lengths



Bond angles

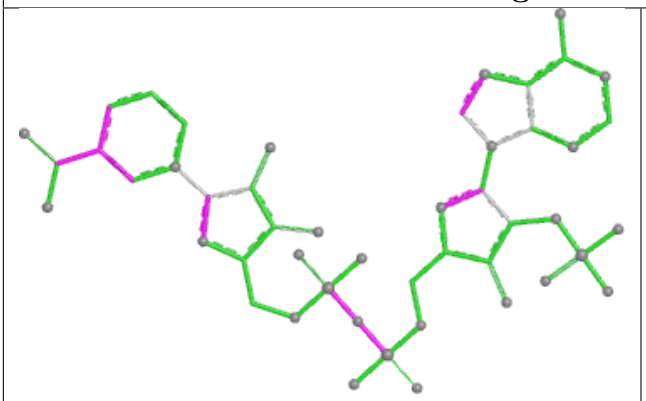


Torsions



Rings

Ligand NAP A 1001



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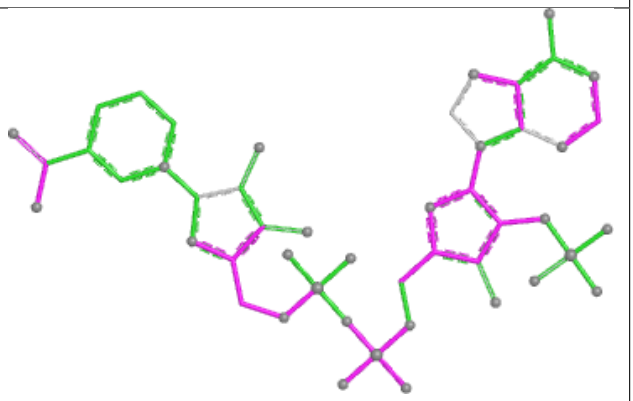
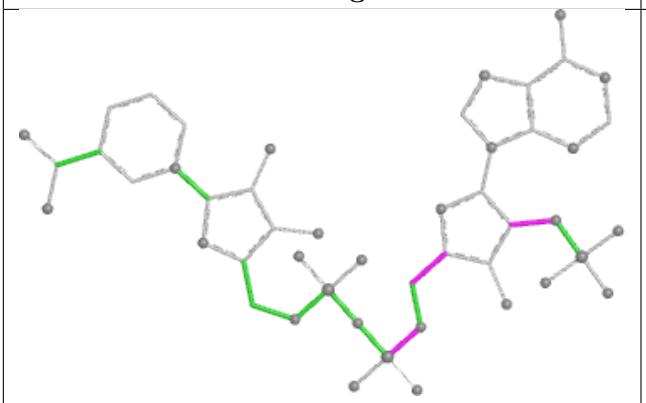


Bond angles



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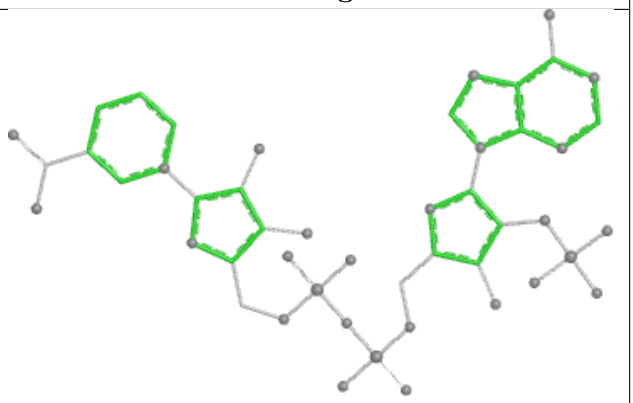
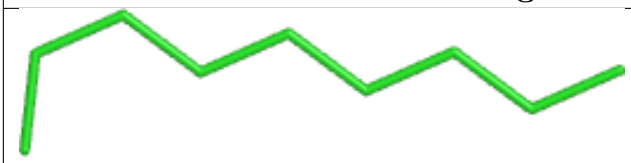


Rings

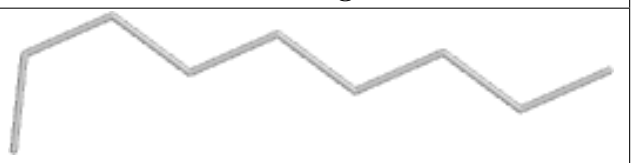
Ligand PGW B 506



Bond lengths

Bond angles

Torsions



Rings

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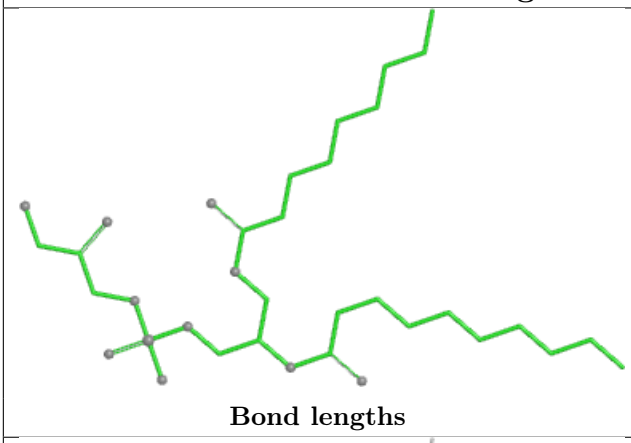

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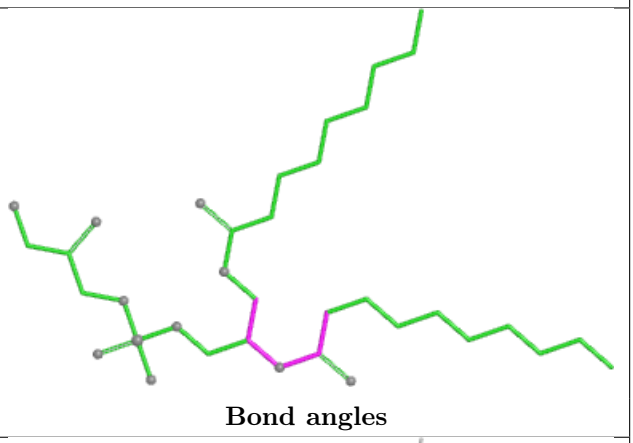

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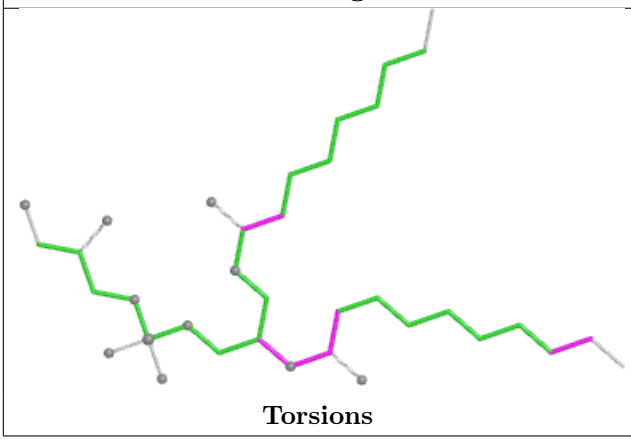

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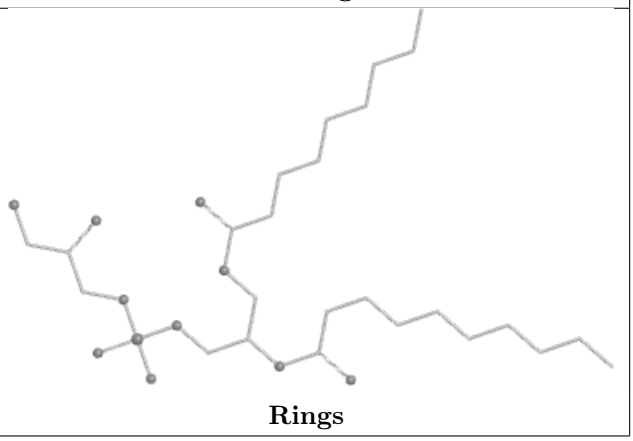
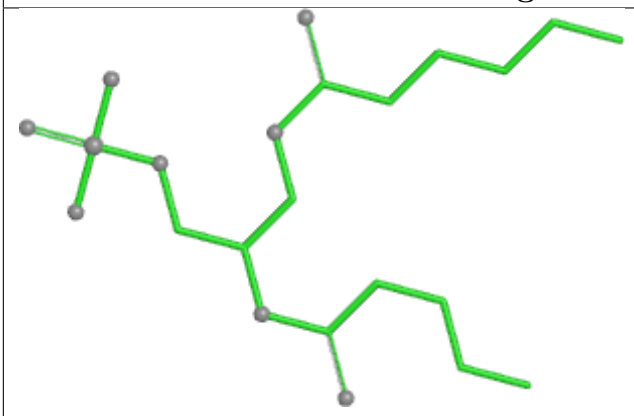


Rings

Ligand PGW B 514



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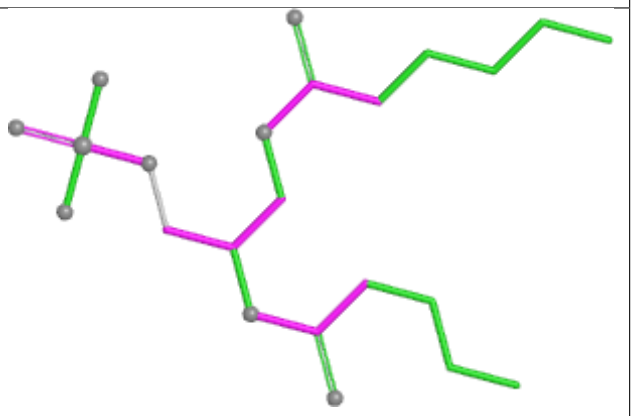
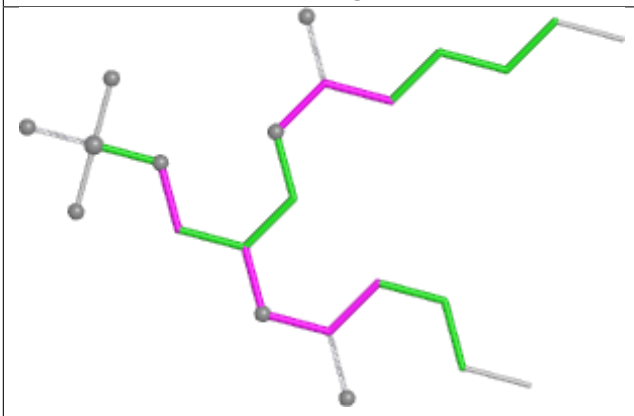


Bond angles



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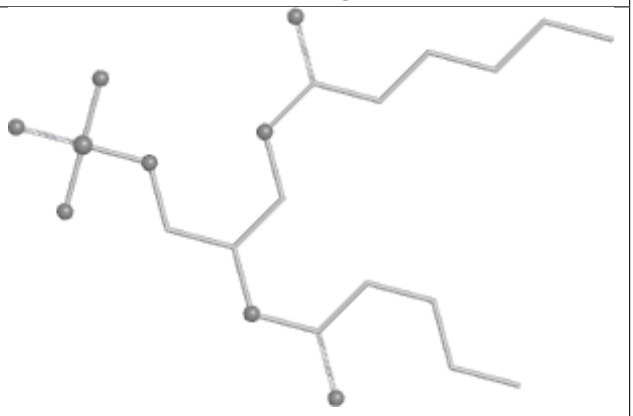
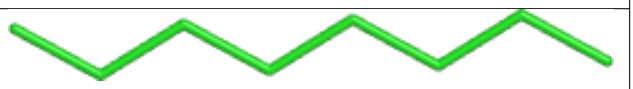


Rings

Ligand PGW B 515

Bond lengths

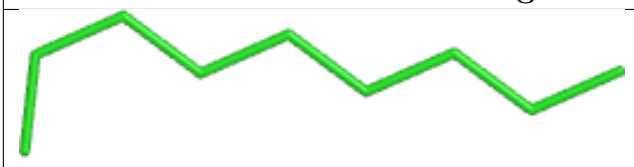


Bond angles

Torsions

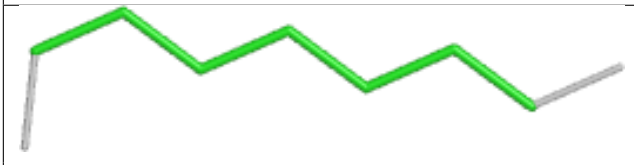
Rings

Ligand PGW B 507



Bond lengths

Bond angles



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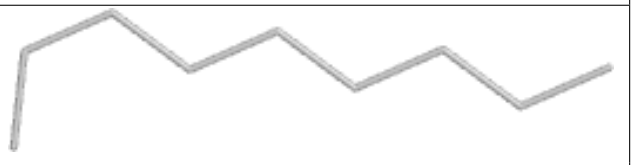
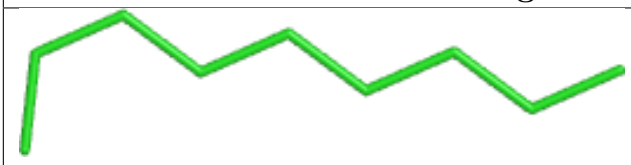
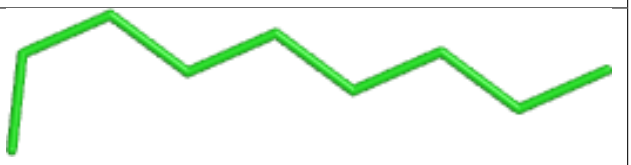
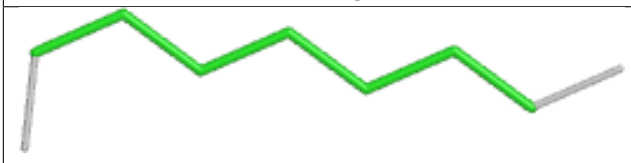
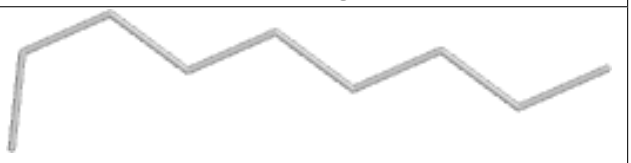
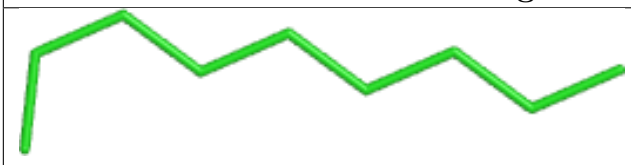
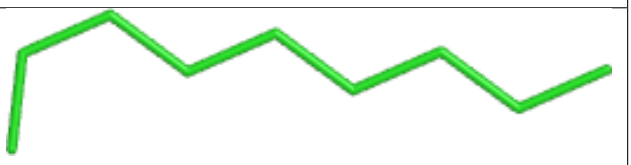
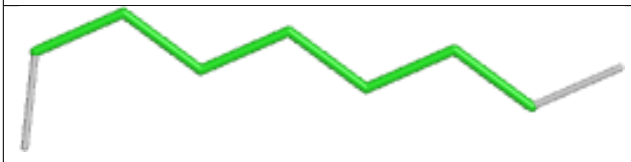
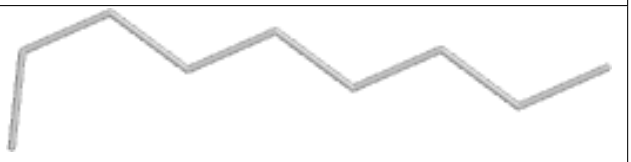
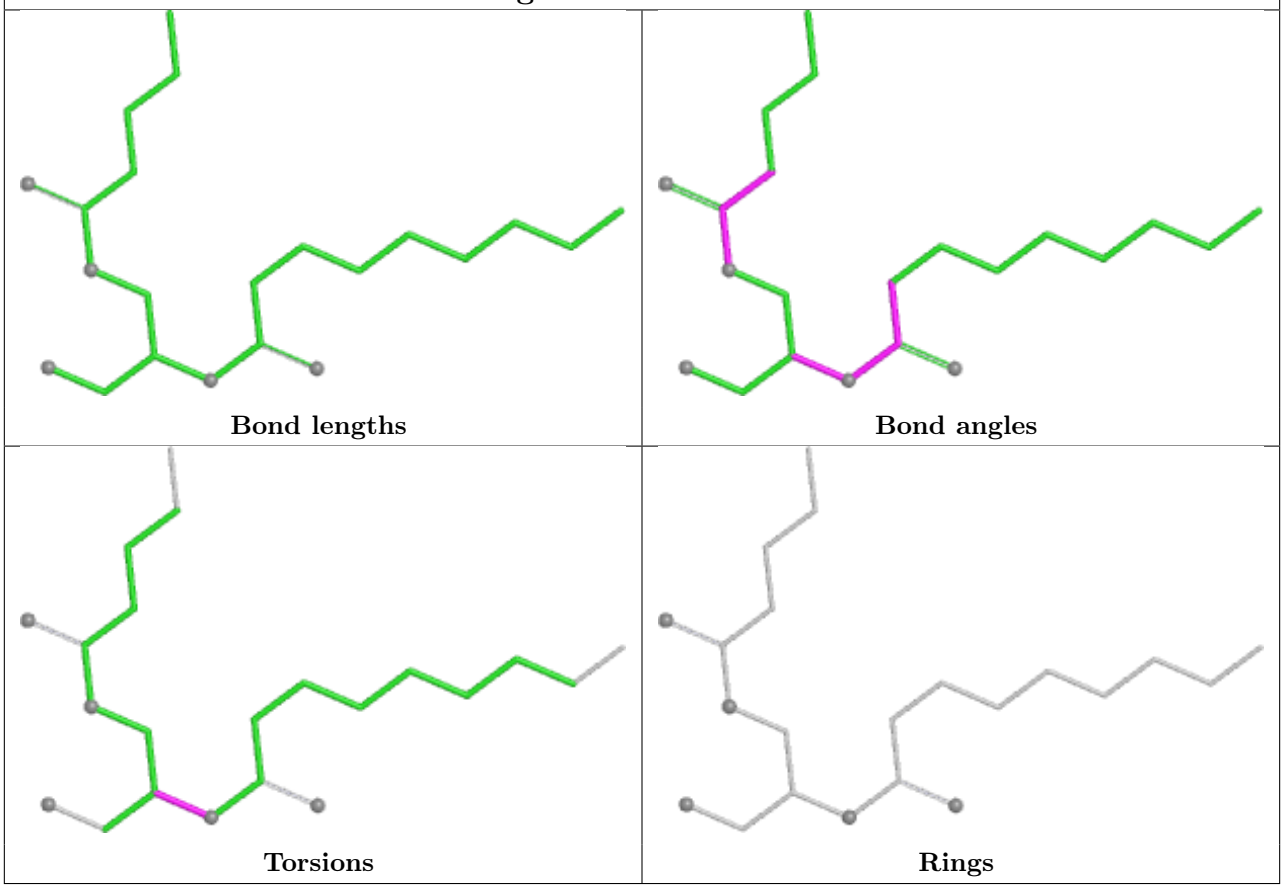


Rings

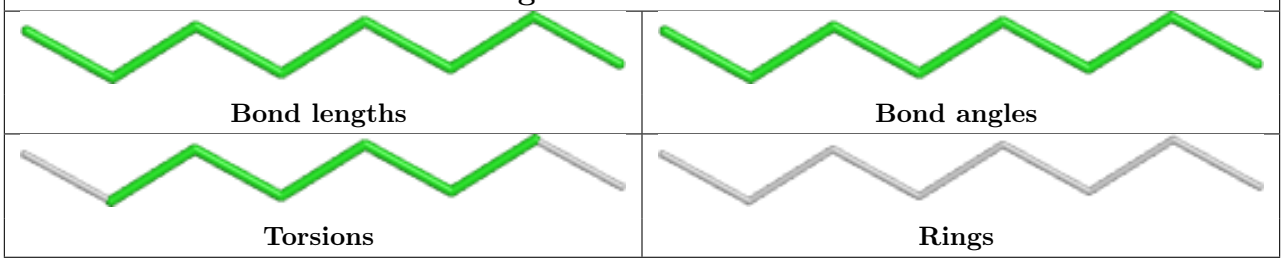
Ligand PGW B 510	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGW B 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PGW H 504



Ligand PGW B 518



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%)	0.22	6 (1%) 68 75	17, 33, 60, 83	0
1	G	326/333 (97%)	0.14	6 (1%) 68 75	21, 39, 72, 96	0
2	B	386/514 (75%)	0.88	62 (16%) 1 2	25, 66, 110, 125	0
2	H	363/514 (70%)	3.03	158 (43%) 0 0	38, 115, 185, 204	0
3	Y	36/37 (97%)	6.72	36 (100%) 0 0	102, 107, 122, 126	36 (100%)
All	All	1437/1731 (83%)	1.25	268 (18%) 1 1	17, 56, 176, 204	36 (2%)

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	272	LEU	21.4
2	H	218	PHE	19.2
2	H	280	LEU	17.0
2	H	248	ALA	16.8
2	H	214	GLN	16.1
2	H	217	SER	13.5
2	H	205	TYR	12.4
2	H	211	GLY	12.4
2	H	241	PHE	12.3
3	Y	5	VAL	12.2
2	H	288	VAL	12.0
2	H	212	TYR	12.0
2	H	246	SER	11.8
2	H	206	SER	11.7
3	Y	6	SER	11.2
2	H	281	GLN	11.1
2	H	279	VAL	11.1
3	Y	17	CYS	10.9
2	H	270	ILE	10.8
2	H	244	CYS	10.6

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Mol	Chain	Res	Type	RSRZ
2	H	269	THR	10.6
3	Y	3	THR	10.6
2	H	242	PHE	10.5
2	H	254	ILE	10.5
3	Y	28	CYS	10.4
2	H	224	ILE	10.3
3	Y	29	MET	10.1
2	H	225	VAL	9.7
2	H	250	PHE	9.6
2	H	282	PHE	9.5
2	H	251	PHE	9.3
2	H	210	ILE	9.3
2	H	153	PHE	9.1
2	H	229	CYS	9.0
3	Y	8	THR	8.9
2	H	289	VAL	8.9
2	H	283	GLN	8.8
2	H	235	PHE	8.7
2	H	168	VAL	8.7
2	H	247	LYS	8.7
3	Y	36	TYR	8.6
2	H	271	PHE	8.6
3	Y	16	VAL	8.3
2	H	245	PRO	8.3
3	Y	27	LYS	8.2
2	H	240	ARG	8.2
2	H	149	VAL	8.2
3	Y	14	TRP	8.1
2	H	172	VAL	8.1
2	H	228	LEU	8.1
2	H	164	ILE	7.9
3	Y	7	CYS	7.9
2	H	183	GLU	7.9
2	H	215	SER	7.9
3	Y	9	THR	7.8
3	Y	12	GLU	7.8
2	H	188	PHE	7.8
2	H	238	LEU	7.7
2	H	216	THR	7.7
3	Y	24	SER	7.7
2	H	222	PHE	7.6
2	H	221	PRO	7.6

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Mol	Chain	Res	Type	RSRZ
2	H	249	GLY	7.5
2	H	231	ILE	7.5
3	Y	2	PHE	7.4
3	Y	21	HIS	7.3
2	H	220	ASP	7.0
2	H	302	LYS	6.9
2	H	252	THR	6.9
2	H	273	THR	6.8
2	H	267	TYR	6.7
2	H	167	ILE	6.7
2	H	262	ALA	6.7
2	H	284	ASN	6.7
2	H	230	ILE	6.6
2	H	151	LEU	6.5
3	Y	4	ASN	6.5
2	H	286	ARG	6.4
2	H	219	THR	6.4
2	H	285	VAL	6.4
3	Y	10	SER	6.4
3	Y	30	ASN	6.3
2	B	193	GLU	6.2
2	H	209	THR	6.2
2	H	260	ILE	6.2
3	Y	13	CYS	6.2
2	B	161	PRO	6.1
3	Y	33	CYS	6.1
2	H	233	PHE	6.1
2	H	409	PHE	6.0
2	H	207	GLN	5.9
2	H	165	ILE	5.9
3	Y	35	CYS	5.9
3	Y	23	THR	5.8
2	H	146	GLN	5.8
2	H	415	ARG	5.8
2	H	257	ILE	5.8
2	H	203	HIS	5.8
2	H	303	LEU	5.7
2	H	161	PRO	5.7
2	H	414	HIS	5.6
3	Y	34	ARG	5.6
2	H	417	THR	5.6
3	Y	37	SER	5.6

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Mol	Chain	Res	Type	RSRZ
2	H	213	GLN	5.6
2	B	153	PHE	5.5
2	H	263	ILE	5.4
2	H	145	PHE	5.4
2	H	232	TRP	5.3
2	H	266	TYR	5.3
2	H	276	ASN	5.3
2	H	277	LYS	5.2
3	Y	15	SER	5.0
2	H	290	GLN	5.0
2	H	416	GLU	5.0
2	H	261	VAL	4.7
2	H	173	ILE	4.7
2	H	413	TYR	4.7
2	H	410	ASN	4.7
2	H	237	PHE	4.7
2	H	255	MET	4.6
2	H	150	TRP	4.6
3	Y	26	GLY	4.6
2	H	295	MET	4.6
2	H	265	PRO	4.6
2	H	170	VAL	4.5
2	B	151	LEU	4.5
2	H	152	LEU	4.5
2	B	219	THR	4.4
2	H	253	ASN	4.4
2	H	155	TYR	4.3
2	H	157	GLU	4.3
2	H	275	SER	4.3
2	H	190	ASP	4.3
1	G	36	LEU	4.2
2	H	159	SER	4.2
2	H	187	ILE	4.1
2	H	202	PHE	4.1
2	B	132	TYR	4.1
2	H	223	PHE	4.1
2	H	171	MET	4.1
2	H	125	MET	4.0
2	B	192	ASN	4.0
3	Y	31	LYS	3.9
1	G	360	TYR	3.9
3	Y	32	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	182	LEU	3.9
2	H	236	GLU	3.8
2	H	226	GLU	3.8
2	H	306	HIS	3.8
2	H	208	SER	3.8
3	Y	20	LEU	3.8
2	H	350	ARG	3.7
1	A	360	TYR	3.7
2	H	63	LYS	3.7
2	B	149	VAL	3.7
2	B	157	GLU	3.7
2	H	287	ARG	3.6
2	H	308	LYS	3.6
2	H	156	PRO	3.6
2	H	381	ILE	3.6
2	B	164	ILE	3.5
2	H	106	LEU	3.5
2	H	181	CYS	3.5
2	B	162	ALA	3.5
2	H	204	THR	3.5
2	H	278	SER	3.4
3	Y	18	GLN	3.4
2	H	158	SER	3.4
2	H	128	GLU	3.3
2	H	177	ILE	3.3
2	H	163	ARG	3.3
2	B	213	GLN	3.3
2	B	218	PHE	3.3
2	B	286	ARG	3.2
2	B	125	MET	3.2
2	H	299	ARG	3.2
2	B	216	THR	3.1
2	B	163	ARG	3.1
2	H	114	ARG	3.1
2	H	154	GLU	3.1
2	H	234	SER	3.1
2	H	162	ALA	3.1
3	Y	25	ARG	3.0
2	H	179	SER	3.0
2	H	239	VAL	3.0
2	B	152	LEU	3.0
2	B	241	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	145	PHE	3.0
1	A	36	LEU	3.0
1	A	262	TYR	2.9
2	B	344	PHE	2.9
2	H	243	ALA	2.9
2	H	227	THR	2.9
2	B	197	GLY	2.9
2	H	174	LEU	2.9
2	H	119	GLY	2.8
2	B	251	PHE	2.8
2	B	201	THR	2.8
2	H	310	LEU	2.7
1	A	250	ILE	2.7
2	B	188	PHE	2.7
2	H	148	GLN	2.7
2	B	249	GLY	2.7
2	H	274	GLU	2.7
2	H	258	ILE	2.7
2	B	140	LEU	2.7
2	H	175	ILE	2.7
2	B	415	ARG	2.6
2	B	168	VAL	2.6
2	H	160	GLY	2.6
1	A	265	ALA	2.6
2	B	120	GLU	2.6
2	H	264	ILE	2.6
2	B	150	TRP	2.6
2	B	160	GLY	2.5
2	B	195	MET	2.5
1	G	349	HIS	2.5
2	B	158	SER	2.5
2	B	252	THR	2.5
2	B	308	LYS	2.5
2	B	282	PHE	2.5
1	G	300	GLY	2.5
2	H	121	GLU	2.5
2	B	190	ASP	2.4
3	Y	22	ASN	2.4
2	B	397	THR	2.4
2	B	196	HIS	2.4
2	B	400	LEU	2.4
2	H	312	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	147	ARG	2.4
2	B	159	SER	2.4
2	H	307	SER	2.4
2	H	124	GLU	2.4
2	B	396	LEU	2.4
2	B	398	ILE	2.4
2	B	250	PHE	2.4
2	B	285	VAL	2.4
1	A	205	PHE	2.4
2	B	399	ALA	2.4
1	G	361	SER	2.4
2	H	412	PHE	2.3
2	B	231	ILE	2.3
1	G	299	LEU	2.3
2	B	198	GLY	2.2
2	H	405	ILE	2.2
2	B	215	SER	2.2
2	H	111	GLU	2.2
2	H	191	GLU	2.2
2	H	109	PHE	2.2
2	B	411	TYR	2.2
2	B	124	GLU	2.2
2	B	155	TYR	2.1
2	H	411	TYR	2.1
2	B	191	GLU	2.1
2	B	413	TYR	2.1
2	H	305	ARG	2.1
2	H	36	VAL	2.1
2	B	106	LEU	2.1
2	B	271	PHE	2.1
2	B	232	TRP	2.1
3	Y	11	LYS	2.1
2	B	136	GLU	2.0
2	H	322	ARG	2.0
2	B	141	PRO	2.0
2	B	337	LEU	2.0
3	Y	19	ARG	2.0
2	B	129	ASP	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	0.71	0.42	125,126,126,126	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	512	9/51	0.22	1.17	126,128,128,128	0
6	PGW	H	504	22/51	0.42	0.84	142,147,149,149	0
6	PGW	B	518	8/51	0.44	0.87	102,105,107,107	0
6	PGW	B	504	22/51	0.48	0.68	85,102,113,114	0
6	PGW	B	515	8/51	0.53	0.53	81,87,91,91	0
6	PGW	B	508	9/51	0.56	0.47	100,102,102,102	0
6	PGW	B	517	7/51	0.56	0.49	63,66,68,69	0
6	PGW	B	516	36/51	0.58	0.39	107,125,141,141	0
6	PGW	B	507	9/51	0.62	0.58	94,96,98,98	0
6	PGW	B	506	9/51	0.62	0.41	87,90,91,91	0
6	PGW	B	519	8/51	0.64	0.39	97,99,100,100	0
6	PGW	B	505	9/51	0.64	0.36	79,82,84,85	0
6	PGW	B	513	8/51	0.65	0.46	74,78,79,79	0
6	PGW	B	514	23/51	0.70	0.31	109,119,123,124	0
6	PGW	B	510	9/51	0.79	0.45	106,107,109,109	0
6	PGW	B	509	9/51	0.81	0.52	82,86,89,89	0
6	PGW	B	511	7/51	0.85	0.20	70,73,73,73	0
5	CS	B	502	1/1	0.88	0.12	43,43,43,43	1
5	CS	H	505	1/1	0.92	0.39	126,126,126,126	1
5	CS	B	503	1/1	0.93	0.14	101,101,101,101	1
5	CS	H	503	1/1	0.94	0.24	75,75,75,75	1

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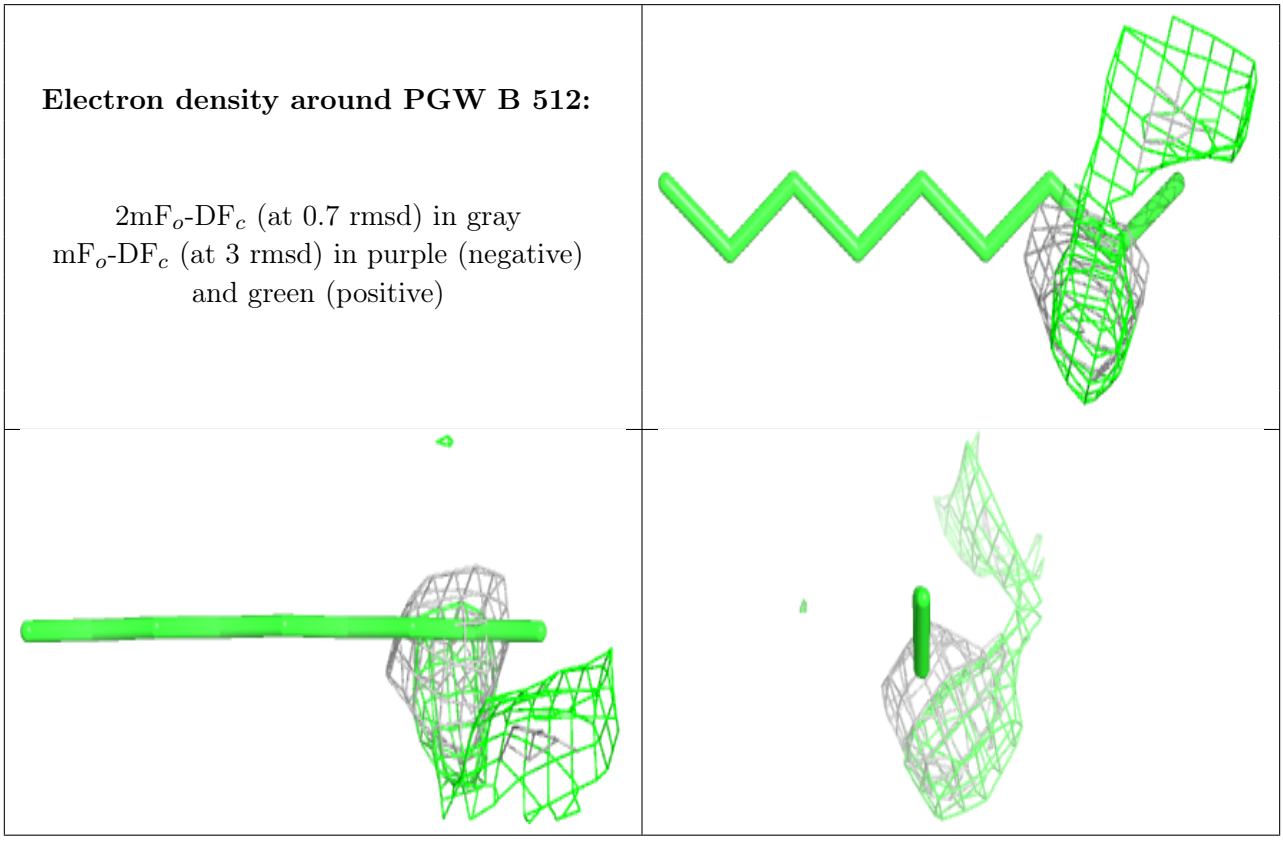
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CS	B	501	1/1	0.95	0.19	45,45,45,45	1
4	NAP	G	1001	48/48	0.95	0.20	25,39,51,51	0
4	NAP	A	1001	48/48	0.96	0.18	23,33,43,47	0
5	CS	H	501	1/1	0.97	0.22	85,85,85,85	1
5	CS	H	502	1/1	0.98	0.22	74,74,74,74	1
5	CS	B	520	1/1	1.00	0.21	61,61,61,61	1

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.

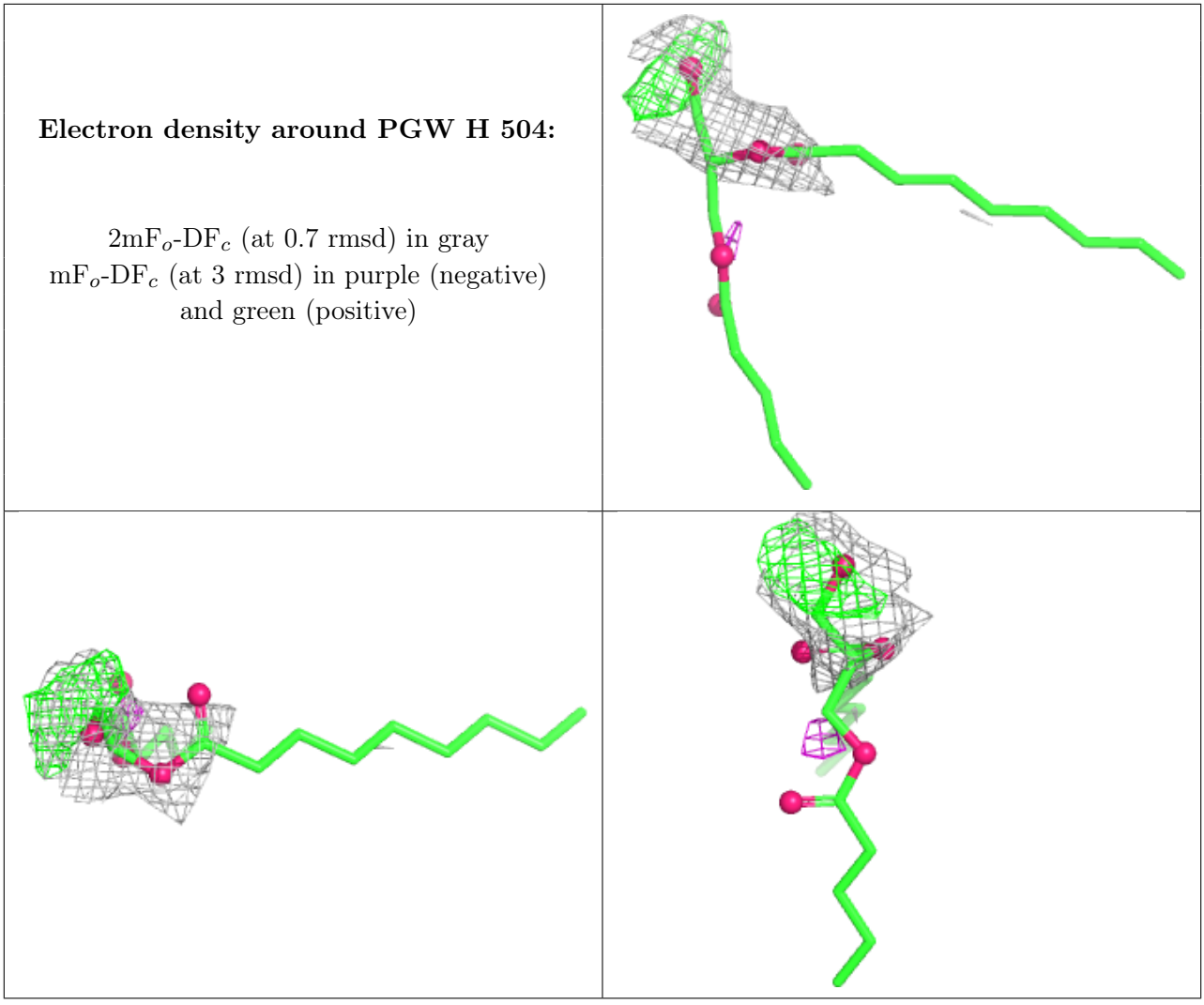
Electron density around PGW B 512:

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



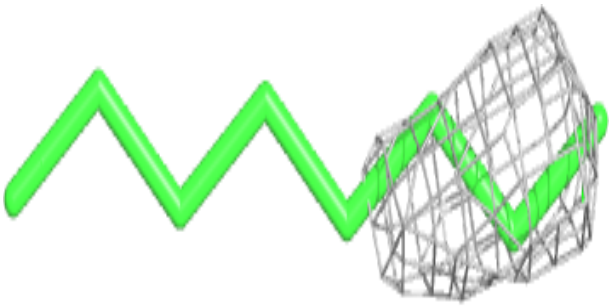
Electron density around PGW H 504:

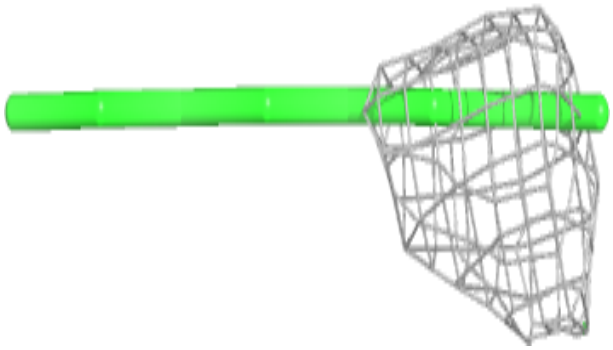
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

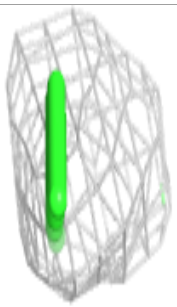


Electron density around PGW B 518:

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

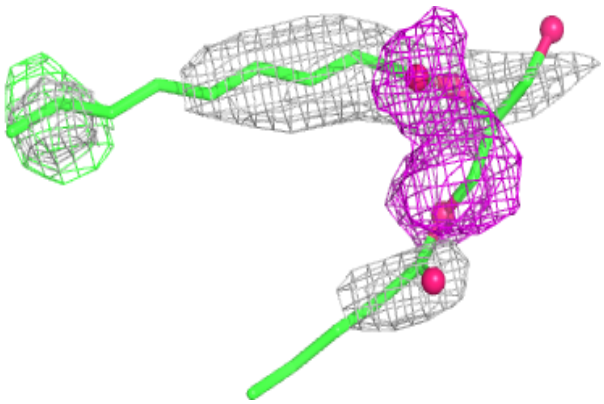


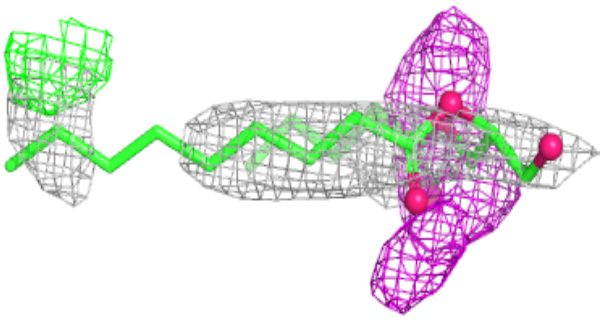


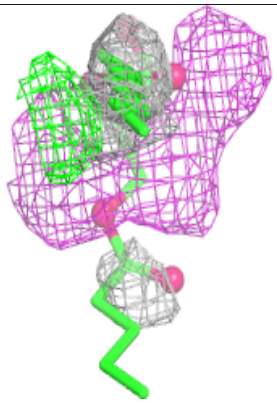


Electron density around PGW B 504:

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

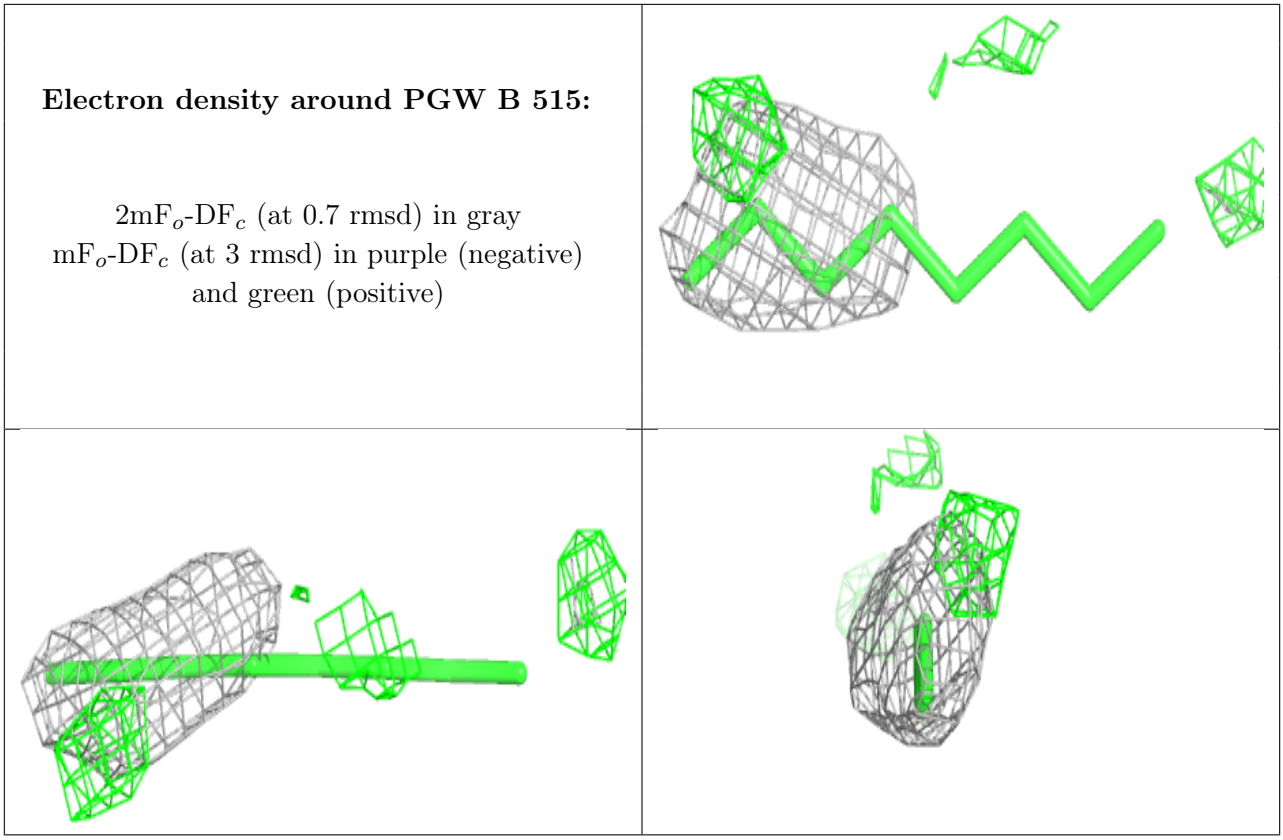






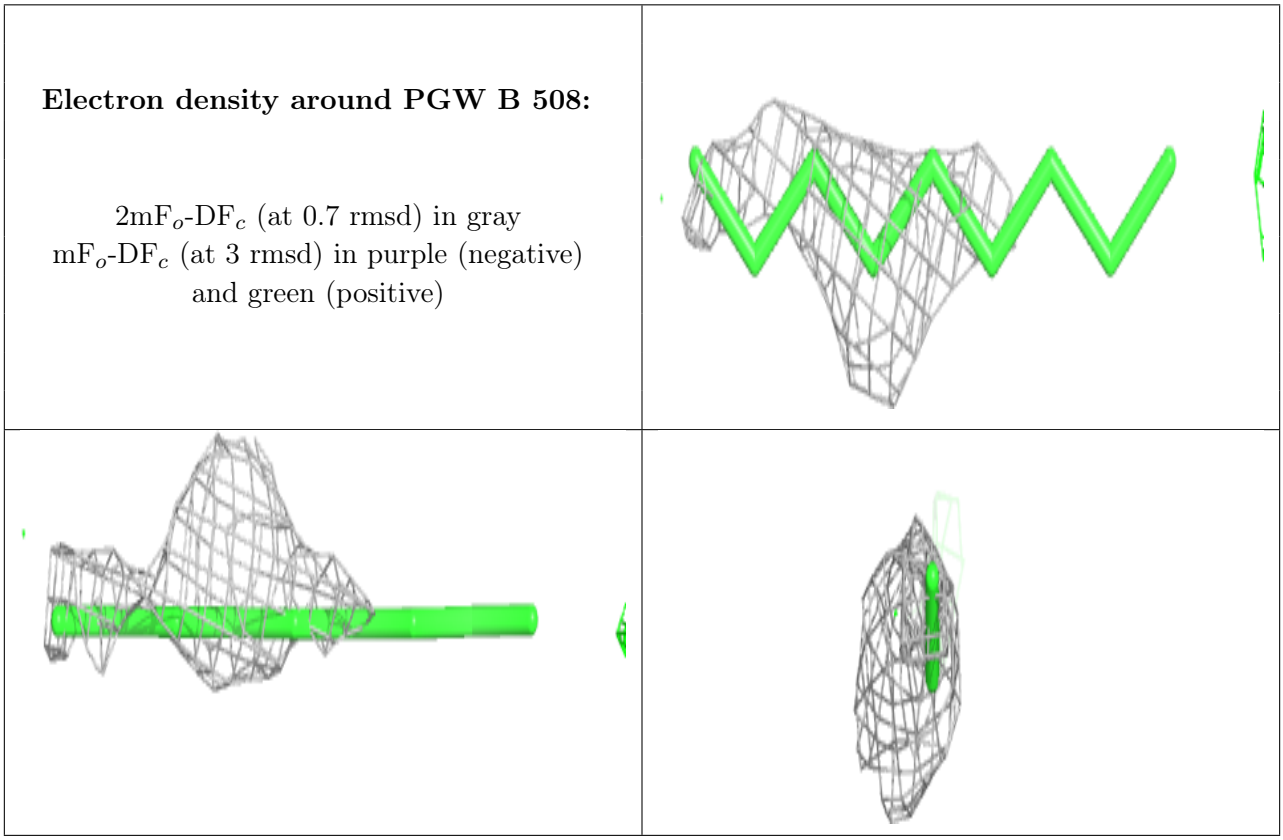
Electron density around PGW B 515:

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



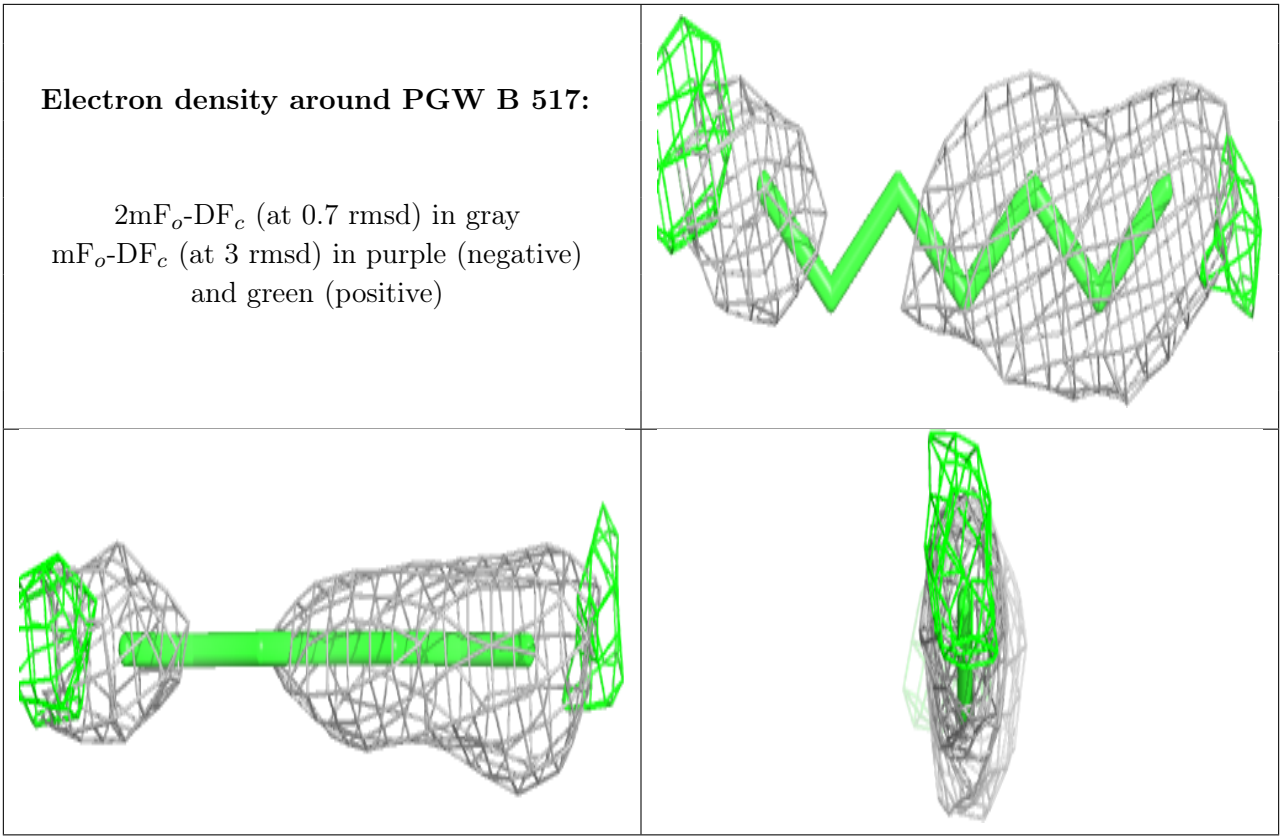
Electron density around PGW B 508:

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



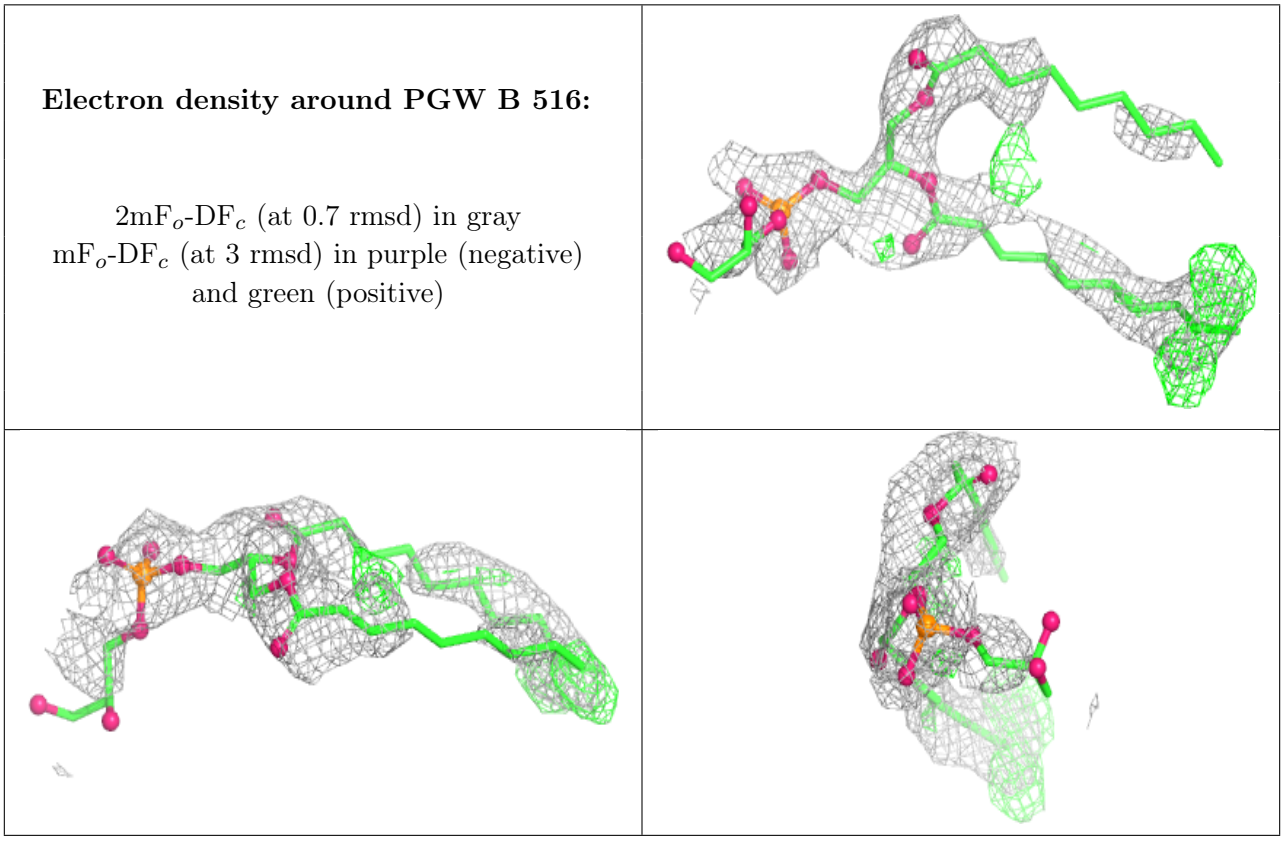
Electron density around PGW B 517:

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



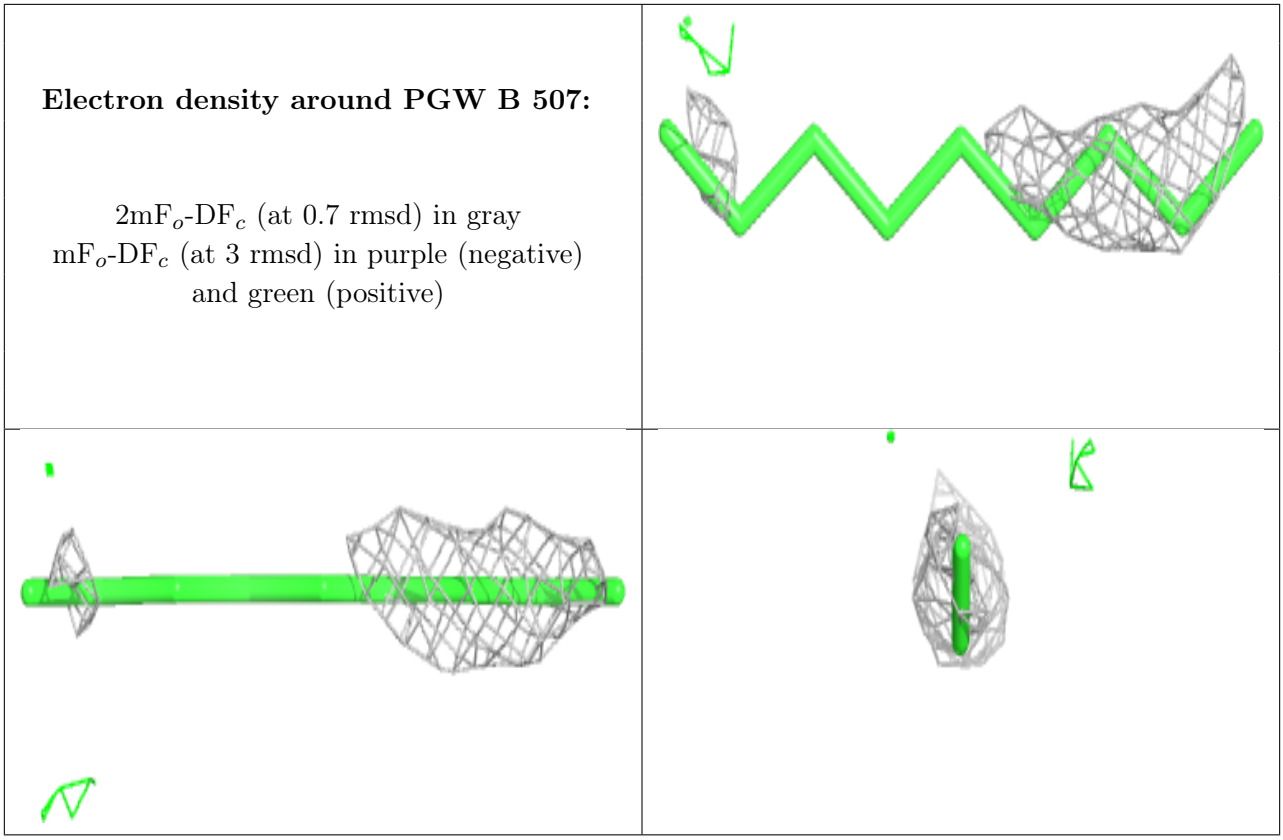
Electron density around PGW B 516:

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



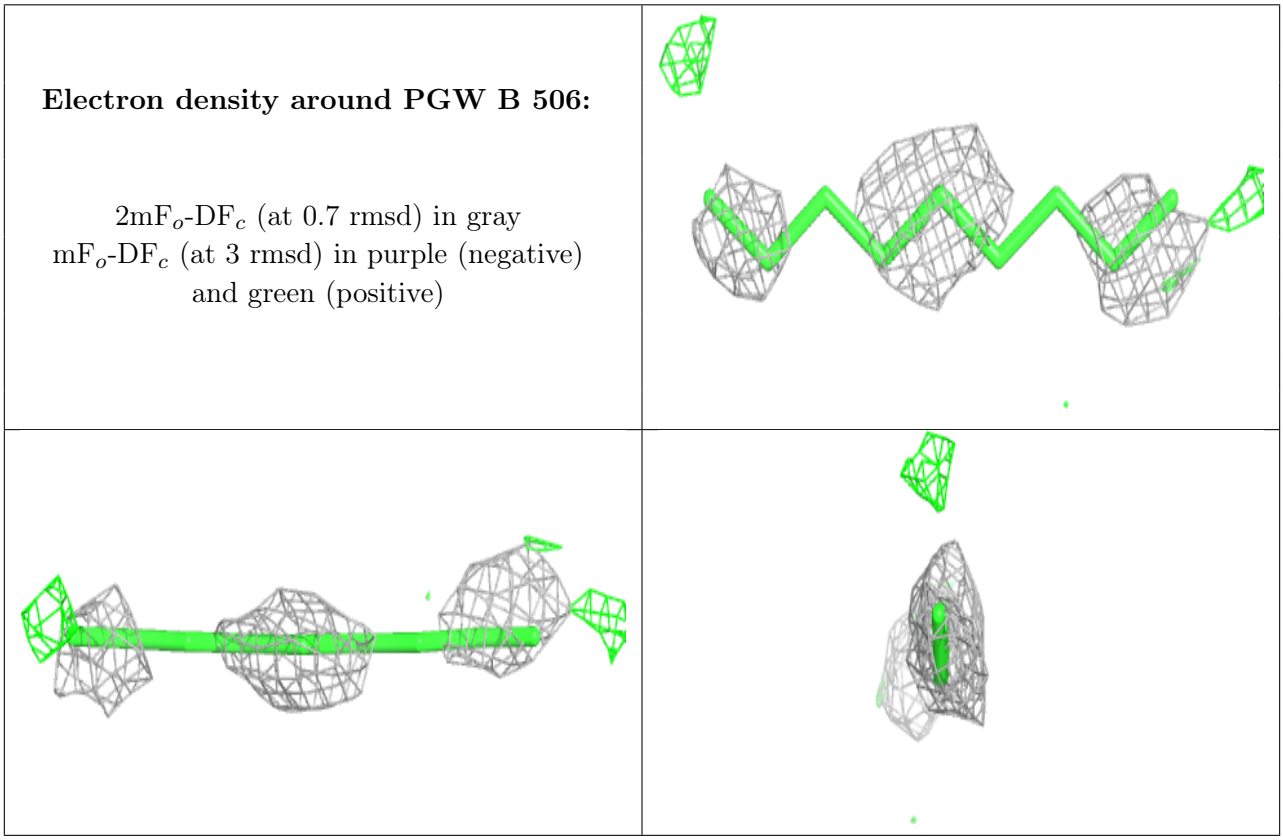
Electron density around PGW B 507:

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



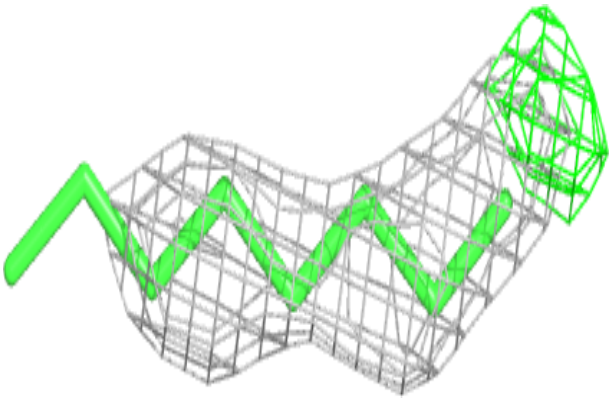
Electron density around PGW B 506:

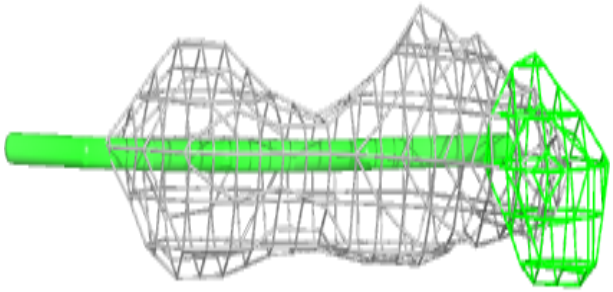
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

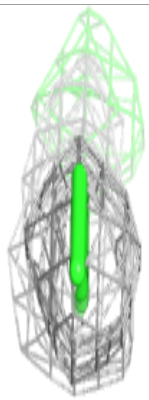


Electron density around PGW B 513:

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

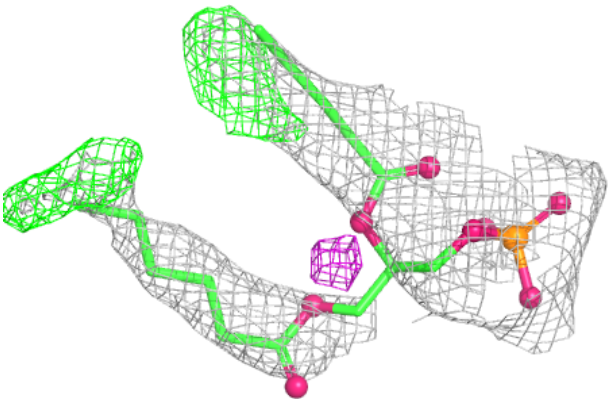


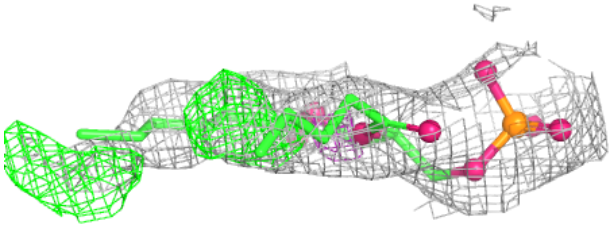


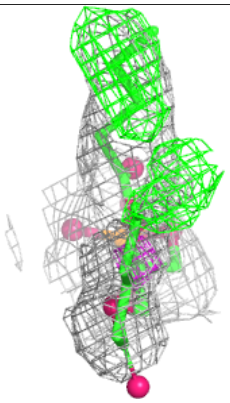


Electron density around PGW B 514:

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

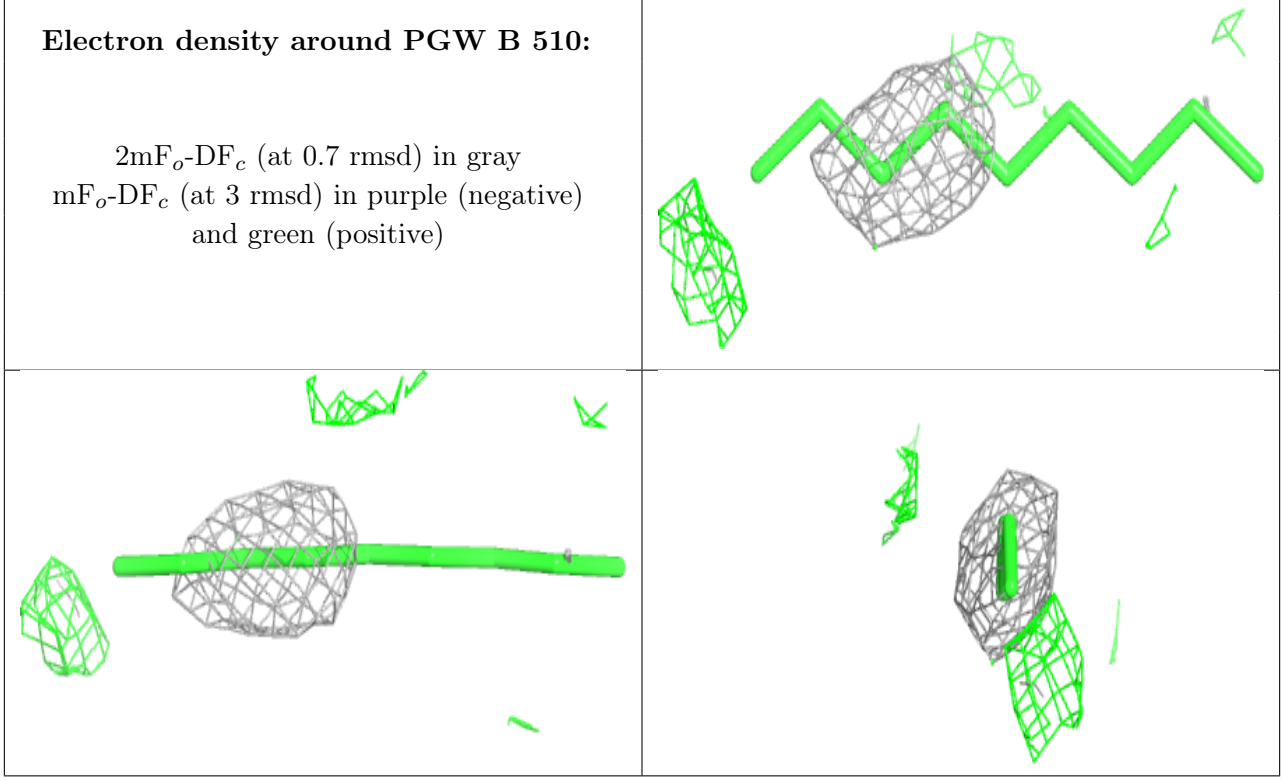






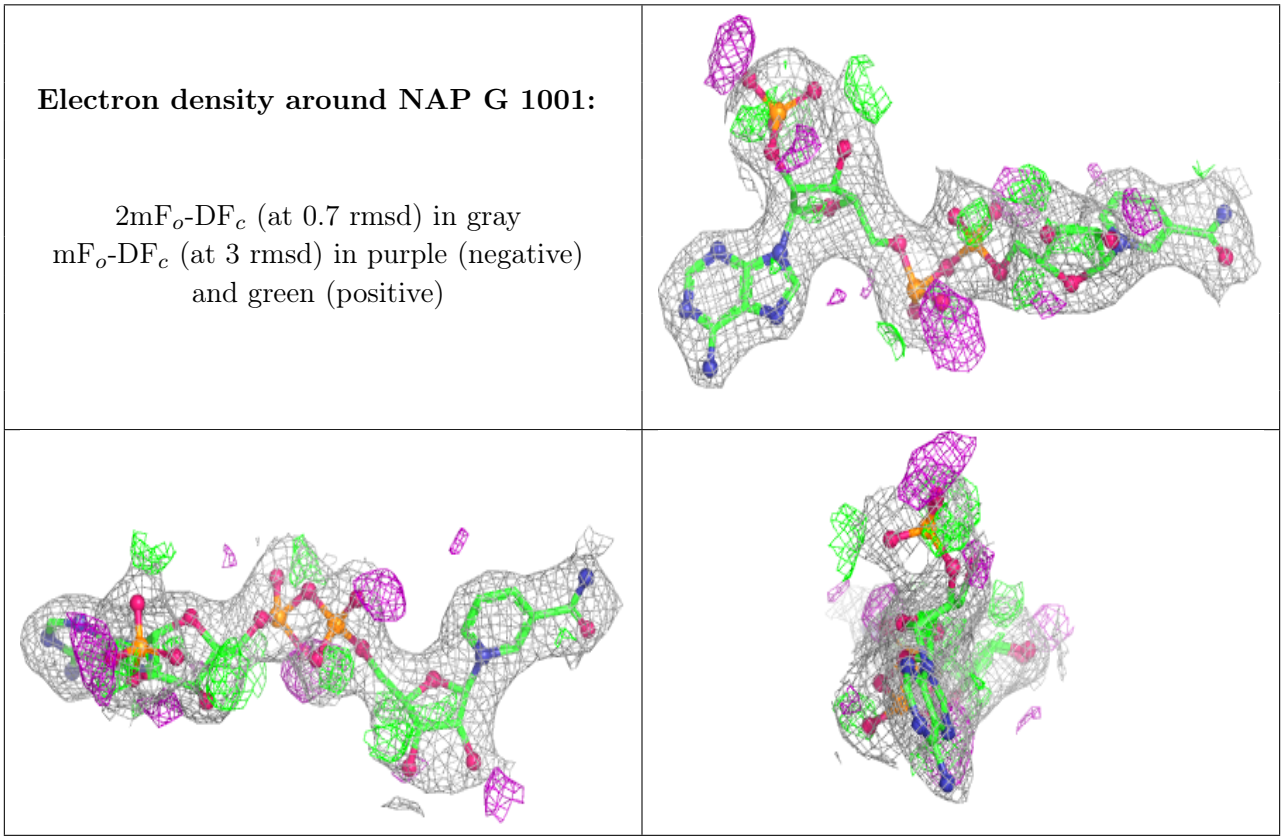
Electron density around PGW B 510:

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



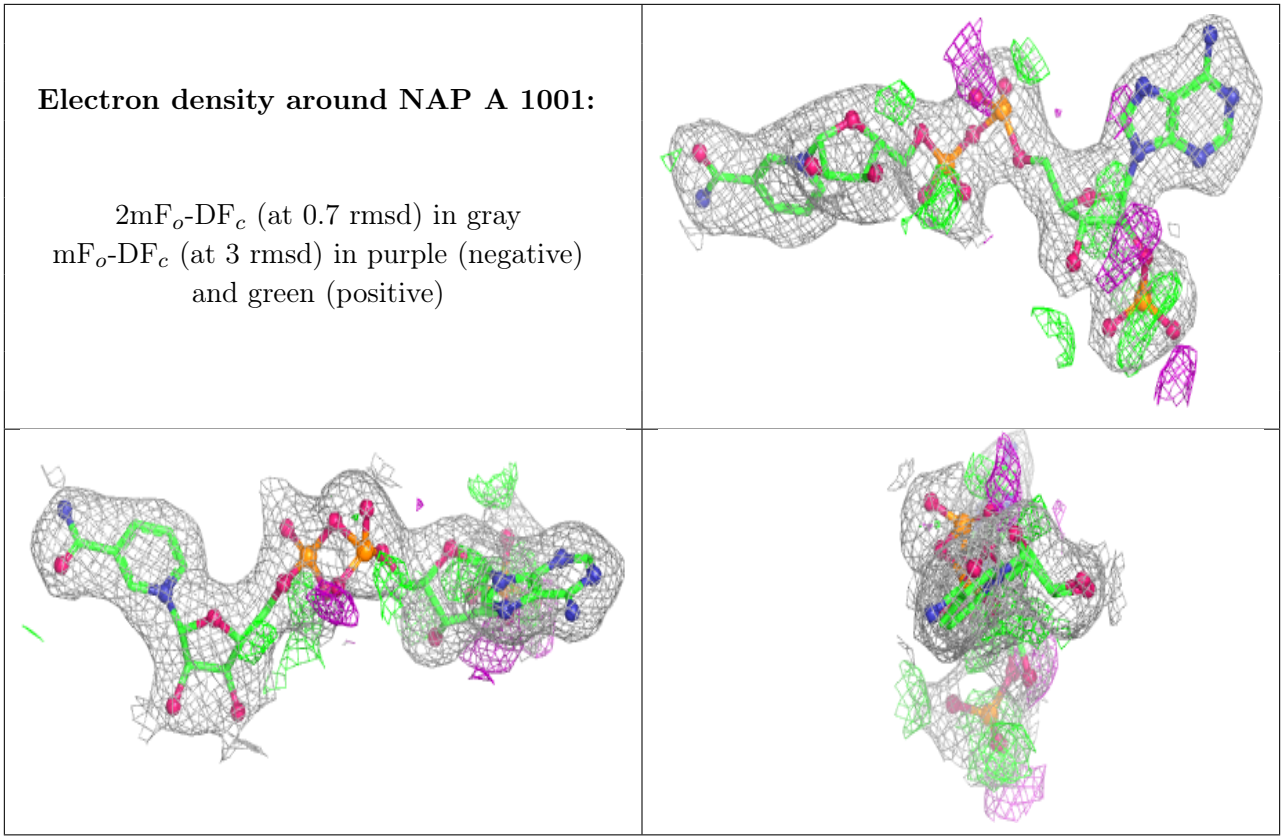
Electron density around NAP G 1001:

$2mF_o$-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.