



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 02:56 AM EST

PDB ID : 4JTA
Title : Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Charyb-dotoxin
Authors : MacKinnon, R.; Banerjee, A.; Lee, A.; Campbell, E.
Deposited on : 2013-03-23
Resolution : 2.50 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

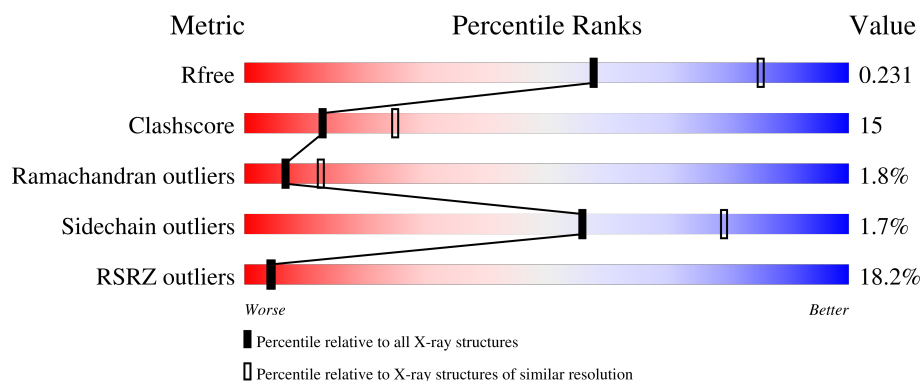
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	P	333	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
2	B	514	<div> <div>12%</div> <div>51%</div> <div>24%</div> <div>25%</div> </div>
2	Q	514	<div> <div>28%</div> <div>40%</div> <div>29%</div> <div>29%</div> </div>
3	Y	37	<div> <div>97%</div> <div>49%</div> <div>43%</div> <div>8%</div> </div>

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	508	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	518	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12106 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	P	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
P	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	Q	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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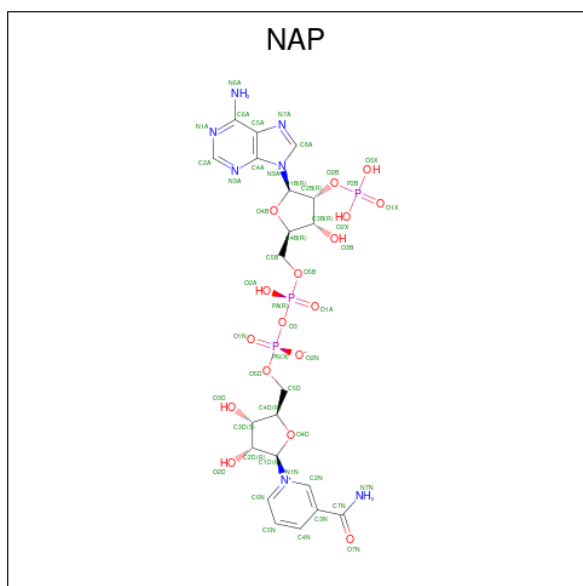
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P63142
B	-8	HIS	-	expression tag	UNP P63142
B	-7	HIS	-	expression tag	UNP P63142
B	-6	GLY	-	expression tag	UNP P63142
B	-5	LEU	-	expression tag	UNP P63142
B	-4	VAL	-	expression 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
Q	-18	MET	-	expression tag	UNP P63142
Q	-17	ALA	-	expression tag	UNP P63142
Q	-16	HIS	-	expression tag	UNP P63142
Q	-15	HIS	-	expression tag	UNP P63142
Q	-14	HIS	-	expression tag	UNP P63142
Q	-13	HIS	-	expression tag	UNP P63142
Q	-12	HIS	-	expression tag	UNP P63142
Q	-11	HIS	-	expression tag	UNP P63142
Q	-10	HIS	-	expression tag	UNP P63142
Q	-9	HIS	-	expression tag	UNP P63142
Q	-8	HIS	-	expression tag	UNP P63142
Q	-7	HIS	-	expression tag	UNP P63142
Q	-6	GLY	-	expression tag	UNP P63142
Q	-5	LEU	-	expression tag	UNP P63142
Q	-4	VAL	-	expression tag	UNP P63142
Q	-3	PRO	-	expression tag	UNP P63142
Q	-2	ARG	-	expression tag	UNP P63142
Q	-1	GLY	-	expression tag	UNP P63142
Q	0	SER	-	expression tag	UNP P63142
Q	31	SER	CYS	engineered mutation	UNP P63142
Q	32	SER	CYS	engineered mutation	UNP P63142
Q	207	GLN	ASN	engineered mutation	UNP P63142
Q	431	SER	CYS	engineered mutation	UNP P63142
Q	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: $C_{21}H_{28}N_7O_{17}P_3$).

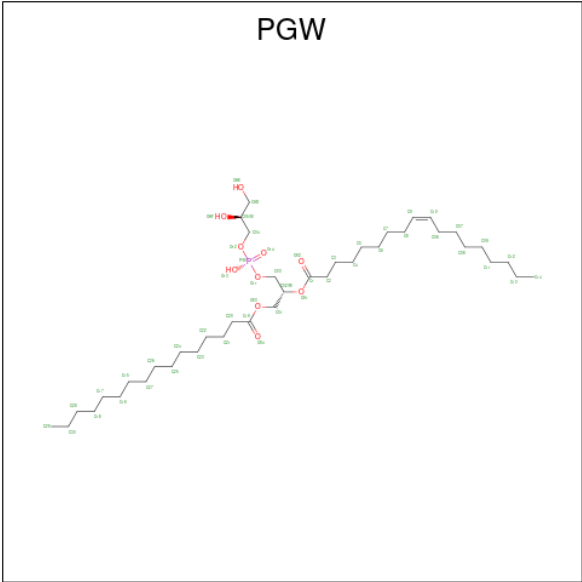


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total 3 K 3	0	0
5	Q	3	Total 3 K 3	0	0

- 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 12 12	0	0
6	B	1	Total C O P 23 14 8 1	0	0
6	B	1	Total C 12 12	0	0
6	B	1	Total C O P 37 26 10 1	0	0
6	B	1	Total C 10 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C 12 12	0	0
6	B	1	Total C 12 12	0	0
6	Q	1	Total C O 22 17 5	0	0

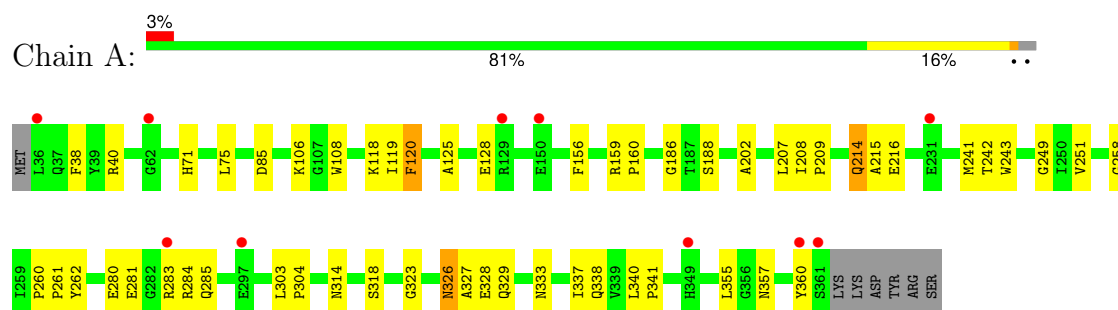
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	140	Total O 140 140	0	0
7	B	53	Total O 53 53	0	0
7	P	102	Total O 102 102	0	0
7	Q	23	Total O 23 23	0	0

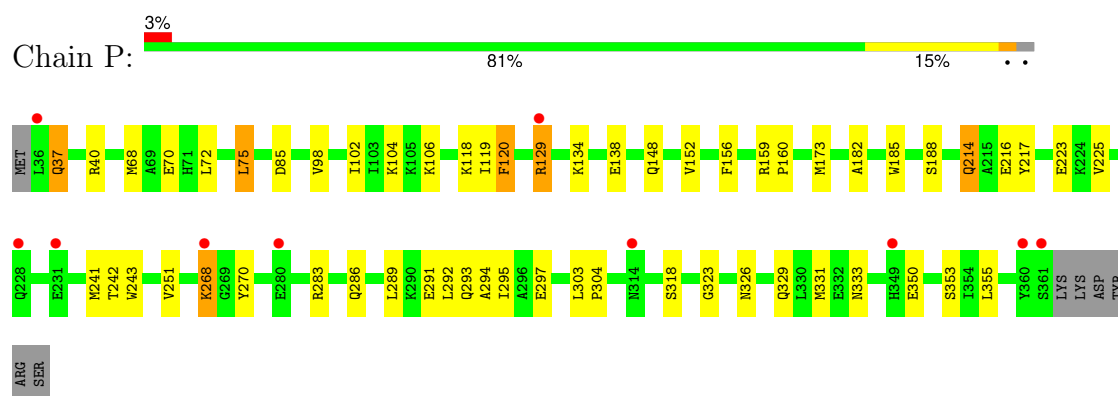
3 Residue-property plots [i](#)

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.

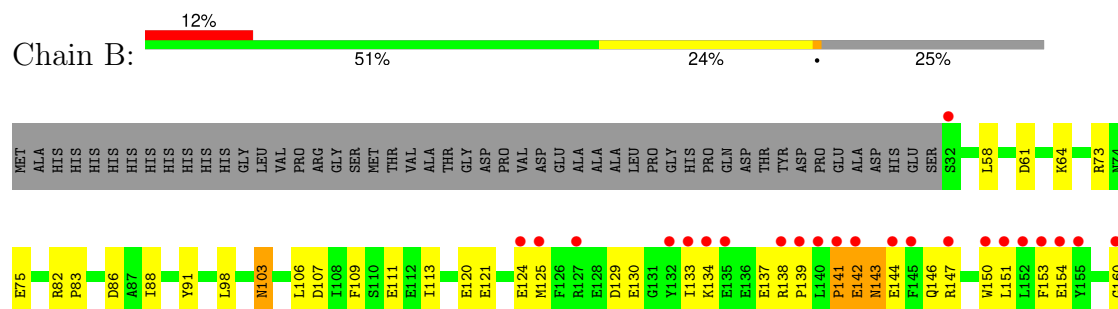
- Molecule 1: Voltage-gated potassium channel subunit beta-2

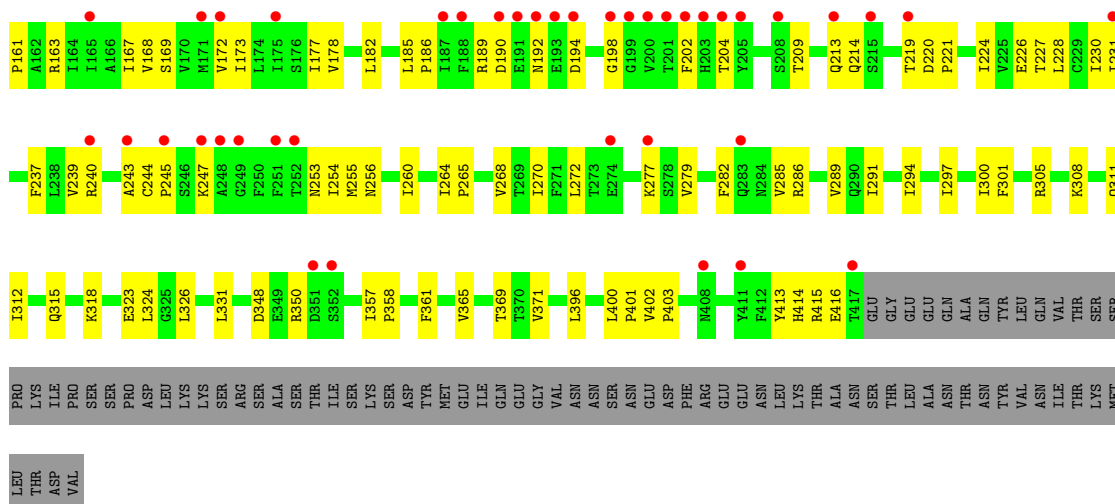


- Molecule 1: Voltage-gated potassium channel subunit beta-2

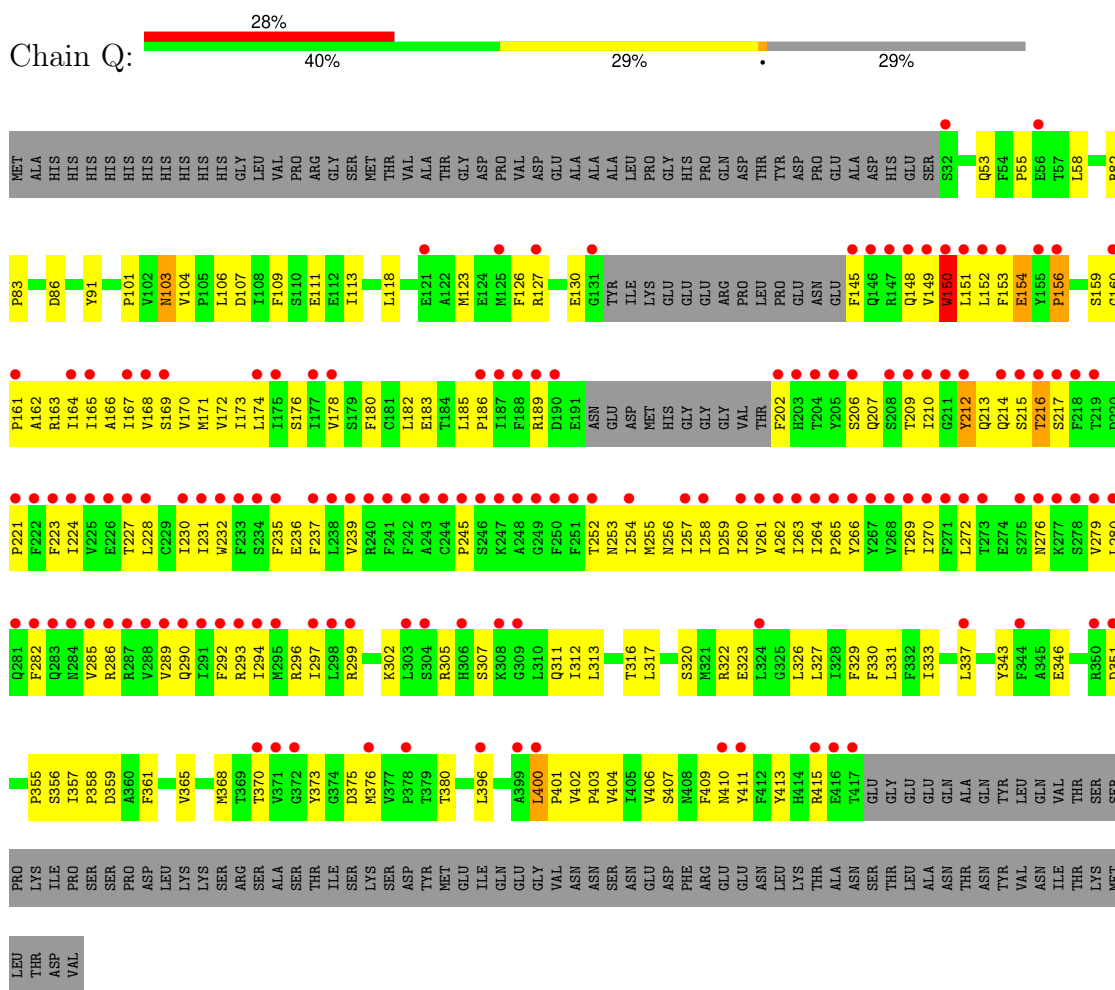


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1





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



- 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	144.40Å 144.40Å 284.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-2.50) 92.6 (50.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.236 0.207 , 0.231	Depositor DCC
R_{free} test set	4873 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12106	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCA, PGW, K, 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	0.36	0/2608	0.58	0/3524
1	P	0.36	0/2608	0.56	0/3524
2	B	0.35	0/3169	0.53	0/4292
2	Q	0.32	0/3036	0.50	0/4114
3	Y	0.26	0/292	0.46	0/389
All	All	0.35	0/11713	0.54	0/15843

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	270	TYR	Sidechain

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	42	0
1	P	2556	0	2582	46	0
2	B	3088	0	3034	91	0
2	Q	2959	0	2956	142	0
3	Y	295	0	282	19	0
4	A	48	0	25	3	0
4	P	48	0	25	3	0
5	B	3	0	0	0	0
5	Q	3	0	0	0	0
6	B	210	0	291	19	0
6	Q	22	0	25	7	0
7	A	140	0	0	2	0
7	B	53	0	0	1	0
7	P	102	0	0	0	0
7	Q	23	0	0	1	0
All	All	12106	0	11802	349	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 15.

The worst 5 of 349 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)
6:B:510:PGW:H2A	6:B:515:PGW:H21A	1.42	0.98
2:Q:400:LEU:HB2	2:Q:401:PRO:HD3	1.52	0.89
1:P:333:ASN:HD21	4:P:1001:NAP:H61A	1.21	0.88
2:Q:312:ILE:HD13	2:Q:413:TYR:HA	1.59	0.83
2:Q:227:THR:HA	2:Q:230:ILE:HG22	1.61	0.82

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%)	313 (97%)	10 (3%)	1 (0%)	37	56
1	P	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	37	56
2	B	384/514 (75%)	350 (91%)	21 (6%)	13 (3%)	3	4
2	Q	357/514 (70%)	311 (87%)	37 (10%)	9 (2%)	4	7
3	Y	35/37 (95%)	19 (54%)	15 (43%)	1 (3%)	3	6
All	All	1424/1731 (82%)	1306 (92%)	93 (6%)	25 (2%)	7	12

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	LYS
2	B	137	GLU
2	B	138	ARG
2	B	139	PRO
2	B	143	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%)	70	87
1	P	273/280 (98%)	266 (97%)	7 (3%)	41	68
2	B	332/459 (72%)	327 (98%)	5 (2%)	60	82
2	Q	324/459 (71%)	320 (99%)	4 (1%)	67	86
3	Y	35/35 (100%)	33 (94%)	2 (6%)	17	35
All	All	1237/1513 (82%)	1216 (98%)	21 (2%)	56	79

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	283	ARG
2	Q	212	TYR
3	Y	18	GLN

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Mol	Chain	Res	Type
2	Q	351	ASP
2	Q	150	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	163	ASN
1	P	286	GLN
2	Q	213	GLN
1	P	271	GLN
1	P	293	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	0.98	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 25 ligands modelled in this entry, 6 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	505	-	8,8,50	0.36	0	7,7,56	0.54	0
6	PGW	B	512	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.54	0
4	NAP	A	1001	-	46,52,52	1.43	7 (15%)	61,80,80	1.03	2 (3%)
6	PGW	B	513	-	11,11,50	0.35	0	10,10,56	0.59	0
6	PGW	B	511	-	6,6,50	0.36	0	5,5,56	0.48	0
6	PGW	B	515	-	11,11,50	0.35	0	10,10,56	0.59	0
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.54	0
6	PGW	B	514	-	22,22,50	0.80	0	25,27,56	1.28	4 (16%)
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.55	0
4	NAP	P	1001	-	46,52,52	1.54	8 (17%)	61,80,80	1.05	1 (1%)
6	PGW	B	504	-	21,21,50	0.61	0	23,23,56	1.22	3 (13%)
6	PGW	B	517	-	9,9,50	0.36	0	8,8,56	0.56	0
6	PGW	B	518	-	11,11,50	0.35	0	10,10,56	0.57	0
6	PGW	B	506	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	519	-	11,11,50	0.35	0	10,10,56	0.57	0
6	PGW	B	516	-	36,36,50	0.65	0	39,42,56	0.90	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGW	Q	504	-	21,21,50	0.61	0	23,23,56	1.21	4 (17%)
6	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGW	B	505	-	-	0/6/6/55	-
6	PGW	B	512	-	-	0/6/6/55	-
6	PGW	B	507	-	-	0/6/6/55	-
4	NAP	A	1001	-	-	4/31/67/67	0/5/5/5
6	PGW	B	513	-	-	0/9/9/55	-
6	PGW	B	511	-	-	0/4/4/55	-
6	PGW	B	515	-	-	0/9/9/55	-
6	PGW	B	509	-	-	0/6/6/55	-
6	PGW	B	514	-	-	7/24/24/55	-
6	PGW	B	510	-	-	0/6/6/55	-
4	NAP	P	1001	-	-	3/31/67/67	0/5/5/5
6	PGW	B	504	-	-	1/23/23/55	-
6	PGW	B	517	-	-	0/7/7/55	-
6	PGW	B	518	-	-	0/9/9/55	-
6	PGW	B	506	-	-	0/6/6/55	-
6	PGW	B	519	-	-	0/9/9/55	-
6	PGW	B	516	-	-	7/41/41/55	-
6	PGW	Q	504	-	-	1/23/23/55	-
6	PGW	B	508	-	-	0/6/6/55	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1001	NAP	C6N-N1N	4.24	1.45	1.35
4	A	1001	NAP	C6N-N1N	4.02	1.44	1.35
4	P	1001	NAP	C4N-C3N	3.73	1.45	1.39
4	A	1001	NAP	C4N-C3N	3.68	1.45	1.39
4	P	1001	NAP	PA-O3	3.68	1.63	1.59

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	504	PGW	O01-C1-C2	3.31	118.64	111.48
6	B	504	PGW	O01-C1-C2	3.29	118.59	111.48
6	B	514	PGW	O01-C1-C2	2.98	117.92	111.48
4	P	1001	NAP	C6N-N1N-C2N	-2.93	119.38	121.88
6	B	514	PGW	C03-C02-C01	-2.92	104.99	111.78

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAP	PN-O3-PA-O5B
4	A	1001	NAP	O4D-C1D-N1N-C6N
4	P	1001	NAP	PN-O3-PA-O5B
4	P	1001	NAP	O4D-C1D-N1N-C6N
6	B	514	PGW	C02-C03-O11-P

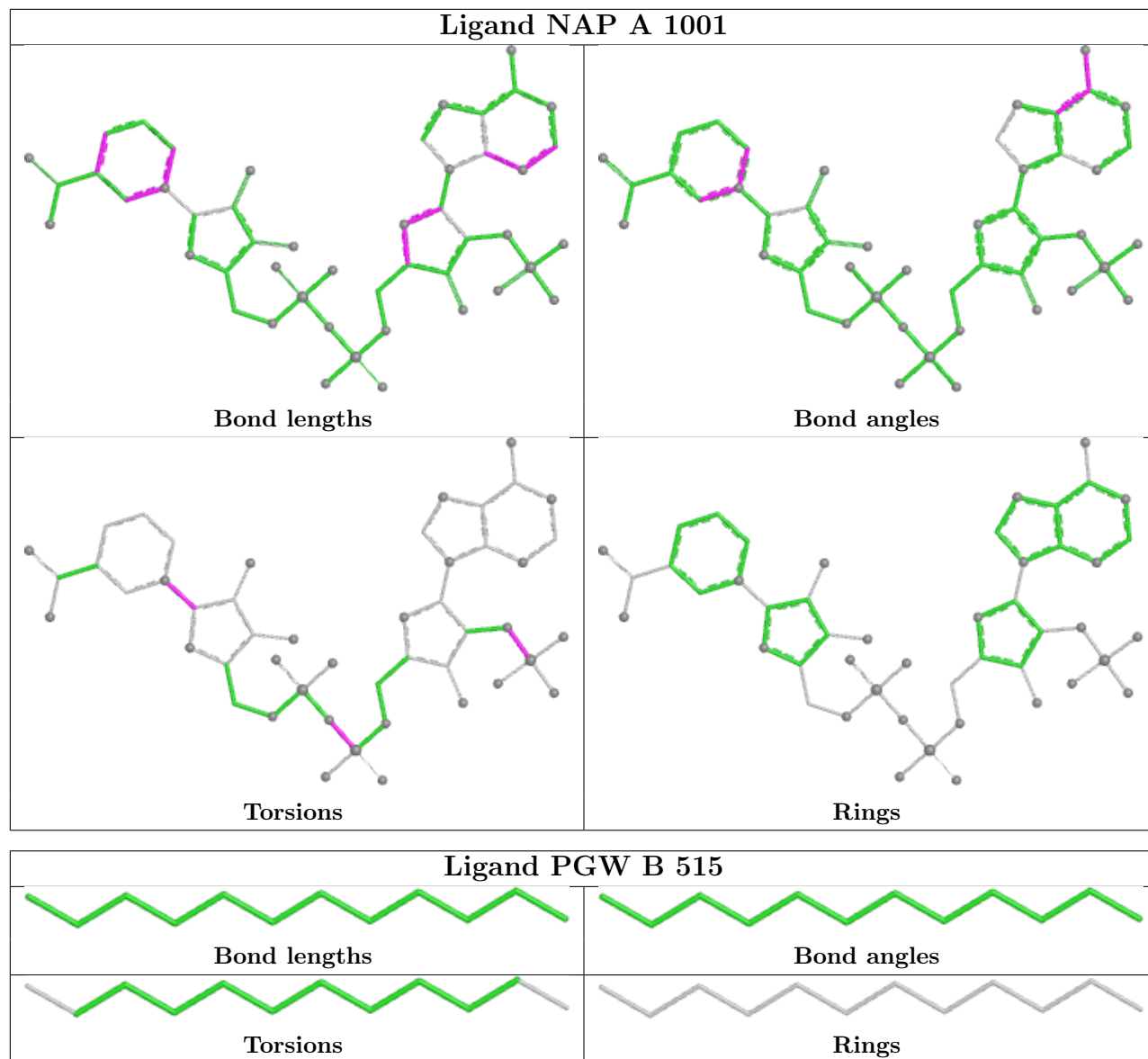
There are no ring outliers.

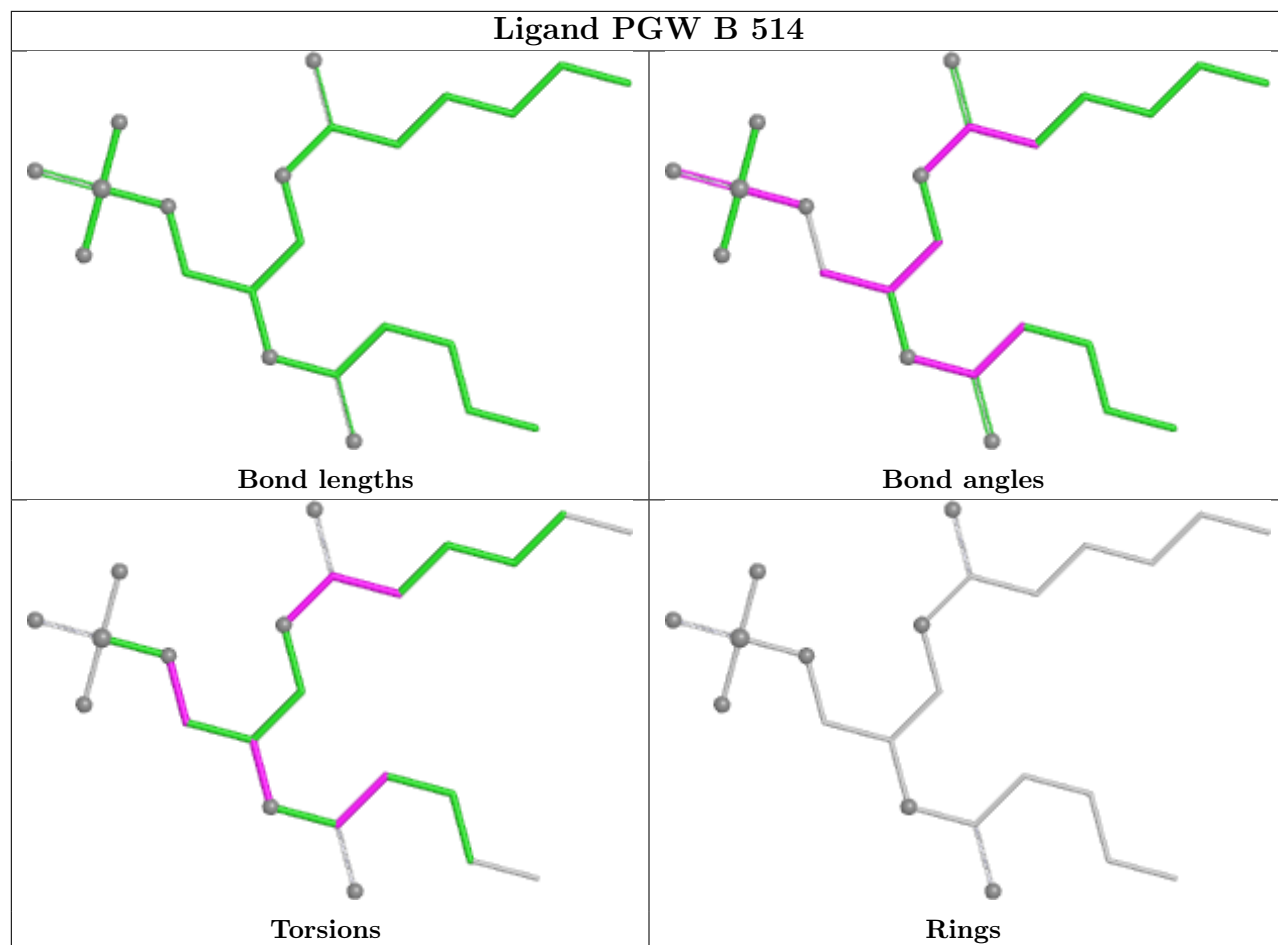
11 monomers are involved in 32 short contacts:

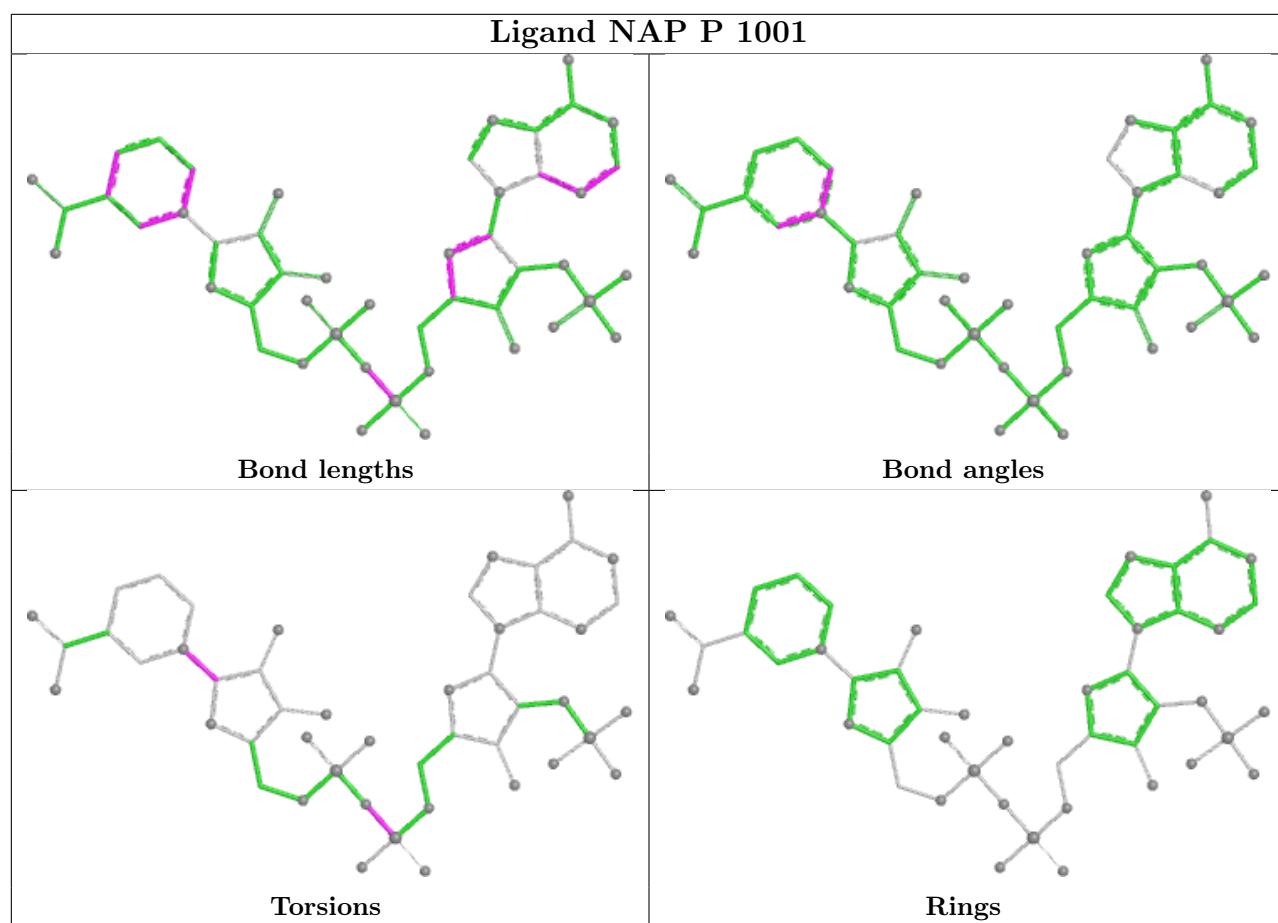
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	507	PGW	1	0
4	A	1001	NAP	3	0
6	B	513	PGW	1	0
6	B	515	PGW	2	0
6	B	509	PGW	1	0
6	B	514	PGW	1	0
6	B	510	PGW	2	0
4	P	1001	NAP	3	0
6	B	504	PGW	4	0
6	B	516	PGW	9	0
6	Q	504	PGW	7	0

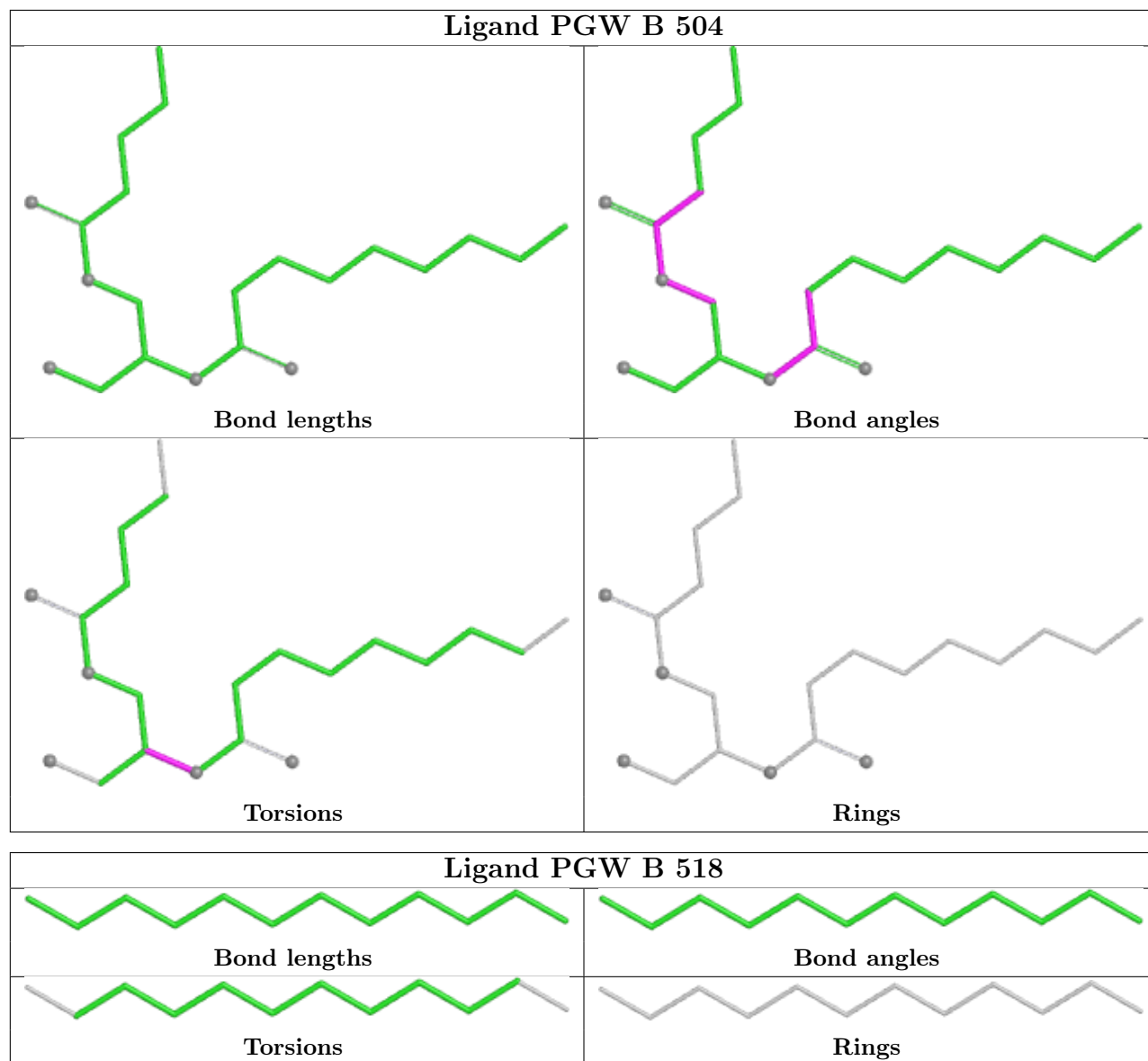
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

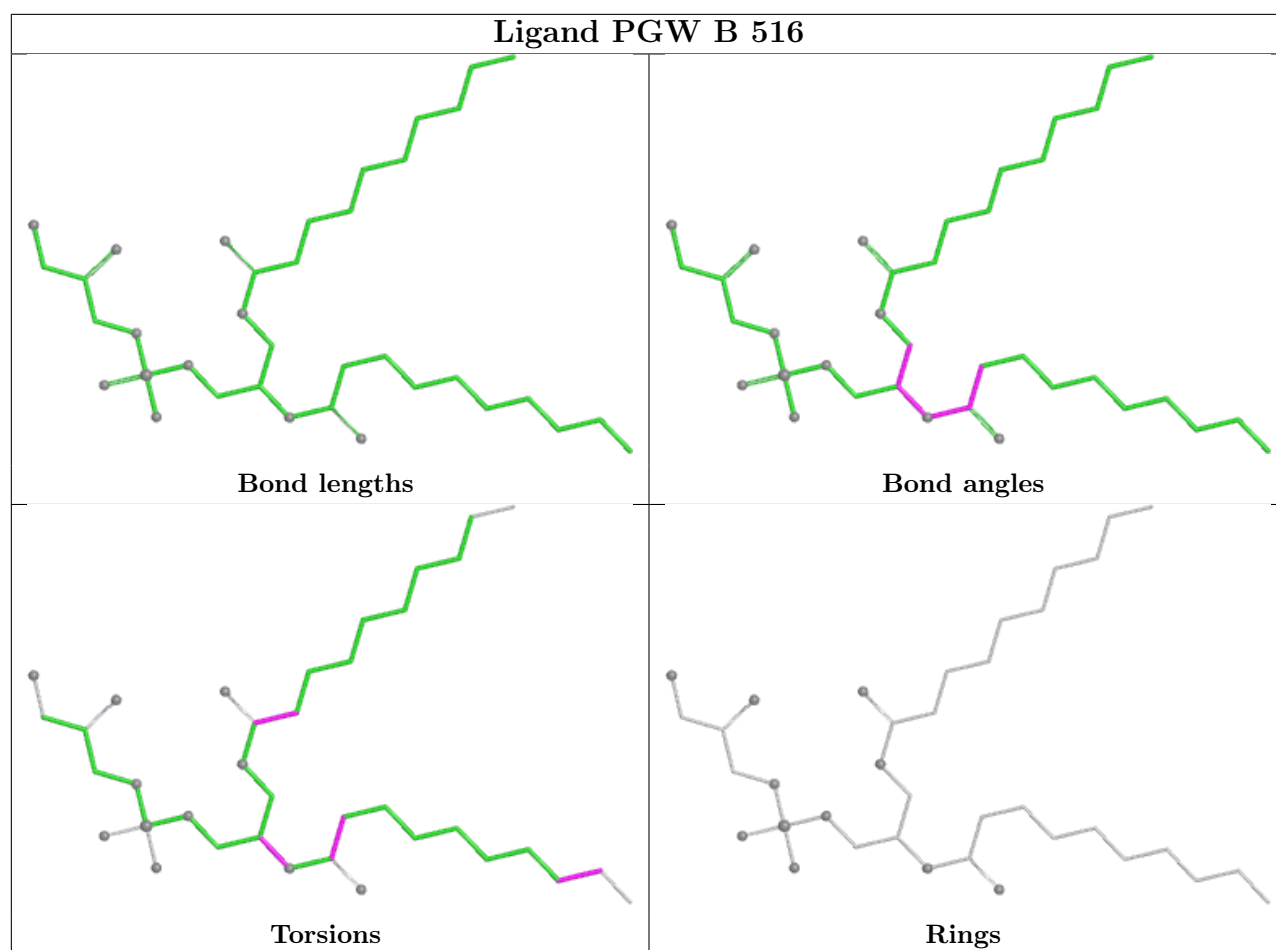
equivalents in the CSD to analyse the geometry.

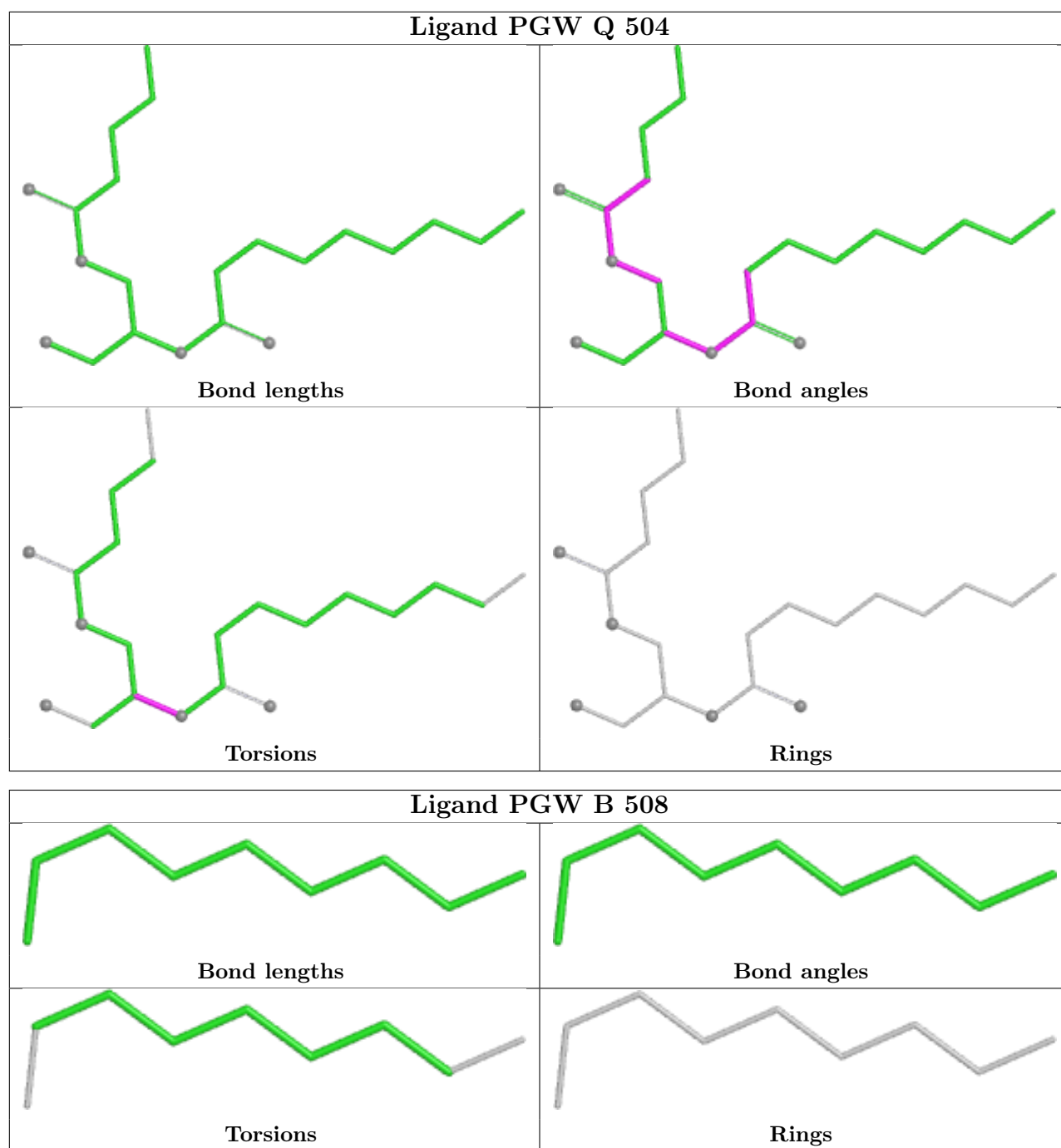












5.7 Other polymers [i](#)

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(Å²)	Q<0.9
1	A	326/333 (97%)	-0.21	10 (3%)	51	48	25, 41, 64, 92	0
1	P	326/333 (97%)	-0.07	10 (3%)	51	48	26, 44, 77, 101	0
2	B	386/514 (75%)	0.88	63 (16%)	5	5	32, 67, 119, 128	0
2	Q	363/514 (70%)	1.94	143 (39%)	1	1	39, 102, 196, 208	0
3	Y	36/37 (97%)	8.36	36 (100%)	0	0	21, 23, 24, 24	36 (100%)
All	All	1437/1731 (83%)	0.87	262 (18%)	4	4	21, 58, 182, 208	36 (2%)

The worst 5 of 262 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	15	SER	27.2
3	Y	19	ARG	24.3
3	Y	18	GLN	22.7
3	Y	20	LEU	18.4
3	Y	22	ASN	15.9

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	0.77	0.20	88,88,89,89	8

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

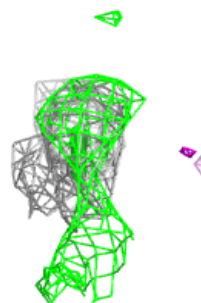
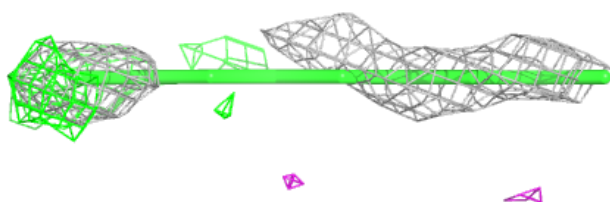
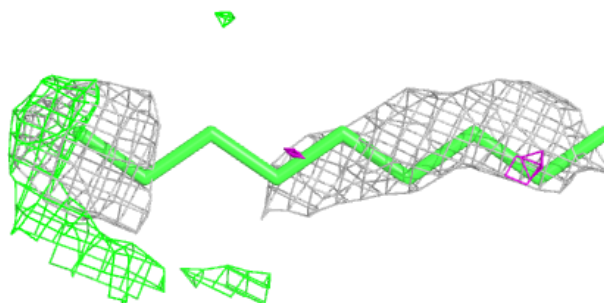
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	508	9/51	0.69	0.43	104,106,107,107	0
6	PGW	B	504	22/51	0.70	0.39	76,86,90,91	0
6	PGW	B	516	37/51	0.72	0.31	108,129,144,145	0
6	PGW	Q	504	22/51	0.72	0.35	100,113,118,119	0
6	PGW	B	506	9/51	0.73	0.37	95,96,96,97	0
6	PGW	B	514	23/51	0.73	0.34	136,139,148,149	0
6	PGW	B	515	12/51	0.76	0.42	84,90,94,94	0
6	PGW	B	512	9/51	0.77	0.32	91,91,92,93	0
6	PGW	B	519	12/51	0.77	0.38	102,104,105,105	0
6	PGW	B	513	12/51	0.77	0.37	74,80,83,84	0
6	PGW	B	517	10/51	0.79	0.32	77,78,80,81	0
6	PGW	B	518	12/51	0.80	0.40	113,116,117,117	0
6	PGW	B	507	9/51	0.81	0.36	100,101,102,103	0
6	PGW	B	511	7/51	0.85	0.31	86,87,87,87	0
6	PGW	B	505	9/51	0.85	0.34	98,99,102,102	0
6	PGW	B	510	9/51	0.86	0.30	90,93,97,98	0
6	PGW	B	509	9/51	0.87	0.30	80,81,81,82	0
5	K	Q	503	1/1	0.90	0.14	38,38,38,38	1
5	K	Q	501	1/1	0.90	0.09	50,50,50,50	1
5	K	Q	502	1/1	0.94	0.13	62,62,62,62	1
5	K	B	503	1/1	0.96	0.12	27,27,27,27	1
5	K	B	501	1/1	0.97	0.18	23,23,23,23	1
4	NAP	P	1001	48/48	0.98	0.07	35,41,50,51	0
4	NAP	A	1001	48/48	0.98	0.06	34,39,45,47	0
5	K	B	502	1/1	0.98	0.09	27,27,27,27	1

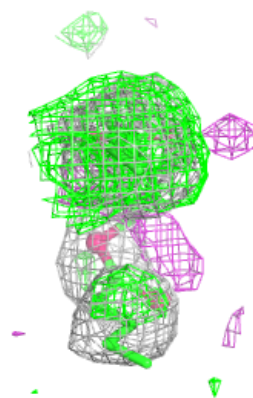
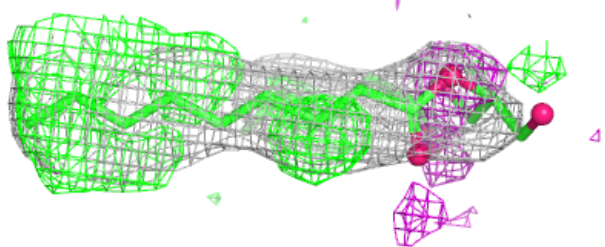
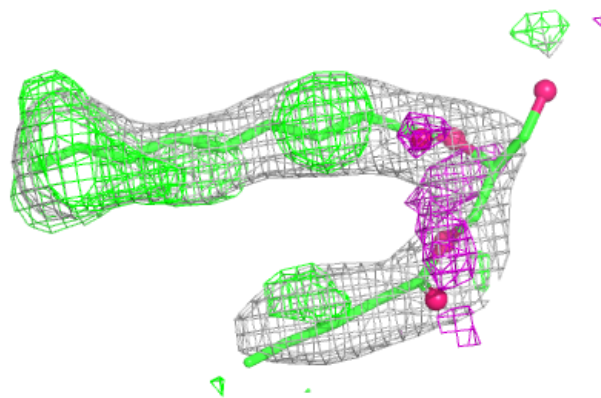
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGW B 508:

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

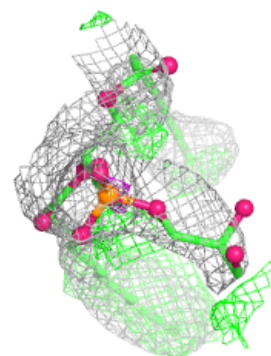
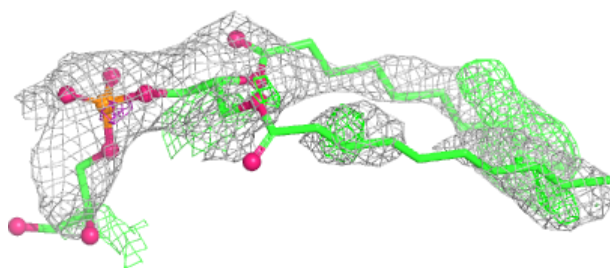
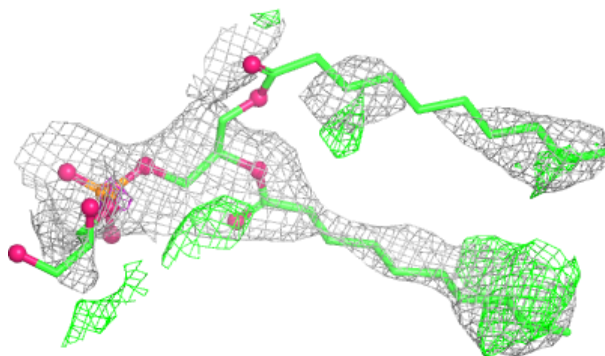
**Electron density around PGW B 504:**

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

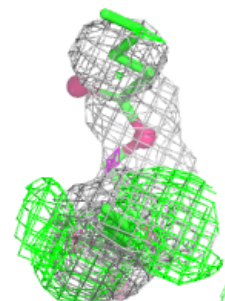
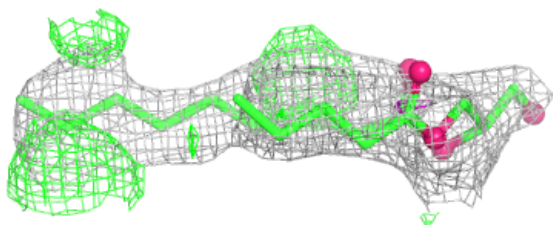
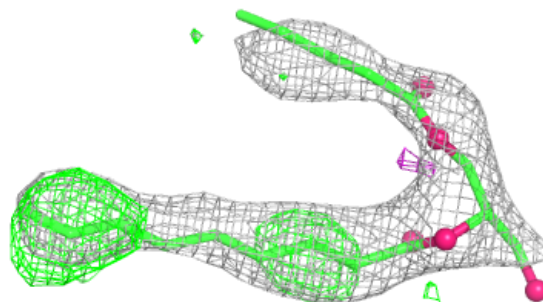


Electron density around PGW B 516:

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

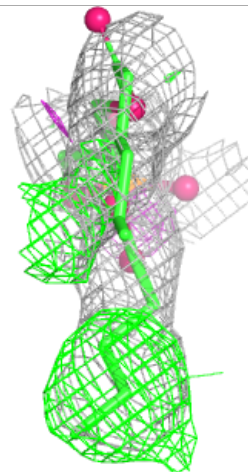
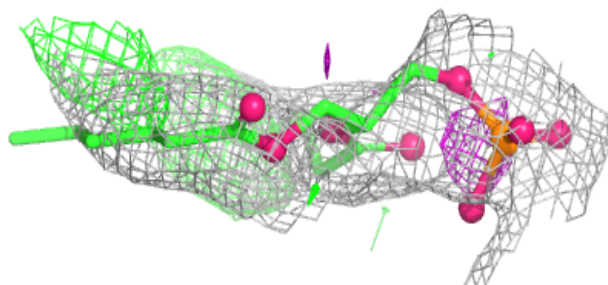
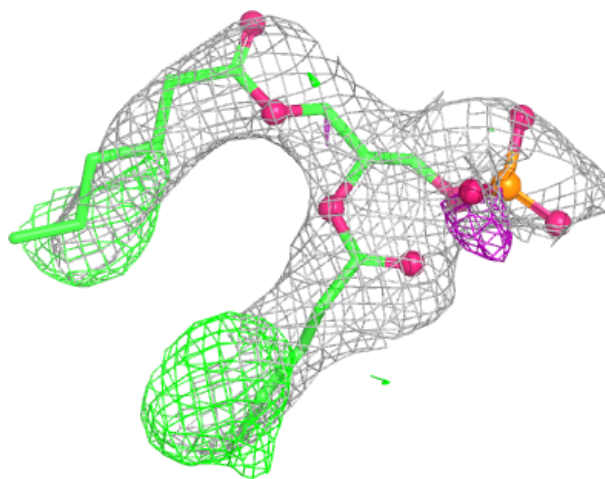
**Electron density around PGW Q 504:**

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



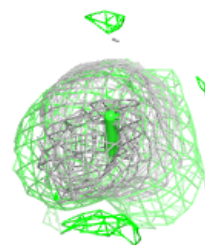
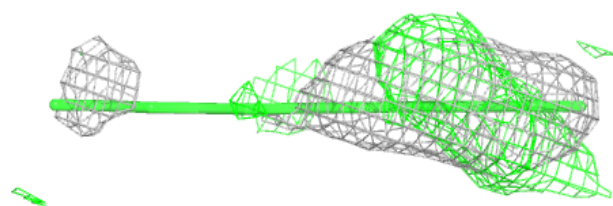
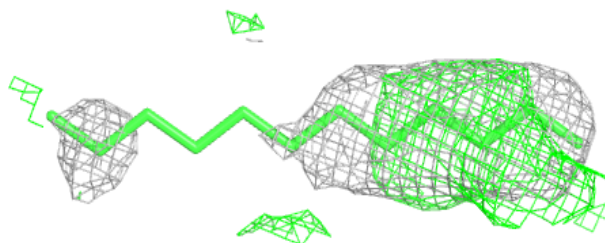
Electron density around PGW B 514:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

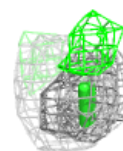
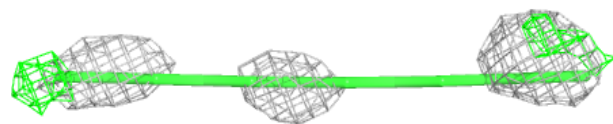
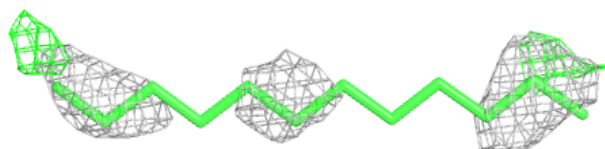


Electron density around PGW B 515:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

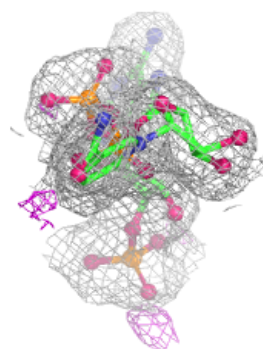
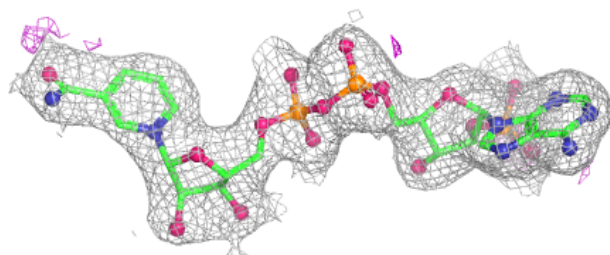
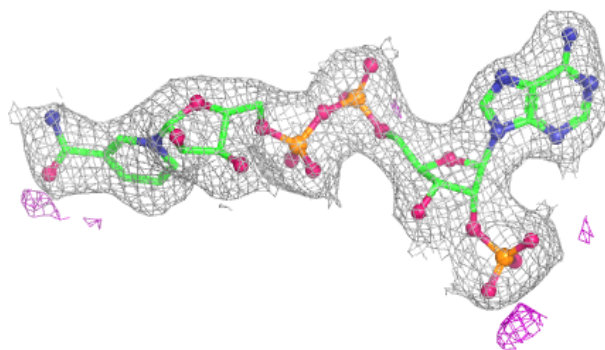
**Electron density around PGW B 518:**

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and green (positive)

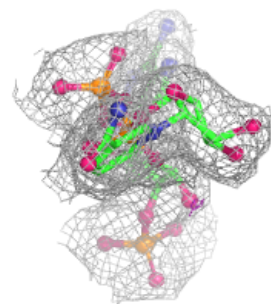
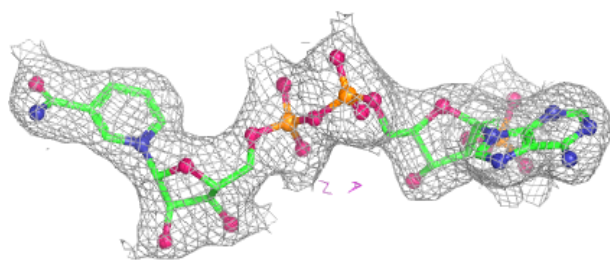
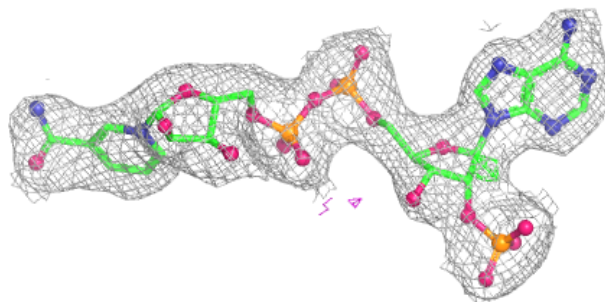


Electron density around NAP P 1001:

$2mF_o-DF_c$ (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.