Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 09:23 PM JST

PDB ID	:	6JXI
Title	:	Rb+-bound E2-MgF state of the gastric proton pump (Tyr799Trp)
Authors	:	Abe, K.; Irie, K.
Deposited on	:	2019-04-23
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

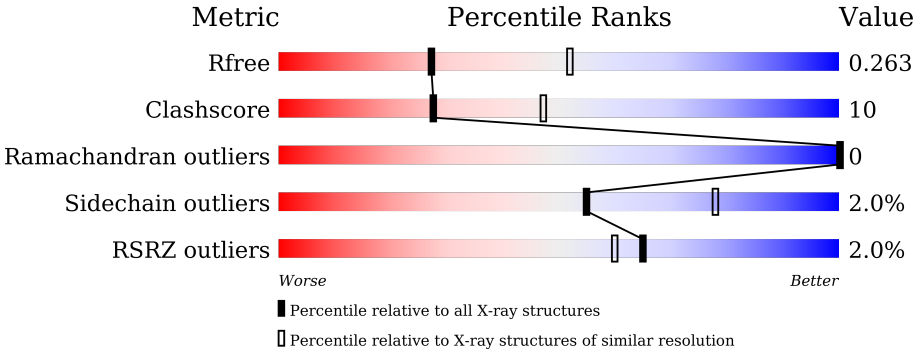
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	987	2% 77% 22% •
2	B	289	3% 75% 14% • 9%

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
4	PCW	A	1112	-	-	-	X
8	NAG	B	305	-	-	-	X
9	CLR	B	304	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 10470 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
			Total	C	N	O	S			
1	A	987	7661	4892	1293	1422	54	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP P19156
A	220	CYS	ARG	engineered mutation	UNP P19156
A	593	CYS	SER	engineered mutation	UNP P19156
A	799	TRP	TYR	engineered mutation	UNP P19156
A	1005	SER	GLY	engineered mutation	UNP P19156

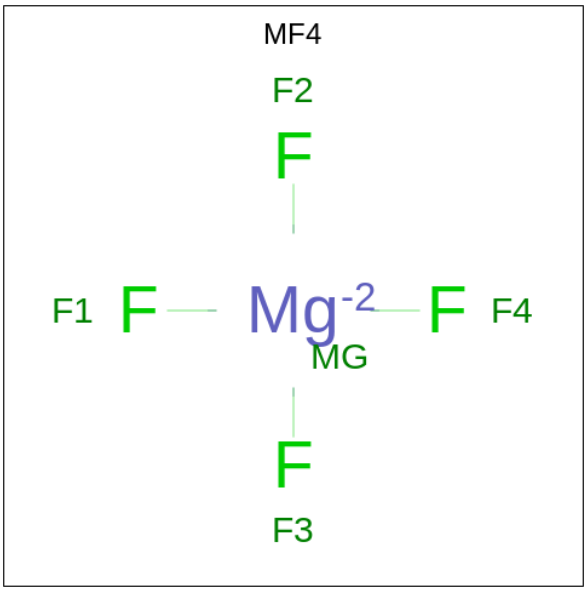
- Molecule 2 is a protein called Potassium-transporting ATPase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	262	2100	1364	348	376	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

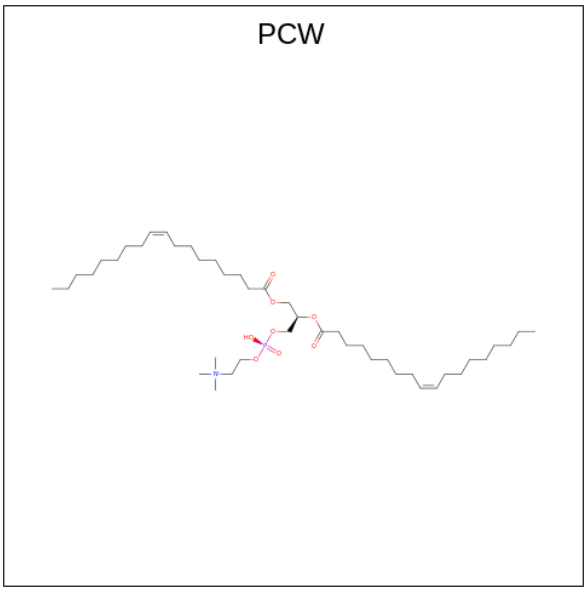
Chain	Residue	Modelled	Actual	Comment	Reference
B	287	LYS	-	expression tag	UNP P18434
B	288	ILE	-	expression tag	UNP P18434
B	289	GLN	-	expression tag	UNP P18434
B	290	LYS	-	expression tag	UNP P18434

- Molecule 3 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	F	Mg		
3	A	1	5	4	1	0	0

- 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
			Total	C	N	O	P		
4	A	1	46	36	1	8	1	0	0
			Total	C	N	O	P		
4	A	1	47	37	1	8	1	0	0

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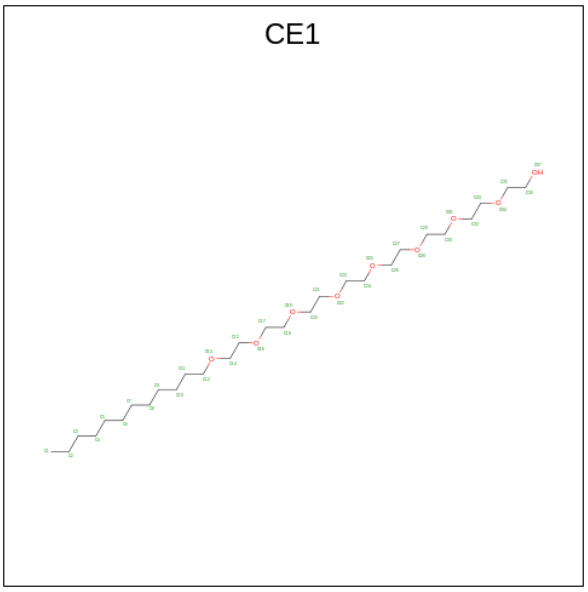
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	54	44	1	8	1	0	0
4	B	1	54	44	1	8	1	0	0

- Molecule 5 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	37	28	9	0	0

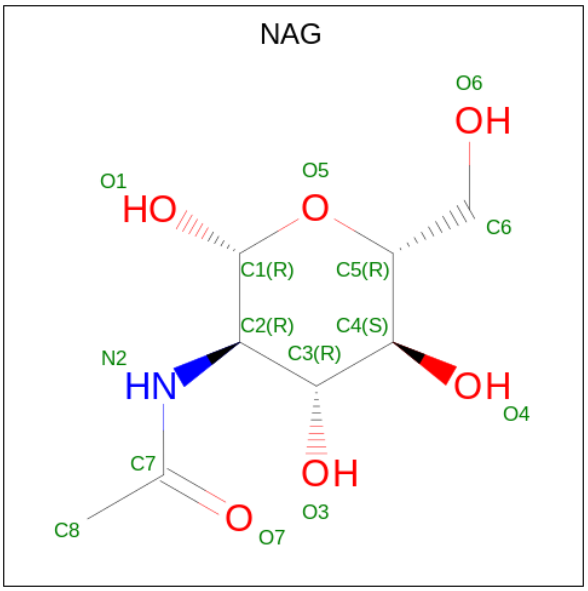
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

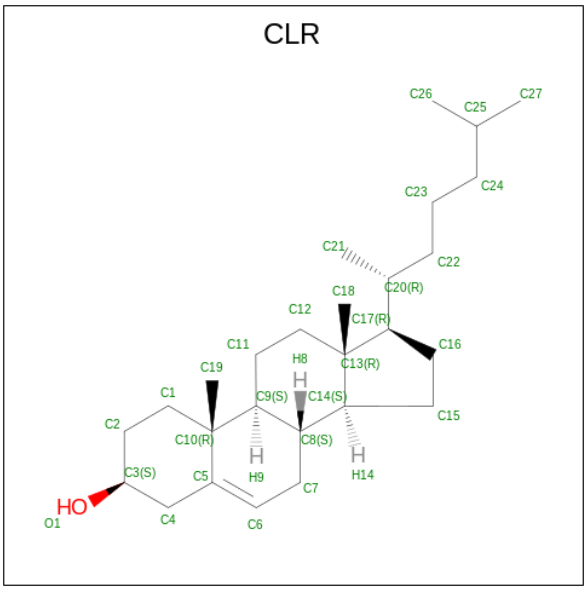
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Rb		
7	A	6	6	6	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	28	27	1	0	0

- Molecule 10 is water.

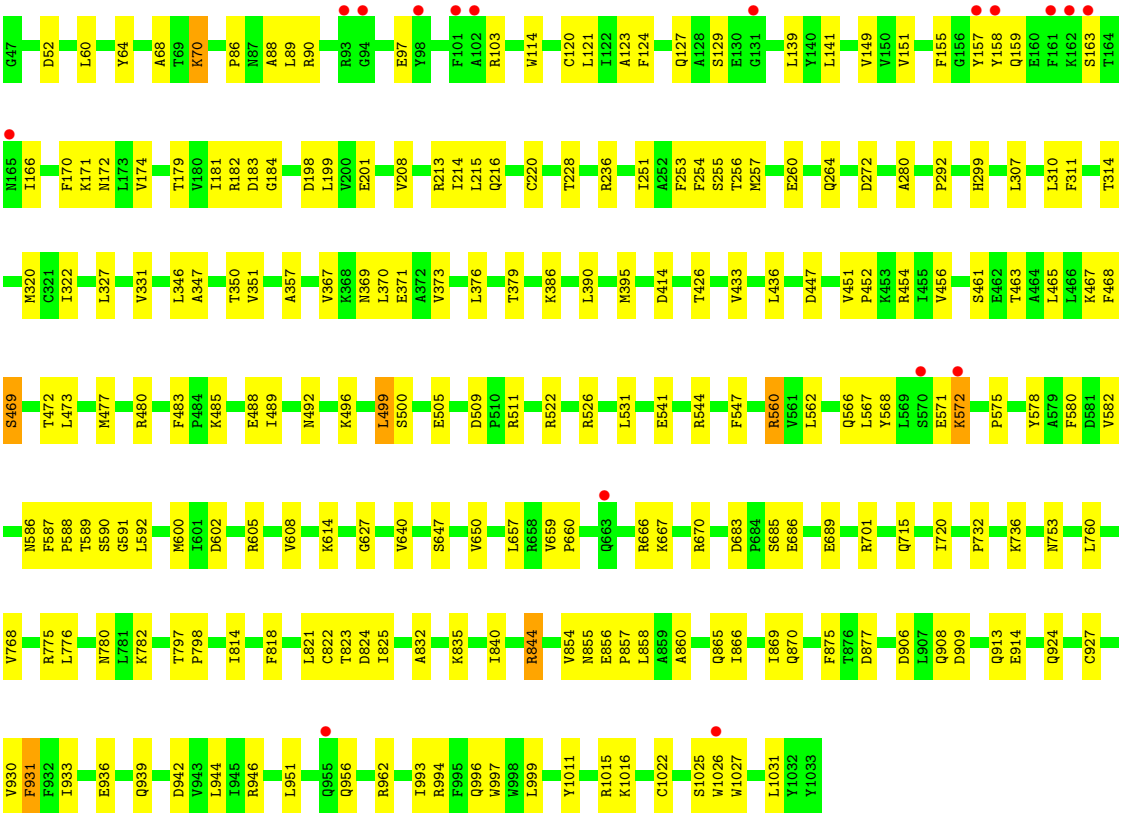
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	294	294	294	0	0
			Total	O		
10	B	67	67	67	0	0

3 Residue-property plots (i)

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.

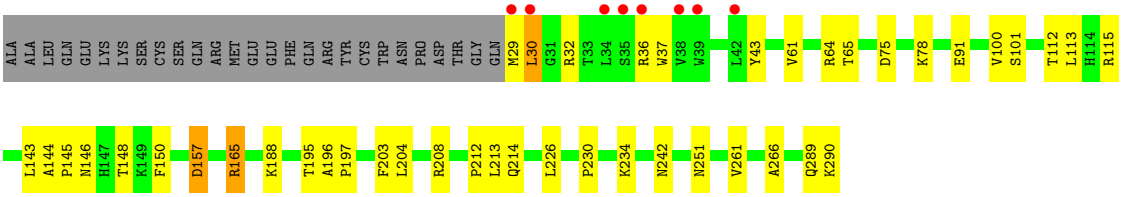
• Molecule 1: Potassium-transporting ATPase alpha chain 1

Chain A: 2% 77% 22%



• Molecule 2: Potassium-transporting ATPase subunit beta

Chain B: 3% 75% 14% 9%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.38Å 103.38Å 369.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.67 – 2.60 47.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	89.0 (47.67-2.60) 88.9 (47.67-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.13_2998, PHENIX 1.13_2998	Depositor
R, R_{free}	0.206 , 0.263 0.206 , 0.263	Depositor DCC
R_{free} test set	3355 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10470	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, CLR, MF4, NAG, CE1, MG, 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	0.47	0/7820	0.64	2/10623 (0.0%)
2	B	0.46	0/2167	0.60	0/2947
All	All	0.47	0/9987	0.63	2/13570 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	MET	CA-CB-CG	-5.31	104.28	113.30
1	A	499	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	7661	0	7687	169	0
2	B	2100	0	2044	32	0
3	A	5	0	0	1	0
4	A	147	0	217	7	0
4	B	54	0	84	2	0
5	A	37	0	58	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	6	0	0	0	0
8	B	70	0	65	2	0
9	B	28	0	46	3	0
10	A	294	0	0	13	0
10	B	67	0	0	3	0
All	All	10470	0	10201	203	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 (203) 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:578:TYR:HE2	1:A:586:ASN:ND2	1.44	1.11
1:A:123:ALA:O	1:A:127:GLN:OE1	1.73	1.06
1:A:578:TYR:HE2	1:A:586:ASN:HD22	1.03	0.99
1:A:578:TYR:CE2	1:A:586:ASN:ND2	2.34	0.87
1:A:477:MET:HG2	1:A:480:ARG:HH21	1.41	0.85
1:A:485:LYS:HD2	1:A:488:GLU:HB2	1.63	0.79
1:A:447:ASP:HA	1:A:454:ARG:HH21	1.48	0.77
1:A:447:ASP:HA	1:A:454:ARG:NH2	2.02	0.74
2:B:289:GLN:HB3	8:B:301:NAG:H82	1.70	0.72
1:A:89:LEU:H	1:A:171:LYS:HZ3	1.39	0.70
1:A:566:GLN:NE2	10:A:1202:HOH:O	2.22	0.69
1:A:89:LEU:H	1:A:171:LYS:NZ	1.90	0.69
1:A:526:ARG:NH1	1:A:589:THR:O	2.24	0.69
1:A:667:LYS:O	1:A:667:LYS:NZ	2.20	0.68
2:B:197:PRO:HB3	2:B:266:ALA:HB2	1.77	0.67
2:B:204:LEU:HD13	2:B:261:VAL:HG21	1.77	0.66
1:A:451:VAL:HA	1:A:454:ARG:HD2	1.78	0.66
1:A:854:VAL:HG13	1:A:858:LEU:HD22	1.77	0.65
1:A:933:ILE:HG13	1:A:993:ILE:HD11	1.78	0.65
1:A:70:LYS:HD3	1:A:183:ASP:HA	1.77	0.64
1:A:580:PHE:HA	1:A:586:ASN:HD21	1.63	0.64
1:A:103:ARG:NH2	10:A:1205:HOH:O	2.31	0.63
2:B:37:TRP:CZ3	9:B:304:CLR:H193	2.34	0.63
1:A:477:MET:HG2	1:A:480:ARG:NH2	2.14	0.62
1:A:216:GLN:HG3	1:A:264:GLN:HB2	1.80	0.62
1:A:860:ALA:HB1	9:B:304:CLR:H6	1.80	0.62
1:A:86:PRO:HD2	1:A:90:ARG:HH22	1.65	0.61
2:B:61:VAL:O	2:B:65:THR:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:LYS:HB2	1:A:522:ARG:HH11	1.63	0.61
1:A:456:VAL:HB	1:A:463:THR:HG23	1.83	0.61
2:B:37:TRP:HZ3	9:B:304:CLR:H193	1.66	0.61
1:A:844:ARG:NH1	10:A:1206:HOH:O	2.32	0.59
1:A:159:GLN:NE2	1:A:371:GLU:HG3	2.16	0.59
2:B:30:LEU:O	2:B:37:TRP:NE1	2.27	0.59
1:A:426:THR:HA	1:A:531:LEU:HD23	1.85	0.58
1:A:1015:ARG:HD2	1:A:1031:LEU:O	2.04	0.57
1:A:541:GLU:OE1	1:A:544:ARG:NH2	2.37	0.57
2:B:100:VAL:HG22	2:B:290:LYS:HA	1.84	0.57
2:B:143:LEU:HB2	2:B:150:PHE:HE2	1.69	0.57
1:A:395:MET:HG2	10:A:1424:HOH:O	2.04	0.57
1:A:685:SER:O	1:A:689:GLU:HG2	2.05	0.56
1:A:715:GLN:OE1	1:A:736:LYS:NZ	2.27	0.56
1:A:182:ARG:NH2	1:A:198:ASP:OD2	2.37	0.56
1:A:602:ASP:HB3	10:A:1245:HOH:O	2.06	0.56
1:A:560:ARG:HD3	1:A:600:MET:HE2	1.87	0.56
1:A:208:VAL:HB	1:A:253:PHE:O	2.06	0.56
1:A:1015:ARG:HA	1:A:1027:TRP:HZ2	1.70	0.56
1:A:930:VAL:HG23	1:A:997:TRP:HB3	1.88	0.56
1:A:120:CYS:SG	1:A:141:LEU:HD23	2.47	0.55
1:A:824:ASP:OD2	1:A:939:GLN:HG3	2.05	0.55
1:A:567:LEU:HB2	1:A:592:LEU:HD23	1.88	0.55
1:A:386:LYS:HA	1:A:390:LEU:HD12	1.90	0.54
1:A:52:ASP:HB3	1:A:60:LEU:HD21	1.90	0.53
1:A:567:LEU:HD12	1:A:568:TYR:H	1.74	0.53
1:A:571:GLU:OE1	1:A:571:GLU:N	2.26	0.53
1:A:469:SER:O	1:A:473:LEU:HD23	2.09	0.53
2:B:143:LEU:HB2	2:B:150:PHE:CE2	2.44	0.52
1:A:875:PHE:CD2	4:B:303:PCW:H431	2.45	0.52
2:B:112:THR:HG22	2:B:115:ARG:NH1	2.23	0.52
1:A:346:LEU:O	1:A:350:THR:HG23	2.10	0.52
1:A:436:LEU:HD11	1:A:483:PHE:HD1	1.74	0.52
1:A:181:ILE:HB	1:A:199:LEU:HD23	1.91	0.52
1:A:627:GLY:O	1:A:701:ARG:HD2	2.10	0.52
1:A:657:LEU:O	1:A:659:VAL:HG23	2.10	0.51
2:B:214:GLN:H	2:B:251:ASN:HB2	1.75	0.51
1:A:216:GLN:CG	1:A:264:GLN:HB2	2.41	0.51
1:A:114:TRP:CE2	1:A:149:VAL:HG11	2.46	0.51
1:A:496:LYS:HB2	1:A:522:ARG:HD3	1.91	0.51
1:A:310:LEU:O	1:A:314:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LYS:NZ	10:A:1209:HOH:O	2.37	0.51
2:B:165:ARG:NH1	10:B:404:HOH:O	2.43	0.51
1:A:52:ASP:OD2	1:A:64:TYR:OH	2.21	0.51
1:A:461:SER:HB2	1:A:560:ARG:NH2	2.26	0.51
1:A:151:VAL:O	1:A:155:PHE:HD1	1.94	0.51
1:A:1015:ARG:HA	1:A:1027:TRP:CZ2	2.45	0.50
1:A:994:ARG:HG3	1:A:997:TRP:CZ3	2.47	0.50
1:A:307:LEU:O	1:A:311:PHE:HD2	1.94	0.50
1:A:650:VAL:HG21	1:A:666:ARG:HD3	1.94	0.50
1:A:426:THR:HG23	1:A:531:LEU:HB3	1.93	0.50
1:A:605:ARG:HB2	1:A:608:VAL:HG23	1.93	0.50
4:A:1102:PCW:H51	10:A:1238:HOH:O	2.10	0.50
1:A:823:THR:HB	1:A:936:GLU:OE2	2.12	0.50
1:A:159:GLN:NE2	1:A:369:ASN:HB2	2.27	0.50
1:A:798:PRO:HG3	1:A:931:PHE:CZ	2.46	0.49
1:A:395:MET:HG2	1:A:600:MET:HE3	1.95	0.49
1:A:906:ASP:O	1:A:914:GLU:HG2	2.13	0.49
1:A:166:ILE:HD12	1:A:753:ASN:HB2	1.95	0.49
1:A:908:GLN:HA	1:A:913:GLN:O	2.12	0.49
1:A:814:ILE:HB	10:A:1318:HOH:O	2.12	0.49
1:A:70:LYS:HD2	1:A:70:LYS:C	2.33	0.49
1:A:489:ILE:O	1:A:489:ILE:HG13	2.13	0.49
1:A:499:LEU:HD23	1:A:500:SER:N	2.28	0.49
1:A:347:ALA:O	1:A:351:VAL:HG23	2.14	0.48
1:A:930:VAL:CG2	1:A:997:TRP:HB3	2.43	0.48
1:A:90:ARG:HG2	1:A:272:ASP:OD2	2.13	0.48
1:A:877:ASP:CG	1:A:930:VAL:HG22	2.33	0.48
1:A:924:GLN:O	1:A:927:CYS:HB2	2.14	0.48
1:A:483:PHE:CE2	1:A:505:GLU:HB2	2.48	0.48
2:B:144:ALA:HB3	2:B:148:THR:HG22	1.96	0.48
1:A:1022:CYS:HB3	1:A:1025:SER:HB2	1.96	0.47
1:A:452:PRO:O	1:A:467:LYS:NZ	2.48	0.47
1:A:1011:TYR:HH	2:B:43:TYR:HH	1.60	0.47
1:A:560:ARG:HD3	1:A:600:MET:CE	2.44	0.47
1:A:818:PHE:O	1:A:822:CYS:HB3	2.15	0.47
2:B:212:PRO:O	2:B:251:ASN:ND2	2.48	0.47
1:A:683:ASP:HB2	1:A:686:GLU:HG3	1.96	0.47
1:A:68:ALA:HB1	1:A:215:LEU:HD13	1.95	0.47
1:A:322:ILE:HD11	4:A:1112:PCW:H351	1.97	0.47
1:A:865:GLN:O	1:A:869:ILE:HG13	2.15	0.47
2:B:195:THR:OG1	2:B:196:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HA	1:A:171:LYS:NZ	2.31	0.46
1:A:732:PRO:O	10:A:1201:HOH:O	2.20	0.46
1:A:877:ASP:OD2	1:A:930:VAL:HG22	2.15	0.46
1:A:86:PRO:HD2	1:A:90:ARG:NH2	2.30	0.46
1:A:780:ASN:ND2	1:A:832:ALA:O	2.46	0.46
1:A:942:ASP:O	1:A:946:ARG:HG2	2.15	0.46
2:B:157:ASP:OD2	10:B:401:HOH:O	2.20	0.46
1:A:213:ARG:HA	1:A:251:ILE:HD13	1.96	0.46
2:B:145:PRO:O	2:B:148:THR:HB	2.15	0.46
2:B:91:GLU:HA	2:B:91:GLU:OE1	2.16	0.45
1:A:485:LYS:HD2	1:A:488:GLU:CB	2.41	0.45
1:A:575:PRO:HD2	1:A:578:TYR:HD1	1.80	0.45
1:A:567:LEU:HD12	1:A:568:TYR:N	2.30	0.45
1:A:608:VAL:HG12	1:A:640:VAL:CG2	2.46	0.45
1:A:996:GLN:HG2	4:A:1102:PCW:H52	1.98	0.45
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.69	0.45
1:A:199:LEU:HA	10:A:1254:HOH:O	2.16	0.45
1:A:855:ASN:ND2	1:A:857:PRO:HD2	2.32	0.45
1:A:776:LEU:HA	1:A:776:LEU:HD23	1.73	0.45
2:B:101:SER:OG	2:B:290:LYS:O	2.34	0.45
1:A:509:ASP:OD2	1:A:511:ARG:HD3	2.17	0.45
1:A:299:HIS:HE1	10:A:1427:HOH:O	1.99	0.45
1:A:367:VAL:HG12	1:A:369:ASN:H	1.82	0.44
2:B:75:ASP:O	2:B:78:LYS:HE3	2.17	0.44
2:B:188:LYS:HA	2:B:230:PRO:HB2	1.99	0.44
1:A:159:GLN:HE21	1:A:369:ASN:HB2	1.81	0.44
4:A:1104:PCW:H63	4:A:1104:PCW:H42	1.81	0.44
1:A:214:ILE:CD1	1:A:236:ARG:HB3	2.47	0.44
1:A:939:GLN:NE2	1:A:939:GLN:HA	2.33	0.44
1:A:994:ARG:HA	5:A:1103:CE1:H232	1.99	0.44
1:A:456:VAL:CB	1:A:463:THR:HG23	2.48	0.44
1:A:208:VAL:O	1:A:254:PHE:O	2.34	0.44
1:A:775:ARG:HB3	1:A:840:ILE:HD11	1.99	0.44
1:A:782:LYS:HB3	1:A:782:LYS:HE3	1.80	0.44
1:A:1026:TRP:HD1	2:B:36:ARG:HH12	1.66	0.44
1:A:97:GLU:HG3	1:A:157:TYR:OH	2.17	0.43
1:A:798:PRO:HB2	10:A:1306:HOH:O	2.17	0.43
1:A:88:ALA:HA	1:A:171:LYS:HZ1	1.81	0.43
1:A:182:ARG:HG3	10:A:1216:HOH:O	2.18	0.43
1:A:70:LYS:HG2	1:A:184:GLY:CA	2.49	0.43
1:A:578:TYR:OH	1:A:586:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:MET:HB3	2:B:32:ARG:O	2.18	0.43
1:A:170:PHE:CD2	1:A:280:ALA:HB2	2.53	0.43
1:A:866:ILE:O	1:A:870:GLN:HG3	2.19	0.43
1:A:951:LEU:O	1:A:1016:LYS:HE3	2.18	0.43
1:A:909:ASP:OD1	1:A:909:ASP:C	2.57	0.43
1:A:587:PHE:HB2	1:A:588:PRO:HD2	2.01	0.43
1:A:835:LYS:HD2	1:A:835:LYS:HA	1.71	0.43
1:A:236:ARG:NH1	1:A:251:ILE:O	2.52	0.43
1:A:254:PHE:C	1:A:254:PHE:CD1	2.92	0.43
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.79	0.43
1:A:157:TYR:HD2	1:A:158:TYR:CD1	2.37	0.42
1:A:414:ASP:OD1	1:A:414:ASP:N	2.52	0.42
2:B:146:ASN:HD21	8:B:307:NAG:C7	2.32	0.42
4:A:1104:PCW:H152	4:A:1112:PCW:H361	2.01	0.42
1:A:220:CYS:HA	1:A:260:GLU:O	2.19	0.42
1:A:821:LEU:HA	1:A:825:ILE:HD11	1.99	0.42
1:A:1027:TRP:CZ3	1:A:1031:LEU:HD12	2.54	0.42
1:A:228:THR:O	3:A:1101:MF4:F1	2.28	0.42
1:A:590:SER:OG	1:A:591:GLY:N	2.53	0.42
2:B:113:LEU:HD23	2:B:113:LEU:HA	1.84	0.42
1:A:370:LEU:O	1:A:373:VAL:HB	2.20	0.42
1:A:376:LEU:HA	1:A:379:THR:OG1	2.20	0.42
1:A:468:PHE:O	1:A:472:THR:HG23	2.20	0.42
4:A:1104:PCW:H382	4:B:303:PCW:H382	2.00	0.42
1:A:89:LEU:N	1:A:171:LYS:HZ3	2.13	0.42
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.80	0.42
1:A:797:THR:OG1	1:A:798:PRO:HD3	2.19	0.42
1:A:489:ILE:HG22	1:A:582:VAL:CG1	2.50	0.41
1:A:70:LYS:HD2	1:A:70:LYS:O	2.20	0.41
1:A:856:GLU:H	1:A:856:GLU:HG2	1.64	0.41
2:B:204:LEU:HD13	2:B:261:VAL:CG2	2.49	0.41
1:A:647:SER:OG	1:A:670:ARG:HD3	2.20	0.41
2:B:203:PHE:CE2	2:B:213:LEU:HB2	2.55	0.41
2:B:251:ASN:O	2:B:251:ASN:OD1	2.39	0.41
1:A:174:VAL:HG13	1:A:254:PHE:CZ	2.56	0.41
1:A:614:LYS:HB3	1:A:768:VAL:HG21	2.02	0.41
1:A:395:MET:CG	1:A:600:MET:HE3	2.50	0.41
2:B:234:LYS:HA	10:B:413:HOH:O	2.19	0.41
1:A:572:LYS:O	1:A:572:LYS:HG3	2.21	0.41
1:A:292:PRO:HG3	1:A:720:ILE:HD13	2.03	0.41
1:A:999:LEU:HB3	4:A:1102:PCW:H141	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:LEU:HD23	2:B:226:LEU:HA	1.89	0.41
1:A:357:ALA:HB2	1:A:373:VAL:HG21	2.03	0.41
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.78	0.40
1:A:256:THR:H	1:A:256:THR:HG23	1.58	0.40
1:A:547:PHE:CD1	1:A:547:PHE:C	2.94	0.40
1:A:179:THR:OG1	1:A:201:GLU:HB3	2.22	0.40
1:A:465:LEU:HA	1:A:465:LEU:HD23	1.91	0.40
1:A:124:PHE:CD1	1:A:139:LEU:HB2	2.56	0.40
1:A:327:LEU:O	1:A:331:VAL:HG23	2.22	0.40
1:A:433:VAL:CG2	1:A:566:GLN:HG3	2.51	0.40
1:A:944:LEU:HD23	1:A:944:LEU:HA	1.85	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	985/987 (100%)	967 (98%)	18 (2%)	0	100	100
2	B	260/289 (90%)	258 (99%)	2 (1%)	0	100	100
All	All	1245/1276 (98%)	1225 (98%)	20 (2%)	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	834/834 (100%)	819 (98%)	15 (2%)	59	80
2	B	229/253 (90%)	223 (97%)	6 (3%)	46	72
All	All	1063/1087 (98%)	1042 (98%)	21 (2%)	55	78

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

Mol	Chain	Res	Type
1	A	70	LYS
1	A	129	SER
1	A	163	SER
1	A	172	ASN
1	A	255	SER
1	A	320	MET
1	A	469	SER
1	A	492	ASN
1	A	560	ARG
1	A	572	LYS
1	A	660	PRO
1	A	844	ARG
1	A	931	PHE
1	A	956	GLN
1	A	962	ARG
2	B	30	LEU
2	B	64	ARG
2	B	157	ASP
2	B	165	ARG
2	B	208	ARG
2	B	242	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	172	ASN
1	A	865	GLN
1	A	870	GLN
1	A	939	GLN
2	B	74	GLN
2	B	251	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
8	NAG	B	305	2	14,14,15	0.23	0	17,19,21	0.39	0
8	NAG	B	302	2	14,14,15	0.41	0	17,19,21	0.86	1 (5%)
5	CE1	A	1103	-	36,36,36	0.56	0	35,35,35	0.41	0
8	NAG	B	301	2	14,14,15	0.53	0	17,19,21	0.48	0
4	PCW	A	1102	-	45,45,53	1.07	2 (4%)	51,53,61	0.96	2 (3%)
4	PCW	A	1104	-	46,46,53	1.08	2 (4%)	52,54,61	0.85	1 (1%)
4	PCW	A	1112	-	53,53,53	0.96	2 (3%)	59,61,61	0.90	2 (3%)
4	PCW	B	303	-	53,53,53	0.91	2 (3%)	59,61,61	1.05	3 (5%)
8	NAG	B	306	2	14,14,15	1.03	1 (7%)	17,19,21	0.72	0
8	NAG	B	307	2	14,14,15	0.65	0	17,19,21	0.39	0
3	MF4	A	1101	1	0,4,4	-	-	-		
9	CLR	B	304	-	31,31,31	0.62	0	48,48,48	1.17	3 (6%)

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
8	NAG	B	302	2	-	0/6/23/26	0/1/1/1
5	CE1	A	1103	-	-	11/34/34/34	-
8	NAG	B	301	2	-	2/6/23/26	0/1/1/1
4	PCW	A	1102	-	-	25/49/49/57	-
4	PCW	A	1104	-	-	21/50/50/57	-
4	PCW	A	1112	-	-	18/57/57/57	-
4	PCW	B	303	-	-	14/57/57/57	-
8	NAG	B	306	2	-	2/6/23/26	0/1/1/1
8	NAG	B	307	2	-	2/6/23/26	0/1/1/1
8	NAG	B	305	2	-	0/6/23/26	0/1/1/1
9	CLR	B	304	-	-	5/10/68/68	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	PCW	O3-C11	4.56	1.46	1.33
4	A	1104	PCW	O3-C11	4.54	1.46	1.33
4	A	1104	PCW	O2-C31	4.43	1.46	1.34
4	A	1112	PCW	O2-C31	4.32	1.46	1.34
4	A	1102	PCW	O2-C31	4.31	1.46	1.34
4	A	1112	PCW	O3-C11	4.19	1.45	1.33
4	B	303	PCW	O3-C11	4.16	1.45	1.33
4	B	303	PCW	O2-C31	3.98	1.45	1.34
8	B	306	NAG	C1-C2	3.43	1.57	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	303	PCW	O2-C31-C32	3.96	120.05	111.50
4	A	1102	PCW	O2-C31-C32	3.76	119.59	111.50
4	A	1112	PCW	O2-C31-C32	3.70	119.47	111.50
4	A	1104	PCW	O2-C31-C32	3.35	118.72	111.50
9	B	304	CLR	C8-C7-C6	-3.01	108.41	112.73
9	B	304	CLR	C19-C10-C5	-2.99	103.50	108.34
9	B	304	CLR	C9-C10-C5	2.97	114.30	109.65
4	B	303	PCW	O3-C11-C12	2.85	120.85	111.91
4	A	1102	PCW	O3-C11-C12	2.80	120.70	111.91
4	B	303	PCW	C2-O2-C31	-2.61	111.38	117.79
8	B	302	NAG	C1-O5-C5	2.59	115.70	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1112	PCW	O3-C11-C12	2.21	118.84	111.91

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1104	PCW	O2-C2-C3-O3
4	A	1104	PCW	C1-O3P-P-O2P
4	A	1104	PCW	C4-O4P-P-O1P
4	A	1112	PCW	C2-C1-O3P-P
4	A	1112	PCW	O4P-C4-C5-N
4	A	1112	PCW	C1-O3P-P-O2P
4	A	1112	PCW	C4-O4P-P-O1P
4	B	303	PCW	O4P-C4-C5-N
4	B	303	PCW	C4-O4P-P-O2P
4	A	1112	PCW	O11-C11-O3-C3
4	A	1112	PCW	C12-C11-O3-C3
8	B	306	NAG	O5-C5-C6-O6
8	B	307	NAG	O5-C5-C6-O6
8	B	307	NAG	C4-C5-C6-O6
8	B	306	NAG	C4-C5-C6-O6
4	A	1102	PCW	C4-C5-N-C8
5	A	1103	CE1	O19-C20-C21-O22
9	B	304	CLR	C17-C20-C22-C23
5	A	1103	CE1	O22-C23-C24-O25
9	B	304	CLR	C21-C20-C22-C23
4	A	1102	PCW	C4-C5-N-C7
9	B	304	CLR	C20-C22-C23-C24
4	A	1112	PCW	C31-C32-C33-C34
4	A	1102	PCW	C4-O4P-P-O3P
4	A	1104	PCW	C1-O3P-P-O4P
4	A	1104	PCW	C4-O4P-P-O3P
4	A	1112	PCW	C1-O3P-P-O4P
4	A	1112	PCW	C4-O4P-P-O3P
4	A	1104	PCW	C23-C24-C25-C26
9	B	304	CLR	C23-C24-C25-C27
4	A	1102	PCW	C34-C35-C36-C37
5	A	1103	CE1	C11-C10-C9-C8
4	A	1112	PCW	C32-C31-O2-C2
4	A	1112	PCW	C36-C37-C38-C39
4	A	1112	PCW	C40-C41-C42-C43
4	A	1102	PCW	C4-C5-N-C6

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Mol	Chain	Res	Type	Atoms
9	B	304	CLR	C23-C24-C25-C26
4	B	303	PCW	C33-C34-C35-C36
5	A	1103	CE1	C2-C3-C4-C5
4	A	1102	PCW	C12-C13-C14-C15
4	A	1104	PCW	C36-C37-C38-C39
4	A	1112	PCW	O31-C31-O2-C2
4	A	1102	PCW	C22-C23-C24-C25
4	A	1102	PCW	C21-C22-C23-C24
4	A	1104	PCW	C12-C11-O3-C3
4	A	1102	PCW	C23-C24-C25-C26
5	A	1103	CE1	O16-C17-C18-O19
4	A	1104	PCW	C20-C21-C22-C23
4	A	1104	PCW	C31-C32-C33-C34
4	A	1102	PCW	C32-C31-O2-C2
4	A	1102	PCW	O31-C31-O2-C2
4	B	303	PCW	C20-C21-C22-C23
4	A	1102	PCW	C32-C33-C34-C35
4	A	1104	PCW	O11-C11-O3-C3
4	A	1104	PCW	O3P-C1-C2-C3
4	A	1104	PCW	C1-C2-C3-O3
4	A	1104	PCW	C25-C26-C27-C28
5	A	1103	CE1	C3-C4-C5-C6
4	A	1102	PCW	C13-C14-C15-C16
4	A	1104	PCW	C32-C33-C34-C35
4	B	303	PCW	C12-C11-O3-C3
4	A	1102	PCW	O2-C2-C3-O3
4	A	1104	PCW	C2-C1-O3P-P
4	A	1102	PCW	C1-C2-C3-O3
4	A	1102	PCW	C25-C26-C27-C28
4	B	303	PCW	O11-C11-O3-C3
4	A	1102	PCW	C33-C34-C35-C36
5	A	1103	CE1	O34-C35-C36-O37
5	A	1103	CE1	C32-C33-O34-C35
4	B	303	PCW	C34-C35-C36-C37
4	A	1102	PCW	C4-O4P-P-O2P
4	A	1104	PCW	C1-O3P-P-O1P
8	B	301	NAG	C4-C5-C6-O6
4	A	1104	PCW	O3P-C1-C2-O2
4	A	1102	PCW	O4P-C4-C5-N
4	A	1104	PCW	O4P-C4-C5-N
4	A	1112	PCW	C33-C34-C35-C36
4	B	303	PCW	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1102	PCW	C1-O3P-P-O4P
4	B	303	PCW	C1-O3P-P-O4P
4	B	303	PCW	C4-O4P-P-O3P
5	A	1103	CE1	C24-C23-O22-C21
4	B	303	PCW	O31-C31-O2-C2
4	A	1112	PCW	C11-C12-C13-C14
8	B	301	NAG	O5-C5-C6-O6
4	A	1102	PCW	C14-C15-C16-C17
4	A	1102	PCW	C3-C2-O2-C31
4	A	1102	PCW	C17-C18-C19-C20
4	A	1104	PCW	C21-C22-C23-C24
4	B	303	PCW	C32-C33-C34-C35
4	A	1112	PCW	C37-C38-C39-C40
4	A	1104	PCW	O2-C31-C32-C33
4	A	1112	PCW	C13-C14-C15-C16
4	B	303	PCW	C43-C44-C45-C46
4	A	1112	PCW	C19-C20-C21-C22
5	A	1103	CE1	C1-C2-C3-C4
4	B	303	PCW	C19-C20-C21-C22
4	A	1102	PCW	C1-O3P-P-O2P
4	A	1102	PCW	C1-C2-O2-C31
5	A	1103	CE1	O13-C14-C15-O16

There are no ring outliers.

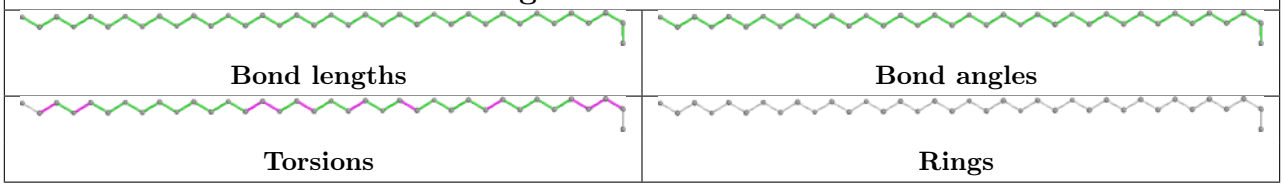
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1103	CE1	1	0
8	B	301	NAG	1	0
4	A	1102	PCW	3	0
4	A	1104	PCW	3	0
4	A	1112	PCW	2	0
4	B	303	PCW	2	0
8	B	307	NAG	1	0
3	A	1101	MF4	1	0
9	B	304	CLR	3	0

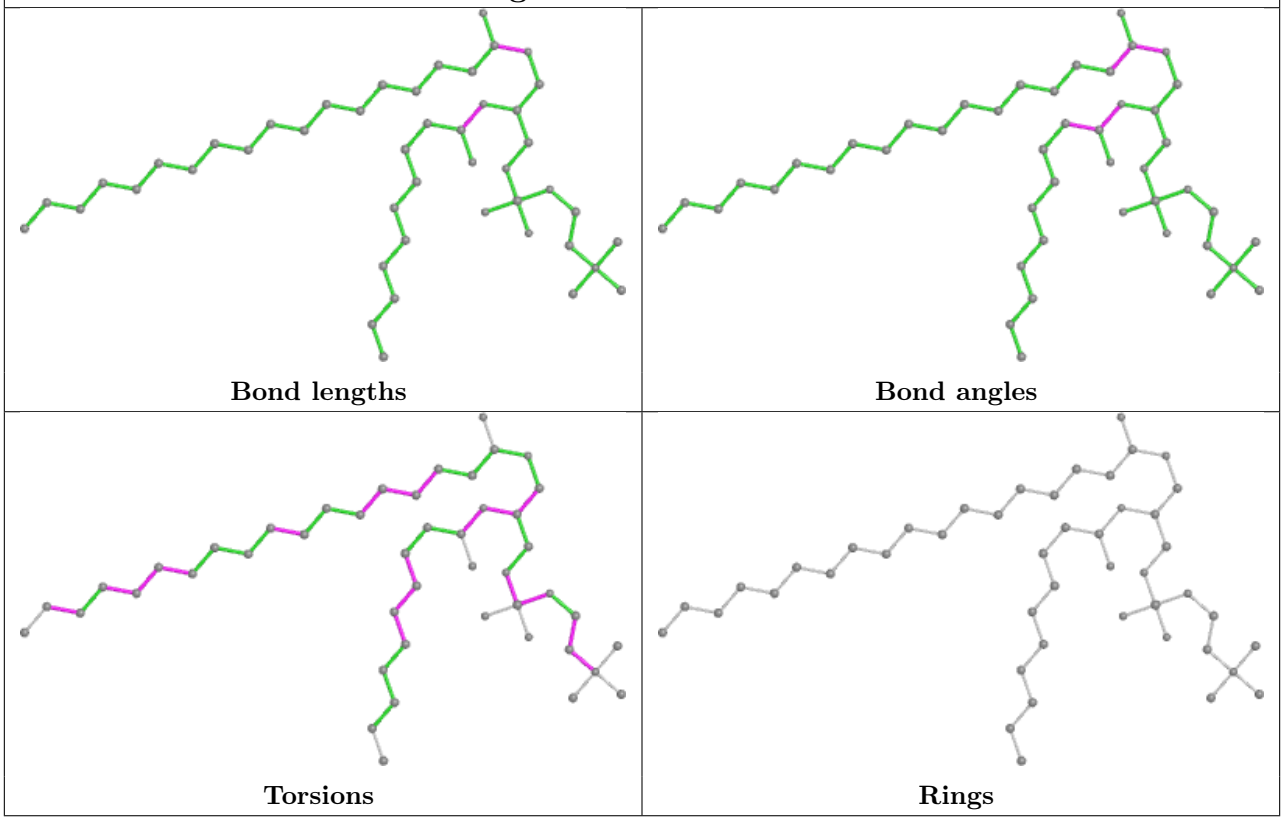
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

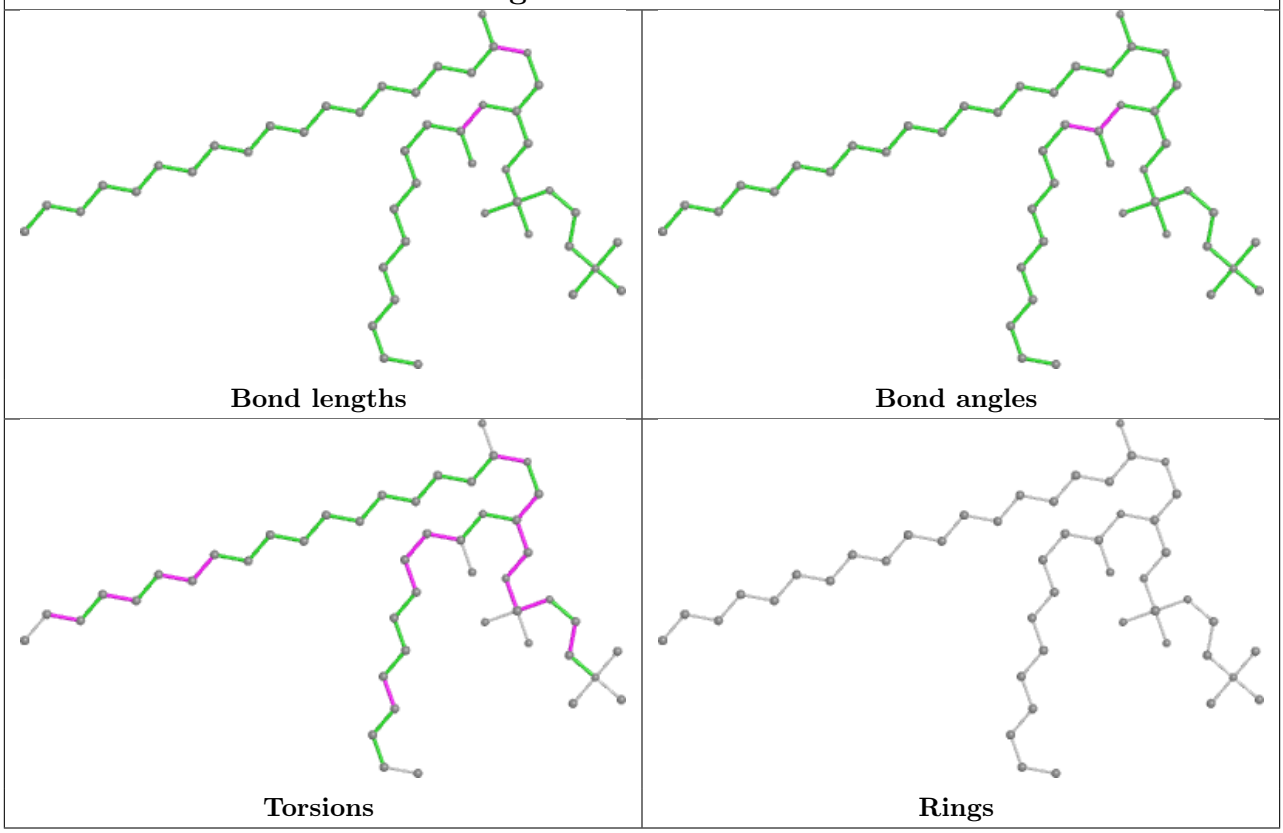
Ligand CE1 A 1103



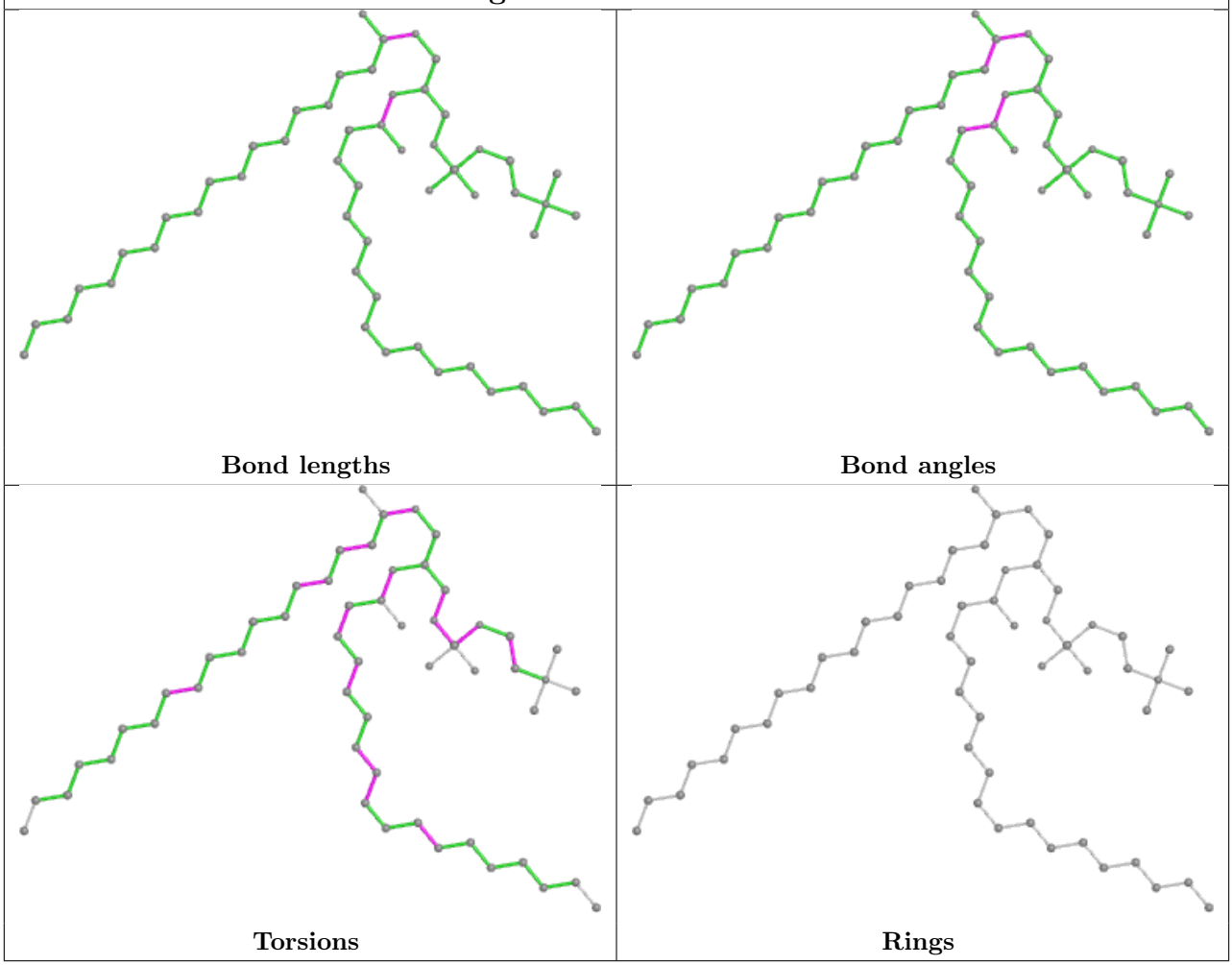
Ligand PCW A 1102



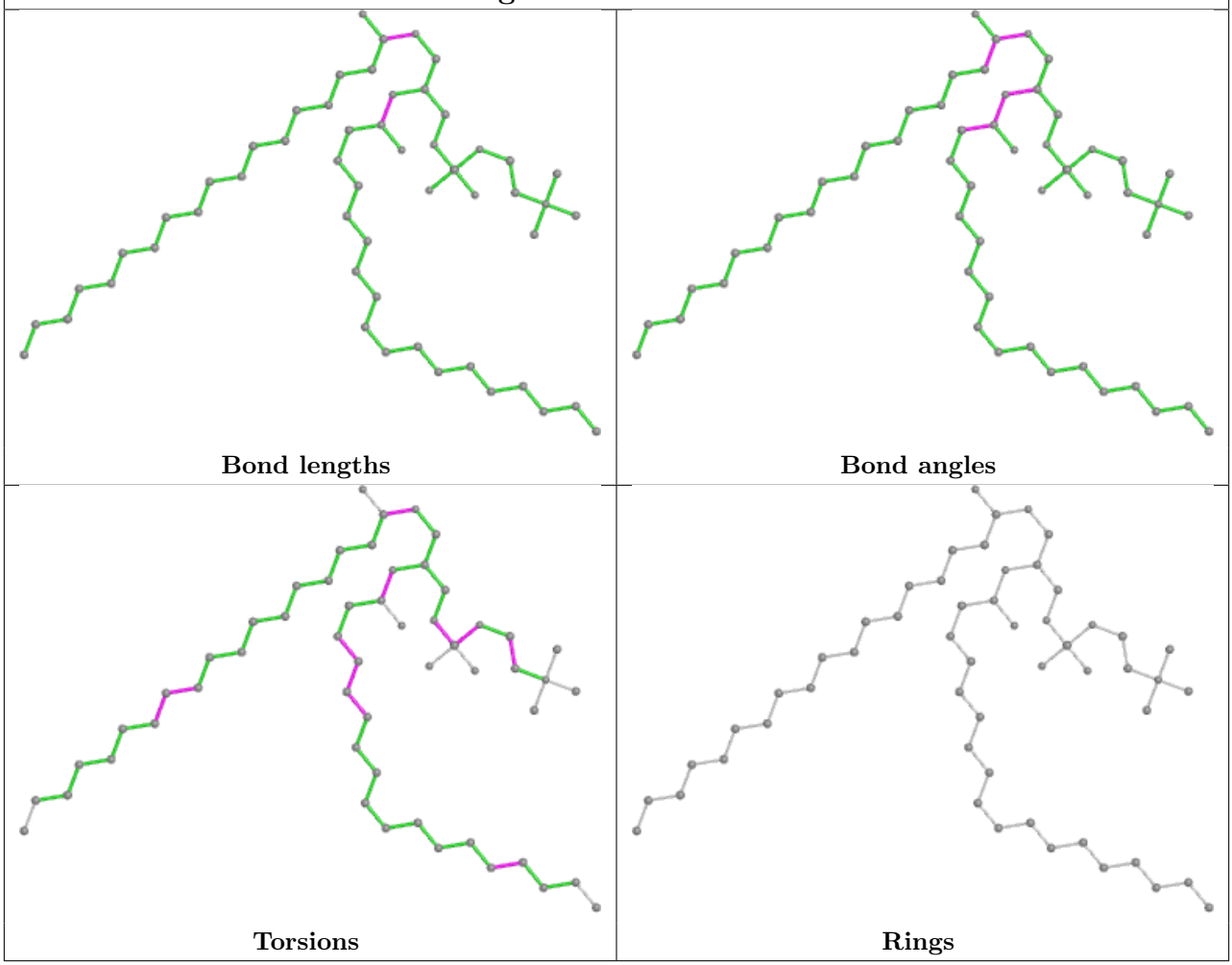
Ligand PCW A 1104



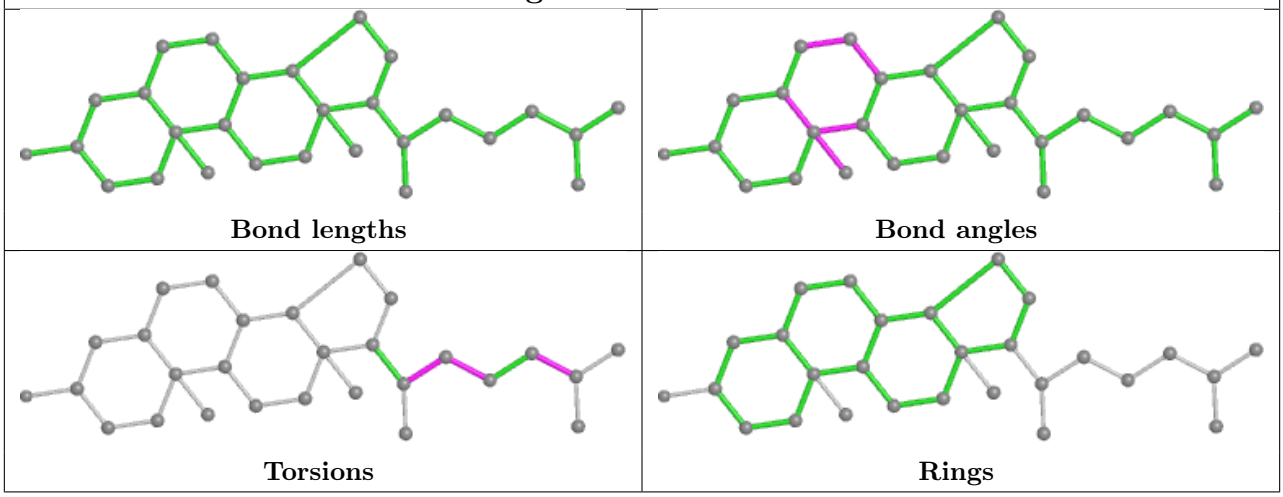
Ligand PCW A 1112



Ligand PCW B 303



Ligand CLR B 304



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 (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	987/987 (100%)	-0.43	17 (1%)	70	66	26, 52, 105, 185	0
2	B	262/289 (90%)	-0.45	8 (3%)	49	42	36, 61, 109, 156	0
All	All	1249/1276 (97%)	-0.43	25 (2%)	65	60	26, 54, 108, 185	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	4.3
1	A	572	LYS	4.2
1	A	165	ASN	4.0
1	A	1026	TRP	3.7
2	B	34	LEU	3.1
1	A	101	PHE	3.1
1	A	131	GLY	2.9
2	B	38	VAL	2.9
1	A	663	GLN	2.8
1	A	102	ALA	2.8
1	A	94	GLY	2.8
1	A	163	SER	2.7
1	A	162	LYS	2.7
2	B	39	TRP	2.6
1	A	93	ARG	2.5
1	A	158	TYR	2.5
1	A	570	SER	2.5
2	B	35	SER	2.4
2	B	30	LEU	2.4
1	A	157	TYR	2.3
2	B	29	MET	2.3
1	A	161	PHE	2.1
2	B	42	LEU	2.1
2	B	36	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	955	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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.

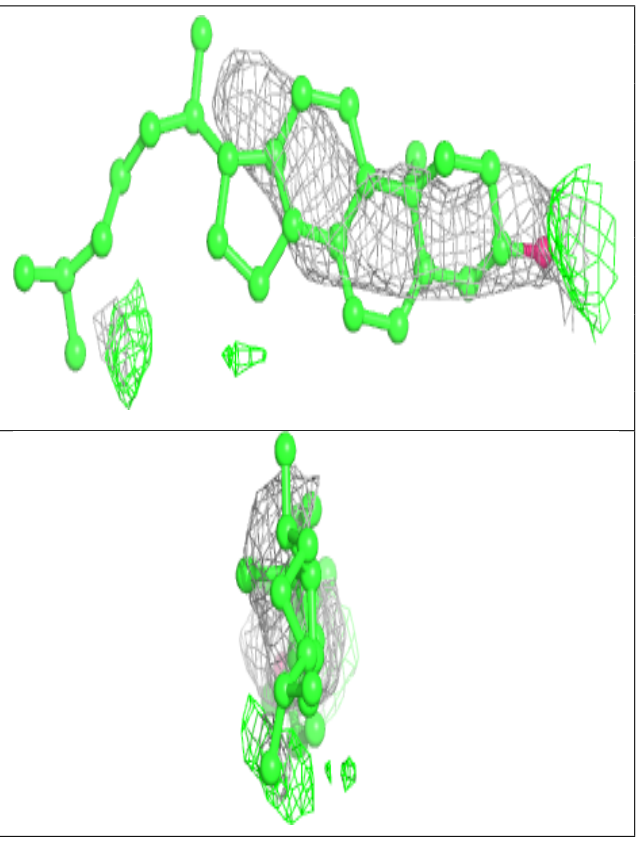
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	CLR	B	304	28/28	0.62	0.67	145,166,174,178	0
4	PCW	A	1104	47/54	0.71	0.36	63,91,170,175	0
8	NAG	B	305	14/15	0.74	0.58	154,163,169,169	0
4	PCW	A	1102	46/54	0.74	0.34	77,120,139,148	0
4	PCW	A	1112	54/54	0.76	0.54	73,107,178,186	0
5	CE1	A	1103	37/37	0.77	0.26	51,97,128,130	0
8	NAG	B	306	14/15	0.87	0.23	128,141,147,154	0
8	NAG	B	307	14/15	0.88	0.39	127,144,149,152	0
7	RB	A	1110	1/1	0.90	0.06	151,151,151,151	0
8	NAG	B	302	14/15	0.90	0.15	79,97,101,104	0
4	PCW	B	303	54/54	0.90	0.27	47,83,123,136	0
8	NAG	B	301	14/15	0.95	0.13	84,97,105,112	0
3	MF4	A	1101	5/5	0.97	0.18	28,33,41,59	0
7	RB	A	1109	1/1	0.98	0.08	81,81,81,81	0
7	RB	A	1108	1/1	0.99	0.14	48,48,48,48	0
6	MG	A	1105	1/1	0.99	0.17	44,44,44,44	0
7	RB	A	1107	1/1	0.99	0.09	90,90,90,90	0
7	RB	A	1106	1/1	1.00	0.11	75,75,75,75	0
7	RB	A	1111	1/1	1.00	0.16	45,45,45,45	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.

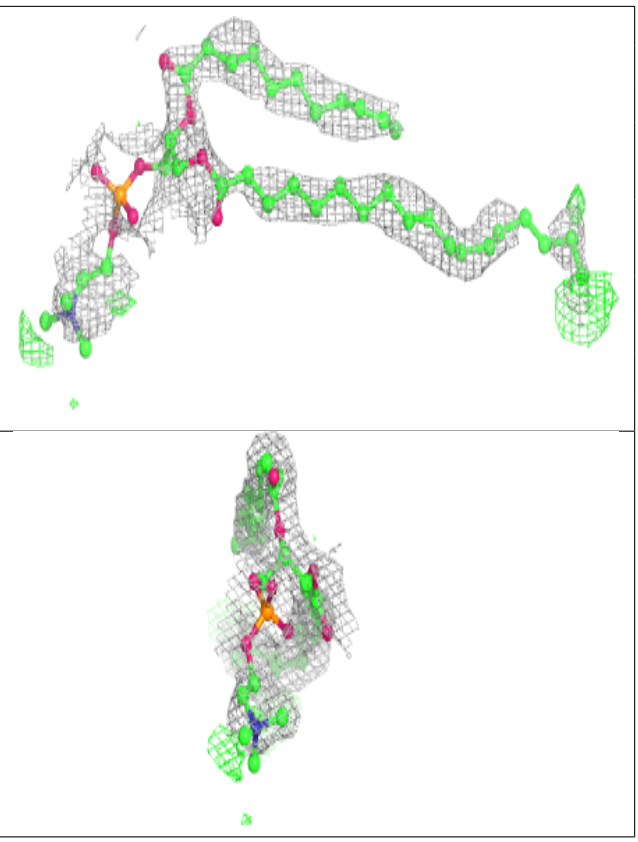
Electron density around CLR B 304:

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



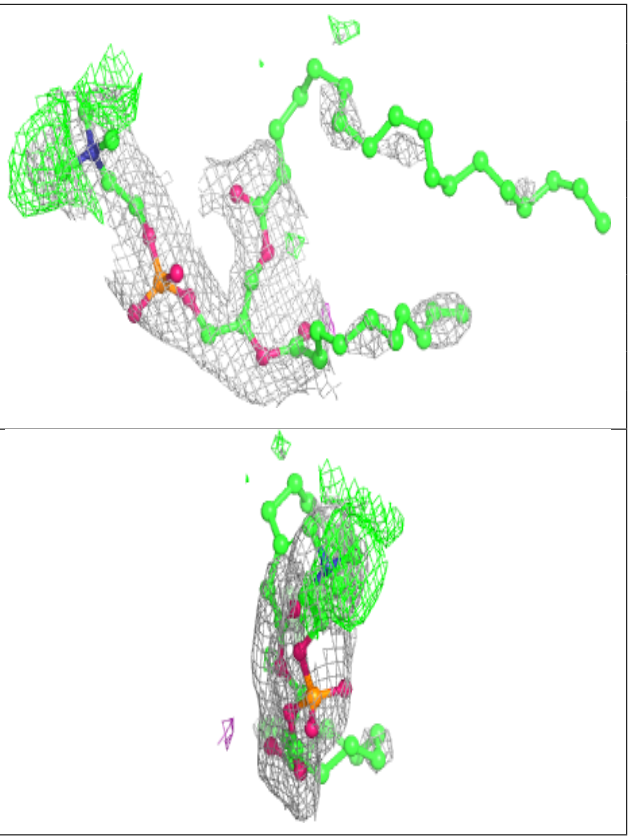
Electron density around PCW A 1104:

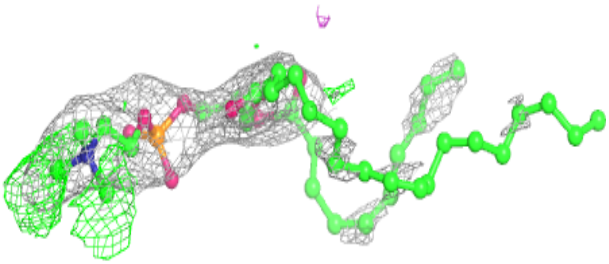
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PCW A 1102:

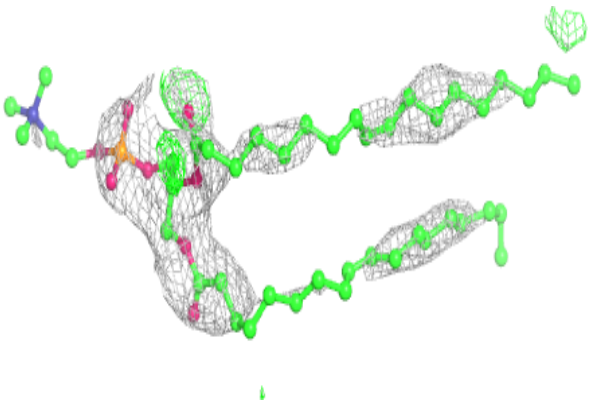
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

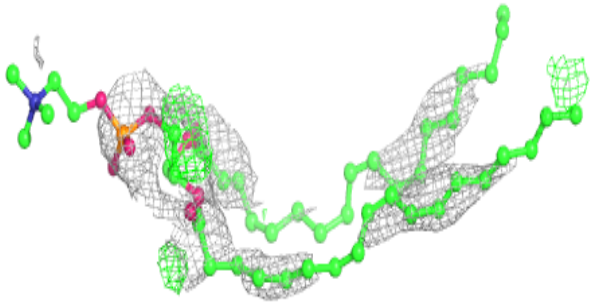


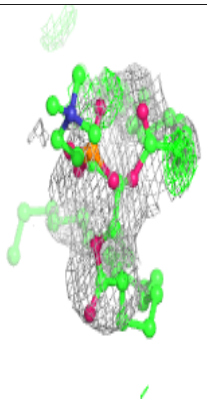


Electron density around PCW A 1112:

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

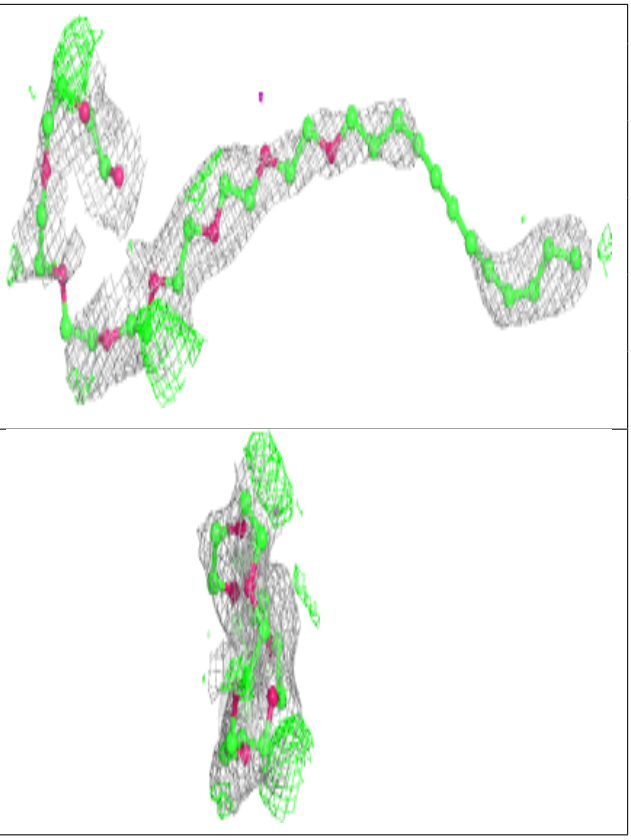


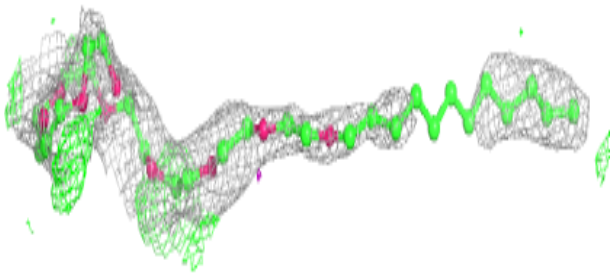




Electron density around CE1 A 1103:

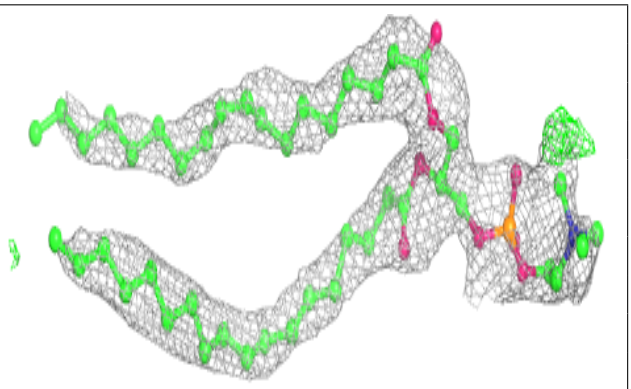
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

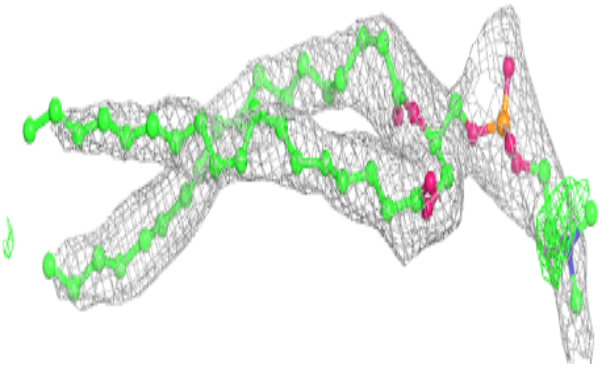


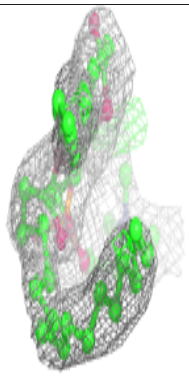


Electron density around PCW B 303:

$2mF_o$-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.