



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 29, 2021 – 12:32 AM JST

PDB ID : 7W48
Title : Crystal structure of the gastric proton pump complexed with PF-03716556
Authors : Abe, K.; Tanaka, S.
Deposited on : 2021-11-26
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.25
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) : 2.25

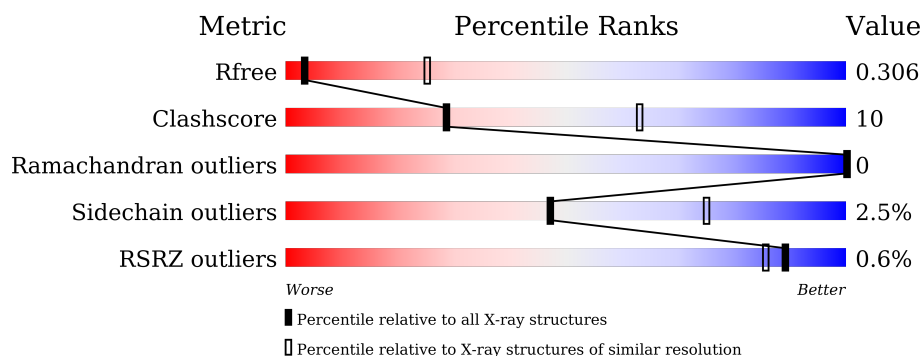
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	 71% 24% 5%
2	B	290	 74% 16% 10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9916 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	987	Total	Be	C	F	N	O	S	0	0	0
			7663	1	4890	3	1292	1423	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

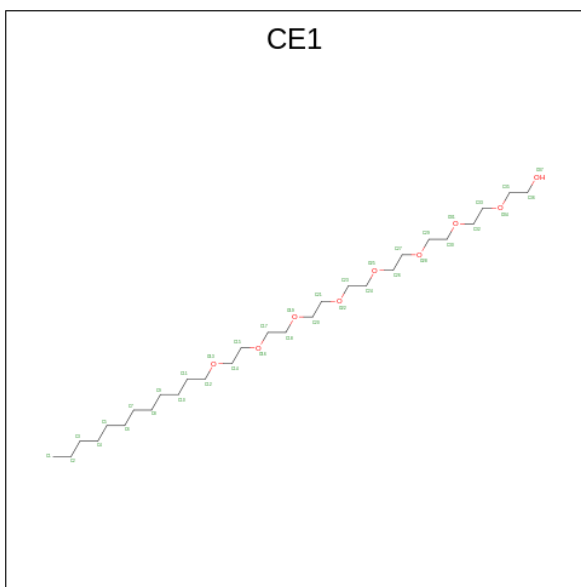
- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2076	1350	341	374	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: C₂₈H₅₈O₉).

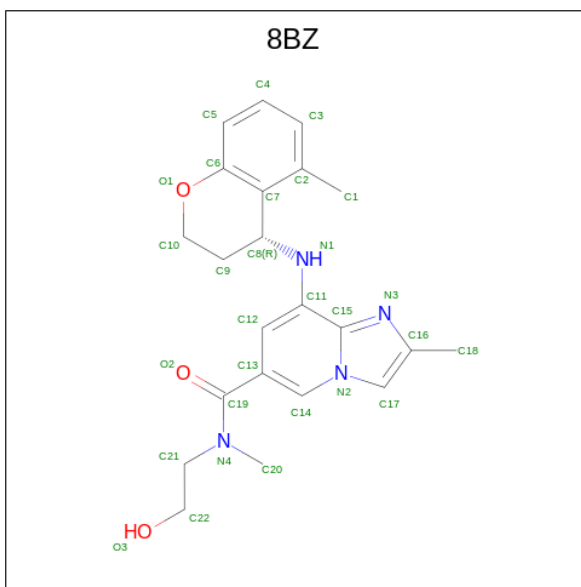


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	23	6		
4	A	1	Total	C	O	0	0
			19	16	3		

- Molecule 5 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

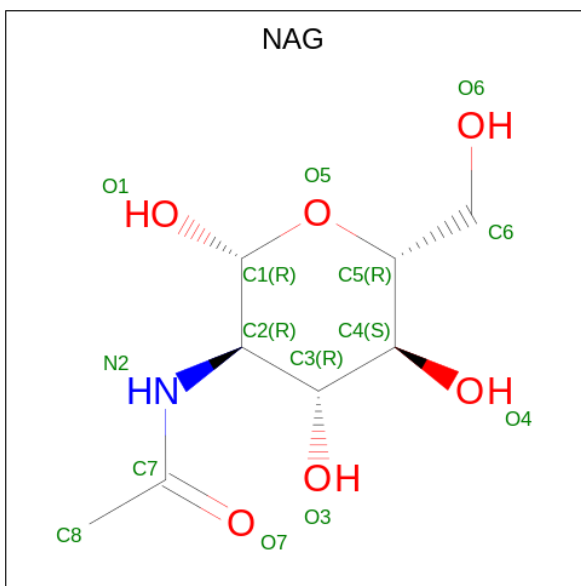
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Rb	0	0
			3	3		

- Molecule 6 is N-(2-hydroxyethyl)-N,2-dimethyl-8-[[[(4R)-5-methyl-3,4-dihydro-2H-chromen-4-yl]amino]imidazo[1,2-a]pyridine-6-carboxamide (three-letter code: 8BZ) (formula: C₂₂H₂₆N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			29	22	4	3		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



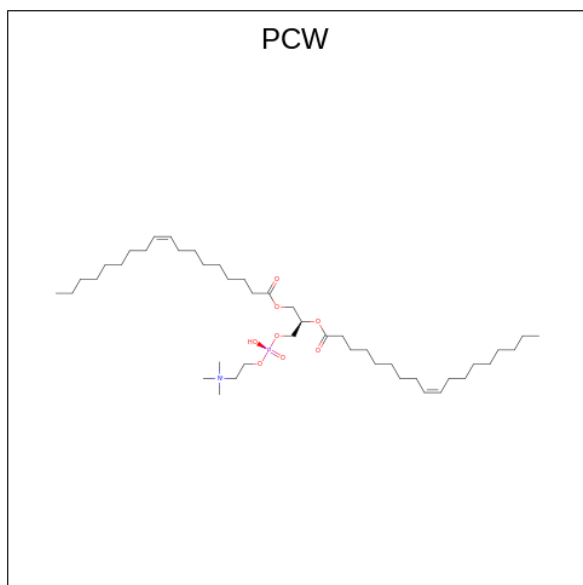
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

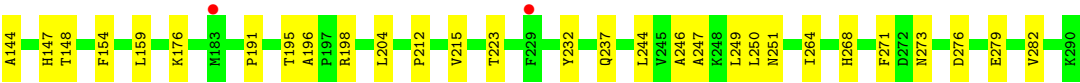
- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



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

- Molecule 1: Potassium-transporting ATPase alpha chain 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.75Å 104.75Å 368.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.18 – 3.50 48.18 – 3.24	Depositor EDS
% Data completeness (in resolution range)	75.4 (48.18-3.50) 61.6 (48.18-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.252 , 0.306 0.252 , 0.306	Depositor DCC
R_{free} test set	1237 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 10.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.128 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9916	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: PCW, MG, NAG, CE1, BFD, 8BZ, RB

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	0.28	0/7808	0.50	1/10604 (0.0%)
2	B	0.28	0/2143	0.52	0/2918
All	All	0.28	0/9951	0.51	1/13522 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	331	VAL	CG1-CB-CG2	6.02	120.53	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	204	LEU	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	7663	0	7683	168	0
2	B	2076	0	2003	28	0
3	A	1	0	0	0	0
4	A	48	0	78	2	0
5	A	3	0	0	0	0
6	A	29	0	0	3	0
7	B	42	0	39	0	0
8	B	54	0	84	3	0
All	All	9916	0	9887	192	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 (192) 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:539:LEU:HD12	1:A:544:ARG:NE	1.86	0.89
1:A:539:LEU:CD1	1:A:544:ARG:NE	2.36	0.87
1:A:1016:LYS:HA	1:A:1019:VAL:HG12	1.61	0.83
2:B:59:ILE:HD11	8:B:304:PCW:H132	1.63	0.81
1:A:328:ARG:HA	1:A:331:VAL:HG12	1.63	0.79
1:A:539:LEU:HD12	1:A:544:ARG:HE	1.48	0.78
1:A:883:ALA:HB1	2:B:66:ILE:HD13	1.68	0.74
1:A:995:PHE:HB2	4:A:1102:CE1:H201	1.71	0.73
1:A:372:ALA:HB1	1:A:739:ILE:HD12	1.70	0.73
1:A:777:ILE:O	1:A:781:LEU:N	2.25	0.68
2:B:212:PRO:O	2:B:251:ASN:ND2	2.27	0.68
1:A:292:PRO:HA	1:A:295:ILE:HD12	1.77	0.66
1:A:524:LEU:HD22	1:A:547:PHE:CD1	2.31	0.65
1:A:854:VAL:HA	1:A:858:LEU:HD23	1.79	0.64
1:A:539:LEU:HD13	1:A:544:ARG:HG2	1.79	0.63
1:A:879:PHE:HB3	1:A:889:PRO:HG3	1.80	0.63
1:A:241:THR:HB	1:A:248:THR:HA	1.81	0.63
1:A:1011:TYR:OH	2:B:43:TYR:OH	2.10	0.63
1:A:812:GLY:HA2	6:A:1107:8BZ:O2	2.00	0.62
1:A:1015:ARG:HA	1:A:1027:TRP:HZ2	1.64	0.61
1:A:792:ASN:ND2	1:A:820:GLU:OE2	2.35	0.60
1:A:236:ARG:NH2	1:A:249:ARG:HA	2.16	0.60
1:A:581:ASP:H	1:A:586:ASN:HD21	1.47	0.60
1:A:581:ASP:H	1:A:586:ASN:ND2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:GLU:HB3	1:A:652:ASP:HB2	1.85	0.59
1:A:331:VAL:HG22	6:A:1107:8BZ:C4	2.33	0.59
1:A:530:ILE:HG12	1:A:532:ILE:HG12	1.85	0.58
1:A:385:BFD:F3	1:A:729:ASN:ND2	2.25	0.58
2:B:191:PRO:HA	2:B:268:HIS:HB2	1.86	0.58
1:A:575:PRO:HD2	1:A:578:TYR:HB2	1.84	0.58
1:A:443:LYS:O	1:A:446:GLN:NE2	2.37	0.58
1:A:925:TYR:C	1:A:991:MET:HE1	2.24	0.57
1:A:539:LEU:HD12	1:A:544:ARG:CZ	2.35	0.57
1:A:902:HIS:O	1:A:905:GLN:NE2	2.38	0.57
1:A:539:LEU:CD1	1:A:544:ARG:HE	2.10	0.57
1:A:398:SER:HB3	1:A:601:ILE:HG22	1.86	0.56
2:B:135:LYS:HG3	2:B:136:TYR:H	1.69	0.56
1:A:280:ALA:O	1:A:284:SER:N	2.32	0.56
1:A:106:ALA:O	1:A:110:GLN:NE2	2.38	0.56
1:A:315:PHE:HA	1:A:318:VAL:HB	1.87	0.56
1:A:616:ARG:NH1	1:A:641:GLY:O	2.32	0.56
2:B:63:MET:HA	2:B:63:MET:HE2	1.88	0.55
1:A:818:PHE:O	1:A:823:THR:HG23	2.06	0.55
1:A:227:LEU:HD21	1:A:276:ILE:HD11	1.87	0.55
1:A:926:THR:N	1:A:991:MET:HE1	2.21	0.55
1:A:699:PHE:HB3	1:A:702:THR:HG21	1.89	0.55
1:A:809:LEU:HD21	6:A:1107:8BZ:O2	2.06	0.55
1:A:945:ILE:HG12	1:A:1012:ASP:HB3	1.89	0.54
1:A:186:LYS:NZ	1:A:201:GLU:OE1	2.34	0.54
1:A:634:LYS:NZ	1:A:652:ASP:OD2	2.40	0.54
1:A:993:ILE:HG12	1:A:997:TRP:HE3	1.73	0.54
1:A:400:LEU:HG	1:A:598:VAL:HG13	1.91	0.52
1:A:704:PRO:HG3	1:A:729:ASN:HA	1.90	0.52
1:A:280:ALA:HA	1:A:283:ALA:HB3	1.91	0.52
1:A:794:PRO:HG3	1:A:870:GLN:HB2	1.91	0.52
1:A:308:ALA:HB1	1:A:337:VAL:HA	1.91	0.52
1:A:426:THR:HG23	1:A:531:LEU:HB3	1.90	0.52
1:A:124:PHE:HD2	1:A:135:THR:HG22	1.75	0.52
1:A:673:VAL:HG13	1:A:698:VAL:HG12	1.92	0.52
1:A:375:THR:O	1:A:379:THR:OG1	2.21	0.52
2:B:176:LYS:HA	2:B:249:LEU:O	2.09	0.52
1:A:357:ALA:HB2	1:A:373:VAL:HG21	1.92	0.52
1:A:779:ASP:O	1:A:783:LYS:HG3	2.09	0.52
2:B:271:PHE:HA	2:B:279:GLU:O	2.10	0.51
1:A:676:GLY:O	1:A:706:GLN:NE2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:VAL:HG13	1:A:737:ALA:HB2	1.91	0.51
2:B:144:ALA:HB3	2:B:148:THR:C	2.31	0.51
1:A:761:ASP:N	1:A:761:ASP:OD1	2.43	0.51
1:A:927:CYS:HA	1:A:930:VAL:HG12	1.93	0.51
1:A:981:CYS:SG	1:A:982:PRO:HD2	2.51	0.51
1:A:925:TYR:O	1:A:928:TYR:HB2	2.11	0.51
2:B:82:VAL:HG23	2:B:282:VAL:HG13	1.92	0.50
1:A:935:ILE:O	1:A:939:GLN:N	2.38	0.50
2:B:59:ILE:HA	2:B:62:LEU:HB3	1.93	0.50
1:A:315:PHE:CD2	1:A:800:LEU:HD22	2.46	0.50
1:A:781:LEU:O	1:A:785:ILE:N	2.32	0.50
1:A:136:ASP:HB3	1:A:140:TYR:CE2	2.46	0.50
1:A:882:MET:O	1:A:887:TRP:N	2.40	0.50
1:A:61:GLU:HB2	1:A:66:THR:O	2.11	0.50
1:A:120:CYS:HB3	1:A:142:ALA:HB2	1.94	0.50
1:A:812:GLY:O	1:A:816:ILE:HG23	2.12	0.49
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.95	0.49
1:A:213:ARG:NH1	1:A:214:ILE:O	2.46	0.49
1:A:516:MET:HB3	1:A:565:CYS:SG	2.53	0.49
2:B:82:VAL:HG11	2:B:264:ILE:HD13	1.94	0.48
1:A:356:THR:CG2	1:A:773:GLN:HB3	2.43	0.48
1:A:796:LEU:HG	1:A:800:LEU:HG	1.96	0.48
2:B:195:THR:HG22	2:B:196:ALA:H	1.78	0.48
1:A:427:TRP:CZ2	1:A:431:CYS:HB2	2.49	0.48
1:A:539:LEU:HD13	1:A:539:LEU:O	2.13	0.48
1:A:581:ASP:N	1:A:586:ASN:HD21	2.12	0.48
1:A:245:PRO:HA	1:A:248:THR:HG22	1.95	0.48
1:A:180:VAL:HG23	1:A:200:VAL:HG12	1.96	0.47
1:A:511:ARG:HB2	1:A:569:LEU:O	2.14	0.47
1:A:391:THR:HA	1:A:604:PRO:HA	1.95	0.47
1:A:1000:VAL:HA	4:A:1102:CE1:H51	1.96	0.47
2:B:176:LYS:HG2	2:B:250:LEU:HA	1.96	0.47
1:A:891:LEU:HG	1:A:895:LEU:HD12	1.97	0.47
1:A:731:SER:HA	1:A:734:LEU:HB2	1.96	0.47
1:A:870:GLN:HG2	1:A:938:CYS:HB3	1.96	0.47
1:A:412:THR:HB	1:A:606:ALA:HB2	1.96	0.47
1:A:916:THR:HG21	2:B:276:ASP:OD2	2.15	0.47
1:A:407:HIS:HB3	1:A:420:PHE:HB2	1.96	0.46
2:B:129:ILE:HD11	2:B:131:CYS:SG	2.54	0.46
1:A:875:PHE:CD2	8:B:304:PCW:H432	2.50	0.46
1:A:777:ILE:HA	1:A:780:ASN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:TYR:HB2	1:A:961:ASN:HD21	1.80	0.46
1:A:367:VAL:HG11	1:A:373:VAL:HG23	1.97	0.46
1:A:769:THR:O	1:A:773:GLN:HG2	2.15	0.46
1:A:581:ASP:O	1:A:586:ASN:ND2	2.48	0.46
1:A:858:LEU:HB2	1:A:1033:TYR:HB2	1.98	0.46
1:A:961:ASN:HB3	1:A:964:LEU:HB3	1.97	0.46
1:A:528:SER:OG	1:A:591:GLY:HA2	2.15	0.46
1:A:563:GLY:HA2	1:A:597:LEU:HD23	1.97	0.46
2:B:45:VAL:O	2:B:49:VAL:HG13	2.16	0.46
1:A:210:ALA:HA	1:A:254:PHE:HD1	1.81	0.45
1:A:317:ILE:HD13	1:A:317:ILE:HA	1.86	0.45
1:A:716:ARG:HB2	1:A:716:ARG:CZ	2.46	0.45
1:A:649:THR:HG22	1:A:652:ASP:OD2	2.17	0.45
1:A:734:LEU:HD22	1:A:755:ALA:HB2	1.99	0.45
1:A:489:ILE:HD12	1:A:499:LEU:HD22	1.98	0.45
1:A:291:THR:HG21	1:A:371:GLU:HB3	1.99	0.44
1:A:587:PHE:HB2	1:A:588:PRO:HD2	2.00	0.44
1:A:802:TYR:CE2	1:A:896:ARG:HG3	2.53	0.44
1:A:308:ALA:O	1:A:337:VAL:HG12	2.18	0.44
1:A:427:TRP:CH2	1:A:431:CYS:HB2	2.52	0.44
1:A:141:LEU:HD12	1:A:817:LEU:HD11	2.00	0.44
1:A:330:MET:O	1:A:333:PHE:HB3	2.18	0.44
1:A:383:CYS:O	1:A:723:VAL:HA	2.17	0.44
1:A:778:PHE:CZ	1:A:846:ARG:HD3	2.53	0.43
1:A:218:GLN:HB2	1:A:262:THR:HG23	2.00	0.43
1:A:372:ALA:HA	1:A:375:THR:OG1	2.19	0.43
1:A:879:PHE:CZ	8:B:304:PCW:H372	2.53	0.43
2:B:147:HIS:O	2:B:147:HIS:CG	2.72	0.43
2:B:198:ARG:HG2	2:B:223:THR:HG22	1.99	0.43
2:B:159:LEU:HD22	2:B:246:ALA:HB2	2.00	0.43
1:A:235:THR:C	1:A:236:ARG:HD2	2.39	0.43
1:A:813:CYS:HA	1:A:816:ILE:HG12	2.00	0.43
1:A:956:GLN:HB3	1:A:960:ARG:HD2	2.00	0.43
2:B:215:VAL:HG11	2:B:247:ALA:HB1	2.00	0.43
1:A:858:LEU:HD13	1:A:1033:TYR:HB2	2.00	0.43
2:B:232:TYR:HB2	2:B:237:GLN:NE2	2.34	0.43
1:A:225:SER:OG	1:A:393:ASN:ND2	2.47	0.43
1:A:659:VAL:HG12	1:A:660:PRO:HD2	2.00	0.43
1:A:797:THR:N	1:A:798:PRO:HD2	2.33	0.43
1:A:799:TYR:HA	1:A:802:TYR:HB3	2.00	0.43
1:A:1015:ARG:HG3	1:A:1031:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PHE:HA	1:A:303:ILE:HB	1.99	0.43
1:A:449:VAL:HG13	1:A:454:ARG:HG2	2.00	0.43
1:A:585:MET:SD	1:A:589:THR:HG21	2.59	0.42
1:A:559:GLU:HG2	1:A:601:ILE:HB	1.99	0.42
2:B:154:PHE:CE1	2:B:244:LEU:HB2	2.54	0.42
1:A:446:GLN:OE1	1:A:455:ILE:HD12	2.19	0.42
1:A:993:ILE:HG12	1:A:997:TRP:CE3	2.53	0.42
1:A:539:LEU:CD1	1:A:539:LEU:O	2.67	0.42
1:A:745:ILE:HB	1:A:762:ASP:OD2	2.19	0.42
1:A:824:ASP:OD2	1:A:939:GLN:NE2	2.46	0.42
1:A:376:LEU:O	1:A:771:VAL:HG22	2.20	0.42
1:A:276:ILE:HD13	1:A:728:VAL:HG21	2.01	0.42
1:A:811:LEU:HG	1:A:816:ILE:HG22	2.01	0.42
1:A:853:LEU:HA	1:A:853:LEU:HD23	1.80	0.42
1:A:963:ILE:H	1:A:963:ILE:HD12	1.84	0.42
2:B:46:ALA:HA	2:B:49:VAL:HG22	2.01	0.42
1:A:376:LEU:HD12	1:A:770:GLY:HA3	2.02	0.42
1:A:1013:GLU:O	1:A:1017:LEU:N	2.50	0.42
1:A:1015:ARG:HA	1:A:1027:TRP:CZ2	2.50	0.41
1:A:296:GLU:HB3	1:A:853:LEU:HB2	2.03	0.41
1:A:178:ALA:HB2	1:A:209:PRO:CB	2.50	0.41
1:A:887:TRP:HH2	1:A:915:TRP:CD2	2.37	0.41
1:A:127:GLN:HB3	1:A:132:ASP:HB2	2.02	0.41
1:A:907:LEU:HD12	1:A:908:GLN:H	1.86	0.41
1:A:388:GLY:HA3	1:A:726:ASP:OD2	2.21	0.41
1:A:539:LEU:CD1	1:A:544:ARG:CD	2.98	0.41
1:A:328:ARG:CZ	1:A:328:ARG:HB2	2.50	0.41
1:A:799:TYR:CE2	1:A:803:ILE:HD11	2.55	0.41
1:A:884:GLN:HG2	2:B:73:TYR:HD1	1.85	0.41
1:A:370:LEU:O	1:A:373:VAL:HB	2.20	0.41
1:A:525:GLU:HG3	1:A:526:ARG:HG3	2.03	0.41
1:A:654:ALA:HB2	1:A:664:VAL:HG21	2.03	0.41
1:A:723:VAL:CG2	1:A:734:LEU:HA	2.51	0.41
1:A:945:ILE:HD12	1:A:945:ILE:HA	1.92	0.41
2:B:249:LEU:HD23	2:B:249:LEU:HA	1.93	0.41
1:A:790:THR:HG22	1:A:862:SER:HB3	2.03	0.40
1:A:124:PHE:CG	1:A:139:LEU:HD21	2.56	0.40
1:A:231:SER:HB3	1:A:387:THR:HG23	2.02	0.40
1:A:431:CYS:SG	1:A:473:LEU:HD12	2.61	0.40
1:A:786:ALA:HB2	1:A:858:LEU:HD11	2.03	0.40
2:B:273:ASN:ND2	2:B:276:ASP:HB3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:O	1:A:286:VAL:HG23	2.21	0.40
1:A:991:MET:HB2	1:A:991:MET:HE3	1.73	0.40
1:A:398:SER:OG	1:A:399:HIS:N	2.55	0.40
1:A:855:ASN:OD1	1:A:855:ASN:N	2.53	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	984/1034 (95%)	951 (97%)	33 (3%)	0	100	100
2	B	259/290 (89%)	237 (92%)	22 (8%)	0	100	100
All	All	1243/1324 (94%)	1188 (96%)	55 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	833/869 (96%)	809 (97%)	24 (3%)	42	71
2	B	224/254 (88%)	222 (99%)	2 (1%)	78	90
All	All	1057/1123 (94%)	1031 (98%)	26 (2%)	47	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	ARG
1	A	98	TYR
1	A	124	PHE
1	A	129	SER
1	A	198	ASP
1	A	202	MET
1	A	216	GLN
1	A	226	SER
1	A	236	ARG
1	A	244	SER
1	A	316	PHE
1	A	354	SER
1	A	431	CYS
1	A	439	ARG
1	A	516	MET
1	A	547	PHE
1	A	586	ASN
1	A	822	CYS
1	A	826	PHE
1	A	849	LYS
1	A	852	ARG
1	A	853	LEU
1	A	931	PHE
1	A	981	CYS
2	B	37	TRP
2	B	39	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	ASN
1	A	586	ASN
2	B	251	ASN

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	8,11,12	5.59	3 (37%)	3,15,17	0.96	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	-	3/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	385	BFD	F3-BE	9.31	1.76	1.54
1	A	385	BFD	F2-BE	8.99	1.76	1.54
1	A	385	BFD	F1-BE	8.89	1.75	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	385	BFD	O-C-CA-CB
1	A	385	BFD	CA-CB-CG-OD2
1	A	385	BFD	CA-CB-CG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	8BZ	A	1107	-	29,32,32	1.19	2 (6%)	32,46,46	3.43	13 (40%)
7	NAG	B	303	2	14,14,15	0.56	0	17,19,21	1.00	1 (5%)
7	NAG	B	302	2	14,14,15	1.64	2 (14%)	17,19,21	1.22	2 (11%)
8	PCW	B	304	-	53,53,53	0.94	2 (3%)	59,61,61	0.95	3 (5%)
4	CE1	A	1106	-	18,18,36	0.32	0	17,17,35	0.53	0
4	CE1	A	1102	-	28,28,36	0.36	0	27,27,35	0.55	0
7	NAG	B	301	2	14,14,15	0.31	0	17,19,21	0.70	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	8BZ	A	1107	-	-	12/15/25/25	0/4/4/4
7	NAG	B	303	2	-	2/6/23/26	0/1/1/1
7	NAG	B	302	2	-	4/6/23/26	0/1/1/1
8	PCW	B	304	-	-	20/57/57/57	-
4	CE1	A	1106	-	-	4/16/16/34	-
4	CE1	A	1102	-	-	13/26/26/34	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	301	2	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	302	NAG	C1-C2	5.45	1.60	1.52
6	A	1107	8BZ	C11-C15	4.60	1.50	1.42
8	B	304	PCW	O2-C31	4.15	1.46	1.34
8	B	304	PCW	O3-C11	4.14	1.45	1.33
6	A	1107	8BZ	C15-N3	3.39	1.36	1.33
7	B	302	NAG	C3-C2	2.15	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1107	8BZ	C15-C11-N1	13.22	125.30	116.74
6	A	1107	8BZ	C18-C16-N3	6.20	134.36	119.98
6	A	1107	8BZ	C10-O1-C6	5.57	123.26	113.65
6	A	1107	8BZ	C18-C16-C17	-5.16	115.49	129.07
6	A	1107	8BZ	C12-C11-N1	-4.25	115.41	121.96
6	A	1107	8BZ	C13-C19-N4	3.86	124.57	118.54
6	A	1107	8BZ	C7-C8-N1	3.82	116.16	110.48
7	B	303	NAG	C1-O5-C5	3.60	117.07	112.19
7	B	302	NAG	C4-C3-C2	3.59	116.28	111.02
6	A	1107	8BZ	C1-C2-C3	-3.44	113.60	120.31
8	B	304	PCW	O2-C31-C32	3.37	118.75	111.50
8	B	304	PCW	O3-C11-C12	3.06	121.51	111.91
6	A	1107	8BZ	O2-C19-C13	-2.94	114.51	120.23
7	B	302	NAG	O5-C5-C4	-2.90	103.76	110.83
7	B	301	NAG	C1-O5-C5	2.47	115.53	112.19
8	B	304	PCW	O3-C11-O11	-2.39	117.55	123.59
6	A	1107	8BZ	C1-C2-C7	2.36	126.37	122.80
6	A	1107	8BZ	O1-C10-C9	-2.23	105.83	111.86
6	A	1107	8BZ	C21-N4-C19	2.19	126.06	120.32
6	A	1107	8BZ	C6-C7-C8	-2.16	116.11	119.77

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1107	8BZ	C12-C11-N1-C8

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Mol	Chain	Res	Type	Atoms
6	A	1107	8BZ	C15-C11-N1-C8
6	A	1107	8BZ	C14-C13-C19-N4
6	A	1107	8BZ	C14-C13-C19-O2
6	A	1107	8BZ	C13-C19-N4-C20
6	A	1107	8BZ	C13-C19-N4-C21
6	A	1107	8BZ	O2-C19-N4-C20
6	A	1107	8BZ	O2-C19-N4-C21
6	A	1107	8BZ	C22-C21-N4-C19
6	A	1107	8BZ	C22-C21-N4-C20
8	B	304	PCW	C1-O3P-P-O2P
8	B	304	PCW	C4-O4P-P-O1P
7	B	303	NAG	O5-C5-C6-O6
7	B	302	NAG	O5-C5-C6-O6
7	B	302	NAG	C4-C5-C6-O6
7	B	302	NAG	C1-C2-N2-C7
7	B	303	NAG	C4-C5-C6-O6
7	B	301	NAG	O5-C5-C6-O6
8	B	304	PCW	C4-O4P-P-O3P
4	A	1102	CE1	O22-C23-C24-O25
4	A	1102	CE1	C10-C11-C12-O13
6	A	1107	8BZ	C12-C13-C19-O2
7	B	301	NAG	C4-C5-C6-O6
8	B	304	PCW	C12-C13-C14-C15
6	A	1107	8BZ	C12-C13-C19-N4
4	A	1106	CE1	C5-C6-C7-C8
4	A	1102	CE1	O19-C20-C21-O22
4	A	1102	CE1	C2-C3-C4-C5
8	B	304	PCW	C20-C21-C22-C23
8	B	304	PCW	C34-C35-C36-C37
4	A	1106	CE1	C2-C3-C4-C5
8	B	304	PCW	C32-C33-C34-C35
8	B	304	PCW	C14-C15-C16-C17
4	A	1102	CE1	C5-C6-C7-C8
8	B	304	PCW	C15-C16-C17-C18
8	B	304	PCW	C41-C42-C43-C44
4	A	1102	CE1	C24-C23-O22-C21
4	A	1102	CE1	C27-C26-O25-C24
8	B	304	PCW	O4P-C4-C5-N
4	A	1102	CE1	C11-C12-O13-C14
8	B	304	PCW	C16-C17-C18-C19
8	B	304	PCW	O3P-C1-C2-O2
4	A	1102	CE1	C15-C14-O13-C12

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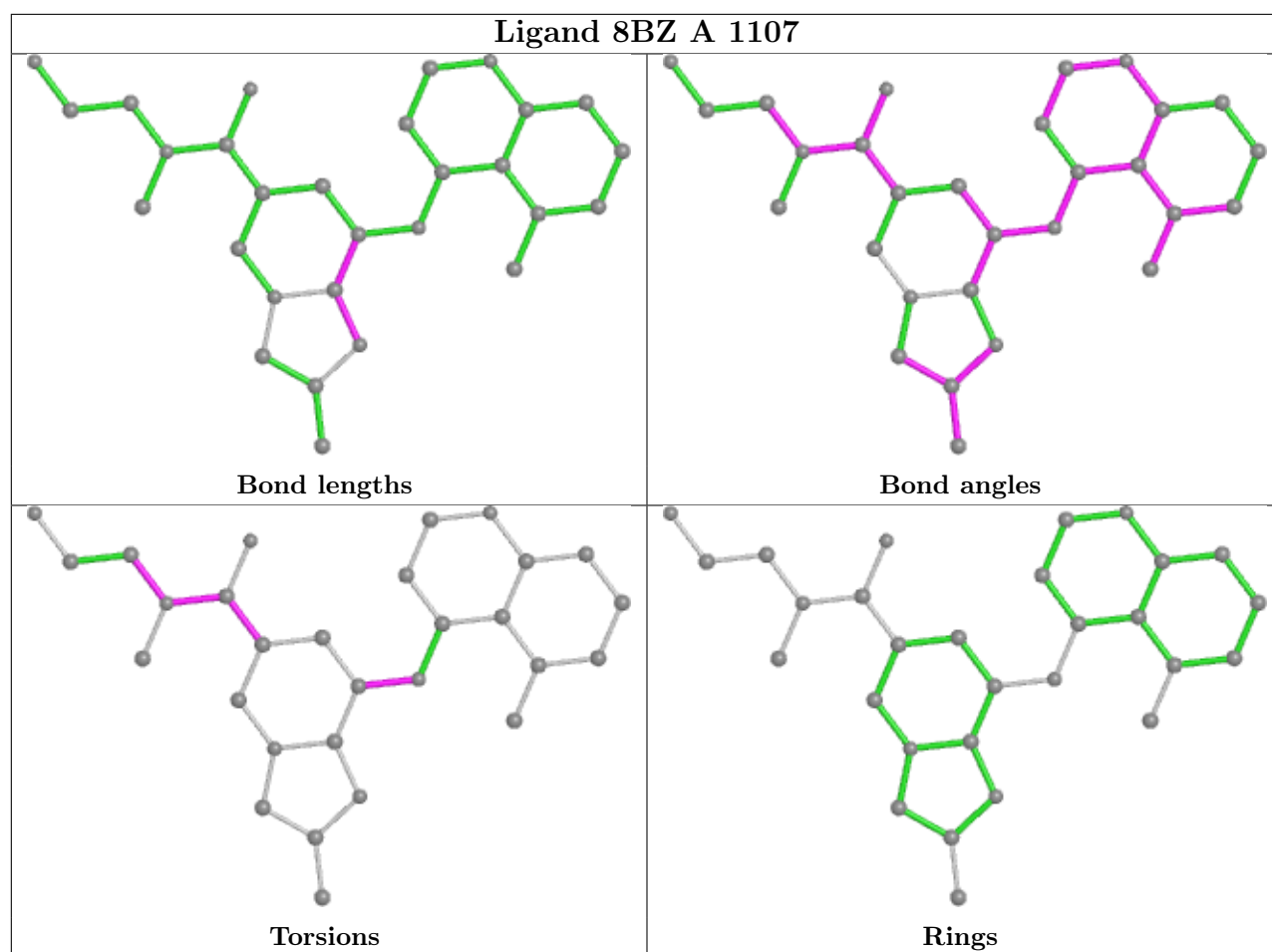
Mol	Chain	Res	Type	Atoms
8	B	304	PCW	C1-O3P-P-O4P
7	B	302	NAG	C3-C2-N2-C7
4	A	1102	CE1	C21-C20-O19-C18
4	A	1106	CE1	C18-C17-O16-C15
4	A	1106	CE1	C14-C15-O16-C17
8	B	304	PCW	O3-C11-C12-C13
4	A	1102	CE1	C1-C2-C3-C4
8	B	304	PCW	C22-C23-C24-C25
8	B	304	PCW	C17-C18-C19-C20
4	A	1102	CE1	C6-C7-C8-C9
8	B	304	PCW	O11-C11-C12-C13
8	B	304	PCW	O11-C11-O3-C3
8	B	304	PCW	C24-C25-C26-C27
4	A	1102	CE1	O13-C14-C15-O16

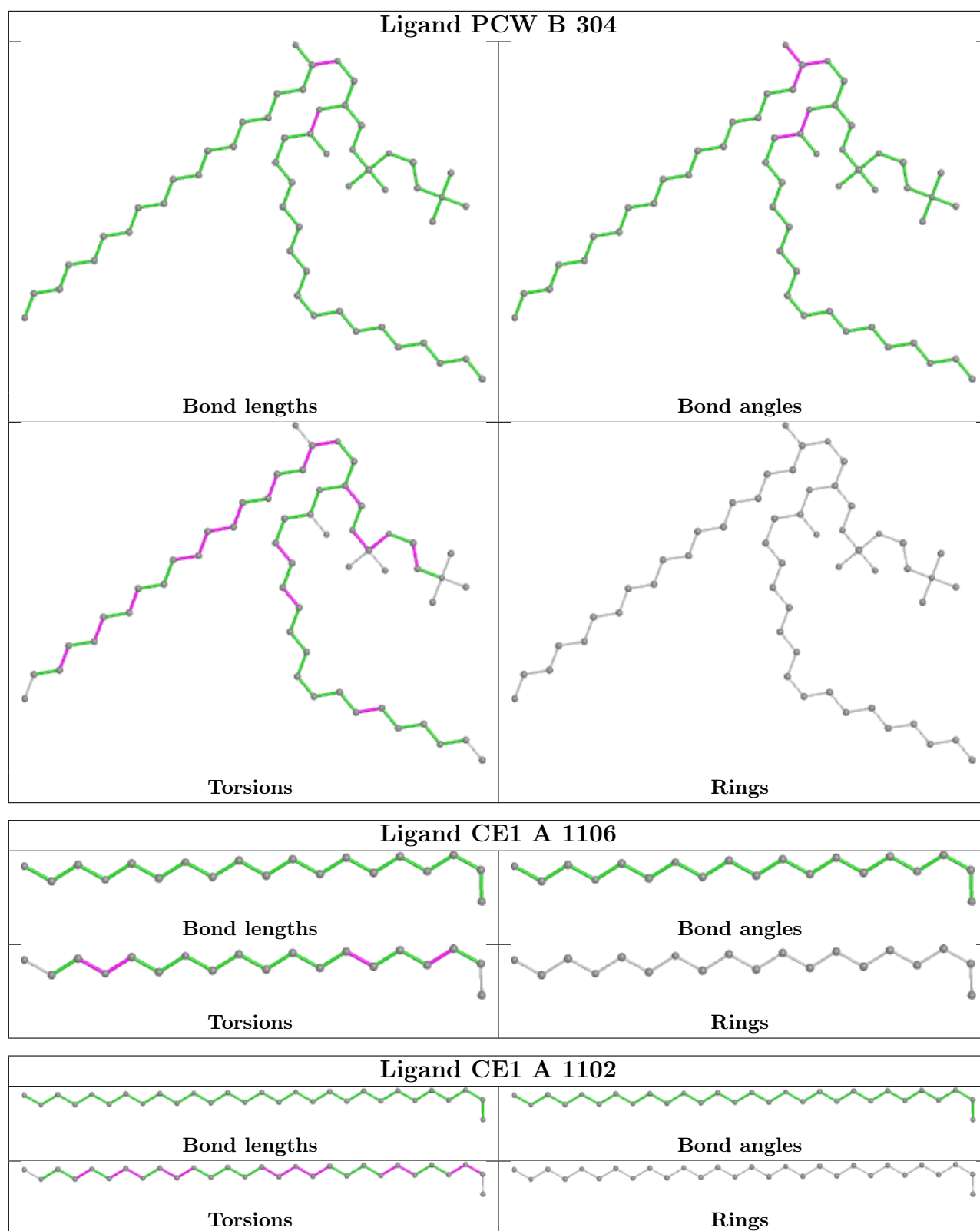
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1107	8BZ	3	0
8	B	304	PCW	3	0
4	A	1102	CE1	2	0

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





5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	986/1034 (95%)	-0.67	5 (0%)	91 88	43, 75, 116, 174	0
2	B	261/290 (90%)	-0.44	2 (0%)	86 81	62, 93, 144, 178	0
All	All	1247/1324 (94%)	-0.62	7 (0%)	89 86	43, 79, 123, 178	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1025	SER	4.2
1	A	173	LEU	2.9
1	A	494	THR	2.8
2	B	229	PHE	2.8
1	A	172	ASN	2.8
1	A	133	LEU	2.4
2	B	183	MET	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	0.92	0.26	55,61,71,74	0

6.3 Carbohydrates [i](#)

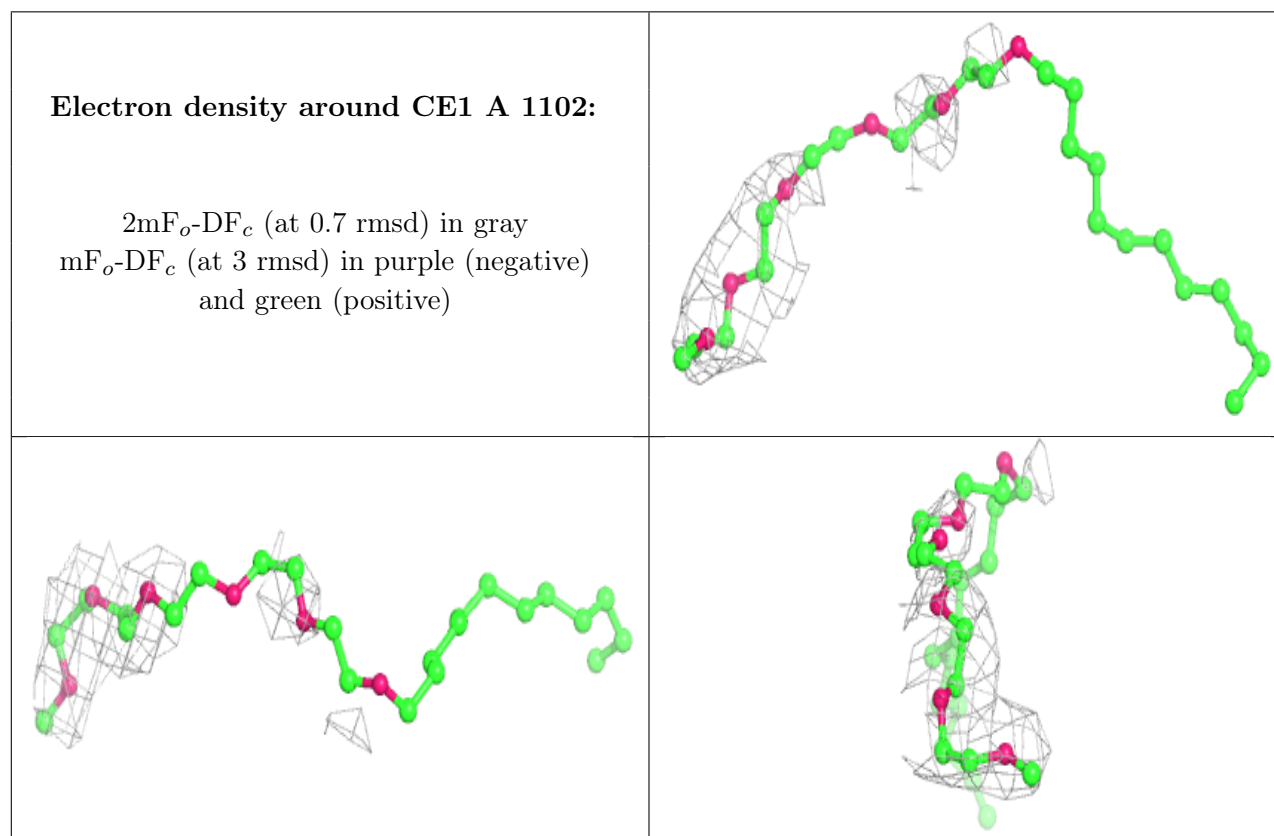
There are no monosaccharides in this entry.

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.

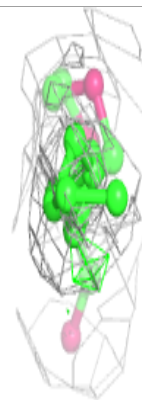
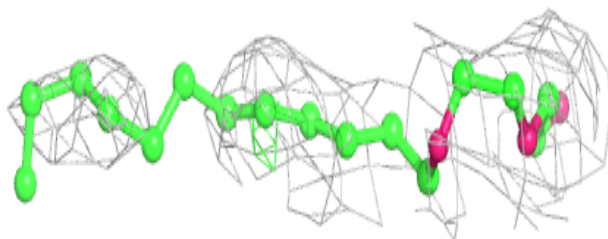
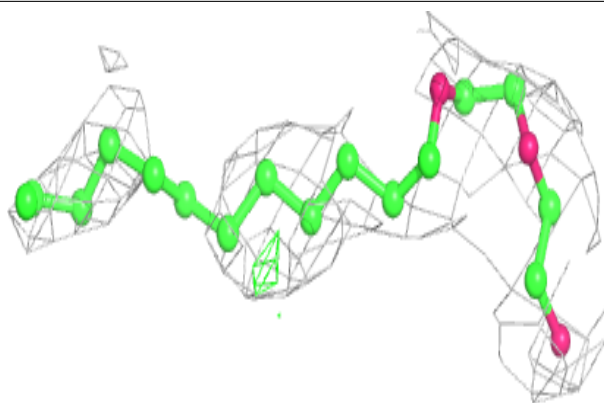
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	RB	A	1103	1/1	0.75	0.16	159,159,159,159	0
5	RB	A	1104	1/1	0.76	0.10	145,145,145,145	0
4	CE1	A	1102	29/37	0.80	0.48	93,112,145,146	0
4	CE1	A	1106	19/37	0.81	0.24	85,99,118,118	0
7	NAG	B	302	14/15	0.82	0.32	113,133,142,143	0
8	PCW	B	304	54/54	0.82	0.46	55,114,152,166	0
3	MG	A	1101	1/1	0.83	0.63	156,156,156,156	0
7	NAG	B	303	14/15	0.89	0.23	81,109,120,121	0
7	NAG	B	301	14/15	0.92	0.19	74,85,92,92	0
6	8BZ	A	1107	29/29	0.93	0.21	67,87,96,98	0
5	RB	A	1105	1/1	0.97	0.04	116,116,116,116	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.

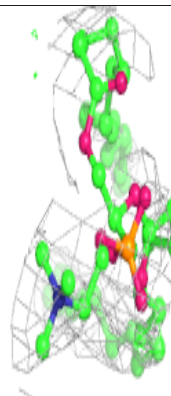
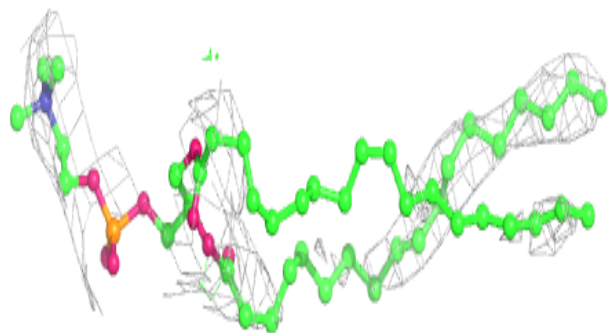
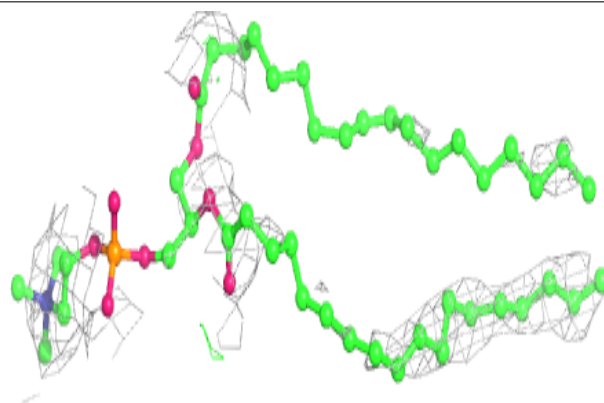


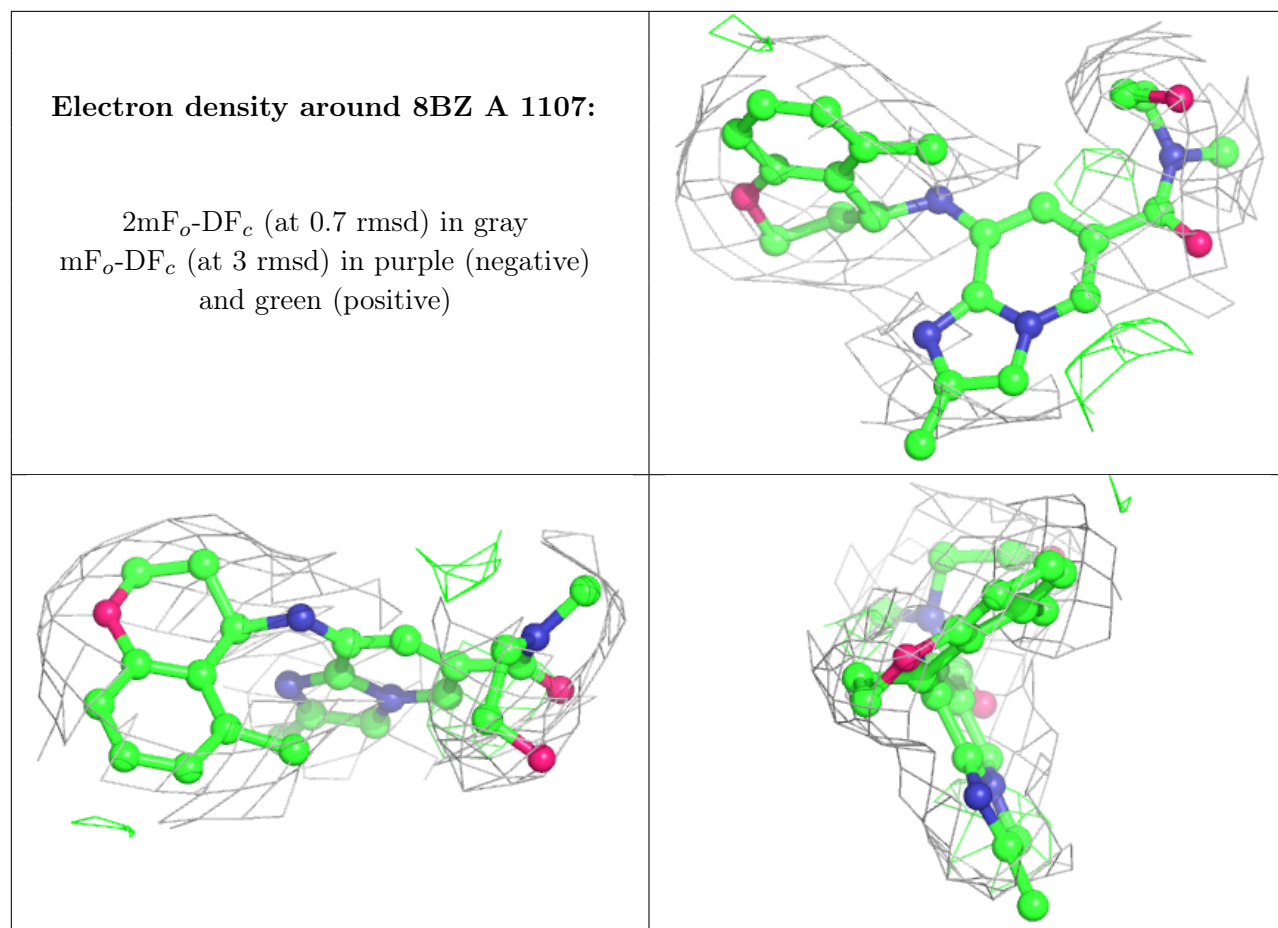
Electron density around CE1 A 1106:

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

**Electron density around PCW 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.