



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:06 AM UTC

PDB ID : 4JTA / pdb_00004jta
Title : Crystal structure of Kv1.2-2.1 paddle chimera channel in complex with Charyb-dotoxin
Authors : MacKinnon, R.; Banerjee, A.; Lee, A.; Campbell, E.
Deposited on : 2013-03-23
Resolution : 2.50 Å(reported)

This is a 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

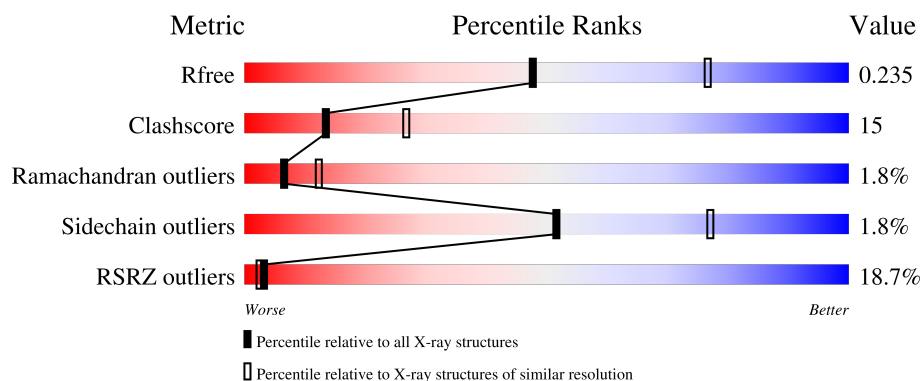
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	333	3% 80% 16% ..
1	P	333	3% 78% 17% ..
2	B	514	13% 49% 24% • 25%
2	Q	514	29% 39% 30% • 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	508	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	518	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There are 48 discrepancies between the modelled and reference sequences:

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

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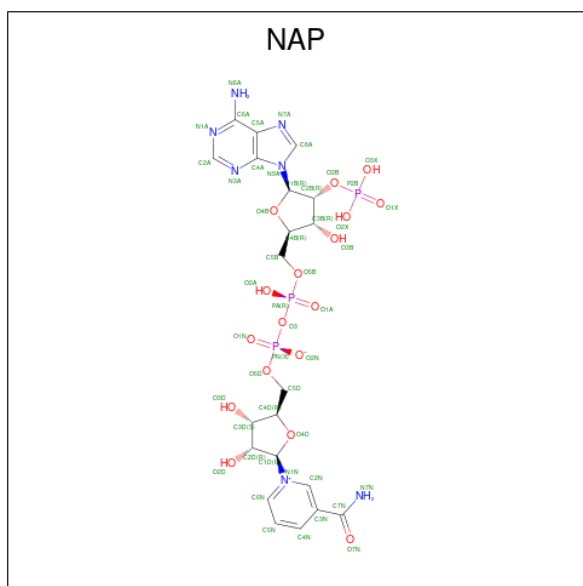
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP P63142
B	-8	HIS	-	expression tag	UNP P63142
B	-7	HIS	-	expression tag	UNP P63142
B	-6	GLY	-	expression tag	UNP P63142
B	-5	LEU	-	expression tag	UNP P63142
B	-4	VAL	-	expression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

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

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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

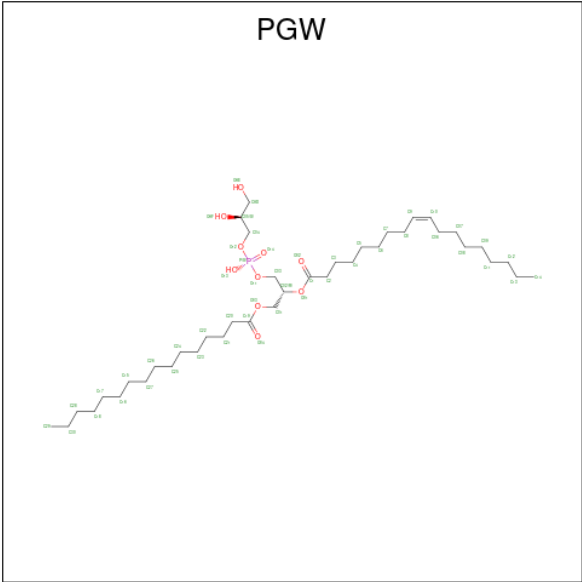


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

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

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula: $C_{40}H_{77}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 22 17 5	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 7 7	0	0
6	B	1	Total C 9 9	0	0
6	B	1	Total C 12 12	0	0
6	B	1	Total C O P 23 14 8 1	0	0
6	B	1	Total C 12 12	0	0
6	B	1	Total C O P 37 26 10 1	0	0
6	B	1	Total C 10 10	0	0

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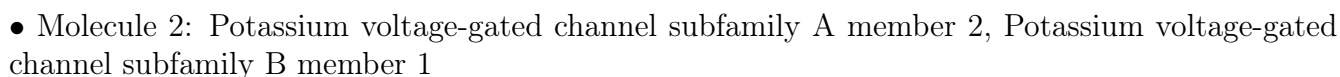
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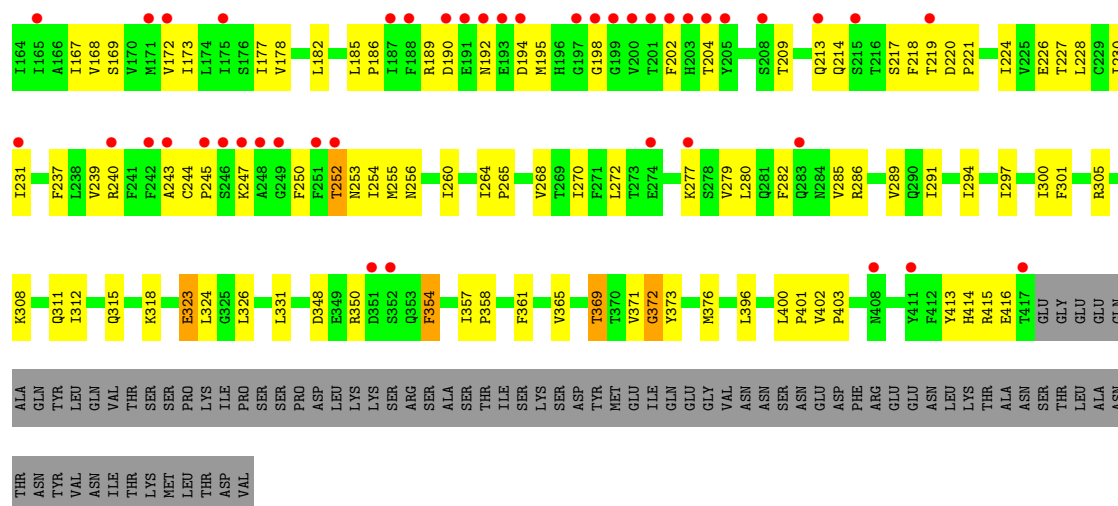
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C 12 12	0	0
6	B	1	Total C 12 12	0	0
6	Q	1	Total C O 22 17 5	0	0

- Molecule 7 is water.

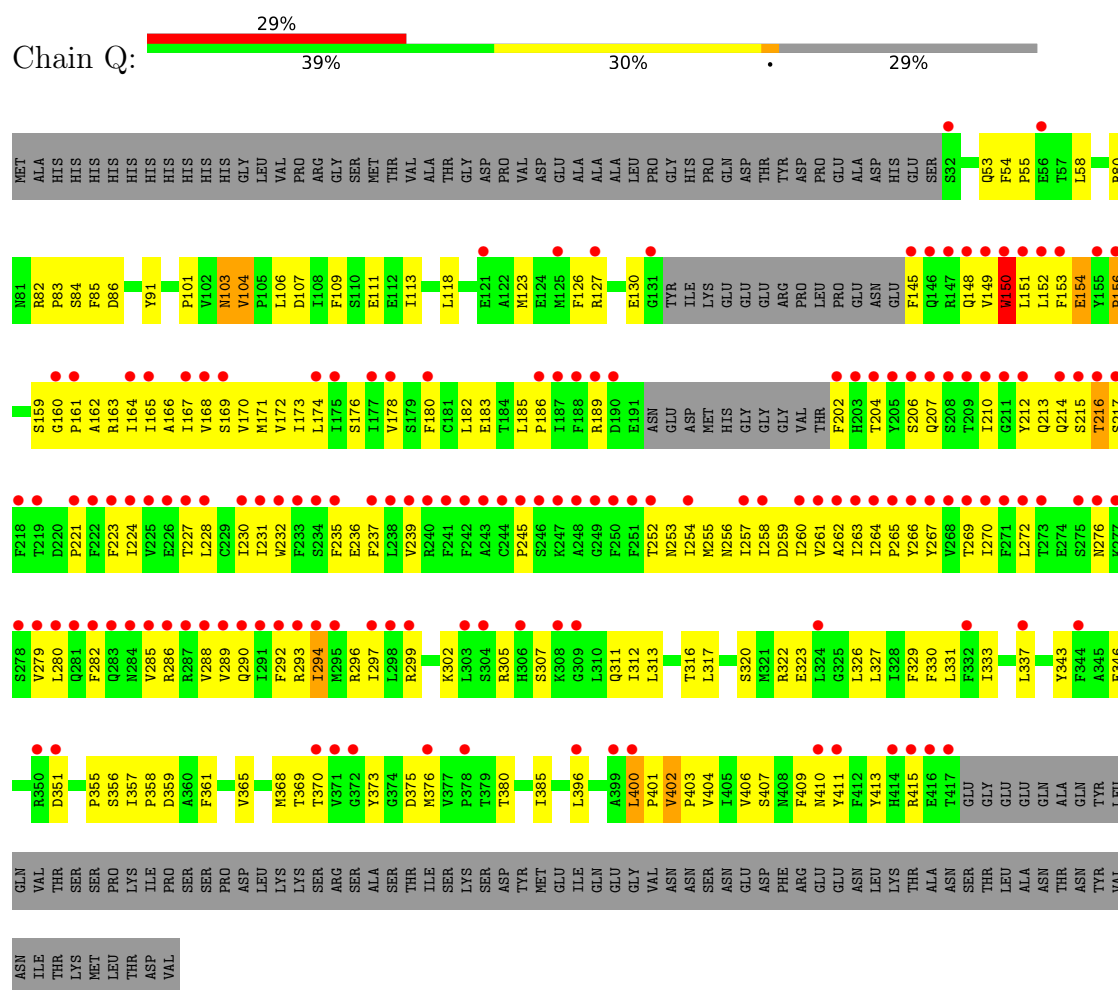
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	140	Total O 140 140	0	0
7	B	53	Total O 53 53	0	0
7	P	102	Total O 102 102	0	0
7	Q	23	Total O 23 23	0	0

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

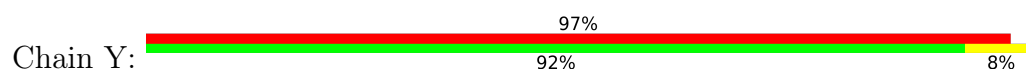




- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1



- Molecule 3: Potassium channel toxin alpha-KTx 1.1



Q1	F2	T3	N4	V5	S6	C7	T8	T9	S10	K11	E12	C13	W14	S15	V16	C17	Q18	R19	L20	H21	N22	T23	S24	R25	G26	K27	C28	M29	N30	K31	K32	C33	R34	C35	Y36	S37
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4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.40Å 144.40Å 284.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-2.50) 92.6 (50.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.236 0.212 , 0.235	Depositor DCC
R_{free} test set	5335 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12106	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.43	0/2608	0.86	1/3524 (0.0%)
1	P	0.42	0/2608	0.88	6/3524 (0.2%)
2	B	0.39	0/3169	0.87	7/4292 (0.2%)
2	Q	0.34	0/3036	0.86	10/4114 (0.2%)
3	Y	0.28	0/292	0.62	0/389
All	All	0.39	0/11713	0.86	24/15843 (0.2%)

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

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

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	ALA	N-CA-C	-7.02	97.79	108.67
1	P	157	ALA	N-CA-C	-6.97	97.87	108.67
2	B	372	GLY	N-CA-C	6.79	123.40	113.48
2	Q	369	THR	N-CA-C	-6.63	105.30	113.19
1	P	227	VAL	N-CA-C	6.41	117.07	111.56
2	Q	54	PHE	CA-C-N	6.35	127.78	119.84
2	Q	54	PHE	C-N-CA	6.35	127.78	119.84
1	P	269	GLY	N-CA-C	-6.06	107.27	114.48
2	B	354	PHE	CA-C-N	6.00	125.88	119.28
2	B	354	PHE	C-N-CA	6.00	125.88	119.28
2	B	252	THR	N-CA-C	-5.98	105.64	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	204	THR	N-CA-C	-5.92	107.05	114.56
2	B	140	LEU	CA-C-N	5.89	127.21	119.84
2	B	140	LEU	C-N-CA	5.89	127.21	119.84
2	B	369	THR	N-CA-C	-5.78	106.21	113.20
1	P	208	ILE	N-CA-C	5.48	113.91	107.77
1	P	228	GLN	N-CA-C	5.42	118.35	111.69
2	Q	104	VAL	N-CA-C	5.30	113.78	107.73
2	Q	85	PHE	N-CA-C	5.23	118.45	111.75
2	Q	402	VAL	CB-CA-C	-5.23	108.73	113.70
1	P	236	ILE	N-CA-C	5.11	117.02	112.17
2	Q	84	SER	N-CA-C	5.08	116.50	111.07
2	Q	385	ILE	N-CA-C	-5.04	105.93	110.82
2	Q	294	ILE	N-CA-C	-5.00	106.26	113.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	270	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2556	0	2582	44	0
1	P	2556	0	2582	48	0
2	B	3088	0	3034	101	0
2	Q	2959	0	2956	145	0
3	Y	295	0	282	0	0
4	A	48	0	25	3	0
4	P	48	0	25	3	0
5	B	3	0	0	0	0
5	Q	3	0	0	0	0
6	B	210	0	291	19	0
6	Q	22	0	25	7	0
7	A	140	0	0	2	0
7	B	53	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	102	0	0	0	0
7	Q	23	0	0	1	0
All	All	12106	0	11802	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (347) 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:Q:255:MET:HE1	2:Q:305:ARG:HA	1.41	1.00
6:B:510:PGW:H2A	6:B:515:PGW:H21A	1.42	0.98
2:Q:400:LEU:HB2	2:Q:401:PRO:HD3	1.52	0.89
1:P:333:ASN:HD21	4:P:1001:NAP:H61A	1.21	0.88
2:Q:312:ILE:HD13	2:Q:413:TYR:HA	1.59	0.83
2:Q:227:THR:HA	2:Q:230:ILE:HG22	1.61	0.82
2:Q:152:LEU:HD22	2:Q:161:PRO:HB2	1.62	0.81
2:Q:103:ASN:H	2:Q:103:ASN:HD22	1.29	0.80
1:A:118:LYS:HG3	1:A:156:PHE:HB2	1.63	0.80
2:B:400:LEU:HB2	2:B:401:PRO:HD3	1.62	0.79
2:B:350:ARG:HH11	2:B:350:ARG:HB3	1.48	0.78
1:P:40:ARG:HD2	1:P:318:SER:O	1.85	0.76
2:B:311:GLN:HG2	6:B:516:PGW:H3	1.69	0.74
1:P:75:LEU:HG	1:P:331:MET:HE3	1.70	0.73
1:P:295:ILE:HD12	1:P:295:ILE:H	1.53	0.71
6:B:510:PGW:H4A	6:B:515:PGW:H23A	1.72	0.71
2:B:192:ASN:O	2:B:195:MET:HE2	1.92	0.69
2:Q:103:ASN:HD22	2:Q:103:ASN:N	1.86	0.69
2:B:350:ARG:HB3	2:B:350:ARG:NH1	2.08	0.69
2:Q:260:ILE:HG22	2:Q:264:ILE:HD11	1.74	0.69
2:Q:361:PHE:HB2	6:Q:504:PGW:H2	1.73	0.69
1:P:268:LYS:NZ	1:P:268:LYS:HB3	2.08	0.69
2:Q:264:ILE:HB	2:Q:265:PRO:HD3	1.75	0.68
2:B:361:PHE:HB2	6:B:504:PGW:H2	1.76	0.68
2:Q:307:SER:O	2:Q:311:GLN:HG3	1.94	0.67
2:Q:262:ALA:HB1	2:Q:302:LYS:HE2	1.76	0.67
2:Q:361:PHE:CB	6:Q:504:PGW:H2	2.25	0.67
2:Q:103:ASN:H	2:Q:103:ASN:ND2	1.89	0.66
1:A:333:ASN:HD21	4:A:1001:NAP:H61A	1.43	0.66
1:A:280:GLU:HA	1:A:283:ARG:NH1	2.10	0.66
2:Q:167:ILE:O	2:Q:171:MET:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:265:PRO:HA	2:Q:292:PHE:HD2	1.59	0.66
2:Q:293:ARG:HA	2:Q:296:ARG:HD3	1.78	0.66
2:B:294:ILE:O	2:B:297:ILE:HG22	1.97	0.65
1:P:104:LYS:NZ	1:P:148:GLN:HE22	1.93	0.65
2:Q:101:PRO:HB2	2:Q:104:VAL:HG23	1.79	0.65
1:A:258:GLY:O	1:A:260:PRO:HD3	1.97	0.64
2:B:103:ASN:H	2:B:103:ASN:HD22	1.44	0.64
2:B:58:LEU:HD23	2:B:58:LEU:C	2.23	0.63
2:B:213:GLN:HB3	2:B:220:ASP:HB2	1.78	0.63
1:P:293:GLN:HE21	1:P:297:GLU:HG3	1.64	0.63
2:Q:230:ILE:HG12	2:Q:266:TYR:CD2	2.34	0.63
2:Q:259:ASP:HA	2:Q:302:LYS:NZ	2.15	0.62
2:B:82:ARG:HB2	2:B:83:PRO:HD3	1.80	0.62
6:Q:504:PGW:H01	6:Q:504:PGW:O02	1.99	0.61
2:Q:262:ALA:CB	2:Q:302:LYS:HE2	2.31	0.61
2:B:226:GLU:O	2:B:230:ILE:HD13	2.01	0.61
1:A:326:ASN:ND2	1:A:329:GLN:H	1.98	0.61
2:B:147:ARG:O	2:B:151:LEU:HG	2.00	0.61
2:Q:316:THR:HG21	2:Q:409:PHE:HB2	1.83	0.60
2:Q:411:TYR:CZ	2:Q:415:ARG:HD3	2.36	0.60
1:A:251:VAL:O	1:A:251:VAL:HG12	2.01	0.60
2:Q:174:LEU:O	2:Q:178:VAL:HG23	2.02	0.60
2:Q:230:ILE:HG21	2:Q:266:TYR:CZ	2.36	0.60
1:A:280:GLU:HG2	1:A:284:ARG:HH12	1.65	0.60
1:A:159:ARG:HA	1:A:188:SER:O	2.02	0.60
2:Q:212:TYR:HB2	2:Q:223:PHE:HB2	1.84	0.60
2:B:141:PRO:C	2:B:143:ASN:H	2.10	0.59
2:B:227:THR:O	2:B:231:ILE:HG12	2.02	0.59
2:Q:227:THR:O	2:Q:231:ILE:HG12	2.01	0.59
2:B:120:GLU:O	2:B:124:GLU:HG3	2.03	0.59
2:B:414:HIS:C	2:B:416:GLU:H	2.10	0.59
2:Q:260:ILE:O	2:Q:264:ILE:HG13	2.01	0.59
2:Q:86:ASP:HB2	7:Q:616:HOH:O	2.03	0.59
2:B:221:PRO:HB2	6:B:513:PGW:H23	1.85	0.58
2:Q:357:ILE:HB	2:Q:358:PRO:HD3	1.86	0.58
2:Q:294:ILE:O	2:Q:297:ILE:HG22	2.04	0.58
2:Q:207:GLN:HE21	2:Q:213:GLN:HB2	1.68	0.58
2:B:121:GLU:O	2:B:125:MET:HG2	2.03	0.58
2:Q:293:ARG:HA	2:Q:296:ARG:CD	2.34	0.58
2:Q:113:ILE:HG23	2:Q:118:LEU:HD12	1.86	0.58
2:Q:163:ARG:O	2:Q:167:ILE:HG12	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:148:GLN:NE2	2:Q:151:LEU:HD12	2.18	0.57
2:Q:82:ARG:HB2	2:Q:83:PRO:HD3	1.86	0.57
1:P:118:LYS:HG2	1:P:156:PHE:HB2	1.86	0.57
1:P:295:ILE:HD12	1:P:295:ILE:N	2.20	0.57
2:B:255:MET:CE	2:B:305:ARG:HA	2.35	0.57
1:P:214:GLN:HA	1:P:241:MET:O	2.05	0.57
2:Q:169:SER:O	2:Q:173:ILE:HG13	2.05	0.57
6:B:516:PGW:O02	6:B:516:PGW:H03A	2.05	0.56
2:Q:322:ARG:HG3	2:Q:322:ARG:HH11	1.68	0.56
2:Q:402:VAL:O	2:Q:406:VAL:HG23	2.05	0.56
1:P:268:LYS:HB3	1:P:268:LYS:HZ3	1.69	0.56
2:B:365:VAL:HG21	6:B:504:PGW:H6A	1.87	0.56
1:A:303:LEU:HB3	1:A:304:PRO:HD3	1.88	0.56
2:B:255:MET:HE1	2:B:305:ARG:HA	1.87	0.56
6:B:504:PGW:H01	6:B:504:PGW:O02	2.05	0.56
2:B:103:ASN:H	2:B:103:ASN:ND2	2.03	0.56
2:Q:145:PHE:CZ	2:Q:149:VAL:HG21	2.41	0.56
2:Q:148:GLN:HE22	2:Q:151:LEU:HD12	1.71	0.55
2:Q:53:GLN:C	2:Q:55:PRO:HD3	2.31	0.55
2:Q:235:PHE:O	2:Q:239:VAL:HG23	2.06	0.55
1:A:280:GLU:HG2	1:A:284:ARG:NH1	2.22	0.55
1:A:340:LEU:HB3	1:A:341:PRO:HD3	1.88	0.55
2:Q:400:LEU:O	2:Q:403:PRO:HD2	2.07	0.55
2:Q:168:VAL:O	2:Q:172:VAL:HG23	2.08	0.54
1:P:217:TYR:HB2	1:P:225:VAL:HG21	1.89	0.54
1:A:73:MET:HE3	1:A:84:PHE:CD2	2.43	0.54
2:Q:282:PHE:CZ	2:Q:289:VAL:HG21	2.43	0.54
1:P:251:VAL:HG12	1:P:251:VAL:O	2.06	0.54
1:A:71:HIS:CD2	1:A:327:ALA:HB2	2.43	0.54
1:P:152:VAL:O	1:P:182:ALA:HA	2.07	0.54
2:Q:227:THR:CA	2:Q:230:ILE:HG22	2.34	0.54
1:P:173:MET:HG3	1:P:185:TRP:CE3	2.44	0.53
2:Q:221:PRO:HA	2:Q:224:ILE:HD12	1.90	0.53
2:Q:232:TRP:O	2:Q:236:GLU:HG3	2.07	0.53
6:B:514:PGW:O11	6:B:514:PGW:O02	2.25	0.53
1:P:159:ARG:HB2	1:P:160:PRO:HD2	1.90	0.53
2:Q:272:LEU:HD13	2:Q:285:VAL:HG21	1.90	0.53
1:P:73:MET:HE3	1:P:84:PHE:CD2	2.43	0.53
2:B:253:ASN:HB3	2:B:256:ASN:ND2	2.24	0.53
2:B:177:ILE:HD13	2:B:300:ILE:HD12	1.89	0.53
2:Q:355:PRO:HB2	2:Q:359:ASP:OD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:GLU:CD	2:B:323:GLU:H	2.16	0.52
2:B:214:GLN:HE22	2:B:270:ILE:HA	1.75	0.52
2:B:318:LYS:HD2	6:B:516:PGW:H21A	1.91	0.52
2:B:357:ILE:HB	2:B:358:PRO:HD3	1.91	0.52
2:Q:227:THR:HA	2:Q:230:ILE:CG2	2.36	0.52
2:Q:280:LEU:H	2:Q:280:LEU:HD12	1.73	0.52
2:B:254:ILE:HD12	6:B:516:PGW:H24A	1.92	0.52
1:P:37:GLN:HE21	1:P:37:GLN:N	2.07	0.52
2:Q:53:GLN:O	2:Q:55:PRO:HD3	2.10	0.52
2:Q:375:ASP:O	2:Q:376:MET:HG3	2.10	0.52
2:Q:178:VAL:O	2:Q:182:LEU:HG	2.10	0.52
2:Q:259:ASP:HA	2:Q:302:LYS:HZ3	1.73	0.52
2:Q:285:VAL:HG13	2:Q:285:VAL:O	2.10	0.52
2:B:277:LYS:HG3	2:B:277:LYS:O	2.10	0.51
2:Q:150:TRP:CE3	2:Q:150:TRP:HA	2.44	0.51
2:Q:224:ILE:O	2:Q:228:LEU:HG	2.11	0.51
2:Q:368:MET:C	2:Q:370:THR:H	2.17	0.51
2:Q:152:LEU:O	2:Q:165:ILE:HD12	2.10	0.51
2:Q:58:LEU:HD23	2:Q:58:LEU:C	2.36	0.51
1:P:120:PHE:CD1	1:P:159:ARG:HG3	2.46	0.51
2:Q:152:LEU:HD13	2:Q:165:ILE:CD1	2.41	0.51
2:Q:166:ALA:O	2:Q:170:VAL:HG23	2.10	0.51
2:B:177:ILE:CD1	2:B:300:ILE:HD12	2.41	0.51
2:B:150:TRP:O	2:B:154:GLU:HB3	2.10	0.51
2:Q:402:VAL:HB	2:Q:403:PRO:HD3	1.94	0.50
2:Q:150:TRP:HA	2:Q:150:TRP:HE3	1.76	0.50
1:P:326:ASN:OD1	1:P:329:GLN:HG3	2.12	0.50
1:P:333:ASN:ND2	4:P:1001:NAP:H61A	2.01	0.50
2:Q:161:PRO:O	2:Q:165:ILE:HG13	2.10	0.50
2:Q:206:SER:O	2:Q:210:ILE:HD12	2.11	0.50
2:Q:237:PHE:CE1	2:Q:260:ILE:HG12	2.45	0.50
2:Q:254:ILE:O	2:Q:258:ILE:HG13	2.12	0.50
1:P:134:LYS:O	1:P:138:GLU:HG3	2.12	0.49
1:P:286:GLN:NE2	1:P:289:LEU:HD12	2.27	0.49
2:B:106:LEU:HD13	2:B:130:GLU:HG2	1.93	0.49
2:B:189:ARG:HG3	2:B:189:ARG:HH11	1.77	0.49
2:B:312:ILE:HD13	2:B:413:TYR:HA	1.94	0.49
1:P:303:LEU:HB3	1:P:304:PRO:HD3	1.94	0.49
2:Q:186:PRO:HB3	2:Q:189:ARG:NH2	2.27	0.49
2:Q:411:TYR:CE2	2:Q:415:ARG:HD3	2.48	0.49
1:P:295:ILE:H	1:P:295:ILE:CD1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.42	0.49
1:A:281:GLU:O	1:A:285:GLN:HG3	2.11	0.49
2:B:308:LYS:O	2:B:312:ILE:HG13	2.12	0.49
2:Q:106:LEU:CD1	2:Q:130:GLU:HG2	2.42	0.49
2:B:178:VAL:O	2:B:182:LEU:HG	2.13	0.49
2:B:186:PRO:O	2:B:190:ASP:HB2	2.13	0.49
2:Q:176:SER:HB2	2:Q:299:ARG:HH11	1.78	0.49
1:P:333:ASN:HD22	1:P:333:ASN:N	2.10	0.49
2:Q:327:LEU:O	2:Q:331:LEU:HD13	2.12	0.49
2:Q:323:GLU:OE1	2:Q:404:VAL:HG11	2.14	0.48
2:B:260:ILE:O	2:B:264:ILE:HG13	2.13	0.48
2:Q:280:LEU:HD12	2:Q:280:LEU:N	2.28	0.48
2:B:348:ASP:HB2	7:B:646:HOH:O	2.13	0.48
2:B:107:ASP:O	2:B:111:GLU:HG3	2.13	0.48
2:B:214:GLN:NE2	2:B:270:ILE:HG12	2.28	0.48
2:B:415:ARG:HH11	2:B:415:ARG:HG2	1.76	0.48
2:Q:326:LEU:HG	2:Q:330:PHE:CE2	2.49	0.48
2:Q:91:TYR:CE2	2:Q:118:LEU:HD22	2.48	0.48
2:Q:107:ASP:O	2:Q:111:GLU:HG3	2.14	0.48
2:B:285:VAL:O	2:B:285:VAL:HG22	2.14	0.47
2:Q:253:ASN:HB3	2:Q:256:ASN:ND2	2.29	0.47
1:A:355:LEU:HB3	1:A:357:ASN:OD1	2.14	0.47
2:B:169:SER:O	2:B:173:ILE:HG13	2.15	0.47
2:Q:396:LEU:O	2:Q:400:LEU:HG	2.14	0.47
2:B:291:ILE:HG23	6:B:507:PGW:H5	1.95	0.47
2:Q:101:PRO:HB2	2:Q:104:VAL:CG2	2.44	0.47
2:Q:171:MET:N	2:Q:171:MET:HE2	2.29	0.47
1:A:326:ASN:ND2	1:A:328:GLU:HB2	2.29	0.47
2:B:109:PHE:O	2:B:113:ILE:HG13	2.13	0.47
6:Q:504:PGW:O02	6:Q:504:PGW:C01	2.60	0.47
2:Q:346:GLU:OE2	2:Q:380:THR:HG23	2.15	0.47
2:Q:365:VAL:HG21	6:Q:504:PGW:H6A	1.96	0.47
2:B:305:ARG:HH11	2:B:305:ARG:HG3	1.80	0.46
1:P:68:MET:O	1:P:72:LEU:HG	2.15	0.46
1:P:102:ILE:O	1:P:106:LYS:HG2	2.15	0.46
1:P:104:LYS:HZ3	1:P:148:GLN:HE22	1.61	0.46
2:Q:320:SER:HA	2:Q:323:GLU:HG2	1.96	0.46
1:P:119:ILE:O	1:P:120:PHE:HB2	2.15	0.46
2:Q:123:MET:O	2:Q:126:PHE:HB3	2.15	0.46
1:A:214:GLN:HA	1:A:241:MET:O	2.15	0.46
2:Q:215:SER:O	2:Q:216:THR:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ILE:O	2:B:268:VAL:HG23	2.16	0.46
6:B:504:PGW:O02	6:B:504:PGW:H03A	2.16	0.46
2:Q:152:LEU:HA	2:Q:162:ALA:HB2	1.98	0.46
2:B:168:VAL:O	2:B:172:VAL:HG23	2.16	0.46
1:P:291:GLU:O	1:P:294:ALA:HB3	2.16	0.46
2:Q:407:SER:O	2:Q:410:ASN:HB3	2.16	0.46
2:B:402:VAL:HB	2:B:403:PRO:HD3	1.97	0.46
1:P:350:GLU:O	1:P:353:SER:HB2	2.16	0.46
2:Q:152:LEU:CD2	2:Q:161:PRO:HB2	2.41	0.46
2:Q:185:LEU:O	2:Q:189:ARG:HG2	2.16	0.46
2:Q:361:PHE:HB3	6:Q:504:PGW:H2	1.97	0.46
1:A:106:LYS:HG3	1:A:108:TRP:CH2	2.51	0.45
2:B:264:ILE:HB	2:B:265:PRO:HD3	1.98	0.45
2:Q:127:ARG:HG2	2:Q:127:ARG:HH11	1.81	0.45
2:Q:337:LEU:C	2:Q:337:LEU:HD23	2.42	0.45
1:A:326:ASN:HD22	1:A:328:GLU:N	2.15	0.45
2:Q:255:MET:HE3	2:Q:305:ARG:NH1	2.32	0.45
2:Q:257:ILE:HD13	2:Q:260:ILE:HD12	1.98	0.45
2:Q:272:LEU:HD13	2:Q:285:VAL:CG2	2.46	0.45
2:Q:152:LEU:CB	2:Q:162:ALA:HB2	2.47	0.45
2:Q:153:PHE:O	2:Q:154:GLU:HB2	2.16	0.45
1:A:120:PHE:CD1	1:A:159:ARG:HG3	2.52	0.45
2:B:142:GLU:O	2:B:143:ASN:C	2.59	0.45
2:Q:227:THR:O	2:Q:230:ILE:HG22	2.17	0.45
2:Q:368:MET:C	2:Q:370:THR:N	2.73	0.45
1:A:85:ASP:OD1	1:A:118:LYS:NZ	2.47	0.45
1:A:314:ASN:HB2	7:A:1166:HOH:O	2.16	0.45
2:B:178:VAL:HG22	6:B:509:PGW:H8	1.99	0.45
2:Q:254:ILE:HG23	2:Q:255:MET:N	2.32	0.45
2:B:153:PHE:CD2	2:B:239:VAL:HG11	2.52	0.45
2:B:414:HIS:C	2:B:416:GLU:N	2.75	0.45
1:A:360:TYR:HD1	1:A:360:TYR:H	1.65	0.44
2:B:318:LYS:HD2	6:B:516:PGW:C22	2.47	0.44
2:Q:156:PRO:HA	2:Q:162:ALA:HB1	1.99	0.44
2:Q:400:LEU:CB	2:Q:401:PRO:HD3	2.35	0.44
2:Q:253:ASN:HB3	2:Q:256:ASN:HD22	1.82	0.44
2:Q:255:MET:HE1	2:Q:305:ARG:CA	2.30	0.44
1:A:326:ASN:HD21	1:A:329:GLN:H	1.63	0.44
2:Q:260:ILE:HG22	2:Q:264:ILE:CD1	2.45	0.44
2:Q:270:ILE:O	2:Q:270:ILE:HG22	2.17	0.44
2:Q:322:ARG:HG3	2:Q:322:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:337:LEU:HD23	2:Q:337:LEU:O	2.18	0.44
2:B:244:CYS:SG	2:B:247:LYS:HG2	2.58	0.44
2:Q:286:ARG:HH12	2:Q:290:GLN:NE2	2.16	0.44
2:Q:202:PHE:HB2	2:Q:279:VAL:CG2	2.47	0.44
2:B:141:PRO:C	2:B:143:ASN:N	2.75	0.44
2:B:318:LYS:HD2	6:B:516:PGW:C21	2.48	0.44
6:Q:504:PGW:O02	6:Q:504:PGW:H03A	2.17	0.44
2:B:163:ARG:O	2:B:167:ILE:HG12	2.18	0.44
2:B:192:ASN:ND2	2:B:194:ASP:H	2.16	0.44
1:P:120:PHE:O	1:P:129:ARG:HA	2.18	0.44
1:P:251:VAL:O	1:P:251:VAL:CG1	2.65	0.44
1:P:323:GLY:HA3	4:P:1001:NAP:H51A	2.00	0.43
2:Q:176:SER:HB2	2:Q:299:ARG:NH1	2.33	0.43
2:B:192:ASN:HD22	2:B:204:THR:HG21	1.81	0.43
2:Q:214:GLN:NE2	2:Q:269:THR:HG22	2.33	0.43
1:A:327:ALA:HB1	1:A:331:MET:HE2	1.99	0.43
2:B:237:PHE:CE1	2:B:260:ILE:HG12	2.53	0.43
1:A:159:ARG:HB2	1:A:160:PRO:HD2	1.99	0.43
1:A:280:GLU:HA	1:A:283:ARG:HH11	1.80	0.43
2:B:323:GLU:CD	2:B:323:GLU:N	2.75	0.43
1:P:104:LYS:HZ2	1:P:148:GLN:HE22	1.64	0.43
2:Q:154:GLU:O	2:Q:156:PRO:HD3	2.19	0.43
2:Q:313:LEU:O	2:Q:317:LEU:HG	2.19	0.43
2:Q:329:PHE:O	2:Q:333:ILE:HG12	2.18	0.43
2:Q:170:VAL:HB	2:Q:171:MET:HE2	2.01	0.43
2:Q:276:ASN:ND2	2:Q:285:VAL:HG11	2.34	0.43
2:Q:297:ILE:C	2:Q:299:ARG:N	2.74	0.43
2:B:318:LYS:HB2	6:B:516:PGW:H23A	2.01	0.43
1:P:217:TYR:HB3	1:P:242:THR:HB	2.00	0.43
1:A:156:PHE:HA	1:A:186:GLY:O	2.19	0.42
2:B:240:ARG:HH11	2:B:240:ARG:HG3	1.84	0.42
2:B:250:PHE:C	2:B:252:THR:H	2.27	0.42
2:B:350:ARG:HH11	2:B:350:ARG:CB	2.24	0.42
1:A:202:ALA:HA	1:A:207:LEU:HB2	2.00	0.42
1:P:70:GLU:HA	1:P:102:ILE:HD13	2.02	0.42
2:Q:109:PHE:CE2	2:Q:113:ILE:HD11	2.54	0.42
2:B:240:ARG:O	2:B:244:CYS:HB3	2.19	0.42
1:P:85:ASP:OD1	1:P:118:LYS:NZ	2.50	0.42
2:Q:236:GLU:HA	2:Q:239:VAL:CG2	2.49	0.42
2:Q:261:VAL:HG12	2:Q:261:VAL:O	2.20	0.42
2:Q:316:THR:CG2	2:Q:409:PHE:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:HD12	2:B:331:LEU:HA	1.83	0.42
1:P:104:LYS:HE2	1:P:104:LYS:HB3	1.86	0.42
1:P:216:GLU:HB2	1:P:243:TRP:CH2	2.54	0.42
1:P:216:GLU:HB2	1:P:243:TRP:CZ2	2.55	0.42
1:P:292:LEU:HD11	1:P:355:LEU:HD21	2.02	0.42
1:A:38:PHE:HE1	1:A:337:ILE:CD1	2.33	0.42
2:B:255:MET:SD	6:B:516:PGW:H2A	2.60	0.42
2:Q:172:VAL:HG12	2:Q:172:VAL:O	2.20	0.42
2:Q:286:ARG:C	2:Q:288:VAL:H	2.27	0.42
1:A:261:PRO:O	1:A:262:TYR:HB2	2.19	0.42
1:A:333:ASN:ND2	4:A:1001:NAP:H61A	2.15	0.42
2:B:98:LEU:HD21	2:B:113:ILE:HD13	2.01	0.42
2:B:272:LEU:HD22	2:B:285:VAL:HG21	2.01	0.42
2:Q:160:GLY:H	2:Q:161:PRO:CD	2.32	0.42
1:A:40:ARG:HD2	1:A:318:SER:O	2.20	0.42
2:B:256:ASN:O	2:B:260:ILE:HG13	2.19	0.42
2:B:369:THR:OG1	2:B:371:VAL:HG23	2.20	0.41
2:B:396:LEU:O	2:B:400:LEU:HG	2.20	0.41
2:Q:297:ILE:C	2:Q:299:ARG:H	2.27	0.41
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.92	0.41
1:P:268:LYS:HD2	1:P:268:LYS:C	2.44	0.41
2:Q:160:GLY:N	2:Q:161:PRO:CD	2.83	0.41
2:Q:230:ILE:HD11	2:Q:263:ILE:HG22	2.01	0.41
1:A:119:ILE:O	1:A:120:PHE:HB2	2.20	0.41
1:A:323:GLY:HA3	4:A:1001:NAP:H51A	2.02	0.41
2:Q:202:PHE:CD1	2:Q:279:VAL:HG22	2.55	0.41
2:B:143:ASN:O	2:B:144:GLU:C	2.63	0.41
2:B:217:SER:O	2:B:218:PHE:C	2.63	0.41
2:B:253:ASN:HB3	2:B:256:ASN:HD22	1.85	0.41
2:B:300:ILE:HG23	2:B:301:PHE:N	2.34	0.41
1:P:159:ARG:HA	1:P:188:SER:O	2.21	0.41
1:A:38:PHE:CD1	1:A:337:ILE:HD13	2.56	0.41
2:B:326:LEU:HD12	2:B:326:LEU:HA	1.83	0.41
2:Q:267:TYR:C	2:Q:269:THR:N	2.77	0.41
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.79	0.41
2:B:202:PHE:HB2	2:B:279:VAL:HG22	2.03	0.41
2:B:282:PHE:HA	2:B:285:VAL:HG12	2.03	0.41
2:Q:164:ILE:O	2:Q:168:VAL:HG23	2.20	0.41
2:Q:305:ARG:HH11	2:Q:305:ARG:HG3	1.86	0.41
2:B:73:ARG:HB2	2:B:75:GLU:HG2	2.03	0.41
2:B:160:GLY:N	2:B:161:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HB3	1:A:128:GLU:HG3	2.01	0.41
1:A:249:GLY:HA3	7:A:1140:HOH:O	2.21	0.41
2:B:61:ASP:OD2	2:B:64:LYS:HG3	2.20	0.41
2:B:88:ILE:O	2:B:91:TYR:HB3	2.21	0.41
2:B:189:ARG:HG3	2:B:189:ARG:NH1	2.36	0.41
2:B:209:THR:HG21	2:B:286:ARG:HG3	2.03	0.41
2:B:213:GLN:HE22	2:B:219:THR:HB	1.86	0.41
2:B:318:LYS:HD2	6:B:516:PGW:H22	2.01	0.41
2:B:354:PHE:CD1	2:B:376:MET:HE2	2.56	0.41
2:B:415:ARG:HG2	2:B:415:ARG:NH1	2.36	0.41
2:Q:236:GLU:HA	2:Q:239:VAL:HG23	2.02	0.41
2:Q:252:THR:HG22	2:Q:252:THR:O	2.21	0.41
1:A:251:VAL:O	1:A:251:VAL:CG1	2.68	0.41
1:A:360:TYR:N	1:A:360:TYR:CD1	2.89	0.41
1:P:73:MET:HE3	1:P:84:PHE:CG	2.56	0.41
1:P:98:VAL:O	1:P:102:ILE:HG13	2.21	0.41
2:Q:400:LEU:C	2:Q:403:PRO:HD2	2.46	0.41
2:B:58:LEU:C	2:B:58:LEU:CD2	2.94	0.40
2:B:224:ILE:O	2:B:228:LEU:HG	2.20	0.40
2:Q:170:VAL:O	2:Q:173:ILE:HB	2.21	0.40
1:A:216:GLU:HB2	1:A:243:TRP:CZ2	2.56	0.40
1:P:292:LEU:HA	1:P:295:ILE:HD13	2.02	0.40
2:Q:343:TYR:CE1	2:Q:356:SER:HA	2.56	0.40
2:B:311:GLN:O	2:B:315:GLN:HG3	2.21	0.40
2:Q:106:LEU:HD11	2:Q:130:GLU:HG2	2.03	0.40
2:Q:180:PHE:HA	2:Q:183:GLU:OE2	2.21	0.40
1:A:215:ALA:O	1:A:242:THR:HA	2.21	0.40
2:B:285:VAL:O	2:B:289:VAL:HG23	2.21	0.40
2:B:372:GLY:O	2:B:373:TYR:C	2.65	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%)	313 (97%)	10 (3%)	1 (0%)	36	55
1	P	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	36	55
2	B	384/514 (75%)	350 (91%)	21 (6%)	13 (3%)	3	4
2	Q	357/514 (70%)	311 (87%)	37 (10%)	9 (2%)	4	7
3	Y	35/37 (95%)	19 (54%)	15 (43%)	1 (3%)	3	5
All	All	1424/1731 (82%)	1306 (92%)	93 (6%)	25 (2%)	6	12

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	134	LYS
2	B	137	GLU
2	B	138	ARG
2	B	139	PRO
2	B	143	ASN
2	Q	154	GLU
1	A	120	PHE
2	B	133	ILE
2	B	144	GLU
1	P	120	PHE
2	Q	150	TRP
2	Q	159	SER
2	Q	216	THR
2	Q	217	SER
2	B	245	PRO
2	B	142	GLU
2	B	146	GLN
2	B	243	ALA
2	Q	373	TYR
3	Y	10	SER
2	Q	245	PRO
2	B	141	PRO
2	B	198	GLY
2	Q	156	PRO
2	Q	400	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/280 (98%)	270 (99%)	3 (1%)	65	84
1	P	273/280 (98%)	265 (97%)	8 (3%)	37	65
2	B	332/459 (72%)	327 (98%)	5 (2%)	57	80
2	Q	324/459 (71%)	320 (99%)	4 (1%)	63	83
3	Y	35/35 (100%)	33 (94%)	2 (6%)	18	39
All	All	1237/1513 (82%)	1215 (98%)	22 (2%)	51	77

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	326	ASN
1	A	360	TYR
2	B	103	ASN
2	B	185	LEU
2	B	280	LEU
2	B	323	GLU
2	B	324	LEU
1	P	37	GLN
1	P	73	MET
1	P	75	LEU
1	P	129	ARG
1	P	214	GLN
1	P	223	GLU
1	P	268	LYS
1	P	283	ARG
2	Q	80	ARG
2	Q	103	ASN
2	Q	150	TRP
2	Q	351	ASP
3	Y	14	TRP
3	Y	18	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS

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Mol	Chain	Res	Type
1	A	148	GLN
1	A	206	ASN
1	A	228	GLN
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	53	GLN
2	B	74	ASN
2	B	103	ASN
2	B	192	ASN
2	B	196	HIS
2	B	213	GLN
2	B	214	GLN
2	B	290	GLN
2	B	306	HIS
2	B	315	GLN
2	B	414	HIS
1	P	37	GLN
1	P	71	HIS
1	P	148	GLN
1	P	163	ASN
1	P	204	GLN
1	P	271	GLN
1	P	286	GLN
1	P	293	GLN
1	P	333	ASN
2	Q	53	GLN
2	Q	103	ASN
2	Q	146	GLN
2	Q	148	GLN
2	Q	207	GLN
2	Q	213	GLN
2	Q	290	GLN
2	Q	315	GLN
2	Q	353	GLN
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	0.98	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGW	B	512	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	504	-	21,21,50	0.61	0	23,23,56	1.22	3 (13%)
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.54	0
6	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.54	0
6	PGW	B	515	-	11,11,50	0.35	0	10,10,56	0.59	0
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.55	0
6	PGW	B	516	-	36,36,50	0.65	0	39,42,56	0.90	2 (5%)
6	PGW	B	506	-	8,8,50	0.36	0	7,7,56	0.53	0
6	PGW	B	513	-	11,11,50	0.35	0	10,10,56	0.59	0
4	NAP	A	1001	-	50,52,52	1.33	6 (12%)	71,80,80	0.95	2 (2%)
6	PGW	B	505	-	8,8,50	0.36	0	7,7,56	0.54	0
6	PGW	B	511	-	6,6,50	0.36	0	5,5,56	0.48	0
6	PGW	B	518	-	11,11,50	0.35	0	10,10,56	0.57	0
4	NAP	P	1001	-	50,52,52	1.43	7 (14%)	71,80,80	0.98	2 (2%)
6	PGW	B	517	-	9,9,50	0.36	0	8,8,56	0.56	0
6	PGW	B	519	-	11,11,50	0.35	0	10,10,56	0.57	0
6	PGW	B	514	-	22,22,50	0.80	0	25,27,56	1.28	4 (16%)
6	PGW	Q	504	-	21,21,50	0.61	0	23,23,56	1.21	4 (17%)

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	512	-	-	0/6/6/55	-
6	PGW	B	504	-	-	1/23/23/55	-
6	PGW	B	507	-	-	0/6/6/55	-
6	PGW	B	508	-	-	0/6/6/55	-
6	PGW	B	509	-	-	0/6/6/55	-
6	PGW	B	515	-	-	0/9/9/55	-
6	PGW	B	510	-	-	0/6/6/55	-
6	PGW	B	516	-	-	7/41/41/55	-
6	PGW	B	506	-	-	0/6/6/55	-
6	PGW	B	513	-	-	0/9/9/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	A	1001	-	-	4/35/67/67	0/5/5/5
6	PGW	B	505	-	-	0/6/6/55	-
6	PGW	B	511	-	-	0/4/4/55	-
6	PGW	B	518	-	-	0/9/9/55	-
4	NAP	P	1001	-	-	3/35/67/67	0/5/5/5
6	PGW	B	517	-	-	0/7/7/55	-
6	PGW	B	519	-	-	0/9/9/55	-
6	PGW	B	514	-	-	7/24/24/55	-
6	PGW	Q	504	-	-	1/23/23/55	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1001	NAP	C6N-N1N	4.24	1.45	1.35
4	A	1001	NAP	C6N-N1N	4.02	1.44	1.35
4	P	1001	NAP	C4N-C3N	3.73	1.45	1.39
4	A	1001	NAP	C4N-C3N	3.68	1.45	1.39
4	P	1001	NAP	PA-O3	3.68	1.63	1.59
4	P	1001	NAP	C4A-N3A	3.01	1.40	1.34
4	A	1001	NAP	C4A-N3A	2.58	1.39	1.34
4	A	1001	NAP	C2N-N1N	2.47	1.37	1.35
4	A	1001	NAP	C5A-N7A	-2.38	1.34	1.39
4	P	1001	NAP	C5A-N7A	-2.35	1.34	1.39
4	P	1001	NAP	O4B-C4B	2.17	1.49	1.45
4	A	1001	NAP	O4B-C4B	2.06	1.49	1.45
4	P	1001	NAP	C2N-N1N	2.01	1.37	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	504	PGW	O01-C1-C2	3.31	118.64	111.48
6	B	504	PGW	O01-C1-C2	3.29	118.59	111.48
6	B	514	PGW	O01-C1-C2	2.98	117.92	111.48
4	P	1001	NAP	C6N-N1N-C2N	-2.93	119.38	121.88
6	B	514	PGW	C03-C02-C01	-2.92	104.99	111.78
4	A	1001	NAP	C6N-N1N-C2N	-2.82	119.48	121.88
4	A	1001	NAP	C2A-N1A-C6A	2.46	122.76	118.73
6	B	504	PGW	O03-C19-C20	2.39	119.11	111.83
6	B	516	PGW	O01-C1-C2	2.38	116.63	111.48
6	B	514	PGW	O11-P-O14	2.34	112.76	106.44
6	Q	504	PGW	O03-C19-C20	2.34	118.95	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	514	PGW	O03-C19-C20	2.31	118.89	111.83
4	P	1001	NAP	C2A-N1A-C6A	2.29	122.49	118.73
6	Q	504	PGW	C02-O01-C1	-2.05	112.89	117.80
6	B	504	PGW	C01-O03-C19	-2.02	109.72	117.12
6	B	516	PGW	O01-C02-C01	-2.01	101.13	108.34
6	Q	504	PGW	C01-O03-C19	-2.00	109.79	117.12

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAP	PN-O3-PA-O5B
4	A	1001	NAP	O4D-C1D-N1N-C6N
4	P	1001	NAP	PN-O3-PA-O5B
4	P	1001	NAP	O4D-C1D-N1N-C6N
6	B	514	PGW	C02-C03-O11-P
6	B	516	PGW	C7-C8-C9-C10
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	Q	504	PGW	C01-C02-O01-C1
6	B	516	PGW	C01-C02-O01-C1
4	A	1001	NAP	O4D-C1D-N1N-C2N
4	P	1001	NAP	O4D-C1D-N1N-C2N
6	B	516	PGW	C03-C02-O01-C1
6	B	516	PGW	O03-C19-C20-C21
6	B	514	PGW	O01-C1-C2-C3
6	B	516	PGW	O01-C1-C2-C3
6	B	514	PGW	C01-C02-O01-C1
6	B	514	PGW	O03-C19-C20-C21
4	A	1001	NAP	C2B-O2B-P2B-O1X
6	B	516	PGW	O04-C19-C20-C21
6	B	514	PGW	O02-C1-C2-C3
6	B	516	PGW	O02-C1-C2-C3

There are no ring outliers.

11 monomers are involved in 32 short contacts:

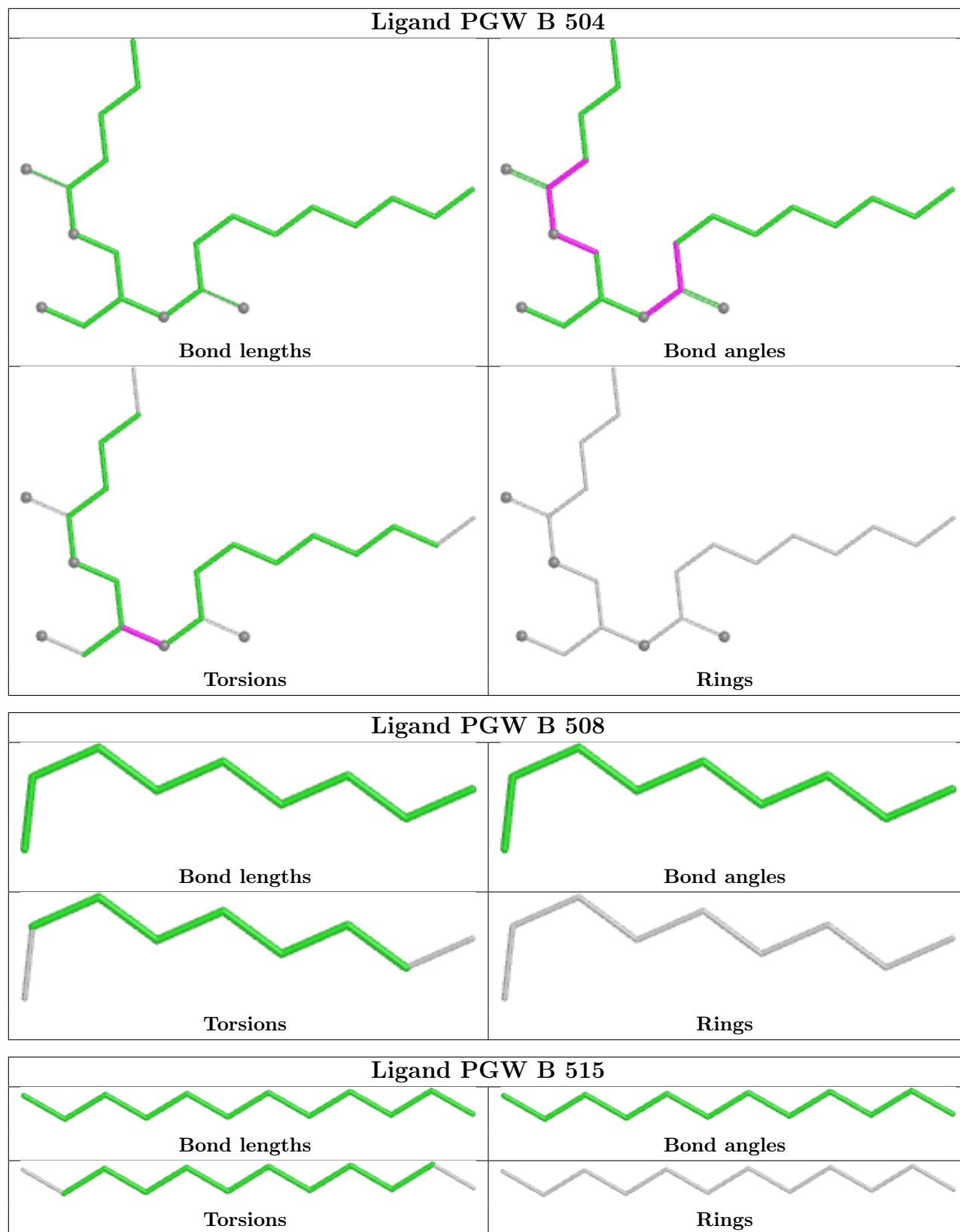
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	504	PGW	4	0
6	B	507	PGW	1	0

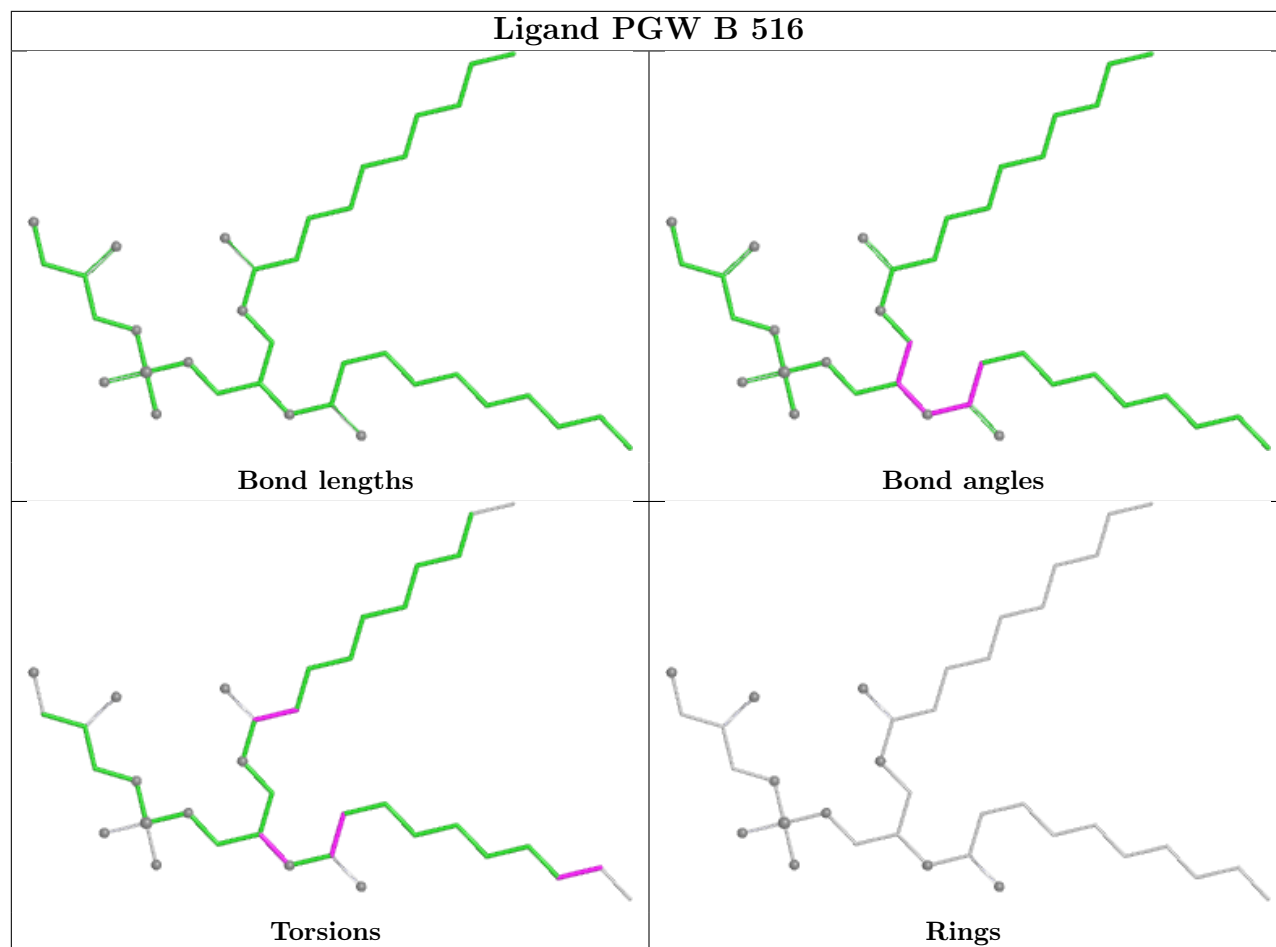
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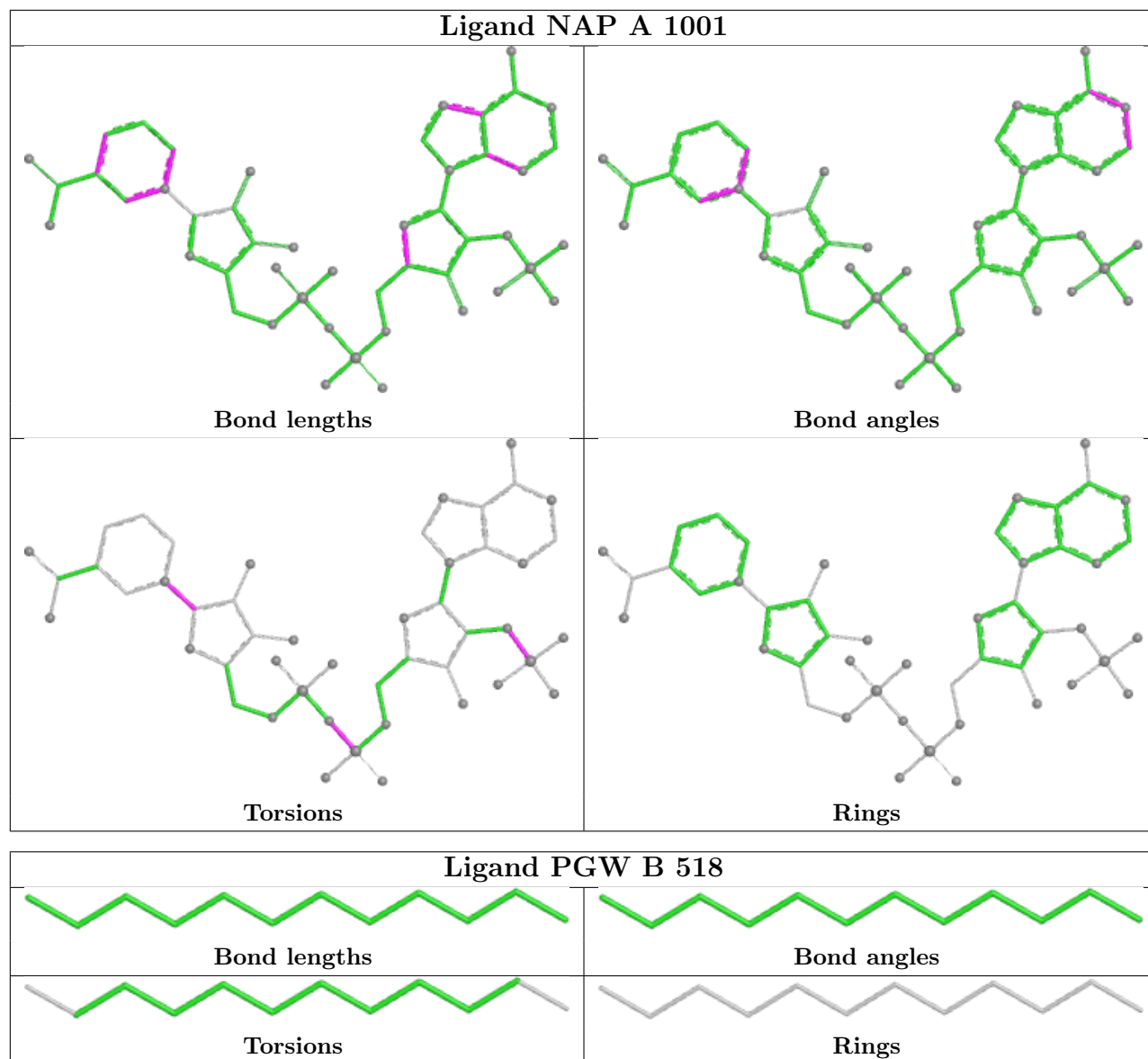
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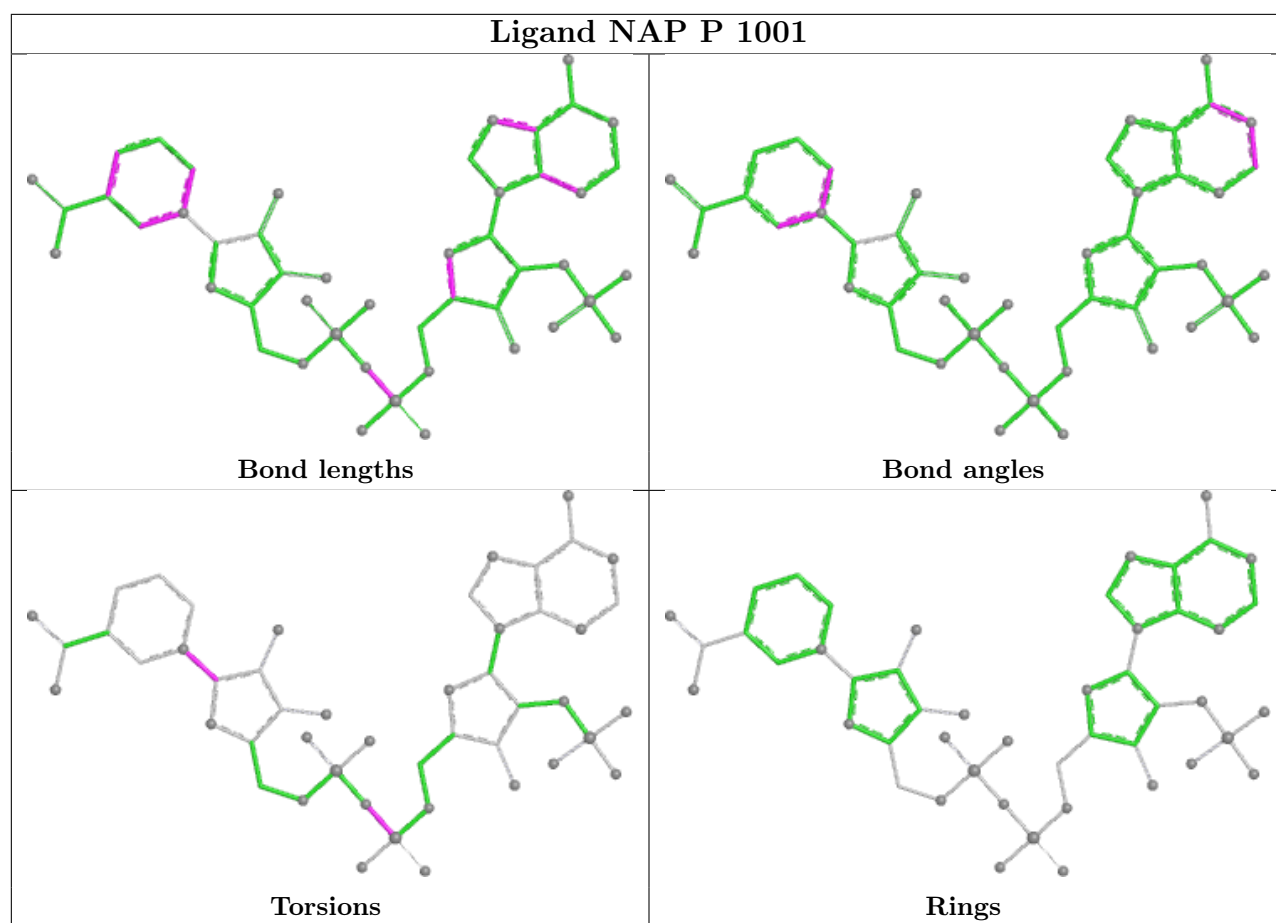
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	509	PGW	1	0
6	B	515	PGW	2	0
6	B	510	PGW	2	0
6	B	516	PGW	9	0
6	B	513	PGW	1	0
4	A	1001	NAP	3	0
4	P	1001	NAP	3	0
6	B	514	PGW	1	0
6	Q	504	PGW	7	0

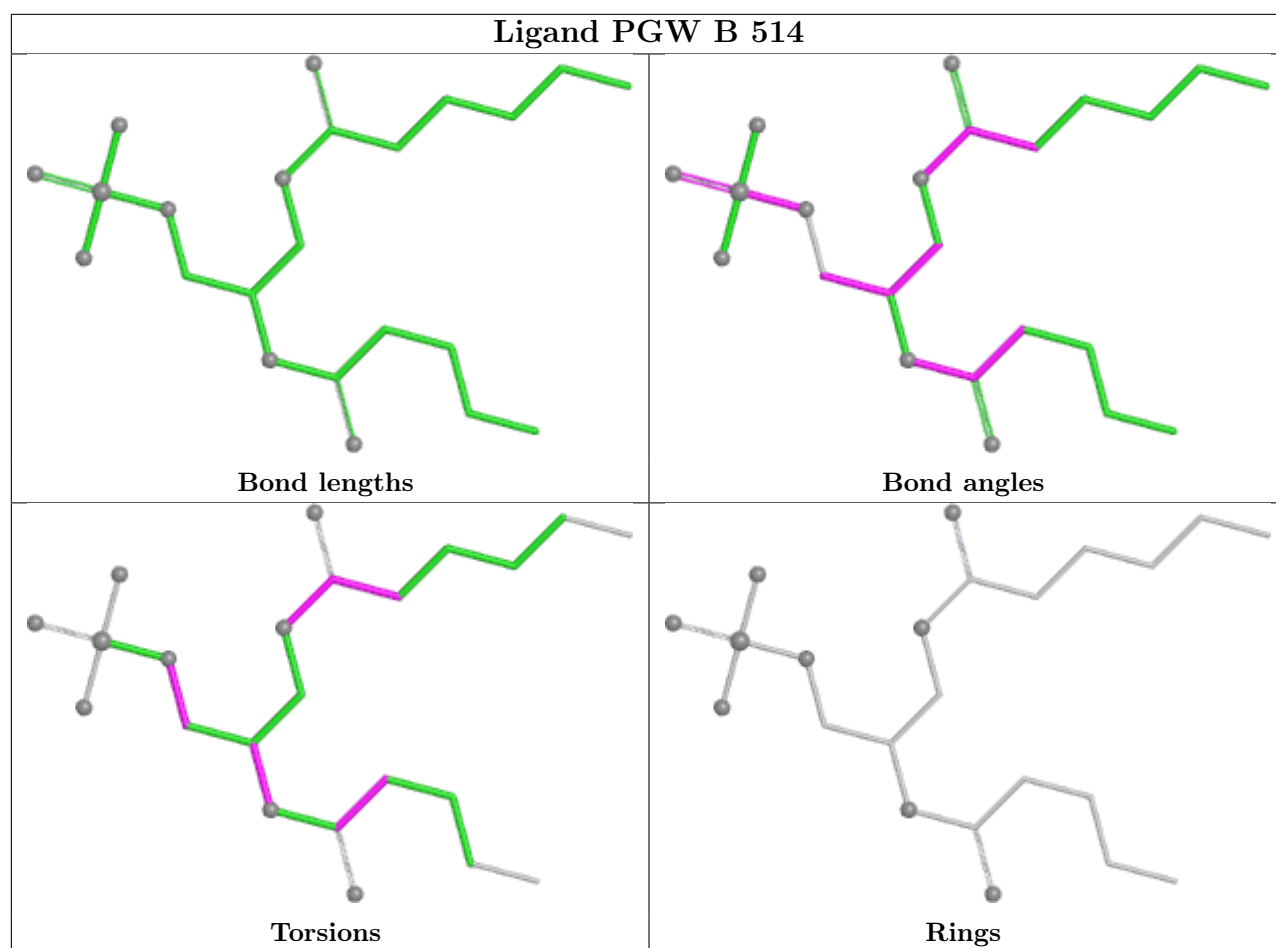
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

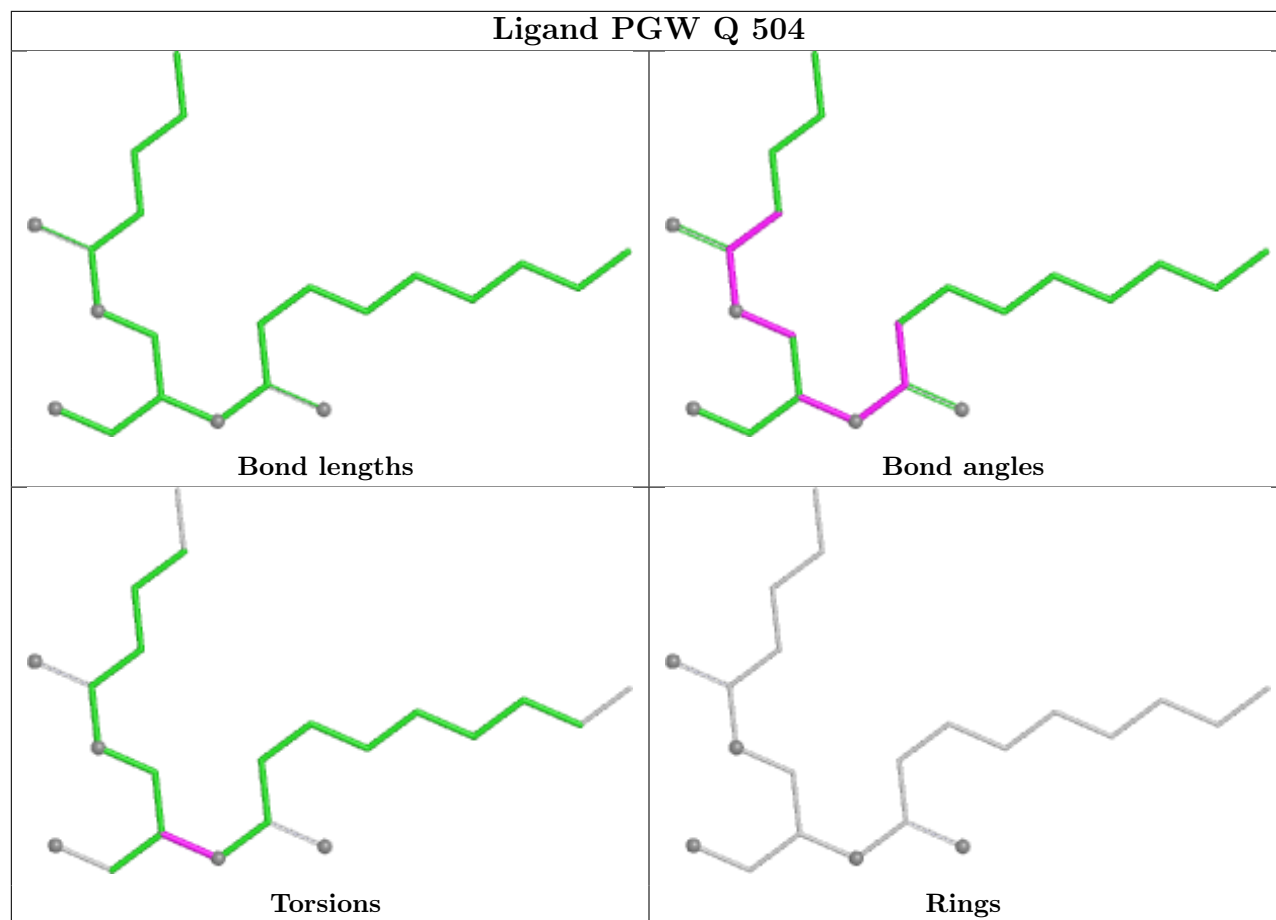












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.10	10 (3%)	51	47	25, 41, 64, 92	0
1	P	326/333 (97%)	0.03	10 (3%)	51	47	26, 44, 77, 101	0
2	B	386/514 (75%)	0.97	66 (17%)	4	3	32, 67, 119, 128	0
2	Q	363/514 (70%)	2.02	147 (40%)	0	0	39, 102, 196, 208	0
3	Y	36/37 (97%)	8.33	36 (100%)	0	0	21, 23, 24, 24	36 (100%)
All	All	1437/1731 (83%)	0.96	269 (18%)	3	2	21, 58, 182, 208	36 (2%)

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Y	15	SER	26.9
3	Y	19	ARG	23.3
3	Y	18	GLN	22.3
3	Y	20	LEU	18.5
3	Y	22	ASN	15.7
3	Y	23	THR	14.1
3	Y	4	ASN	13.1
3	Y	11	LYS	11.8
3	Y	9	THR	10.6
3	Y	24	SER	9.8
2	Q	280	LEU	9.2
3	Y	37	SER	9.0
3	Y	8	THR	8.8
3	Y	21	HIS	7.9
3	Y	6	SER	6.9
3	Y	14	TRP	6.9
3	Y	3	THR	6.9
2	Q	238	LEU	6.7
2	Q	153	PHE	6.5
2	Q	294	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
2	Q	288	VAL	6.2
2	Q	210	ILE	6.1
3	Y	28	CYS	6.1
2	Q	209	THR	6.0
3	Y	36	TYR	6.0
2	Q	214	GLN	5.9
2	Q	272	LEU	5.9
2	Q	131	GLY	5.8
3	Y	30	ASN	5.8
2	Q	254	ILE	5.7
3	Y	25	ARG	5.6
2	Q	149	VAL	5.5
2	Q	282	PHE	5.5
2	Q	145	PHE	5.4
2	Q	291	ILE	5.4
2	Q	237	PHE	5.4
2	Q	167	ILE	5.4
1	P	36	LEU	5.3
2	B	200	VAL	5.3
2	B	193	GLU	5.3
2	Q	279	VAL	5.2
2	Q	248	ALA	5.2
2	Q	164	ILE	5.2
2	Q	205	TYR	5.2
2	Q	243	ALA	5.2
2	Q	231	ILE	5.2
3	Y	17	CYS	5.1
2	Q	268	VAL	5.1
2	Q	228	LEU	5.1
3	Y	33	CYS	5.0
2	Q	266	TYR	5.0
2	Q	240	ARG	5.0
2	B	199	GLY	5.0
3	Y	12	GLU	5.0
2	Q	222	PHE	4.9
2	B	417	THR	4.9
2	Q	257	ILE	4.9
2	B	141	PRO	4.9
2	Q	232	TRP	4.8
1	A	36	LEU	4.8
2	Q	270	ILE	4.7
2	Q	277	LYS	4.7

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Mol	Chain	Res	Type	RSRZ
2	Q	250	PHE	4.7
2	Q	242	PHE	4.7
2	Q	219	THR	4.6
2	Q	239	VAL	4.6
3	Y	13	CYS	4.5
2	Q	147	ARG	4.5
2	B	203	HIS	4.5
2	Q	235	PHE	4.5
2	Q	190	ASP	4.4
3	Y	16	VAL	4.4
2	Q	271	PHE	4.4
3	Y	5	VAL	4.3
2	Q	252	THR	4.3
2	Q	204	THR	4.2
2	Q	417	THR	4.2
2	Q	415	ARG	4.2
2	Q	264	ILE	4.2
2	Q	202	PHE	4.2
2	Q	218	PHE	4.1
3	Y	10	SER	4.1
2	Q	247	LYS	4.1
3	Y	7	CYS	4.1
2	Q	278	SER	4.0
2	Q	206	SER	4.0
1	P	361	SER	4.0
2	Q	152	LEU	4.0
2	Q	289	VAL	4.0
2	B	145	PHE	3.9
3	Y	27	LYS	3.9
2	Q	281	GLN	3.9
1	A	360	TYR	3.9
2	Q	284	ASN	3.9
2	Q	187	ILE	3.9
2	Q	267	TYR	3.9
2	Q	233	PHE	3.9
2	Q	221	PRO	3.8
2	B	140	LEU	3.8
2	Q	261	VAL	3.8
2	Q	262	ALA	3.8
1	P	360	TYR	3.8
2	Q	212	TYR	3.8
2	B	133	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
3	Y	34	ARG	3.7
2	Q	223	PHE	3.7
2	B	213	GLN	3.7
2	Q	273	THR	3.7
2	Q	216	THR	3.7
3	Y	2	PHE	3.7
3	Y	29	MET	3.7
2	B	251	PHE	3.6
2	Q	244	CYS	3.6
2	Q	245	PRO	3.6
2	Q	251	PHE	3.6
2	Q	287	ARG	3.6
2	Q	150	TRP	3.6
2	B	215	SER	3.6
2	Q	165	ILE	3.6
2	Q	260	ILE	3.6
2	B	138	ARG	3.5
2	B	155	TYR	3.5
2	Q	241	PHE	3.5
2	B	142	GLU	3.5
2	B	205	TYR	3.5
2	Q	148	GLN	3.5
2	Q	285	VAL	3.5
2	Q	263	ILE	3.5
2	Q	295	MET	3.4
2	Q	151	LEU	3.4
2	Q	411	TYR	3.4
3	Y	32	LYS	3.4
2	B	152	LEU	3.3
2	B	139	PRO	3.3
2	B	151	LEU	3.3
2	Q	225	VAL	3.3
2	B	201	THR	3.3
2	Q	269	THR	3.3
2	B	32	SER	3.2
2	Q	125	MET	3.2
2	Q	286	ARG	3.2
2	Q	370	THR	3.2
2	Q	283	GLN	3.2
2	Q	292	PHE	3.2
3	Y	26	GLY	3.2
1	P	314	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	P	280	GLU	3.1
1	A	361	SER	3.1
2	Q	324	LEU	3.1
2	Q	371	VAL	3.1
2	Q	174	LEU	3.1
2	Q	211	GLY	3.1
1	P	268	LYS	3.0
2	B	160	GLY	3.0
2	B	249	GLY	3.0
2	Q	215	SER	3.0
2	Q	297	ILE	3.0
2	Q	230	ILE	3.0
2	B	154	GLU	3.0
2	B	277	LYS	3.0
3	Y	31	LYS	3.0
2	Q	234	SER	3.0
1	P	349	HIS	2.9
2	Q	246	SER	2.9
2	Q	203	HIS	2.9
2	B	274	GLU	2.9
2	Q	399	ALA	2.9
2	Q	56	GLU	2.9
2	B	147	ARG	2.8
2	Q	258	ILE	2.8
2	Q	249	GLY	2.8
2	Q	350	ARG	2.8
2	Q	208	SER	2.8
2	B	175	ILE	2.8
3	Y	35	CYS	2.8
2	Q	372	GLY	2.7
2	Q	224	ILE	2.7
2	Q	155	TYR	2.7
2	Q	168	VAL	2.7
2	B	132	TYR	2.7
2	B	124	GLU	2.7
2	B	187	ILE	2.7
2	B	194	ASP	2.7
2	B	247	LYS	2.7
2	Q	298	LEU	2.7
2	Q	175	ILE	2.6
2	Q	265	PRO	2.6
2	Q	344	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	Q	275	SER	2.6
2	B	153	PHE	2.6
2	B	125	MET	2.6
1	A	150	GLU	2.6
2	B	351	ASP	2.6
2	Q	309	GLY	2.6
2	B	171	MET	2.6
2	Q	306	HIS	2.6
2	Q	160	GLY	2.5
2	B	231	ILE	2.5
2	Q	226	GLU	2.5
2	B	411	TYR	2.5
2	Q	186	PRO	2.5
2	Q	378	PRO	2.5
2	B	219	THR	2.5
2	Q	293	ARG	2.5
2	Q	400	LEU	2.5
2	B	144	GLU	2.5
2	B	150	TRP	2.5
2	B	188	PHE	2.5
2	Q	376	MET	2.5
2	Q	308	LYS	2.4
2	Q	303	LEU	2.4
2	Q	146	GLN	2.4
2	Q	290	GLN	2.4
2	Q	127	ARG	2.4
2	Q	156	PRO	2.4
2	B	190	ASP	2.4
2	Q	337	LEU	2.4
2	Q	217	SER	2.4
2	Q	351	ASP	2.4
2	Q	189	ARG	2.4
2	Q	188	PHE	2.4
2	Q	410	ASN	2.4
2	Q	304	SER	2.4
2	Q	276	ASN	2.4
2	B	243	ALA	2.4
2	B	165	ILE	2.3
2	Q	396	LEU	2.3
1	P	231	GLU	2.3
2	B	240	ARG	2.3
1	A	349	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	283	GLN	2.3
2	B	252	THR	2.3
1	A	231	GLU	2.3
2	Q	161	PRO	2.3
2	B	208	SER	2.3
2	Q	32	SER	2.3
2	B	204	THR	2.2
1	A	62	GLY	2.2
1	A	297	GLU	2.2
2	B	191	GLU	2.2
2	Q	121	GLU	2.2
2	B	198	GLY	2.2
2	Q	299	ARG	2.2
2	B	202	PHE	2.2
2	Q	169	SER	2.2
1	A	283	ARG	2.2
2	B	172	VAL	2.1
2	Q	178	VAL	2.1
2	B	245	PRO	2.1
1	P	228	GLN	2.1
2	B	248	ALA	2.1
2	Q	227	THR	2.1
2	Q	416	GLU	2.1
2	B	192	ASN	2.1
2	Q	177	ILE	2.1
2	B	134	LYS	2.1
2	B	352	SER	2.1
2	B	408	ASN	2.1
2	B	197	GLY	2.1
2	B	135	GLU	2.1
2	Q	414	HIS	2.1
2	Q	332	PHE	2.0
1	A	129	ARG	2.0
1	P	129	ARG	2.0
2	B	127	ARG	2.0
2	B	246	SER	2.0
2	Q	207	GLN	2.0
2	B	242	PHE	2.0
2	Q	180	PHE	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	0.77	0.20	88,88,89,89	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.

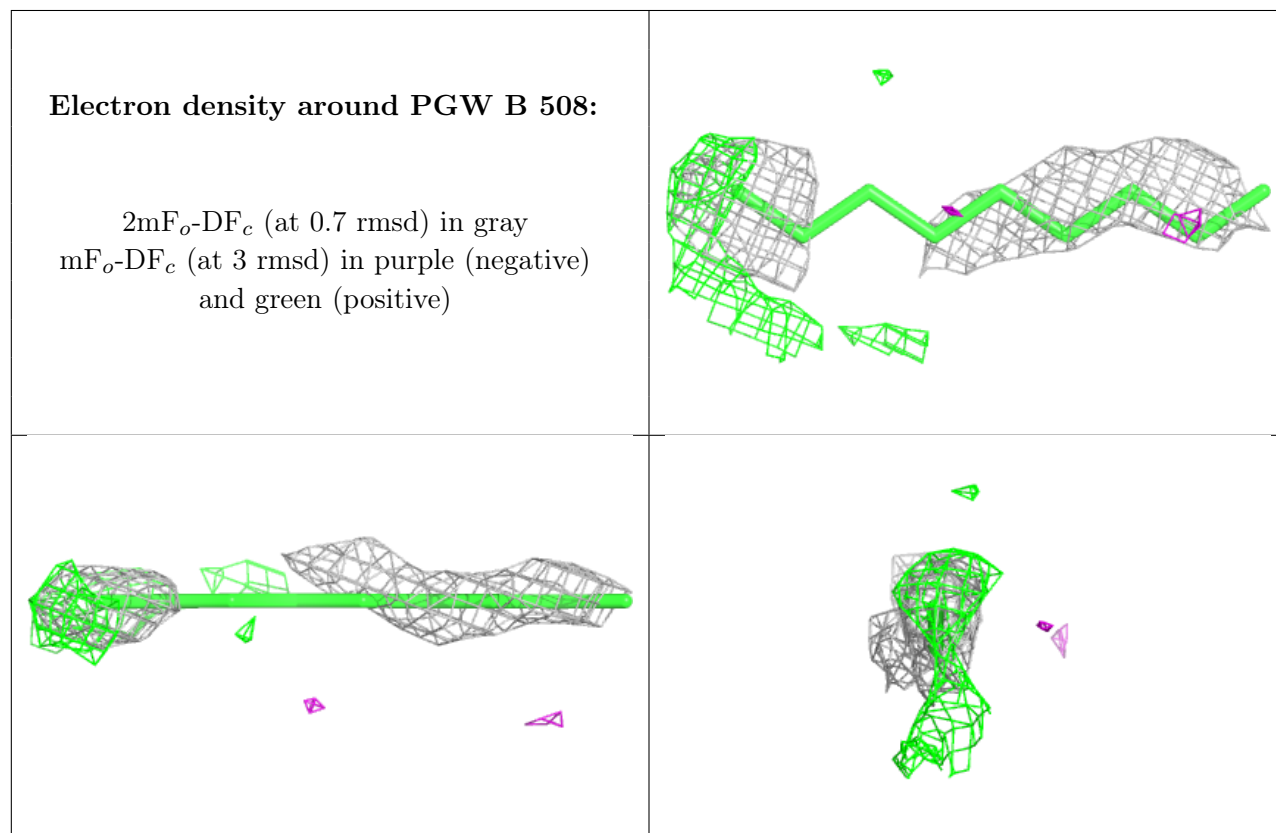
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PGW	B	508	9/51	0.69	0.43	104,106,107,107	0
6	PGW	B	504	22/51	0.70	0.39	76,86,90,91	0
6	PGW	B	516	37/51	0.72	0.31	108,129,144,145	0
6	PGW	Q	504	22/51	0.72	0.35	100,113,118,119	0
6	PGW	B	506	9/51	0.73	0.37	95,96,96,97	0
6	PGW	B	514	23/51	0.73	0.34	136,139,148,149	0
6	PGW	B	515	12/51	0.76	0.42	84,90,94,94	0
6	PGW	B	512	9/51	0.77	0.32	91,91,92,93	0
6	PGW	B	519	12/51	0.77	0.38	102,104,105,105	0
6	PGW	B	513	12/51	0.77	0.37	74,80,83,84	0
6	PGW	B	517	10/51	0.79	0.32	77,78,80,81	0
6	PGW	B	518	12/51	0.80	0.40	113,116,117,117	0
6	PGW	B	507	9/51	0.81	0.36	100,101,102,103	0
6	PGW	B	511	7/51	0.85	0.31	86,87,87,87	0
6	PGW	B	505	9/51	0.85	0.34	98,99,102,102	0
6	PGW	B	510	9/51	0.86	0.30	90,93,97,98	0
6	PGW	B	509	9/51	0.87	0.30	80,81,81,82	0
5	K	Q	503	1/1	0.90	0.14	38,38,38,38	1
5	K	Q	501	1/1	0.90	0.09	50,50,50,50	1
5	K	Q	502	1/1	0.94	0.13	62,62,62,62	1
5	K	B	503	1/1	0.95	0.12	27,27,27,27	1

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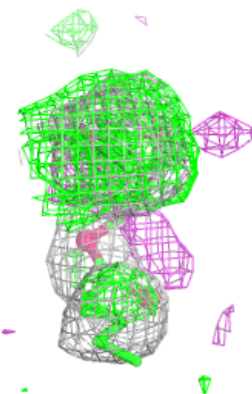
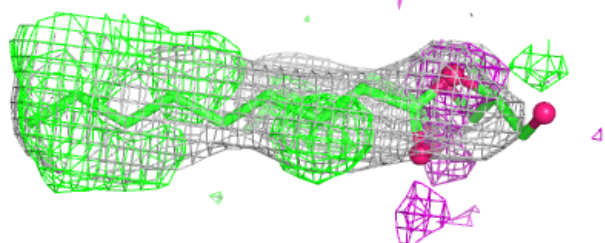
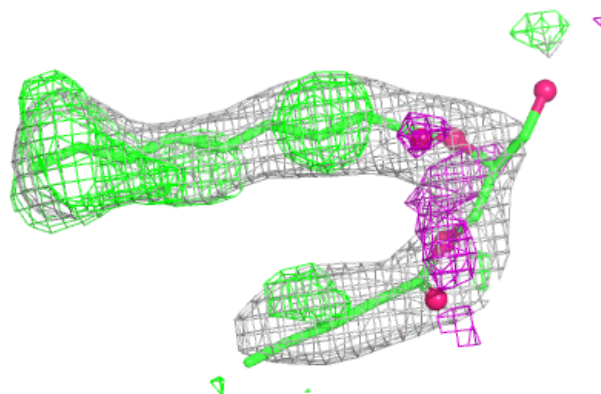
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	K	B	501	1/1	0.97	0.18	23,23,23,23	1
4	NAP	P	1001	48/48	0.98	0.07	35,41,50,51	0
4	NAP	A	1001	48/48	0.98	0.06	34,39,45,47	0
5	K	B	502	1/1	0.98	0.09	27,27,27,27	1

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

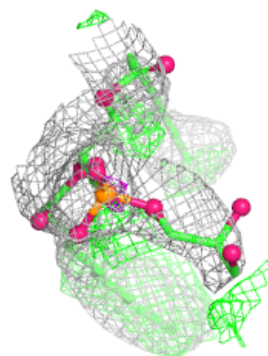
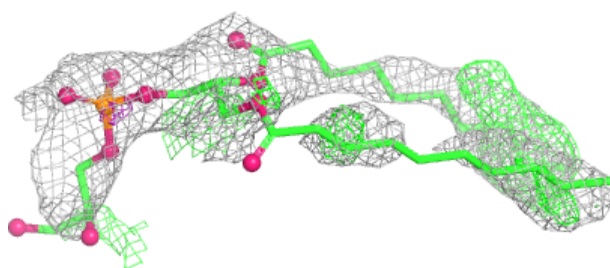
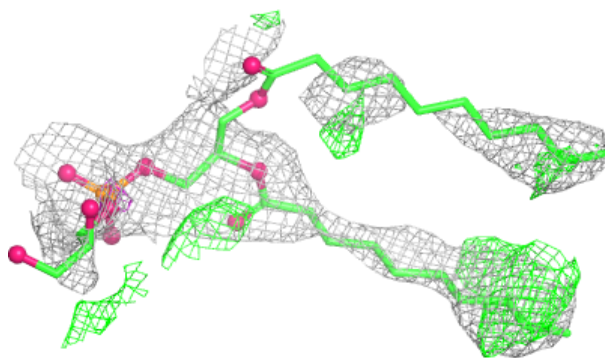


Electron density around PGW B 504:

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

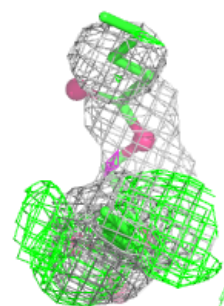
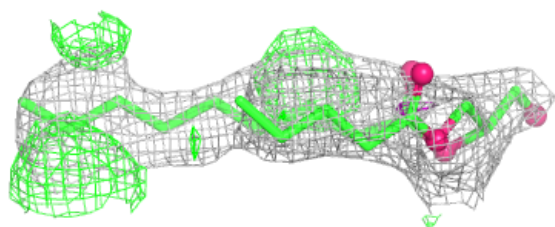
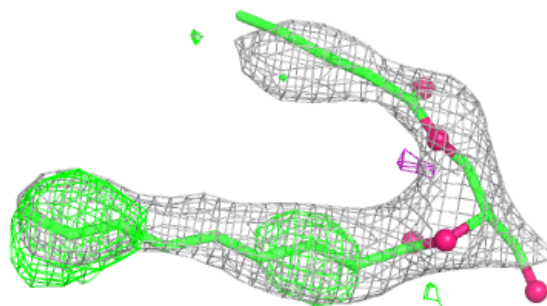
**Electron density around PGW B 516:**

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



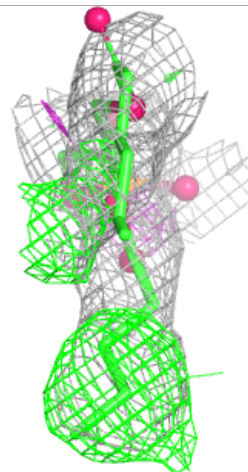
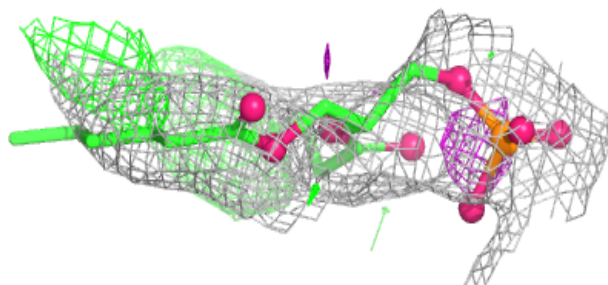
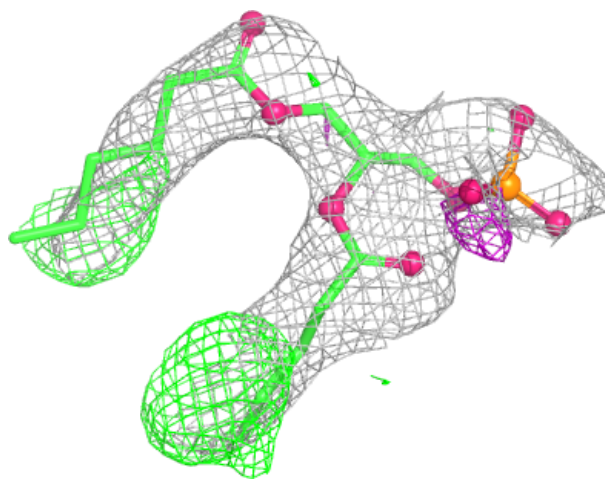
Electron density around PGW Q 504:

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



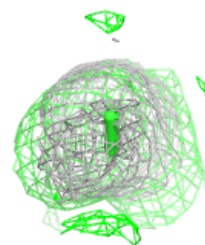
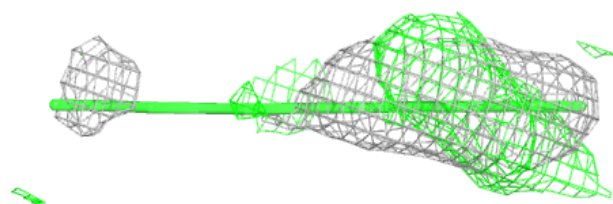
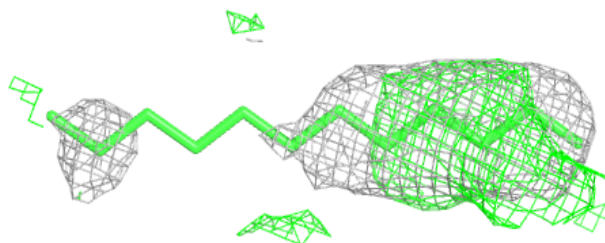
Electron density around PGW B 514:

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

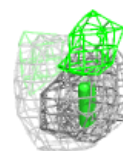
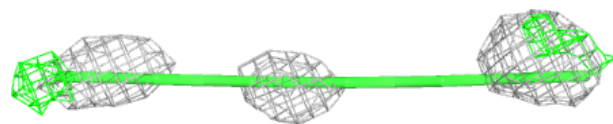
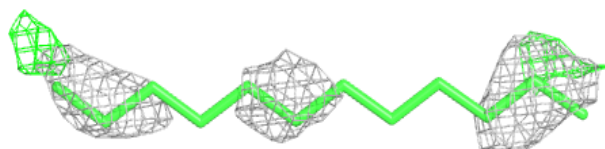


Electron density around PGW B 515:

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

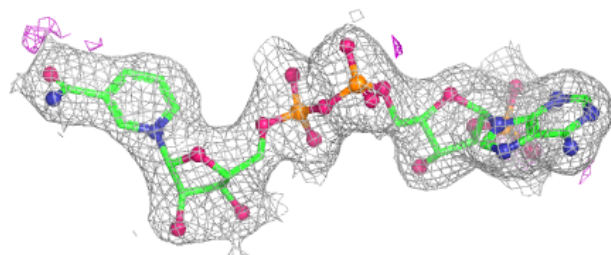
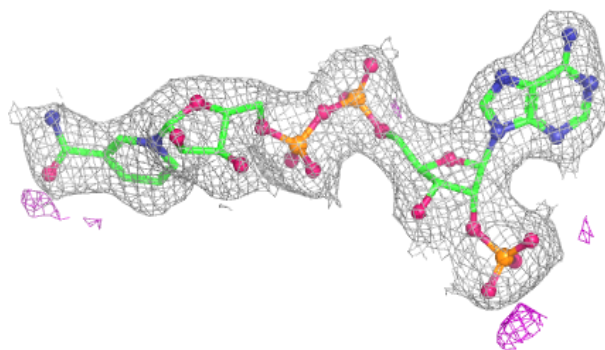
**Electron density around PGW B 518:**

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

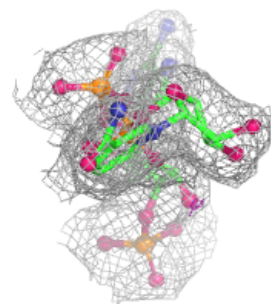
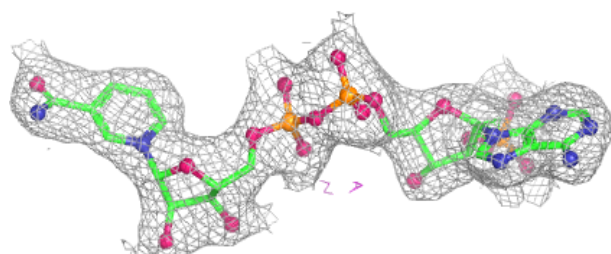
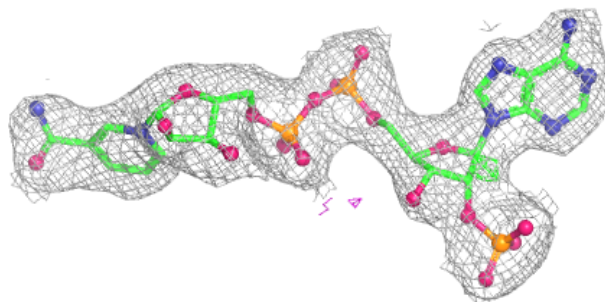


Electron density around NAP P 1001:

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

**Electron density around NAP A 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.