Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 05:44 PM EDT

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

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

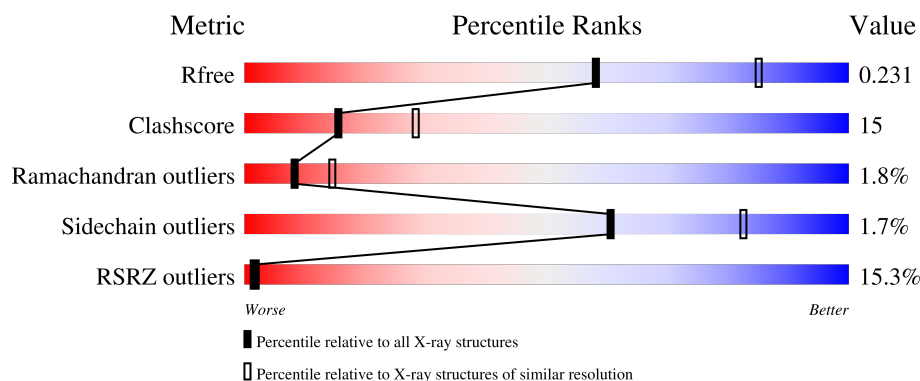|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
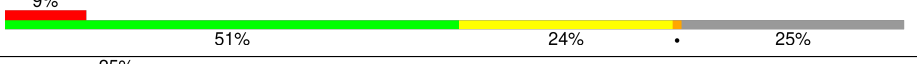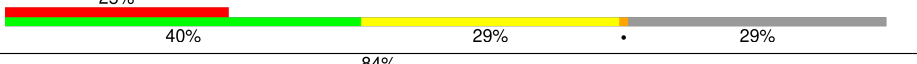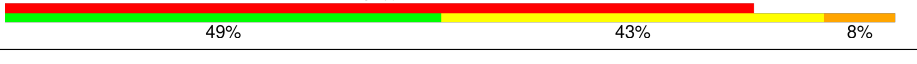*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Rfree		0.231
Clashscore		15
Ramachandran outliers		1.8%
Sidechain outliers		1.7%
RSRZ outliers		15.3%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	2% 81% 16% ··
1	P	333	2% 81% 15% ··
2	B	514	9% 51% 24% · 25%
2	Q	514	25% 40% 29% · 29%
3	Y	37	84% 49% 43% 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	509	-	-	-	X
6	PGW	B	510	-	-	-	X
6	PGW	B	515	-	-	-	X
6	PGW	B	518	-	-	-	X
6	PGW	B	519	-	-	-	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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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 295	C 176	N 57	O 55	S 7	0	0	0

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

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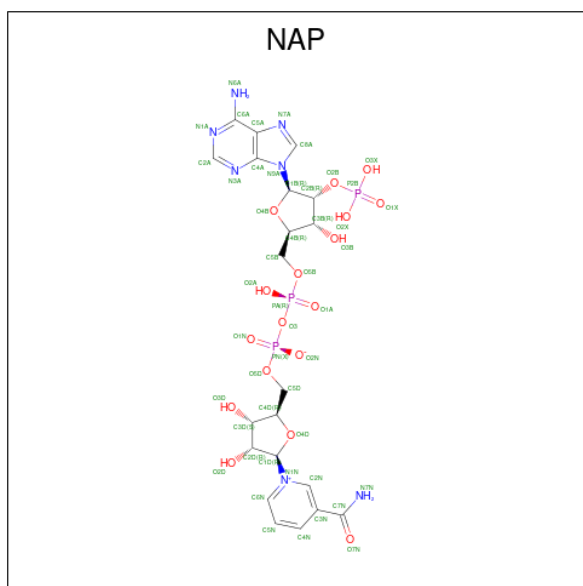
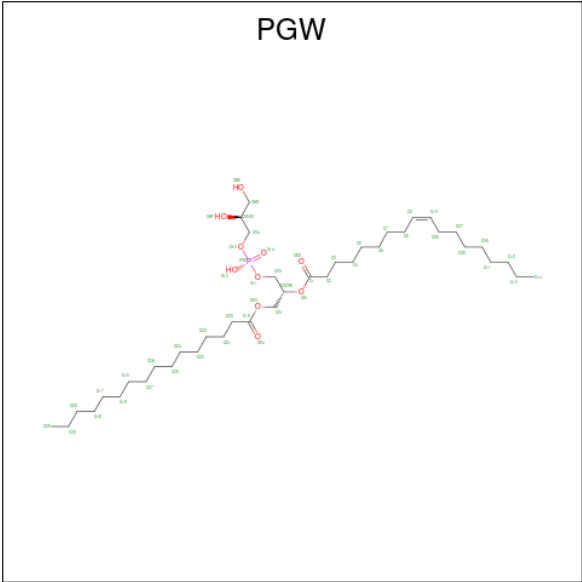| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	P	1	Total 48	C 21	N 7	O 17	P 3	0	0

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

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

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

PGW

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

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

- Molecule 7 is water.

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

3 Residue-property plots ⓘ

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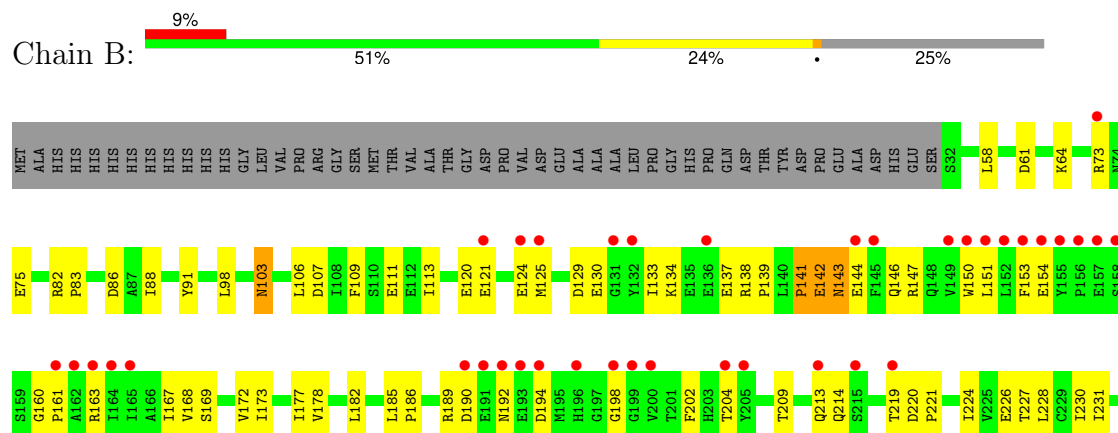
- Molecule 1: Voltage-gated potassium channel subunit beta-2
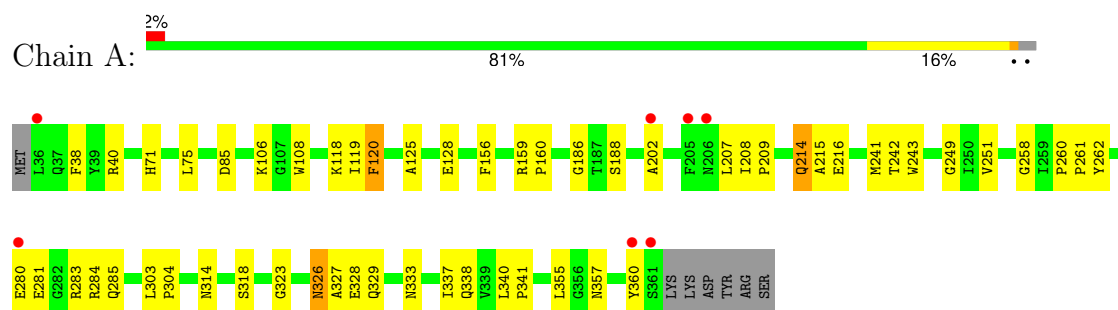
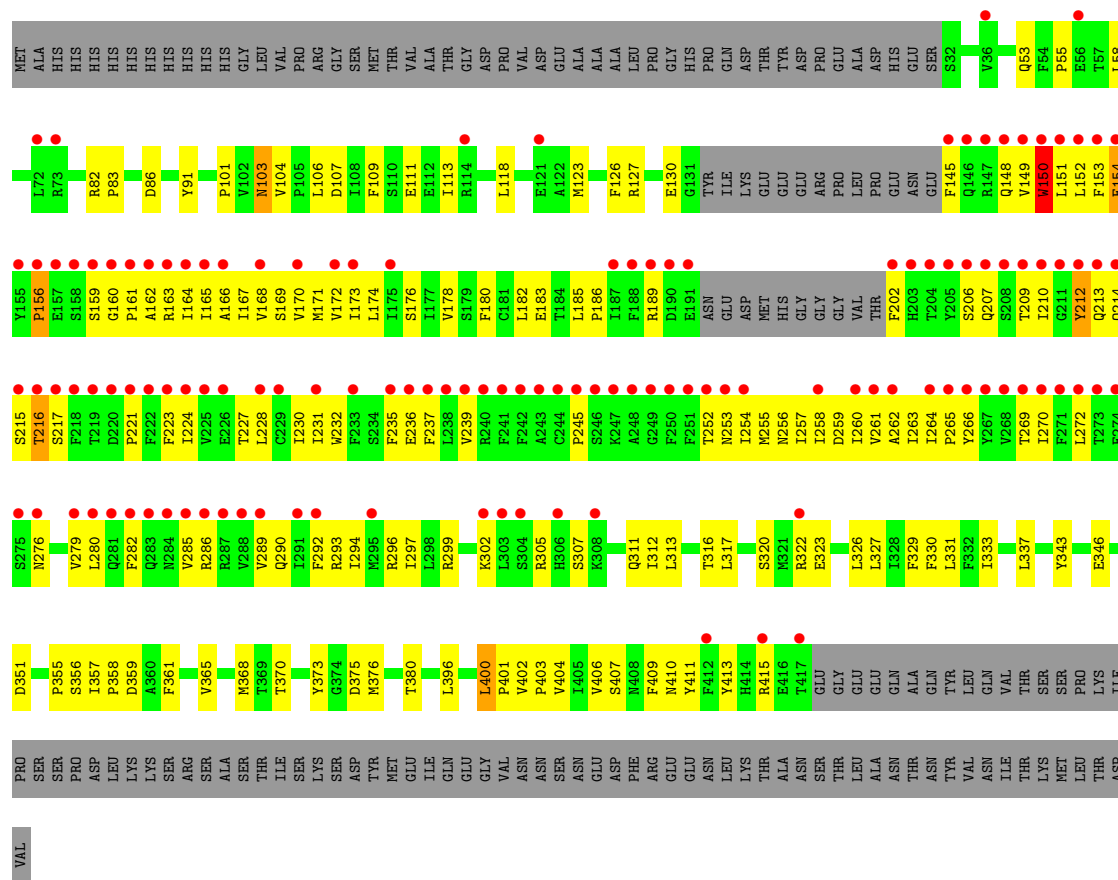- Molecule 1: Voltage-gated potassium channel subunit beta-2
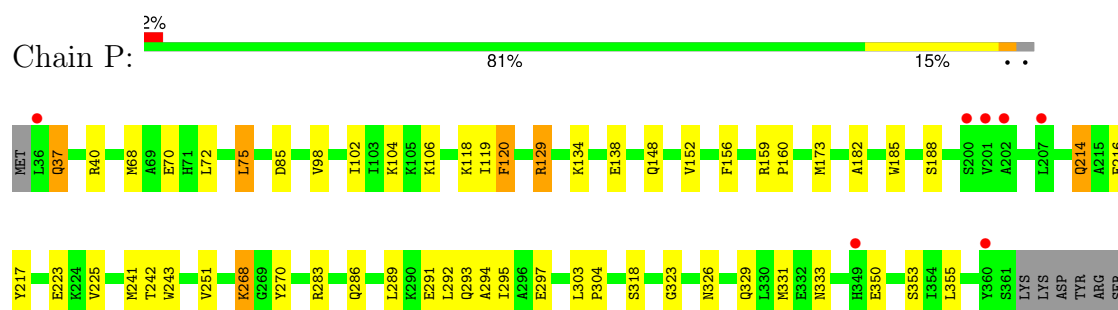
- Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1
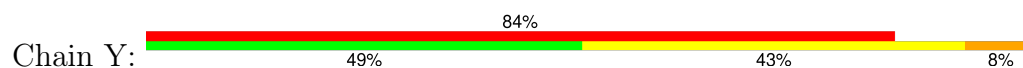
• Molecule 2: Potassium voltage-gated channel subfamily A member 2, Potassium voltage-gated channel subfamily B member 1

• Molecule 3: Potassium channel toxin alpha-KTx 1.1

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	144.40Å 144.40Å 284.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.6 (50.00-2.50) 86.0 (49.65-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.236 0.207 , 0.231	Depositor DCC
R_{free} test set	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)	0.33 , 64.8	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.36	0/2608	0.58	0/3524
1	P	0.36	0/2608	0.56	0/3524
2	B	0.35	0/3169	0.53	0/4292
2	Q	0.32	0/3036	0.50	0/4114
3	Y	0.26	0/292	0.46	0/389
All	All	0.35	0/11713	0.54	0/15843

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	270	TYR	Sidechain

5.2   Too-close contacts ⓘ

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

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2556	0	2582	42	0
1	P	2556	0	2582	46	0
2	B	3088	0	3034	91	0
2	Q	2959	0	2956	142	0
3	Y	295	0	282	19	0
4	A	48	0	25	3	0
4	P	48	0	25	3	0
5	B	3	0	0	0	0
5	Q	3	0	0	0	0
6	B	210	0	291	19	0
6	Q	22	0	25	7	0
7	A	140	0	0	2	0
7	B	53	0	0	1	0
7	P	102	0	0	0	0
7	Q	23	0	0	1	0
All	All	12106	0	11802	349	0

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

All (349) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:510:PGW:H2A	6:B:515:PGW:H21A	1.42	0.98
2:Q:400:LEU:HB2	2:Q:401:PRO:HD3	1.52	0.89
1:P:333:ASN:HD21	4:P:1001:NAP:H61A	1.21	0.88
2:Q:312:ILE:HD13	2:Q:413:TYR:HA	1.59	0.83
2:Q:227:THR:HA	2:Q:230:ILE:HG22	1.61	0.82
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
3:Y:4:ASN:HA	3:Y:32:LYS:HD3	1.63	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:295:ILE:HD12	1:P:295:ILE:H	1.53	0.71
2:Q:103:ASN:H	2:Q:103:ASN:ND2	1.89	0.71
6:B:510:PGW:H4A	6:B:515:PGW:H23A	1.72	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:26:GLY:HA3	3:Y:35:CYS:HA	1.77	0.67
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
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
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: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: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:Q:260:ILE:O	2:Q:264:ILE:HG13	2.01	0.59
2:B:58:LEU:HD23	2:B:58:LEU:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:14:TRP:HA	3:Y:14:TRP:CE3	2.38	0.58
2:Q:294:ILE:O	2:Q:297:ILE:HG22	2.04	0.58
3:Y:14:TRP:HA	3:Y:14:TRP:HE3	1.68	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
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
2:Q:170:VAL:HB	2:Q:171:MET:HE2	1.86	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
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
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:B:255:MET:HE3	2:B:305:ARG:HA	1.87	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:255:MET:CE	2:Q:305:ARG:HA	2.37	0.55
2:Q:259:ASP:HA	2:Q:302:LYS:HZ3	1.70	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
1:P:75:LEU:HG	1:P:331:MET:HE3	1.88	0.55
2:B:141:PRO:C	2:B:143:ASN:H	2.10	0.55
2:Q:400:LEU:O	2:Q:403:PRO:HD2	2.07	0.55
2:B:414:HIS:C	2:B:416:GLU:H	2.10	0.54
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
2:Q:282:PHE:CZ	2:Q:289:VAL:HG21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:29:MET:C	3:Y:31:LYS:H	2.11	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
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
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
3:Y:17:CYS:O	3:Y:21:HIS:HB2	2.09	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:152:LEU:O	2:Q:165:ILE:HD12	2.10	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:53:GLN:C	2:Q:55:PRO:HD3	2.31	0.51
2:Q:402:VAL:HB	2:Q:403:PRO:HD3	1.94	0.50
3:Y:10:SER:C	3:Y:12:GLU:H	2.15	0.50
2:Q:150:TRP:HA	2:Q:150:TRP:HE3	1.76	0.50
3:Y:27:LYS:CG	3:Y:28:CYS:N	2.72	0.50
1:P:326:ASN:OD1	1:P:329:GLN:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:202:PHE:HB2	2:B:279:VAL:CG2	2.42	0.49
3:Y:27:LYS:HG3	3:Y:28:CYS:N	2.28	0.49
3:Y:29:MET:HG3	3:Y:31:LYS:HB3	1.94	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:323:GLU:CD	2:B:323:GLU:H	2.16	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
1:P:268:LYS:HB3	1:P:268:LYS:HZ3	1.77	0.47
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
2:Q:368:MET:C	2:Q:370:THR:H	2.17	0.47
1:A:355:LEU:HB3	1:A:357:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:Y:20:LEU:N	3:Y:20:LEU:HD12	2.30	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:58:LEU:HD23	2:Q:58:LEU:C	2.36	0.46
2:Q:320:SER:HA	2:Q:323:GLU:HG2	1.96	0.46
3:Y:26:GLY:HA2	3:Y:36:TYR:HD1	1.80	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: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
1:P:75:LEU:HG	1:P:331:MET:CE	2.46	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
1:A:326:ASN:HD22	1:A:328:GLU:N	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:227:THR:O	2:Q:230:ILE:HG22	2.17	0.45
3:Y:28:CYS:SG	3:Y:29:MET:N	2.90	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
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
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
2:Q:337:LEU:O	2:Q:337:LEU:HD23	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
3:Y:2:PHE:HZ	3:Y:31:LYS:HE2	1.83	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
2:Q:255:MET:HE1	2:Q:305:ARG:HA	2.00	0.44
3:Y:7:CYS:HA	3:Y:12:GLU:OE1	2.18	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
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
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
3:Y:2:PHE:CZ	3:Y:31:LYS:HE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:276:ASN:ND2	2:Q:285:VAL:HG11	2.34	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:350:ARG:HH11	2:B:350:ARG:CB	2.24	0.42
3:Y:18:GLN:NE2	3:Y:18:GLN:C	2.72	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:368:MET:C	2:Q:370:THR:N	2.73	0.42
3:Y:11:LYS:HA	3:Y:14:TRP:CD1	2.54	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
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
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
1:A:208:ILE:HA	1:A:209:PRO:HD3	1.92	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:Q:215:SER:O	2:Q:216:THR:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:Q:209:THR:HG22	2:Q:209:THR:O	2.21	0.41
2:Q:297:ILE:C	2:Q:299:ARG:N	2.74	0.41
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: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
2:Q:337:LEU:HD23	2:Q:337:LEU:C	2.42	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:98:VAL:O	1:P:102:ILE:HG13	2.21	0.41
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
3:Y:26:GLY:HA2	3:Y:36:TYR:CD1	2.56	0.40
2:Q:255:MET:HE3	2:Q:305:ARG:HG3	2.03	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:142:GLU:O	2:B:143:ASN:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:VAL:O	2:B:289:VAL:HG23	2.21	0.40
2:Q:171:MET:HE2	2:Q:171:MET:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	41	61
1	P	324/333 (97%)	313 (97%)	10 (3%)	1 (0%)	41	61
2	B	384/514 (75%)	350 (91%)	21 (6%)	13 (3%)	3	5
2	Q	357/514 (70%)	311 (87%)	37 (10%)	9 (2%)	5	8
3	Y	35/37 (95%)	19 (54%)	15 (43%)	1 (3%)	4	6
All	All	1424/1731 (82%)	1306 (92%)	93 (6%)	25 (2%)	8	14

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

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Mol	Chain	Res	Type
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%)	73	89
1	P	273/280 (98%)	266 (97%)	7 (3%)	46	72
2	B	332/459 (72%)	327 (98%)	5 (2%)	65	85
2	Q	324/459 (71%)	320 (99%)	4 (1%)	71	88
3	Y	35/35 (100%)	33 (94%)	2 (6%)	20	39
All	All	1237/1513 (82%)	1216 (98%)	21 (2%)	60	82

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

Mol	Chain	Res	Type
1	A	214	GLN
1	A	326	ASN
1	A	338	GLN
2	B	86	ASP
2	B	103	ASN
2	B	129	ASP

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Mol	Chain	Res	Type
2	B	185	LEU
2	B	324	LEU
1	P	37	GLN
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	103	ASN
2	Q	150	TRP
2	Q	212	TYR
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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	148	GLN
1	A	286	GLN
1	A	326	ASN
1	A	333	ASN
1	A	338	GLN
2	B	53	GLN
2	B	103	ASN
2	B	192	ASN
2	B	213	GLN
2	B	214	GLN
2	B	414	HIS
1	P	37	GLN
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	148	GLN

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Mol	Chain	Res	Type
2	Q	207	GLN
2	Q	213	GLN
2	Q	290	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 monosaccharides 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	518	-	11,11,50	0.35	0	10,10,56	0.57	0
6	PGW	B	511	-	6,6,50	0.36	0	5,5,56	0.48	0
6	PGW	B	509	-	8,8,50	0.36	0	7,7,56	0.54	0
6	PGW	B	510	-	8,8,50	0.36	0	7,7,56	0.55	0
6	PGW	B	519	-	11,11,50	0.35	0	10,10,56	0.57	0
6	PGW	B	513	-	11,11,50	0.35	0	10,10,56	0.59	0
6	PGW	B	512	-	8,8,50	0.36	0	7,7,56	0.52	0
6	PGW	B	507	-	8,8,50	0.36	0	7,7,56	0.54	0
4	NAP	P	1001	-	46,52,52	1.54	8 (17%)	61,80,80	1.05	1 (1%)
6	PGW	B	514	-	22,22,50	0.80	0	25,27,56	1.28	4 (16%)
6	PGW	B	508	-	8,8,50	0.36	0	7,7,56	0.53	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	Q	504	-	21,21,50	0.61	0	23,23,56	1.21	4 (17%)
6	PGW	B	517	-	9,9,50	0.36	0	8,8,56	0.56	0
6	PGW	B	515	-	11,11,50	0.35	0	10,10,56	0.59	0
6	PGW	B	504	-	21,21,50	0.61	0	23,23,56	1.22	3 (13%)
6	PGW	B	505	-	8,8,50	0.36	0	7,7,56	0.54	0
4	NAP	A	1001	-	46,52,52	1.43	7 (15%)	61,80,80	1.03	2 (3%)

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1001	NAP	C6N-N1N	4.24	1.45	1.35
4	A	1001	NAP	C6N-N1N	4.02	1.44	1.35
4	P	1001	NAP	C4N-C3N	3.73	1.45	1.39
4	A	1001	NAP	C4N-C3N	3.68	1.45	1.39
4	P	1001	NAP	PA-O3	3.68	1.63	1.59
4	A	1001	NAP	O4B-C1B	3.59	1.45	1.40
4	P	1001	NAP	C2A-N3A	3.43	1.37	1.32
4	P	1001	NAP	O4B-C1B	3.42	1.45	1.40
4	P	1001	NAP	C4A-N3A	3.25	1.40	1.35
4	A	1001	NAP	C2A-N3A	2.98	1.36	1.32
4	A	1001	NAP	C4A-N3A	2.67	1.39	1.35
4	A	1001	NAP	C2N-N1N	2.47	1.37	1.35
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 (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
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
6	B	514	PGW	O03-C19-C20	2.31	118.89	111.83
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
4	A	1001	NAP	C5A-C6A-N6A	2.01	123.38	120.31
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

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

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

Ligand PGW B 518

Bond lengths	Bond angles
Torsions	Rings

Ligand PGW B 509

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW B 510

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW B 519

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP P 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW B 514

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW B 516

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW Q 504

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW B 515

Bond lengths

Bond angles

Torsions

Rings

Ligand PGW B 504

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 1001

Bond lengths

Bond angles

Torsions

Rings

5.7　Other polymers ⓘ

There are no such residues in this entry.

5.8　Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.04	7 (2%)	63	66	25, 41, 64, 92	0
1	P	326/333 (97%)	0.02	7 (2%)	63	66	26, 44, 77, 101	0
2	B	386/514 (75%)	0.66	48 (12%)	4	3	32, 67, 119, 128	0
2	Q	363/514 (70%)	2.33	127 (34%)	0	0	39, 102, 196, 208	0
3	Y	36/37 (97%)	4.64	31 (86%)	0	0	83, 90, 98, 98	36 (100%)
All	All	1437/1731 (83%)	0.89	220 (15%)	2	1	25, 59, 182, 208	36 (2%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	214	GLN	15.6
3	Y	20	LEU	13.9
2	Q	153	PHE	13.3
2	Q	210	ILE	13.0
2	Q	280	LEU	12.9
2	Q	279	VAL	12.8
2	Q	216	THR	12.7
2	Q	281	GLN	12.5
2	Q	218	PHE	12.3
2	Q	282	PHE	12.2
2	Q	250	PHE	12.1
3	Y	4	ASN	11.2
2	Q	247	LYS	10.8
2	Q	272	LEU	10.8
2	Q	242	PHE	10.6
2	Q	244	CYS	10.2
2	Q	206	SER	10.0
2	Q	205	TYR	9.9
2	Q	240	ARG	9.7
2	Q	249	GLY	9.6

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Mol	Chain	Res	Type	RSRZ
2	Q	161	PRO	9.6
2	Q	245	PRO	9.5
2	Q	150	TRP	9.5
2	Q	273	THR	9.4
2	Q	251	PHE	9.3
2	Q	248	ALA	9.2
2	Q	246	SER	9.2
2	Q	215	SER	9.1
2	Q	225	VAL	9.1
2	Q	212	TYR	9.1
2	Q	202	PHE	9.0
2	Q	149	VAL	9.0
3	Y	21	HIS	8.9
2	Q	164	ILE	8.7
2	Q	223	PHE	8.5
1	P	36	LEU	8.3
2	Q	285	VAL	8.1
2	Q	288	VAL	8.1
2	Q	208	SER	8.0
2	Q	283	GLN	7.6
2	Q	190	ASP	7.6
3	Y	28	CYS	7.4
2	B	152	LEU	7.4
2	Q	209	THR	7.4
2	Q	241	PHE	7.3
2	Q	203	HIS	7.0
3	Y	16	VAL	7.0
2	Q	284	ASN	7.0
2	Q	152	LEU	6.9
2	Q	165	ILE	6.8
2	Q	243	ALA	6.8
2	Q	156	PRO	6.7
3	Y	15	SER	6.6
2	Q	145	PHE	6.5
3	Y	17	CYS	6.4
2	Q	415	ARG	6.4
2	Q	217	SER	6.2
2	Q	158	SER	6.1
2	Q	252	THR	6.1
2	Q	275	SER	6.1
2	Q	271	PHE	6.1
1	A	360	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
2	Q	238	LEU	6.1
2	Q	235	PHE	6.1
2	Q	213	GLN	6.1
2	Q	151	LEU	6.0
2	Q	269	THR	5.9
2	Q	229	CYS	5.8
3	Y	23	THR	5.7
2	Q	155	TYR	5.7
3	Y	8	THR	5.7
2	Q	237	PHE	5.6
3	Y	3	THR	5.5
3	Y	12	GLU	5.5
2	Q	168	VAL	5.5
2	B	153	PHE	5.5
3	Y	22	ASN	5.4
2	Q	219	THR	5.4
2	Q	265	PRO	5.4
3	Y	19	ARG	5.4
2	Q	160	GLY	5.3
2	Q	286	ARG	5.3
2	Q	159	SER	5.3
2	Q	276	ASN	5.2
1	P	360	TYR	5.2
2	B	193	GLU	5.1
2	B	145	PHE	5.1
3	Y	24	SER	5.0
3	Y	18	GLN	5.0
2	Q	233	PHE	5.0
3	Y	36	TYR	4.9
2	Q	154	GLU	4.8
2	Q	268	VAL	4.8
2	Q	287	ARG	4.8
3	Y	6	SER	4.8
2	Q	163	ARG	4.7
2	Q	146	GLN	4.7
2	B	156	PRO	4.7
2	B	199	GLY	4.5
3	Y	34	ARG	4.4
2	Q	222	PHE	4.4
2	Q	224	ILE	4.4
2	B	251	PHE	4.3
2	Q	303	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
2	Q	291	ILE	4.3
2	Q	231	ILE	4.2
2	B	219	THR	4.2
2	B	136	GLU	4.2
2	B	191	GLU	4.2
2	Q	162	ALA	4.1
3	Y	9	THR	4.1
2	B	155	TYR	4.1
2	Q	261	VAL	4.0
2	Q	258	ILE	4.0
2	Q	207	GLN	4.0
2	Q	172	VAL	4.0
2	B	151	LEU	3.9
3	Y	29	MET	3.9
2	Q	166	ALA	3.9
3	Y	5	VAL	3.9
2	Q	221	PRO	3.8
3	Y	14	TRP	3.8
2	Q	226	GLU	3.7
2	Q	189	ARG	3.6
2	Q	204	THR	3.6
1	A	36	LEU	3.6
2	B	190	ASP	3.5
2	B	158	SER	3.5
3	Y	26	GLY	3.5
2	Q	147	ARG	3.5
2	Q	191	GLU	3.5
2	Q	157	GLU	3.4
2	Q	289	VAL	3.4
2	Q	302	LYS	3.4
2	B	165	ILE	3.4
2	Q	220	ASP	3.3
2	Q	267	TYR	3.3
2	B	204	THR	3.3
2	Q	264	ILE	3.3
2	B	157	GLU	3.3
2	B	194	ASP	3.3
3	Y	7	CYS	3.3
2	B	192	ASN	3.2
2	B	248	ALA	3.2
2	Q	187	ILE	3.2
2	Q	253	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	Q	266	TYR	3.2
2	B	161	PRO	3.1
2	Q	274	GLU	3.1
2	Q	148	GLN	3.1
2	Q	306	HIS	3.1
2	B	150	TRP	3.0
2	B	125	MET	3.0
2	B	252	THR	2.9
2	B	205	TYR	2.9
2	B	215	SER	2.9
3	Y	25	ARG	2.9
2	Q	260	ILE	2.9
3	Y	10	SER	2.8
2	B	162	ALA	2.8
2	Q	262	ALA	2.8
2	Q	170	VAL	2.8
2	B	241	PHE	2.8
3	Y	31	LYS	2.8
1	A	280	GLU	2.8
2	Q	173	ILE	2.8
2	Q	295	MET	2.8
2	Q	254	ILE	2.7
2	B	154	GLU	2.7
2	B	200	VAL	2.7
2	Q	322	ARG	2.7
2	Q	175	ILE	2.7
2	B	132	TYR	2.7
2	B	124	GLU	2.6
2	B	164	ILE	2.6
1	P	349	HIS	2.6
2	B	213	GLN	2.6
2	B	370	THR	2.6
2	B	351	ASP	2.6
2	Q	292	PHE	2.6
2	Q	36	VAL	2.5
2	B	163	ARG	2.5
3	Y	13	CYS	2.5
3	Y	33	CYS	2.5
2	Q	114	ARG	2.5
2	Q	308	LYS	2.5
2	Q	188	PHE	2.5
2	B	121	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	149	VAL	2.4
2	Q	417	THR	2.4
1	A	205	PHE	2.4
2	B	371	VAL	2.4
2	Q	73	ARG	2.4
1	P	207	LEU	2.4
2	Q	304	SER	2.4
2	B	242	PHE	2.3
2	B	144	GLU	2.3
2	Q	228	LEU	2.3
1	P	202	ALA	2.3
3	Y	37	SER	2.2
2	B	417	THR	2.2
2	B	73	ARG	2.2
2	B	272	LEU	2.2
1	P	201	VAL	2.2
1	P	200	SER	2.2
3	Y	27	LYS	2.1
2	Q	239	VAL	2.1
2	Q	236	GLU	2.1
2	Q	412	PHE	2.1
2	Q	72	LEU	2.1
1	A	206	ASN	2.1
2	Q	270	ILE	2.1
1	A	361	SER	2.1
2	B	131	GLY	2.1
1	A	202	ALA	2.1
2	Q	121	GLU	2.1
2	Q	211	GLY	2.1
2	B	198	GLY	2.0
2	Q	56	GLU	2.0
2	B	196	HIS	2.0

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

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	0.84	0.22	88,88,89,89	8

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
6	PGW	B	508	9/51	0.35	0.36	104,106,107,107	0
6	PGW	B	518	12/51	0.35	0.51	113,116,117,117	0
6	PGW	B	516	37/51	0.38	0.37	108,129,144,145	0
6	PGW	B	504	22/51	0.50	0.43	76,86,90,91	0
6	PGW	Q	504	22/51	0.51	0.34	100,113,118,119	0
6	PGW	B	515	12/51	0.55	0.54	84,90,94,94	0
6	PGW	B	514	23/51	0.56	0.40	136,139,148,149	0
6	PGW	B	519	12/51	0.58	0.44	102,104,105,105	0
6	PGW	B	507	9/51	0.65	0.28	100,101,102,103	0
6	PGW	B	513	12/51	0.66	0.35	74,80,83,84	0
6	PGW	B	506	9/51	0.69	0.30	95,96,96,97	0
6	PGW	B	505	9/51	0.69	0.29	98,99,102,102	0
6	PGW	B	512	9/51	0.72	0.26	91,91,92,93	0
6	PGW	B	517	10/51	0.73	0.31	77,78,80,81	0
6	PGW	B	510	9/51	0.78	0.54	90,93,97,98	0
6	PGW	B	509	9/51	0.80	0.40	80,81,81,82	0
6	PGW	B	511	7/51	0.81	0.23	86,87,87,87	0
5	K	Q	501	1/1	0.92	0.23	50,50,50,50	1
5	K	Q	503	1/1	0.97	0.34	38,38,38,38	1
4	NAP	P	1001	48/48	0.98	0.15	35,41,50,51	0
4	NAP	A	1001	48/48	0.99	0.14	34,39,45,47	0
5	K	Q	502	1/1	0.99	0.24	62,62,62,62	1
5	K	B	502	1/1	0.99	0.20	27,27,27,27	1
5	K	B	503	1/1	0.99	0.27	27,27,27,27	1
5	K	B	501	1/1	1.00	0.31	23,23,23,23	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 518:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
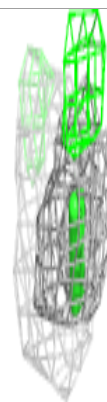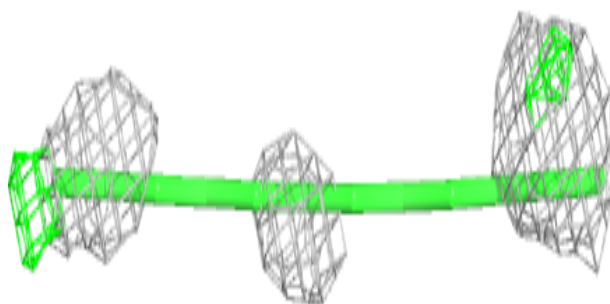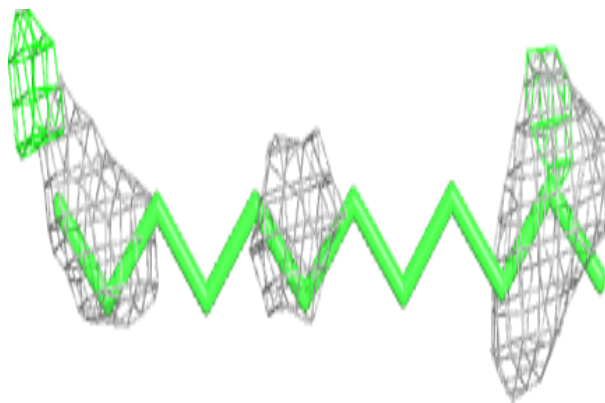
Electron density around PGW B 516:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
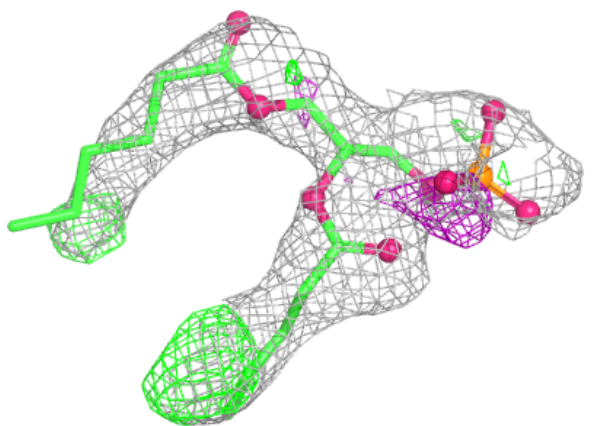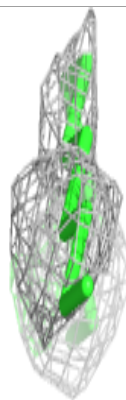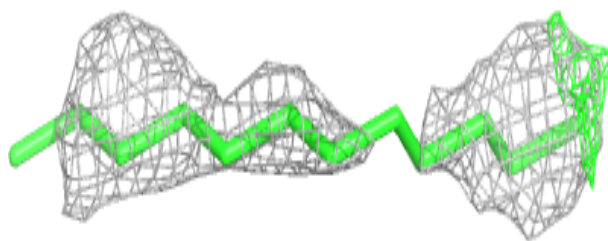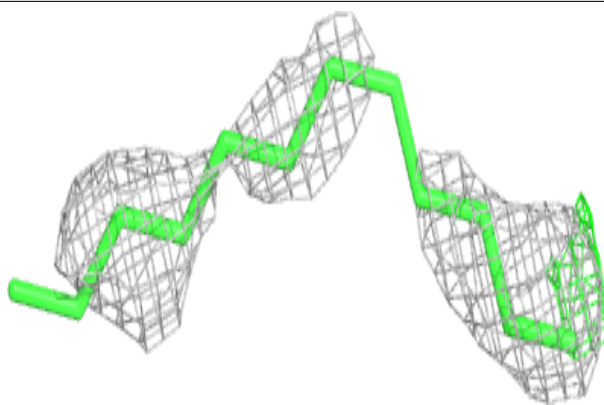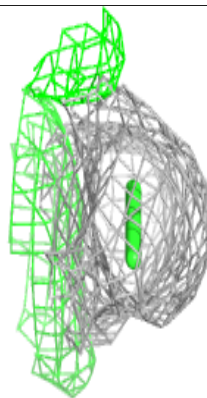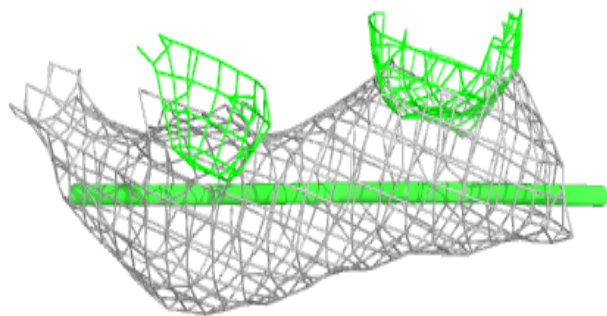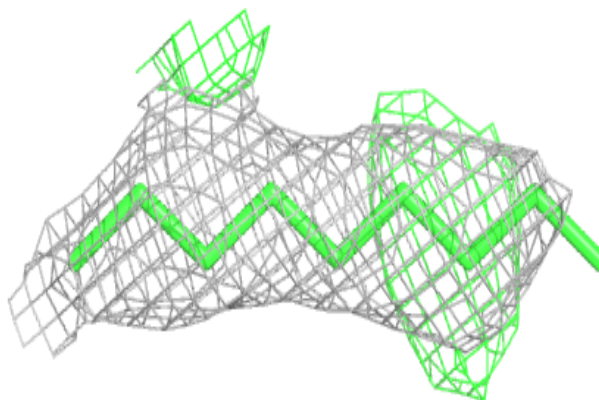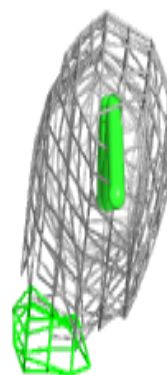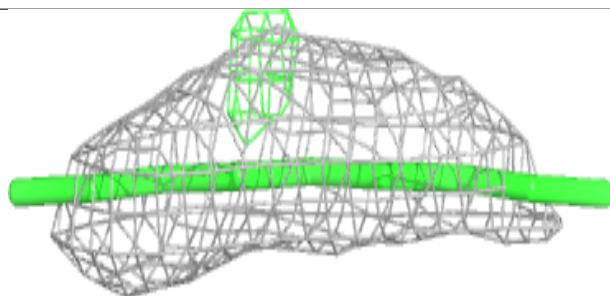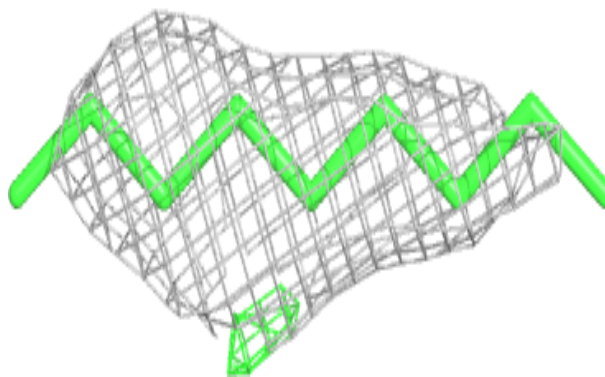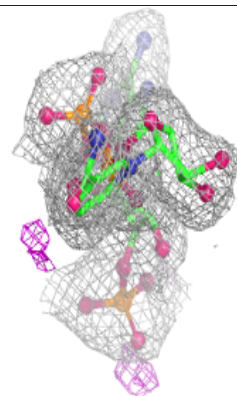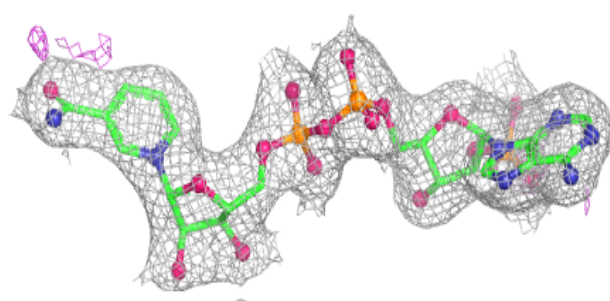$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
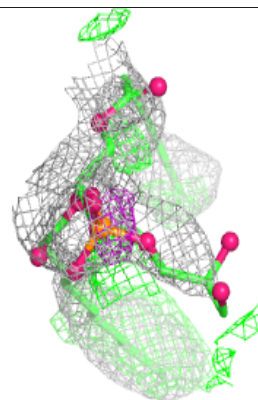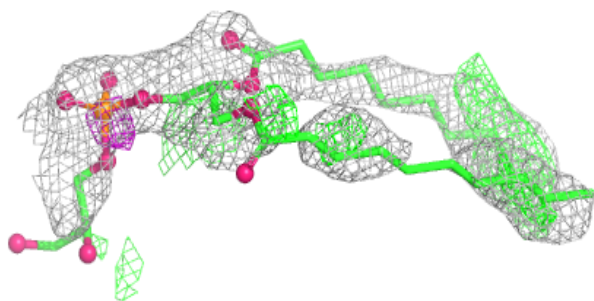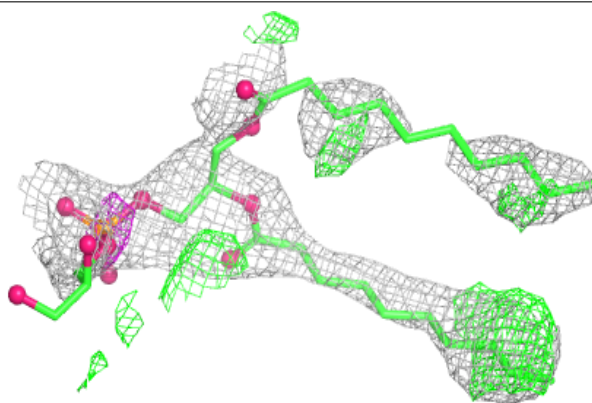
Electron density around PGW B 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
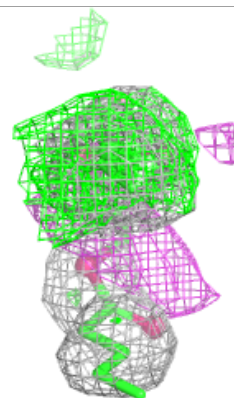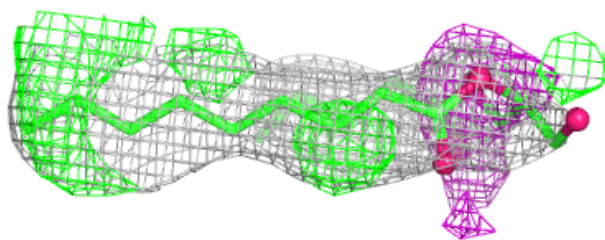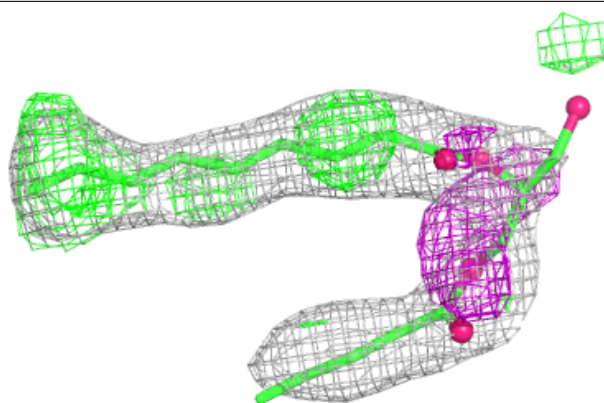
Electron density around PGW Q 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
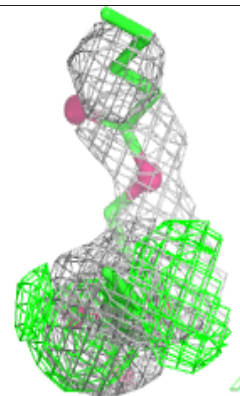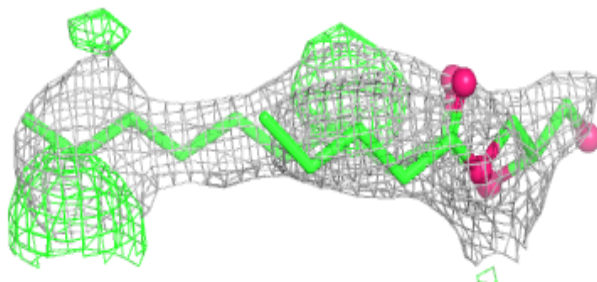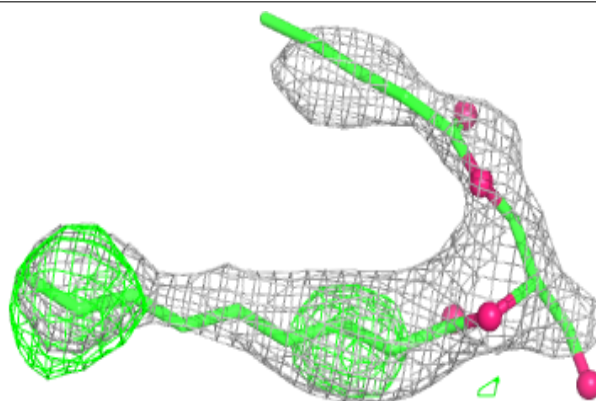
Electron density around PGW B 515:

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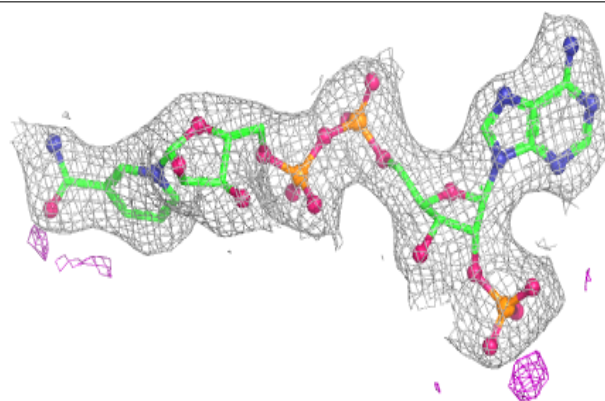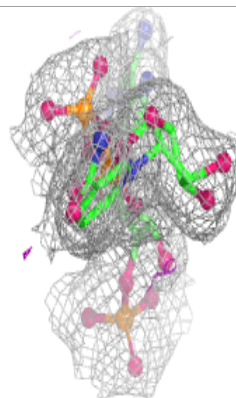mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
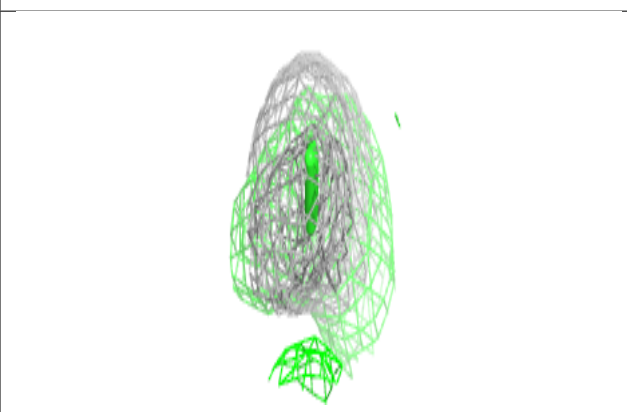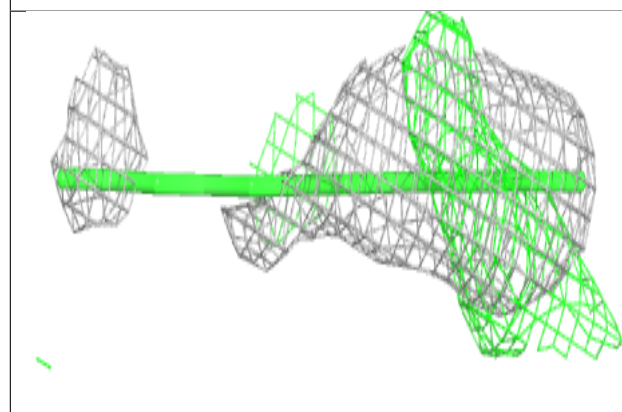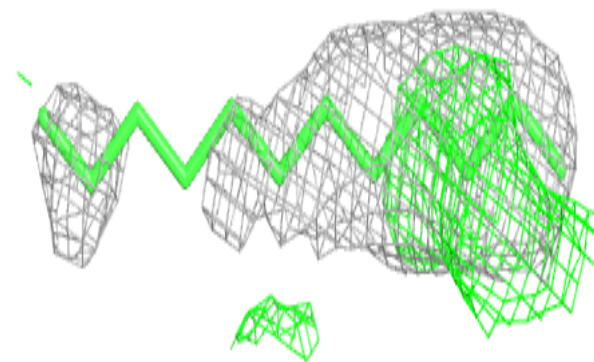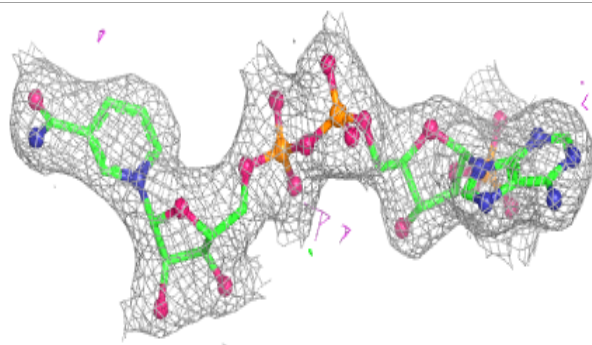

Electron density around PGW B 514:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
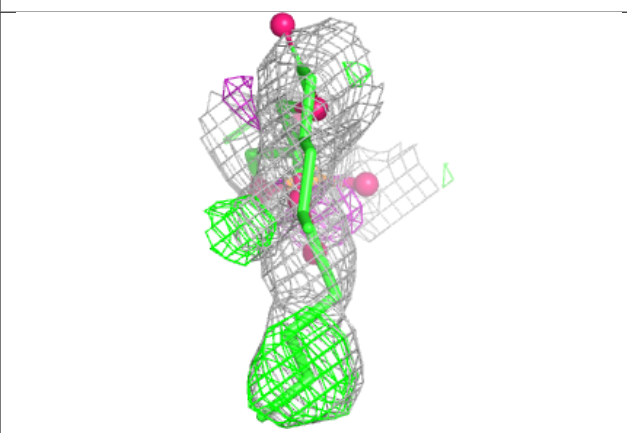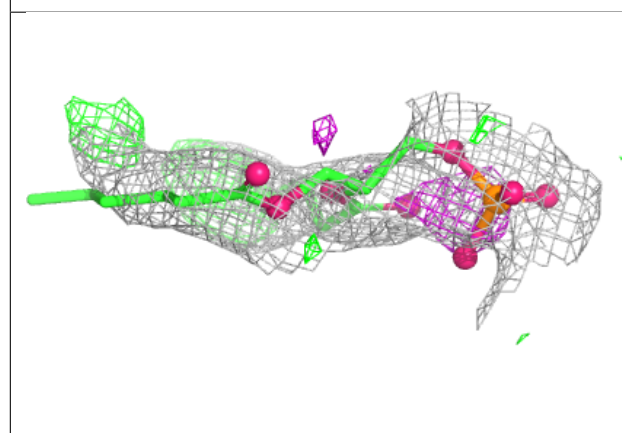
Electron density around PGW B 519:

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

Electron density around PGW B 510:

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

Electron density around PGW B 509:

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

Electron density around NAP P 1001:

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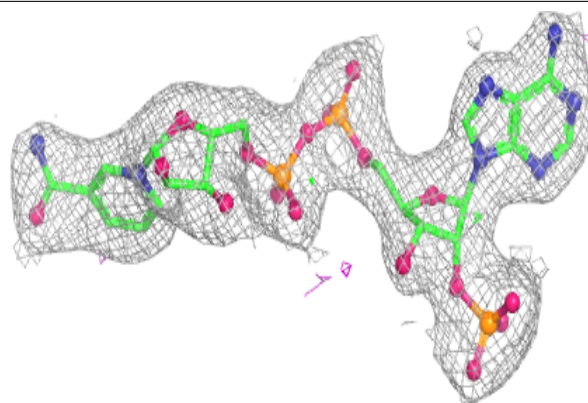$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

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 ⓘ

There are no such residues in this entry.