



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:31 AM UTC

PDB ID : 4JTC / pdb_00004jtc
Title : Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Charyb-dotoxin in Cs+
Authors : Banerjee, A.; Lee, A.; Campbell, E.; MacKinnon, R.
Deposited on : 2013-03-23
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

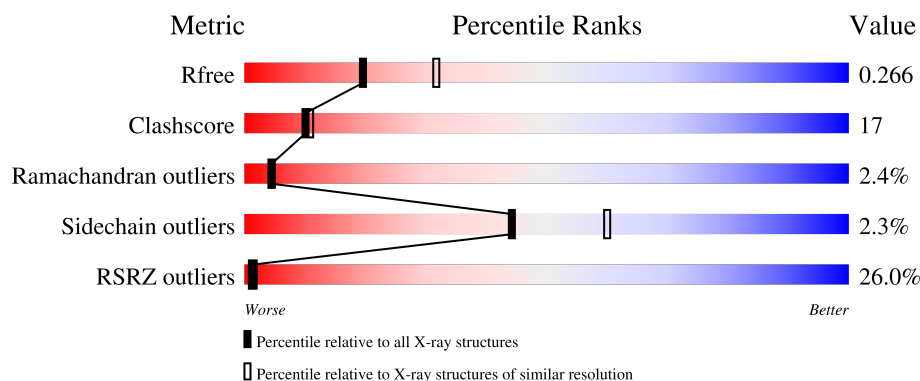
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 77% 19% ..
1	G	333	5% 77% 20% ..
2	B	514	17% 45% 27% • 25%
2	H	514	43% 36% 32% • 29%
3	Y	37	97% 92% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PGW	B	504	-	-	-	X
6	PGW	B	506	-	-	-	X
6	PGW	B	508	-	-	-	X
6	PGW	B	512	-	-	-	X
6	PGW	B	517	-	-	-	X
6	PGW	B	519	-	-	-	X
6	PGW	H	504	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11770 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Voltage-gated potassium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			
1	G	326	Total	C	N	O	S	0	0	0
			2556	1627	443	470	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP P62483
G	35	MET	-	expression tag	UNP P62483

- Molecule 2 is a protein called Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	386	Total	C	N	O	S	0	0	0
			3088	2022	504	548	14			
2	H	363	Total	C	N	O	S	0	0	0
			2959	1950	478	518	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	expression tag	UNP P63142
B	-17	ALA	-	expression tag	UNP P63142
B	-16	HIS	-	expression tag	UNP P63142
B	-15	HIS	-	expression tag	UNP P63142
B	-14	HIS	-	expression tag	UNP P63142
B	-13	HIS	-	expression tag	UNP P63142
B	-12	HIS	-	expression tag	UNP P63142
B	-11	HIS	-	expression tag	UNP P63142
B	-10	HIS	-	expression tag	UNP P63142

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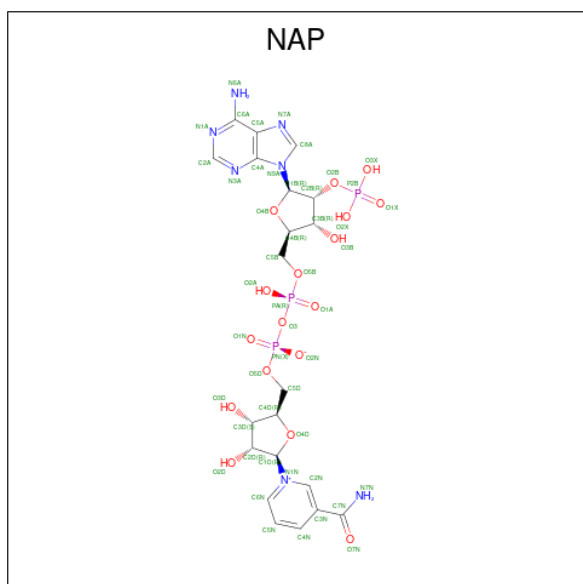
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P63142
B	-8	HIS	-	expression tag	UNP P63142
B	-7	HIS	-	expression tag	UNP P63142
B	-6	GLY	-	expression tag	UNP P63142
B	-5	LEU	-	expression tag	UNP P63142
B	-4	VAL	-	expression tag	UNP P63142
B	-3	PRO	-	expression tag	UNP P63142
B	-2	ARG	-	expression tag	UNP P63142
B	-1	GLY	-	expression tag	UNP P63142
B	0	SER	-	expression tag	UNP P63142
B	31	SER	CYS	engineered mutation	UNP P63142
B	32	SER	CYS	engineered mutation	UNP P63142
B	207	GLN	ASN	engineered mutation	UNP P63142
B	431	SER	CYS	engineered mutation	UNP P63142
B	478	SER	CYS	engineered mutation	UNP P63142
H	-18	MET	-	expression tag	UNP P63142
H	-17	ALA	-	expression tag	UNP P63142
H	-16	HIS	-	expression tag	UNP P63142
H	-15	HIS	-	expression tag	UNP P63142
H	-14	HIS	-	expression tag	UNP P63142
H	-13	HIS	-	expression tag	UNP P63142
H	-12	HIS	-	expression tag	UNP P63142
H	-11	HIS	-	expression tag	UNP P63142
H	-10	HIS	-	expression tag	UNP P63142
H	-9	HIS	-	expression tag	UNP P63142
H	-8	HIS	-	expression tag	UNP P63142
H	-7	HIS	-	expression tag	UNP P63142
H	-6	GLY	-	expression tag	UNP P63142
H	-5	LEU	-	expression tag	UNP P63142
H	-4	VAL	-	expression tag	UNP P63142
H	-3	PRO	-	expression tag	UNP P63142
H	-2	ARG	-	expression tag	UNP P63142
H	-1	GLY	-	expression tag	UNP P63142
H	0	SER	-	expression tag	UNP P63142
H	31	SER	CYS	engineered mutation	UNP P63142
H	32	SER	CYS	engineered mutation	UNP P63142
H	207	GLN	ASN	engineered mutation	UNP P63142
H	431	SER	CYS	engineered mutation	UNP P63142
H	478	SER	CYS	engineered mutation	UNP P63142

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	37	Total	C	N	O	S	0	0	0
			295	176	57	55	7			

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).

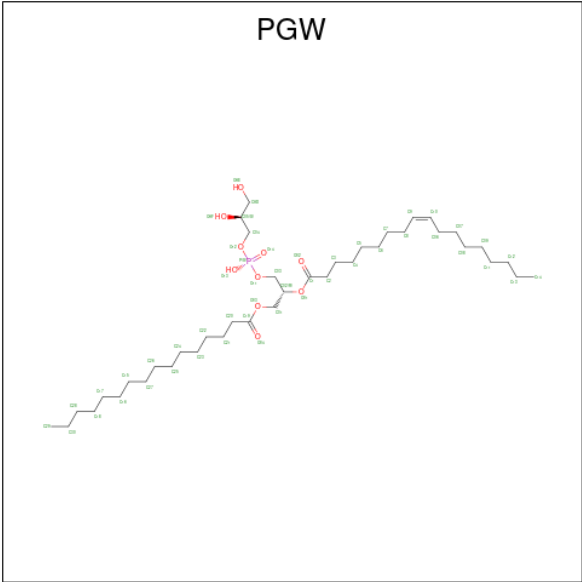


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is CESIUM ION (CCD ID: CS) (formula: Cs).

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

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 22 17 5	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 7 7	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C O P 23 14 8 1	0	0
6	B	1	Total C 8 8	0	0
6	B	1	Total C O P 36 25 10 1	0	0
6	B	1	Total C 7 7	0	0

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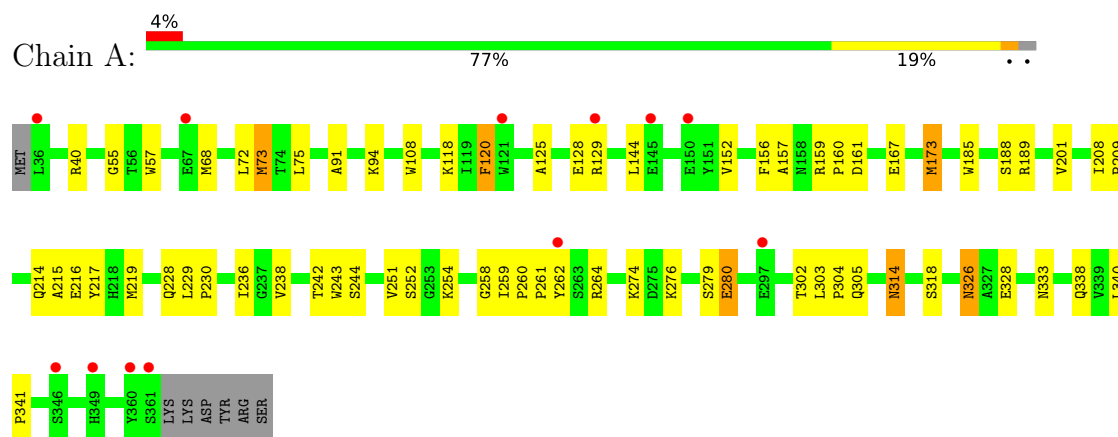
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C		0	0
			8	8			
6	B	1	Total	C		0	0
			8	8			
6	H	1	Total	C	O	0	0
			22	17	5		

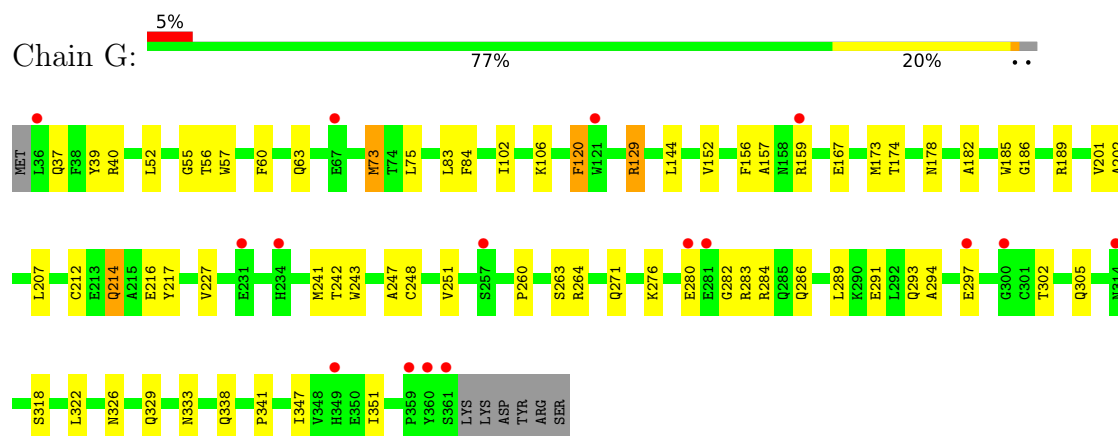
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

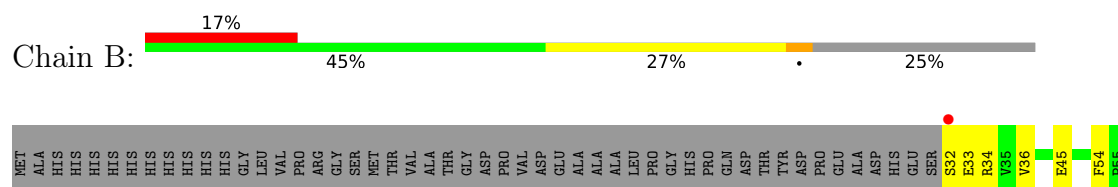
- Molecule 1: Voltage-gated potassium channel subunit beta-2

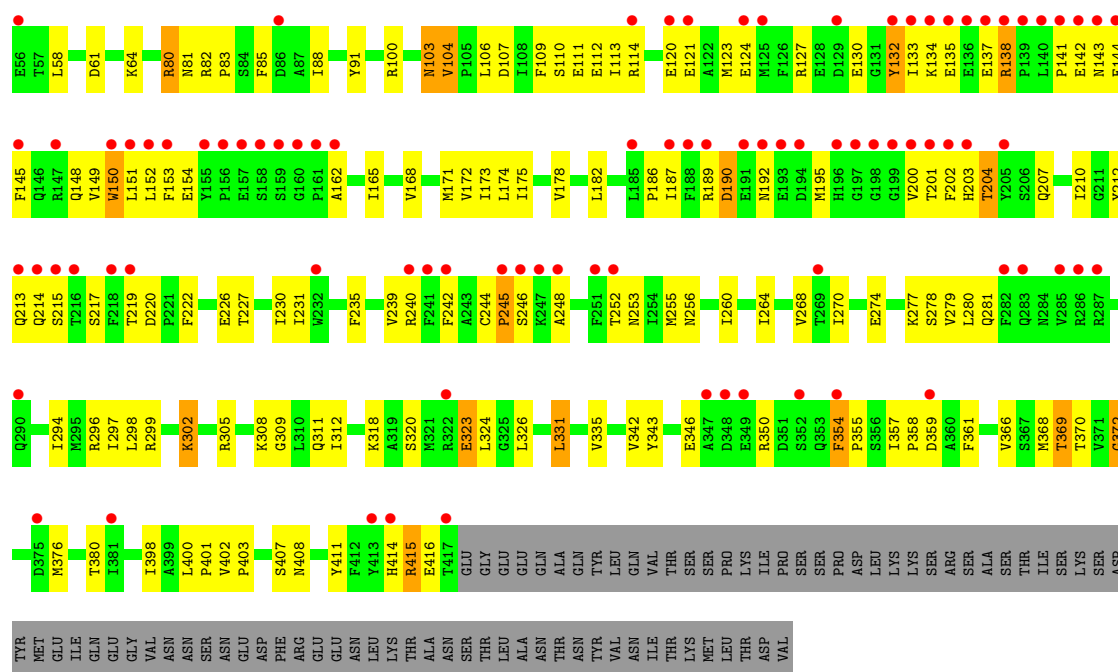


- Molecule 1: Voltage-gated potassium channel subunit beta-2

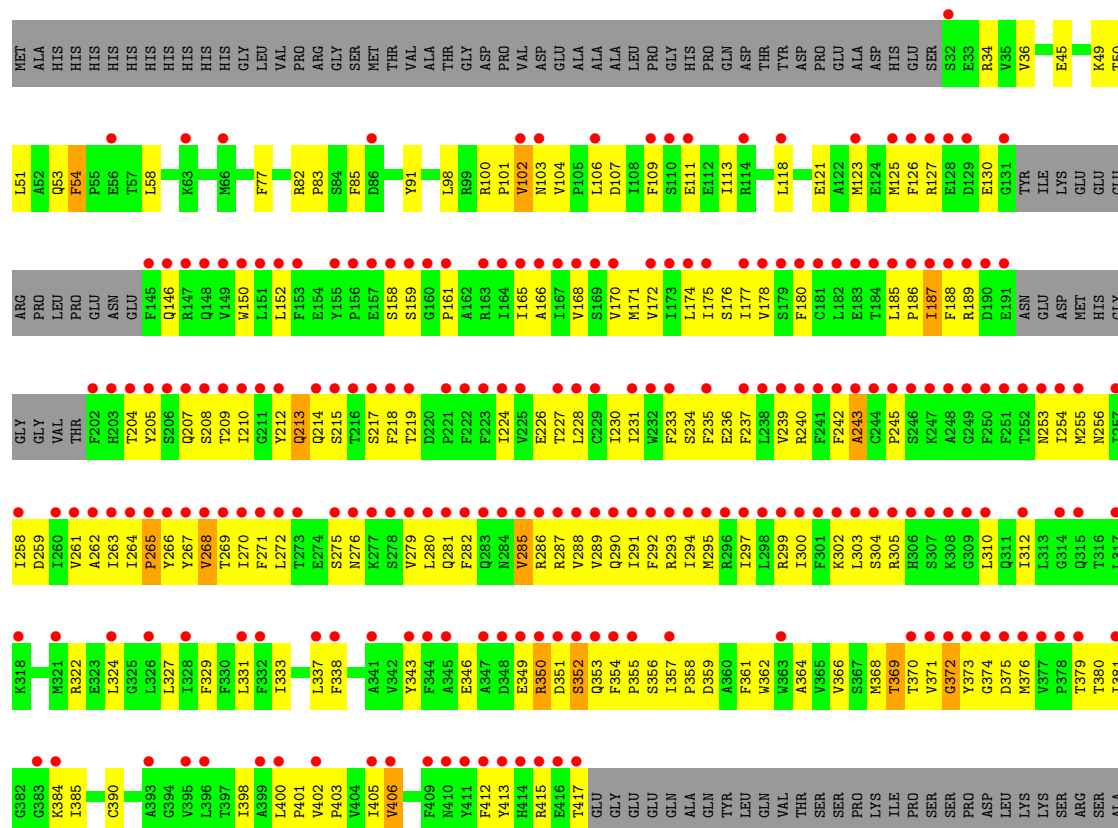


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



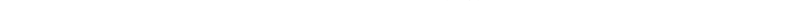


- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



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

- Molecule 3: Potassium channel toxin alpha-KTx 1.1

Chain Y: 

Q1	F2	T3	N4	V5	S6	C7	T8	T9	S10	K11	E12	C13	W14	S15	V16	C17	R18	R19	L20	H21	N22	T23	S24	R25	G26	K27	C28	M29	N30	K31	K32	C33	R34	C35	V36	S37
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	145.43Å 145.43Å 285.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 50.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	91.9 (50.00-2.56) 91.9 (50.00-2.56)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.262 0.238 , 0.266	Depositor DCC
R_{free} test set	4652 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11770	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.52	0/2608	0.92	6/3524 (0.2%)
1	G	0.47	0/2608	0.90	3/3524 (0.1%)
2	B	0.42	0/3169	0.92	12/4292 (0.3%)
2	H	0.34	0/3036	0.84	8/4114 (0.2%)
3	Y	0.27	0/292	0.65	0/389
All	All	0.43	0/11713	0.89	29/15843 (0.2%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	PHE	N-CA-C	7.49	120.40	111.33
2	H	369	THR	N-CA-C	-7.44	104.34	113.19
2	B	204	THR	N-CA-C	-7.25	104.96	113.88
1	G	227	VAL	N-CA-C	7.16	117.70	111.90
1	A	280	GLU	N-CA-C	-6.89	103.70	111.14
2	B	369	THR	N-CA-C	-6.80	105.09	113.19
1	A	157	ALA	N-CA-C	-6.67	98.33	108.67
1	G	157	ALA	N-CA-C	-6.54	97.88	108.41
2	B	354	PHE	CA-C-N	6.36	126.11	119.05
2	B	354	PHE	C-N-CA	6.36	126.11	119.05
2	B	252	THR	N-CA-C	-6.20	104.68	112.93
1	A	228	GLN	N-CA-C	6.13	120.93	112.90
2	H	85	PHE	N-CA-C	6.08	119.53	111.75
1	G	63	GLN	N-CA-C	5.98	118.58	111.71
2	H	293	ARG	N-CA-C	-5.71	106.66	113.97
2	B	54	PHE	CA-C-N	5.68	126.94	119.84
2	B	54	PHE	C-N-CA	5.68	126.94	119.84
2	H	54	PHE	CA-C-N	5.59	126.83	119.84
2	H	54	PHE	C-N-CA	5.59	126.83	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	VAL	N-CA-C	5.59	114.10	107.73
2	B	138	ARG	CA-C-N	5.59	125.90	119.92
2	B	138	ARG	C-N-CA	5.59	125.90	119.92
2	H	385	ILE	N-CA-C	-5.56	106.28	111.45
1	A	161	ASP	CA-C-N	5.50	125.17	119.56
1	A	161	ASP	C-N-CA	5.50	125.17	119.56
1	A	173	MET	N-CA-C	-5.45	105.42	111.36
2	H	77	PHE	N-CA-C	5.42	117.80	109.07
2	B	210	ILE	N-CA-C	5.39	116.45	111.81
2	H	295	MET	N-CA-C	-5.07	106.94	113.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2556	0	2582	45	0
1	G	2556	0	2582	48	0
2	B	3088	0	3034	130	0
2	H	2959	0	2956	172	0
3	Y	295	0	282	0	0
4	A	48	0	25	11	0
4	G	48	0	25	12	0
5	B	4	0	0	0	0
5	H	4	0	0	0	0
6	B	190	0	251	18	0
6	H	22	0	25	7	0
All	All	11770	0	11762	407	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.43	1.00
2:B:255:MET:HE1	2:B:305:ARG:HA	1.50	0.94
1:G:55:GLY:HA3	4:G:1001:NAP:O3D	1.68	0.93
2:H:213:GLN:HE21	2:H:215:SER:HB3	1.31	0.91
2:H:146:GLN:HB3	2:H:243:ALA:HA	1.51	0.90
1:A:55:GLY:HA3	4:A:1001:NAP:O3D	1.73	0.89
1:A:314:ASN:H	1:A:314:ASN:ND2	1.69	0.88
2:H:350:ARG:HH11	2:H:350:ARG:HB3	1.40	0.87
1:G:333:ASN:HD21	4:G:1001:NAP:H61A	1.22	0.87
2:H:358:PRO:HB3	6:H:504:PGW:H20A	1.61	0.83
1:G:40:ARG:HD2	1:G:318:SER:O	1.77	0.82
1:A:314:ASN:H	1:A:314:ASN:HD22	1.26	0.81
2:H:185:LEU:HD12	2:H:186:PRO:HD2	1.63	0.80
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.31	0.78
1:G:189:ARG:HH21	4:G:1001:NAP:H71N	1.32	0.78
2:H:358:PRO:HB3	6:H:504:PGW:C20	2.14	0.78
2:H:349:GLU:HB2	2:H:352:SER:HB2	1.66	0.76
2:B:311:GLN:HG2	6:B:516:PGW:H3	1.67	0.75
2:H:213:GLN:HE21	2:H:215:SER:CB	2.01	0.73
1:G:293:GLN:O	1:G:297:GLU:HG3	1.89	0.72
2:H:412:PHE:HD1	2:H:415:ARG:HH21	1.34	0.72
2:B:400:LEU:O	2:B:403:PRO:HD2	1.88	0.72
2:B:227:THR:O	2:B:231:ILE:HG12	1.88	0.72
1:G:129:ARG:HB3	1:G:129:ARG:HH11	1.53	0.72
2:H:113:ILE:HG23	2:H:118:LEU:HD12	1.72	0.71
2:B:253:ASN:ND2	2:B:255:MET:HB2	2.04	0.71
2:H:177:ILE:HD11	2:H:300:ILE:HA	1.71	0.71
2:H:270:ILE:HD12	2:H:270:ILE:H	1.55	0.71
2:H:366:VAL:HG12	2:H:372:GLY:HA2	1.73	0.71
2:B:103:ASN:H	2:B:103:ASN:HD22	1.39	0.70
2:H:400:LEU:HB2	2:H:401:PRO:HD3	1.72	0.70
2:H:375:ASP:O	2:H:376:MET:HG3	1.92	0.70
2:B:120:GLU:O	2:B:124:GLU:HG3	1.92	0.69
1:A:258:GLY:O	1:A:260:PRO:HD3	1.92	0.69
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.72	0.69
2:H:364:ALA:O	2:H:368:MET:HG3	1.93	0.67
2:B:100:ARG:NH1	2:B:106:LEU:HB2	2.10	0.67
2:B:226:GLU:O	2:B:230:ILE:HD13	1.94	0.67
2:H:109:PHE:CE2	2:H:113:ILE:HD11	2.28	0.66
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.11	0.66
1:A:314:ASN:HD22	1:A:314:ASN:N	1.92	0.65
2:H:230:ILE:HG12	2:H:266:TYR:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1001:NAP:H52A	4:G:1001:NAP:H8A	1.77	0.65
1:G:338:GLN:O	1:G:341:PRO:HD2	1.96	0.65
2:H:350:ARG:HH11	2:H:350:ARG:CB	2.09	0.65
4:A:1001:NAP:H8A	4:A:1001:NAP:H52A	1.79	0.65
2:B:61:ASP:HB3	2:B:64:LYS:HB2	1.79	0.65
2:B:366:VAL:HG12	2:B:372:GLY:HA2	1.80	0.64
2:B:416:GLU:HA	6:B:516:PGW:HADA	1.78	0.64
2:B:414:HIS:C	2:B:416:GLU:H	2.04	0.63
2:B:323:GLU:CD	2:B:323:GLU:H	2.06	0.63
2:H:276:ASN:HB3	2:H:282:PHE:HB2	1.80	0.63
1:G:83:LEU:HD21	1:G:241:MET:HE2	1.79	0.63
2:H:276:ASN:OD1	2:H:281:GLN:HG2	1.99	0.63
2:H:253:ASN:HD21	2:H:255:MET:HE3	1.64	0.63
2:B:253:ASN:HD21	2:B:255:MET:HB2	1.63	0.62
2:H:213:GLN:NE2	2:H:215:SER:HB3	2.09	0.62
2:H:402:VAL:O	2:H:406:VAL:HG23	1.99	0.62
2:H:207:GLN:HE21	2:H:213:GLN:HA	1.64	0.62
2:B:58:LEU:HD12	2:B:64:LYS:HB3	1.80	0.62
2:H:270:ILE:HD12	2:H:270:ILE:N	2.15	0.62
2:H:305:ARG:HH11	2:H:305:ARG:HG2	1.65	0.62
2:B:149:VAL:C	2:B:151:LEU:H	2.07	0.62
2:H:210:ILE:HD11	2:H:214:GLN:N	2.15	0.62
2:H:354:PHE:CE1	2:H:376:MET:HE2	2.35	0.62
2:B:400:LEU:CB	2:B:401:PRO:HD3	2.25	0.61
2:H:331:LEU:HD11	2:H:398:ILE:HG12	1.82	0.61
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.15	0.61
2:H:362:TRP:HB2	6:H:504:PGW:H2A	1.82	0.61
2:H:302:LYS:HA	2:H:302:LYS:HE2	1.82	0.61
2:H:230:ILE:HD12	2:H:230:ILE:N	2.16	0.61
2:B:187:ILE:HG21	6:B:512:PGW:H2A	1.82	0.61
2:H:294:ILE:O	2:H:297:ILE:HG22	2.01	0.61
2:B:100:ARG:HH11	2:B:106:LEU:HB2	1.65	0.60
2:H:381:ILE:HD12	2:H:381:ILE:H	1.65	0.60
2:B:331:LEU:O	2:B:335:VAL:HG23	2.01	0.60
1:A:91:ALA:O	1:A:94:LYS:HB2	2.01	0.60
2:H:58:LEU:C	2:H:58:LEU:HD23	2.25	0.60
1:G:302:THR:OG1	1:G:305:GLN:HG3	2.02	0.59
2:H:212:TYR:O	2:H:213:GLN:HB2	2.01	0.59
2:B:186:PRO:O	2:B:190:ASP:HB2	2.02	0.59
2:H:36:VAL:HG22	2:H:45:GLU:HG3	1.83	0.59
2:H:357:ILE:HB	2:H:358:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:398:ILE:HG22	2:H:398:ILE:O	2.03	0.58
1:G:55:GLY:HA3	4:G:1001:NAP:HO3N	1.69	0.58
2:H:264:ILE:HB	2:H:265:PRO:HD3	1.86	0.58
2:H:381:ILE:HD12	2:H:381:ILE:N	2.18	0.58
6:B:516:PGW:O02	6:B:516:PGW:H03A	2.04	0.58
2:H:161:PRO:O	2:H:165:ILE:HG13	2.04	0.58
2:B:171:MET:O	2:B:175:ILE:HG13	2.03	0.58
1:G:120:PHE:CD1	1:G:159:ARG:HG3	2.39	0.57
2:H:402:VAL:HB	2:H:403:PRO:HD3	1.86	0.57
2:H:207:GLN:NE2	2:H:213:GLN:HG3	2.18	0.57
2:H:231:ILE:O	2:H:235:PHE:HB2	2.04	0.57
2:B:142:GLU:O	2:B:144:GLU:N	2.34	0.57
2:H:415:ARG:HG2	2:H:415:ARG:HH11	1.69	0.57
1:A:259:ILE:HG13	1:A:274:LYS:HE3	1.86	0.57
2:B:201:THR:HB	2:B:204:THR:OG1	2.05	0.57
2:B:222:PHE:CE1	6:B:513:PGW:H15A	2.39	0.57
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.40	0.56
2:B:213:GLN:HE22	2:B:219:THR:HB	1.70	0.56
1:G:280:GLU:HG2	1:G:284:ARG:NH1	2.19	0.56
1:A:251:VAL:O	1:A:251:VAL:HG12	2.05	0.56
2:B:152:LEU:N	2:B:152:LEU:HD12	2.21	0.56
1:A:125:ALA:HB3	1:A:128:GLU:HG3	1.85	0.56
2:H:152:LEU:HD22	2:H:161:PRO:HG2	1.87	0.56
2:H:400:LEU:O	2:H:403:PRO:HD2	2.06	0.56
2:B:152:LEU:HA	2:B:162:ALA:HB1	1.87	0.56
2:H:354:PHE:CD1	2:H:376:MET:HE2	2.40	0.56
2:H:346:GLU:HG2	2:H:380:THR:CG2	2.35	0.56
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.40	0.56
2:B:278:SER:OG	2:B:281:GLN:HG3	2.06	0.55
2:B:400:LEU:HB2	2:B:401:PRO:CD	2.27	0.55
1:G:214:GLN:HA	1:G:241:MET:O	2.06	0.55
2:H:91:TYR:CE2	2:H:118:LEU:HD22	2.42	0.55
2:H:101:PRO:HB2	2:H:104:VAL:HG23	1.89	0.55
2:H:82:ARG:HB2	2:H:83:PRO:HD3	1.87	0.55
2:H:171:MET:HE1	2:H:174:LEU:HD12	1.89	0.55
1:A:159:ARG:HA	1:A:188:SER:O	2.06	0.55
2:H:180:PHE:CE2	2:H:297:ILE:HD13	2.42	0.55
2:H:355:PRO:HB2	2:H:359:ASP:OD2	2.07	0.55
2:B:277:LYS:HG3	2:B:277:LYS:O	2.07	0.55
2:H:368:MET:C	2:H:370:THR:H	2.15	0.55
2:B:103:ASN:HD22	2:B:103:ASN:N	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:286:GLN:HA	1:G:289:LEU:HD12	1.88	0.54
6:B:514:PGW:O11	6:B:514:PGW:O02	2.26	0.54
1:G:144:LEU:HD21	1:G:152:VAL:HG13	1.89	0.54
2:H:121:GLU:O	2:H:125:MET:HB2	2.08	0.54
2:H:327:LEU:O	2:H:331:LEU:HD13	2.08	0.54
2:H:230:ILE:HG12	2:H:266:TYR:CB	2.38	0.54
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.89	0.54
2:H:152:LEU:O	2:H:165:ILE:HD12	2.08	0.54
2:H:285:VAL:HG22	2:H:285:VAL:O	2.08	0.54
2:B:354:PHE:CD1	2:B:376:MET:HE2	2.43	0.54
2:H:107:ASP:O	2:H:111:GLU:HG3	2.07	0.54
1:G:216:GLU:HB2	1:G:243:TRP:CH2	2.43	0.54
1:G:264:ARG:NH2	4:G:1001:NAP:H4B	2.22	0.54
1:A:276:LYS:O	1:A:279:SER:HB3	2.08	0.54
2:H:253:ASN:HB3	2:H:256:ASN:OD1	2.08	0.54
2:B:355:PRO:HB2	2:B:359:ASP:OD2	2.08	0.53
1:G:251:VAL:HG12	1:G:251:VAL:O	2.08	0.53
2:H:267:TYR:C	2:H:269:THR:H	2.16	0.53
2:H:236:GLU:HA	2:H:239:VAL:CG2	2.38	0.53
2:H:324:LEU:HD13	2:H:405:ILE:HD13	1.91	0.53
2:B:246:SER:C	2:B:248:ALA:H	2.17	0.53
2:B:201:THR:HG22	2:B:202:PHE:N	2.23	0.53
1:G:280:GLU:HG2	1:G:284:ARG:HH12	1.73	0.53
2:B:127:ARG:HG2	2:B:132:TYR:HB2	1.90	0.53
2:B:294:ILE:O	2:B:297:ILE:HG22	2.09	0.53
2:B:36:VAL:HG22	2:B:45:GLU:HG2	1.92	0.52
2:B:88:ILE:O	2:B:91:TYR:HB3	2.10	0.52
2:H:210:ILE:HD11	2:H:213:GLN:C	2.35	0.52
2:H:224:ILE:O	2:H:228:LEU:HG	2.09	0.52
2:H:374:GLY:C	2:H:376:MET:H	2.18	0.52
2:H:287:ARG:HG2	2:H:290:GLN:OE1	2.10	0.52
2:H:303:LEU:O	2:H:310:LEU:HD23	2.10	0.52
2:H:361:PHE:HB3	6:H:504:PGW:H4	1.91	0.52
1:G:247:ALA:O	1:G:248:CYS:HB2	2.10	0.52
1:G:120:PHE:O	1:G:129:ARG:HA	2.10	0.52
2:H:210:ILE:HG21	2:H:269:THR:HG23	1.91	0.52
2:B:110:SER:O	2:B:114:ARG:HG3	2.10	0.51
2:H:230:ILE:HD12	2:H:230:ILE:H	1.73	0.51
2:B:153:PHE:CE1	2:B:165:ILE:HD13	2.45	0.51
2:B:368:MET:C	2:B:370:THR:H	2.18	0.51
1:G:291:GLU:O	1:G:294:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:268:VAL:HG12	2:H:268:VAL:O	2.10	0.51
6:H:504:PGW:H01	6:H:504:PGW:O02	2.09	0.51
1:A:302:THR:OG1	1:A:305:GLN:HG3	2.10	0.51
2:B:178:VAL:O	2:B:182:LEU:HG	2.10	0.51
1:G:37:GLN:NE2	1:G:37:GLN:HA	2.25	0.51
2:H:279:VAL:HG12	2:H:279:VAL:O	2.11	0.51
2:B:255:MET:CE	2:B:305:ARG:HA	2.32	0.51
2:H:381:ILE:H	2:H:381:ILE:CD1	2.24	0.51
6:B:510:PGW:H2	6:B:515:PGW:H16	1.93	0.51
2:H:168:VAL:O	2:H:172:VAL:HG23	2.11	0.51
2:H:210:ILE:HD12	2:H:212:TYR:CE1	2.46	0.50
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.94	0.50
2:B:203:HIS:HE1	2:B:277:LYS:NZ	2.09	0.50
2:B:414:HIS:O	2:B:416:GLU:N	2.39	0.50
1:G:217:TYR:HB3	1:G:242:THR:HB	1.93	0.50
2:B:107:ASP:O	2:B:111:GLU:HG3	2.12	0.50
2:H:205:TYR:CE2	2:H:279:VAL:HG13	2.47	0.50
1:A:216:GLU:HB2	1:A:243:TRP:CH2	2.45	0.50
6:B:504:PGW:H01	6:B:504:PGW:O02	2.12	0.50
1:G:189:ARG:NH2	4:G:1001:NAP:H71N	2.04	0.50
2:H:213:GLN:HG2	2:H:215:SER:HB3	1.94	0.50
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.76	0.50
2:H:152:LEU:HD22	2:H:161:PRO:CG	2.42	0.50
2:H:353:GLN:O	2:H:355:PRO:HD3	2.10	0.50
2:H:150:TRP:HB2	2:H:243:ALA:HB1	1.93	0.49
2:H:415:ARG:C	2:H:417:THR:H	2.20	0.49
1:A:144:LEU:HD21	1:A:152:VAL:HG13	1.93	0.49
1:A:217:TYR:HB3	1:A:242:THR:HB	1.95	0.49
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.94	0.49
2:H:322:ARG:HG3	2:H:322:ARG:HH11	1.77	0.49
1:A:120:PHE:O	1:A:129:ARG:HA	2.13	0.49
6:B:510:PGW:C2	6:B:515:PGW:H16	2.42	0.49
1:G:55:GLY:CA	4:G:1001:NAP:O3D	2.50	0.49
1:A:55:GLY:CA	4:A:1001:NAP:O3D	2.52	0.49
2:B:152:LEU:HA	2:B:162:ALA:CB	2.42	0.49
2:H:106:LEU:HD11	2:H:130:GLU:HG2	1.92	0.49
2:H:176:SER:HB2	2:H:299:ARG:NH1	2.27	0.49
2:H:177:ILE:O	2:H:180:PHE:HB3	2.12	0.49
2:H:302:LYS:C	2:H:304:SER:H	2.20	0.49
2:B:145:PHE:O	2:B:148:GLN:HB3	2.13	0.49
2:B:297:ILE:C	2:B:299:ARG:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:GLN:HG3	2:H:242:PHE:O	2.12	0.49
2:H:212:TYR:CE2	2:H:226:GLU:HG2	2.46	0.49
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.93	0.49
2:B:299:ARG:O	2:B:302:LYS:HB2	2.12	0.49
2:B:320:SER:O	2:B:324:LEU:HB2	2.12	0.49
2:B:369:THR:HA	2:B:398:ILE:HD11	1.94	0.49
2:B:150:TRP:CE2	2:B:154:GLU:HG2	2.48	0.49
2:B:361:PHE:HB2	6:B:504:PGW:H2	1.94	0.49
1:G:73:MET:HE3	1:G:84:PHE:CD2	2.47	0.49
2:H:259:ASP:CG	2:H:305:ARG:HH21	2.21	0.49
1:A:57:TRP:HB3	4:A:1001:NAP:H3D	1.93	0.49
2:B:109:PHE:CE2	2:B:113:ILE:HD11	2.48	0.49
6:H:504:PGW:O02	6:H:504:PGW:H03A	2.12	0.49
2:H:187:ILE:HG22	2:H:187:ILE:O	2.13	0.48
2:H:224:ILE:HD12	2:H:224:ILE:N	2.27	0.48
1:A:326:ASN:HD22	1:A:328:GLU:H	1.61	0.48
2:B:110:SER:HB2	2:B:123:MET:HE1	1.94	0.48
2:H:127:ARG:HH11	2:H:127:ARG:HG2	1.78	0.48
2:B:414:HIS:C	2:B:416:GLU:N	2.69	0.48
2:B:260:ILE:O	2:B:264:ILE:HG13	2.14	0.48
2:H:287:ARG:HH11	2:H:287:ARG:HB3	1.79	0.48
2:B:318:LYS:HD2	6:B:516:PGW:H22	1.95	0.48
6:B:510:PGW:C1	6:B:515:PGW:H16	2.43	0.48
1:G:52:LEU:HD13	1:G:322:LEU:HD11	1.95	0.48
1:G:333:ASN:ND2	4:G:1001:NAP:H61A	2.01	0.48
2:H:171:MET:HB3	2:H:175:ILE:HD12	1.96	0.48
2:B:235:PHE:O	2:B:239:VAL:HG23	2.13	0.48
2:H:123:MET:O	2:H:127:ARG:HG3	2.13	0.48
2:B:153:PHE:CE2	2:B:239:VAL:HG11	2.48	0.48
1:G:156:PHE:HA	1:G:186:GLY:O	2.13	0.48
2:H:234:SER:HA	2:H:237:PHE:HB2	1.96	0.48
2:H:152:LEU:HA	2:H:158:SER:OG	2.14	0.48
2:H:204:THR:HG23	2:H:208:SER:OG	2.13	0.47
2:B:127:ARG:CG	2:B:132:TYR:HB2	2.43	0.47
1:A:229:LEU:N	1:A:230:PRO:CD	2.77	0.47
2:B:240:ARG:NH2	2:B:305:ARG:HD3	2.29	0.47
2:H:231:ILE:O	2:H:231:ILE:HG22	2.13	0.47
2:H:280:LEU:HD12	2:H:280:LEU:N	2.30	0.47
2:H:358:PRO:HB3	6:H:504:PGW:H20	1.94	0.47
2:B:215:SER:C	2:B:217:SER:H	2.22	0.47
2:B:309:GLY:HA2	2:B:312:ILE:HD12	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:180:PHE:HE2	2:H:297:ILE:HD13	1.77	0.47
2:B:311:GLN:HA	6:B:516:PGW:H5	1.96	0.47
4:A:1001:NAP:H52N	4:A:1001:NAP:H6N	1.97	0.47
2:B:149:VAL:C	2:B:151:LEU:N	2.73	0.47
1:G:329:GLN:OE1	4:G:1001:NAP:H2B	2.14	0.47
2:H:127:ARG:HG2	2:H:127:ARG:NH1	2.30	0.47
2:B:246:SER:C	2:B:248:ALA:N	2.73	0.47
2:H:253:ASN:ND2	2:H:255:MET:HE3	2.28	0.47
2:H:327:LEU:HD11	2:H:398:ILE:HG23	1.97	0.47
2:B:264:ILE:O	2:B:268:VAL:HG23	2.15	0.47
2:B:366:VAL:CG1	2:B:372:GLY:HA2	2.44	0.47
2:B:174:LEU:O	2:B:178:VAL:HG23	2.15	0.46
2:H:175:ILE:HG22	2:H:175:ILE:O	2.14	0.46
2:H:366:VAL:O	2:H:372:GLY:N	2.45	0.46
2:H:369:THR:OG1	2:H:371:VAL:HG23	2.15	0.46
2:B:240:ARG:HH21	2:B:305:ARG:HD3	1.81	0.46
1:A:215:ALA:O	1:A:242:THR:HA	2.15	0.46
2:B:173:ILE:HD13	2:B:302:LYS:HB3	1.98	0.46
2:B:200:VAL:HG23	2:B:200:VAL:O	2.15	0.46
2:B:350:ARG:NH1	2:B:350:ARG:CB	2.79	0.46
1:G:37:GLN:HA	1:G:37:GLN:HE21	1.80	0.46
2:H:254:ILE:C	2:H:256:ASN:H	2.23	0.46
2:B:80:ARG:NH1	2:B:112:GLU:OE1	2.48	0.46
2:B:368:MET:C	2:B:370:THR:N	2.73	0.46
1:G:167:GLU:HA	1:G:201:VAL:HG11	1.97	0.46
2:H:53:GLN:HB3	2:H:54:PHE:CD1	2.51	0.46
1:A:188:SER:O	1:A:189:ARG:HB2	2.16	0.46
2:B:202:PHE:HB2	2:B:279:VAL:HG22	1.98	0.46
2:B:320:SER:HA	2:B:323:GLU:OE2	2.16	0.46
1:G:37:GLN:HG3	1:G:39:TYR:O	2.16	0.46
2:H:240:ARG:HH12	2:H:305:ARG:CD	2.29	0.46
2:H:312:ILE:HD13	2:H:413:TYR:HA	1.98	0.46
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.31	0.46
2:H:98:LEU:HD21	2:H:113:ILE:HD13	1.97	0.46
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.52	0.45
1:A:254:LYS:HE3	4:A:1001:NAP:N3A	2.32	0.45
2:B:207:GLN:O	2:B:207:GLN:HG2	2.17	0.45
2:B:212:TYR:CE2	2:B:226:GLU:HG2	2.51	0.45
1:G:173:MET:HG3	1:G:185:TRP:CE3	2.52	0.45
2:H:337:LEU:C	2:H:337:LEU:HD23	2.41	0.45
2:H:368:MET:C	2:H:370:THR:N	2.71	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:262:ALA:HB1	2:H:302:LYS:HD2	1.98	0.45
2:H:286:ARG:HH11	2:H:286:ARG:HG2	1.81	0.45
2:H:291:ILE:HG22	2:H:291:ILE:O	2.16	0.45
2:H:400:LEU:C	2:H:403:PRO:HD2	2.40	0.45
1:A:189:ARG:HH21	4:A:1001:NAP:H71N	1.64	0.45
2:B:168:VAL:O	2:B:172:VAL:HG23	2.17	0.45
2:H:51:LEU:C	2:H:53:GLN:H	2.25	0.45
1:A:252:SER:OG	1:A:254:LYS:HG2	2.16	0.45
1:G:260:PRO:HG2	1:G:263:SER:HB3	1.98	0.45
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.82	0.45
1:G:251:VAL:O	1:G:251:VAL:CG1	2.65	0.45
2:H:276:ASN:HD21	2:H:285:VAL:HG11	1.81	0.45
2:H:230:ILE:HG23	2:H:263:ILE:HG22	1.99	0.45
2:H:288:VAL:HG12	2:H:288:VAL:O	2.17	0.45
2:B:149:VAL:O	2:B:151:LEU:N	2.50	0.44
2:H:204:THR:HG22	2:H:204:THR:O	2.17	0.44
2:H:219:THR:HG22	2:H:219:THR:O	2.16	0.44
2:H:270:ILE:H	2:H:270:ILE:CD1	2.27	0.44
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.98	0.44
2:H:305:ARG:HG2	2:H:305:ARG:NH1	2.30	0.44
2:H:346:GLU:HG2	2:H:380:THR:HG23	2.00	0.44
2:B:270:ILE:O	2:B:274:GLU:HG2	2.17	0.44
2:B:350:ARG:CB	2:B:350:ARG:HH11	2.29	0.44
1:G:57:TRP:HB3	4:G:1001:NAP:H3D	1.99	0.44
2:H:276:ASN:ND2	2:H:285:VAL:HG11	2.33	0.44
1:A:40:ARG:HD2	1:A:318:SER:O	2.17	0.44
2:B:242:PHE:C	2:B:244:CYS:H	2.26	0.44
1:G:189:ARG:NE	4:G:1001:NAP:N7N	2.66	0.44
2:H:285:VAL:HG23	2:H:288:VAL:HG21	1.99	0.44
2:H:227:THR:HG23	2:H:231:ILE:HG13	1.99	0.44
2:B:357:ILE:HB	2:B:358:PRO:HD3	2.00	0.44
2:B:411:TYR:CE1	2:B:415:ARG:HD3	2.53	0.44
1:G:56:THR:HB	1:G:60:PHE:HB2	1.98	0.44
2:H:106:LEU:CD1	2:H:130:GLU:HG2	2.48	0.44
2:H:287:ARG:HB3	2:H:287:ARG:NH1	2.32	0.44
1:G:202:ALA:HA	1:G:207:LEU:HB2	1.99	0.44
2:H:102:VAL:HG23	2:H:102:VAL:O	2.17	0.44
2:H:258:ILE:O	2:H:258:ILE:HG22	2.18	0.44
2:H:343:TYR:HE1	2:H:355:PRO:O	2.01	0.44
2:H:178:VAL:C	2:H:180:PHE:H	2.26	0.43
2:H:351:ASP:O	2:H:352:SER:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:NH2	4:A:1001:NAP:H4B	2.33	0.43
2:B:296:ARG:HE	2:B:299:ARG:NH2	2.16	0.43
2:H:152:LEU:HB3	2:H:159:SER:OG	2.17	0.43
2:H:174:LEU:O	2:H:178:VAL:HG23	2.18	0.43
2:H:343:TYR:CE1	2:H:356:SER:HA	2.53	0.43
1:G:152:VAL:O	1:G:182:ALA:HA	2.18	0.43
2:B:214:GLN:O	2:B:215:SER:HB2	2.18	0.43
2:H:189:ARG:HG3	2:H:189:ARG:HH11	1.84	0.43
2:H:322:ARG:HG3	2:H:322:ARG:NH1	2.33	0.43
1:A:125:ALA:HB3	1:A:128:GLU:CG	2.48	0.43
2:B:81:ASN:OD1	2:B:83:PRO:HD2	2.19	0.43
2:B:152:LEU:HB3	2:B:165:ILE:HD12	2.01	0.43
2:B:106:LEU:CD1	2:B:130:GLU:HG2	2.49	0.43
2:B:149:VAL:HA	2:B:152:LEU:HD13	2.00	0.43
2:H:172:VAL:HG12	2:H:233:PHE:CZ	2.54	0.43
1:A:73:MET:HE2	1:A:108:TRP:CZ3	2.54	0.42
2:B:308:LYS:O	2:B:312:ILE:HG13	2.19	0.42
2:H:271:PHE:O	2:H:271:PHE:CG	2.72	0.42
2:B:415:ARG:O	6:B:516:PGW:HADA	2.19	0.42
2:H:212:TYR:OH	2:H:269:THR:HG21	2.19	0.42
2:H:230:ILE:H	2:H:230:ILE:CD1	2.32	0.42
2:H:329:PHE:O	2:H:333:ILE:HG12	2.19	0.42
1:A:173:MET:HG3	1:A:185:TRP:CE3	2.54	0.42
2:H:379:THR:HA	2:H:384:LYS:HE3	2.01	0.42
1:A:244:SER:HA	4:A:1001:NAP:O3	2.19	0.42
2:H:261:VAL:HA	2:H:264:ILE:CD1	2.50	0.42
2:B:192:ASN:O	2:B:195:MET:HE2	2.19	0.42
2:H:338:PHE:CE2	2:H:390:CYS:HA	2.55	0.42
2:B:100:ARG:HG3	2:B:109:PHE:CG	2.55	0.42
2:B:106:LEU:HD13	2:B:130:GLU:HG2	2.01	0.42
2:H:213:GLN:C	2:H:215:SER:H	2.27	0.42
2:H:287:ARG:C	2:H:289:VAL:H	2.26	0.42
2:B:80:ARG:NH1	2:B:112:GLU:OE2	2.52	0.42
2:B:350:ARG:HB3	2:B:350:ARG:CZ	2.50	0.42
6:B:504:PGW:O02	6:B:504:PGW:H03A	2.20	0.42
1:G:347:ILE:O	1:G:351:ILE:HG13	2.20	0.42
2:H:230:ILE:HG21	2:H:266:TYR:HB3	2.02	0.42
1:G:73:MET:HE3	1:G:84:PHE:CE2	2.55	0.41
2:H:170:VAL:HG12	2:H:171:MET:HE2	2.01	0.41
1:G:276:LYS:O	1:G:282:GLY:HA3	2.19	0.41
2:H:100:ARG:HB2	2:H:126:PHE:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186:PRO:C	2:H:188:PHE:H	2.28	0.41
2:B:311:GLN:CG	6:B:516:PGW:H3	2.43	0.41
2:B:318:LYS:CD	6:B:516:PGW:H22	2.50	0.41
2:B:407:SER:O	2:B:408:ASN:C	2.62	0.41
2:H:312:ILE:CD1	2:H:413:TYR:HD1	2.32	0.41
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.83	0.41
2:B:32:SER:O	2:B:33:GLU:C	2.63	0.41
2:B:297:ILE:C	2:B:299:ARG:N	2.79	0.41
2:H:49:LYS:HG3	2:H:50:THR:N	2.36	0.41
2:H:166:ALA:O	2:H:170:VAL:HG23	2.20	0.41
2:H:272:LEU:CD2	2:H:289:VAL:HG22	2.50	0.41
2:B:109:PHE:O	2:B:113:ILE:HG13	2.21	0.41
2:B:342:VAL:CG1	2:B:343:TYR:N	2.84	0.41
2:H:236:GLU:HA	2:H:239:VAL:HG23	2.02	0.41
1:A:333:ASN:ND2	4:A:1001:NAP:H61A	2.09	0.41
1:A:261:PRO:O	1:A:262:TYR:HB2	2.20	0.41
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.51	0.41
2:B:203:HIS:HE1	2:B:277:LYS:HZ2	1.68	0.41
2:H:264:ILE:O	2:H:268:VAL:HG23	2.21	0.41
2:B:83:PRO:HB2	2:B:104:VAL:HG22	2.03	0.41
2:B:150:TRP:O	2:B:150:TRP:CG	2.73	0.41
2:B:215:SER:C	2:B:217:SER:N	2.79	0.41
2:B:280:LEU:C	2:B:280:LEU:HD23	2.46	0.41
2:B:346:GLU:OE2	2:B:380:THR:HG23	2.21	0.41
1:G:174:THR:HG22	1:G:178:ASN:ND2	2.36	0.41
1:A:236:ILE:HG13	1:A:238:VAL:HG23	2.02	0.40
2:B:202:PHE:C	2:B:204:THR:H	2.29	0.40
1:A:167:GLU:HA	1:A:201:VAL:HG11	2.03	0.40
2:B:187:ILE:HG21	6:B:512:PGW:C2	2.49	0.40
2:H:261:VAL:HA	2:H:264:ILE:HD12	2.02	0.40
2:H:297:ILE:C	2:H:299:ARG:N	2.79	0.40
2:B:80:ARG:NH1	2:B:112:GLU:CD	2.79	0.40
1:G:102:ILE:O	1:G:106:LYS:HG2	2.22	0.40
1:G:326:ASN:OD1	1:G:329:GLN:HG3	2.21	0.40
1:A:68:MET:O	1:A:72:LEU:HG	2.20	0.40
2:B:244:CYS:HA	2:B:245:PRO:HD3	1.90	0.40
2:H:172:VAL:O	2:H:176:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/333 (97%)	308 (95%)	14 (4%)	2 (1%)	21	28
1	G	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	36	44
2	B	384/514 (75%)	344 (90%)	27 (7%)	13 (3%)	3	2
2	H	357/514 (70%)	280 (78%)	60 (17%)	17 (5%)	2	1
3	Y	35/37 (95%)	17 (49%)	17 (49%)	1 (3%)	3	3
All	All	1424/1731 (82%)	1262 (89%)	128 (9%)	34 (2%)	4	4

All (34) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains ⓘ

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%)	266 (97%)	7 (3%)	40	57
1	G	273/280 (98%)	266 (97%)	7 (3%)	40	57
2	B	332/459 (72%)	322 (97%)	10 (3%)	36	51
2	H	324/459 (71%)	321 (99%)	3 (1%)	70	80
3	Y	35/35 (100%)	33 (94%)	2 (6%)	18	28
All	All	1237/1513 (82%)	1208 (98%)	29 (2%)	44	60

All (29) 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	280	GLU
1	A	314	ASN
1	A	326	ASN

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Mol	Chain	Res	Type
1	A	338	GLN
2	B	34	ARG
2	B	80	ARG
2	B	82	ARG
2	B	103	ASN
2	B	121	GLU
2	B	190	ASP
2	B	302	LYS
2	B	323	GLU
2	B	326	LEU
2	B	331	LEU
1	G	73	MET
1	G	75	LEU
1	G	129	ARG
1	G	212	CYS
1	G	214	GLN
1	G	271	GLN
1	G	283	ARG
2	H	34	ARG
2	H	292	PHE
2	H	350	ARG
3	Y	14	TRP
3	Y	18	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	158	ASN
1	A	175	HIS
1	A	204	GLN
1	A	206	ASN
1	A	286	GLN
1	A	293	GLN
1	A	314	ASN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	53	GLN
2	B	103	ASN
2	B	203	HIS
2	B	207	GLN

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Mol	Chain	Res	Type
2	B	213	GLN
2	B	253	ASN
2	B	256	ASN
1	G	37	GLN
1	G	63	GLN
1	G	71	HIS
1	G	148	GLN
1	G	178	ASN
1	G	204	GLN
1	G	333	ASN
2	H	53	GLN
2	H	207	GLN
2	H	213	GLN
2	H	284	ASN
2	H	306	HIS
2	H	315	GLN
2	H	408	ASN
3	Y	18	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PCA	Y	1	3	7,8,9	0.62	0	9,10,12	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	Y	1	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	PGW	B	506	-	8,8,50	0.36	0	7,7,56	0.50	0
6	PGW	B	517	-	6,6,50	0.37	0	5,5,56	0.43	0
6	PGW	B	505	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	515	-	7,7,50	0.36	0	6,6,56	0.50	0
4	NAP	G	1001	-	50,52,52	2.51	10 (20%)	71,80,80	2.61	20 (28%)
4	NAP	A	1001	-	50,52,52	2.81	9 (18%)	71,80,80	2.63	19 (26%)
6	PGW	B	518	-	7,7,50	0.36	0	6,6,56	0.51	0
6	PGW	B	513	-	7,7,50	0.37	0	6,6,56	0.51	0
6	PGW	B	516	-	35,35,50	0.66	0	38,41,56	0.91	2 (5%)
6	PGW	B	514	-	22,22,50	0.80	0	25,27,56	1.26	4 (16%)
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	511	-	6,6,50	0.37	0	5,5,56	0.47	0
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.55	0
6	PGW	B	504	-	21,21,50	0.61	0	23,23,56	1.24	3 (13%)
6	PGW	H	504	-	21,21,50	0.61	0	23,23,56	1.29	3 (13%)
6	PGW	B	512	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	519	-	7,7,50	0.36	0	6,6,56	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PGW	B	506	-	-	0/6/6/55	-
6	PGW	B	517	-	-	0/4/4/55	-
6	PGW	B	505	-	-	0/6/6/55	-
6	PGW	B	515	-	-	0/5/5/55	-
4	NAP	G	1001	-	-	4/35/67/67	0/5/5/5
4	NAP	A	1001	-	-	4/35/67/67	0/5/5/5
6	PGW	B	518	-	-	0/5/5/55	-
6	PGW	B	513	-	-	0/5/5/55	-
6	PGW	B	516	-	-	9/40/40/55	-
6	PGW	B	514	-	-	9/24/24/55	-
6	PGW	B	510	-	-	0/6/6/55	-
6	PGW	B	509	-	-	0/6/6/55	-
6	PGW	B	508	-	-	0/6/6/55	-
6	PGW	B	511	-	-	0/4/4/55	-
6	PGW	B	507	-	-	0/6/6/55	-
6	PGW	B	504	-	-	1/23/23/55	-
6	PGW	H	504	-	-	1/23/23/55	-
6	PGW	B	512	-	-	0/6/6/55	-
6	PGW	B	519	-	-	0/5/5/55	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAP	PN-O3	15.70	1.76	1.59
4	G	1001	NAP	PN-O3	13.80	1.74	1.59
4	A	1001	NAP	PA-O3	6.45	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAP	O4D-C1D	4.96	1.47	1.40
4	G	1001	NAP	PA-O3	4.73	1.64	1.59
4	G	1001	NAP	O4D-C1D	4.11	1.46	1.40
4	A	1001	NAP	C2N-C3N	3.36	1.44	1.39
4	A	1001	NAP	O4B-C1B	3.16	1.49	1.42
4	G	1001	NAP	O4B-C1B	3.13	1.49	1.42
4	G	1001	NAP	C2N-C3N	2.65	1.43	1.39
4	A	1001	NAP	C5A-N7A	-2.56	1.34	1.39
4	G	1001	NAP	C4N-C3N	2.55	1.43	1.39
4	A	1001	NAP	C5A-C4A	2.54	1.43	1.39
4	G	1001	NAP	C5A-C4A	2.40	1.43	1.39
4	G	1001	NAP	C5A-N7A	-2.35	1.34	1.39
4	G	1001	NAP	P2B-O2B	2.33	1.63	1.59
4	G	1001	NAP	O3D-C3D	-2.21	1.37	1.43
4	A	1001	NAP	C4N-C3N	2.15	1.42	1.39
4	A	1001	NAP	C3N-C7N	-2.02	1.47	1.50

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	NAP	O3-PA-O1A	-11.38	76.46	110.70
4	A	1001	NAP	O3-PA-O1A	-10.93	77.84	110.70
4	A	1001	NAP	C2B-C1B-N9A	-7.83	100.87	113.75
4	G	1001	NAP	C2B-C1B-N9A	-6.77	102.61	113.75
4	A	1001	NAP	O2A-PA-O3	-6.58	89.48	107.27
4	G	1001	NAP	O2A-PA-O3	-6.24	90.39	107.27
4	A	1001	NAP	O4B-C1B-N9A	5.86	119.35	108.09
4	A	1001	NAP	C5A-C4A-N3A	-5.82	118.70	126.72
4	G	1001	NAP	O4B-C1B-N9A	5.77	119.17	108.09
4	G	1001	NAP	C5A-C4A-N3A	-5.69	118.88	126.72
4	A	1001	NAP	N3A-C4A-N9A	4.66	135.10	127.17
4	G	1001	NAP	N3A-C4A-N9A	4.58	134.96	127.17
4	G	1001	NAP	N3A-C2A-N1A	-4.46	121.83	128.58
4	A	1001	NAP	N3A-C2A-N1A	-4.28	122.10	128.58
4	A	1001	NAP	C2B-C3B-C4B	3.88	110.34	101.99
4	G	1001	NAP	C2B-C3B-C4B	3.86	110.28	101.99
4	G	1001	NAP	C2A-N3A-C4A	3.84	121.22	111.83
4	A	1001	NAP	C5A-N7A-C8A	3.81	109.44	103.45
4	A	1001	NAP	C2A-N3A-C4A	3.80	121.10	111.83
4	A	1001	NAP	O2B-C2B-C3B	3.78	125.22	111.68
4	G	1001	NAP	C5A-N7A-C8A	3.76	109.36	103.45
6	H	504	PGW	O01-C1-C2	3.55	119.17	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1001	NAP	PN-O5D-C5D	-3.55	101.00	121.35
4	A	1001	NAP	PN-O5D-C5D	-3.37	102.06	121.35
6	B	504	PGW	O01-C1-C2	3.34	118.70	111.48
4	G	1001	NAP	O2B-C2B-C3B	3.30	123.51	111.68
4	A	1001	NAP	O4B-C4B-C5B	-2.96	99.86	109.33
4	A	1001	NAP	C4A-C5A-N7A	-2.95	107.21	110.58
4	G	1001	NAP	O4B-C4B-C5B	-2.94	99.92	109.33
4	G	1001	NAP	C4A-C5A-N7A	-2.91	107.25	110.58
6	B	514	PGW	O01-C1-C2	2.78	117.50	111.48
6	B	514	PGW	C03-C02-C01	-2.71	105.47	111.78
6	H	504	PGW	O03-C19-C20	2.55	119.61	111.83
6	B	516	PGW	O01-C1-C2	2.46	116.81	111.48
6	B	504	PGW	O03-C19-C20	2.46	119.33	111.83
6	B	514	PGW	O03-C19-C20	2.45	119.31	111.83
6	B	514	PGW	O11-P-O14	2.32	112.72	106.44
4	G	1001	NAP	C5D-C4D-C3D	-2.26	107.08	115.21
4	A	1001	NAP	O2A-PA-O5B	2.26	117.80	107.57
4	G	1001	NAP	O5B-PA-O1A	2.23	117.76	108.94
4	A	1001	NAP	O7N-C7N-N7N	-2.21	119.43	122.62
4	A	1001	NAP	C5D-C4D-C3D	-2.20	107.30	115.21
4	A	1001	NAP	O5B-PA-O1A	2.12	117.33	108.94
4	G	1001	NAP	O7N-C7N-N7N	-2.11	119.56	122.62
4	G	1001	NAP	O2A-PA-O5B	2.11	117.12	107.57
6	H	504	PGW	C02-O01-C1	-2.10	112.76	117.80
6	B	516	PGW	O01-C02-C01	-2.10	100.81	108.34
6	B	504	PGW	C02-O01-C1	-2.06	112.87	117.80
4	A	1001	NAP	O4D-C4D-C3D	2.05	109.22	105.15
4	G	1001	NAP	O2A-PA-O1A	2.04	121.92	112.44
4	G	1001	NAP	O4D-C4D-C3D	2.02	109.16	105.15

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAP	C5B-O5B-PA-O1A
4	G	1001	NAP	C5B-O5B-PA-O1A
6	B	514	PGW	C02-C03-O11-P
4	G	1001	NAP	C1B-C2B-O2B-P2B
4	A	1001	NAP	C1B-C2B-O2B-P2B
4	A	1001	NAP	C3B-C2B-O2B-P2B
4	G	1001	NAP	C3B-C2B-O2B-P2B
6	B	514	PGW	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
6	B	516	PGW	C7-C8-C9-C10
6	B	514	PGW	O02-C1-O01-C02
6	B	514	PGW	C20-C19-O03-C01
6	B	514	PGW	O04-C19-O03-C01
6	B	504	PGW	C01-C02-O01-C1
6	B	516	PGW	C01-C02-O01-C1
6	H	504	PGW	C01-C02-O01-C1
6	B	516	PGW	O02-C1-O01-C02
6	B	514	PGW	O01-C1-C2-C3
6	B	516	PGW	C2-C1-O01-C02
6	B	516	PGW	O01-C1-C2-C3
6	B	516	PGW	O03-C19-C20-C21
6	B	514	PGW	C01-C02-O01-C1
6	B	516	PGW	C03-C02-O01-C1
4	A	1001	NAP	O4B-C4B-C5B-O5B
4	G	1001	NAP	O4B-C4B-C5B-O5B
6	B	514	PGW	O03-C19-C20-C21
6	B	514	PGW	O02-C1-C2-C3
6	B	516	PGW	O04-C19-C20-C21
6	B	516	PGW	O02-C1-C2-C3

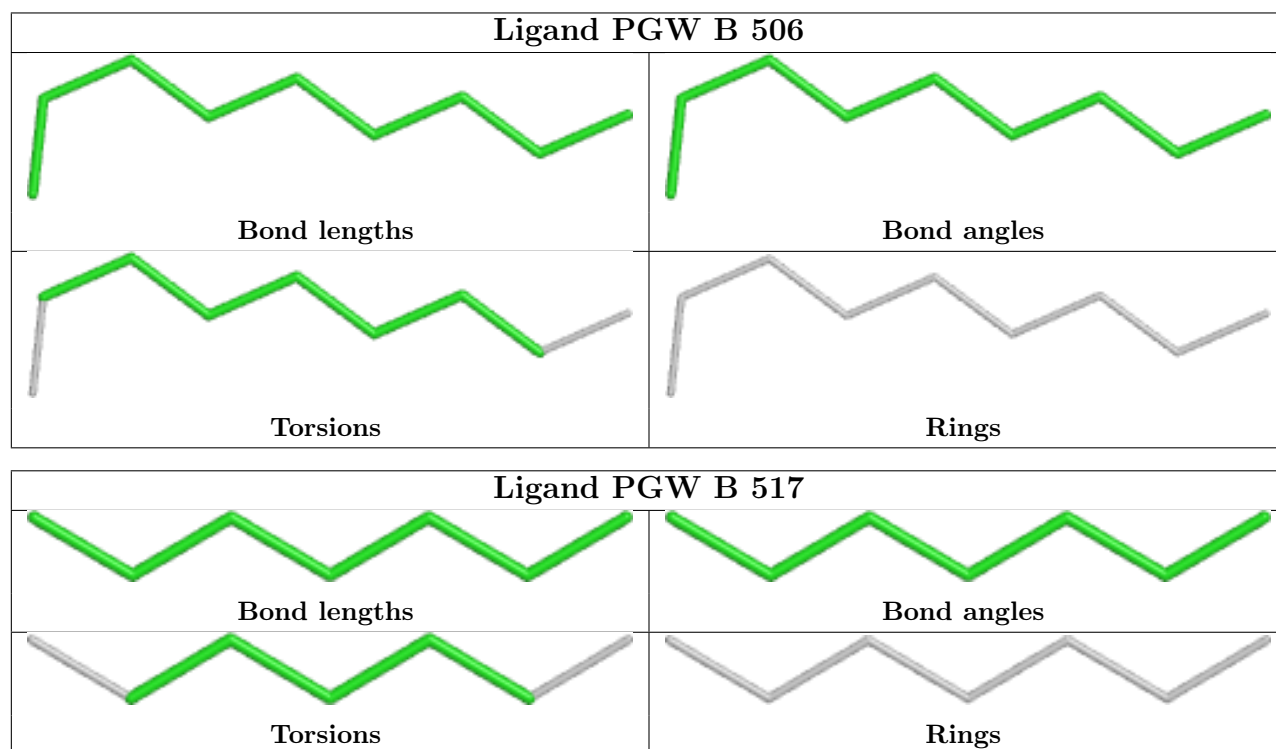
There are no ring outliers.

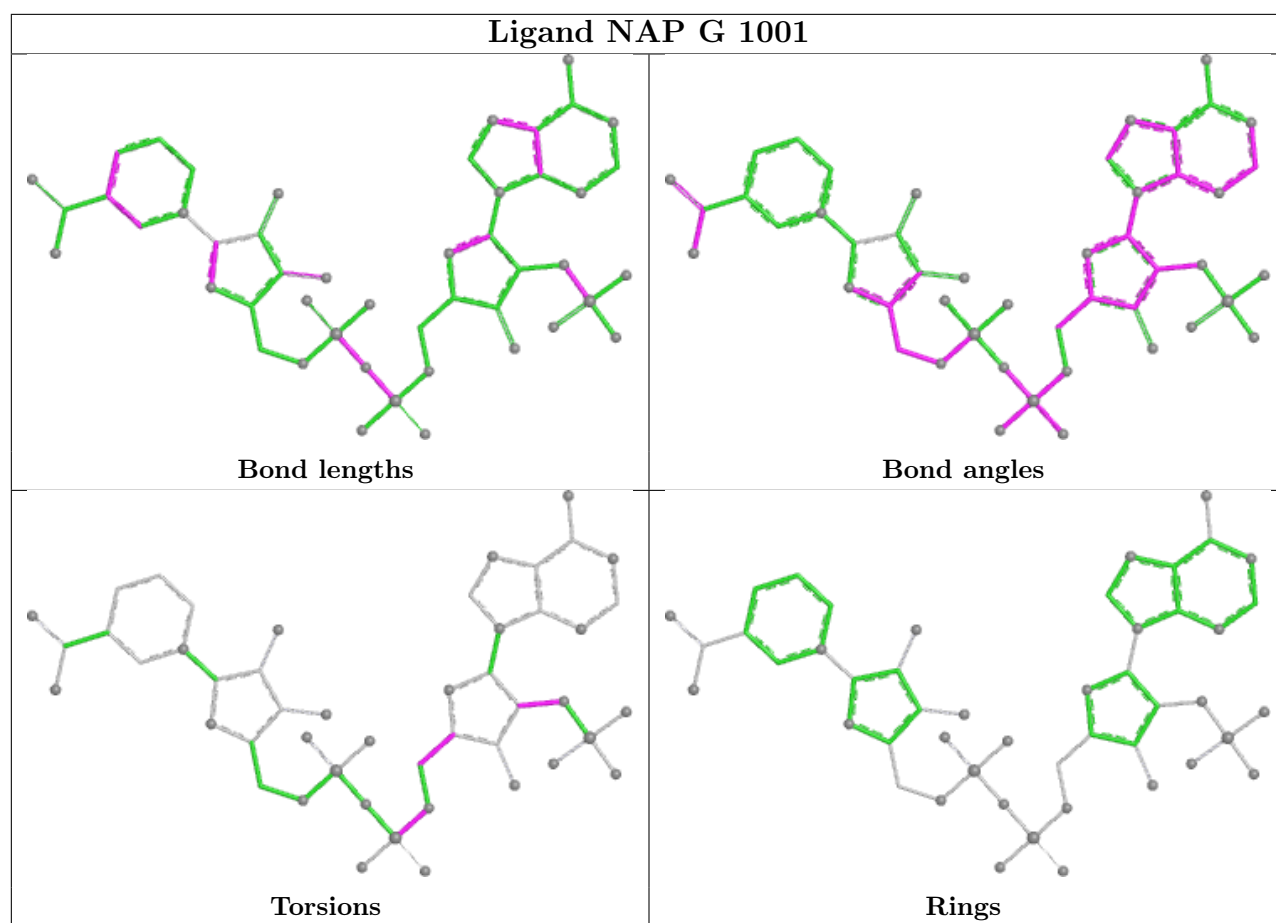
10 monomers are involved in 48 short contacts:

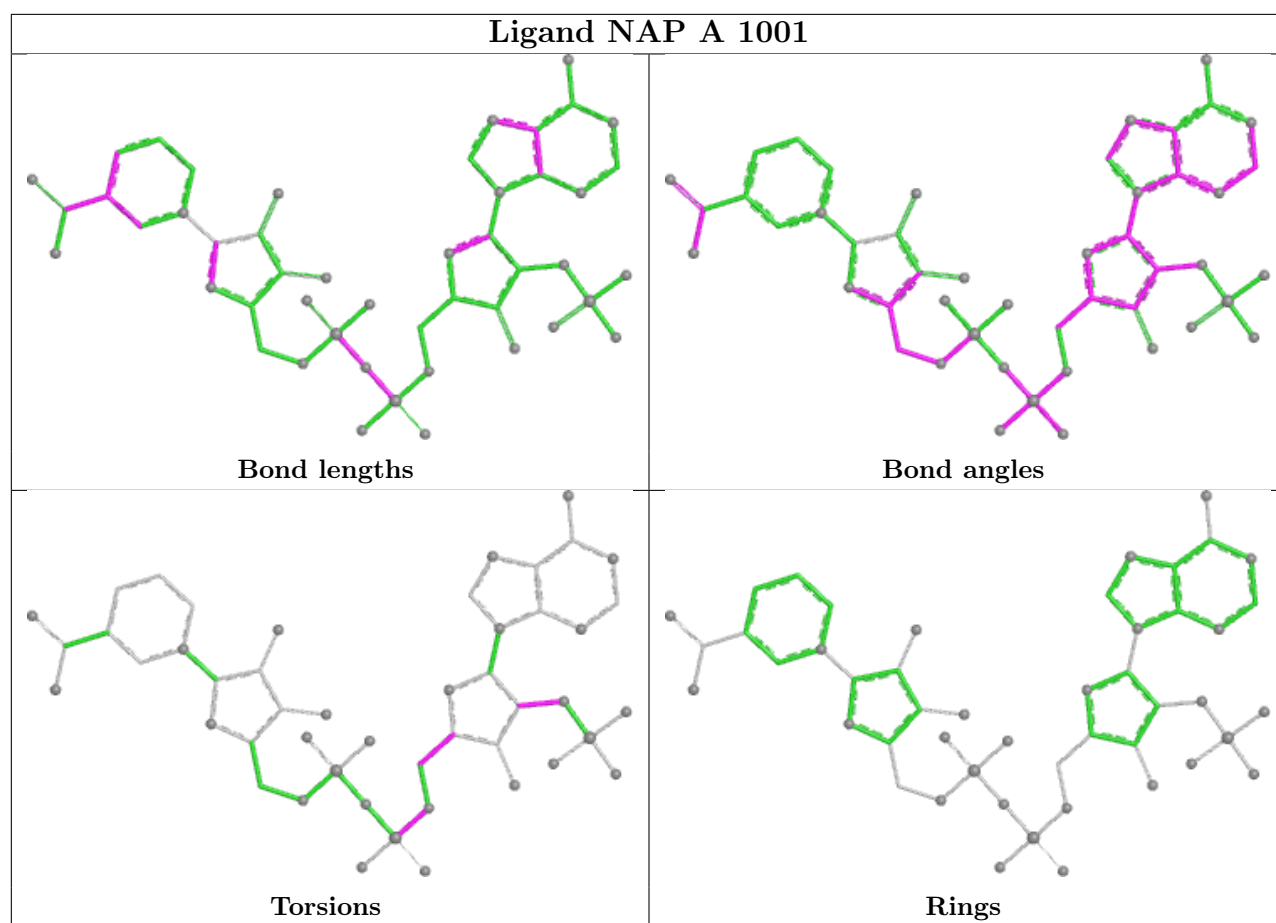
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	515	PGW	3	0
4	G	1001	NAP	12	0
4	A	1001	NAP	11	0
6	B	513	PGW	1	0
6	B	516	PGW	8	0
6	B	514	PGW	1	0
6	B	510	PGW	3	0
6	B	504	PGW	3	0
6	H	504	PGW	7	0
6	B	512	PGW	2	0

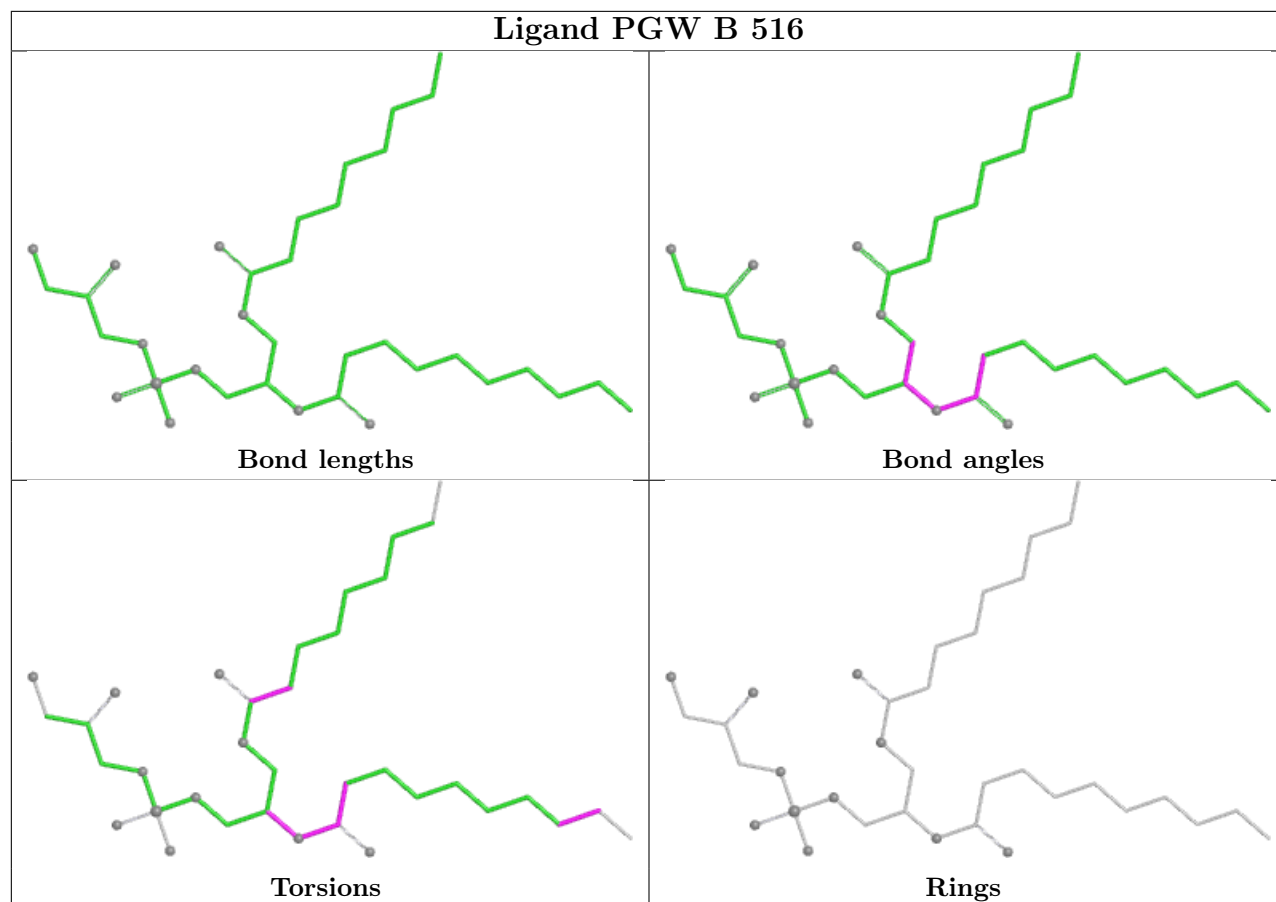
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

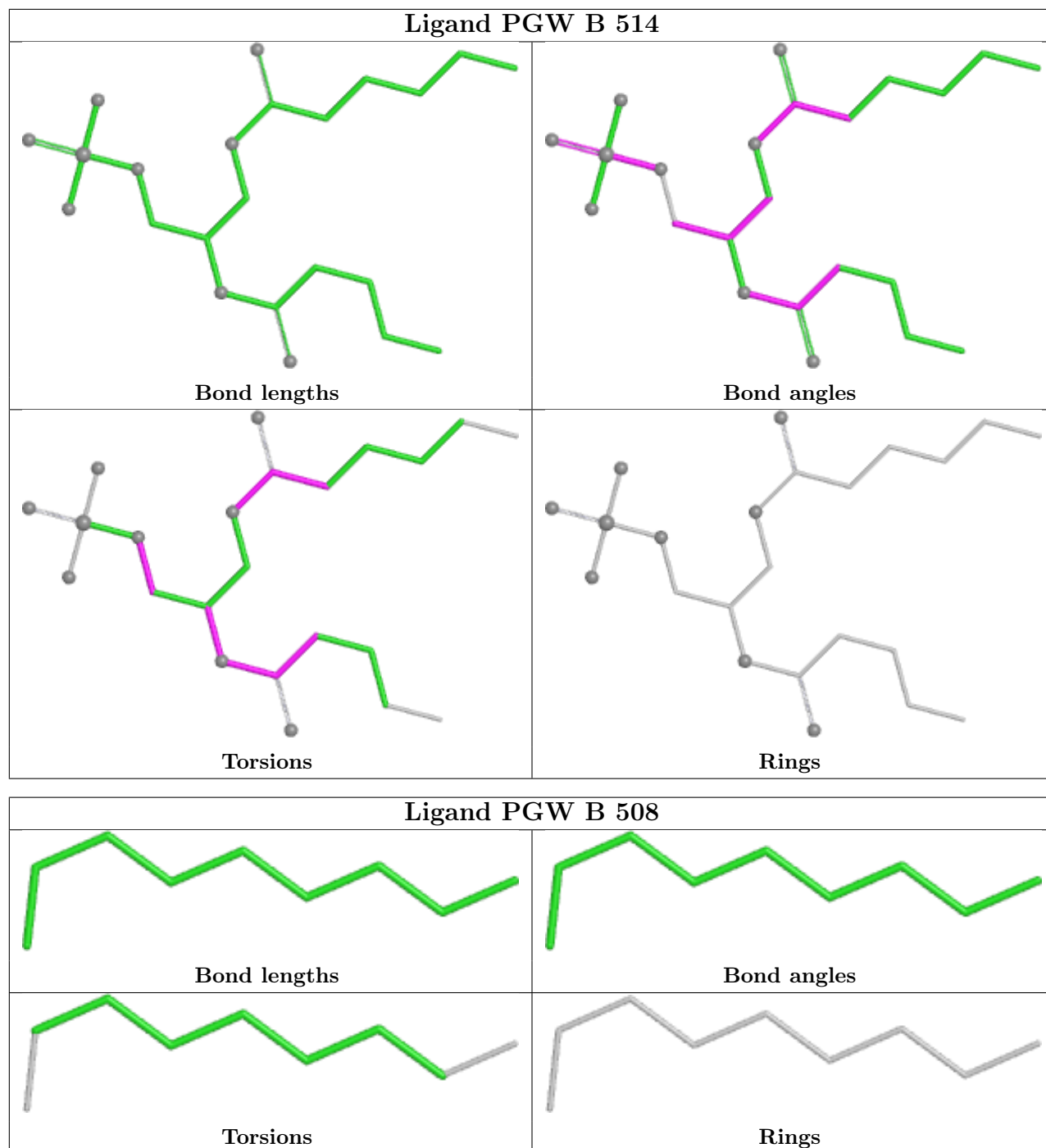
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

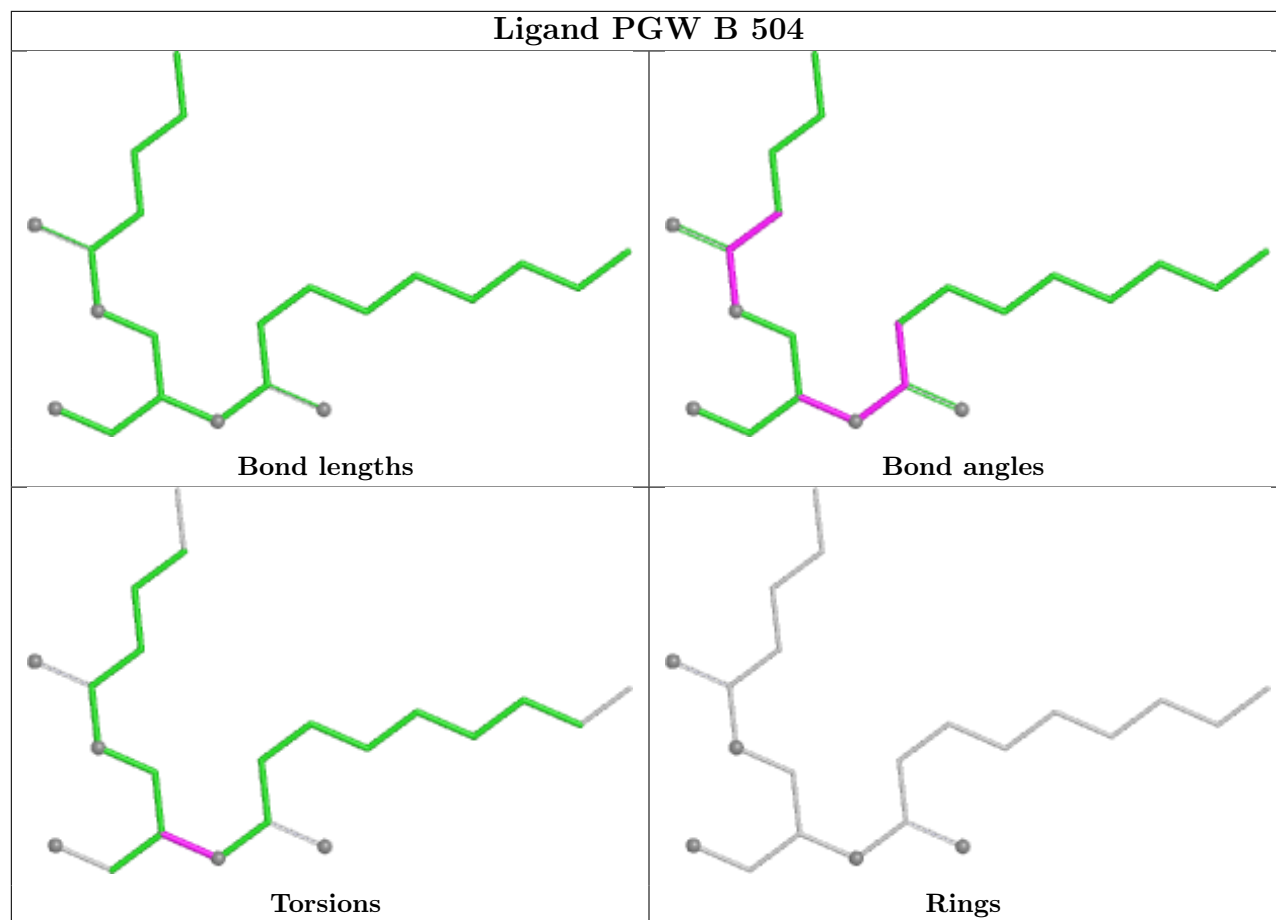


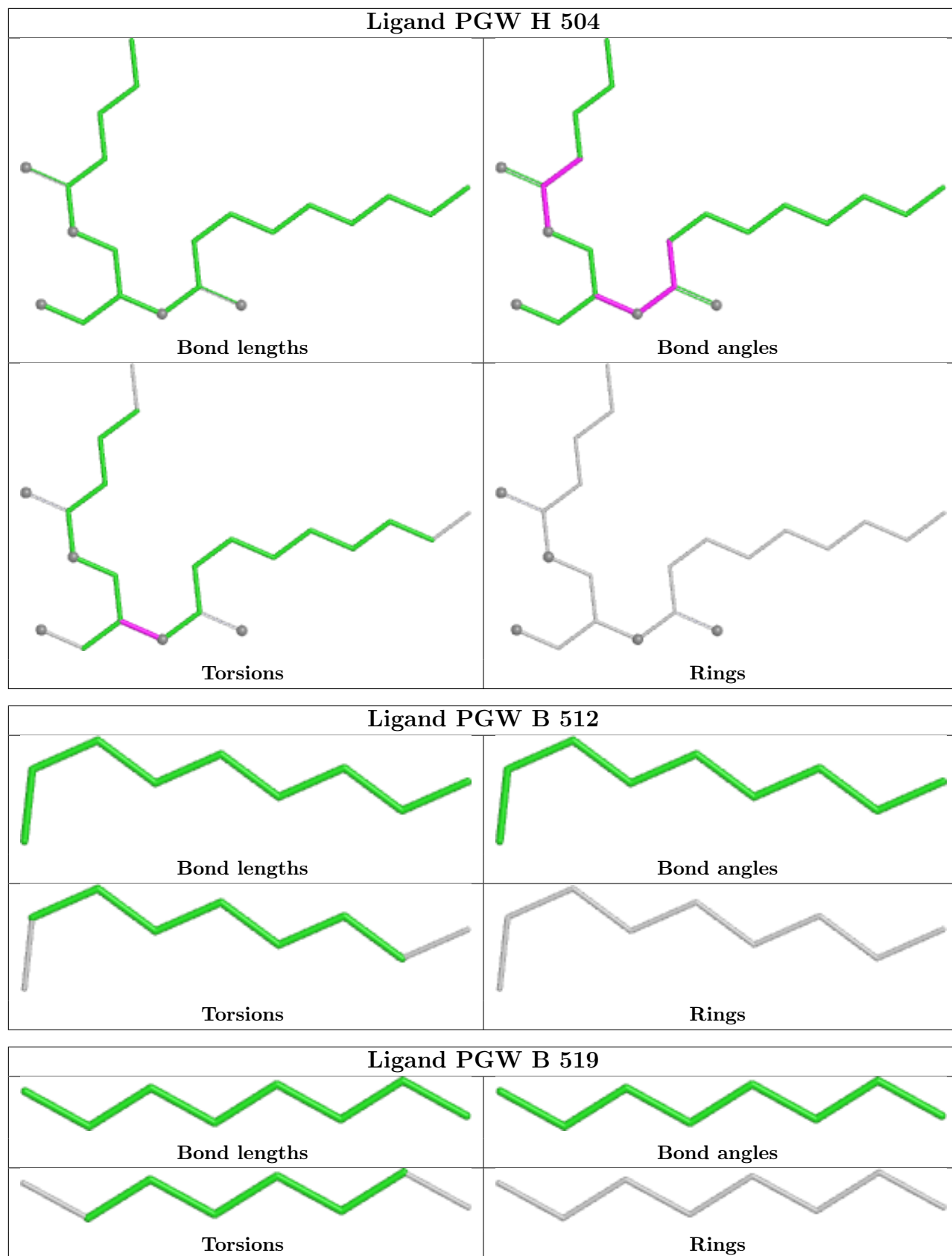












5.7 Other polymers

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, 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%)	-0.03	12 (3%) 45 46	17, 33, 60, 83	0
1	G	326/333 (97%)	0.14	16 (4%) 35 35	21, 39, 72, 96	0
2	B	386/514 (75%)	1.22	88 (22%) 2 2	25, 66, 110, 125	0
2	H	363/514 (70%)	2.81	221 (60%) 0 0	38, 115, 185, 204	0
3	Y	36/37 (97%)	11.89	36 (100%) 0 0	25, 27, 31, 31	36 (100%)
All	All	1437/1731 (83%)	1.36	373 (25%) 1 1	17, 53, 176, 204	36 (2%)

All (373) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	15	SER	28.2
3	Y	20	LEU	26.0
3	Y	18	GLN	23.9
3	Y	4	ASN	18.5
3	Y	22	ASN	18.5
3	Y	23	THR	18.4
3	Y	11	LYS	17.7
3	Y	9	THR	16.8
3	Y	19	ARG	15.7
3	Y	14	TRP	14.4
3	Y	8	THR	14.1
3	Y	37	SER	14.1
3	Y	3	THR	13.2
3	Y	24	SER	12.8
3	Y	21	HIS	12.2
3	Y	5	VAL	11.8
2	H	280	LEU	11.3
2	H	272	LEU	10.9
3	Y	7	CYS	10.6
3	Y	6	SER	10.0

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Mol	Chain	Res	Type	RSRZ
2	H	187	ILE	9.8
3	Y	25	ARG	9.7
3	Y	17	CYS	9.5
3	Y	36	TYR	9.5
3	Y	30	ASN	8.6
2	H	288	VAL	8.6
3	Y	28	CYS	8.6
3	Y	12	GLU	8.5
2	B	193	GLU	8.2
3	Y	26	GLY	8.1
3	Y	29	MET	8.1
3	Y	16	VAL	7.9
2	H	268	VAL	7.7
2	H	270	ILE	7.6
2	H	254	ILE	7.2
3	Y	13	CYS	7.0
2	H	242	PHE	6.9
2	H	291	ILE	6.7
2	H	131	GLY	6.6
2	H	248	ALA	6.6
3	Y	2	PHE	6.6
2	H	250	PHE	6.6
2	H	164	ILE	6.5
2	H	285	VAL	6.4
2	H	241	PHE	6.4
3	Y	33	CYS	6.3
2	H	188	PHE	6.2
3	Y	10	SER	6.2
2	B	161	PRO	6.2
2	H	289	VAL	6.1
2	H	156	PRO	6.1
3	Y	27	LYS	6.1
2	B	200	VAL	6.1
2	H	279	VAL	6.1
2	H	287	ARG	6.0
2	B	199	GLY	6.0
2	H	245	PRO	6.0
2	H	271	PHE	6.0
2	B	198	GLY	6.0
2	B	417	THR	6.0
2	H	252	THR	6.0
2	H	381	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	187	ILE	5.9
2	H	211	GLY	5.9
2	H	283	GLN	5.9
2	H	145	PHE	5.8
2	H	147	ARG	5.8
2	B	197	GLY	5.8
2	H	238	LEU	5.8
2	B	157	GLU	5.8
2	H	257	ILE	5.8
2	H	237	PHE	5.7
3	Y	32	LYS	5.7
3	Y	35	CYS	5.6
2	H	151	LEU	5.6
2	H	228	LEU	5.6
2	H	417	THR	5.6
2	H	218	PHE	5.5
2	H	353	GLN	5.4
2	H	190	ASP	5.4
1	G	36	LEU	5.4
2	H	149	VAL	5.4
2	H	292	PHE	5.3
2	H	278	SER	5.3
2	H	284	ASN	5.3
2	H	255	MET	5.3
2	H	290	GLN	5.2
2	H	210	ILE	5.2
2	H	216	THR	5.2
2	H	214	GLN	5.2
2	H	416	GLU	5.1
2	H	205	TYR	5.1
2	H	415	ARG	5.1
2	H	235	PHE	5.1
2	H	273	THR	5.0
2	H	244	CYS	5.0
2	H	219	THR	5.0
2	H	231	ILE	5.0
2	H	222	PHE	4.9
2	H	221	PRO	4.9
2	H	209	THR	4.9
2	H	155	TYR	4.8
2	H	372	GLY	4.8
2	B	213	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
2	H	264	ILE	4.7
2	H	277	LYS	4.7
2	H	350	ARG	4.7
2	H	269	THR	4.7
2	B	132	TYR	4.6
2	H	240	ARG	4.6
3	Y	34	ARG	4.6
2	H	282	PHE	4.6
2	H	183	GLU	4.6
2	H	224	ILE	4.6
3	Y	31	LYS	4.6
2	H	167	ILE	4.5
2	H	153	PHE	4.5
2	H	246	SER	4.5
2	H	267	TYR	4.4
2	H	160	GLY	4.4
2	H	186	PRO	4.4
2	H	225	VAL	4.4
2	H	275	SER	4.4
2	H	363	TRP	4.4
2	H	32	SER	4.4
2	H	258	ILE	4.3
2	H	301	PHE	4.3
1	A	360	TYR	4.3
2	H	203	HIS	4.3
2	H	286	ARG	4.3
1	A	36	LEU	4.3
2	H	345	ALA	4.3
2	H	206	SER	4.3
2	H	370	THR	4.3
2	H	409	PHE	4.2
2	H	373	TYR	4.2
2	B	201	THR	4.1
2	H	260	ILE	4.1
2	H	251	PHE	4.1
2	B	192	ASN	4.1
2	H	191	GLU	4.1
2	H	202	PHE	4.1
2	H	374	GLY	4.0
2	H	175	ILE	4.0
2	H	414	HIS	4.0
2	H	262	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	314	ASN	4.0
2	H	300	ILE	4.0
2	H	217	SER	4.0
1	A	121	TRP	3.9
2	H	239	VAL	3.9
2	H	181	CYS	3.9
2	H	376	MET	3.8
2	H	378	PRO	3.8
2	B	251	PHE	3.8
2	H	189	ARG	3.8
2	H	308	LYS	3.8
2	H	152	LEU	3.8
2	B	133	ILE	3.8
2	H	294	ILE	3.8
2	H	168	VAL	3.7
2	H	182	LEU	3.7
2	H	303	LEU	3.7
2	B	286	ARG	3.7
2	B	219	THR	3.7
1	G	361	SER	3.7
2	B	215	SER	3.7
2	B	139	PRO	3.7
2	H	351	ASP	3.7
2	B	140	LEU	3.6
2	H	174	LEU	3.6
2	H	337	LEU	3.6
2	H	253	ASN	3.6
2	B	205	TYR	3.6
2	H	298	LEU	3.6
2	H	265	PRO	3.6
2	B	252	THR	3.5
2	H	318	LYS	3.5
2	B	191	GLU	3.5
2	H	261	VAL	3.5
2	B	194	ASP	3.5
1	G	360	TYR	3.5
2	H	247	LYS	3.5
1	A	150	GLU	3.5
2	B	120	GLU	3.5
2	B	147	ARG	3.5
2	H	63	LYS	3.5
1	A	361	SER	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	352	SER	3.4
2	H	352	SER	3.4
2	B	188	PHE	3.4
2	H	306	HIS	3.4
2	H	161	PRO	3.4
2	H	281	GLN	3.4
2	B	196	HIS	3.4
2	H	293	ARG	3.4
2	H	341	ALA	3.4
2	H	410	ASN	3.3
2	H	185	LEU	3.3
2	H	157	GLU	3.3
2	H	233	PHE	3.3
2	H	371	VAL	3.3
2	B	137	GLU	3.3
2	H	332	PHE	3.3
1	G	280	GLU	3.3
2	B	414	HIS	3.3
2	B	158	SER	3.2
2	H	354	PHE	3.2
2	H	296	ARG	3.2
2	H	128	GLU	3.2
2	H	309	GLY	3.2
2	H	150	TRP	3.2
2	H	328	ILE	3.2
2	B	125	MET	3.2
2	B	240	ARG	3.1
2	H	114	ARG	3.1
2	H	344	PHE	3.1
2	H	412	PHE	3.1
2	H	413	TYR	3.1
2	H	229	CYS	3.1
2	H	321	MET	3.1
2	H	204	THR	3.1
2	H	347	ALA	3.1
2	H	125	MET	3.1
2	H	302	LYS	3.1
2	H	357	ILE	3.1
2	H	295	MET	3.0
2	H	208	SER	3.0
2	H	297	ILE	3.0
2	H	399	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	155	TYR	3.0
2	B	282	PHE	3.0
2	B	203	HIS	2.9
2	B	145	PHE	2.9
2	H	249	GLY	2.9
2	B	152	LEU	2.9
2	H	170	VAL	2.9
2	H	266	TYR	2.9
2	B	159	SER	2.9
2	B	359	ASP	2.9
2	H	111	GLU	2.9
2	H	304	SER	2.8
2	H	177	ILE	2.8
2	H	400	LEU	2.8
2	B	381	ILE	2.8
2	B	134	LYS	2.8
2	B	32	SER	2.8
1	G	231	GLU	2.8
2	H	305	ARG	2.8
2	H	110	SER	2.7
2	B	151	LEU	2.7
2	H	184	THR	2.7
2	H	396	LEU	2.7
2	B	135	GLU	2.7
2	H	179	SER	2.7
2	H	411	TYR	2.7
2	H	166	ALA	2.7
1	G	300	GLY	2.7
2	H	383	GLY	2.7
2	H	165	ILE	2.7
2	H	317	LEU	2.7
2	H	232	TRP	2.7
2	H	379	THR	2.7
2	H	180	PHE	2.6
2	B	136	GLU	2.6
2	B	202	PHE	2.6
2	H	109	PHE	2.6
2	H	310	LEU	2.6
1	A	297	GLU	2.6
2	H	102	VAL	2.6
2	H	315	GLN	2.6
1	G	234	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	153	PHE	2.6
2	H	169	SER	2.6
2	B	413	TYR	2.6
2	B	156	PRO	2.6
2	H	127	ARG	2.6
2	H	348	ASP	2.6
2	H	123	MET	2.6
2	H	173	ILE	2.6
1	G	121	TRP	2.5
2	B	129	ASP	2.5
2	B	160	GLY	2.5
2	B	348	ASP	2.5
2	B	143	ASN	2.5
2	H	146	GLN	2.5
2	H	377	VAL	2.5
1	G	349	HIS	2.5
2	H	215	SER	2.5
2	H	393	ALA	2.5
2	B	269	THR	2.5
2	H	212	TYR	2.5
2	H	314	GLY	2.5
2	H	375	ASP	2.5
2	H	324	LEU	2.5
2	H	384	LYS	2.5
2	H	349	GLU	2.5
2	H	355	PRO	2.5
2	B	124	GLU	2.5
2	H	129	ASP	2.5
2	H	405	ILE	2.5
2	B	185	LEU	2.5
2	H	402	VAL	2.5
2	B	287	ARG	2.5
2	H	243	ALA	2.5
1	G	297	GLU	2.4
2	H	331	LEU	2.4
2	H	207	GLN	2.4
2	H	172	VAL	2.4
1	G	281	GLU	2.4
2	B	141	PRO	2.4
2	B	86	ASP	2.4
2	B	354	PHE	2.4
1	A	145	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	56	GLU	2.4
2	H	126	PHE	2.4
2	H	307	SER	2.3
1	G	159	ARG	2.3
2	H	326	LEU	2.3
2	H	395	VAL	2.3
2	H	163	ARG	2.3
2	H	299	ARG	2.3
2	B	283	GLN	2.3
2	H	148	GLN	2.3
2	H	223	PHE	2.3
1	A	262	TYR	2.3
2	H	276	ASN	2.3
2	B	162	ALA	2.3
2	B	246	SER	2.3
2	B	375	ASP	2.3
2	B	121	GLU	2.3
2	B	349	GLU	2.3
2	B	322	ARG	2.3
2	H	158	SER	2.3
2	B	150	TRP	2.3
1	G	67	GLU	2.3
2	B	218	PHE	2.3
2	B	285	VAL	2.3
2	B	248	ALA	2.2
2	H	106	LEU	2.2
2	B	245	PRO	2.2
2	H	178	VAL	2.2
2	H	159	SER	2.2
2	H	312	ILE	2.2
2	B	114	ARG	2.2
2	B	247	LYS	2.2
2	B	241	PHE	2.2
2	B	216	THR	2.2
1	A	67	GLU	2.2
2	H	338	PHE	2.2
2	H	227	THR	2.1
2	H	263	ILE	2.1
2	B	290	GLN	2.1
2	H	66	MET	2.1
1	A	129	ARG	2.1
1	G	257	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	349	HIS	2.1
2	B	214	GLN	2.1
2	H	103	ASN	2.1
2	B	189	ARG	2.1
2	B	142	GLU	2.1
2	B	144	GLU	2.1
2	H	56	GLU	2.1
2	B	242	PHE	2.0
2	B	138	ARG	2.0
2	H	343	TYR	2.0
2	H	406	VAL	2.0
2	B	347	ALA	2.0
2	H	118	LEU	2.0
2	B	232	TRP	2.0
1	G	359	PRO	2.0
2	H	86	ASP	2.0
1	A	346	SER	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCA	Y	1	8/9	0.66	0.36	125,126,126,126	8

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

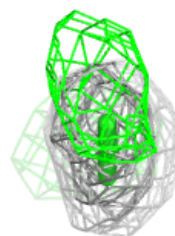
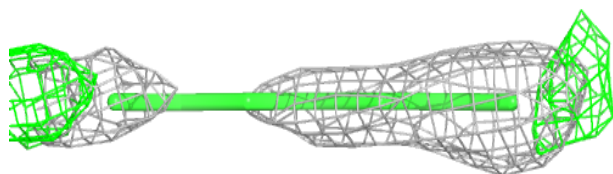
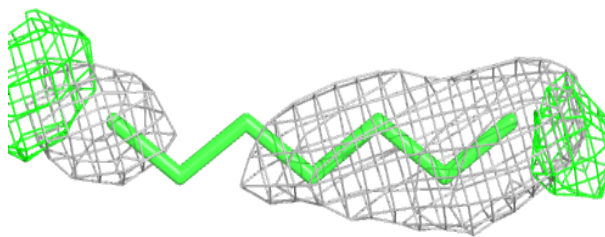
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	PGW	B	517	7/51	0.62	0.41	63,66,68,69	0
6	PGW	B	512	9/51	0.63	0.71	126,128,128,128	0
6	PGW	B	504	22/51	0.64	0.47	85,102,113,114	0
6	PGW	H	504	22/51	0.65	0.51	142,147,149,149	0
6	PGW	B	506	9/51	0.67	0.51	87,90,91,91	0
6	PGW	B	516	36/51	0.74	0.33	107,125,141,141	0
6	PGW	B	519	8/51	0.75	0.50	97,99,100,100	0
6	PGW	B	514	23/51	0.75	0.31	109,119,123,124	0
6	PGW	B	513	8/51	0.78	0.35	74,78,79,79	0
6	PGW	B	508	9/51	0.79	0.43	100,102,102,102	0
6	PGW	B	505	9/51	0.79	0.39	79,82,84,85	0
6	PGW	B	515	8/51	0.81	0.41	81,87,91,91	0
6	PGW	B	518	8/51	0.82	0.48	102,105,107,107	0
6	PGW	B	511	7/51	0.83	0.27	70,73,73,73	0
6	PGW	B	507	9/51	0.83	0.37	94,96,98,98	0
6	PGW	B	509	9/51	0.84	0.34	82,86,89,89	0
6	PGW	B	510	9/51	0.85	0.40	106,107,109,109	0
5	CS	B	502	1/1	0.86	0.08	43,43,43,43	1
5	CS	H	503	1/1	0.91	0.10	75,75,75,75	1
5	CS	B	501	1/1	0.92	0.08	45,45,45,45	1
5	CS	B	503	1/1	0.92	0.32	101,101,101,101	1
4	NAP	G	1001	48/48	0.93	0.12	25,39,51,51	0
4	NAP	A	1001	48/48	0.95	0.10	23,33,43,47	0
5	CS	H	505	1/1	0.96	0.18	126,126,126,126	1
5	CS	H	501	1/1	0.97	0.07	85,85,85,85	1
5	CS	H	502	1/1	0.98	0.07	74,74,74,74	1
5	CS	B	520	1/1	0.99	0.07	61,61,61,61	1

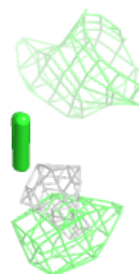
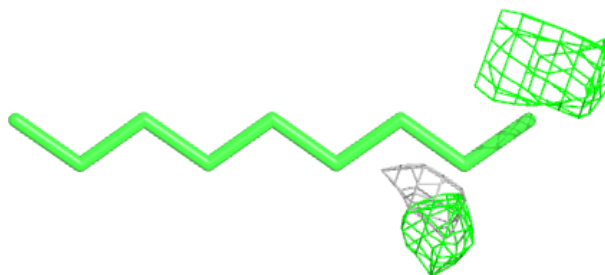
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PGW B 517:

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

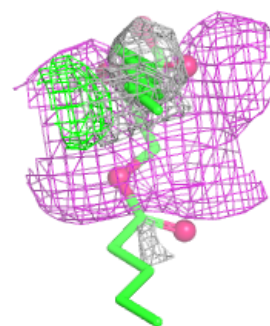
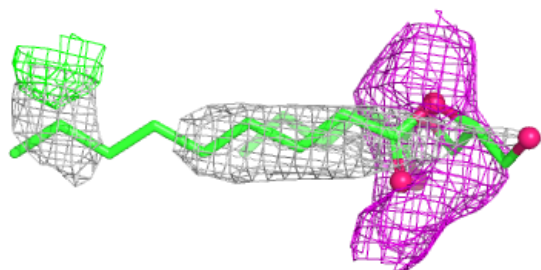
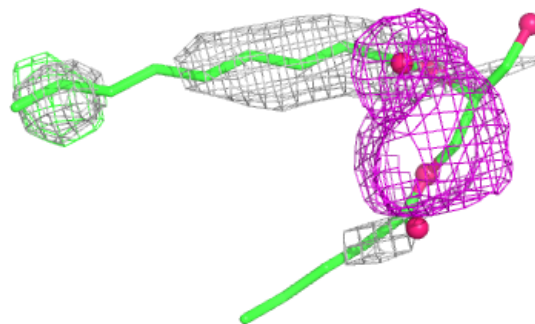
**Electron density around PGW B 512:**

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



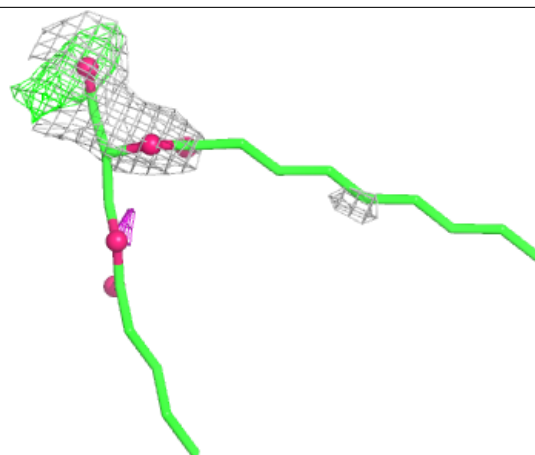
Electron density around PGW B 504:

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

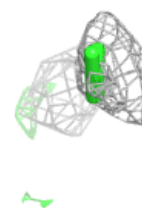
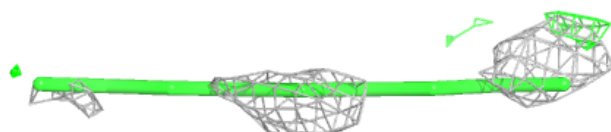
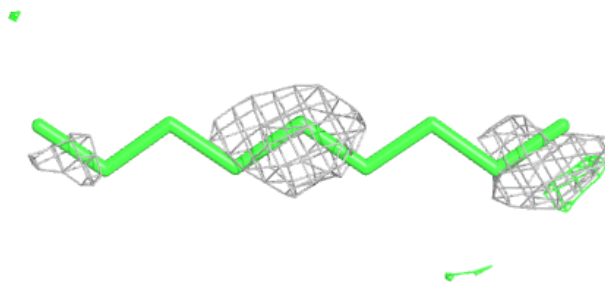


Electron density around PGW H 504:

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

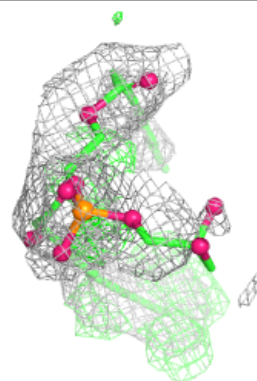
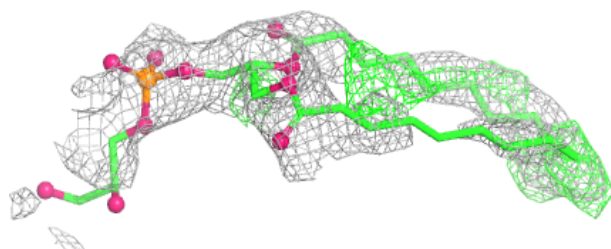
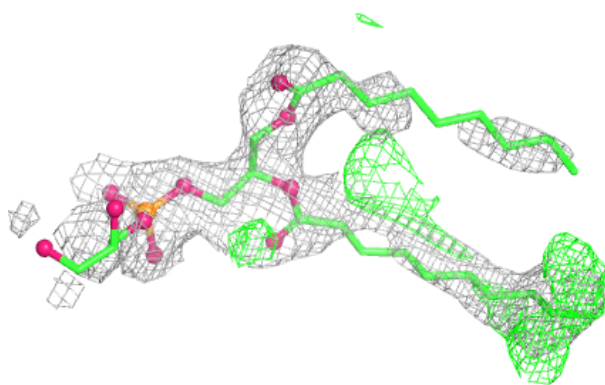
**Electron density around PGW B 506:**

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

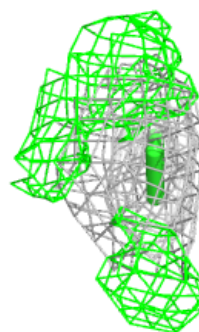
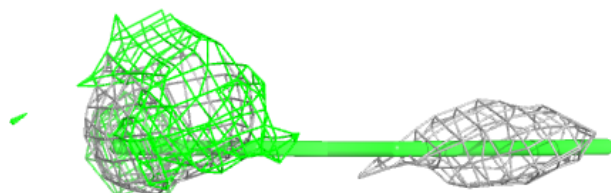
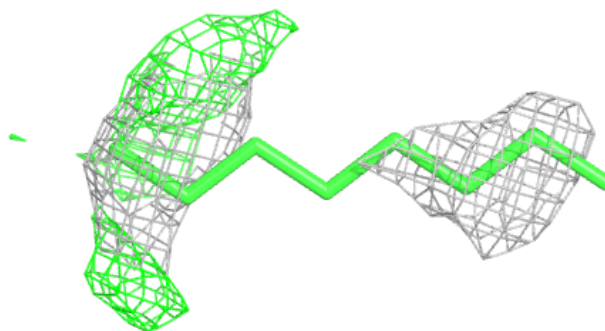


Electron density around PGW B 516:

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

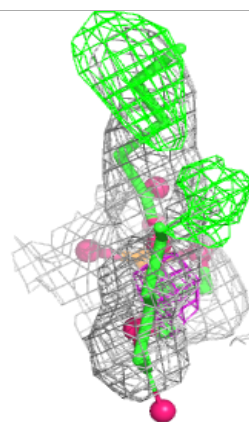
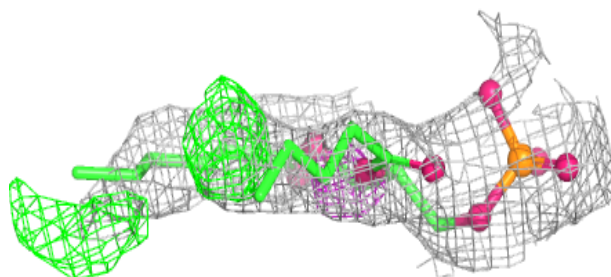
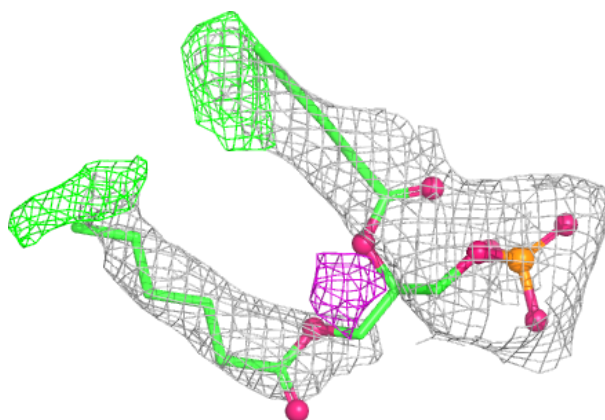
**Electron density around PGW B 519:**

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



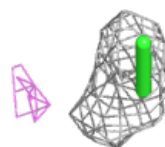
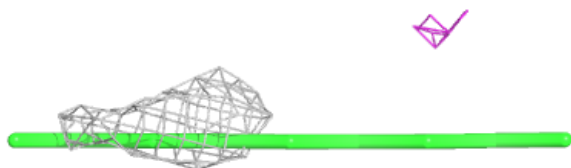
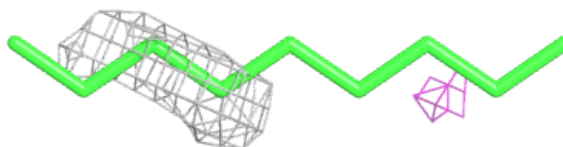
Electron density around PGW B 514:

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

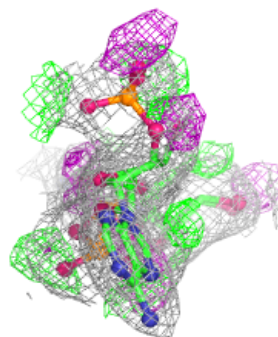
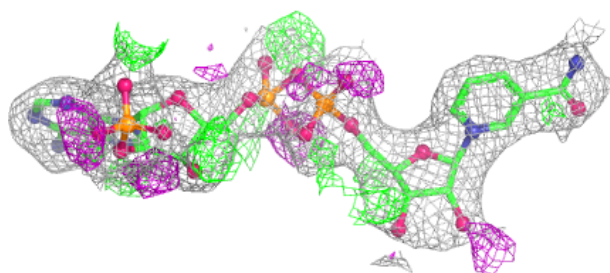
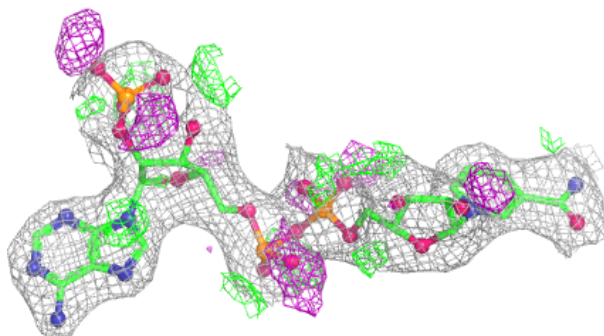


Electron density around PGW B 508:

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

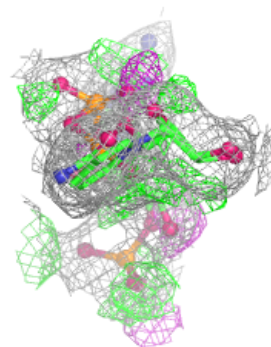
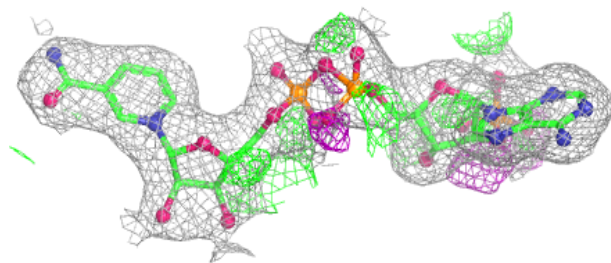
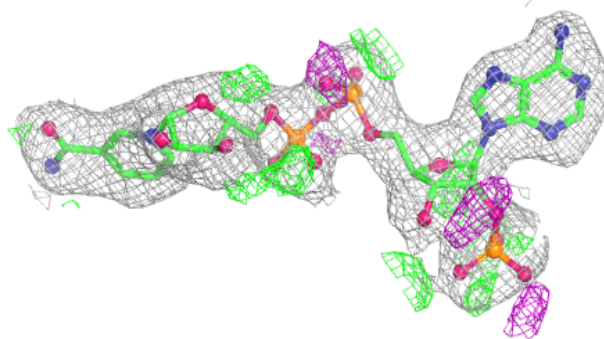
**Electron density around NAP G 1001:**

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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)



6.5 Other polymers [i](#)

There are no such residues in this entry.