



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:35 AM UTC

PDB ID : 5YLU / pdb_00005ylu
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

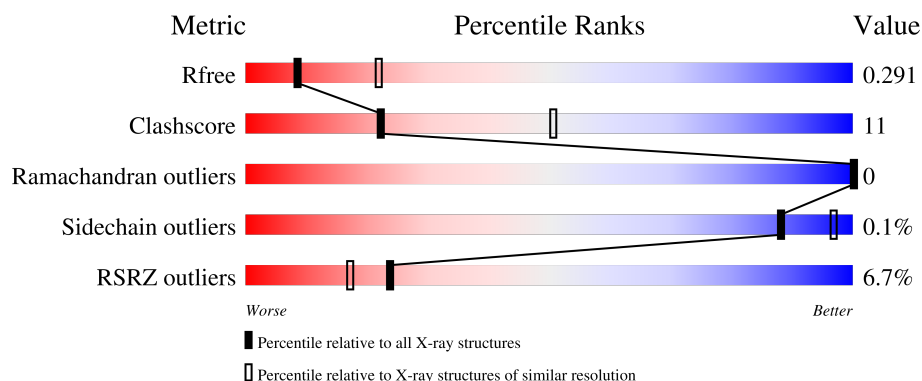
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1034	
2	B	289	

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	-

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			

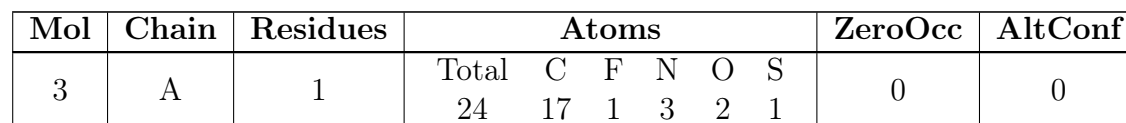
There are 3 discrepancies between the modelled and reference sequences:

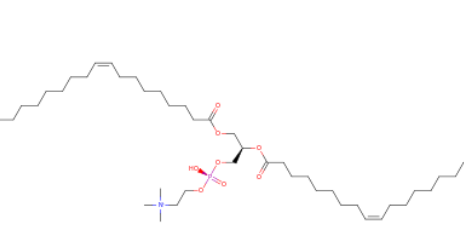
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	CYS	ARG	engineered mutation	UNP P19156
A	593	CYS	SER	engineered mutation	UNP P19156
A	1005	SER	GLY	engineered mutation	UNP P19156

- 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 (CCD ID: HKT) (formula: C₁₇H₁₆FN₃O₂S).



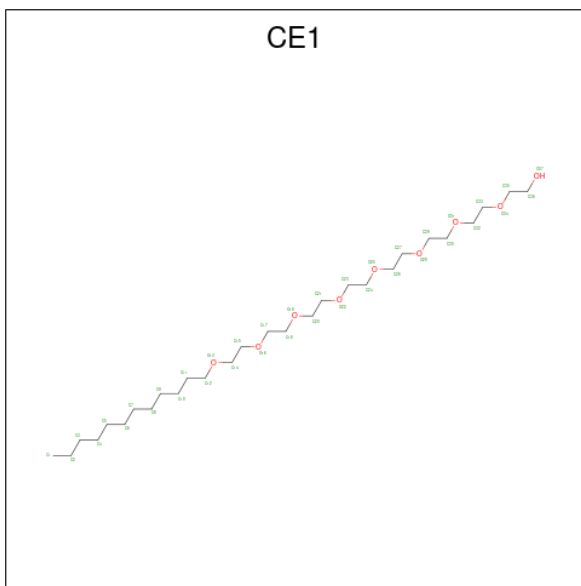
- PCW
- 
- The chemical structure shows a long, wavy hydrocarbon chain with two double bonds, representing a polyunsaturated fatty acid. This chain is esterified to a central carbon atom. This central carbon is also bonded to a phosphate group (PO₄) and a methyl group. The phosphate group is further esterified to a second long, wavy hydrocarbon chain, also containing two double bonds. The entire structure is shown in a perspective view, with the chains extending outwards and the central carbon atom at the junction.

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 (CCD ID: MG) (formula: Mg).

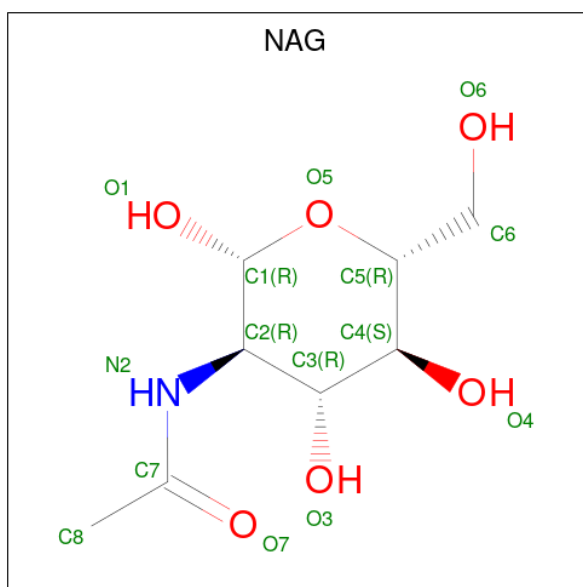
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: C₂₈H₅₈O₉).



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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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		

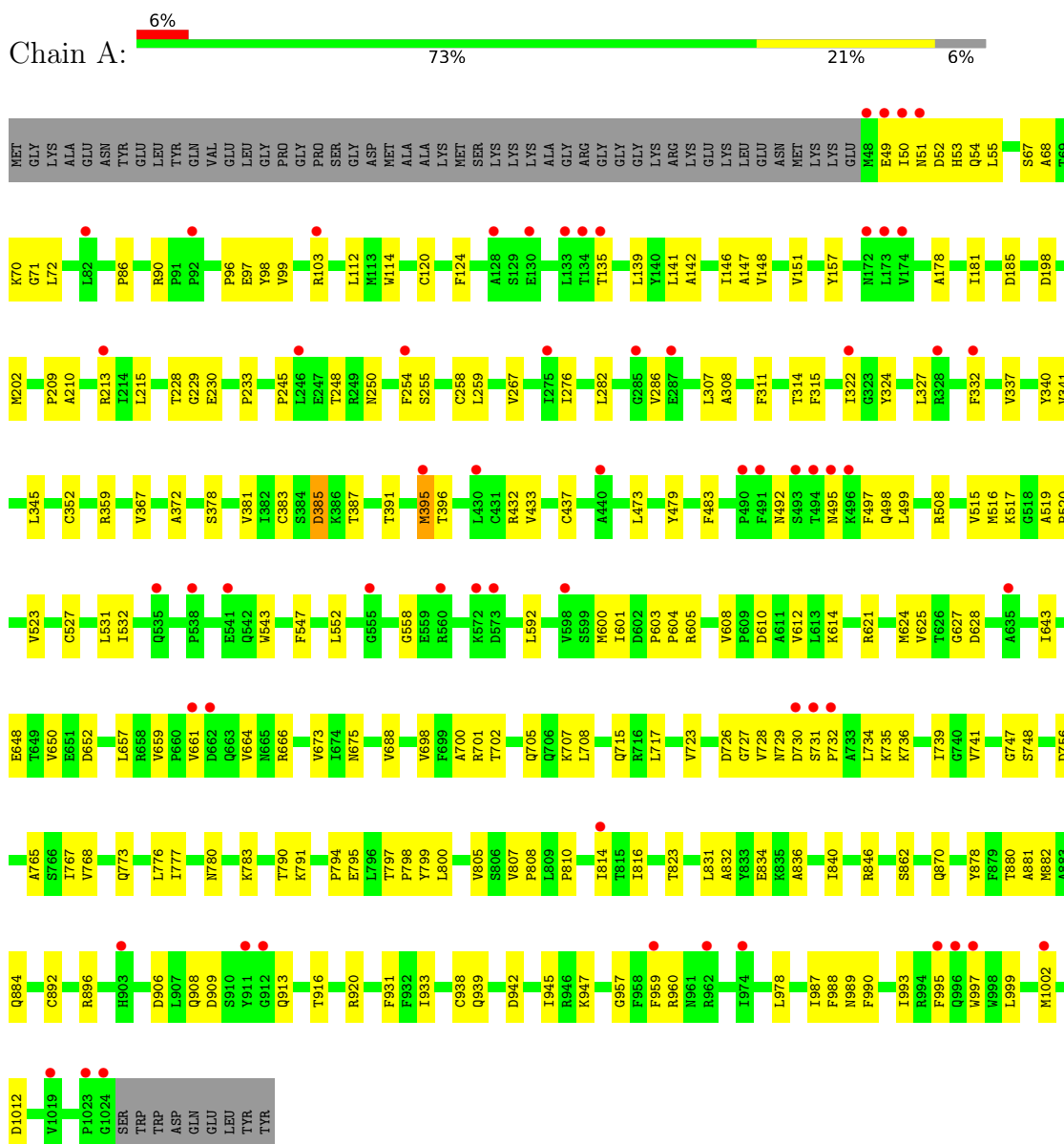
- Molecule 8 is water.

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

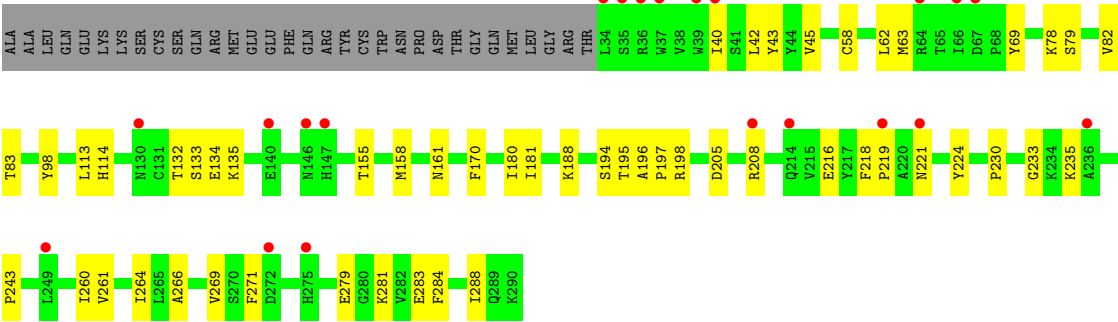
3 Residue-property plots

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: Potassium-transporting ATPase alpha chain 1



- Molecule 2: Potassium-transporting ATPase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 0.239 , 0.291	Depositor DCC
R_{free} test set	2610 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	40.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9884	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HKT, BFD, PCW, NAG, 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	0/7705	0.71	2/10463 (0.0%)
2	B	0.52	1/2125 (0.0%)	0.71	1/2893 (0.0%)
All	All	0.54	1/9830 (0.0%)	0.71	3/13356 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	233	GLY	C-O	-5.58	1.16	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASP	N-CA-C	11.29	123.59	111.28
1	A	823	THR	N-CA-C	6.28	118.20	111.36
2	B	233	GLY	N-CA-C	5.32	117.00	111.95

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	174	0
2	B	2058	0	1993	33	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	210	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 11.

All (210) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:332:PHE:HD1	1:A:799:TYR:HH	1.46	0.63
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: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:527:CYS:HB2	1:A:592:LEU:C	2.28	0.58
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.85	0.58
1:A:67:SER:HG	1:A:71:GLY:H	1.52	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:882:MET:HE3	1:A:892:CYS:SG	2.47	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
1:A:731:SER:HG	1:A:732:PRO:HD3	1.73	0.54
1:A:880:THR:HG22	1:A:997:TRP:CZ3	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:516:MET:HE2	1:A:523:VAL:HG22	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:808:PRO:HG2	1:A:882:MET:HE1	1.91	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:791:LYS:C	1:A:794:PRO:HD2	2.37	0.50
1:A:916:THR:O	1:A:920:ARG:HG3	2.12	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:HG13	1:A:625:VAL:O	2.13	0.49
1:A:202:MET:HE3	1:A:258:CYS:HB2	1.95	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: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:791:LYS:HG2	1:A:939:GLN:CD	2.38	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
2:B:62:LEU:HG	2:B:63:MET:HE2	1.96	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:HB2	1:A:508:ARG:HH11	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: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:CD1	1:A:959:PHE:N	2.85	0.45
1:A:657:LEU:HB3	1:A:659:VAL:HG23	1.98	0.45
1:A:547:PHE:CD1	1:A:547:PHE:C	2.95	0.45
2:B:161:ASN:HB2	2:B:218:PHE:CZ	2.52	0.45
1:A:230:GLU:HA	1:A:628:ASP:OD1	2.17	0.45
1:A:945:ILE:HB	1:A:1012:ASP:OD2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:THR:HG21	4:A:1102:PCW:H472	1.99	0.45
4:A:1102:PCW:H42	4:A:1102:PCW:H63	1.71	0.44
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:HD12	1:A:345:LEU:HA	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:395:MET:SD	1:A:600:MET:HE3	2.57	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:O	1:A:322:ILE:HG22	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:HD12	1:A:708:LEU:O	2.19	0.43
1:A:814:ILE:HD13	1:A:989:ASN:ND2	2.33	0.43
1:A:836:ALA:HB1	1:A:840:ILE:CG1	2.49	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:229:GLY:HA3	1:A:627:GLY:C	2.43	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:HA	1:A:307:LEU:HD23	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
1:A:49:GLU:C	1:A:49:GLU:CD	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:HIS:CE1	2:B:170:PHE:CE1	3.07	0.42
1:A:327:LEU:HD12	1:A:327:LEU:HA	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
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:96:PRO:HD2	1:A:99:VAL:HG11	2.01	0.41
1:A:276:ILE:HA	1:A:276:ILE:HD13	1.86	0.41
1:A:98:TYR:CD1	1:A:98:TYR:C	2.99	0.41
1:A:707:LYS:NZ	1:A:730:ASP:CG	2.73	0.41
1:A:960:ARG:HD3	1:A:960:ARG:N	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:50:ILE:HG22	1:A:54:GLN:NE2	2.30	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:777:ILE:HD12	1:A:777:ILE:HA	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
1:A:135:THR:H	1:A:135:THR:HG23	1.60	0.40
6:A:1105:CE1:C14	6:B:304:CE1:H112	2.51	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:610:ASP:OD1	1:A:614:LYS:NZ	2.54	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	974/1034 (94%)	918 (94%)	56 (6%)	0	100	100
2	B	255/289 (88%)	230 (90%)	25 (10%)	0	100	100
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%)	823 (100%)	1 (0%)	88	97
2	B	224/253 (88%)	224 (100%)	0	100	100
All	All	1048/1122 (93%)	1047 (100%)	1 (0%)	88	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	MET

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

Mol	Chain	Res	Type
1	A	177	GLN
1	A	663	GLN
1	A	753	ASN
1	A	989	ASN
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	5.78	3 (37%)	2,15,17	1.22	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	10.56	1.77	1.54
1	A	385	BFD	F1-BE	8.87	1.74	1.54
1	A	385	BFD	F2-BE	8.52	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 oligosaccharides 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$
3	HKT	A	1101	-	24,26,26	2.31	3 (12%)	31,37,37	3.35	14 (45%)
7	NAG	B	301	2	14,14,15	1.01	1 (7%)	17,19,21	0.94	1 (5%)
4	PCW	A	1102	-	53,53,53	1.00	2 (3%)	59,61,61	0.84	2 (3%)
7	NAG	B	302	2	14,14,15	1.96	2 (14%)	17,19,21	1.52	3 (17%)
7	NAG	B	303	2	14,14,15	0.57	0	17,19,21	1.15	2 (11%)
4	PCW	A	1103	-	53,53,53	1.04	2 (3%)	59,61,61	1.01	4 (6%)
6	CE1	A	1105	-	28,28,36	0.45	0	27,27,35	0.49	0
6	CE1	B	304	-	18,18,36	0.39	0	17,17,35	0.52	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	HKT	A	1101	-	-	1/19/19/19	0/3/3/3
7	NAG	B	301	2	-	4/6/23/26	0/1/1/1
4	PCW	A	1102	-	-	11/57/57/57	-
7	NAG	B	302	2	-	4/6/23/26	0/1/1/1
7	NAG	B	303	2	-	1/6/23/26	0/1/1/1
4	PCW	A	1103	-	-	21/57/57/57	-
6	CE1	A	1105	-	-	13/26/26/34	-
6	CE1	B	304	-	-	4/16/16/34	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	HKT	CAN-SAA	-9.55	1.63	1.76
7	B	302	NAG	C1-C2	6.44	1.61	1.52
4	A	1103	PCW	O3-C11	4.65	1.46	1.33
4	A	1102	PCW	O3-C11	4.49	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
3	A	1101	HKT	CAO-NAI	-3.66	1.34	1.39
3	A	1101	HKT	SAA-NAI	-3.63	1.62	1.69
7	B	301	NAG	O5-C1	-3.30	1.38	1.43
7	B	302	NAG	O5-C1	3.20	1.49	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	HKT	OAD-SAA-OAC	-10.57	103.10	119.59
3	A	1101	HKT	CAO-NAI-CAL	7.35	114.22	108.09
3	A	1101	HKT	CAM-CAL-NAI	5.00	129.21	124.29
3	A	1101	HKT	CAN-SAA-NAI	4.80	109.87	104.56
4	A	1103	PCW	O2-C31-C32	4.78	121.82	111.48
3	A	1101	HKT	CAW-CAR-CAM	-4.36	118.37	123.07
3	A	1101	HKT	CAQ-CAL-NAI	-4.26	104.63	107.02
3	A	1101	HKT	OAD-SAA-CAN	3.80	112.82	108.10
3	A	1101	HKT	OAD-SAA-NAI	3.60	112.10	105.77
3	A	1101	HKT	CAP-CAO-NAI	-3.46	105.70	109.76
7	B	302	NAG	C1-O5-C5	-3.39	107.64	112.19
3	A	1101	HKT	OAC-SAA-CAN	3.32	112.23	108.10
4	A	1102	PCW	O2-C31-C32	3.18	118.37	111.48
4	A	1103	PCW	O3-C11-C12	2.95	120.82	111.83
7	B	302	NAG	O3-C3-C2	-2.88	103.41	109.40
3	A	1101	HKT	CAS-CAM-CAR	2.85	119.86	116.70
7	B	301	NAG	C1-O5-C5	-2.63	108.66	112.19
7	B	302	NAG	C1-C2-N2	2.61	114.55	110.43
3	A	1101	HKT	CAU-CAN-CAT	-2.59	115.99	118.91
7	B	303	NAG	C3-C4-C5	2.57	114.89	110.23
7	B	303	NAG	C1-O5-C5	2.54	115.59	112.19
4	A	1102	PCW	O3-C11-C12	2.46	119.33	111.83
3	A	1101	HKT	CBA-NAJ-CAT	2.44	121.12	116.85
4	A	1103	PCW	C2-O2-C31	-2.37	112.12	117.80
3	A	1101	HKT	CAZ-CAX-CAS	-2.35	117.33	120.24
4	A	1103	PCW	O2-C31-O31	-2.19	118.58	123.70

There are no chirality outliers.

All (59) 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
4	A	1103	PCW	C4-O4P-P-O1P
4	A	1103	PCW	C4-O4P-P-O3P
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
6	A	1105	CE1	C11-C10-C9-C8
6	A	1105	CE1	C7-C8-C9-C10
4	A	1103	PCW	C13-C14-C15-C16
7	B	302	NAG	C4-C5-C6-O6
4	A	1102	PCW	C13-C14-C15-C16
6	A	1105	CE1	O13-C14-C15-O16
4	A	1103	PCW	C14-C15-C16-C17
4	A	1102	PCW	C36-C37-C38-C39
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
4	A	1103	PCW	C16-C17-C18-C19
6	A	1105	CE1	C3-C4-C5-C6
7	B	301	NAG	O5-C5-C6-O6
6	A	1105	CE1	C21-C20-O19-C18
6	A	1105	CE1	C14-C15-O16-C17
4	A	1102	PCW	C41-C42-C43-C44
4	A	1102	PCW	O31-C31-O2-C2
4	A	1103	PCW	O3P-C1-C2-O2
4	A	1102	PCW	C32-C31-O2-C2
6	B	304	CE1	C15-C14-O13-C12
4	A	1103	PCW	O4P-C4-C5-N
6	B	304	CE1	C10-C11-C12-O13
6	A	1105	CE1	C9-C10-C11-C12
7	B	301	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	A	1103	PCW	C15-C16-C17-C18
3	A	1101	HKT	CAO-NAI-SAA-OAD
6	A	1105	CE1	C15-C14-O13-C12
4	A	1103	PCW	C32-C33-C34-C35
4	A	1103	PCW	C22-C23-C24-C25
4	A	1102	PCW	O3P-C1-C2-O2
4	A	1102	PCW	C35-C36-C37-C38
6	B	304	CE1	C9-C10-C11-C12
7	B	301	NAG	C1-C2-N2-C7
4	A	1102	PCW	C1-C2-C3-O3
4	A	1103	PCW	C17-C18-C19-C20
6	B	304	CE1	C3-C4-C5-C6
4	A	1103	PCW	C37-C38-C39-C40
6	A	1105	CE1	C4-C5-C6-C7
7	B	303	NAG	C4-C5-C6-O6
6	A	1105	CE1	C11-C12-O13-C14
6	A	1105	CE1	O22-C23-C24-O25

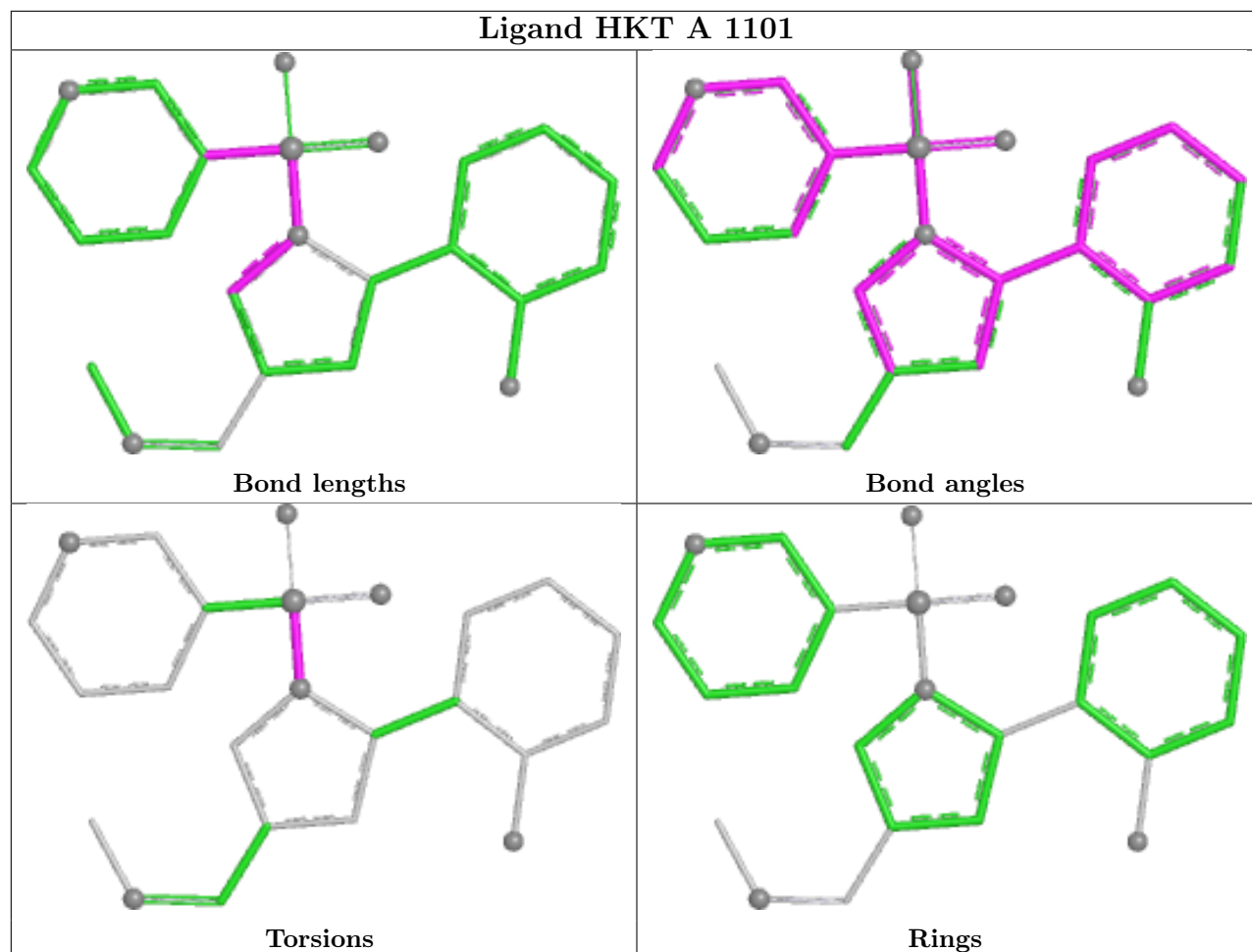
There are no ring outliers.

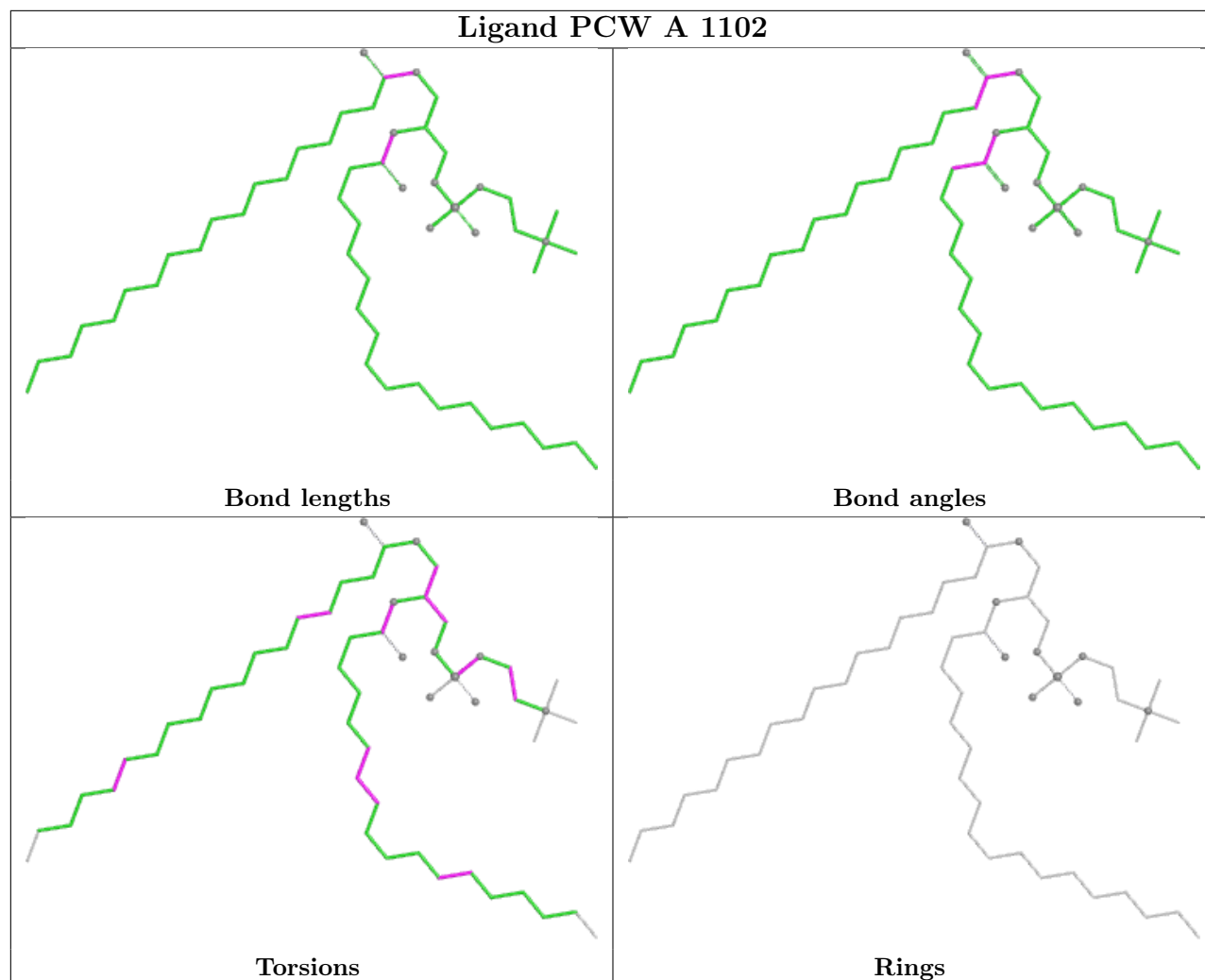
6 monomers are involved in 12 short contacts:

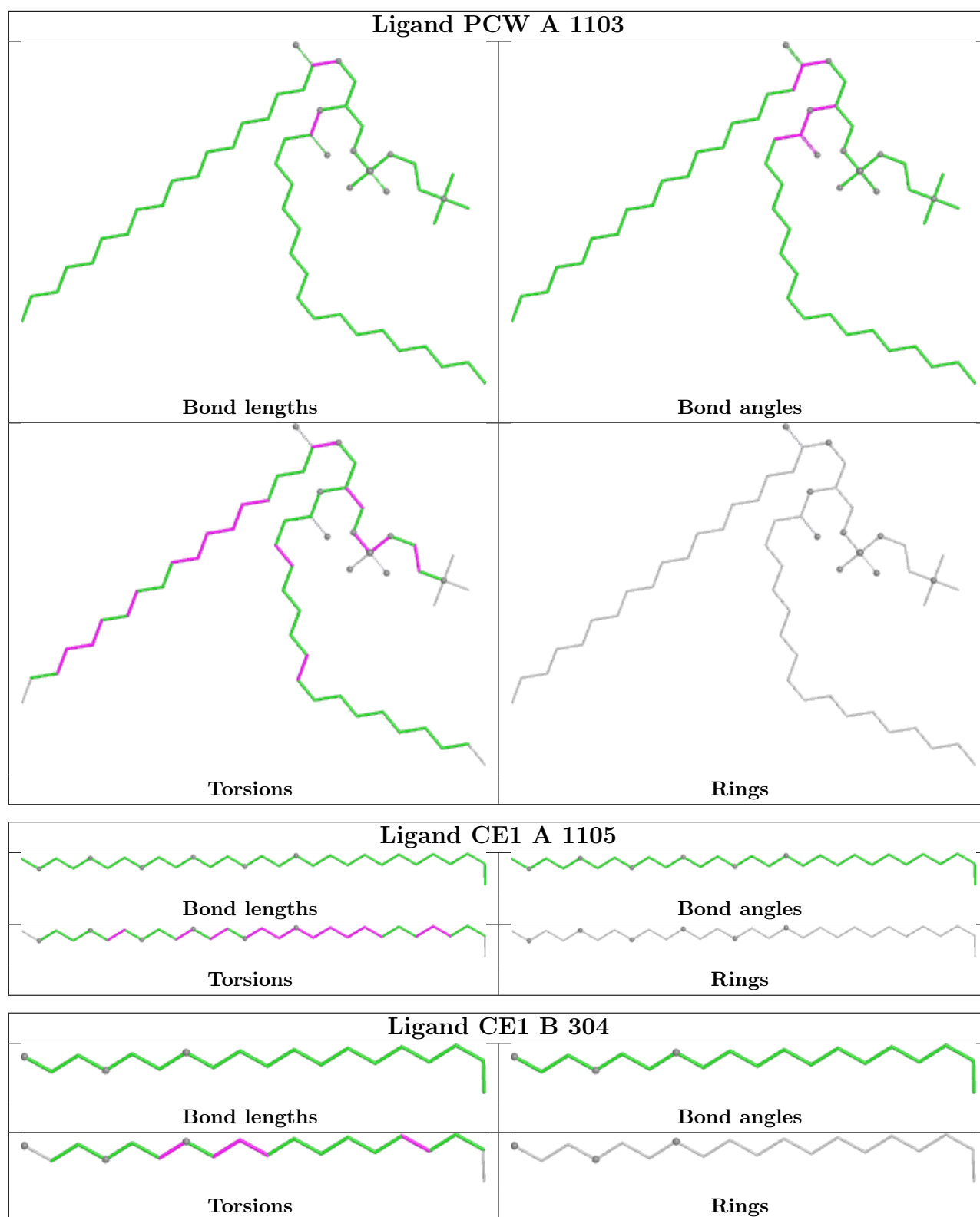
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	PCW	2	0
7	B	302	NAG	1	0
7	B	303	NAG	2	0
4	A	1103	PCW	1	0
6	A	1105	CE1	4	0
6	B	304	CE1	5	0

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 ⓘ

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	976/1034 (94%)	0.51	61 (6%) 26 19	20, 37, 70, 115	0
2	B	257/289 (88%)	0.74	21 (8%) 17 13	26, 45, 71, 113	0
All	All	1233/1323 (93%)	0.56	82 (6%) 24 17	20, 39, 70, 115	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1024	GLY	8.2
1	A	50	ILE	7.2
1	A	49	GLU	7.0
1	A	134	THR	5.7
1	A	133	LEU	5.5
1	A	48	MET	5.2
1	A	730	ASP	5.0
1	A	535	GLN	4.5
1	A	103	ARG	4.5
1	A	51	ASN	4.5
2	B	34	LEU	4.4
1	A	732	PRO	4.3
1	A	135	THR	4.3
2	B	272	ASP	4.0
1	A	213	ARG	3.8
1	A	912	GLY	3.8
1	A	174	VAL	3.7
1	A	173	LEU	3.7
2	B	37	TRP	3.6
2	B	147	HIS	3.6
1	A	572	LYS	3.6
2	B	39	TRP	3.5
1	A	287	GLU	3.4
2	B	130	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	995	PHE	3.2
2	B	40	ILE	3.1
1	A	328	ARG	3.0
1	A	440	ALA	3.0
1	A	1023	PRO	2.9
1	A	814	ILE	2.9
2	B	66	ILE	2.9
1	A	959	PHE	2.8
2	B	35	SER	2.7
1	A	1002	MET	2.7
1	A	332	PHE	2.7
1	A	538	PRO	2.7
1	A	172	ASN	2.6
1	A	246	LEU	2.6
1	A	430	LEU	2.5
1	A	491	PHE	2.5
1	A	254	PHE	2.5
1	A	598	VAL	2.5
1	A	494	THR	2.4
1	A	493	SER	2.4
1	A	541	GLU	2.4
1	A	128	ALA	2.4
1	A	962	ARG	2.4
1	A	997	TRP	2.4
1	A	92	PRO	2.3
1	A	82	LEU	2.3
2	B	221	ASN	2.3
1	A	130	GLU	2.3
2	B	275	HIS	2.3
1	A	662	ASP	2.3
1	A	731	SER	2.3
2	B	67	ASP	2.3
1	A	661	VAL	2.3
2	B	208	ARG	2.2
2	B	249	LEU	2.2
1	A	903	HIS	2.2
2	B	64	ARG	2.2
2	B	146	ASN	2.2
1	A	490	PRO	2.2
1	A	496	LYS	2.2
2	B	140	GLU	2.2
1	A	285	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	395	MET	2.2
1	A	322	ILE	2.2
1	A	573	ASP	2.2
2	B	236	ALA	2.1
1	A	495	ASN	2.1
1	A	275	ILE	2.1
1	A	635	ALA	2.1
1	A	560	ARG	2.1
1	A	996	GLN	2.1
2	B	214	GLN	2.1
1	A	555	GLY	2.1
1	A	911	TYR	2.1
1	A	974	ILE	2.1
2	B	36	ARG	2.1
2	B	219	PRO	2.1
1	A	1019	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	BFD	A	385	12/13	0.91	0.12	23,26,32,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	B	302	14/15	0.21	0.25	90,99,108,111	0

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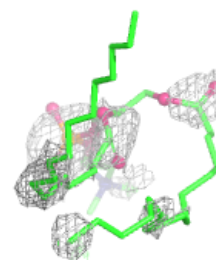
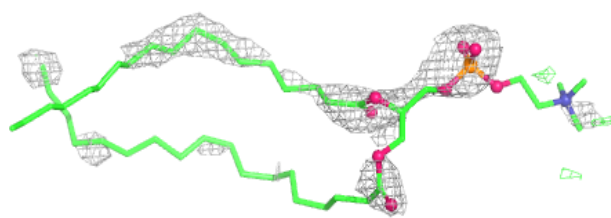
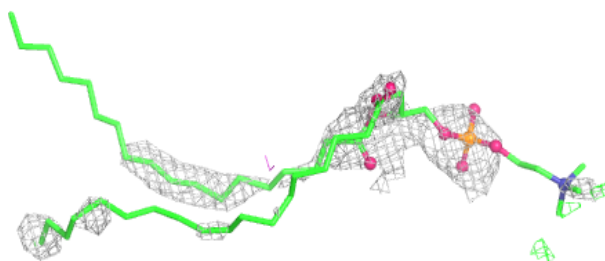
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	B	303	14/15	0.71	0.18	60,71,75,78	0
4	PCW	A	1103	54/54	0.79	0.30	47,84,135,142	0
6	CE1	A	1105	29/37	0.82	0.28	53,72,102,105	0
4	PCW	A	1102	54/54	0.84	0.21	48,69,122,133	0
6	CE1	B	304	19/37	0.86	0.19	40,57,66,67	0
3	HKT	A	1101	24/24	0.89	0.12	40,47,51,59	0
7	NAG	B	301	14/15	0.89	0.14	26,35,45,53	0
5	MG	A	1104	1/1	0.95	0.08	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.

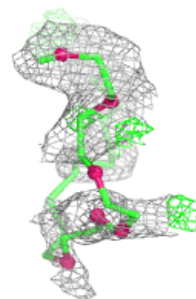
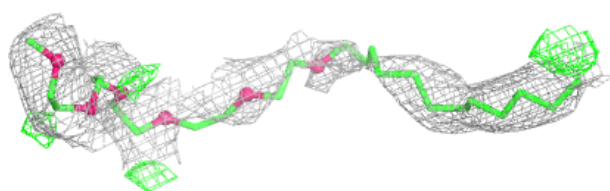
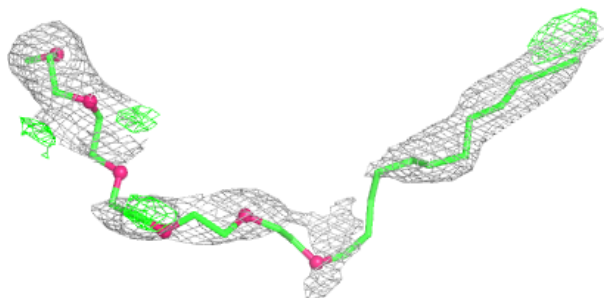
Electron density around PCW A 1103:

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

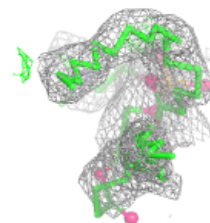
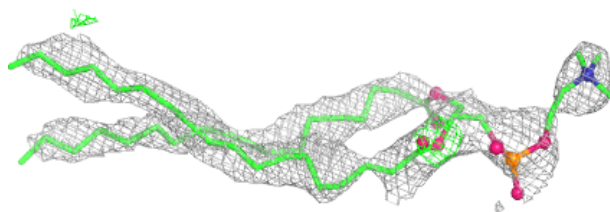
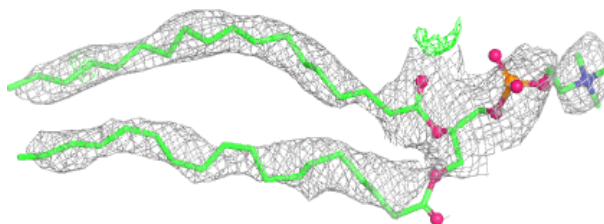


Electron density around CE1 A 1105:

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

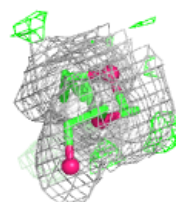
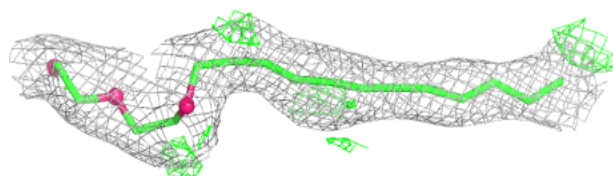
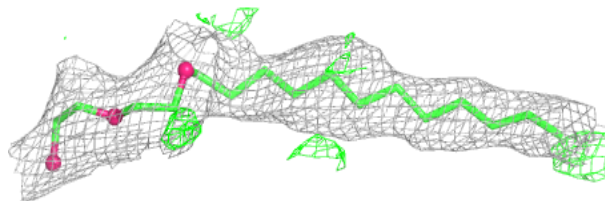
**Electron density around PCW A 1102:**

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



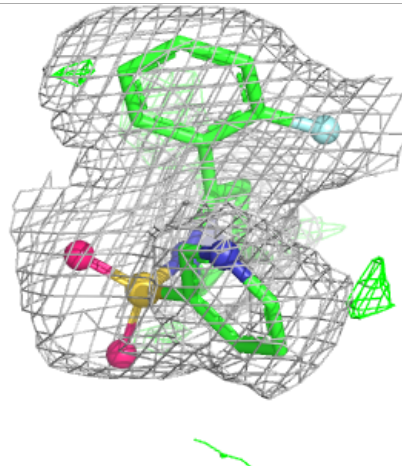
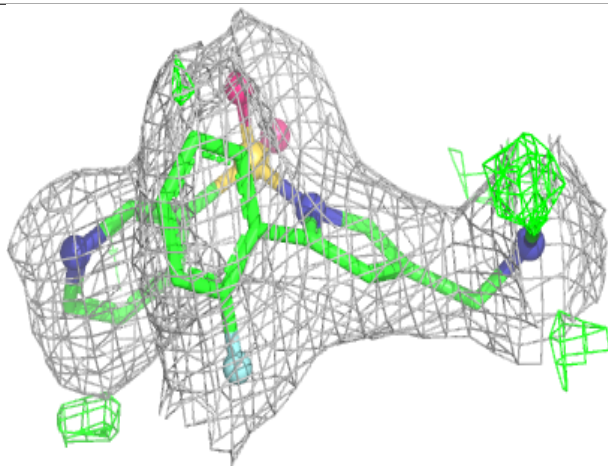
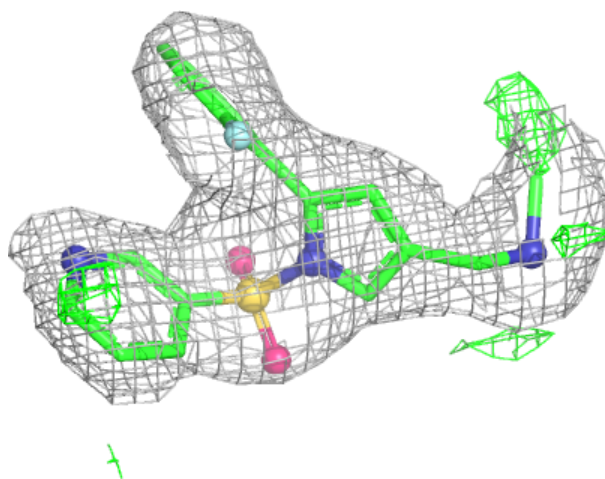
Electron density around CE1 B 304:

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



Electron density around 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 ⓘ

There are no such residues in this entry.