



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:50 PM UTC

PDB ID : 2R9R / pdb_00002r9r
Title : Shaker family voltage dependent potassium channel (kv1.2-kv2.1 paddle chimera channel) in association with beta subunit
Authors : Long, S.B.; Tao, X.; Campbell, E.B.; Mackinnon, R.
Deposited on : 2007-09-13
Resolution : 2.40 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	:	4-5-2 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

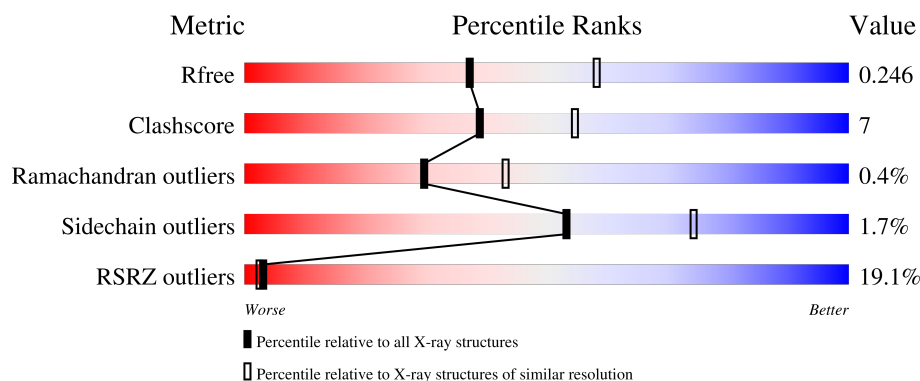
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	2% 87% 10% ..
1	G	333	2% 84% 12% ..
2	B	514	13% 59% 16% 25%
2	H	514	36% 54% 16% 29%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PGW	B	501	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11814 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 Paddle chimera voltage gated potassium channel Kv1.2-Kv2.1.

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			

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

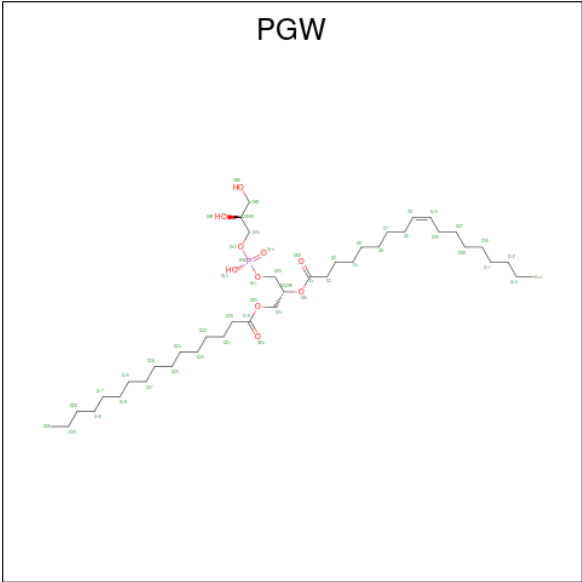


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	G	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 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
5	B	1	Total C O 22 17 5	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 7 7	0	0
5	B	1	Total C 9 9	0	0
5	B	1	Total C 12 12	0	0
5	B	1	Total C O P 23 14 8 1	0	0
5	B	1	Total C 12 12	0	0
5	B	1	Total C O P 37 26 10 1	0	0
5	B	1	Total C 10 10	0	0

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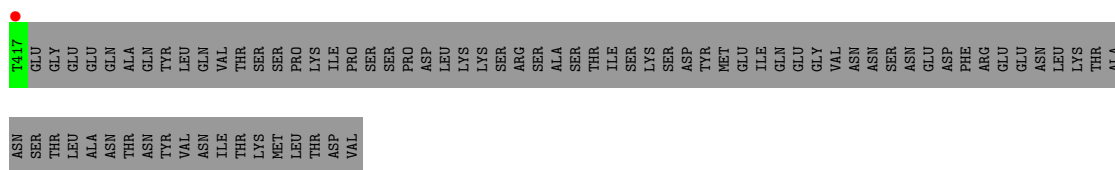
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 12 12	0	0
5	B	1	Total C 12 12	0	0
5	H	1	Total C O 22 17 5	0	0

- Molecule 6 is water.

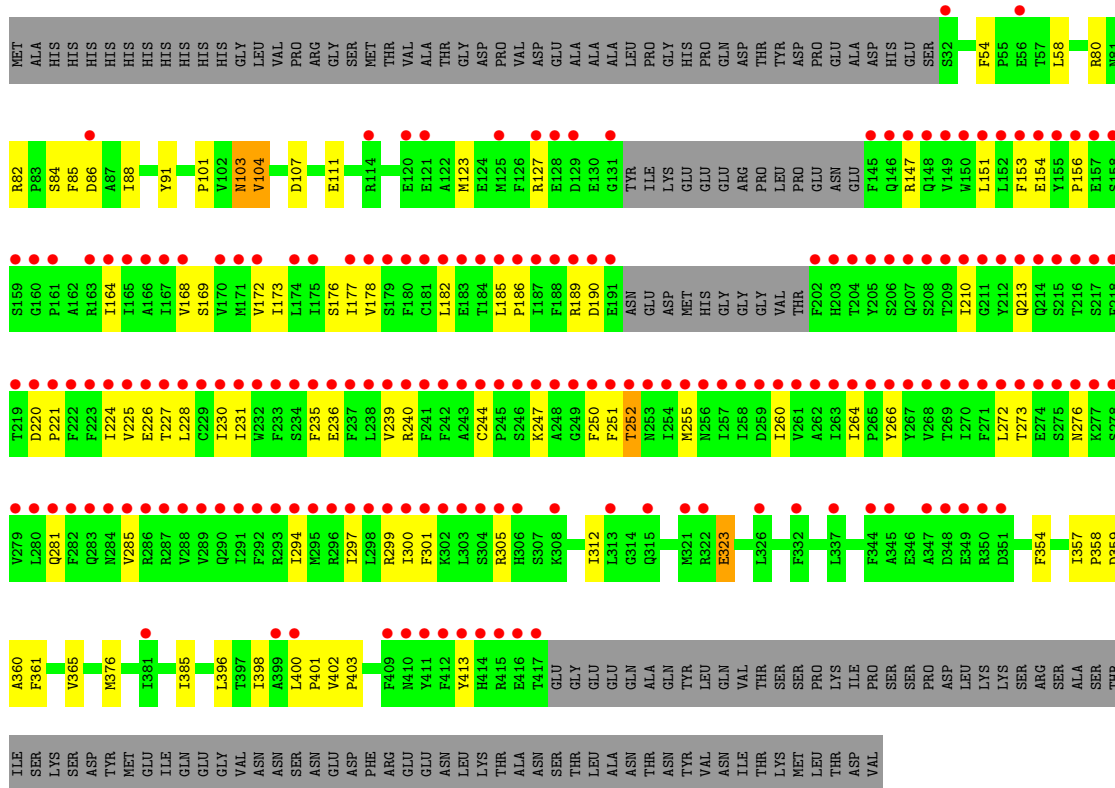
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	141	Total O 141 141	0	0
6	B	52	Total O 52 52	0	0
6	G	102	Total O 102 102	0	0
6	H	24	Total O 24 24	0	0

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





- Molecule 2: Paddle chimera voltage gated potassium channel Kv1.2-Kv2.1



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.05Å 144.05Å 284.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.40 49.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.4 (49.66-2.40) 89.4 (49.66-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.244 0.216 , 0.246	Depositor DCC
R_{free} test set	5746 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	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	0.93	EDS
Total number of atoms	11814	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: PGW, NAP, 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	0.80	0/2608	0.99	3/3524 (0.1%)
1	G	0.78	0/2608	1.00	10/3524 (0.3%)
2	B	0.67	0/3169	0.97	12/4292 (0.3%)
2	H	0.55	0/3036	0.92	7/4114 (0.2%)
All	All	0.70	0/11421	0.97	32/15454 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	136	GLU	N-CA-C	10.35	123.14	110.41
1	G	157	ALA	N-CA-C	-7.82	97.28	109.25
1	A	157	ALA	N-CA-C	-7.80	97.31	109.25
2	B	252	THR	N-CA-C	-6.92	105.37	113.88
1	G	315	GLU	N-CA-C	-6.79	105.14	113.50
2	H	252	THR	N-CA-C	-6.34	106.08	113.88
2	B	54	PHE	CA-C-N	6.34	127.77	119.84
2	B	54	PHE	C-N-CA	6.34	127.77	119.84
2	B	80	ARG	N-CA-C	6.15	118.54	109.69
2	H	54	PHE	CA-C-N	6.06	126.50	119.47
2	H	54	PHE	C-N-CA	6.06	126.50	119.47
2	H	85	PHE	N-CA-C	6.02	118.64	111.71
1	G	323	GLY	N-CA-C	-5.97	101.64	111.38
1	G	228	GLN	N-CA-C	5.96	117.86	111.36
1	A	227	VAL	N-CA-C	5.96	116.93	111.81
2	H	104	VAL	N-CA-C	5.94	114.50	107.73
1	G	269	GLY	N-CA-C	-5.72	107.16	114.37
1	G	208	ILE	N-CA-C	5.71	114.16	107.77
2	H	385	ILE	N-CA-C	-5.63	104.86	111.00
2	B	354	PHE	CA-C-N	5.54	125.38	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	354	PHE	C-N-CA	5.54	125.38	119.28
2	B	119	GLY	N-CA-C	5.37	118.30	112.29
1	A	228	GLN	N-CA-C	5.36	119.90	112.45
2	B	61	ASP	CA-C-N	5.27	125.33	119.32
2	B	61	ASP	C-N-CA	5.27	125.33	119.32
1	G	211	ILE	CB-CA-C	-5.24	105.16	110.93
1	G	241	MET	N-CA-C	-5.24	98.85	108.02
2	B	347	ALA	N-CA-C	5.18	117.32	111.11
2	H	84	SER	N-CA-C	5.10	116.92	111.36
1	G	191	SER	N-CA-C	-5.04	103.75	110.55
2	B	82	ARG	N-CA-C	5.03	120.93	109.81
1	G	236	ILE	N-CA-C	5.01	117.19	111.88

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	23	0
1	G	2556	0	2582	24	0
2	B	3088	0	3033	50	1
2	H	2959	0	2955	57	0
3	A	48	0	25	1	0
3	G	48	0	25	3	0
4	B	4	0	0	0	0
4	H	4	0	0	0	0
5	B	210	0	291	9	0
5	H	22	0	25	6	0
6	A	141	0	0	1	0
6	B	52	0	0	0	0
6	G	102	0	0	0	0
6	H	24	0	0	1	0
All	All	11814	0	11518	157	1

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 7.

All (157) 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:103:ASN:HD22	2:H:103:ASN:H	1.16	0.93
1:G:333:ASN:HD21	3:G:1001:NAP:H61A	1.29	0.79
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.72	0.71
2:B:177:ILE:HD13	2:B:300:ILE:HD12	1.73	0.70
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.72	0.70
2:B:359:ASP:HA	5:B:500:PGW:H02	1.74	0.69
2:B:318:LYS:HD2	5:B:512:PGW:H23A	1.74	0.68
2:H:177:ILE:HD13	2:H:300:ILE:HD12	1.76	0.67
2:B:143:ASN:C	2:B:145:PHE:H	2.01	0.67
1:A:326:ASN:ND2	1:A:329:GLN:H	1.93	0.66
1:G:75:LEU:HG	1:G:331:MET:HE3	1.77	0.66
1:G:295:ILE:H	1:G:295:ILE:HD12	1.62	0.65
1:G:40:ARG:HD2	1:G:318:SER:O	1.98	0.64
2:H:227:THR:O	2:H:231:ILE:HG12	1.98	0.63
2:H:103:ASN:H	2:H:103:ASN:ND2	1.92	0.63
2:H:359:ASP:HA	5:H:500:PGW:H02	1.80	0.63
1:A:40:ARG:HD2	1:A:318:SER:O	2.00	0.62
2:B:323:GLU:H	2:B:323:GLU:CD	2.09	0.60
1:A:333:ASN:HD21	3:A:1001:NAP:H61A	1.49	0.59
2:H:236:GLU:HB3	2:H:240:ARG:NH1	2.19	0.58
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.85	0.57
2:B:177:ILE:CD1	2:B:300:ILE:HD12	2.35	0.57
2:B:227:THR:O	2:B:231:ILE:HG12	2.05	0.56
2:H:236:GLU:HB3	2:H:240:ARG:HH12	1.70	0.56
2:B:103:ASN:H	2:B:103:ASN:HD22	1.54	0.56
2:H:361:PHE:HB2	5:H:500:PGW:H2	1.88	0.55
2:H:186:PRO:O	2:H:190:ASP:HB2	2.07	0.55
2:B:236:GLU:HB3	2:B:240:ARG:NH1	2.22	0.54
1:G:159:ARG:HB2	1:G:160:PRO:HD2	1.89	0.54
2:B:244:CYS:SG	2:B:247:LYS:HD3	2.47	0.54
5:B:500:PGW:H01	5:B:500:PGW:O02	2.06	0.54
2:B:361:PHE:HB2	5:B:500:PGW:H2	1.89	0.54
2:B:103:ASN:H	2:B:103:ASN:ND2	2.05	0.53
2:B:186:PRO:O	2:B:190:ASP:HB2	2.08	0.53
2:H:86:ASP:HB2	6:H:516:HOH:O	2.09	0.53
2:B:121:GLU:O	2:B:125:MET:HG2	2.08	0.53
2:H:153:PHE:CE2	2:H:239:VAL:HG11	2.44	0.52
1:A:258:GLY:O	1:A:260:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ASN:C	2:B:145:PHE:N	2.68	0.52
1:G:214:GLN:HA	1:G:241:MET:O	2.10	0.52
1:A:159:ARG:HA	1:A:188:SER:O	2.11	0.51
2:B:139:PRO:O	2:B:245:PRO:CG	2.59	0.51
2:B:250:PHE:C	2:B:252:THR:H	2.18	0.51
2:H:177:ILE:CD1	2:H:300:ILE:HD12	2.40	0.51
2:H:244:CYS:SG	2:H:247:LYS:HD3	2.50	0.51
2:B:236:GLU:HB3	2:B:240:ARG:HH12	1.75	0.51
2:H:235:PHE:O	2:H:239:VAL:HG23	2.11	0.50
2:H:250:PHE:C	2:H:252:THR:H	2.19	0.50
2:H:323:GLU:H	2:H:323:GLU:CD	2.19	0.50
1:G:333:ASN:ND2	3:G:1001:NAP:H61A	2.05	0.50
1:G:251:VAL:HG12	1:G:251:VAL:O	2.12	0.49
1:G:280:GLU:O	1:G:284:ARG:HG3	2.12	0.49
2:B:113:ILE:HG23	2:B:118:LEU:HD12	1.95	0.49
2:B:311:GLN:HG2	5:B:512:PGW:H3	1.93	0.49
1:A:251:VAL:HG12	1:A:251:VAL:O	2.13	0.49
2:H:169:SER:O	2:H:173:ILE:HG13	2.12	0.49
2:H:312:ILE:HD13	2:H:413:TYR:HA	1.95	0.49
2:H:154:GLU:C	2:H:156:PRO:HD3	2.37	0.49
1:G:247:ALA:O	1:G:248:CYS:HB2	2.13	0.49
2:H:272:LEU:HD22	2:H:285:VAL:HG21	1.95	0.49
2:H:396:LEU:O	2:H:400:LEU:HG	2.13	0.48
2:B:276:ASN:HB3	2:B:281:GLN:HB3	1.94	0.48
2:B:221:PRO:O	2:B:225:VAL:HG23	2.13	0.48
1:A:326:ASN:HD21	1:A:329:GLN:H	1.58	0.48
2:B:396:LEU:O	2:B:400:LEU:HG	2.12	0.48
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.96	0.48
5:H:500:PGW:O02	5:H:500:PGW:H01	2.13	0.48
2:H:354:PHE:CD1	2:H:376:MET:HE2	2.49	0.47
2:H:276:ASN:HB3	2:H:281:GLN:HB3	1.96	0.47
1:G:217:TYR:HB3	1:G:242:THR:HB	1.96	0.47
1:A:314:ASN:HB2	6:A:1068:HOH:O	2.15	0.47
1:A:120:PHE:O	1:A:129:ARG:HA	2.15	0.46
2:H:213:GLN:HB3	2:H:220:ASP:HB2	1.96	0.46
2:H:226:GLU:O	2:H:230:ILE:HD13	2.16	0.46
2:H:365:VAL:HG21	5:H:500:PGW:H6A	1.97	0.46
1:G:217:TYR:HB2	1:G:225:VAL:HG21	1.96	0.46
2:H:255:MET:HE1	2:H:305:ARG:HA	1.98	0.46
2:B:138:ARG:O	2:B:245:PRO:HG2	2.16	0.46
2:H:58:LEU:C	2:H:58:LEU:HD23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:221:PRO:O	2:H:225:VAL:HG23	2.16	0.46
5:B:500:PGW:O02	5:B:500:PGW:C01	2.64	0.46
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.51	0.45
2:B:260:ILE:O	2:B:264:ILE:HG13	2.16	0.45
2:H:255:MET:CE	2:H:305:ARG:HA	2.47	0.45
2:B:312:ILE:HD13	2:B:413:TYR:HA	1.98	0.45
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.99	0.45
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.51	0.45
2:H:107:ASP:O	2:H:111:GLU:HG3	2.17	0.45
1:G:73:MET:HE3	1:G:84:PHE:CG	2.52	0.45
2:B:73:ARG:HB2	2:B:75:GLU:HG2	1.98	0.45
2:H:361:PHE:CB	5:H:500:PGW:H2	2.47	0.45
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.52	0.45
2:B:149:VAL:O	2:B:152:LEU:HD12	2.17	0.45
2:B:235:PHE:O	2:B:239:VAL:HG23	2.16	0.45
1:G:102:ILE:O	1:G:106:LYS:HG2	2.16	0.45
2:H:88:ILE:O	2:H:91:TYR:HB3	2.17	0.45
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.98	0.45
2:B:255:MET:CE	2:B:305:ARG:HA	2.47	0.44
1:G:42:LEU:HD11	1:G:212:CYS:SG	2.56	0.44
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.44
1:G:152:VAL:O	1:G:182:ALA:HA	2.17	0.44
2:B:120:GLU:O	2:B:124:GLU:HG3	2.17	0.44
2:B:178:VAL:HG22	5:B:505:PGW:H8	1.99	0.44
1:G:295:ILE:HD12	1:G:295:ILE:N	2.28	0.44
2:B:365:VAL:HG21	5:B:500:PGW:H6A	1.99	0.44
2:H:224:ILE:O	2:H:228:LEU:HG	2.18	0.44
1:A:73:MET:HE3	1:A:84:PHE:CD2	2.53	0.43
2:H:260:ILE:O	2:H:264:ILE:HG13	2.18	0.43
2:B:58:LEU:C	2:B:58:LEU:HD23	2.43	0.43
2:B:256:ASN:O	2:B:260:ILE:HG13	2.18	0.43
2:H:168:VAL:O	2:H:172:VAL:HG23	2.18	0.43
1:A:215:ALA:O	1:A:242:THR:HA	2.19	0.43
2:B:353:GLN:O	2:B:376:MET:HE3	2.19	0.43
1:G:323:GLY:HA3	3:G:1001:NAP:H51A	2.01	0.43
2:H:210:ILE:HD11	2:H:273:THR:HG21	2.00	0.43
2:H:402:VAL:HB	2:H:403:PRO:HD3	2.01	0.43
2:H:178:VAL:O	2:H:182:LEU:HG	2.19	0.42
2:H:294:ILE:O	2:H:297:ILE:HG22	2.19	0.42
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.92	0.42
2:B:154:GLU:C	2:B:156:PRO:HD3	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:361:PHE:HD2	5:H:500:PGW:H20A	1.85	0.42
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.93	0.42
2:B:323:GLU:CD	2:B:323:GLU:N	2.76	0.42
2:H:354:PHE:CE1	2:H:376:MET:HE2	2.55	0.42
2:H:398:ILE:O	2:H:402:VAL:HG23	2.19	0.42
1:A:159:ARG:HB2	1:A:160:PRO:HD2	2.00	0.42
2:B:255:MET:HE1	2:B:305:ARG:HA	2.01	0.42
2:B:308:LYS:N	5:B:510:PGW:O13	2.53	0.42
2:H:123:MET:O	2:H:127:ARG:HG3	2.20	0.42
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.55	0.41
1:A:217:TYR:HB3	1:A:242:THR:HB	2.01	0.41
2:B:178:VAL:O	2:B:182:LEU:HG	2.19	0.41
2:B:308:LYS:O	2:B:312:ILE:HG13	2.20	0.41
2:H:101:PRO:HB2	2:H:104:VAL:HG23	2.02	0.41
1:G:251:VAL:O	1:G:251:VAL:CG1	2.68	0.41
2:H:164:ILE:O	2:H:168:VAL:HG23	2.20	0.41
2:H:189:ARG:HH11	2:H:189:ARG:HG3	1.84	0.41
1:A:56:THR:HB	1:A:60:PHE:HB2	2.02	0.41
2:B:83:PRO:HB2	2:B:104:VAL:HG22	2.01	0.41
2:H:300:ILE:HG23	2:H:301:PHE:N	2.35	0.41
2:H:154:GLU:O	2:H:156:PRO:HD3	2.20	0.41
2:H:260:ILE:HG22	2:H:264:ILE:HD11	2.03	0.41
2:B:81:ASN:OD1	2:B:83:PRO:HD2	2.21	0.41
2:B:213:GLN:HB3	2:B:220:ASP:HB2	2.03	0.41
1:G:117:THR:HG22	1:G:152:VAL:HG11	2.02	0.41
1:A:73:MET:HE3	1:A:84:PHE:CG	2.56	0.41
2:B:360:ALA:O	2:B:361:PHE:C	2.62	0.41
1:G:104:LYS:NZ	1:G:148:GLN:HE22	2.19	0.41
2:B:272:LEU:HD22	2:B:285:VAL:HG21	2.02	0.40
2:H:176:SER:HB2	2:H:299:ARG:NH1	2.35	0.40
2:H:255:MET:HB3	2:H:305:ARG:NH2	2.36	0.40
1:A:326:ASN:HD21	1:A:329:GLN:HG3	1.87	0.40
2:H:147:ARG:O	2:H:151:LEU:HG	2.22	0.40
2:H:360:ALA:O	2:H:361:PHE:C	2.65	0.40
1:G:205:PHE:O	1:G:206:ASN:HB3	2.21	0.40
2:H:230:ILE:HG21	2:H:266:TYR:CD2	2.56	0.40
1:G:159:ARG:HA	1:G:188:SER:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:GLU:O	2:B:142:GLU:O[8_556]	1.43	0.77

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%)	7 (2%)	1 (0%)	36	50
1	G	324/333 (97%)	317 (98%)	6 (2%)	1 (0%)	36	50
2	B	384/514 (75%)	365 (95%)	16 (4%)	3 (1%)	16	25
2	H	357/514 (70%)	345 (97%)	11 (3%)	1 (0%)	36	50
All	All	1389/1694 (82%)	1343 (97%)	40 (3%)	6 (0%)	30	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
2	B	137	GLU
1	G	120	PHE
2	B	135	GLU
2	B	142	GLU
2	H	251	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/280 (98%)	268 (98%)	5 (2%)	51	73
1	G	273/280 (98%)	266 (97%)	7 (3%)	40	63
2	B	332/459 (72%)	328 (99%)	4 (1%)	63	81
2	H	324/459 (71%)	319 (98%)	5 (2%)	57	77
All	All	1202/1478 (81%)	1181 (98%)	21 (2%)	53	74

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	MET
1	A	75	LEU
1	A	214	GLN
1	A	257	SER
1	A	326	ASN
2	B	86	ASP
2	B	185	LEU
2	B	323	GLU
2	B	337	LEU
1	G	37	GLN
1	G	73	MET
1	G	75	LEU
1	G	214	GLN
1	G	223	GLU
1	G	271	GLN
1	G	283	ARG
2	H	80	ARG
2	H	82	ARG
2	H	103	ASN
2	H	185	LEU
2	H	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	148	GLN
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN

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Mol	Chain	Res	Type
2	B	47	GLN
2	B	53	GLN
2	B	103	ASN
2	B	192	ASN
2	B	290	GLN
2	B	315	GLN
1	G	37	GLN
1	G	148	GLN
1	G	163	ASN
1	G	333	ASN
1	G	338	GLN
2	H	53	GLN
2	H	103	ASN
2	H	290	GLN
2	H	315	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	NAP	G	1001	-	50,52,52	1.50	9 (18%)	71,80,80	1.06	3 (4%)
5	PGW	B	501	-	8,8,50	0.37	0	7,7,56	0.50	0
5	PGW	H	500	-	21,21,50	0.61	0	23,23,56	1.09	1 (4%)
5	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.52	0
5	PGW	B	505	-	8,8,50	0.36	0	7,7,56	0.54	0
5	PGW	B	506	-	8,8,50	0.35	0	7,7,56	0.58	0
5	PGW	B	513	-	9,9,50	0.36	0	8,8,56	0.58	0
5	PGW	B	502	-	8,8,50	0.37	0	7,7,56	0.50	0
5	PGW	B	500	-	21,21,50	0.59	0	23,23,56	1.13	1 (4%)
5	PGW	B	512	-	36,36,50	0.65	0	39,42,56	0.98	3 (7%)
5	PGW	B	514	-	11,11,50	0.36	0	10,10,56	0.54	0
5	PGW	B	507	-	6,6,50	0.37	0	5,5,56	0.48	0
3	NAP	A	1001	-	50,52,52	1.46	9 (18%)	71,80,80	1.03	3 (4%)
5	PGW	B	515	-	11,11,50	0.36	0	10,10,56	0.57	0
5	PGW	B	504	-	8,8,50	0.37	0	7,7,56	0.50	0
5	PGW	B	503	-	8,8,50	0.36	0	7,7,56	0.51	0
5	PGW	B	509	-	11,11,50	0.36	0	10,10,56	0.58	0
5	PGW	B	510	-	22,22,50	0.80	0	25,27,56	1.30	4 (16%)
5	PGW	B	511	-	11,11,50	0.35	0	10,10,56	0.60	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	NAP	G	1001	-	-	2/35/67/67	0/5/5/5
5	PGW	B	501	-	-	0/6/6/55	-
5	PGW	H	500	-	-	3/23/23/55	-
5	PGW	B	508	-	-	0/6/6/55	-
5	PGW	B	505	-	-	0/6/6/55	-
5	PGW	B	506	-	-	0/6/6/55	-
5	PGW	B	513	-	-	0/7/7/55	-
5	PGW	B	502	-	-	0/6/6/55	-
5	PGW	B	500	-	-	3/23/23/55	-
5	PGW	B	512	-	-	9/41/41/55	-
5	PGW	B	514	-	-	0/9/9/55	-
5	PGW	B	507	-	-	0/4/4/55	-
3	NAP	A	1001	-	-	3/35/67/67	0/5/5/5
5	PGW	B	515	-	-	0/9/9/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGW	B	504	-	-	0/6/6/55	-
5	PGW	B	503	-	-	0/6/6/55	-
5	PGW	B	509	-	-	0/9/9/55	-
5	PGW	B	510	-	-	10/24/24/55	-
5	PGW	B	511	-	-	0/9/9/55	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	NAP	C6N-N1N	4.56	1.45	1.35
3	G	1001	NAP	C6N-N1N	4.05	1.44	1.35
3	A	1001	NAP	C4N-C3N	3.77	1.45	1.39
3	G	1001	NAP	PA-O3	3.65	1.63	1.59
3	G	1001	NAP	C4N-C3N	3.09	1.44	1.39
3	G	1001	NAP	C4A-N3A	2.93	1.39	1.34
3	A	1001	NAP	C4A-N3A	2.85	1.39	1.34
3	A	1001	NAP	O4B-C4B	2.83	1.51	1.45
3	G	1001	NAP	O4B-C4B	2.65	1.50	1.45
3	G	1001	NAP	C2A-N3A	2.59	1.38	1.33
3	G	1001	NAP	PN-O3	-2.55	1.56	1.59
3	G	1001	NAP	C5A-N7A	-2.49	1.34	1.39
3	A	1001	NAP	C2N-N1N	2.34	1.37	1.35
3	A	1001	NAP	PN-O3	-2.32	1.57	1.59
3	A	1001	NAP	C5N-C4N	2.17	1.42	1.38
3	G	1001	NAP	C5A-C4A	2.12	1.42	1.39
3	A	1001	NAP	O3D-C3D	-2.11	1.37	1.43
3	A	1001	NAP	PA-O3	2.04	1.61	1.59

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1001	NAP	C6N-N1N-C2N	-3.37	119.01	121.88
5	B	500	PGW	O01-C1-C2	3.26	118.53	111.48
5	B	510	PGW	C03-C02-C01	-3.08	104.59	111.78
5	H	500	PGW	O01-C1-C2	2.95	117.86	111.48
3	A	1001	NAP	C2A-N1A-C6A	2.92	123.53	118.73
5	B	512	PGW	O03-C01-C02	-2.74	100.50	108.40
5	B	512	PGW	O01-C1-C2	2.63	117.17	111.48
3	A	1001	NAP	C6N-N1N-C2N	-2.59	119.67	121.88
5	B	512	PGW	O01-C02-C03	2.49	117.27	108.34
5	B	510	PGW	O01-C1-C2	2.45	116.78	111.48
5	B	510	PGW	O03-C19-C20	2.44	119.27	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	510	PGW	O11-P-O14	2.35	112.80	106.44
3	G	1001	NAP	C2B-C1B-N9A	2.33	117.58	113.75
3	G	1001	NAP	C2A-N1A-C6A	2.23	122.39	118.73
3	A	1001	NAP	N3A-C2A-N1A	-2.05	125.48	128.58

There are no chirality outliers.

All (30) torsion outliers are listed below:

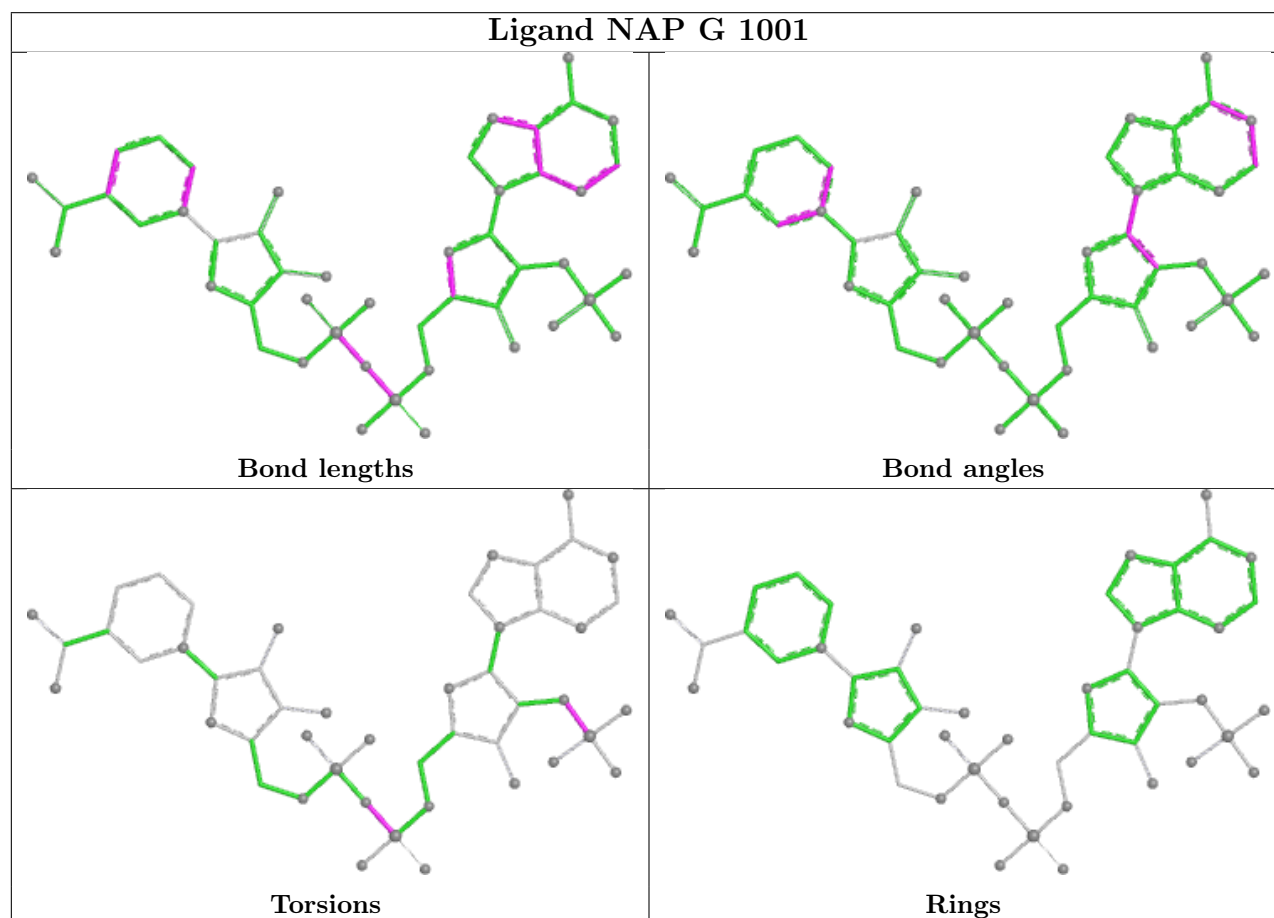
Mol	Chain	Res	Type	Atoms
3	A	1001	NAP	PN-O3-PA-O5B
3	A	1001	NAP	O4D-C1D-N1N-C6N
5	B	510	PGW	C20-C19-O03-C01
5	B	500	PGW	C20-C19-O03-C01
5	B	500	PGW	O04-C19-O03-C01
5	B	510	PGW	O04-C19-O03-C01
5	H	500	PGW	C20-C19-O03-C01
5	H	500	PGW	O04-C19-O03-C01
5	B	510	PGW	C02-C03-O11-P
3	G	1001	NAP	PN-O3-PA-O5B
5	B	512	PGW	O04-C19-O03-C01
5	B	512	PGW	C20-C19-O03-C01
5	B	512	PGW	C7-C8-C9-C10
5	B	500	PGW	C01-C02-O01-C1
5	H	500	PGW	C01-C02-O01-C1
5	B	510	PGW	O03-C01-C02-O01
3	A	1001	NAP	O4D-C1D-N1N-C2N
5	B	510	PGW	O03-C01-C02-C03
5	B	512	PGW	O01-C1-C2-C3
5	B	510	PGW	O01-C1-C2-C3
5	B	512	PGW	O02-C1-O01-C02
5	B	512	PGW	C2-C1-O01-C02
5	B	510	PGW	O02-C1-O01-C02
5	B	512	PGW	O03-C19-C20-C21
5	B	510	PGW	C01-C02-O01-C1
3	G	1001	NAP	C2B-O2B-P2B-O1X
5	B	510	PGW	O02-C1-C2-C3
5	B	512	PGW	O02-C1-C2-C3
5	B	510	PGW	O03-C19-C20-C21
5	B	512	PGW	O04-C19-C20-C21

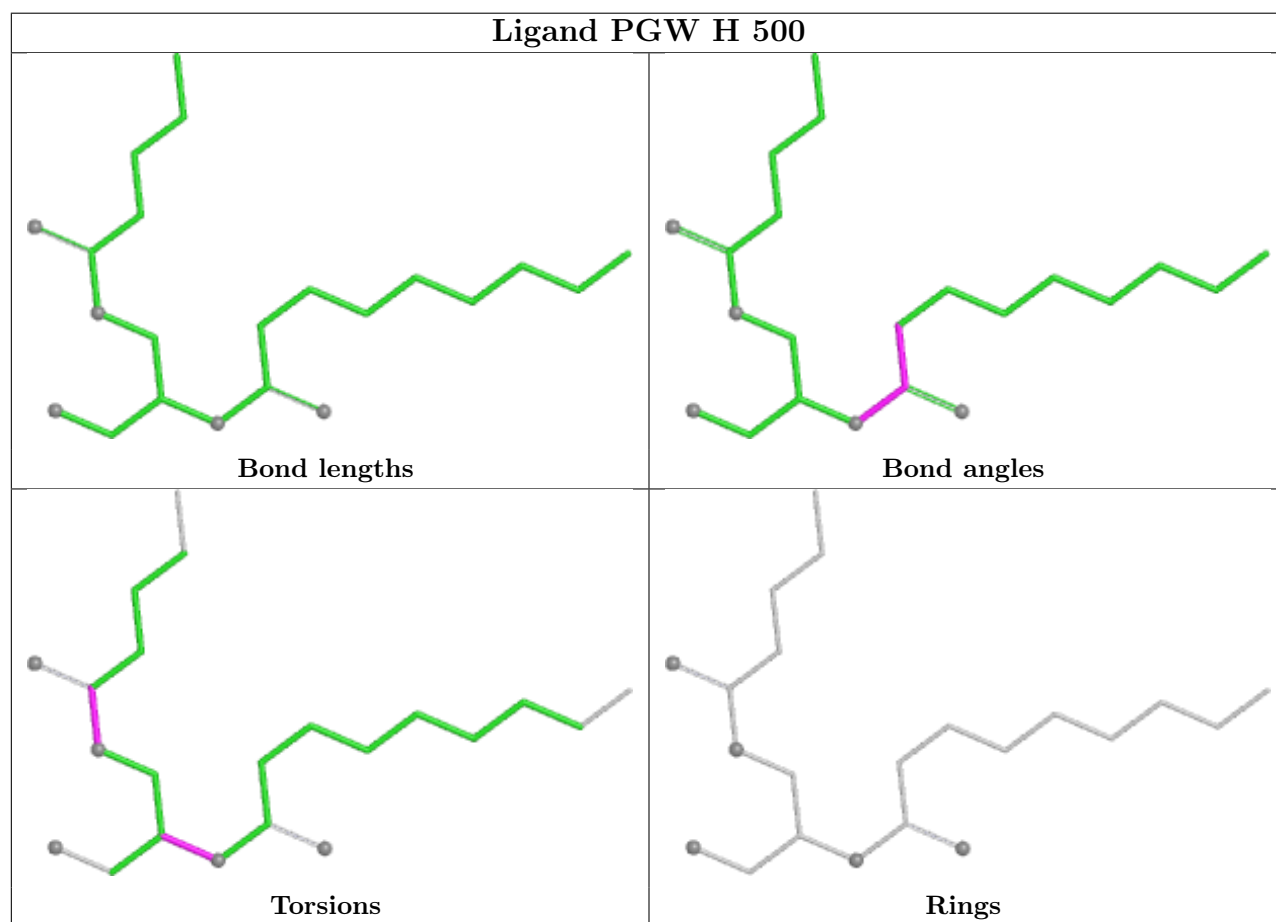
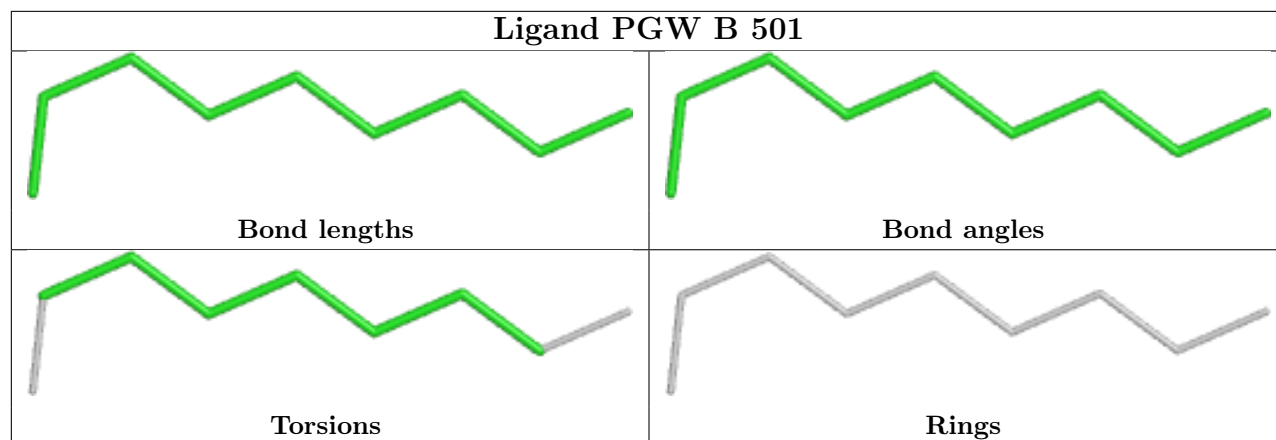
There are no ring outliers.

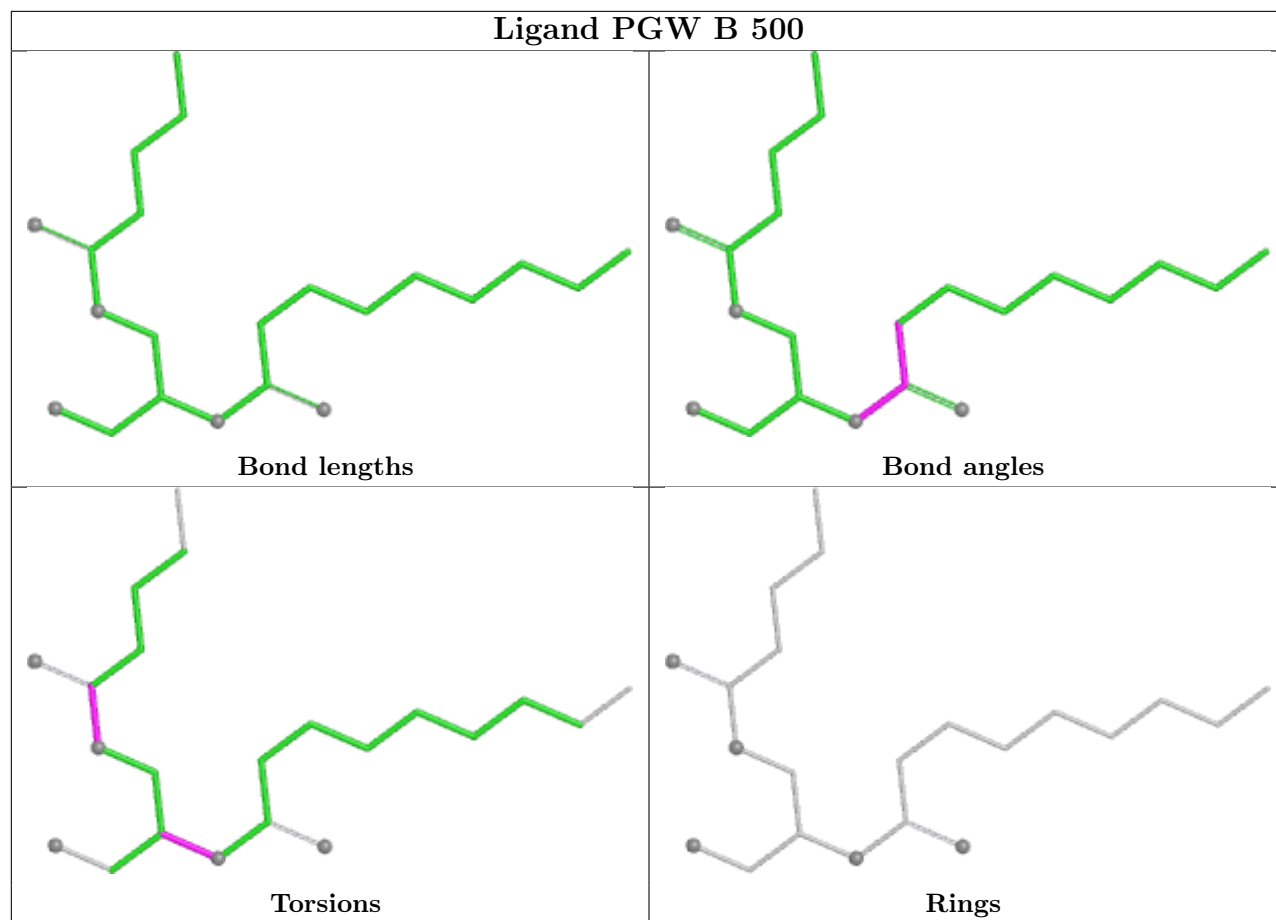
7 monomers are involved in 19 short contacts:

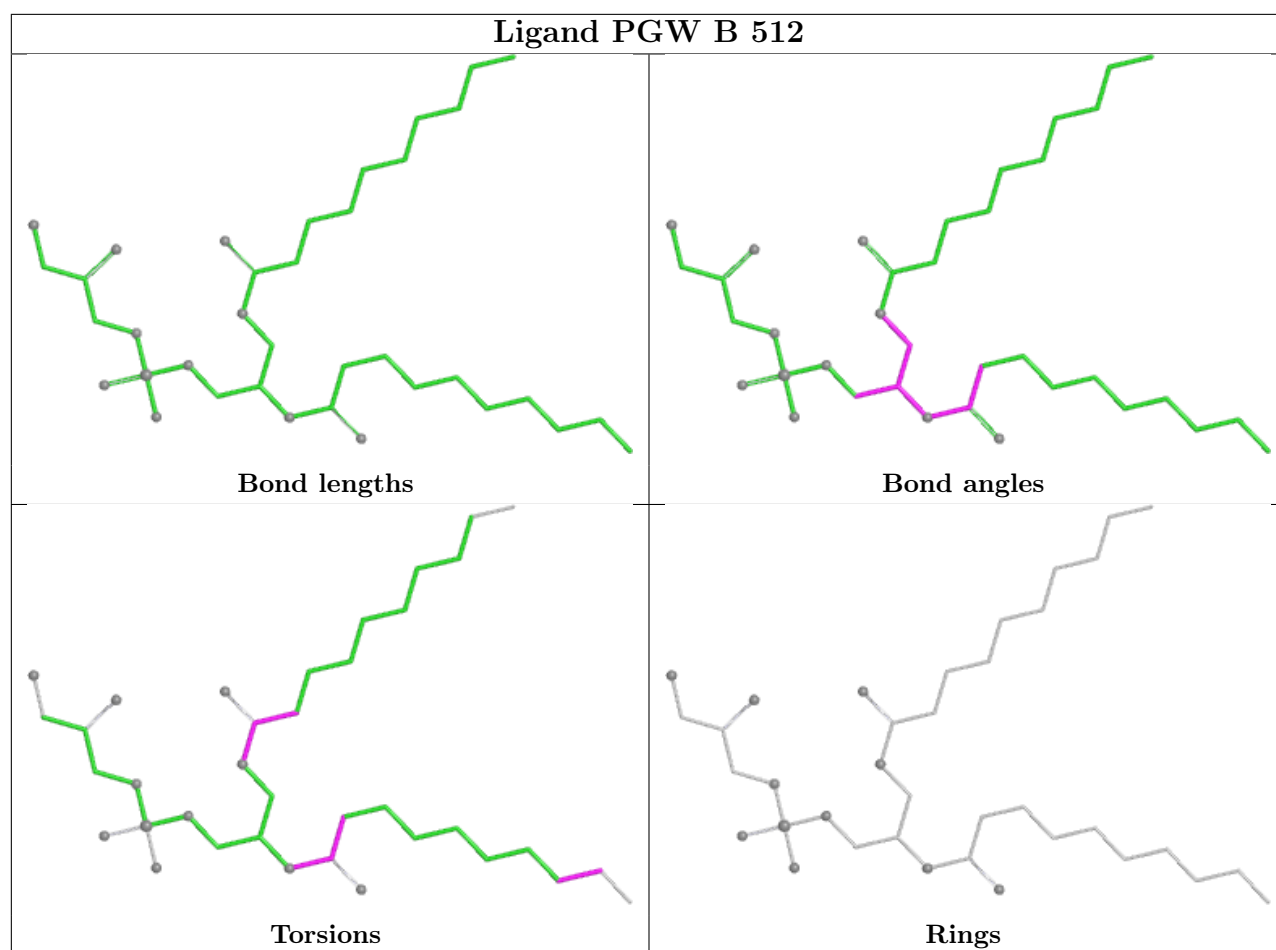
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1001	NAP	3	0
5	H	500	PGW	6	0
5	B	505	PGW	1	0
5	B	500	PGW	5	0
5	B	512	PGW	2	0
3	A	1001	NAP	1	0
5	B	510	PGW	1	0

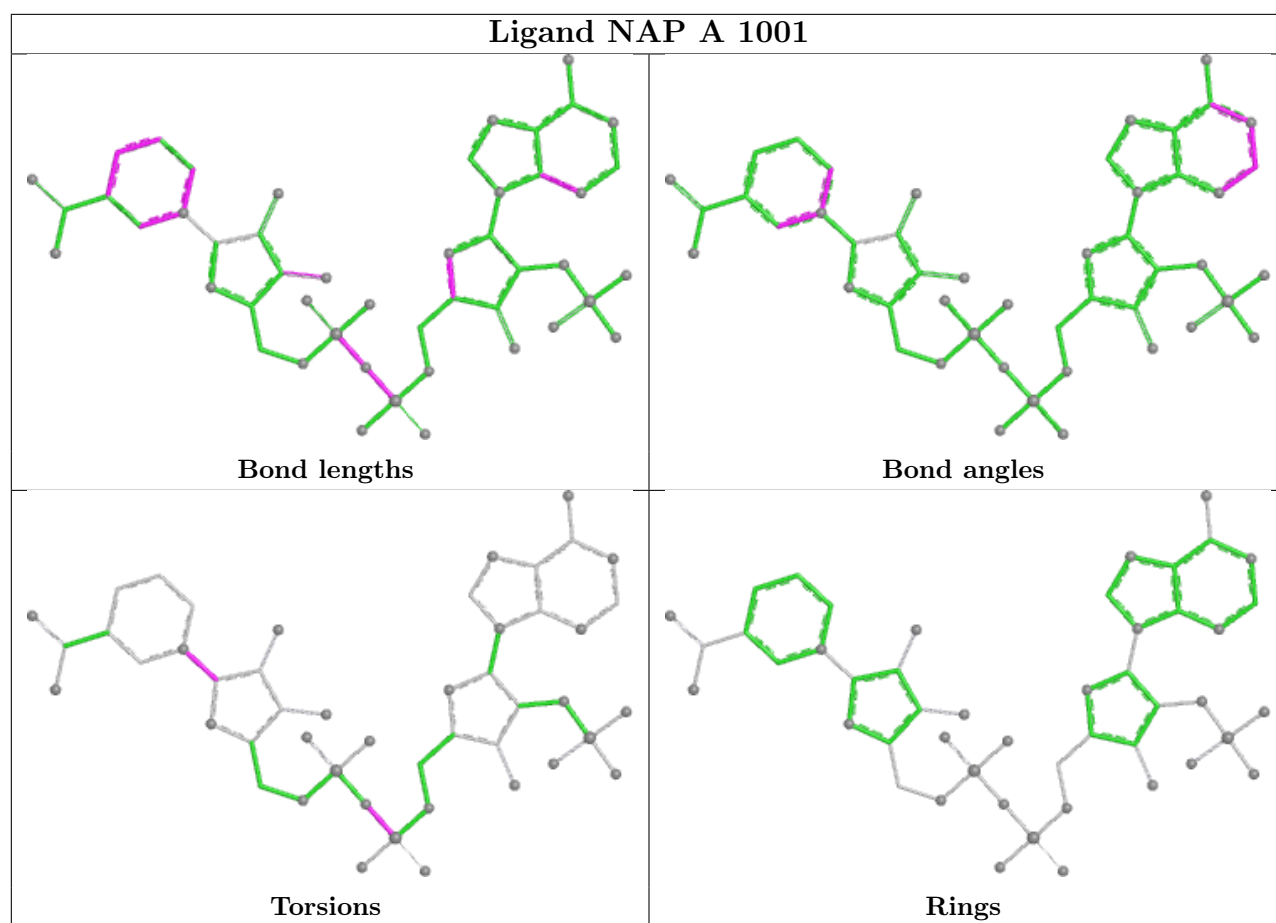
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

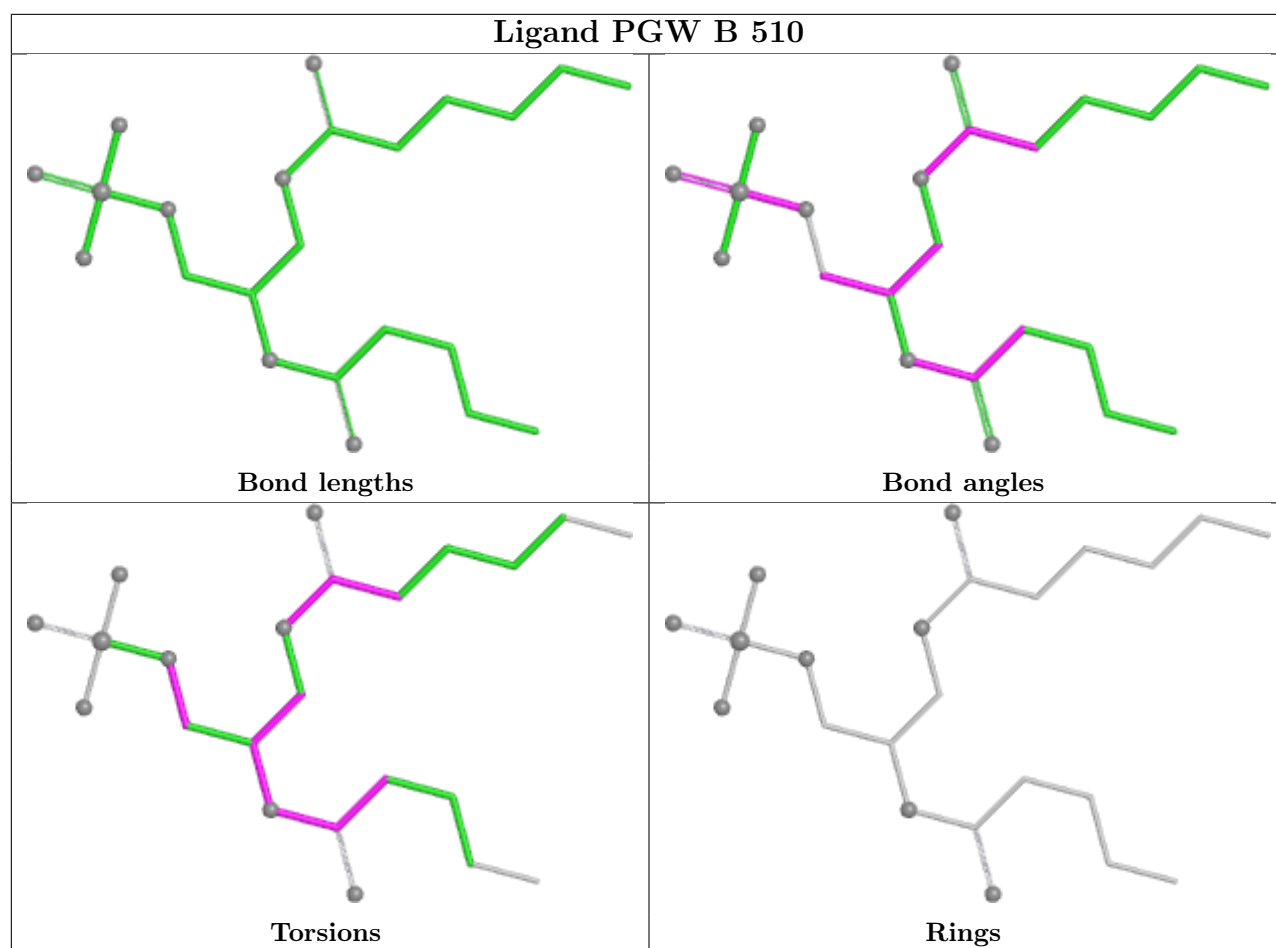












5.7 Other polymers [i](#)

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

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, 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%)	-0.24	7 (2%) 63 59	18, 32, 54, 74	0
1	G	326/333 (97%)	-0.05	8 (2%) 58 54	19, 34, 63, 82	0
2	B	386/514 (75%)	0.87	66 (17%) 4 3	25, 53, 98, 113	0
2	H	363/514 (70%)	2.58	186 (51%) 0 0	30, 85, 176, 185	0
All	All	1401/1694 (82%)	0.84	267 (19%) 3 2	18, 46, 153, 185	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	280	LEU	11.0
2	H	149	VAL	10.3
2	H	205	TYR	9.2
2	H	269	THR	9.2
2	H	272	LEU	9.1
2	B	143	ASN	8.9
2	H	279	VAL	8.3
2	H	282	PHE	8.0
2	H	294	ILE	7.9
2	H	288	VAL	7.9
2	H	153	PHE	7.8
2	H	167	ILE	7.7
2	H	270	ILE	7.5
2	H	273	THR	7.5
2	H	271	PHE	7.3
2	H	151	LEU	7.1
2	H	245	PRO	7.0
2	H	268	VAL	7.0
2	H	214	GLN	6.9
2	H	204	THR	6.9
1	G	360	TYR	6.9

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Mol	Chain	Res	Type	RSRZ
1	A	360	TYR	6.8
2	H	147	ARG	6.8
2	H	266	TYR	6.7
2	B	142	GLU	6.6
2	H	285	VAL	6.5
2	H	252	THR	6.4
2	H	150	TRP	6.4
2	H	238	LEU	6.3
2	H	417	THR	6.3
2	H	160	GLY	6.3
2	H	287	ARG	6.2
2	H	241	PHE	6.2
2	H	265	PRO	6.1
2	H	145	PHE	6.1
2	B	138	ARG	6.1
2	H	244	CYS	6.0
2	H	286	ARG	5.9
2	H	254	ILE	5.9
2	H	291	ILE	5.9
2	H	228	LEU	5.8
2	H	233	PHE	5.8
2	H	231	ILE	5.8
2	H	275	SER	5.7
2	H	161	PRO	5.7
2	H	164	ILE	5.6
2	H	218	PHE	5.6
2	H	219	THR	5.6
2	H	202	PHE	5.5
2	H	187	ILE	5.5
2	H	174	LEU	5.5
2	H	209	THR	5.5
2	B	133	ILE	5.4
2	B	141	PRO	5.4
2	H	267	TYR	5.4
2	B	140	LEU	5.4
2	H	217	SER	5.3
2	H	264	ILE	5.3
2	H	212	TYR	5.3
2	B	154	GLU	5.2
2	H	222	PHE	5.2
2	H	277	LYS	5.2
2	H	232	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
2	B	144	GLU	5.1
2	H	237	PHE	5.1
2	H	215	SER	5.1
2	B	139	PRO	5.0
2	H	156	PRO	5.0
2	H	251	PHE	5.0
2	H	240	ARG	4.9
2	H	257	ILE	4.9
2	H	152	LEU	4.9
2	H	210	ILE	4.9
2	H	242	PHE	4.9
2	H	289	VAL	4.9
2	H	247	LYS	4.8
1	G	36	LEU	4.8
2	H	148	GLN	4.8
2	H	283	GLN	4.7
1	A	36	LEU	4.7
2	H	211	GLY	4.7
2	H	235	PHE	4.7
2	H	350	ARG	4.6
2	H	248	ALA	4.6
2	H	168	VAL	4.6
2	H	239	VAL	4.6
2	H	206	SER	4.5
2	B	203	HIS	4.5
2	H	131	GLY	4.5
2	H	276	ASN	4.5
2	H	203	HIS	4.5
2	H	262	ALA	4.5
2	H	188	PHE	4.5
2	H	411	TYR	4.4
2	H	250	PHE	4.4
2	H	255	MET	4.3
2	H	284	ASN	4.3
2	B	193	GLU	4.3
2	H	295	MET	4.3
2	H	274	GLU	4.3
2	H	416	GLU	4.3
2	H	290	GLN	4.3
2	B	200	VAL	4.3
2	H	297	ILE	4.3
2	B	147	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	417	THR	4.2
2	B	274	GLU	4.2
2	H	292	PHE	4.2
1	G	361	SER	4.1
2	H	225	VAL	4.1
2	B	129	ASP	4.0
2	H	263	ILE	4.0
2	B	155	TYR	4.0
2	B	137	GLU	4.0
2	H	260	ILE	4.0
2	H	155	TYR	4.0
2	H	224	ILE	3.9
2	H	186	PRO	3.9
2	H	190	ASP	3.9
2	H	227	THR	3.9
2	H	293	ARG	3.9
2	H	163	ARG	3.8
2	H	298	LEU	3.8
2	H	178	VAL	3.8
2	H	351	ASP	3.8
2	H	216	THR	3.8
2	H	243	ALA	3.7
2	H	261	VAL	3.7
2	H	182	LEU	3.7
2	H	415	ARG	3.7
2	H	179	SER	3.7
2	H	281	GLN	3.7
2	H	208	SER	3.6
2	H	175	ILE	3.6
2	H	253	ASN	3.6
2	H	345	ALA	3.6
2	H	308	LYS	3.6
2	H	180	PHE	3.6
1	A	361	SER	3.5
2	H	278	SER	3.5
2	H	249	GLY	3.5
2	B	145	PHE	3.5
2	B	158	SER	3.4
2	H	226	GLU	3.4
2	B	194	ASP	3.4
2	H	146	GLN	3.4
2	H	221	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	32	SER	3.4
2	H	223	PHE	3.4
2	H	184	THR	3.4
2	H	414	HIS	3.4
2	H	322	ARG	3.3
2	H	348	ASP	3.3
2	H	191	GLU	3.3
2	B	136	GLU	3.3
2	H	165	ILE	3.3
2	H	300	ILE	3.3
2	H	259	ASP	3.2
2	H	158	SER	3.2
2	H	230	ILE	3.2
2	H	344	PHE	3.2
2	H	258	ILE	3.2
2	B	160	GLY	3.1
2	B	151	LEU	3.1
2	H	189	ARG	3.1
2	H	296	ARG	3.1
2	H	181	CYS	3.1
2	H	306	HIS	3.1
2	H	256	ASN	3.1
2	B	132	TYR	3.1
2	B	134	LYS	3.1
2	H	399	ALA	3.1
2	B	171	MET	3.1
2	H	120	GLU	3.1
2	H	171	MET	3.1
2	H	315	GLN	3.0
2	H	185	LEU	3.0
2	H	166	ALA	3.0
2	H	234	SER	3.0
2	H	183	GLU	3.0
2	B	152	LEU	3.0
2	B	251	PHE	3.0
2	B	199	GLY	3.0
2	H	400	LEU	2.9
2	B	240	ARG	2.9
2	B	146	GLN	2.9
1	G	349	HIS	2.9
2	H	170	VAL	2.9
2	H	409	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	121	GLU	2.9
2	H	349	GLU	2.9
2	H	303	LEU	2.8
2	H	125	MET	2.8
2	B	165	ILE	2.8
2	B	244	CYS	2.8
2	H	246	SER	2.8
2	H	154	GLU	2.8
2	H	207	GLN	2.8
2	H	410	ASN	2.8
2	H	302	LYS	2.8
2	B	205	TYR	2.7
2	B	215	SER	2.7
2	B	150	TRP	2.7
2	B	247	LYS	2.7
2	H	114	ARG	2.7
2	B	252	THR	2.7
2	H	299	ARG	2.6
2	H	305	ARG	2.6
1	A	231	GLU	2.6
2	B	114	ARG	2.6
2	H	213	GLN	2.6
2	B	156	PRO	2.6
2	H	157	GLU	2.6
1	G	314	ASN	2.6
2	H	413	TYR	2.6
2	B	125	MET	2.5
2	H	301	PHE	2.5
2	B	187	ILE	2.5
2	B	410	ASN	2.5
2	H	56	GLU	2.5
2	B	148	GLN	2.5
2	B	243	ALA	2.5
2	B	283	GLN	2.5
2	H	332	PHE	2.5
2	H	86	ASP	2.4
2	H	159	SER	2.4
2	H	129	ASP	2.4
2	H	412	PHE	2.4
2	H	220	ASP	2.4
2	B	213	GLN	2.4
2	B	128	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	381	ILE	2.4
2	B	242	PHE	2.4
2	H	128	GLU	2.4
2	B	351	ASP	2.3
2	B	277	LYS	2.3
2	B	149	VAL	2.3
2	B	287	ARG	2.3
2	B	248	ALA	2.2
2	B	249	GLY	2.2
2	B	231	ILE	2.2
2	B	135	GLU	2.2
2	B	239	VAL	2.2
2	H	229	CYS	2.2
1	A	349	HIS	2.2
2	B	86	ASP	2.2
2	B	157	GLU	2.2
2	H	172	VAL	2.2
1	G	268	LYS	2.2
1	G	280	GLU	2.2
2	B	332	PHE	2.2
2	H	321	MET	2.1
2	H	326	LEU	2.1
1	A	297	GLU	2.1
2	B	127	ARG	2.1
2	H	236	GLU	2.1
1	G	342	LYS	2.1
2	H	347	ALA	2.1
2	B	411	TYR	2.1
2	B	246	SER	2.1
2	H	177	ILE	2.1
2	B	395	VAL	2.1
2	H	337	LEU	2.1
2	H	304	SER	2.1
2	H	127	ARG	2.0
2	H	313	LEU	2.0
1	A	262	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

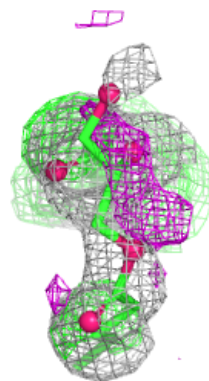
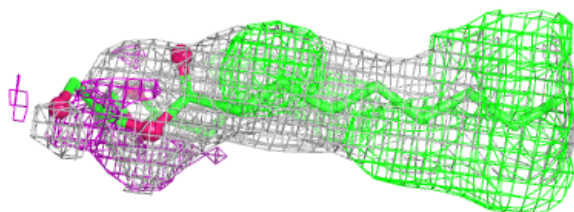
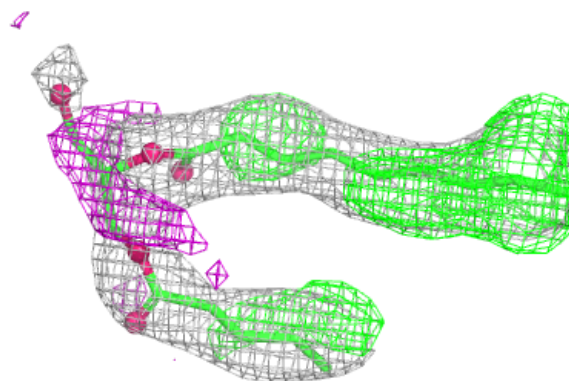
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PGW	B	504	9/51	0.69	0.40	83,84,85,85	0
5	PGW	B	500	22/51	0.70	0.37	61,65,68,69	0
5	PGW	B	512	37/51	0.72	0.30	81,99,121,123	0
5	PGW	H	500	22/51	0.72	0.38	82,90,92,92	0
5	PGW	B	502	9/51	0.74	0.38	83,84,84,84	0
5	PGW	B	501	9/51	0.76	0.41	82,84,86,86	0
5	PGW	B	511	12/51	0.76	0.37	76,79,80,80	0
5	PGW	B	510	23/51	0.77	0.30	100,103,111,111	0
5	PGW	B	515	12/51	0.78	0.36	88,89,89,89	0
5	PGW	B	514	12/51	0.78	0.37	87,88,89,89	0
5	PGW	B	503	9/51	0.79	0.39	90,91,91,91	0
5	PGW	B	513	10/51	0.80	0.30	63,64,66,66	0
5	PGW	B	509	12/51	0.82	0.30	67,67,68,68	0
5	PGW	B	507	7/51	0.82	0.31	72,73,74,74	0
5	PGW	B	506	9/51	0.83	0.30	74,76,79,79	0
5	PGW	B	505	9/51	0.86	0.28	65,66,67,67	0
5	PGW	B	508	9/51	0.87	0.27	76,77,77,77	0
4	K	H	498	1/1	0.91	0.07	51,51,51,51	1
4	K	H	496	1/1	0.92	0.09	49,49,49,49	1
4	K	H	497	1/1	0.94	0.10	51,51,51,51	1
4	K	B	496	1/1	0.95	0.07	38,38,38,38	1
4	K	H	499	1/1	0.98	0.07	51,51,51,51	1
3	NAP	A	1001	48/48	0.98	0.06	26,30,34,34	0
3	NAP	G	1001	48/48	0.98	0.06	27,30,37,37	0
4	K	B	497	1/1	0.99	0.03	35,35,35,35	1
4	K	B	499	1/1	1.00	0.03	35,35,35,35	1
4	K	B	498	1/1	1.00	0.03	29,29,29,29	1

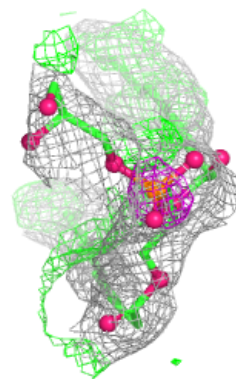
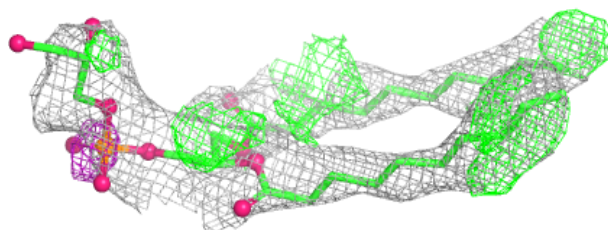
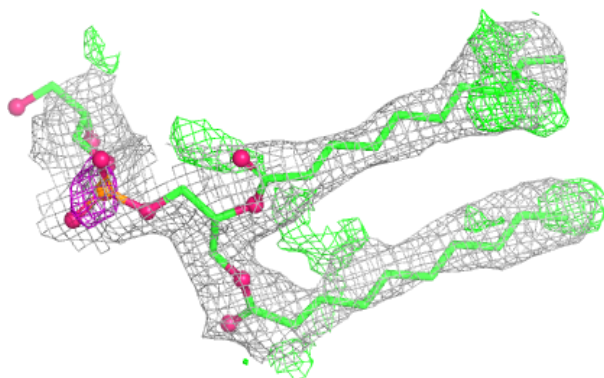
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGW B 500:

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

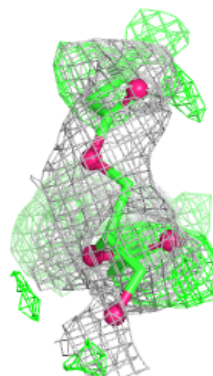
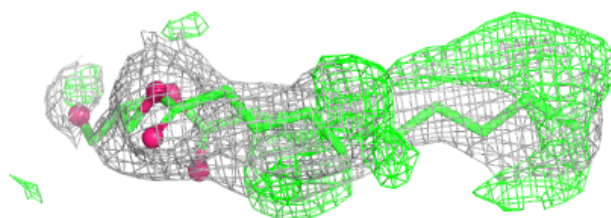
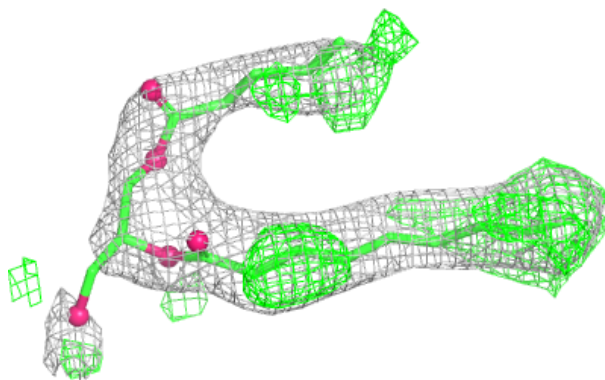
**Electron density around PGW B 512:**

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

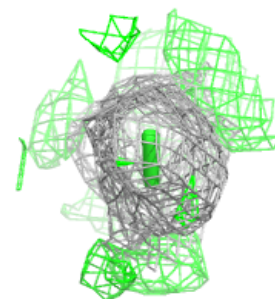
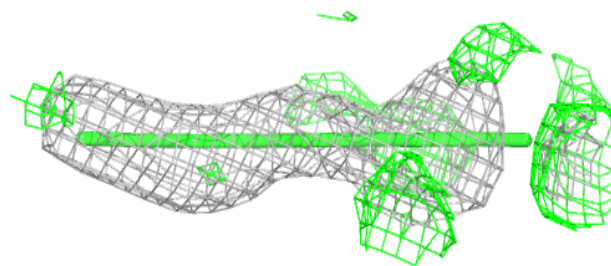
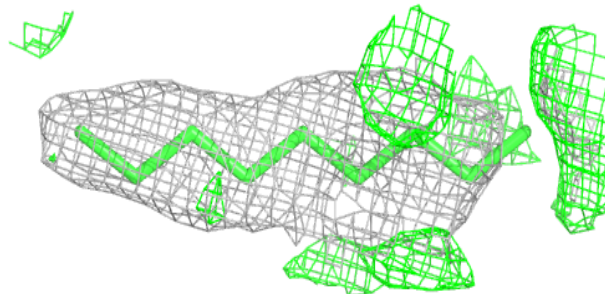


Electron density around PGW H 500:

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

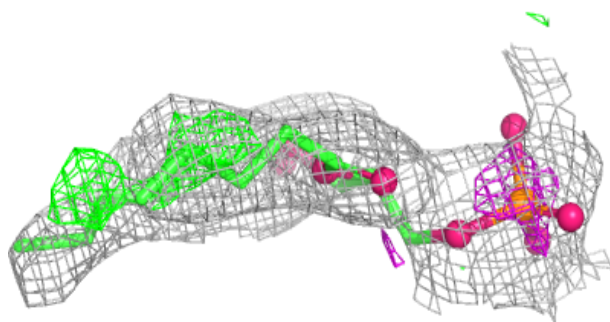
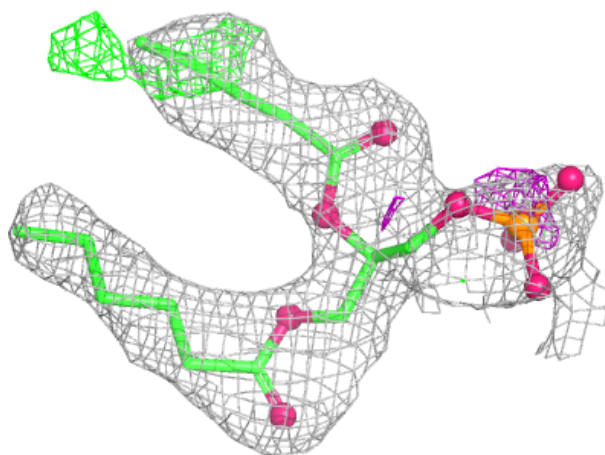
**Electron density around PGW B 501:**

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



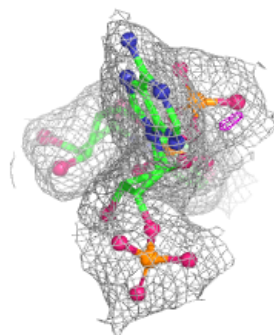
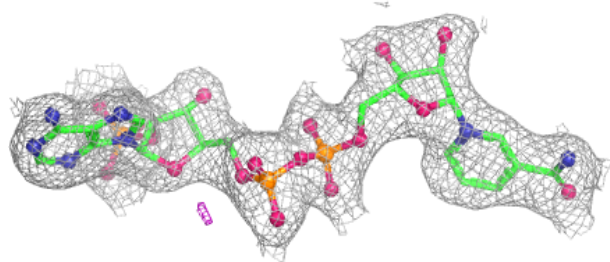
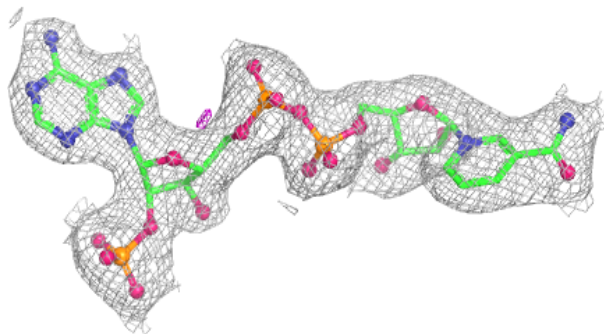
Electron density around PGW B 510:

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

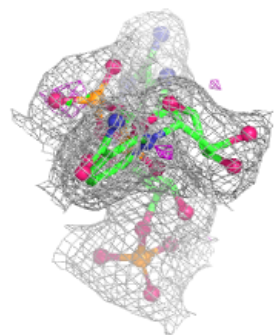
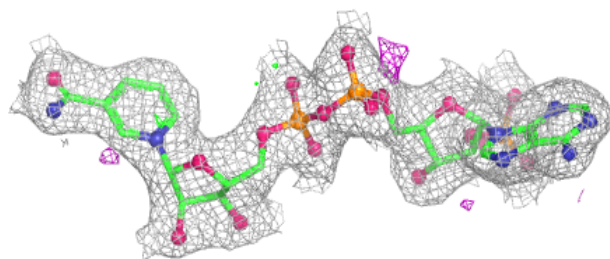
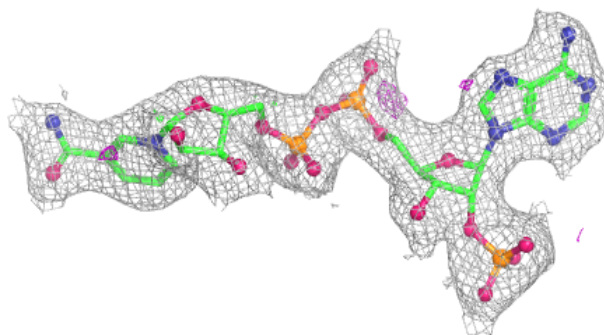


Electron density around NAP A 1001:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.