



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:11 PM UTC

PDB ID : 4JTD / pdb_00004jtd
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

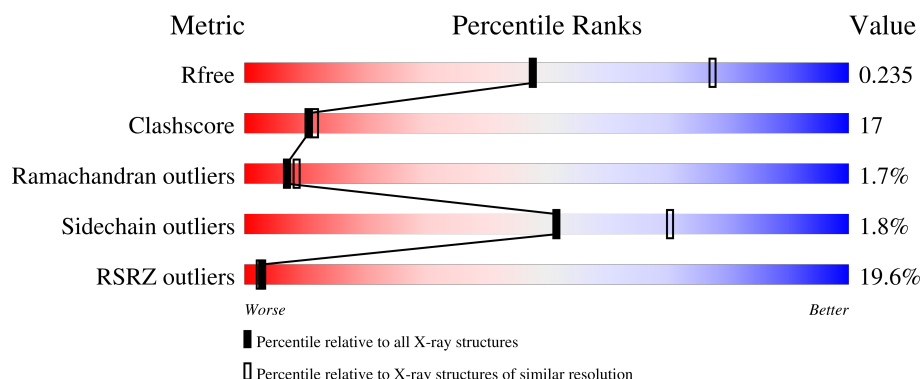
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	3% 75% 22% ..
1	G	333	2% 77% 19% ..
2	B	514	13% 46% 27% • 25%
2	H	514	32% 36% 33% • 29%
3	Y	37	92% 89% 11%

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
6	PGW	B	505	-	-	-	X
6	PGW	B	506	-	-	-	X
6	PGW	B	509	-	-	-	X
6	PGW	B	513	-	-	-	X
6	PGW	B	520	-	-	-	X
6	PGW	H	505	-	-	-	X

2 Entry composition

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

Continued on next page...

Continued from previous page...

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

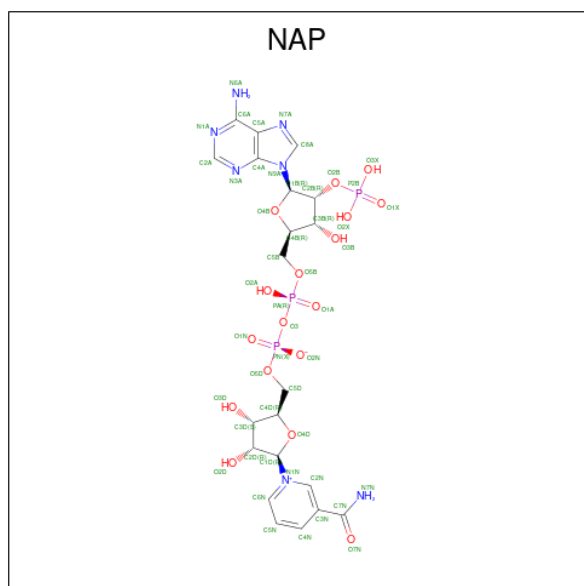
- Molecule 3 is a protein called Potassium channel toxin alpha-KTx 1.1.

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 (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



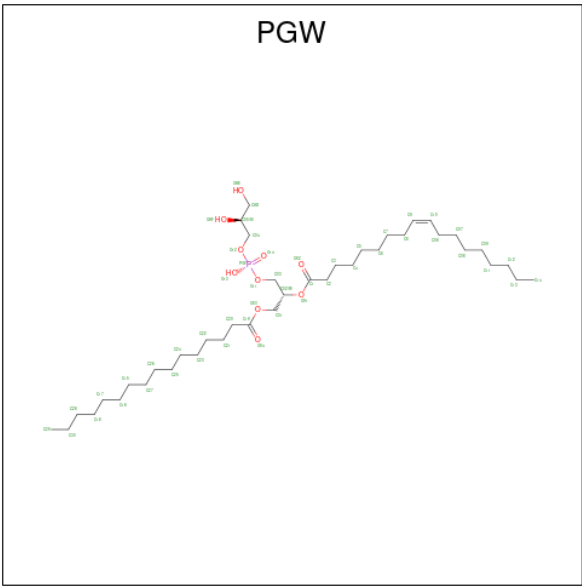
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	G	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

C₄₀H₇₇O₁₀P).



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

Continued on next page...

Continued from previous page...

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

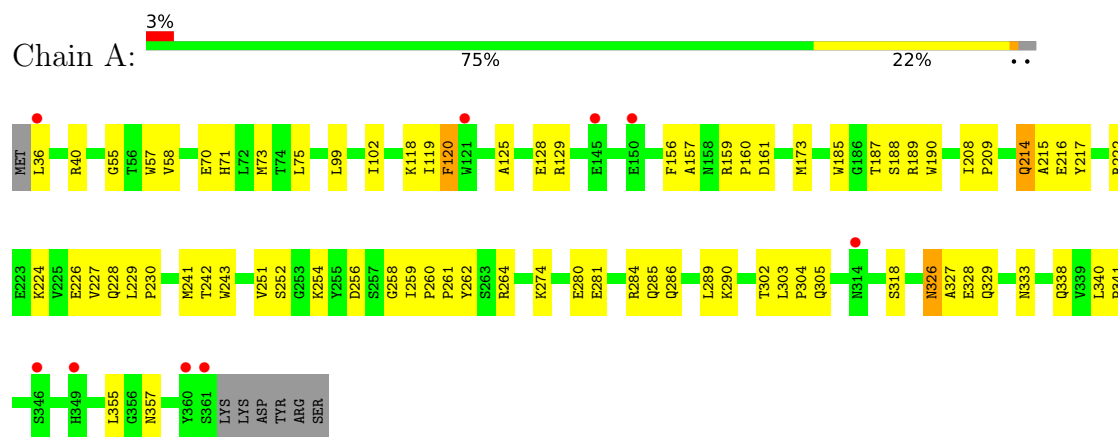
- Molecule 7 is water.

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

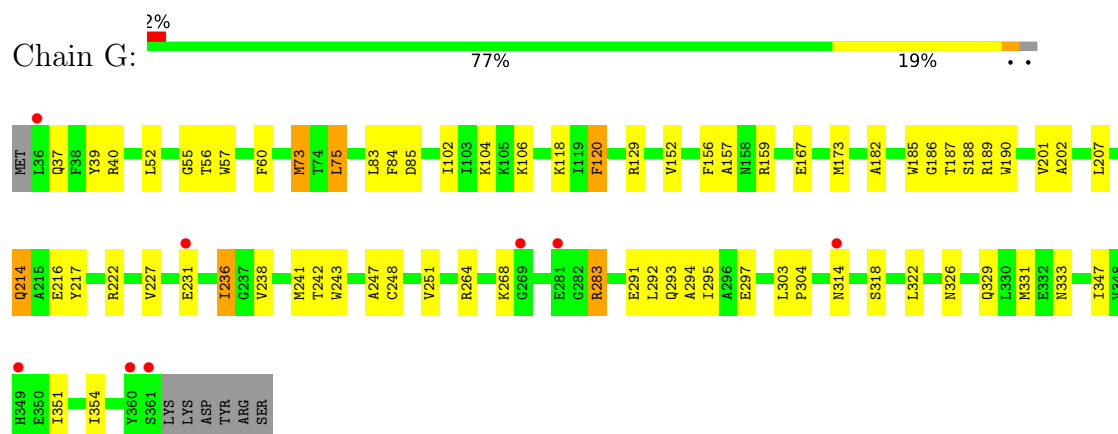
3 Residue-property plots

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.

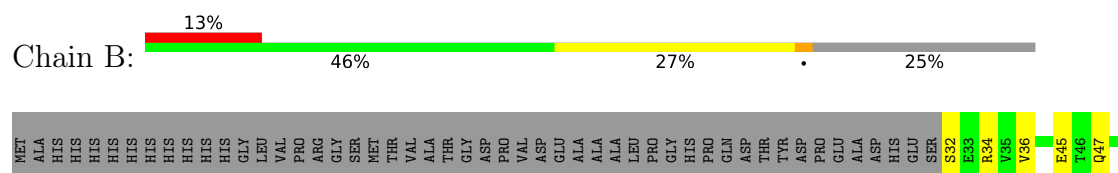
- Molecule 1: Voltage-gated potassium channel subunit beta-2

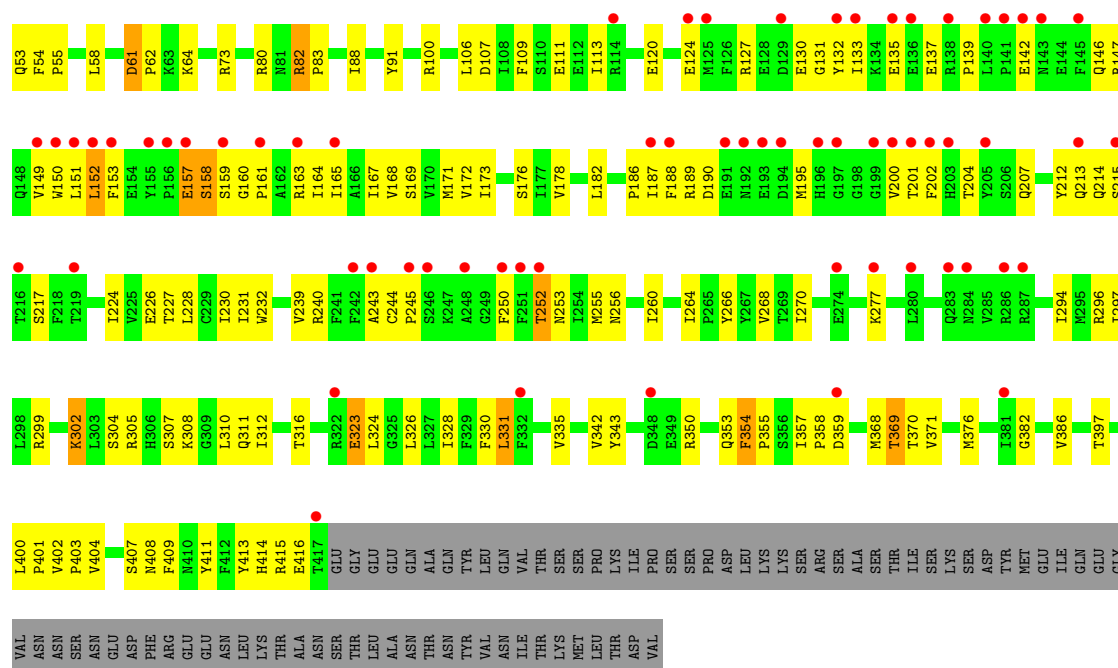


- Molecule 1: Voltage-gated potassium channel subunit beta-2



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



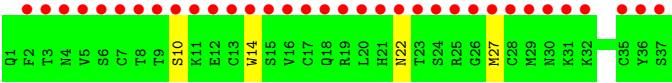
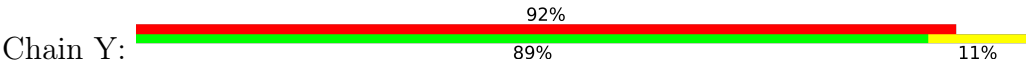


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



GLU
GLY
VAL
ASN
ASN
SER
ASN
GLU
ASP
PHE
ARG
GLU
GLU
ASN
LEU
LYS
THR
ALA
ASN
SER
THR
LEU
ALA
ASN
THR
ASN
TYR
VAL
ASN
ILE
THR
LYS
MET
LEU
THR
ASP
VAL

● Molecule 3: Potassium channel toxin alpha-KTx 1.1



4 Data and refinement statistics

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 50.00 – 2.54	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.54) 93.1 (50.00-2.54)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/2608	0.88	4/3524 (0.1%)
1	G	0.43	0/2608	0.88	4/3524 (0.1%)
2	B	0.39	0/3169	0.89	11/4292 (0.3%)
2	H	0.33	0/3036	0.83	6/4114 (0.1%)
3	Y	0.26	0/291	0.64	0/388
All	All	0.40	0/11712	0.86	25/15842 (0.2%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	369	THR	N-CA-C	-7.46	104.17	113.20
2	B	80	ARG	N-CA-C	6.82	118.86	109.18
1	G	227	VAL	N-CA-C	6.78	117.39	111.56
2	B	54	PHE	CA-C-N	6.75	127.30	119.47
2	B	54	PHE	C-N-CA	6.75	127.30	119.47

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2556	0	2582	54	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2556	0	2582	50	0
2	B	3088	0	3034	101	0
2	H	2959	0	2956	178	0
3	Y	294	0	278	0	0
4	A	48	0	25	11	0
4	G	48	0	25	12	0
5	B	4	0	0	0	0
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	395	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.

The worst 5 of 395 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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

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%)	36	45
1	G	324/333 (97%)	315 (97%)	8 (2%)	1 (0%)	36	45
2	B	384/514 (75%)	348 (91%)	27 (7%)	9 (2%)	5	4
2	H	357/514 (70%)	291 (82%)	55 (15%)	11 (3%)	3	2
3	Y	35/37 (95%)	17 (49%)	16 (46%)	2 (6%)	1	0
All	All	1424/1731 (82%)	1281 (90%)	119 (8%)	24 (2%)	7	8

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/280 (98%)	270 (99%)	3 (1%)	65	79
1	G	273/280 (98%)	266 (97%)	7 (3%)	40	59
2	B	332/459 (72%)	325 (98%)	7 (2%)	47	66
2	H	324/459 (71%)	321 (99%)	3 (1%)	70	82
3	Y	35/35 (100%)	33 (94%)	2 (6%)	18	28
All	All	1237/1513 (82%)	1215 (98%)	22 (2%)	51	70

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	231	GLU
2	H	150	TRP
1	G	314	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	263	ILE
2	B	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	148	GLN
2	H	207	GLN
2	H	281	GLN
2	B	253	ASN
2	B	214	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	0.61	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 oligosaccharides 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	511	-	8,8,50	0.35	0	7,7,56	0.54	0
6	PGW	B	516	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	519	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	512	-	6,6,50	0.37	0	5,5,56	0.47	0
6	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	513	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.53	0
4	NAP	G	1001	-	50,52,52	2.50	8 (16%)	71,80,80	2.58	20 (28%)
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	515	-	22,22,50	0.80	0	25,27,56	1.28	4 (16%)
4	NAP	A	1001	-	50,52,52	2.57	9 (18%)	71,80,80	2.64	20 (28%)
6	PGW	B	505	-	21,21,50	0.61	0	23,23,56	1.25	3 (13%)
6	PGW	B	520	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	506	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGW	B	518	-	6,6,50	0.37	0	5,5,56	0.45	0
6	PGW	B	514	-	7,7,50	0.36	0	6,6,56	0.52	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	511	-	-	0/6/6/55	-
6	PGW	B	516	-	-	0/5/5/55	-
6	PGW	B	519	-	-	0/5/5/55	-
6	PGW	B	512	-	-	0/4/4/55	-
6	PGW	B	508	-	-	0/6/6/55	-
6	PGW	B	513	-	-	0/6/6/55	-
6	PGW	B	509	-	-	0/6/6/55	-
4	NAP	G	1001	-	-	3/35/67/67	0/5/5/5
6	PGW	B	517	-	-	7/40/40/55	-
6	PGW	H	505	-	-	1/23/23/55	-
6	PGW	B	515	-	-	8/24/24/55	-
4	NAP	A	1001	-	-	4/35/67/67	0/5/5/5
6	PGW	B	505	-	-	1/23/23/55	-
6	PGW	B	520	-	-	0/5/5/55	-
6	PGW	B	507	-	-	0/6/6/55	-
6	PGW	B	506	-	-	0/6/6/55	-
6	PGW	B	510	-	-	0/6/6/55	-
6	PGW	B	518	-	-	0/4/4/55	-
6	PGW	B	514	-	-	0/5/5/55	-

The worst 5 of 17 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	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

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C2B-C1B-N9A	-7.66	101.15	113.75
4	G	1001	NAP	C2B-C1B-N9A	-6.84	102.49	113.75
4	A	1001	NAP	O2A-PA-O3	-6.01	91.02	107.27

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

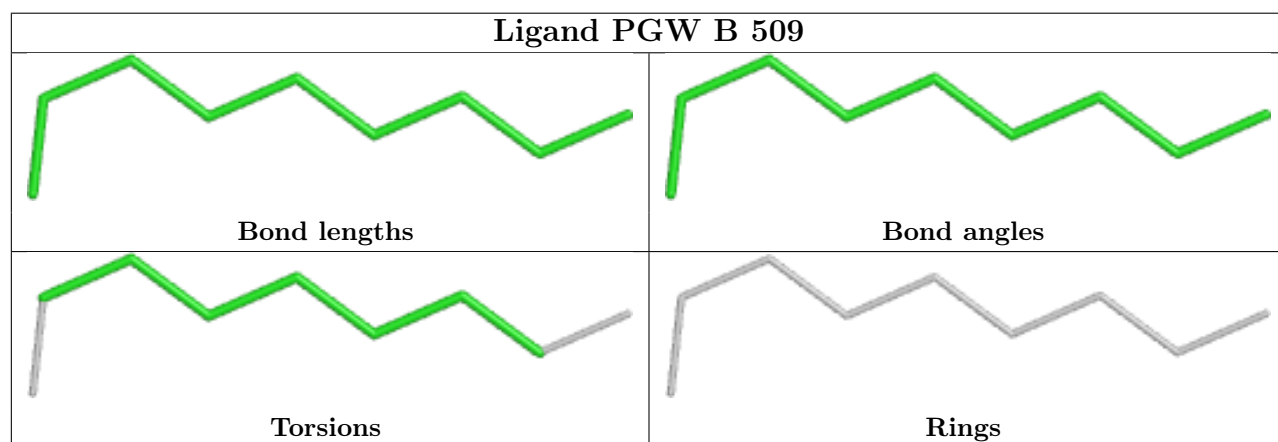
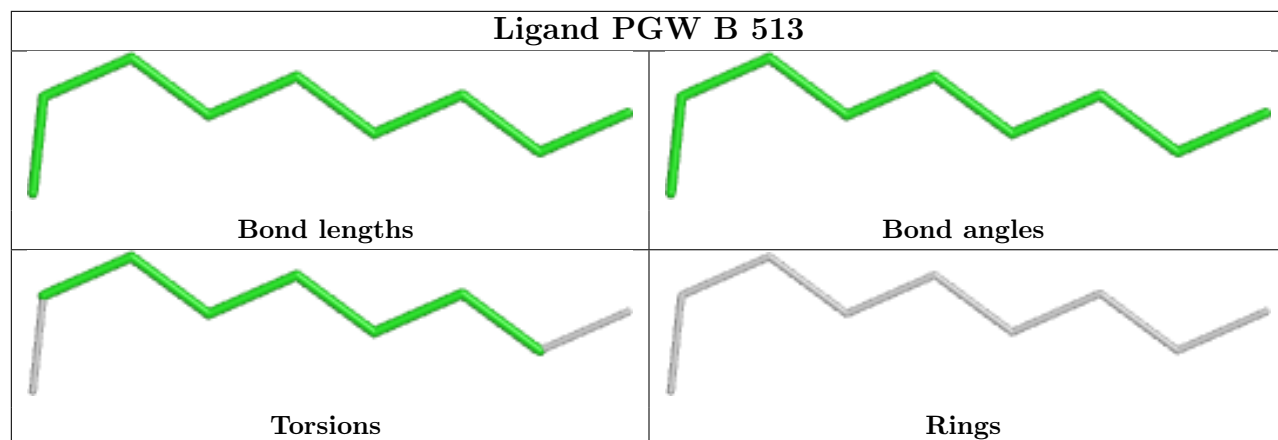
Mol	Chain	Res	Type	Atoms
4	A	1001	NAP	C5B-O5B-PA-O1A
4	G	1001	NAP	C5B-O5B-PA-O1A
6	B	515	PGW	C02-C03-O11-P
4	A	1001	NAP	C1B-C2B-O2B-P2B
4	G	1001	NAP	C1B-C2B-O2B-P2B

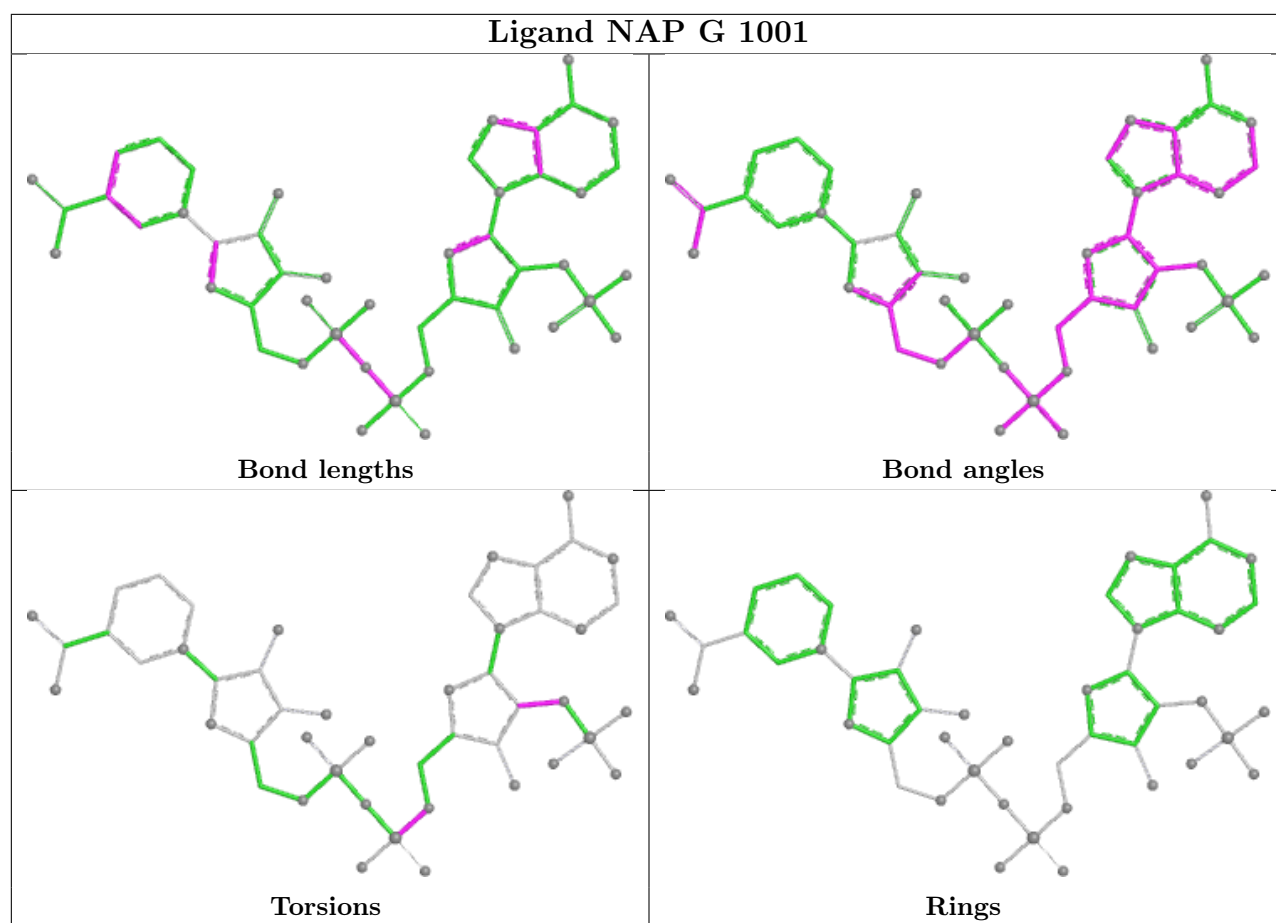
There are no ring outliers.

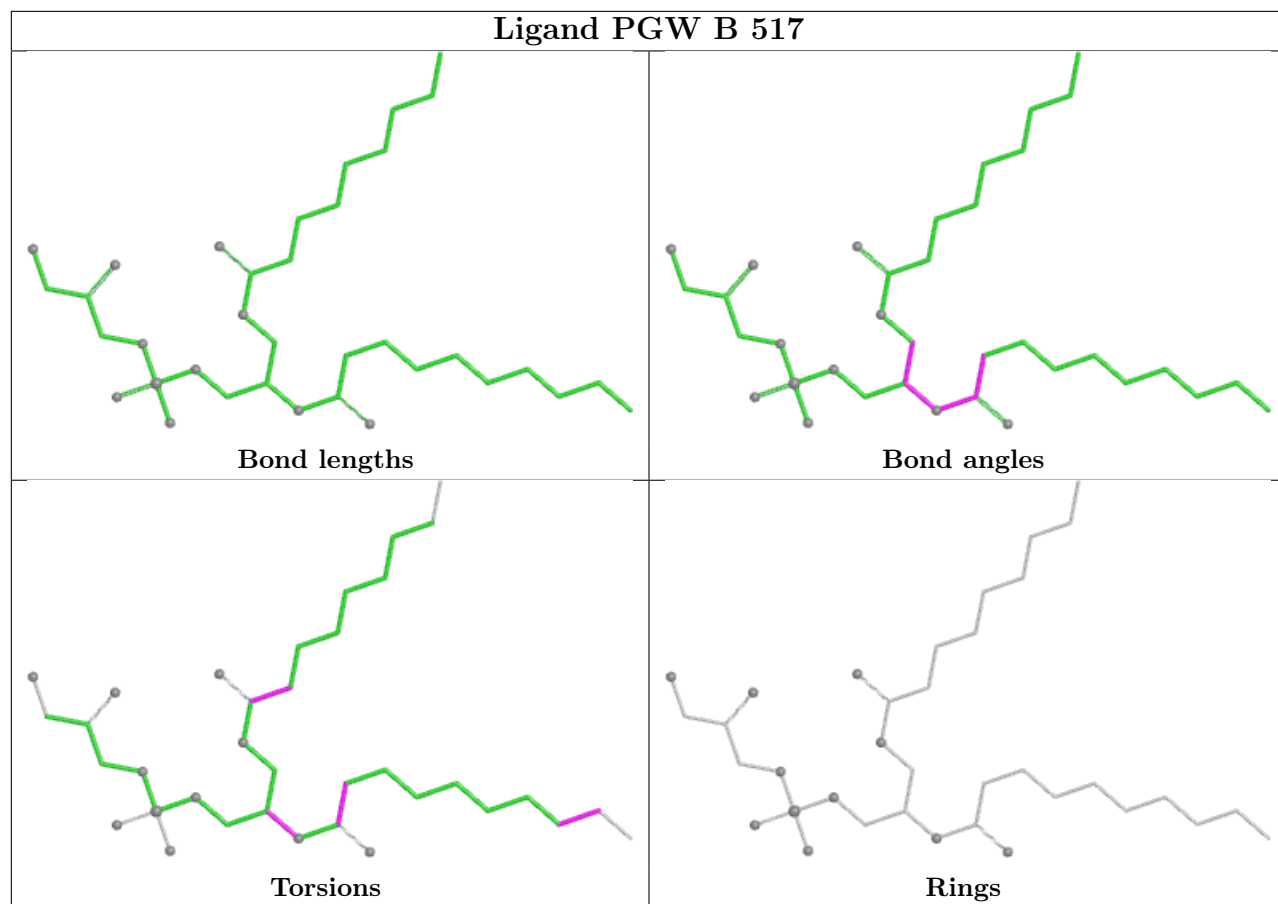
8 monomers are involved in 39 short contacts:

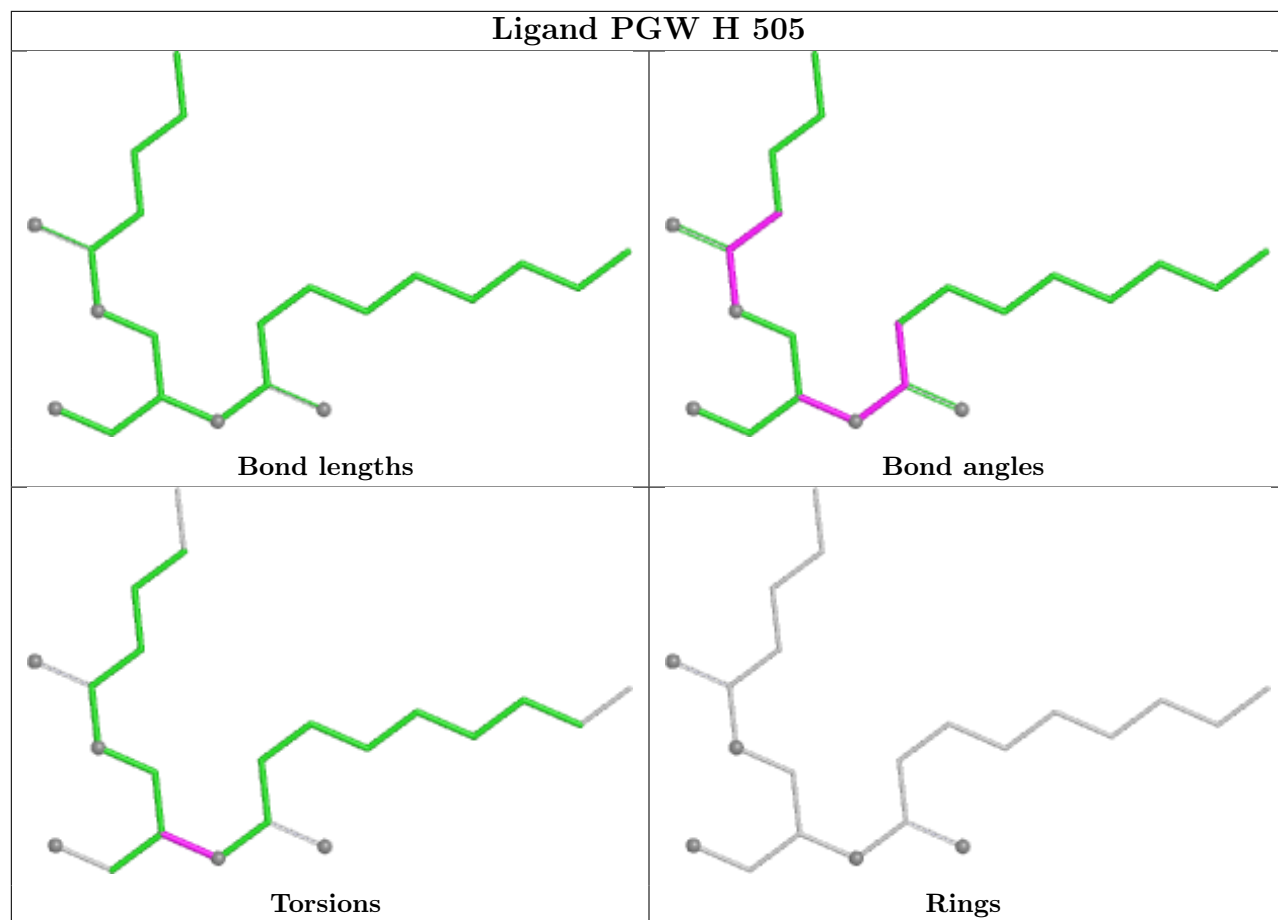
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	511	PGW	3	0
6	B	516	PGW	2	0
4	G	1001	NAP	12	0
6	B	517	PGW	4	0
6	H	505	PGW	5	0
6	B	515	PGW	1	0
4	A	1001	NAP	11	0
6	B	505	PGW	3	0

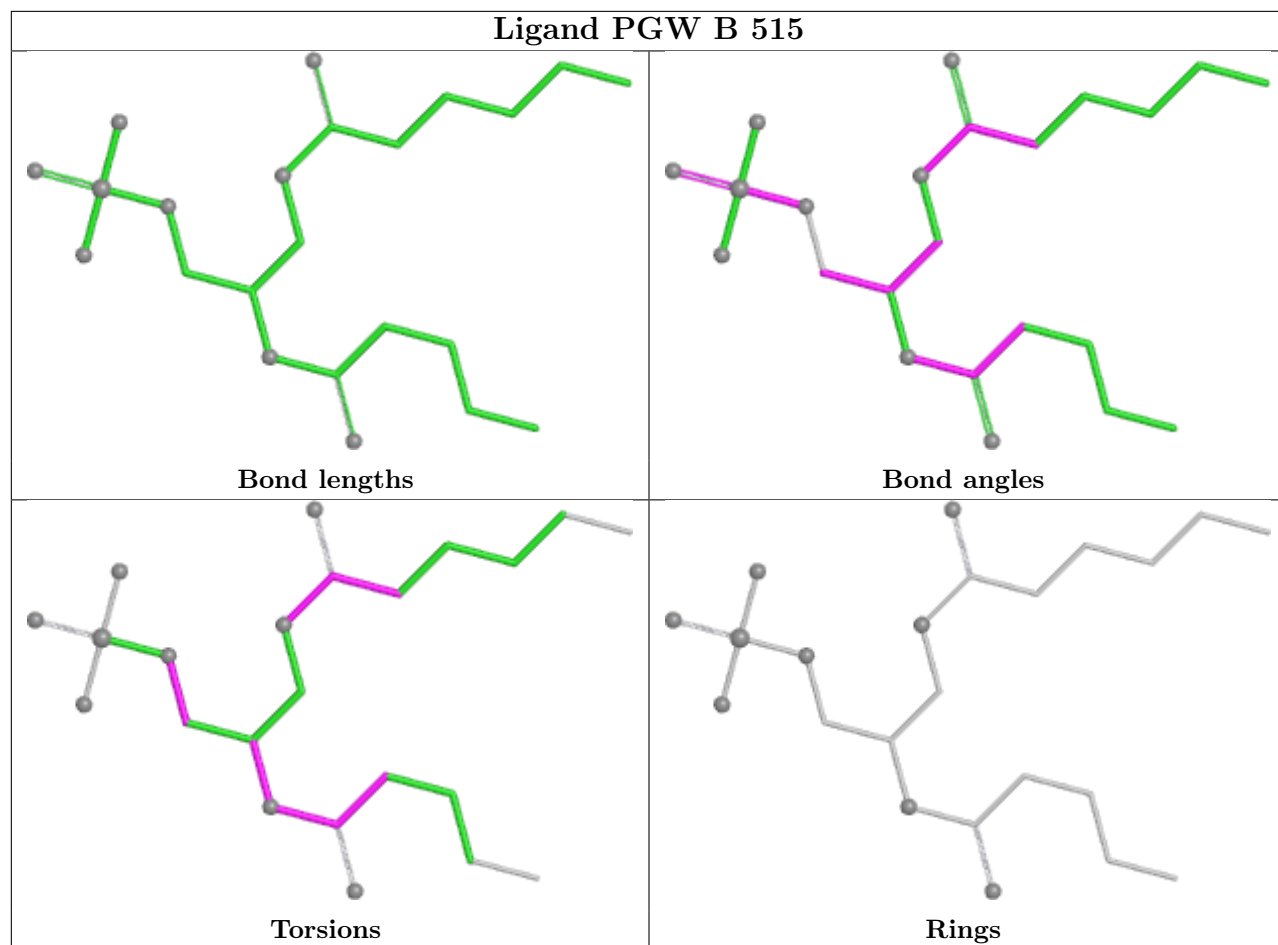
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

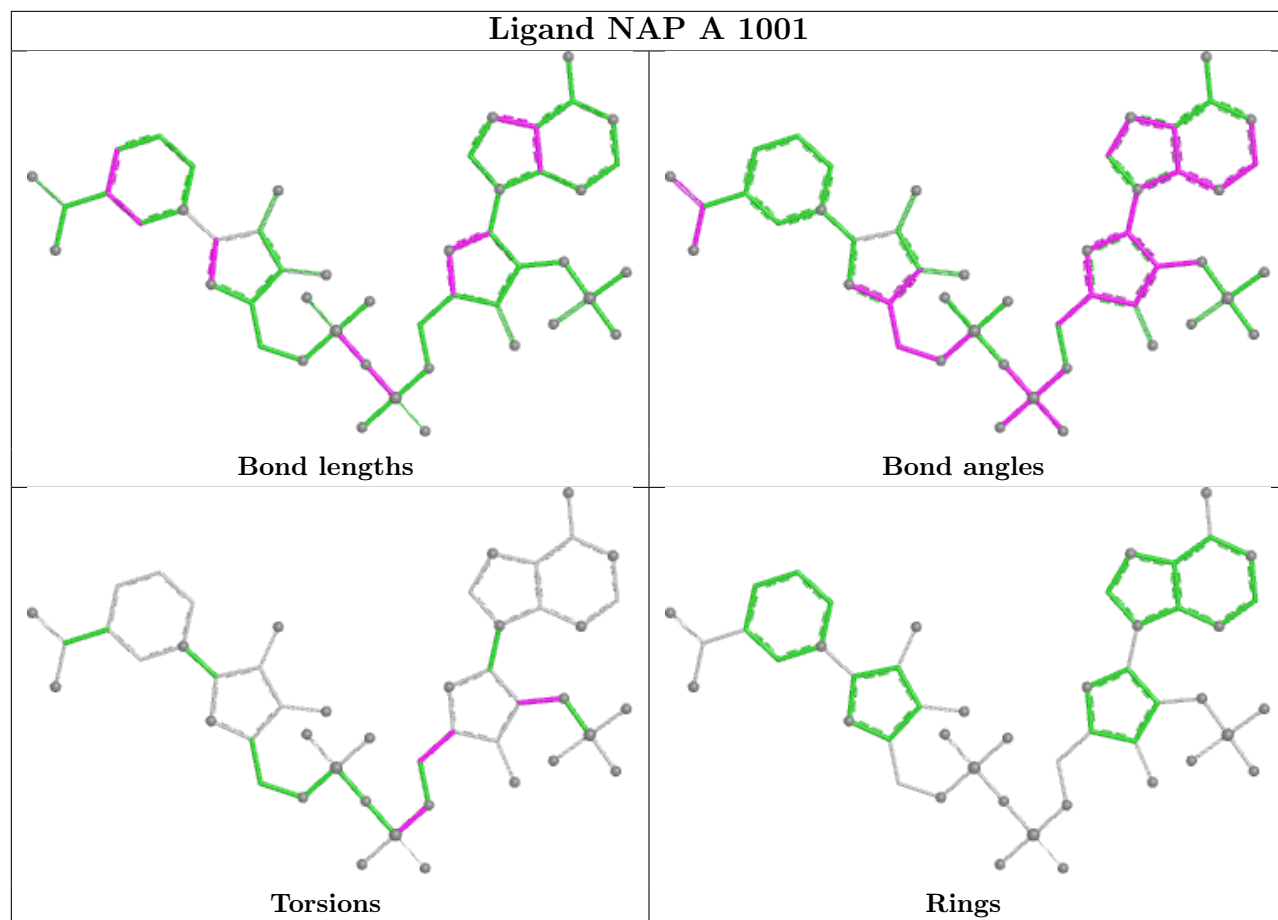


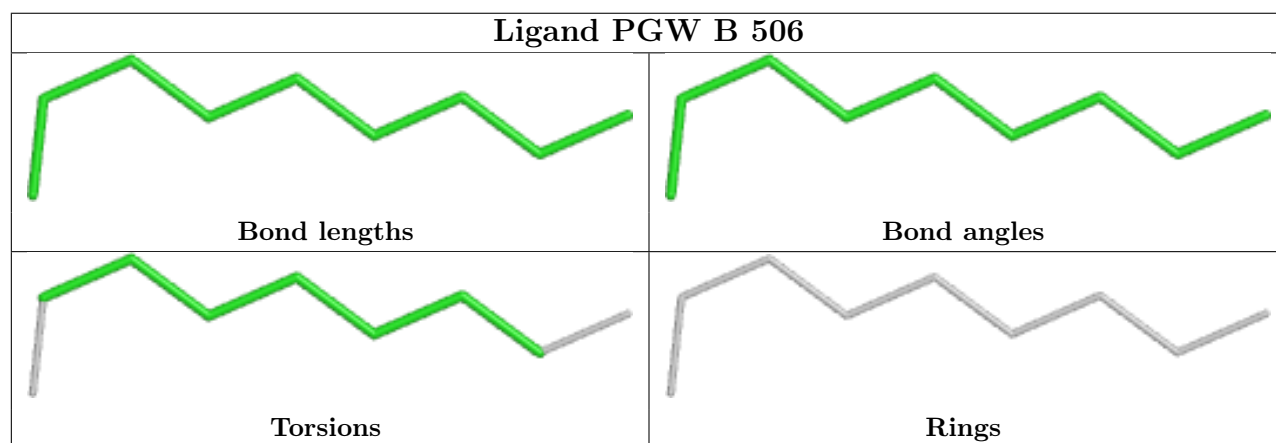
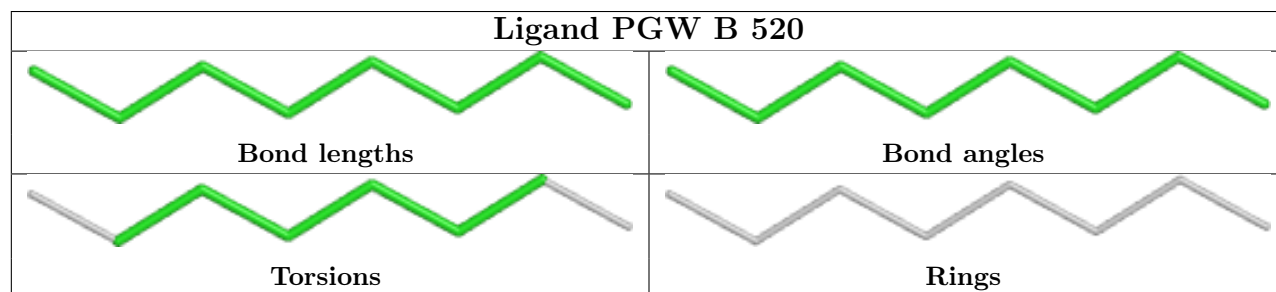
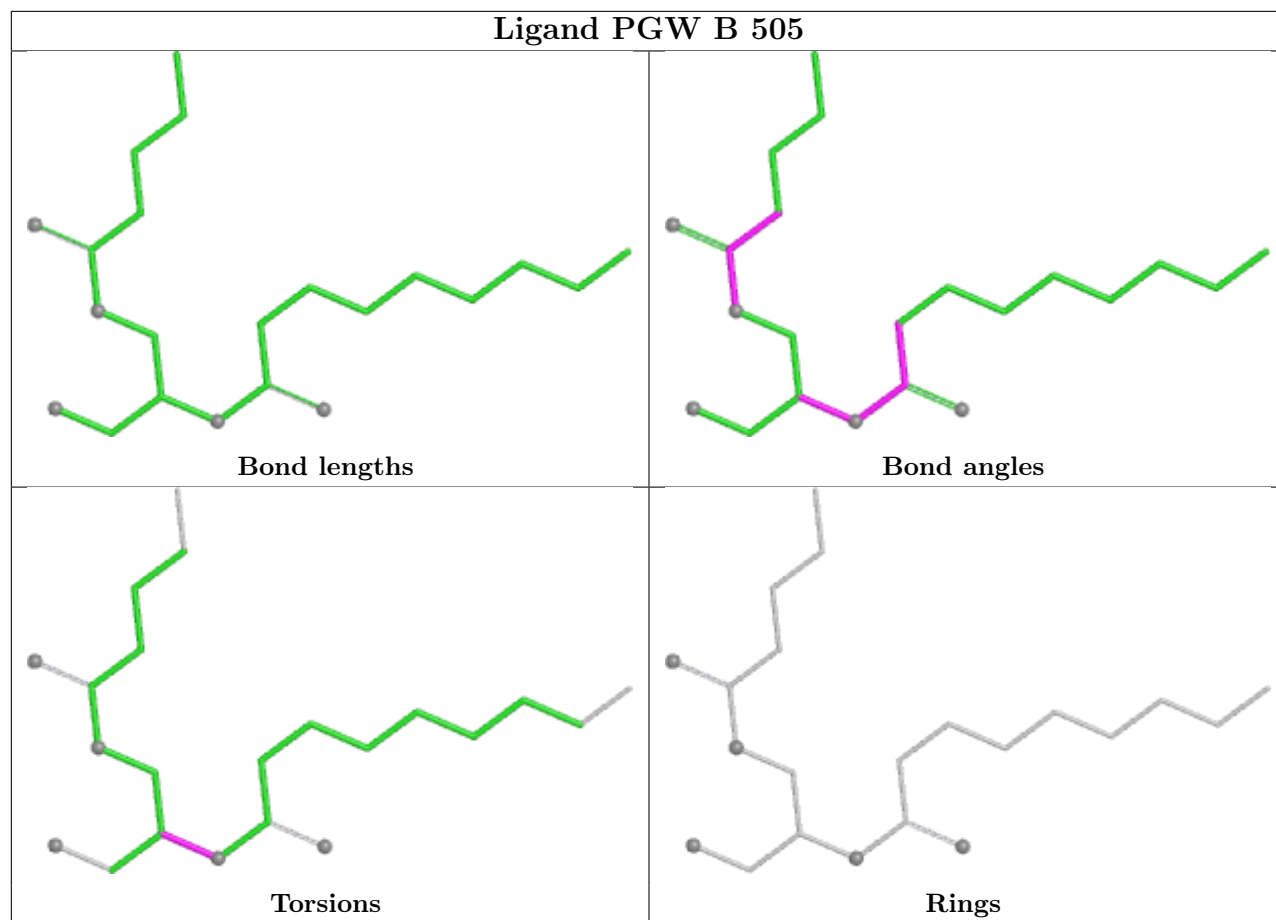












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/333 (97%)	-0.05	9 (2%) 55 56	24, 41, 66, 89	0
1	G	326/333 (97%)	0.01	8 (2%) 58 59	27, 45, 77, 100	0
2	B	386/514 (75%)	0.97	65 (16%) 4 3	34, 70, 120, 128	0
2	H	363/514 (70%)	2.18	165 (45%) 0 0	44, 115, 191, 202	0
3	Y	36/37 (97%)	7.95	34 (94%) 0 0	20, 21, 22, 22	36 (100%)
All	All	1437/1731 (83%)	1.00	281 (19%) 3 2	20, 59, 175, 202	36 (2%)

The worst 5 of 281 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	15	SER	27.0
3	Y	18	GLN	23.6
3	Y	20	LEU	19.2
3	Y	4	ASN	18.0
3	Y	22	ASN	15.4

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCA	Y	1	8/9	0.71	0.22	90,90,90,91	8

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

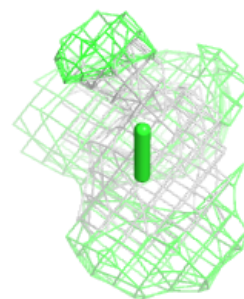
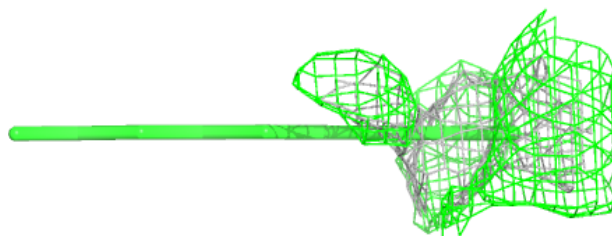
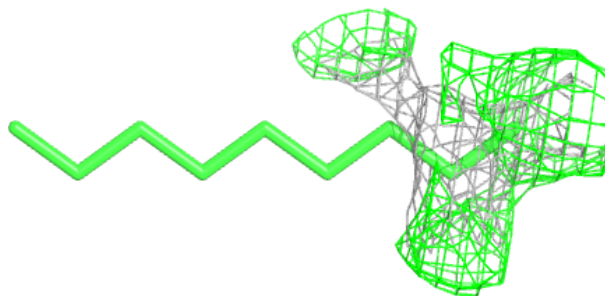
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PGW	B	513	9/51	0.45	0.62	127,129,129,129	0
6	PGW	H	505	22/51	0.64	0.53	139,145,148,148	0
6	PGW	B	505	22/51	0.65	0.49	92,107,120,121	0
5	K	H	504	1/1	0.67	0.19	55,55,55,55	1
6	PGW	B	518	7/51	0.72	0.39	72,74,75,75	0
6	PGW	B	517	36/51	0.72	0.37	117,135,152,152	0
6	PGW	B	520	8/51	0.73	0.47	96,100,103,104	0
6	PGW	B	509	9/51	0.73	0.50	115,115,116,116	0
6	PGW	B	506	9/51	0.75	0.41	81,84,88,88	0
6	PGW	B	507	9/51	0.79	0.39	94,97,98,99	0
6	PGW	B	515	23/51	0.79	0.29	128,136,138,138	0
6	PGW	B	512	7/51	0.79	0.27	76,78,79,79	0
6	PGW	B	516	8/51	0.83	0.40	90,94,99,99	0
6	PGW	B	519	8/51	0.84	0.42	111,114,115,115	0
6	PGW	B	514	8/51	0.85	0.35	80,82,84,85	0
6	PGW	B	510	9/51	0.86	0.37	104,106,107,107	0
5	K	H	503	1/1	0.88	0.13	56,56,56,56	1
6	PGW	B	511	9/51	0.88	0.36	122,123,124,124	0
6	PGW	B	508	9/51	0.88	0.30	96,97,98,99	0
5	K	H	502	1/1	0.88	0.11	55,55,55,55	1
4	NAP	G	1001	48/48	0.93	0.12	26,45,58,63	0
4	NAP	A	1001	48/48	0.94	0.12	32,42,52,55	0
5	K	B	504	1/1	0.95	0.08	39,39,39,39	1
5	K	B	502	1/1	0.96	0.08	39,39,39,39	1
5	K	B	501	1/1	0.96	0.14	42,42,42,42	1
5	K	H	501	1/1	0.97	0.16	53,53,53,53	1
5	K	B	503	1/1	0.98	0.08	34,34,34,34	1

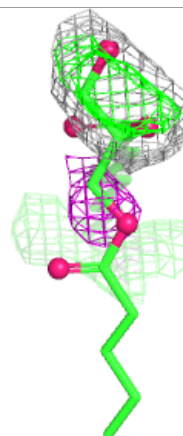
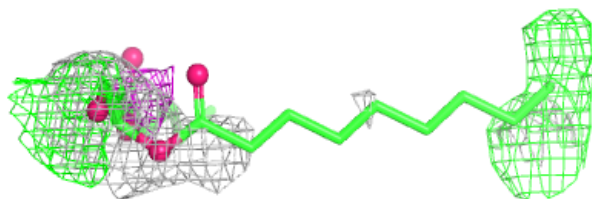
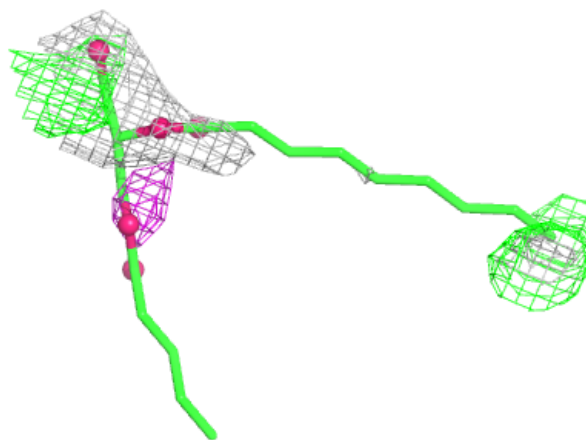
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

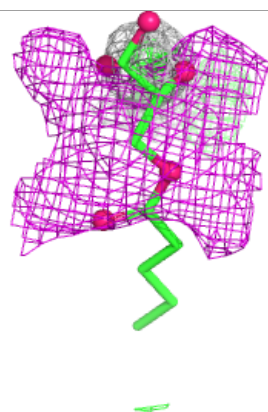
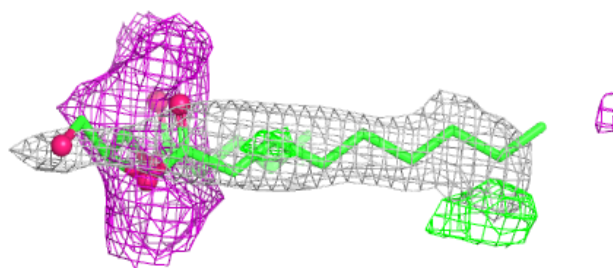
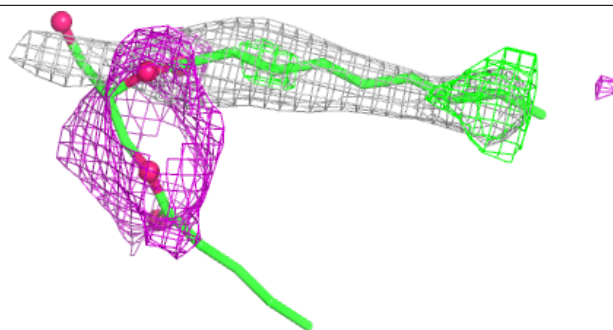
**Electron density around PGW H 505:**

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

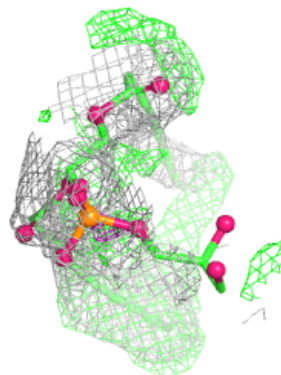
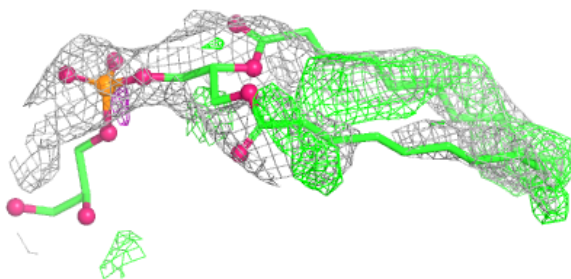
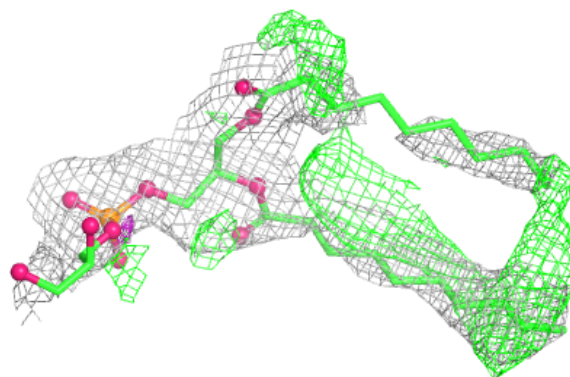


Electron density around PGW B 505:

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

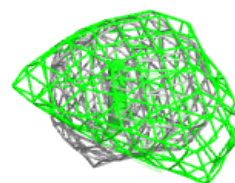
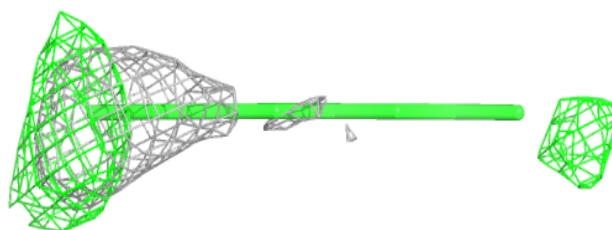
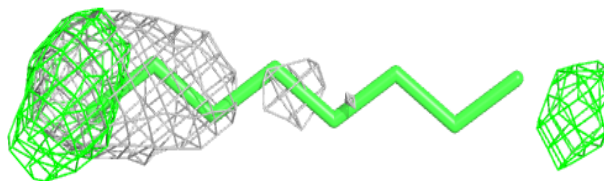
**Electron density around PGW B 517:**

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

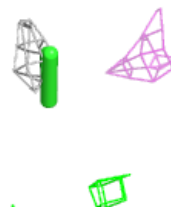
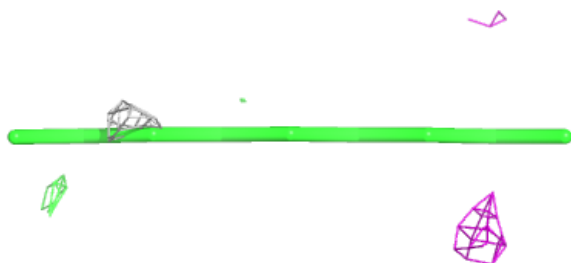
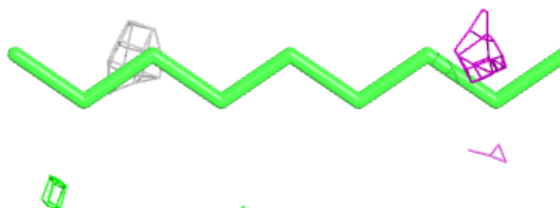


Electron density around PGW B 520:

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

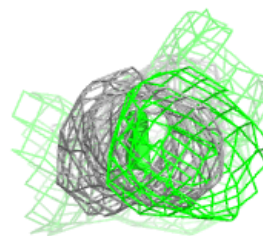
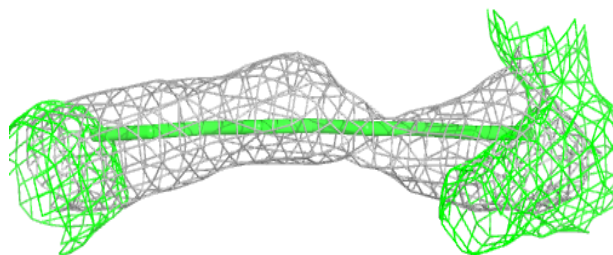
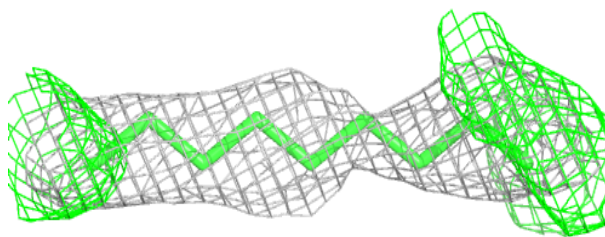
**Electron density around PGW B 509:**

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

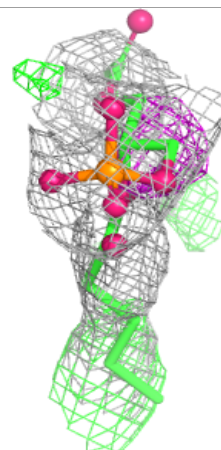
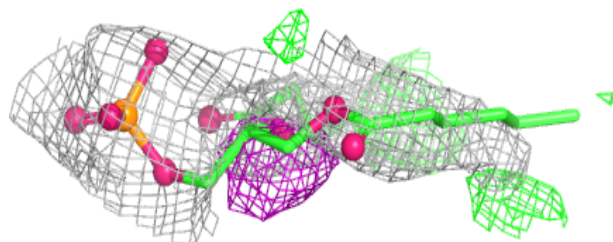
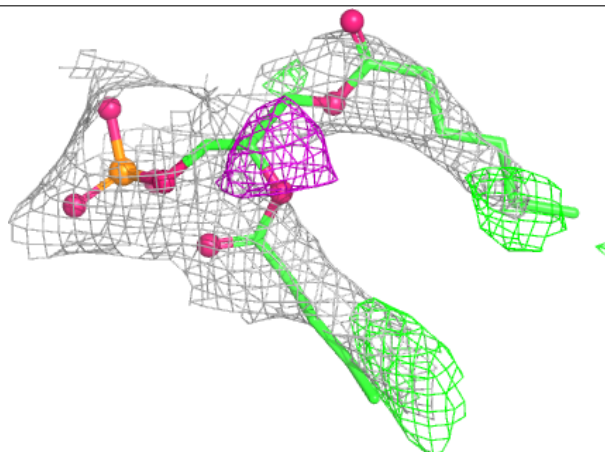


Electron density around PGW B 506:

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

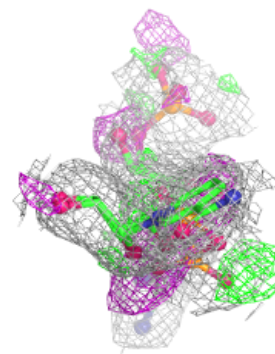
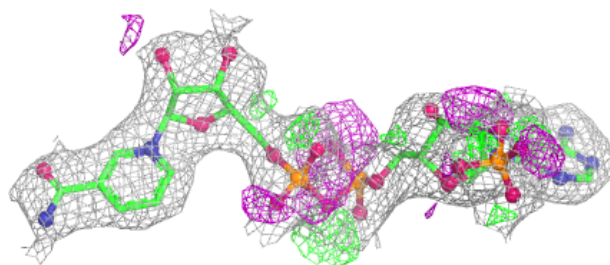
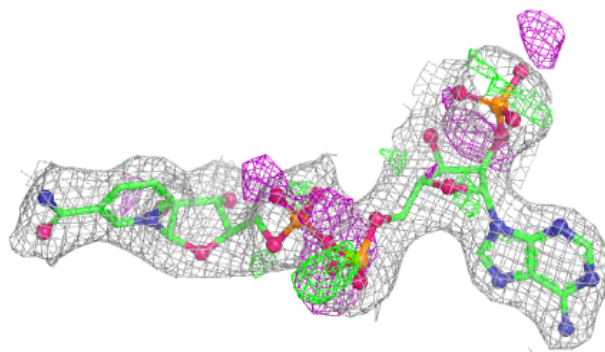
**Electron density around PGW B 515:**

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

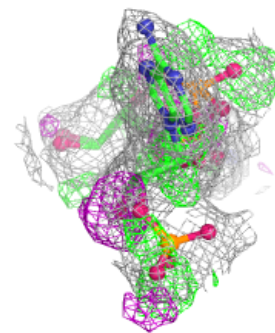
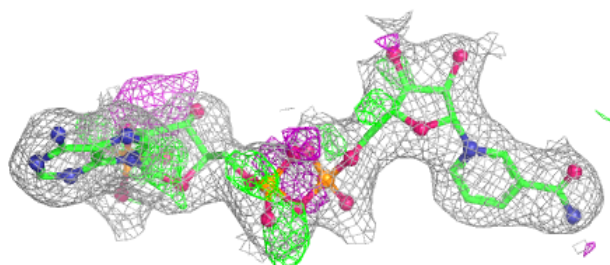
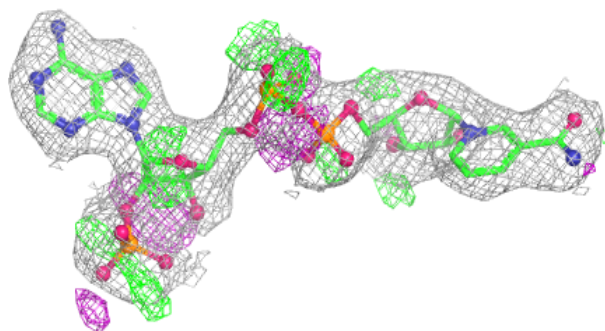


Electron density around NAP G 1001:

$2mF_o-DF_c$ (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.