Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 12:04 AM EDT

PDB ID	:	5WIE
Title	:	Crystal structure of a Kv1.2-2.1 chimera K+ channel V406W mutant in an inactivated state
Authors	:	Pau, V.; Zhou, Y.; Ramu, Y.; Xu, Y.; Lu, Z.
Deposited on	:	2017-07-19
Resolution	:	3.30 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:

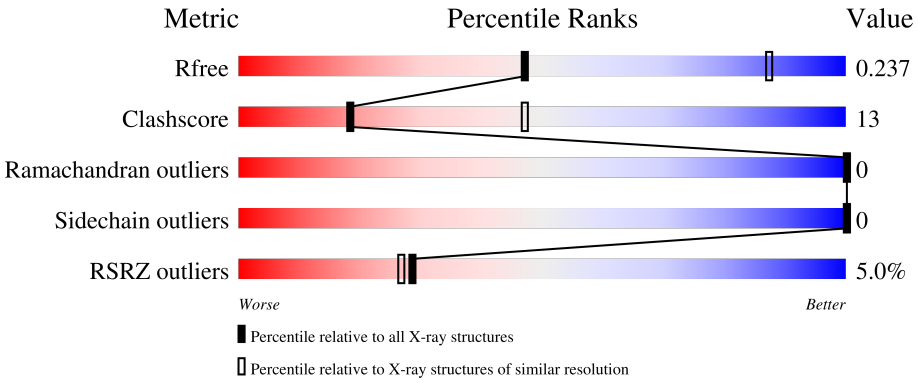
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	82% 16%
1	G	333	77% 20%
2	B	532	4% 48% 25% 27%
2	H	532	8% 37% 24% 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
4	PGW	B	502	-	-	-	X
4	PGW	B	503	-	-	-	X
4	PGW	B	505	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10955 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
			2505	1599	436	454	16			
1	G	326	Total	C	N	O	S	0	0	0
			2515	1603	436	460	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	initiating methionine	UNP P62483
G	35	MET	-	initiating methionine	UNP P62483

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	390	Total	C	N	O	S	0	0	0
			3099	2037	500	548	14			
2	H	328	Total	C	N	O	S	0	0	0
			2652	1757	426	457	12			

There are 148 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-36	MET	-	initiating methionine	UNP P63142
B	-35	SER	-	expression tag	UNP P63142
B	-34	ALA	-	expression tag	UNP P63142
B	-33	TRP	-	expression tag	UNP P63142
B	-32	SER	-	expression tag	UNP P63142
B	-31	HIS	-	expression tag	UNP P63142
B	-30	PRO	-	expression tag	UNP P63142
B	-29	GLN	-	expression tag	UNP P63142
B	-28	PHE	-	expression tag	UNP P63142

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	GLU	-	expression tag	UNP P63142
B	-26	LYS	-	expression tag	UNP P63142
B	-25	GLY	-	expression tag	UNP P63142
B	-24	GLY	-	expression tag	UNP P63142
B	-23	GLY	-	expression tag	UNP P63142
B	-22	SER	-	expression tag	UNP P63142
B	-21	GLY	-	expression tag	UNP P63142
B	-20	GLY	-	expression tag	UNP P63142
B	-19	GLY	-	expression tag	UNP P63142
B	-18	SER	-	expression tag	UNP P63142
B	-17	GLY	-	expression tag	UNP P63142
B	-16	GLY	-	expression tag	UNP P63142
B	-15	SER	-	expression tag	UNP P63142
B	-14	ALA	-	expression tag	UNP P63142
B	-13	TRP	-	expression tag	UNP P63142
B	-12	SER	-	expression tag	UNP P63142
B	-11	HIS	-	expression tag	UNP P63142
B	-10	PRO	-	expression tag	UNP P63142
B	-9	GLN	-	expression tag	UNP P63142
B	-8	PHE	-	expression tag	UNP P63142
B	-7	GLU	-	expression tag	UNP P63142
B	-6	LYS	-	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	15	HIS	LEU	linker	UNP P63142
B	31	SER	CYS	linker	UNP P63142
B	32	SER	CYS	linker	UNP P63142
B	207	GLN	ASN	linker	UNP P63142
B	266	TYR	-	linker	UNP P63142
B	267	TYR	-	linker	UNP P63142
B	268	VAL	-	linker	UNP P63142
B	269	THR	-	linker	UNP P63142
B	270	ILE	-	linker	UNP P63142
B	271	PHE	-	linker	UNP P63142
B	272	LEU	-	linker	UNP P63142
B	273	THR	-	linker	UNP P63142
B	274	GLU	-	linker	UNP P63142
B	275	SER	-	linker	UNP P63142

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Chain	Residue	Modelled	Actual	Comment	Reference
B	276	ASN	ASP	conflict	UNP P63141
B	277	LYS	ALA	conflict	UNP P63141
B	278	SER	GLN	conflict	UNP P63141
B	279	VAL	GLN	conflict	UNP P63141
B	280	LEU	GLY	conflict	UNP P63141
B	282	PHE	GLN	conflict	UNP P63141
B	283	GLN	ALA	conflict	UNP P63141
B	284	ASN	MET	conflict	UNP P63141
B	285	VAL	SER	conflict	UNP P63141
B	286	ARG	LEU	conflict	UNP P63141
B	287	ARG	ALA	conflict	UNP P63141
B	288	VAL	ILE	conflict	UNP P63141
B	289	VAL	LEU	conflict	UNP P63141
B	290	GLN	ARG	conflict	UNP P63141
B	291	ILE	VAL	conflict	UNP P63141
B	292	PHE	ILE	conflict	UNP P63141
B	294	ILE	LEU	conflict	UNP P63141
B	295	MET	VAL	conflict	UNP P63141
B	297	ILE	VAL	conflict	UNP P63141
B	298	LEU	PHE	conflict	UNP P63141
B	406	TRP	VAL	engineered mutation	UNP P63141
B	431	SER	CYS	conflict	UNP P63141
B	478	SER	CYS	conflict	UNP P63141
H	-36	MET	-	initiating methionine	UNP P63142
H	-35	SER	-	expression tag	UNP P63142
H	-34	ALA	-	expression tag	UNP P63142
H	-33	TRP	-	expression tag	UNP P63142
H	-32	SER	-	expression tag	UNP P63142
H	-31	HIS	-	expression tag	UNP P63142
H	-30	PRO	-	expression tag	UNP P63142
H	-29	GLN	-	expression tag	UNP P63142
H	-28	PHE	-	expression tag	UNP P63142
H	-27	GLU	-	expression tag	UNP P63142
H	-26	LYS	-	expression tag	UNP P63142
H	-25	GLY	-	expression tag	UNP P63142
H	-24	GLY	-	expression tag	UNP P63142
H	-23	GLY	-	expression tag	UNP P63142
H	-22	SER	-	expression tag	UNP P63142
H	-21	GLY	-	expression tag	UNP P63142
H	-20	GLY	-	expression tag	UNP P63142
H	-19	GLY	-	expression tag	UNP P63142
H	-18	SER	-	expression tag	UNP P63142

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-17	GLY	-	expression tag	UNP P63142
H	-16	GLY	-	expression tag	UNP P63142
H	-15	SER	-	expression tag	UNP P63142
H	-14	ALA	-	expression tag	UNP P63142
H	-13	TRP	-	expression tag	UNP P63142
H	-12	SER	-	expression tag	UNP P63142
H	-11	HIS	-	expression tag	UNP P63142
H	-10	PRO	-	expression tag	UNP P63142
H	-9	GLN	-	expression tag	UNP P63142
H	-8	PHE	-	expression tag	UNP P63142
H	-7	GLU	-	expression tag	UNP P63142
H	-6	LYS	-	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	15	HIS	LEU	linker	UNP P63142
H	31	SER	CYS	linker	UNP P63142
H	32	SER	CYS	linker	UNP P63142
H	207	GLN	ASN	linker	UNP P63142
H	266	TYR	-	linker	UNP P63142
H	267	TYR	-	linker	UNP P63142
H	268	VAL	-	linker	UNP P63142
H	269	THR	-	linker	UNP P63142
H	270	ILE	-	linker	UNP P63142
H	271	PHE	-	linker	UNP P63142
H	272	LEU	-	linker	UNP P63142
H	273	THR	-	linker	UNP P63142
H	274	GLU	-	linker	UNP P63142
H	275	SER	-	linker	UNP P63142
H	276	ASN	ASP	conflict	UNP P63141
H	277	LYS	ALA	conflict	UNP P63141
H	278	SER	GLN	conflict	UNP P63141
H	279	VAL	GLN	conflict	UNP P63141
H	280	LEU	GLY	conflict	UNP P63141
H	282	PHE	GLN	conflict	UNP P63141
H	283	GLN	ALA	conflict	UNP P63141
H	284	ASN	MET	conflict	UNP P63141
H	285	VAL	SER	conflict	UNP P63141
H	286	ARG	LEU	conflict	UNP P63141

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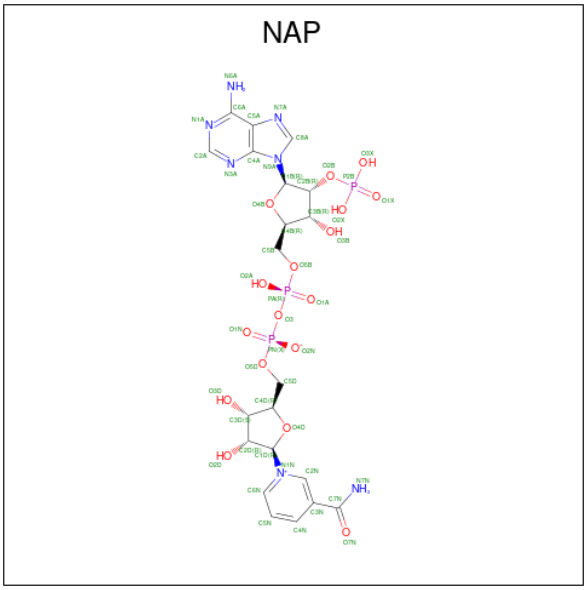
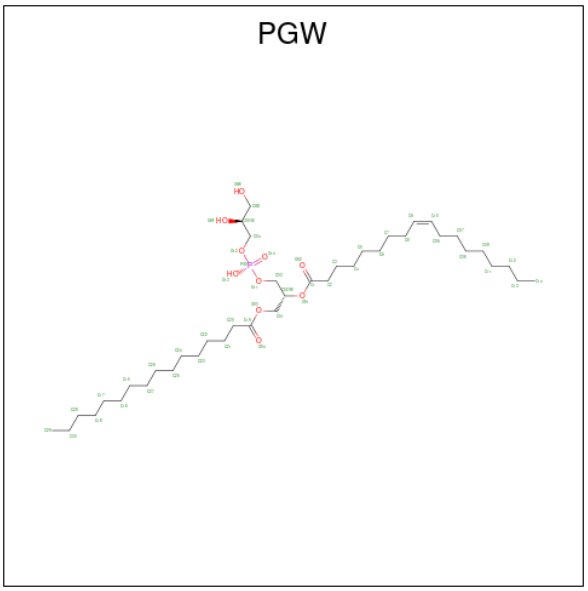
Chain	Residue	Modelled	Actual	Comment	Reference
H	287	ARG	ALA	conflict	UNP P63141
H	288	VAL	ILE	conflict	UNP P63141
H	289	VAL	LEU	conflict	UNP P63141
H	290	GLN	ARG	conflict	UNP P63141
H	291	ILE	VAL	conflict	UNP P63141
H	292	PHE	ILE	conflict	UNP P63141
H	294	ILE	LEU	conflict	UNP P63141
H	295	MET	VAL	conflict	UNP P63141
H	297	ILE	VAL	conflict	UNP P63141
H	298	LEU	PHE	conflict	UNP P63141
H	406	TRP	VAL	engineered mutation	UNP P63141
H	431	SER	CYS	conflict	UNP P63141
H	478	SER	CYS	conflict	UNP P63141

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 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
4	B	1	Total C O 22 17 5	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 9 9	0	0
4	B	1	Total C 9 9	0	0
4	H	1	Total C O 22 17 5	0	0

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

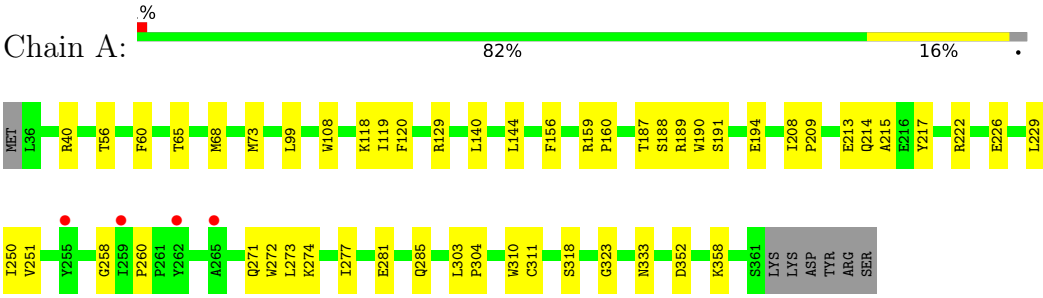
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total K 4 4	0	0
5	H	4	Total K 4 4	0	0

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.

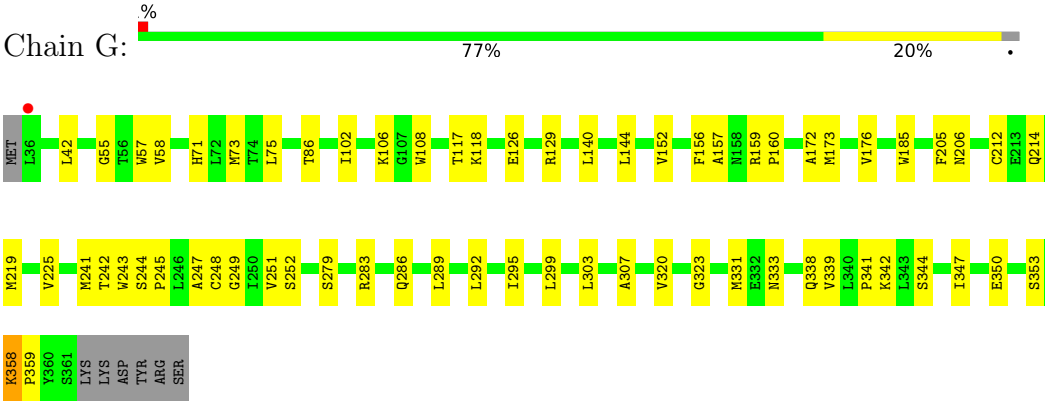
• Molecule 1: Voltage-gated potassium channel subunit beta-2

Chain A:



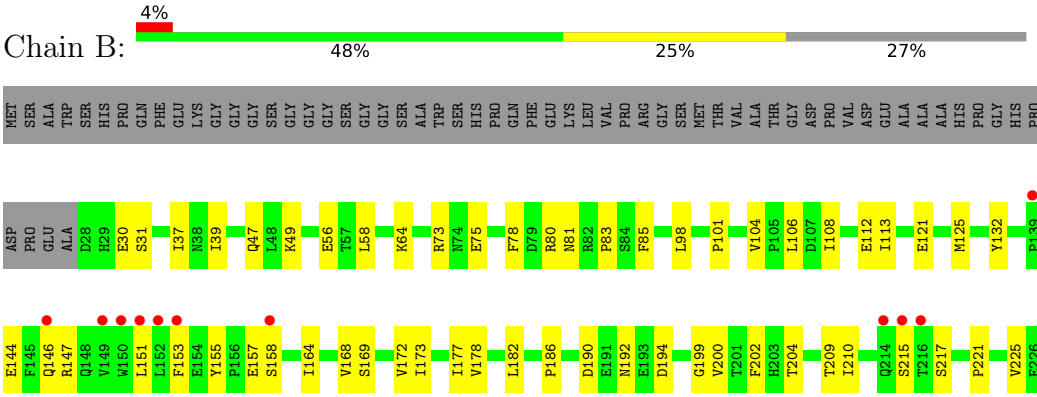
• Molecule 1: Voltage-gated potassium channel subunit beta-2

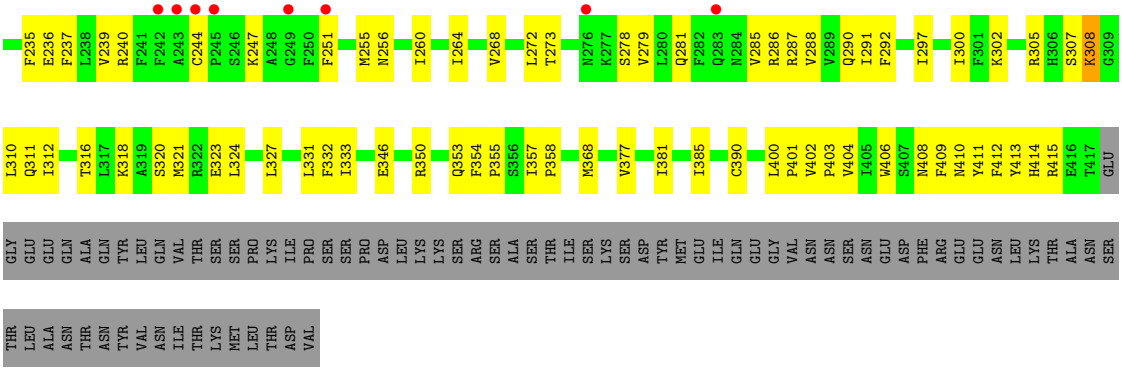
Chain G:



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

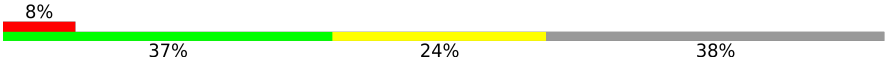
Chain B:

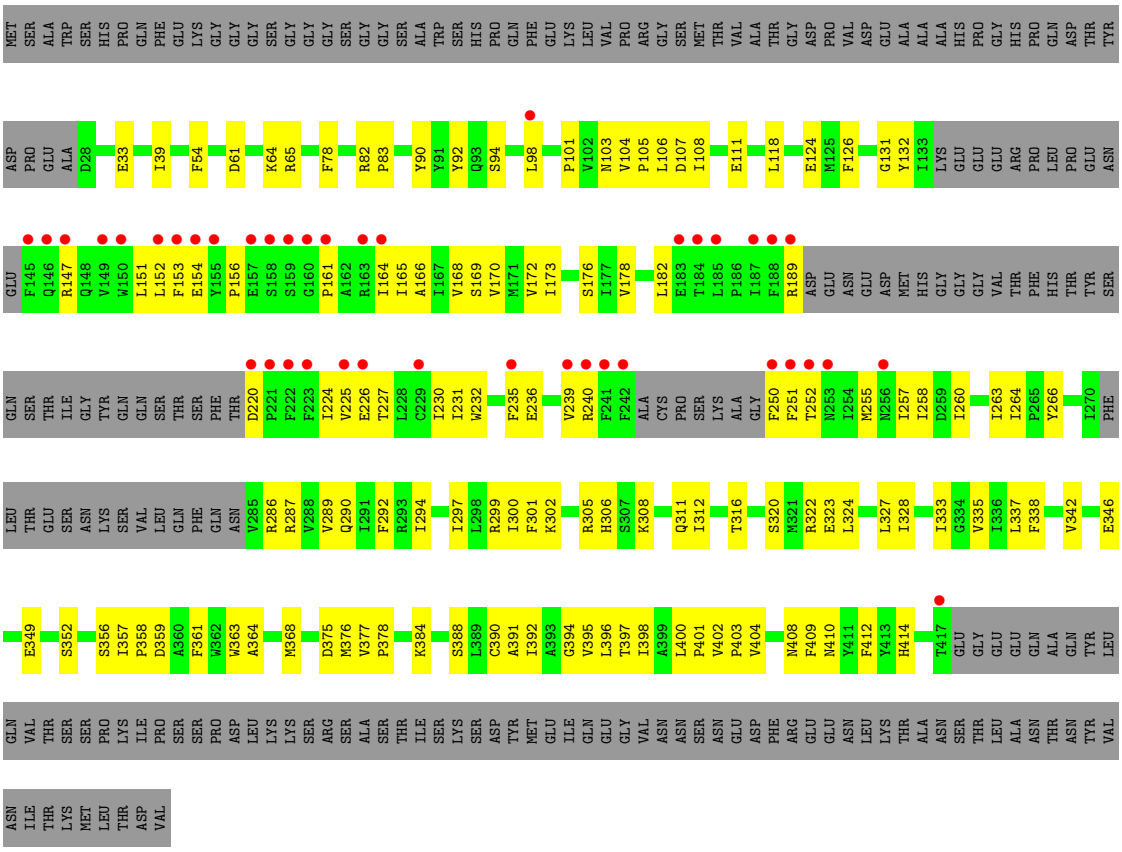




• Molecule 2: Potassium voltage-gated channel subfamily A member 2,Potassium voltage-gated channel subfamily A member 2

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.12Å 143.12Å 284.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 49.82 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.00-3.30) 99.5 (49.82-3.29)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.243 0.227 , 0.237	Depositor DCC
R_{free} test set	2285 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10955	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: NAP, PGW, 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	0.86	0/2556	0.75	0/3458
1	G	0.89	0/2566	0.76	3/3473 (0.1%)
2	B	0.82	1/3183 (0.0%)	0.75	0/4326
2	H	0.72	0/2721	0.70	0/3687
All	All	0.83	1/11026 (0.0%)	0.74	3/14944 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	LYS	C-N	7.54	1.46	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	358	LYS	C-N-CD	5.50	139.95	128.40
1	G	303	LEU	C-N-CD	5.16	139.23	128.40
1	G	157	ALA	N-CA-C	-5.08	97.28	111.00

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	2505	0	2510	38	0
1	G	2515	0	2517	50	0
2	B	3099	0	3017	98	0
2	H	2652	0	2618	101	0
3	A	48	0	25	3	0
3	G	48	0	25	5	0
4	B	58	0	81	1	0
4	H	22	0	25	4	0
5	B	4	0	0	0	0
5	H	4	0	0	0	0
All	All	10955	0	10818	289	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 13.

All (289) 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:H:400:LEU:HB2	2:H:401:PRO:HD3	1.39	1.04
2:B:323:GLU:HG2	2:B:404:VAL:HG21	1.44	0.98
1:G:333:ASN:HD21	3:G:1001:NAP:H61A	1.34	0.76
1:A:118:LYS:HG2	1:A:156:PHE:HB2	1.71	0.71
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.73	0.71
2:B:186:PRO:O	2:B:190:ASP:HB2	1.92	0.69
2:B:327:LEU:HD22	2:B:401:PRO:HG3	1.75	0.69
2:B:381:ILE:O	2:B:385:ILE:HG12	1.93	0.69
2:H:305:ARG:HB3	2:H:306:HIS:HD2	1.58	0.68
2:B:400:LEU:O	2:B:403:PRO:HD2	1.94	0.67
2:H:346:GLU:OE1	2:H:378:PRO:HA	1.95	0.66
2:H:327:LEU:HB2	2:H:401:PRO:HG2	1.76	0.66
2:H:251:PHE:O	2:H:257:ILE:HD11	1.95	0.66
2:B:141:PRO:O	2:B:142:GLU:HB2	1.95	0.66
1:G:295:ILE:H	1:G:295:ILE:HD12	1.61	0.65
2:B:192:ASN:HD22	2:B:204:THR:CG2	2.09	0.65
1:G:338:GLN:O	1:G:341:PRO:HD2	1.97	0.64
2:H:305:ARG:HB3	2:H:306:HIS:CD2	2.32	0.64
2:B:192:ASN:HD22	2:B:204:THR:HG23	1.63	0.64
1:A:40:ARG:HD2	1:A:318:SER:O	1.98	0.64
1:G:247:ALA:O	1:G:248:CYS:HB2	1.97	0.64
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.28	0.63
2:B:39:ILE:HD11	2:B:85:PHE:CE1	2.32	0.63
2:H:169:SER:O	2:H:173:ILE:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:402:VAL:HB	2:H:403:PRO:HD3	1.80	0.63
2:H:106:LEU:O	2:H:106:LEU:HD12	1.98	0.63
2:H:323:GLU:HG2	2:H:404:VAL:HG21	1.80	0.62
1:A:73:MET:HE2	1:A:108:TRP:HZ3	1.62	0.62
2:H:322:ARG:HG3	2:H:322:ARG:HH11	1.64	0.62
1:A:250:ILE:HG12	1:A:277:ILE:HD13	1.82	0.61
2:B:98:LEU:HD21	2:B:113:ILE:HD13	1.80	0.61
2:B:353:GLN:O	2:B:355:PRO:HD3	2.00	0.61
1:A:333:ASN:HD21	3:A:1001:NAP:H61A	1.48	0.61
2:B:412:PHE:HD1	2:B:415:ARG:HH21	1.48	0.61
2:H:400:LEU:HB2	2:H:401:PRO:CD	2.23	0.60
2:B:202:PHE:HB2	2:B:279:VAL:HG22	1.83	0.60
1:A:222:ARG:O	1:A:226:GLU:HG3	2.01	0.60
1:A:188:SER:O	1:A:189:ARG:HB2	2.00	0.60
1:G:279:SER:O	1:G:283:ARG:HG2	2.03	0.59
1:A:65:THR:O	1:A:68:MET:N	2.36	0.58
2:H:236:GLU:HB3	2:H:240:ARG:NH1	2.18	0.58
2:H:305:ARG:CB	2:H:306:HIS:HD2	2.16	0.58
2:B:408:ASN:O	2:B:411:TYR:HB3	2.04	0.58
2:H:260:ILE:HG22	2:H:264:ILE:HD11	1.84	0.58
2:H:342:VAL:HG11	2:H:363:TRP:CZ3	2.39	0.58
2:H:124:GLU:HA	2:H:124:GLU:OE1	2.04	0.57
2:H:161:PRO:HA	2:H:164:ILE:HD12	1.85	0.57
1:G:172:ALA:O	1:G:176:VAL:HG13	2.04	0.57
1:G:214:GLN:HA	1:G:241:MET:O	2.04	0.57
2:B:400:LEU:HB2	2:B:401:PRO:CD	2.34	0.57
2:H:166:ALA:O	2:H:170:VAL:HG23	2.04	0.57
1:G:244:SER:N	1:G:245:PRO:HD3	2.20	0.57
1:G:342:LYS:O	1:G:347:ILE:HD12	2.05	0.57
1:G:245:PRO:HG3	1:G:320:VAL:HG13	1.87	0.56
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.85	0.56
2:B:244:CYS:SG	2:B:247:LYS:HD3	2.45	0.56
2:B:307:SER:O	2:B:311:GLN:NE2	2.38	0.56
2:B:307:SER:HB3	2:B:310:LEU:HB2	1.86	0.56
2:H:236:GLU:HB3	2:H:240:ARG:HH12	1.70	0.56
2:B:227:THR:O	2:B:231:ILE:HG12	2.05	0.56
2:B:39:ILE:HD11	2:B:85:PHE:CZ	2.41	0.56
2:B:155:TYR:N	2:B:155:TYR:CD1	2.73	0.56
2:H:306:HIS:CD2	2:H:306:HIS:N	2.72	0.56
2:H:260:ILE:HG22	2:H:264:ILE:CD1	2.36	0.56
2:B:209:THR:HG21	2:B:286:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLN:OE1	3:A:1001:NAP:N7N	2.36	0.55
2:B:278:SER:HB3	2:B:281:GLN:HG3	1.86	0.55
2:B:141:PRO:HB3	2:B:146:GLN:HB2	1.88	0.55
2:B:200:VAL:HG23	2:B:200:VAL:O	2.07	0.55
2:H:358:PRO:HA	2:H:361:PHE:CE2	2.42	0.55
1:G:339:VAL:HG12	1:G:339:VAL:O	2.06	0.55
1:G:159:ARG:HB2	1:G:160:PRO:HD2	1.89	0.54
2:B:286:ARG:O	2:B:290:GLN:HG3	2.08	0.54
2:B:308:LYS:O	2:B:312:ILE:HG13	2.07	0.54
2:H:384:LYS:O	2:H:388:SER:HB2	2.06	0.54
2:H:358:PRO:HA	2:H:361:PHE:CD2	2.43	0.54
2:H:153:PHE:CE2	2:H:239:VAL:HG11	2.42	0.54
2:B:177:ILE:HD13	2:B:300:ILE:HD12	1.89	0.54
2:B:221:PRO:O	2:B:225:VAL:HG23	2.08	0.54
2:H:255:MET:HB3	2:H:305:ARG:NH2	2.23	0.54
1:A:258:GLY:O	1:A:260:PRO:HD3	2.08	0.53
1:G:299:LEU:HD11	1:G:347:ILE:HD13	1.91	0.53
1:G:140:LEU:O	1:G:144:LEU:HG	2.08	0.53
2:H:391:ALA:O	2:H:395:VAL:HG23	2.09	0.53
2:H:394:GLY:O	2:H:398:ILE:HG13	2.08	0.53
1:G:245:PRO:HG3	1:G:320:VAL:CG1	2.39	0.53
2:H:82:ARG:HB2	2:H:83:PRO:HD3	1.90	0.53
2:B:215:SER:HB2	2:B:217:SER:OG	2.10	0.52
1:G:299:LEU:N	1:G:299:LEU:HD23	2.24	0.52
1:G:214:GLN:OE1	3:G:1001:NAP:N7N	2.38	0.52
2:H:235:PHE:O	2:H:239:VAL:HG23	2.09	0.52
2:H:316:THR:HG21	2:H:409:PHE:HB2	1.90	0.52
4:B:501:PGW:O02	4:B:501:PGW:H03A	2.08	0.52
1:G:342:LYS:O	1:G:347:ILE:CD1	2.58	0.52
2:B:47:GLN:NE2	2:B:49:LYS:HE2	2.25	0.52
2:B:141:PRO:HG2	2:B:147:ARG:HA	1.90	0.52
2:H:338:PHE:CZ	2:H:390:CYS:HA	2.45	0.52
2:B:251:PHE:HE1	2:B:260:ILE:HD11	1.75	0.52
2:B:151:LEU:HB3	2:B:158:SER:OG	2.10	0.52
1:A:187:THR:O	1:A:213:GLU:HA	2.10	0.51
2:B:232:TRP:O	2:B:235:PHE:HB3	2.10	0.51
2:B:144:GLU:HA	2:B:144:GLU:OE1	2.09	0.51
2:B:316:THR:OG1	2:B:409:PHE:HA	2.10	0.51
1:A:217:TYR:HE2	1:A:311:CYS:HA	1.75	0.51
2:B:251:PHE:CE1	2:B:260:ILE:HD11	2.46	0.51
1:G:118:LYS:HG2	1:G:156:PHE:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:SER:O	2:B:49:LYS:HB3	2.11	0.51
2:B:312:ILE:HD13	2:B:413:TYR:HA	1.93	0.51
2:H:90:TYR:CE2	2:H:94:SER:HB3	2.46	0.51
2:H:39:ILE:HD13	2:H:78:PHE:HB2	1.93	0.50
2:B:346:GLU:HG3	2:B:354:PHE:CE2	2.46	0.50
2:H:227:THR:O	2:H:231:ILE:HG12	2.12	0.50
2:B:235:PHE:O	2:B:239:VAL:HG23	2.12	0.50
1:A:73:MET:HE2	1:A:108:TRP:CZ3	2.44	0.50
1:A:273:LEU:O	1:A:277:ILE:HG12	2.10	0.50
2:H:131:GLY:C	2:H:132:TYR:CD1	2.85	0.50
1:A:251:VAL:O	1:A:251:VAL:HG12	2.12	0.50
2:B:81:ASN:ND2	2:B:83:PRO:HD2	2.27	0.50
2:B:39:ILE:HG13	2:B:85:PHE:CG	2.47	0.50
2:H:289:VAL:O	2:H:290:GLN:C	2.50	0.50
2:H:408:ASN:O	2:H:412:PHE:HD2	1.94	0.50
2:B:237:PHE:CE1	2:B:260:ILE:HG12	2.47	0.49
1:G:244:SER:N	1:G:245:PRO:CD	2.75	0.49
2:H:305:ARG:CB	2:H:306:HIS:CD2	2.94	0.49
2:H:61:ASP:O	2:H:65:ARG:HG2	2.12	0.49
2:H:289:VAL:O	2:H:292:PHE:N	2.46	0.49
2:H:287:ARG:O	2:H:290:GLN:N	2.46	0.49
2:H:305:ARG:C	2:H:306:HIS:CD2	2.85	0.49
2:H:266:TYR:CD1	2:H:266:TYR:C	2.85	0.49
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.95	0.49
2:B:168:VAL:O	2:B:172:VAL:HG23	2.13	0.49
2:H:101:PRO:HB2	2:H:104:VAL:HG23	1.95	0.49
2:H:376:MET:O	2:H:377:VAL:HG12	2.13	0.49
1:A:118:LYS:HG2	1:A:156:PHE:CB	2.42	0.48
2:H:392:ILE:O	2:H:396:LEU:HG	2.13	0.48
2:H:320:SER:O	2:H:324:LEU:HG	2.14	0.48
2:B:236:GLU:OE1	2:B:302:LYS:NZ	2.47	0.48
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.49	0.48
1:G:217:TYR:HB3	1:G:242:THR:HB	1.94	0.48
2:H:226:GLU:O	2:H:230:ILE:HD13	2.14	0.48
2:B:320:SER:O	2:B:321:MET:C	2.52	0.48
2:H:98:LEU:HD23	2:H:126:PHE:HB2	1.96	0.48
4:H:501:PGW:H01	4:H:501:PGW:O02	2.13	0.48
2:B:288:VAL:O	2:B:292:PHE:HD1	1.96	0.47
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.95	0.47
1:G:323:GLY:HA3	3:G:1001:NAP:H51A	1.95	0.47
1:G:42:LEU:HD11	1:G:212:CYS:SG	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:333:ILE:O	2:H:337:LEU:HB2	2.14	0.47
2:B:260:ILE:O	2:B:264:ILE:HG13	2.14	0.47
1:G:75:LEU:HB3	1:G:331:MET:HE3	1.97	0.47
1:G:102:ILE:O	1:G:106:LYS:HG2	2.13	0.47
2:H:54:PHE:HE2	2:H:92:TYR:HA	1.80	0.47
2:H:324:LEU:O	2:H:328:ILE:HG12	2.14	0.47
2:H:349:GLU:HB2	2:H:352:SER:HB2	1.95	0.47
2:H:394:GLY:HA2	2:H:397:THR:HG22	1.96	0.47
2:H:107:ASP:O	2:H:111:GLU:HG3	2.15	0.47
2:H:308:LYS:O	2:H:311:GLN:N	2.47	0.47
2:H:361:PHE:CB	4:H:501:PGW:H2	2.45	0.47
1:A:271:GLN:O	1:A:274:LYS:N	2.48	0.47
1:G:217:TYR:HB2	1:G:225:VAL:HG21	1.96	0.47
1:A:73:MET:SD	1:A:99:LEU:HD12	2.55	0.47
2:H:258:ILE:HD13	2:H:258:ILE:HA	1.68	0.46
2:H:305:ARG:C	2:H:306:HIS:HD2	2.18	0.46
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.97	0.46
2:B:121:GLU:O	2:B:125:MET:HG2	2.16	0.46
2:B:255:MET:CE	2:B:305:ARG:HA	2.45	0.46
2:H:154:GLU:C	2:H:156:PRO:HD3	2.35	0.46
1:A:118:LYS:HD3	1:A:214:GLN:OE1	2.15	0.46
2:H:168:VAL:HG11	2:H:232:TRP:CZ3	2.50	0.46
2:H:230:ILE:HG12	2:H:266:TYR:CD2	2.51	0.46
2:B:37:ILE:HG21	2:B:85:PHE:CZ	2.51	0.46
2:H:250:PHE:C	2:H:252:THR:H	2.19	0.46
2:B:108:ILE:O	2:B:112:GLU:HG2	2.16	0.46
2:B:307:SER:OG	2:B:310:LEU:HD23	2.16	0.46
1:A:191:SER:OG	1:A:194:GLU:HG3	2.16	0.46
1:A:217:TYR:HB3	1:A:242:THR:HB	1.97	0.46
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.31	0.46
1:G:71:HIS:O	1:G:75:LEU:HG	2.16	0.46
2:B:327:LEU:O	2:B:331:LEU:HB2	2.16	0.45
2:H:376:MET:C	2:H:377:VAL:CG1	2.85	0.45
1:A:272:TRP:CE3	1:A:273:LEU:N	2.84	0.45
2:B:30:GLU:HA	2:B:30:GLU:OE2	2.16	0.45
2:B:73:ARG:HB2	2:B:75:GLU:HG2	1.98	0.45
2:B:106:LEU:HD21	2:B:132:TYR:HE2	1.81	0.45
1:A:215:ALA:O	1:A:242:THR:HA	2.17	0.45
2:B:324:LEU:HD12	2:B:324:LEU:HA	1.85	0.45
2:H:33:GLU:O	2:H:33:GLU:HG3	2.15	0.45
2:B:308:LYS:O	2:B:311:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:GLU:OE1	1:G:129:ARG:NH2	2.50	0.45
2:H:152:LEU:O	2:H:165:ILE:HD12	2.17	0.45
2:H:356:SER:H	2:H:359:ASP:HB2	1.82	0.45
1:G:333:ASN:ND2	3:G:1001:NAP:H61A	2.08	0.45
1:G:251:VAL:HG12	1:G:251:VAL:O	2.17	0.45
1:G:295:ILE:HD12	1:G:295:ILE:N	2.28	0.45
2:H:105:PRO:HG2	2:H:108:ILE:HD12	1.98	0.45
2:H:312:ILE:HG23	2:H:412:PHE:CB	2.47	0.45
1:G:286:GLN:HA	1:G:289:LEU:HD12	1.99	0.44
2:H:286:ARG:O	2:H:289:VAL:HB	2.17	0.44
2:B:408:ASN:O	2:B:412:PHE:CD2	2.70	0.44
2:H:225:VAL:O	2:H:226:GLU:C	2.55	0.44
1:G:249:GLY:O	1:G:252:SER:HB3	2.17	0.44
2:H:312:ILE:HG23	2:H:412:PHE:HB3	2.00	0.44
2:H:322:ARG:HG3	2:H:322:ARG:NH1	2.32	0.44
2:B:256:ASN:O	2:B:260:ILE:HG13	2.17	0.44
2:H:178:VAL:O	2:H:182:LEU:HG	2.18	0.44
2:H:394:GLY:O	2:H:397:THR:HG22	2.18	0.43
2:B:415:ARG:HG2	2:B:415:ARG:O	2.17	0.43
1:G:358:LYS:HG3	1:G:359:PRO:CD	2.48	0.43
2:H:410:ASN:OD1	2:H:414:HIS:HD2	2.00	0.43
2:B:408:ASN:O	2:B:412:PHE:HD2	2.02	0.43
2:H:294:ILE:O	2:H:297:ILE:HG22	2.18	0.43
2:B:323:GLU:H	2:B:323:GLU:CD	2.21	0.43
2:H:168:VAL:HG11	2:H:232:TRP:CH2	2.53	0.43
2:H:189:ARG:HG3	2:H:189:ARG:HH11	1.83	0.43
1:G:350:GLU:O	1:G:353:SER:HB2	2.18	0.43
1:A:190:TRP:CD1	1:A:190:TRP:N	2.86	0.43
2:B:406:TRP:O	2:B:410:ASN:CB	2.67	0.43
2:B:353:GLN:NE2	2:B:377:VAL:O	2.52	0.43
2:B:236:GLU:HB3	2:B:240:ARG:NH1	2.34	0.43
2:B:318:LYS:O	2:B:321:MET:HG2	2.19	0.43
2:B:368:MET:HG3	2:B:390:CYS:SG	2.59	0.43
2:H:335:VAL:HG13	2:H:364:ALA:HB3	2.01	0.43
2:B:178:VAL:O	2:B:182:LEU:HG	2.18	0.42
2:H:251:PHE:CE1	2:H:260:ILE:HD11	2.53	0.42
2:B:346:GLU:HG3	2:B:354:PHE:HE2	1.84	0.42
2:H:154:GLU:O	2:H:156:PRO:HD3	2.18	0.42
2:H:375:ASP:N	2:H:375:ASP:OD1	2.49	0.42
1:A:250:ILE:HG12	1:A:277:ILE:CD1	2.48	0.42
1:G:86:THR:O	1:G:118:LYS:NZ	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:THR:HG22	1:G:152:VAL:HG11	2.02	0.42
2:H:103:ASN:OD1	2:H:103:ASN:N	2.53	0.42
1:G:219:MET:O	1:G:357:ASN:ND2	2.44	0.42
2:H:300:ILE:HG23	2:H:301:PHE:N	2.34	0.42
1:A:222:ARG:HG2	1:A:310:TRP:HH2	1.84	0.42
2:H:147:ARG:O	2:H:151:LEU:HG	2.20	0.42
2:H:176:SER:HB2	2:H:299:ARG:NH1	2.34	0.42
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.92	0.42
1:A:120:PHE:O	1:A:129:ARG:HA	2.19	0.42
1:A:217:TYR:CE2	1:A:311:CYS:HA	2.54	0.42
2:B:194:ASP:CB	2:B:199:GLY:O	2.68	0.42
1:G:118:LYS:HZ3	1:G:118:LYS:HG3	1.64	0.42
1:A:56:THR:HB	1:A:60:PHE:HB2	2.01	0.42
2:B:331:LEU:HA	2:B:331:LEU:HD12	1.85	0.42
1:G:205:PHE:O	1:G:206:ASN:HB3	2.19	0.42
2:H:118:LEU:HA	2:H:118:LEU:HD23	1.81	0.42
2:B:56:GLU:O	2:B:64:LYS:NZ	2.53	0.42
2:B:140:LEU:HA	2:B:141:PRO:HD3	1.86	0.42
2:B:78:PHE:HB3	2:B:80:ARG:HG3	2.02	0.42
2:H:173:ILE:HD13	2:H:302:LYS:HB3	2.02	0.42
1:G:173:MET:HG3	1:G:185:TRP:CE3	2.54	0.41
2:B:272:LEU:HD22	2:B:285:VAL:HG21	2.01	0.41
1:G:251:VAL:HG11	1:G:307:ALA:HB2	2.02	0.41
1:G:333:ASN:N	1:G:333:ASN:HD22	2.18	0.41
2:H:61:ASP:HB3	2:H:64:LYS:HG3	2.02	0.41
2:H:260:ILE:O	2:H:263:ILE:HG13	2.21	0.41
2:B:30:GLU:OE2	2:B:30:GLU:CA	2.68	0.41
2:B:210:ILE:HD11	2:B:273:THR:HG21	2.02	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.86	0.41
2:B:264:ILE:O	2:B:268:VAL:HG23	2.20	0.41
2:B:101:PRO:HB2	2:B:104:VAL:HG23	2.02	0.41
2:H:176:SER:HB2	2:H:299:ARG:HH11	1.86	0.41
2:H:260:ILE:CG2	2:H:264:ILE:HD11	2.50	0.41
1:A:352:ASP:OD2	1:A:358:LYS:HD2	2.21	0.41
2:B:157:GLU:OE1	2:B:157:GLU:HA	2.20	0.41
2:B:164:ILE:HD13	2:B:164:ILE:HA	1.95	0.41
1:G:292:LEU:HA	1:G:295:ILE:HD13	2.02	0.41
2:B:287:ARG:O	2:B:291:ILE:HG13	2.21	0.41
1:G:57:TRP:CG	1:G:58:VAL:HG23	2.56	0.41
2:H:335:VAL:CG2	2:H:368:MET:HE1	2.51	0.41
1:A:323:GLY:HA3	3:A:1001:NAP:H51A	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:VAL:HG11	1:G:307:ALA:CB	2.51	0.41
2:H:168:VAL:O	2:H:172:VAL:HG23	2.21	0.41
2:H:220:ASP:O	2:H:224:ILE:HG13	2.20	0.41
1:A:119:ILE:HD11	1:A:140:LEU:HA	2.04	0.40
2:B:297:ILE:HD12	2:B:297:ILE:HA	1.90	0.40
2:H:361:PHE:HB3	4:H:501:PGW:H2	2.03	0.40
2:B:58:LEU:HD23	2:B:58:LEU:C	2.41	0.40
2:B:413:TYR:CD1	2:B:413:TYR:C	2.94	0.40
1:G:216:GLU:HB2	1:G:243:TRP:CH2	2.55	0.40
2:H:361:PHE:HB2	4:H:501:PGW:H2	2.03	0.40
1:A:281:GLU:O	1:A:285:GLN:HG3	2.21	0.40
2:B:410:ASN:OD1	2:B:414:HIS:CD2	2.74	0.40
1:G:55:GLY:HA3	3:G:1001:NAP:O3D	2.20	0.40
1:G:344:SER:H	1:G:347:ILE:HD12	1.86	0.40
1:A:229:LEU:N	1:A:230:PRO:CD	2.84	0.40
2:B:157:GLU:OE1	2:B:157:GLU:CA	2.69	0.40
2:B:169:SER:O	2:B:173:ILE:HG13	2.21	0.40
2:B:332:PHE:HD2	2:B:333:ILE:HD13	1.86	0.40
1:G:73:MET:CE	1:G:108:TRP:HZ3	2.35	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%)	316 (98%)	8 (2%)	0	100	100
1	G	324/333 (97%)	315 (97%)	9 (3%)	0	100	100
2	B	388/532 (73%)	364 (94%)	24 (6%)	0	100	100
2	H	318/532 (60%)	308 (97%)	10 (3%)	0	100	100
All	All	1354/1730 (78%)	1303 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	259/280 (92%)	259 (100%)	0	100	100
1	G	263/280 (94%)	263 (100%)	0	100	100
2	B	327/469 (70%)	327 (100%)	0	100	100
2	H	282/469 (60%)	282 (100%)	0	100	100
All	All	1131/1498 (76%)	1131 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	286	GLN
1	A	333	ASN
2	B	47	GLN
2	B	103	ASN
2	B	192	ASN
2	B	414	HIS
1	G	148	GLN
1	G	163	ASN
1	G	293	GLN
1	G	333	ASN
2	H	306	HIS
2	H	414	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	NAP	G	1001	-	45,52,52	1.31	6 (13%)	56,80,80	1.19	3 (5%)
4	PGW	B	503	-	8,8,50	0.36	0	7,7,56	0.70	0
3	NAP	A	1001	-	45,52,52	1.30	8 (17%)	56,80,80	1.18	5 (8%)
4	PGW	B	502	-	8,8,50	0.36	0	7,7,56	0.67	0
4	PGW	B	505	-	8,8,50	0.36	0	7,7,56	0.68	0
4	PGW	B	501	-	21,21,50	1.27	2 (9%)	23,23,56	1.70	4 (17%)
4	PGW	B	504	-	8,8,50	0.35	0	7,7,56	0.80	0
4	PGW	H	501	-	21,21,50	0.60	0	23,23,56	1.08	1 (4%)

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	NAP	G	1001	-	-	2/31/67/67	0/5/5/5
4	PGW	B	503	-	-	0/6/6/55	-
3	NAP	A	1001	-	-	4/31/67/67	0/5/5/5
4	PGW	B	502	-	-	0/6/6/55	-
4	PGW	B	505	-	-	0/6/6/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGW	B	501	-	-	9/23/23/55	-
4	PGW	B	504	-	-	0/6/6/55	-
4	PGW	H	501	-	-	3/23/23/55	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAP	C6N-N1N	3.80	1.44	1.35
4	B	501	PGW	O03-C19	3.43	1.43	1.33
4	B	501	PGW	O01-C1	3.42	1.44	1.34
3	G	1001	NAP	C2A-N3A	3.37	1.37	1.32
3	G	1001	NAP	C6N-N1N	3.33	1.43	1.35
3	A	1001	NAP	C4N-C3N	2.77	1.44	1.39
3	G	1001	NAP	O4B-C1B	2.64	1.44	1.41
3	G	1001	NAP	C4A-N3A	2.53	1.39	1.35
3	A	1001	NAP	O4B-C4B	2.36	1.50	1.45
3	A	1001	NAP	O4B-C1B	2.35	1.44	1.41
3	A	1001	NAP	C4A-N3A	2.34	1.38	1.35
3	G	1001	NAP	C4N-C3N	2.28	1.43	1.39
3	A	1001	NAP	O3D-C3D	-2.25	1.37	1.43
3	G	1001	NAP	O4B-C4B	2.18	1.49	1.45
3	A	1001	NAP	C2A-N3A	2.11	1.35	1.32
3	A	1001	NAP	PA-O2A	-2.10	1.45	1.55

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	PGW	O01-C1-C2	5.08	122.46	111.50
3	G	1001	NAP	C6N-N1N-C2N	-3.34	118.93	121.97
4	B	501	PGW	O03-C19-C20	3.16	121.82	111.91
4	H	501	PGW	O01-C1-C2	2.91	117.77	111.50
3	A	1001	NAP	C2A-N1A-C6A	2.83	123.60	118.75
3	G	1001	NAP	PN-O3-PA	2.72	142.17	132.83
3	A	1001	NAP	PN-O3-PA	2.63	141.86	132.83
3	A	1001	NAP	C6N-N1N-C2N	-2.56	119.64	121.97
4	B	501	PGW	C01-C02-C03	-2.53	105.89	111.80
4	B	501	PGW	O03-C19-O04	-2.25	117.92	123.59
3	G	1001	NAP	C2A-N1A-C6A	2.20	122.52	118.75
3	A	1001	NAP	N3A-C2A-N1A	-2.09	125.41	128.68
3	A	1001	NAP	O7N-C7N-N7N	2.07	125.52	122.58

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	NAP	PN-O3-PA-O5B
3	A	1001	NAP	O4D-C1D-N1N-C6N
4	B	501	PGW	C01-C02-C03-O11
4	B	501	PGW	O01-C02-C03-O11
4	B	501	PGW	C20-C19-O03-C01
4	B	501	PGW	O04-C19-O03-C01
4	B	501	PGW	C4-C5-C6-C7
4	H	501	PGW	C20-C19-O03-C01
4	H	501	PGW	O04-C19-O03-C01
3	G	1001	NAP	PN-O3-PA-O5B
3	A	1001	NAP	C2B-O2B-P2B-O1X
3	G	1001	NAP	C2B-O2B-P2B-O1X
4	B	501	PGW	C03-C02-O01-C1
4	H	501	PGW	C01-C02-O01-C1
4	B	501	PGW	C20-C21-C22-C23
4	B	501	PGW	O01-C1-C2-C3
3	A	1001	NAP	C2B-O2B-P2B-O2X
4	B	501	PGW	O02-C1-C2-C3

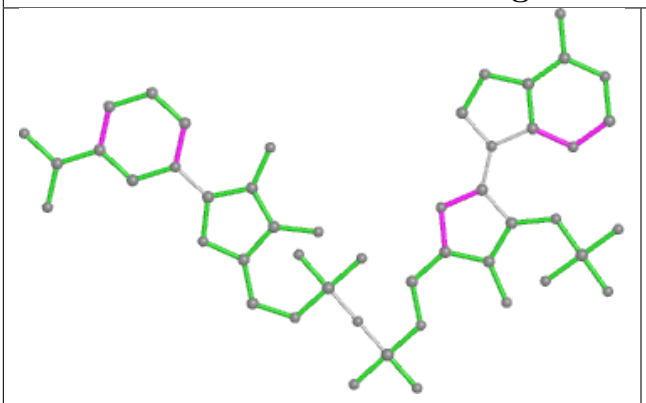
There are no ring outliers.

4 monomers are involved in 13 short contacts:

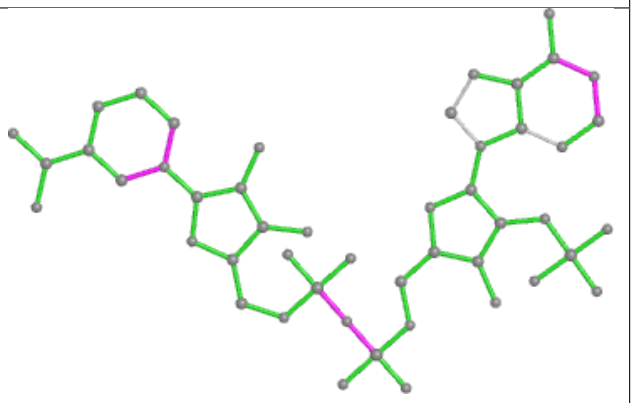
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1001	NAP	5	0
3	A	1001	NAP	3	0
4	B	501	PGW	1	0
4	H	501	PGW	4	0

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.

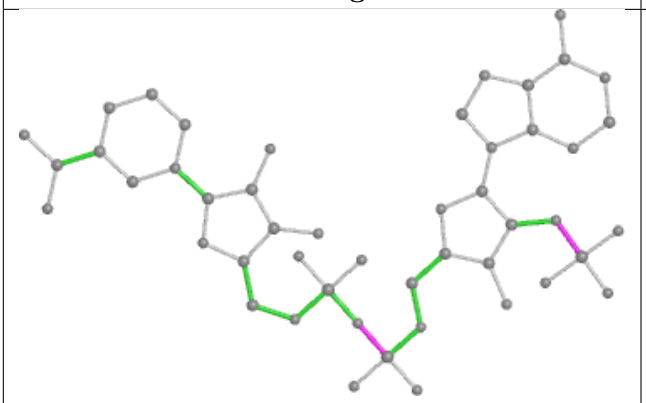
Ligand NAP G 1001



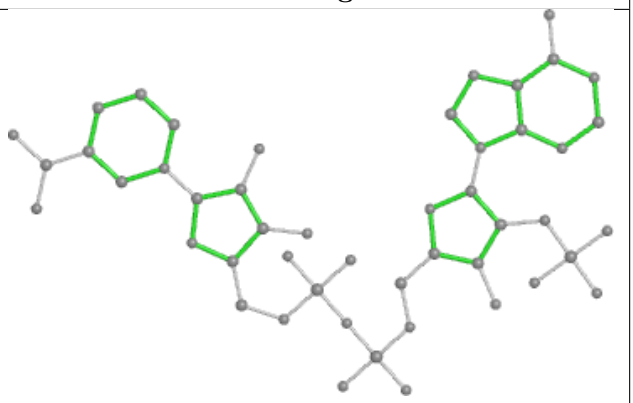
Bond lengths



Bond angles

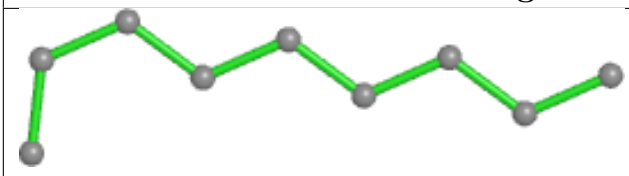


Torsions



Rings

Ligand PGW B 503



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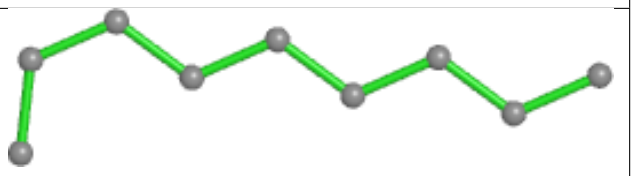

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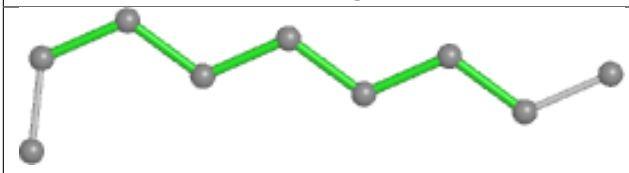

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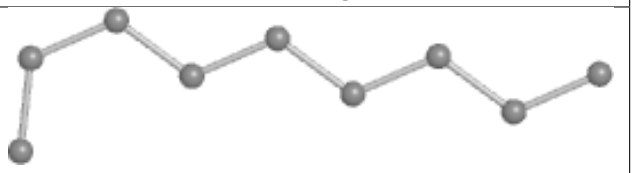
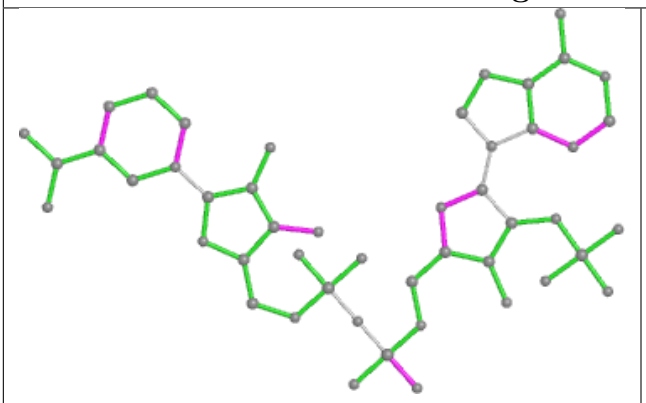


Rings

Ligand NAP A 1001



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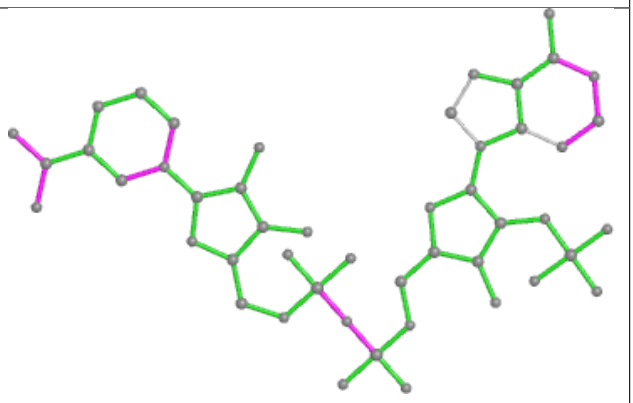

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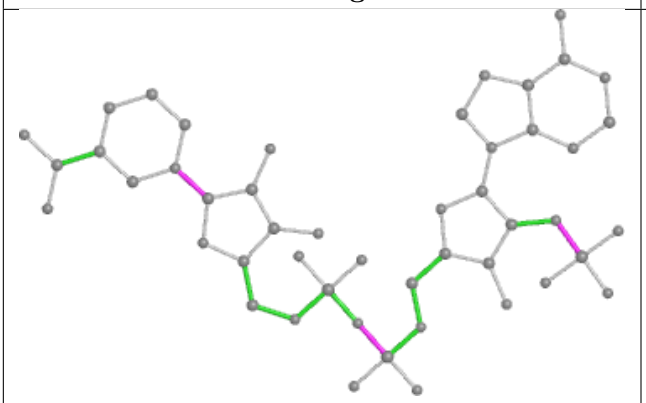

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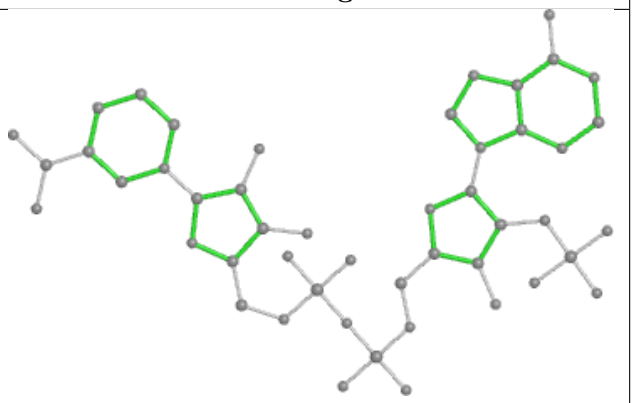
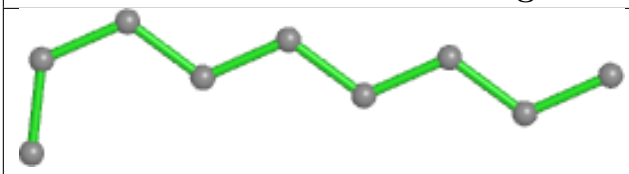


Rings

Ligand PGW B 502



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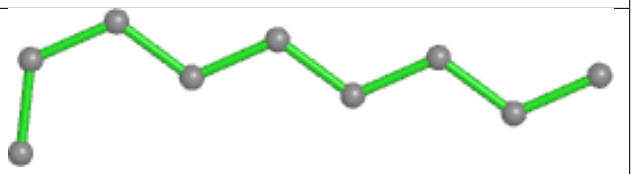

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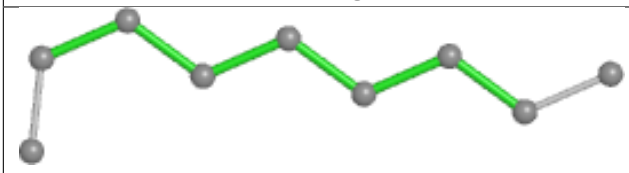

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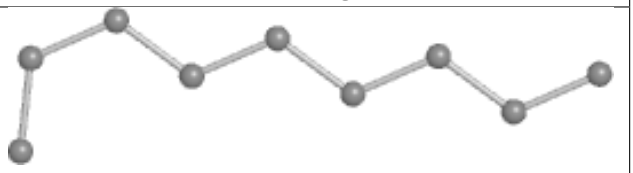

Rings

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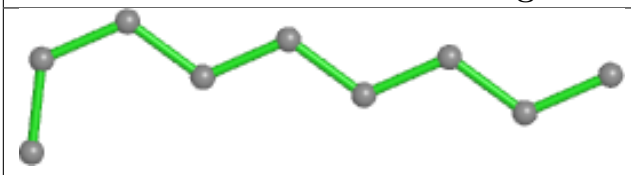

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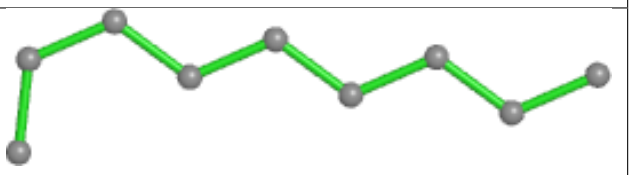

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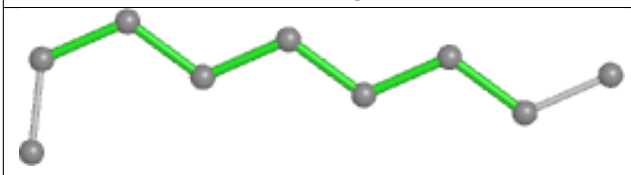

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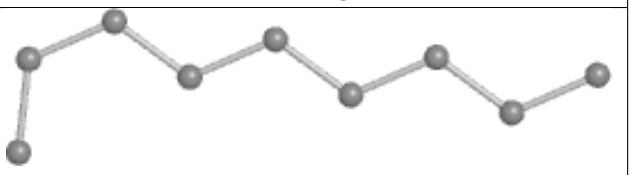

Rings

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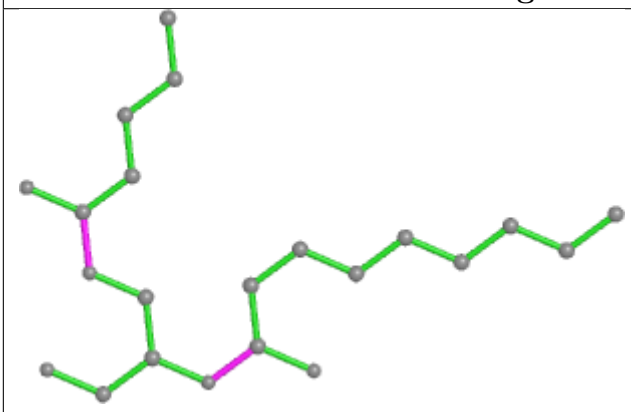

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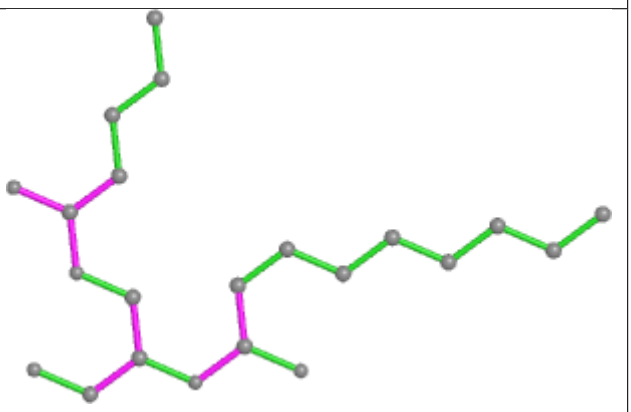
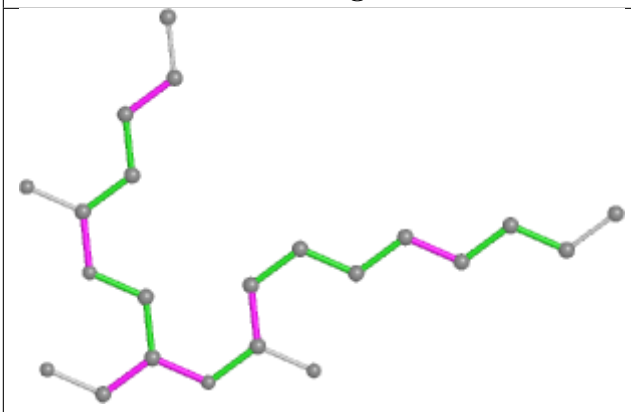
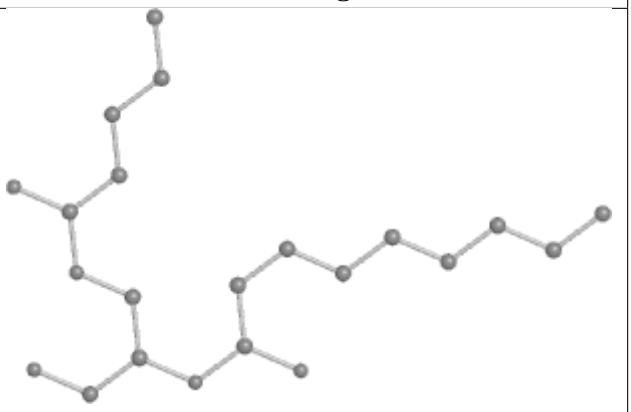


Bond angles

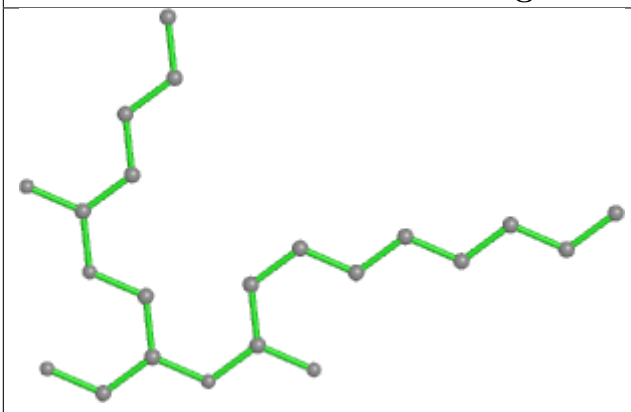


Torsions

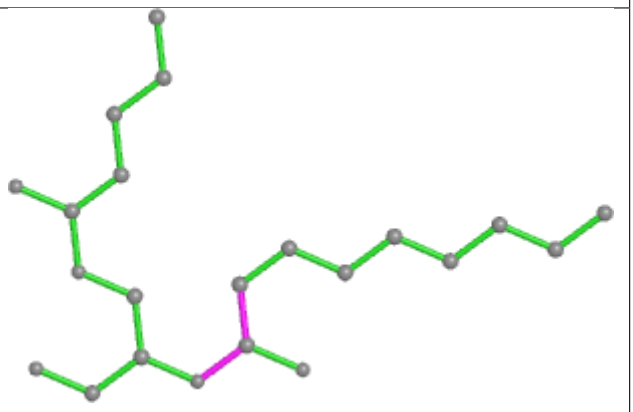


Rings

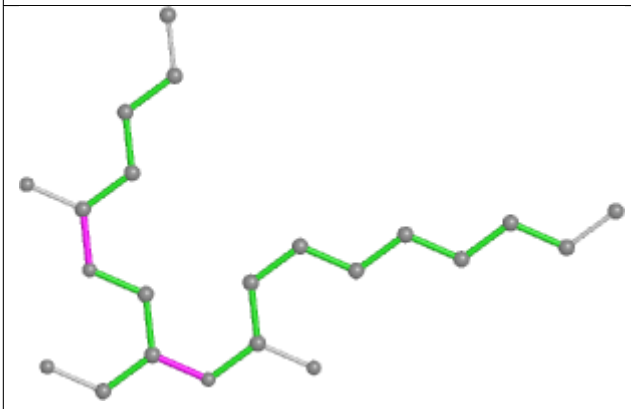
Ligand PGW H 501



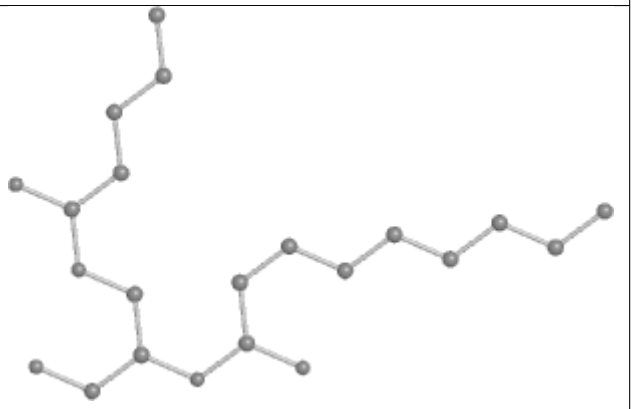
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.17	4 (1%) 79 78	29, 45, 69, 84	0
1	G	326/333 (97%)	-0.18	2 (0%) 89 90	27, 48, 77, 92	0
2	B	390/532 (73%)	0.10	21 (5%) 25 24	35, 60, 104, 125	0
2	H	328/532 (61%)	0.55	41 (12%) 3 3	40, 83, 160, 179	0
All	All	1370/1730 (79%)	0.08	68 (4%) 28 27	27, 55, 123, 179	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	242	PHE	7.5
2	H	149	VAL	6.3
2	H	251	PHE	6.2
2	H	145	PHE	5.9
2	H	153	PHE	5.8
2	H	250	PHE	5.7
2	H	252	THR	5.5
2	H	221	PRO	5.1
2	H	150	TRP	4.9
2	H	189	ARG	4.2
2	H	161	PRO	4.1
2	H	222	PHE	4.0
2	H	188	PHE	3.9
2	B	149	VAL	3.9
2	B	153	PHE	3.8
2	H	164	ILE	3.8
2	H	253	ASN	3.8
2	B	158	SER	3.6
2	H	146	GLN	3.6
2	B	141	PRO	3.5
2	H	152	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	158	SER	3.4
2	H	187	ILE	3.4
2	H	220	ASP	3.4
2	H	159	SER	3.4
2	H	183	GLU	3.3
2	B	244	CYS	3.2
2	H	241	PHE	3.2
2	H	160	GLY	3.2
2	B	243	ALA	3.1
2	H	223	PHE	3.1
2	B	249	GLY	3.1
2	H	163	ARG	3.1
2	H	157	GLU	3.0
2	B	152	LEU	3.0
1	G	36	LEU	3.0
2	B	151	LEU	3.0
2	H	226	GLU	3.0
2	B	214	GLN	2.9
2	H	229	CYS	2.9
2	H	184	THR	2.9
2	B	150	TRP	2.8
2	H	155	TYR	2.7
2	B	242	PHE	2.6
2	B	139	PRO	2.5
1	G	355	LEU	2.5
2	H	240	ARG	2.5
2	B	140	LEU	2.5
2	B	215	SER	2.5
1	A	262	TYR	2.4
1	A	255	TYR	2.4
2	H	235	PHE	2.4
2	H	154	GLU	2.4
2	H	239	VAL	2.3
2	B	251	PHE	2.3
2	B	245	PRO	2.3
2	B	283	GLN	2.3
2	H	225	VAL	2.3
2	B	216	THR	2.2
2	B	146	GLN	2.2
1	A	265	ALA	2.1
2	B	276	ASN	2.1
1	A	259	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	256	ASN	2.1
2	H	417	THR	2.0
2	H	185	LEU	2.0
2	H	98	LEU	2.0
2	H	147	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.

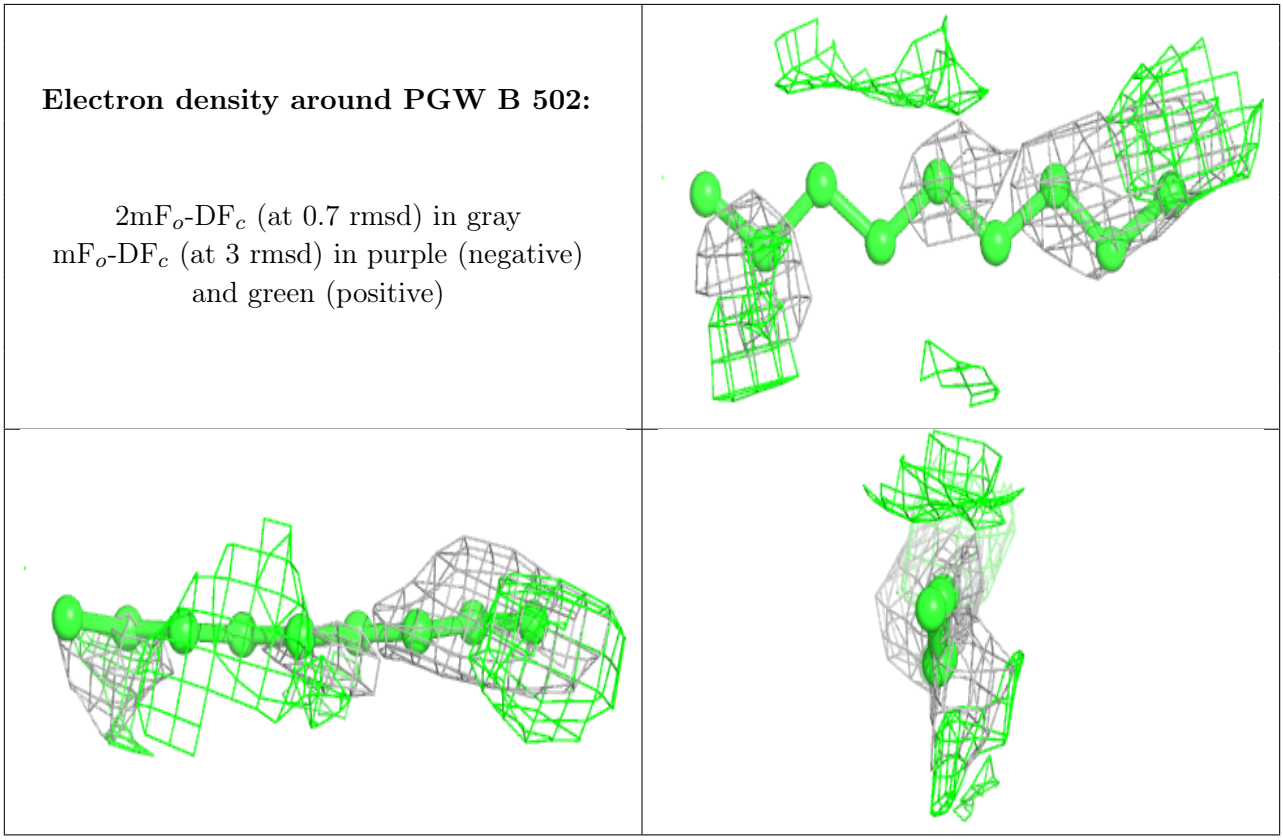
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	K	H	503	1/1	0.32	0.29	84,84,84,84	1
4	PGW	B	502	9/51	0.56	0.56	74,78,81,81	0
4	PGW	B	503	9/51	0.67	0.57	81,82,82,83	0
5	K	H	502	1/1	0.72	0.23	62,62,62,62	1
4	PGW	B	504	9/51	0.78	0.34	61,63,64,65	0
4	PGW	B	505	9/51	0.80	0.59	49,50,52,52	0
4	PGW	B	501	22/51	0.82	0.29	42,50,57,60	0
4	PGW	H	501	22/51	0.84	0.27	64,78,82,83	0
5	K	B	508	1/1	0.91	0.17	33,33,33,33	1
5	K	H	504	1/1	0.91	0.19	58,58,58,58	1
5	K	B	509	1/1	0.92	0.77	93,93,93,93	1
3	NAP	G	1001	48/48	0.95	0.21	46,54,58,61	0
5	K	B	507	1/1	0.96	0.16	38,38,38,38	1
3	NAP	A	1001	48/48	0.97	0.20	38,46,55,55	0
5	K	H	505	1/1	0.98	0.22	68,68,68,68	1
5	K	B	506	1/1	0.99	0.17	60,60,60,60	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.

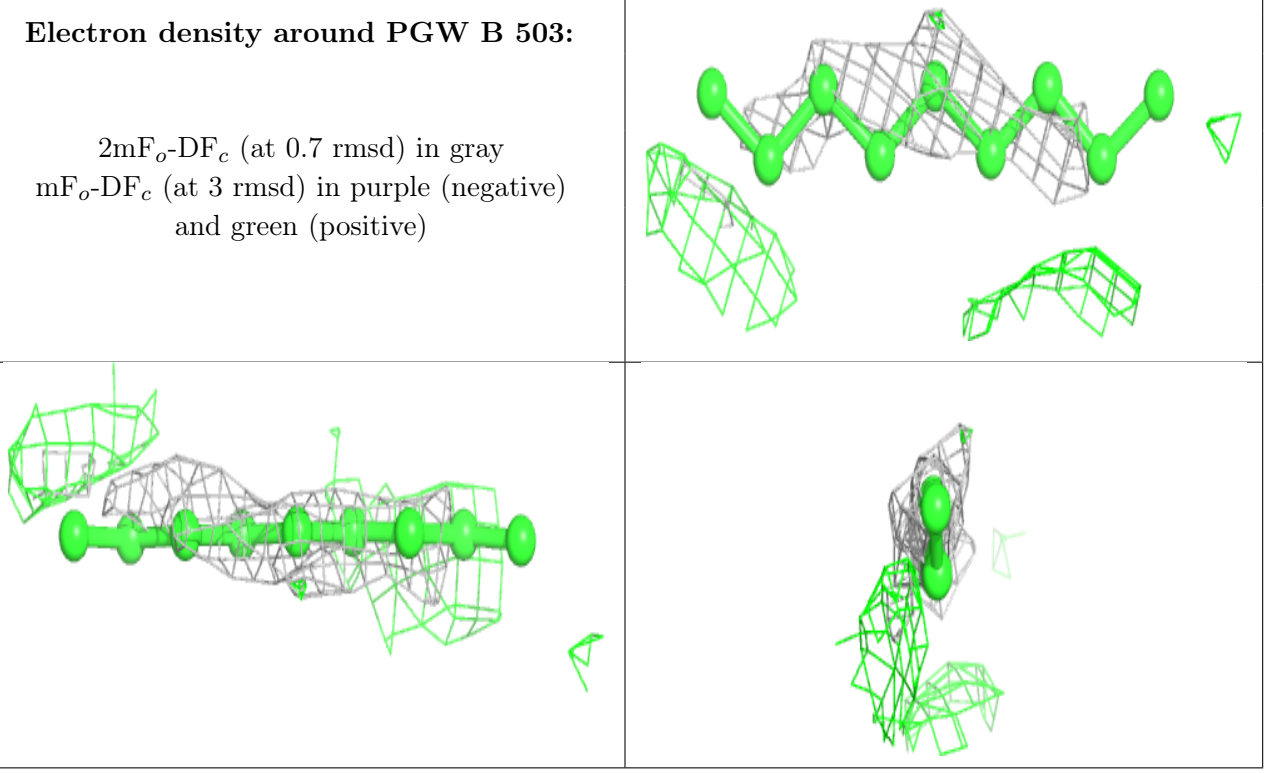
Electron density around PGW B 502:

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



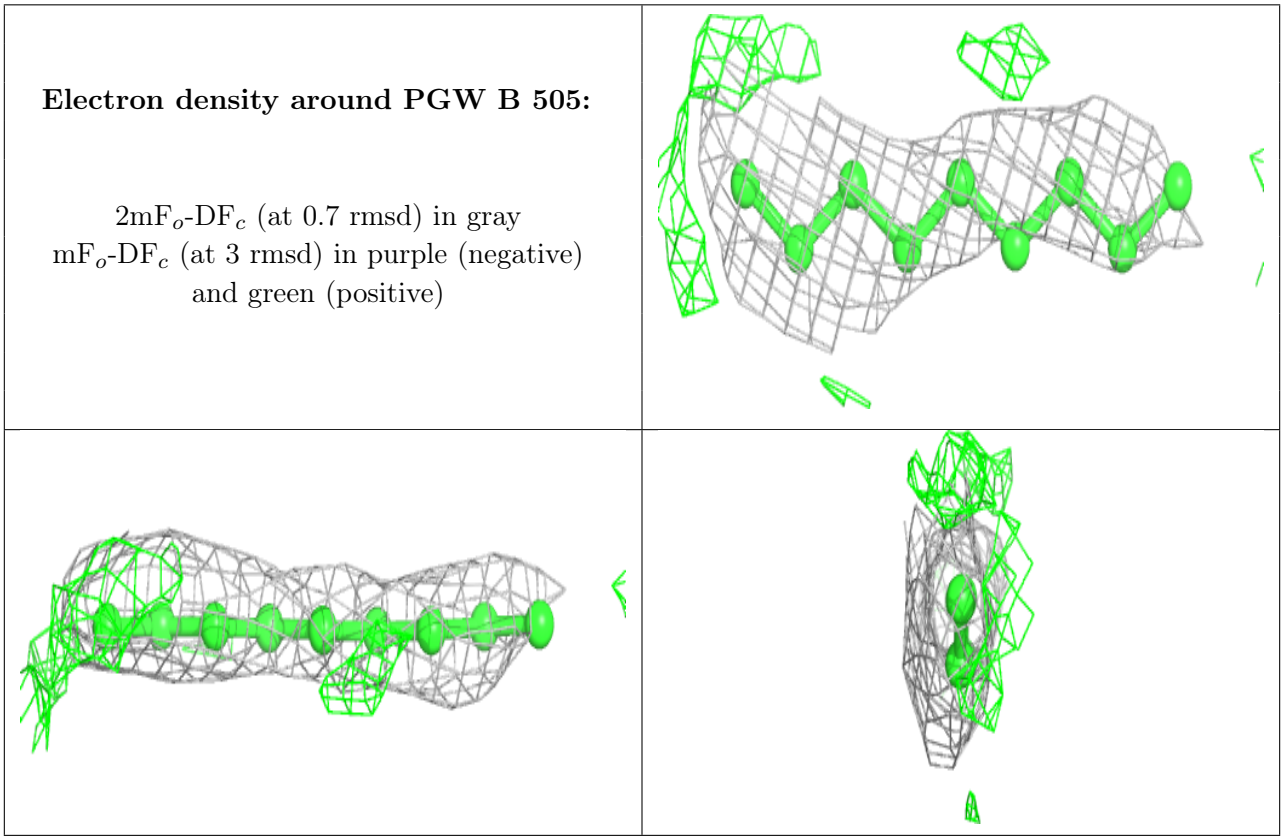
Electron density around PGW B 503:

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



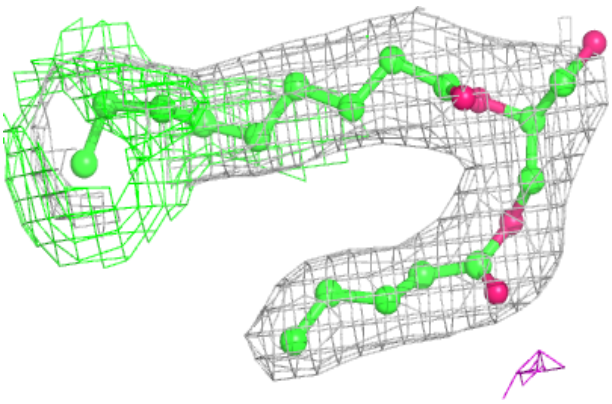
Electron density around PGW B 505:

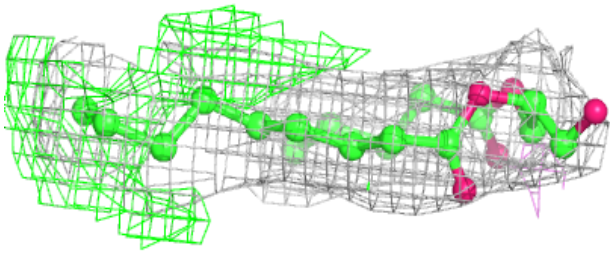
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

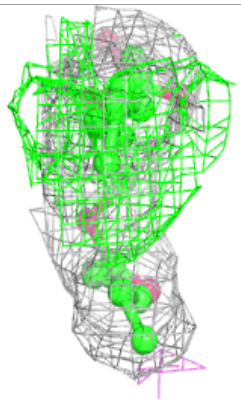


Electron density around PGW B 501:

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

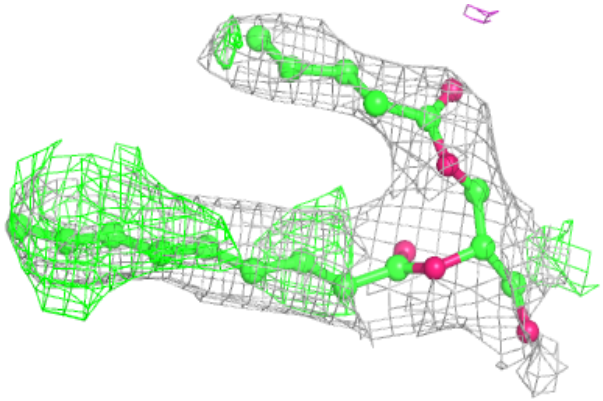


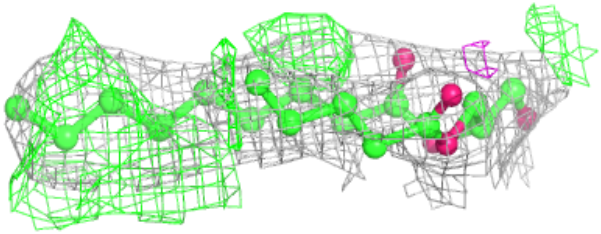


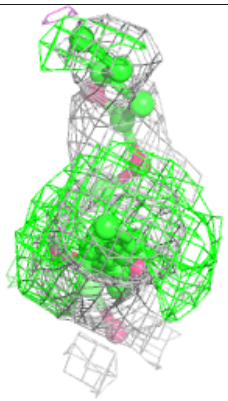


Electron density around PGW H 501:

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

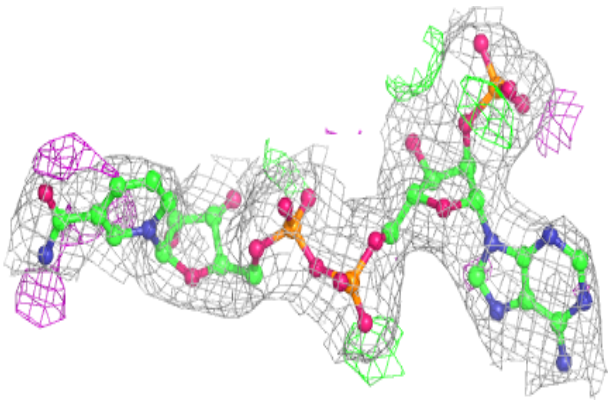


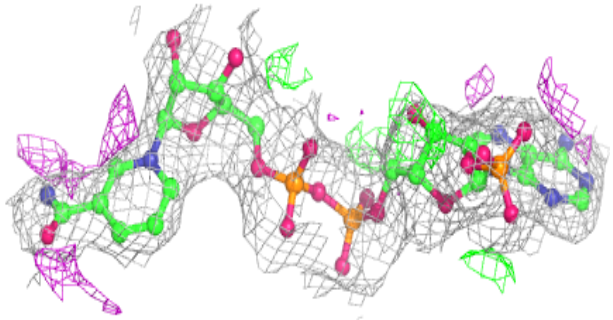


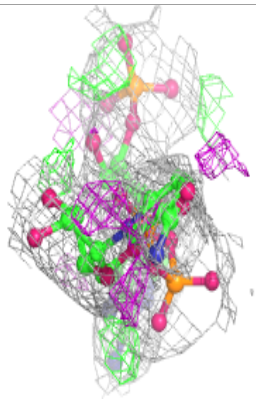


Electron density around NAP G 1001:

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

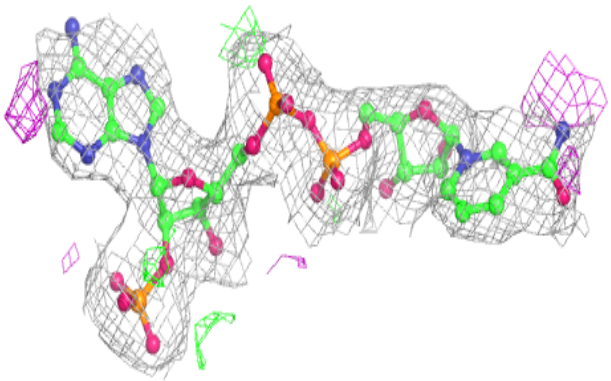


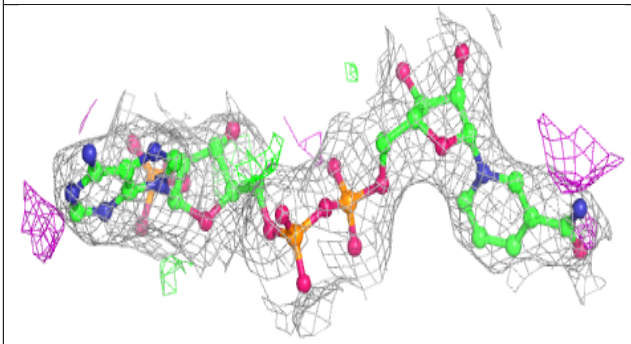


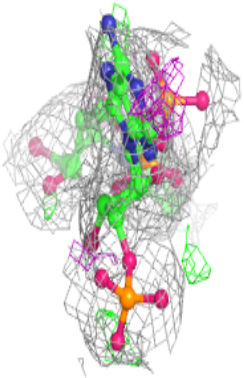


Electron density around NAP A 1001:

$2mF_o$-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.