



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:56 PM BST

PDB ID : 5YLU  
Title : Crystal structure of the gastric proton pump complexed with vonoprazan  
Authors : Abe, K.; Irie, K.; Nakanishi, H.; Fujiyoshi, Y.  
Deposited on : 2017-10-19  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

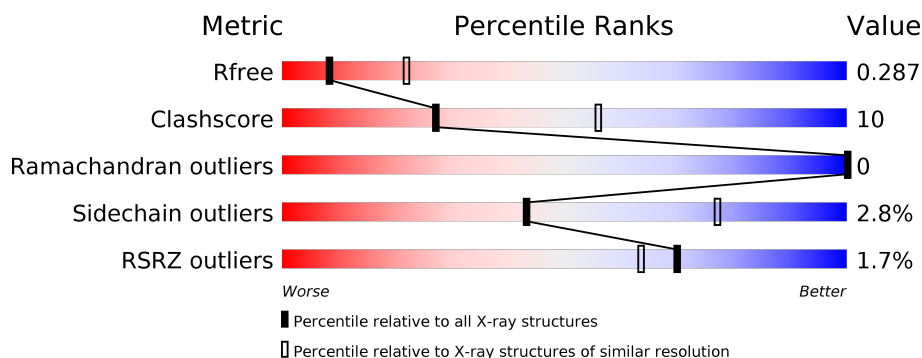
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1034	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 6%</div> </div> </div>
2	B	289	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>11%</div> </div> </div>

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
1	BFD	A	385	-	-	X	-
4	PCW	A	1103	-	-	-	X
7	NAG	B	302	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9884 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 Potassium-transporting ATPase alpha chain 1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	977	Total	Be	C	F	N	O	S	0	0	0
			7566	1	4825	3	1279	1404	54			

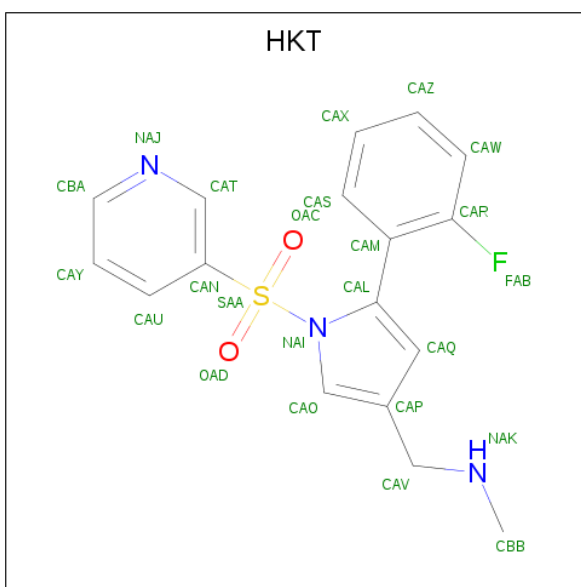
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	CYS	ARG	engineered mutation	UNP P19156
A	593	CYS	SER	engineered mutation	UNP P19156
A	1005	SER	GLY	engineered mutation	UNP P19156

- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

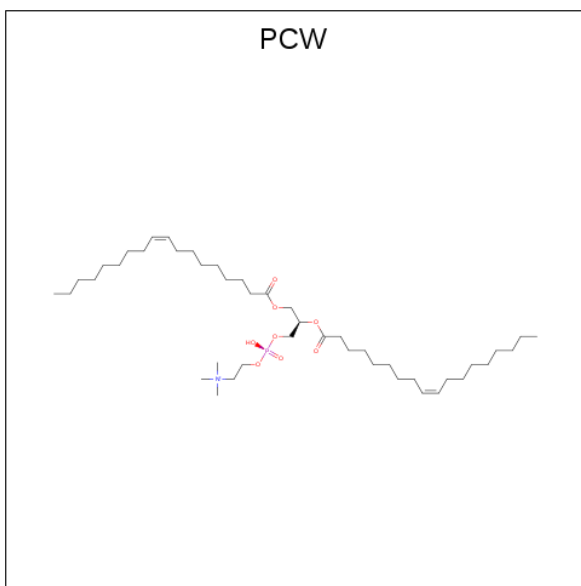
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	257	Total	C	N	O	S	0	0	0
			2058	1338	340	369	11			

- Molecule 3 is 1-[5-(2-fluorophenyl)-1-pyridin-3-ylsulfonyl-pyrrol-3-yl]- {N}-methyl-methanamine (three-letter code: HKT) (formula: C<sub>17</sub>H<sub>16</sub>FN<sub>3</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			24	17	1	3	2	1		

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula:  $C_{44}H_{85}NO_8P$ ).

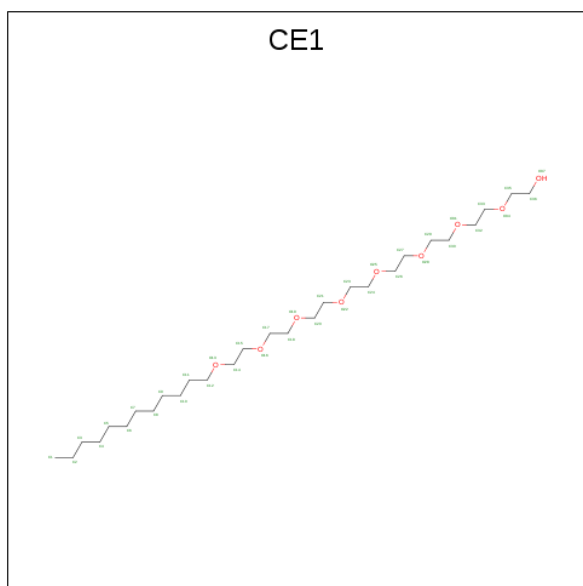


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 54	C 44	N 1	O 8	P 1	0	0
4	A	1	Total 54	C 44	N 1	O 8	P 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

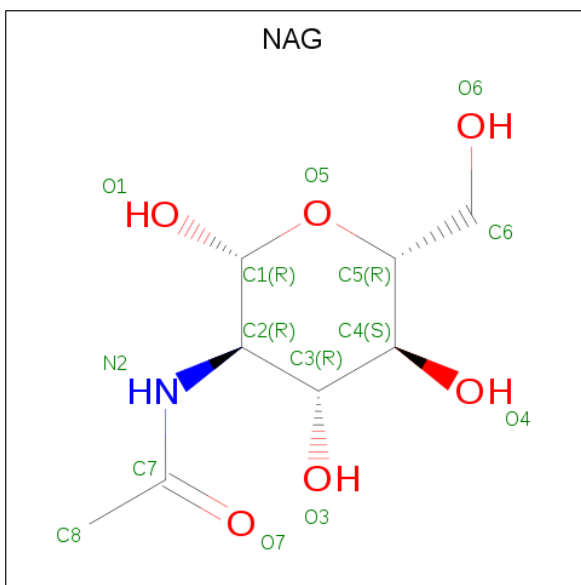
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: C<sub>28</sub>H<sub>58</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			29	23	6		
6	B	1	Total	C	O	0	0
			19	16	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



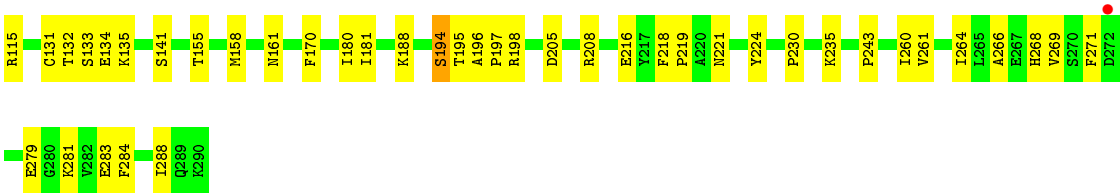
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	30	Total	O	0	0
			30	30		
8	B	7	Total	O	0	0
			7	7		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.82Å 104.82Å 367.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.18 – 2.80 48.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.5 (48.18-2.80) 87.5 (48.18-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.81Å)	Xtriage
Refinement program	phenix.refine 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.237 , 0.288 0.237 , 0.287	Depositor DCC
$R_{free}$ test set	2610 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 26.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	9884	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, NAG, BFD, PCW, HKT, CE1

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	0.55	1/7705 (0.0%)	0.69	4/10463 (0.0%)
2	B	0.56	1/2125 (0.0%)	0.64	0/2893
All	All	0.55	2/9830 (0.0%)	0.68	4/13356 (0.0%)

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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	131	CYS	CB-SG	-5.65	1.72	1.81
1	A	651	GLU	CG-CD	5.08	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	LEU	CA-CB-CG	6.95	131.28	115.30
1	A	136	ASP	CB-CG-OD1	5.29	123.07	118.30
1	A	173	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	527	CYS	CA-CB-SG	5.12	123.22	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	219	PRO	Peptide

## 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	7566	0	7607	165	0
2	B	2058	0	1993	32	0
3	A	24	0	0	0	0
4	A	108	0	168	3	0
5	A	1	0	0	0	0
6	A	29	0	45	4	0
6	B	19	0	33	5	0
7	B	42	0	39	3	0
8	A	30	0	0	1	0
8	B	7	0	0	1	0
All	All	9884	0	9885	200	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 10.

All (200) 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)
1:A:387:THR:O	1:A:726:ASP:OD2	1.76	1.02
1:A:432:ARG:NH1	1:A:483:PHE:CZ	2.31	0.97
1:A:707:LYS:NZ	1:A:730:ASP:OD1	1.97	0.97
1:A:385:BFD:CG	1:A:730:ASP:OD2	2.13	0.96
1:A:723:VAL:HG23	1:A:734:LEU:HD23	1.47	0.95
1:A:385:BFD:HB3	1:A:730:ASP:OD2	1.66	0.95
1:A:723:VAL:CG2	1:A:734:LEU:HD23	1.98	0.93
1:A:385:BFD:CB	1:A:730:ASP:OD2	2.23	0.87
1:A:880:THR:HG22	1:A:997:TRP:HZ3	1.41	0.83
1:A:731:SER:OG	1:A:732:PRO:HD3	1.77	0.82
1:A:909:ASP:OD2	1:A:913:GLN:NE2	2.12	0.82
1:A:432:ARG:NH1	1:A:483:PHE:HZ	1.77	0.81
1:A:795:GLU:HG2	1:A:816:ILE:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:SER:OG	8:B:401:HOH:O	2.09	0.70
1:A:385:BFD:OD1	1:A:730:ASP:OD2	2.08	0.70
1:A:332:PHE:HD1	1:A:799:TYR:HH	1.41	0.69
1:A:181:ILE:HA	1:A:185:ASP:O	1.94	0.68
1:A:783:LYS:HB3	1:A:831:LEU:HD13	1.74	0.68
1:A:993:ILE:HB	1:A:997:TRP:HD1	1.59	0.67
1:A:51:ASN:O	1:A:55:LEU:HD13	1.94	0.67
1:A:68:ALA:HB1	1:A:215:LEU:HD13	1.76	0.66
2:B:224:TYR:HD1	2:B:243:PRO:HB2	1.61	0.66
1:A:50:ILE:CG2	1:A:54:GLN:HE21	2.09	0.66
1:A:50:ILE:HG22	1:A:54:GLN:HE21	1.61	0.65
2:B:197:PRO:HB3	2:B:266:ALA:HB2	1.78	0.65
1:A:881:ALA:HA	1:A:997:TRP:CH2	2.32	0.65
2:B:132:THR:HG21	7:B:302:NAG:H61	1.80	0.64
1:A:765:ALA:O	1:A:768:VAL:HG22	1.98	0.64
1:A:112:LEU:HD21	1:A:341:VAL:HG22	1.80	0.64
2:B:261:VAL:HG22	2:B:283:GLU:HG2	1.81	0.63
1:A:727:GLY:HA2	1:A:748:SER:OG	1.98	0.63
1:A:67:SER:HG	1:A:71:GLY:H	1.47	0.63
1:A:378:SER:OG	1:A:846:ARG:NH1	2.32	0.63
1:A:229:GLY:HA2	1:A:385:BFD:F2	1.90	0.62
1:A:99:VAL:O	1:A:103:ARG:HG3	2.00	0.61
1:A:432:ARG:HH12	1:A:483:PHE:HZ	1.48	0.61
1:A:286:VAL:HG11	1:A:735:LYS:HB3	1.82	0.61
1:A:50:ILE:CG2	1:A:54:GLN:NE2	2.62	0.60
2:B:69:TYR:HE1	2:B:235:LYS:HG2	1.66	0.60
1:A:432:ARG:NH1	1:A:483:PHE:CE2	2.69	0.60
2:B:205:ASP:HB3	2:B:208:ARG:HH22	1.66	0.59
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.85	0.58
1:A:726:ASP:O	1:A:747:GLY:HA2	2.04	0.58
1:A:688:VAL:HG22	1:A:717:LEU:HD11	1.86	0.57
1:A:957:GLY:HA3	1:A:960:ARG:HE	1.69	0.57
1:A:67:SER:OG	1:A:71:GLY:N	2.37	0.56
1:A:908:GLN:HA	1:A:913:GLN:O	2.05	0.55
2:B:134:GLU:O	2:B:135:LYS:HD3	2.06	0.55
1:A:359:ARG:HD2	1:A:773:GLN:OE1	2.06	0.55
1:A:282:LEU:HD11	1:A:705:GLN:HG3	1.88	0.55
1:A:498:GLN:OE1	1:A:517:LYS:HE3	2.04	0.55
1:A:352:CYS:HB3	1:A:777:ILE:HD11	1.88	0.55
1:A:957:GLY:CA	1:A:960:ARG:HE	2.20	0.55
1:A:650:VAL:HG11	1:A:666:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:THR:HG22	1:A:997:TRP:CZ3	2.31	0.54
1:A:97:GLU:HG3	1:A:157:TYR:OH	2.07	0.54
1:A:723:VAL:HG23	1:A:734:LEU:CD2	2.28	0.54
1:A:527:CYS:HB2	1:A:592:LEU:C	2.28	0.54
1:A:508:ARG:NH1	1:A:508:ARG:HB2	2.23	0.53
1:A:67:SER:OG	1:A:70:LYS:N	2.41	0.53
1:A:50:ILE:HG13	1:A:245:PRO:HD3	1.88	0.53
1:A:807:VAL:HG12	1:A:878:TYR:OH	2.09	0.53
1:A:308:ALA:HB1	1:A:337:VAL:HA	1.90	0.53
2:B:62:LEU:HB2	6:B:304:CE1:H22	1.91	0.52
2:B:181:ILE:HG22	2:B:224:TYR:OH	2.10	0.52
1:A:836:ALA:HB1	1:A:840:ILE:HG13	1.91	0.52
1:A:814:ILE:HD13	1:A:989:ASN:HD22	1.73	0.52
1:A:230:GLU:OE2	1:A:701:ARG:NH2	2.43	0.52
1:A:624:MET:HB3	1:A:698:VAL:HG13	1.91	0.52
2:B:98:TYR:CE1	2:B:288:ILE:HG12	2.44	0.52
1:A:383:CYS:O	1:A:723:VAL:HA	2.09	0.51
1:A:332:PHE:HD1	1:A:799:TYR:OH	1.92	0.51
1:A:790:THR:HG23	1:A:862:SER:O	2.10	0.51
1:A:884:GLN:HB2	1:A:997:TRP:HH2	1.75	0.50
2:B:188:LYS:HA	2:B:230:PRO:HB2	1.92	0.50
1:A:367:VAL:CG2	1:A:372:ALA:HB3	2.42	0.50
2:B:194:SER:OG	2:B:195:THR:N	2.44	0.50
1:A:916:THR:O	1:A:920:ARG:HG3	2.12	0.50
1:A:707:LYS:HZ2	1:A:730:ASP:CG	2.07	0.50
1:A:315:PHE:CE2	1:A:800:LEU:HD22	2.47	0.50
1:A:492:ASN:OD1	1:A:495:ASN:N	2.43	0.50
1:A:715:GLN:OE1	1:A:736:LYS:NZ	2.44	0.50
1:A:780:ASN:ND2	1:A:832:ALA:O	2.43	0.50
1:A:286:VAL:CG1	1:A:735:LYS:HB3	2.42	0.49
1:A:707:LYS:CE	1:A:730:ASP:OD1	2.60	0.49
1:A:198:ASP:O	1:A:267:VAL:HG23	2.13	0.49
1:A:741:VAL:HG11	1:A:767:ILE:HD11	1.94	0.49
1:A:805:VAL:HB	1:A:807:VAL:HG23	1.95	0.49
1:A:999:LEU:HA	1:A:1002:MET:SD	2.52	0.49
1:A:625:VAL:O	1:A:625:VAL:HG13	2.13	0.49
2:B:216:GLU:HG2	7:B:303:NAG:H82	1.94	0.49
6:A:1105:CE1:H122	6:B:304:CE1:H101	1.95	0.48
1:A:202:MET:HE3	1:A:258:CYS:HB2	1.95	0.48
1:A:433:VAL:HG22	1:A:515:VAL:HG12	1.94	0.48
1:A:50:ILE:HD12	1:A:50:ILE:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:VAL:HG22	1:A:698:VAL:HB	1.95	0.48
1:A:527:CYS:HB2	1:A:592:LEU:O	2.14	0.48
1:A:558:GLY:O	1:A:601:ILE:HD13	2.14	0.48
1:A:608:VAL:O	1:A:612:VAL:HG23	2.14	0.48
1:A:836:ALA:CB	1:A:840:ILE:HG13	2.44	0.47
2:B:82:VAL:HB	2:B:281:LYS:O	2.14	0.47
1:A:661:VAL:HA	1:A:664:VAL:HG23	1.95	0.47
1:A:210:ALA:O	1:A:254:PHE:HA	2.14	0.47
1:A:978:LEU:HD13	1:A:990:PHE:CE2	2.49	0.47
1:A:213:ARG:HD2	1:A:250:ASN:O	2.15	0.47
1:A:776:LEU:HA	1:A:776:LEU:HD23	1.63	0.47
1:A:906:ASP:HB3	2:B:83:THR:HG21	1.95	0.47
1:A:437:CYS:O	1:A:517:LYS:HE2	2.15	0.47
1:A:324:TYR:OH	1:A:896:ARG:NH2	2.48	0.47
1:A:798:PRO:HG3	1:A:931:PHE:CZ	2.50	0.47
2:B:271:PHE:HA	2:B:279:GLU:O	2.14	0.46
1:A:147:ALA:O	1:A:151:VAL:HG23	2.16	0.46
1:A:473:LEU:HD21	1:A:479:TYR:CD2	2.51	0.46
1:A:731:SER:N	1:A:732:PRO:CD	2.79	0.46
1:A:870:GLN:HG2	1:A:938:CYS:CB	2.46	0.46
2:B:264:ILE:HG22	2:B:269:VAL:HG11	1.97	0.46
1:A:508:ARG:HH11	1:A:508:ARG:HB2	1.79	0.46
2:B:260:ILE:HB	2:B:284:PHE:CE1	2.50	0.46
1:A:114:TRP:CZ3	1:A:146:ILE:HG13	2.50	0.46
1:A:675:ASN:HA	1:A:700:ALA:O	2.15	0.46
1:A:987:ILE:HG23	1:A:988:PHE:CD2	2.51	0.45
1:A:791:LYS:C	1:A:794:PRO:HD2	2.37	0.45
1:A:120:CYS:CB	1:A:142:ALA:HB2	2.45	0.45
1:A:870:GLN:HG2	1:A:938:CYS:HB3	1.97	0.45
1:A:933:ILE:HG13	1:A:993:ILE:HD11	1.98	0.45
1:A:497:PHE:CE1	1:A:499:LEU:HD23	2.50	0.45
1:A:834:GLU:OE2	1:A:947:LYS:HG2	2.17	0.45
1:A:959:PHE:N	1:A:959:PHE:CD1	2.85	0.45
1:A:657:LEU:HB3	1:A:659:VAL:HG23	1.98	0.45
2:B:161:ASN:HB2	2:B:218:PHE:CZ	2.52	0.45
1:A:945:ILE:HB	1:A:1012:ASP:OD2	2.16	0.45
1:A:230:GLU:HA	1:A:628:ASP:OD1	2.17	0.45
1:A:627:GLY:HA2	1:A:702:THR:H	1.81	0.45
1:A:387:THR:HA	1:A:391:THR:OG1	2.17	0.45
1:A:797:THR:HG21	4:A:1102:PCW:H472	1.99	0.45
4:A:1102:PCW:H63	4:A:1102:PCW:H42	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1105:CE1:H142	6:B:304:CE1:H112	1.98	0.44
2:B:196:ALA:HB1	2:B:224:TYR:O	2.17	0.44
2:B:155:THR:O	2:B:158:MET:HG3	2.17	0.44
1:A:391:THR:HA	1:A:604:PRO:HA	1.99	0.44
2:B:40:ILE:O	2:B:43:TYR:HB3	2.17	0.44
1:A:739:ILE:CD1	1:A:756:ASP:HB2	2.48	0.44
1:A:345:LEU:HA	1:A:345:LEU:HD12	1.78	0.44
2:B:58:CYS:O	6:B:304:CE1:H11	2.18	0.43
1:A:233:PRO:HB3	1:A:259:LEU:HD12	1.99	0.43
1:A:648:GLU:HB2	1:A:652:ASP:HB2	2.00	0.43
1:A:798:PRO:HB3	1:A:810:PRO:HB2	1.99	0.43
1:A:120:CYS:HB2	1:A:142:ALA:HB2	2.01	0.43
1:A:311:PHE:O	1:A:314:THR:N	2.52	0.43
1:A:72:LEU:HD12	1:A:72:LEU:HA	1.81	0.43
1:A:90:ARG:HA	1:A:90:ARG:HD2	1.84	0.43
1:A:870:GLN:CG	1:A:938:CYS:HB3	2.49	0.43
1:A:322:ILE:HG22	1:A:322:ILE:O	2.19	0.43
1:A:776:LEU:HD21	1:A:836:ALA:HB2	2.01	0.43
1:A:248:THR:OG1	1:A:250:ASN:OD1	2.23	0.43
1:A:995:PHE:HB2	6:A:1105:CE1:H181	2.01	0.43
2:B:216:GLU:CG	7:B:303:NAG:H82	2.49	0.43
1:A:708:LEU:O	1:A:708:LEU:HD12	2.19	0.43
1:A:836:ALA:HB1	1:A:840:ILE:CG1	2.49	0.43
1:A:814:ILE:HD13	1:A:989:ASN:ND2	2.33	0.43
1:A:53:HIS:HA	1:A:213:ARG:HD3	2.00	0.42
1:A:86:PRO:HD2	1:A:90:ARG:NH2	2.34	0.42
1:A:791:LYS:HG2	1:A:939:GLN:CD	2.38	0.42
1:A:383:CYS:HB2	1:A:723:VAL:HG12	2.01	0.42
1:A:120:CYS:SG	1:A:141:LEU:HD23	2.60	0.42
1:A:228:THR:O	1:A:729:ASN:ND2	2.53	0.42
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.73	0.42
2:B:98:TYR:HE1	2:B:288:ILE:HG12	1.85	0.42
1:A:124:PHE:CE2	1:A:139:LEU:HD13	2.54	0.42
1:A:178:ALA:HB2	1:A:209:PRO:HB3	2.01	0.42
1:A:532:ILE:HD13	1:A:543:TRP:CH2	2.55	0.42
1:A:381:VAL:HA	1:A:621:ARG:O	2.19	0.42
2:B:113:LEU:HD22	2:B:180:ILE:HD13	2.01	0.42
2:B:114:HIS:CE1	2:B:170:PHE:CE1	3.07	0.42
1:A:327:LEU:HA	1:A:327:LEU:HD12	1.80	0.41
1:A:531:LEU:O	1:A:532:ILE:HG13	2.20	0.41
2:B:78:LYS:HG3	2:B:79:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:THR:OG1	1:A:603:PRO:HG3	2.20	0.41
2:B:113:LEU:HA	2:B:113:LEU:HD23	1.82	0.41
1:A:643:ILE:O	8:A:1201:HOH:O	2.22	0.41
1:A:276:ILE:HD13	1:A:276:ILE:HA	1.86	0.41
1:A:96:PRO:HD2	1:A:99:VAL:HG11	2.01	0.41
1:A:960:ARG:N	1:A:960:ARG:HD3	2.35	0.41
1:A:276:ILE:HD12	1:A:728:VAL:HG21	2.02	0.41
1:A:148:VAL:HG12	4:A:1103:PCW:H261	2.02	0.41
1:A:255:SER:HB3	1:A:276:ILE:HG13	2.01	0.41
1:A:552:LEU:HD23	1:A:552:LEU:HA	1.87	0.41
1:A:939:GLN:HA	1:A:942:ASP:HB2	2.03	0.41
1:A:50:ILE:HG22	1:A:54:GLN:NE2	2.30	0.41
1:A:777:ILE:HA	1:A:777:ILE:HD12	1.92	0.41
1:A:794:PRO:HG3	1:A:870:GLN:CB	2.51	0.41
2:B:198:ARG:HD2	2:B:221:ASN:O	2.21	0.41
6:A:1105:CE1:C14	6:B:304:CE1:H112	2.51	0.40
1:A:135:THR:H	1:A:135:THR:HG23	1.60	0.40
2:B:42:LEU:HA	2:B:45:VAL:HG22	2.02	0.40
1:A:834:GLU:OE2	1:A:947:LYS:HE2	2.21	0.40
1:A:519:ALA:HA	1:A:520:PRO:HD3	1.98	0.40
1:A:527:CYS:HB3	1:A:592:LEU:HB2	2.03	0.40
1:A:547:PHE:CD1	1:A:547:PHE:C	2.95	0.40
1:A:308:ALA:HB2	1:A:340:TYR:HB2	2.02	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	974/1034 (94%)	918 (94%)	56 (6%)	0	100	100
2	B	255/289 (88%)	230 (90%)	25 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1229/1323 (93%)	1148 (93%)	81 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	824/869 (95%)	800 (97%)	24 (3%)	42	76
2	B	224/253 (88%)	219 (98%)	5 (2%)	52	83
All	All	1048/1122 (93%)	1019 (97%)	29 (3%)	43	77

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	SER
1	A	90	ARG
1	A	93	ARG
1	A	130	GLU
1	A	163	SER
1	A	255	SER
1	A	273	ARG
1	A	328	ARG
1	A	362	SER
1	A	395	MET
1	A	398	SER
1	A	439	ARG
1	A	508	ARG
1	A	701	ARG
1	A	813	CYS
1	A	824	ASP
1	A	846	ARG
1	A	853	LEU
1	A	855	ASN
1	A	934	SER

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Mol	Chain	Res	Type
1	A	946	ARG
1	A	970	PHE
1	A	1002	MET
1	A	1005	SER
2	B	85	ARG
2	B	115	ARG
2	B	141	SER
2	B	194	SER
2	B	268	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	177	GLN
1	A	792	ASN
1	A	884	GLN
2	B	275	HIS

### 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	$\# Z  > 2$
1	BFD	A	385	1,5	8,11,12	5.32	3 (37%)	3,15,17	1.06	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
1	BFD	A	385	1,5	-	0/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	BFD	F3-BE	9.73	1.77	1.54
1	A	385	BFD	F1-BE	8.16	1.74	1.54
1	A	385	BFD	F2-BE	7.83	1.73	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	385	BFD	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CE1	B	304	-	18,18,36	0.38	0	17,17,35	0.53	0
7	NAG	B	302	2	14,14,15	1.84	2 (14%)	17,19,21	1.52	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HKT	A	1101	-	23,26,26	1.08	3 (13%)	27,37,37	2.15	11 (40%)
4	PCW	A	1102	-	53,53,53	0.99	2 (3%)	59,61,61	0.82	2 (3%)
6	CE1	A	1105	-	28,28,36	0.45	0	27,27,35	0.49	0
4	PCW	A	1103	-	53,53,53	1.04	2 (3%)	59,61,61	0.99	4 (6%)
7	NAG	B	303	2	14,14,15	0.53	0	17,19,21	1.13	2 (11%)
7	NAG	B	301	2	14,14,15	1.05	1 (7%)	17,19,21	0.93	1 (5%)

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	CE1	B	304	-	-	4/16/16/34	-
7	NAG	B	302	2	-	4/6/23/26	0/1/1/1
3	HKT	A	1101	-	-	2/10/19/19	0/3/3/3
4	PCW	A	1102	-	-	13/57/57/57	-
6	CE1	A	1105	-	-	13/26/26/34	-
4	PCW	A	1103	-	-	21/57/57/57	-
7	NAG	B	303	2	-	1/6/23/26	0/1/1/1
7	NAG	B	301	2	-	4/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	302	NAG	C1-C2	5.88	1.61	1.52
4	A	1103	PCW	O3-C11	4.64	1.46	1.33
4	A	1102	PCW	O3-C11	4.48	1.46	1.33
4	A	1103	PCW	O2-C31	4.45	1.46	1.34
4	A	1102	PCW	O2-C31	4.40	1.46	1.34
7	B	301	NAG	O5-C1	-3.48	1.38	1.43
7	B	302	NAG	O5-C1	3.35	1.49	1.43
3	A	1101	HKT	CAN-SAA	-2.91	1.63	1.77
3	A	1101	HKT	CAO-NAI	-2.27	1.34	1.38
3	A	1101	HKT	CAT-CAN	2.27	1.40	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	PCW	O2-C31-C32	4.79	121.82	111.50
3	A	1101	HKT	CAN-SAA-NAI	4.72	109.87	104.95
3	A	1101	HKT	OAD-SAA-OAC	-4.29	103.10	117.71
3	A	1101	HKT	CAW-CAR-CAM	-4.04	118.37	123.30
7	B	302	NAG	C1-O5-C5	-3.36	107.64	112.19
4	A	1102	PCW	O2-C31-C32	3.19	118.37	111.50
7	B	302	NAG	O3-C3-C2	-2.93	103.41	109.47
4	A	1103	PCW	O3-C11-C12	2.84	120.82	111.91
7	B	301	NAG	C1-O5-C5	-2.61	108.66	112.19
3	A	1101	HKT	CAS-CAM-CAR	2.61	119.86	116.10
7	B	303	NAG	C3-C4-C5	2.61	114.89	110.24
3	A	1101	HKT	CAT-CAN-SAA	2.53	122.63	120.21
7	B	303	NAG	C1-O5-C5	2.51	115.59	112.19
3	A	1101	HKT	CBA-NAJ-CAT	2.47	121.12	116.85
3	A	1101	HKT	FAB-CAR-CAM	2.43	122.55	118.89
3	A	1101	HKT	CAU-CAN-CAT	-2.38	115.99	118.65
7	B	302	NAG	C1-C2-N2	2.38	114.55	110.49
4	A	1102	PCW	O3-C11-C12	2.36	119.33	111.91
3	A	1101	HKT	OAD-SAA-CAN	2.30	112.82	107.62
4	A	1103	PCW	C2-O2-C31	-2.30	112.12	117.79
3	A	1101	HKT	CAL-CAQ-CAP	2.25	108.88	105.52
4	A	1103	PCW	O2-C31-O31	-2.12	118.58	123.70
3	A	1101	HKT	OAC-SAA-CAN	2.04	112.23	107.62

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	PCW	O4P-C4-C5-N
4	A	1102	PCW	C4-O4P-P-O2P
4	A	1103	PCW	C1-O3P-P-O1P
4	A	1103	PCW	C1-O3P-P-O2P
4	A	1103	PCW	C1-O3P-P-O4P
7	B	301	NAG	C1-C2-N2-C7
7	B	302	NAG	O5-C5-C6-O6
4	A	1103	PCW	C12-C11-O3-C3
6	A	1105	CE1	O16-C17-C18-O19
7	B	302	NAG	C8-C7-N2-C2
7	B	302	NAG	O7-C7-N2-C2
6	A	1105	CE1	C10-C11-C12-O13
4	A	1103	PCW	O11-C11-O3-C3
4	A	1103	PCW	C4-O4P-P-O3P
6	A	1105	CE1	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
6	A	1105	CE1	C11-C10-C9-C8
4	A	1103	PCW	C14-C15-C16-C17
7	B	302	NAG	C4-C5-C6-O6
4	A	1103	PCW	C13-C14-C15-C16
6	A	1105	CE1	O13-C14-C15-O16
4	A	1102	PCW	C13-C14-C15-C16
4	A	1102	PCW	C36-C37-C38-C39
4	A	1103	PCW	C16-C17-C18-C19
4	A	1103	PCW	O3P-C1-C2-C3
4	A	1103	PCW	C23-C24-C25-C26
4	A	1103	PCW	C20-C21-C22-C23
4	A	1103	PCW	C24-C25-C26-C27
7	B	301	NAG	C4-C5-C6-O6
4	A	1102	PCW	C22-C23-C24-C25
6	A	1105	CE1	C3-C4-C5-C6
4	A	1102	PCW	O31-C31-O2-C2
4	A	1102	PCW	C41-C42-C43-C44
7	B	301	NAG	O5-C5-C6-O6
6	A	1105	CE1	C21-C20-O19-C18
4	A	1102	PCW	C32-C31-O2-C2
6	A	1105	CE1	C14-C15-O16-C17
4	A	1103	PCW	O3P-C1-C2-O2
6	B	304	CE1	C15-C14-O13-C12
6	B	304	CE1	C10-C11-C12-O13
3	A	1101	HKT	CAQ-CAL-CAM-CAR
4	A	1103	PCW	C4-O4P-P-O1P
6	A	1105	CE1	C9-C10-C11-C12
4	A	1103	PCW	O4P-C4-C5-N
4	A	1103	PCW	C15-C16-C17-C18
4	A	1103	PCW	C32-C33-C34-C35
6	A	1105	CE1	C15-C14-O13-C12
4	A	1103	PCW	C22-C23-C24-C25
7	B	301	NAG	C3-C2-N2-C7
4	A	1102	PCW	O3P-C1-C2-O2
4	A	1102	PCW	C1-C2-C3-O3
4	A	1102	PCW	C35-C36-C37-C38
6	B	304	CE1	C9-C10-C11-C12
6	B	304	CE1	C3-C4-C5-C6
4	A	1103	PCW	C37-C38-C39-C40
6	A	1105	CE1	C4-C5-C6-C7
4	A	1103	PCW	C17-C18-C19-C20
7	B	303	NAG	C4-C5-C6-O6

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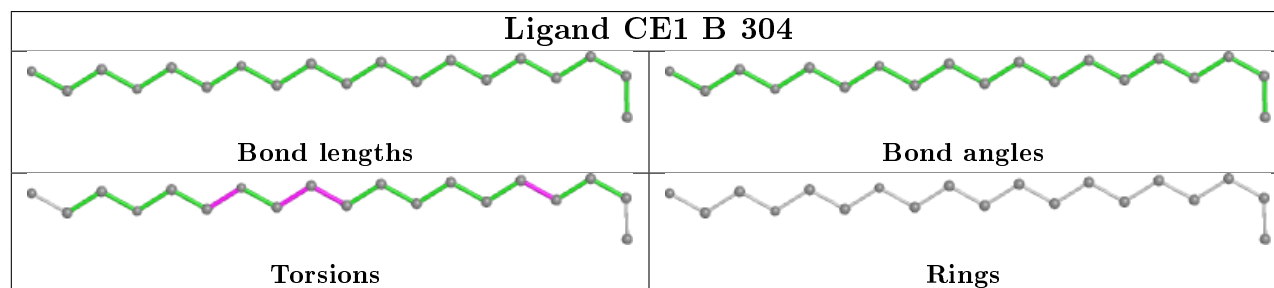
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6	A	1105	CE1	O22-C23-C24-O25
3	A	1101	HKT	NAI-CAL-CAM-CAR
6	A	1105	CE1	C11-C12-O13-C14
4	A	1102	PCW	C17-C18-C19-C20

There are no ring outliers.

6 monomers are involved in 12 short contacts:

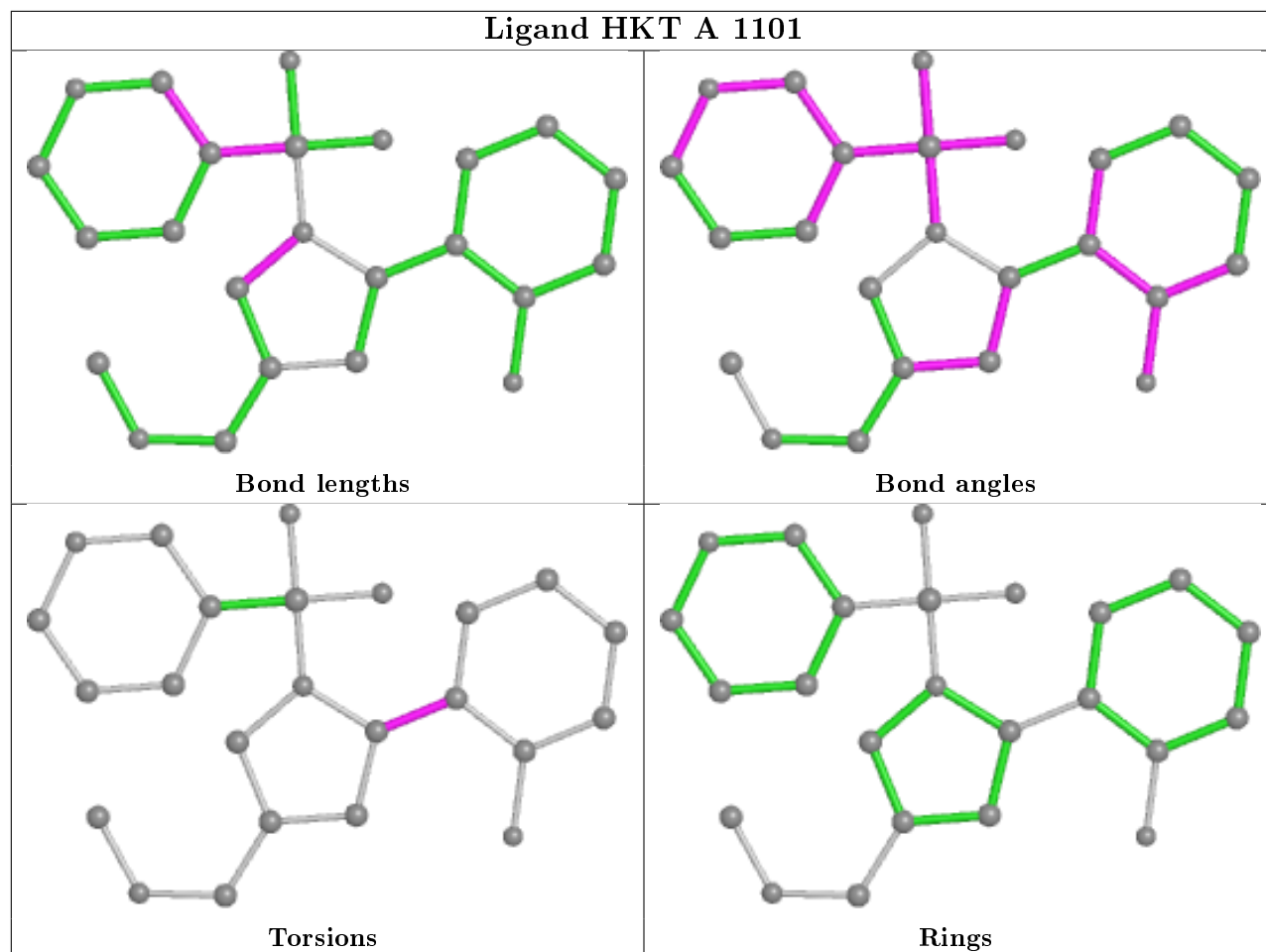
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7	B	302	NAG	1	0
4	A	1102	PCW	2	0
6	A	1105	CE1	4	0
4	A	1103	PCW	1	0
7	B	303	NAG	2	0

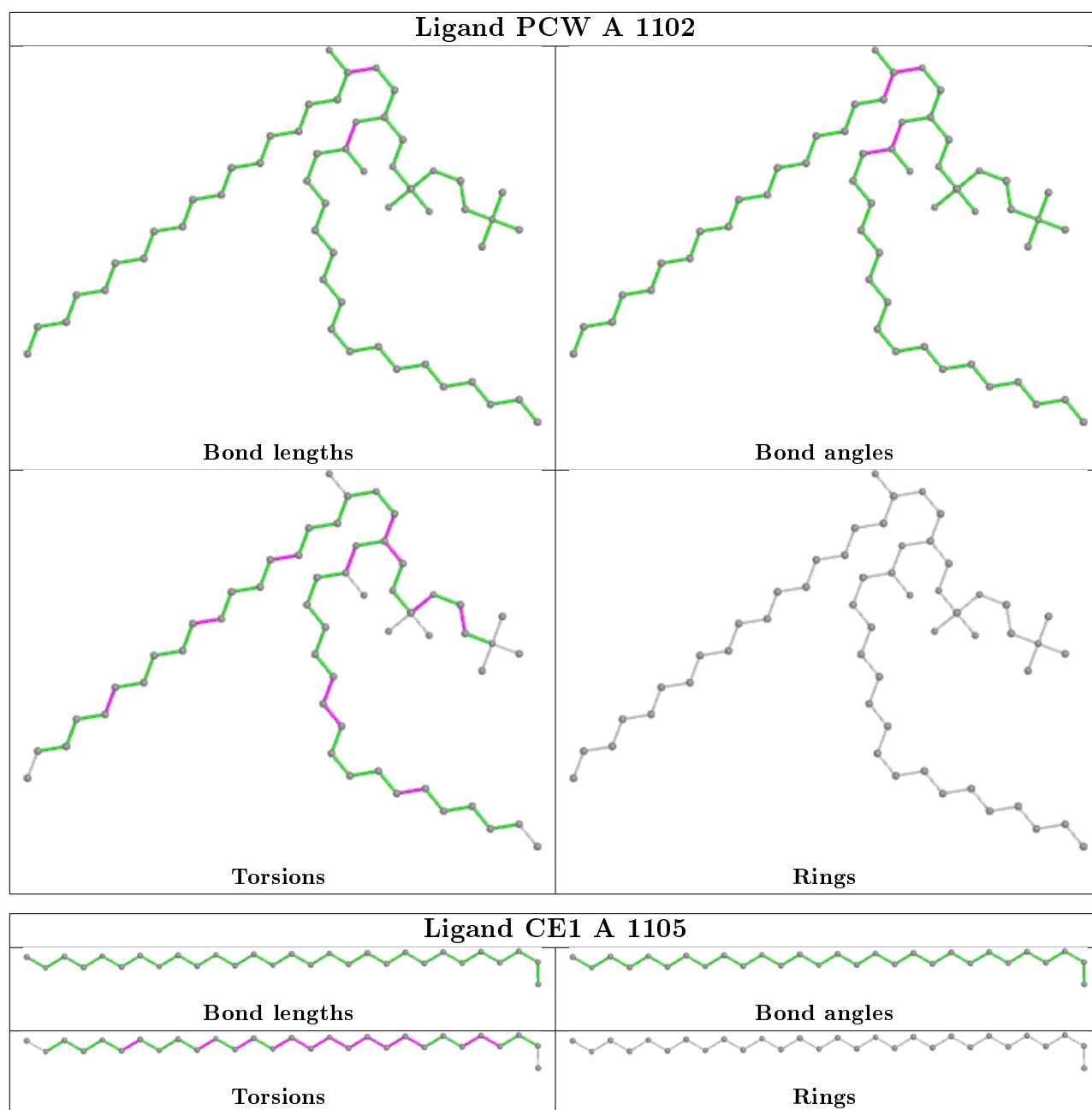
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

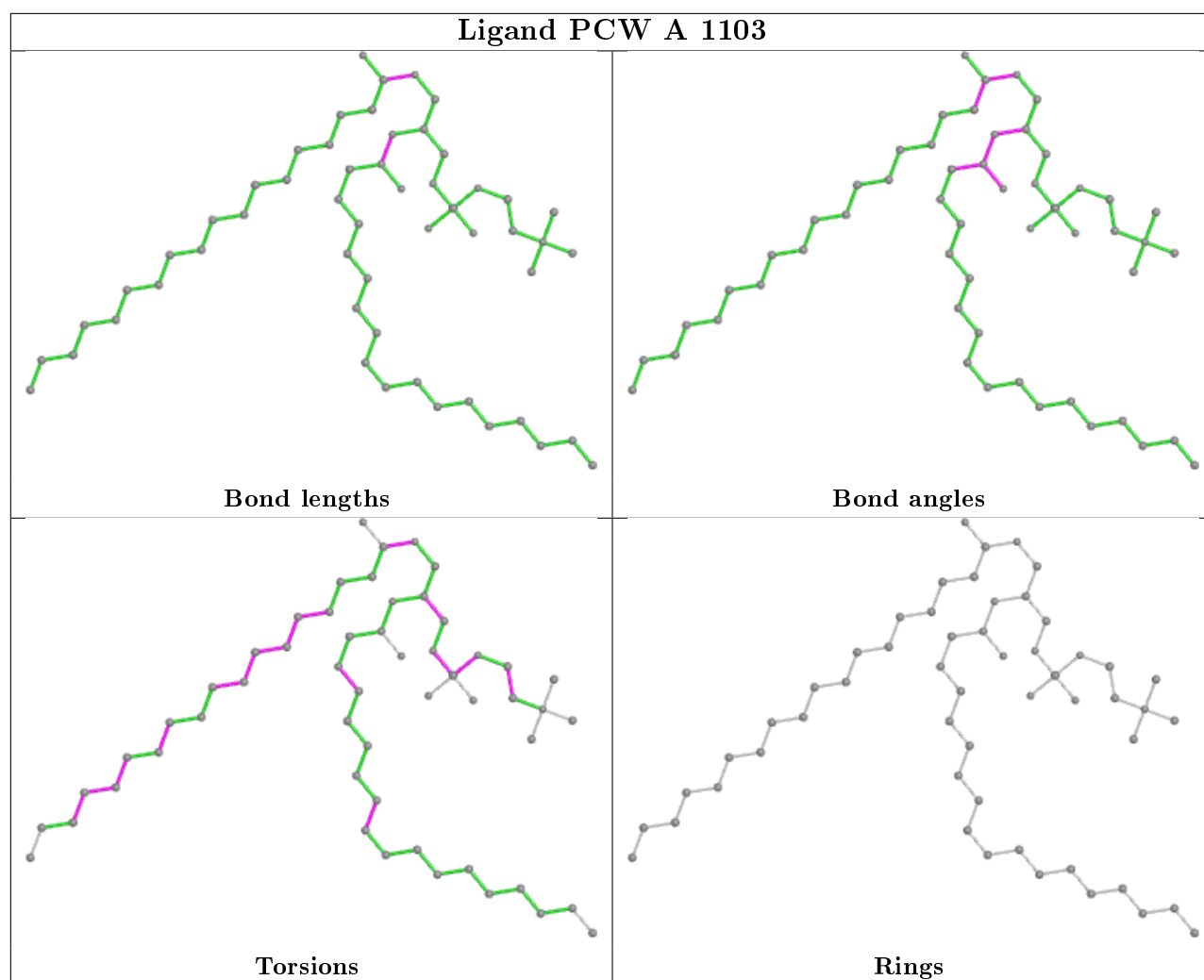




## Ligand HKT A 1101







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	976/1034 (94%)	-0.20	18 (1%) 68 61	20, 37, 70, 115	0
2	B	257/289 (88%)	-0.15	3 (1%) 79 73	26, 45, 71, 113	0
All	All	1233/1323 (93%)	-0.19	21 (1%) 70 63	20, 39, 70, 115	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1024	GLY	5.8
1	A	48	MET	5.7
2	B	34	LEU	4.9
1	A	50	ILE	4.7
1	A	49	GLU	4.3
1	A	174	VAL	3.5
1	A	173	LEU	3.4
1	A	572	LYS	3.1
1	A	132	ASP	2.7
1	A	51	ASN	2.6
2	B	35	SER	2.6
1	A	82	LEU	2.6
2	B	272	ASP	2.6
1	A	94	GLY	2.5
1	A	494	THR	2.5
1	A	172	ASN	2.4
1	A	93	ARG	2.4
1	A	959	PHE	2.4
1	A	538	PRO	2.3
1	A	1023	PRO	2.1
1	A	103	ARG	2.1

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	BFD	A	385	12/13	0.93	0.21	23,26,32,33	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

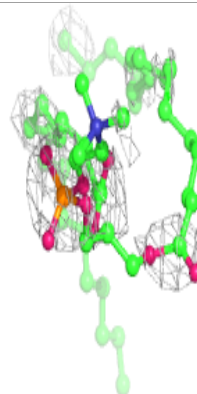
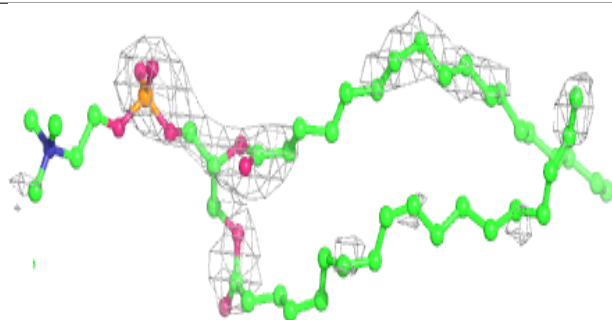
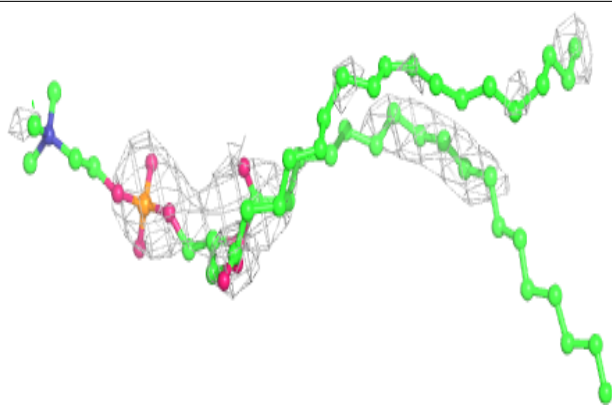
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	B	302	14/15	0.64	0.67	90,99,108,111	0
4	PCW	A	1103	54/54	0.76	0.59	47,84,135,142	0
6	CE1	A	1105	29/37	0.79	0.29	53,72,102,105	0
6	CE1	B	304	19/37	0.85	0.15	40,57,66,67	0
4	PCW	A	1102	54/54	0.85	0.37	48,69,122,133	0
7	NAG	B	303	14/15	0.88	0.21	60,71,75,78	0
3	HKT	A	1101	24/24	0.94	0.15	40,47,51,59	0
7	NAG	B	301	14/15	0.94	0.16	26,35,45,53	0
5	MG	A	1104	1/1	0.99	0.21	56,56,56,56	0

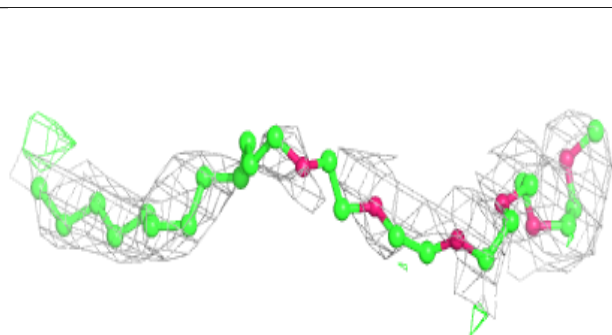
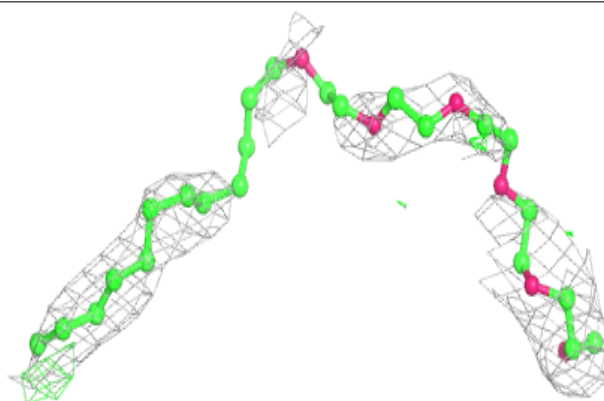
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PCW A 1103:**

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

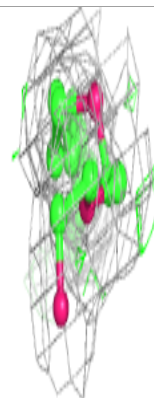
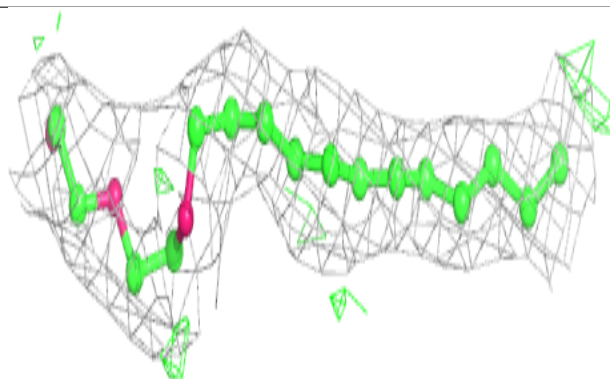
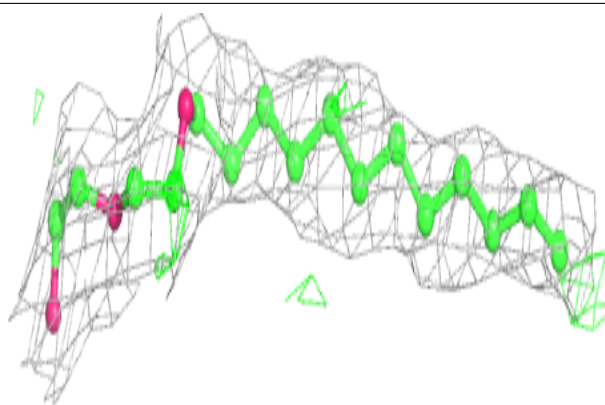
**Electron density around CE1 A 1105:**

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

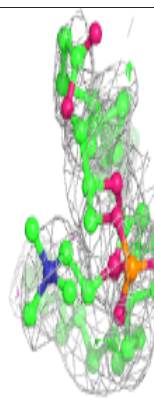
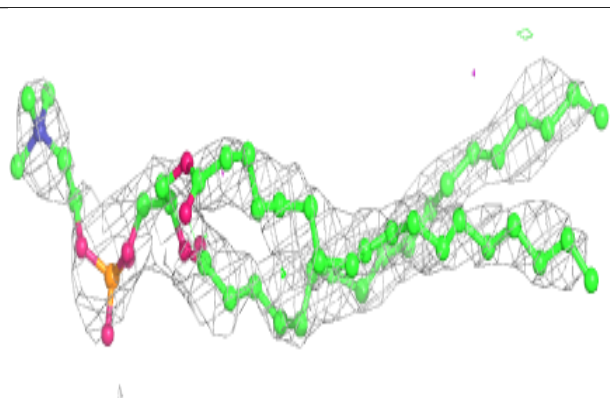
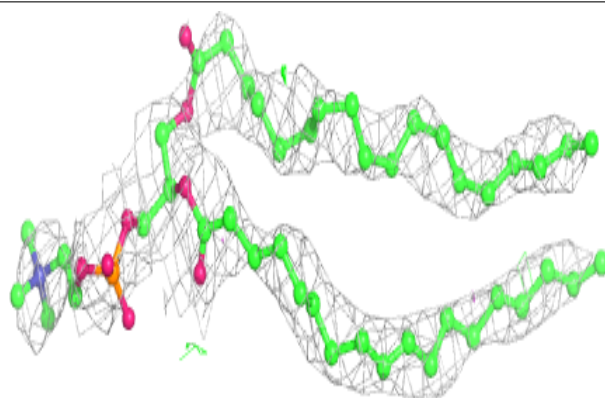


**Electron density around CE1 B 304:**

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

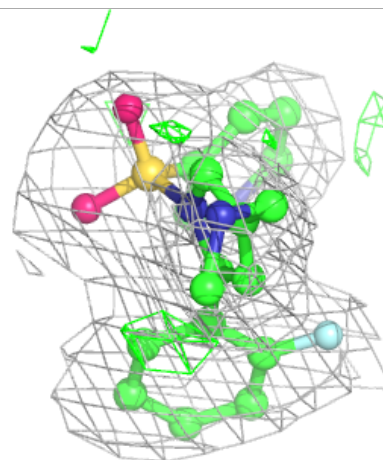
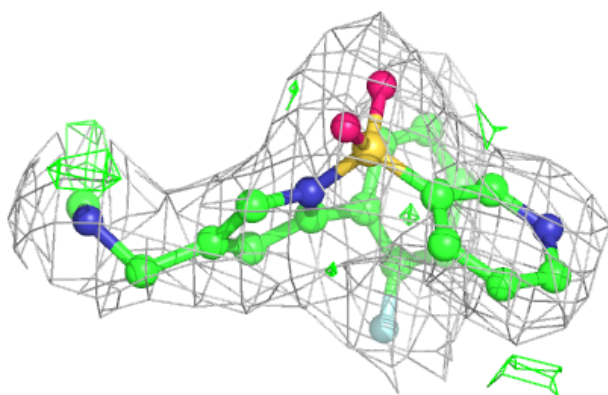
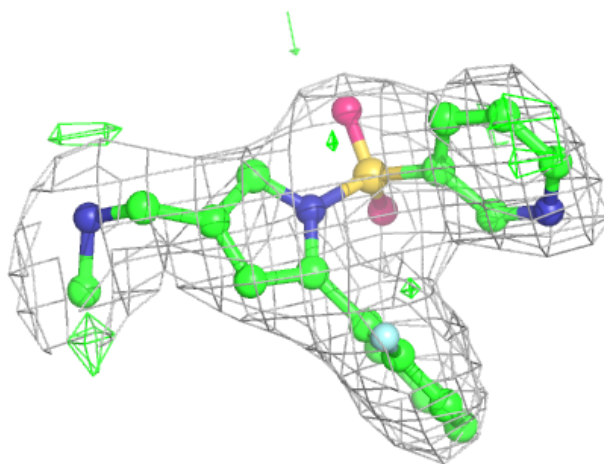
**Electron density around PCW A 1102:**

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



**Electron density around HKT A 1101:**

$2mF_o-DF_c$  (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.