



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:19 AM UTC

PDB ID : 4RET / pdb_00004ret
Title : Crystal structure of the Na,K-ATPase E2P-digoxin complex with bound magnesium
Authors : Gregersen, J.L.; Laursen, M.; Yatime, L.; Nissen, P.; Fedosova, N.U.
Deposited on : 2014-09-23
Resolution : 4.00 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

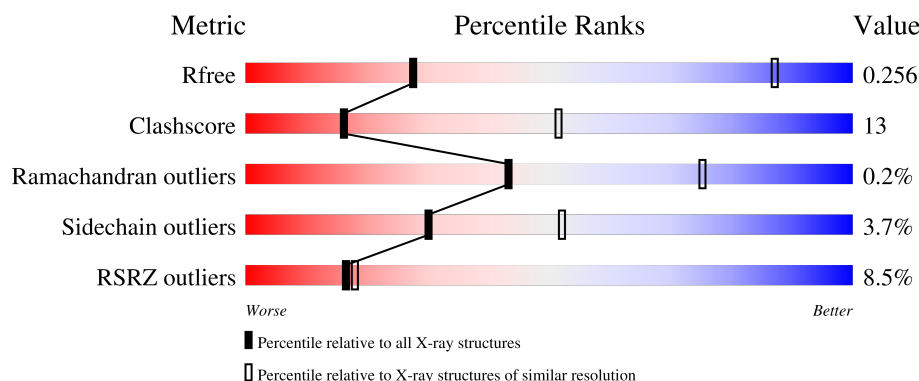
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	1021	6% 69% 27% ..
1	C	1021	10% 69% 27% ..
2	B	303	10% 61% 30% ..
2	D	303	9% 61% 30% 5%
3	E	65	3% 38% 9% 51%

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Mol	Chain	Length	Quality of chain
3	G	65	
4	F	2	
5	H	2	
5	I	2	

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
5	GLC	H	1	-	-	X	-
7	CLR	A	1104	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21123 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			
1	C	996	Total	C	N	O	P	S	0	0	0
			7730	4922	1301	1459	1	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	290	Total	C	N	O	S	0	0	0
			2377	1540	388	436	13			
2	D	288	Total	C	N	O	S	0	0	0
			2357	1525	385	434	13			

- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

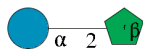
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

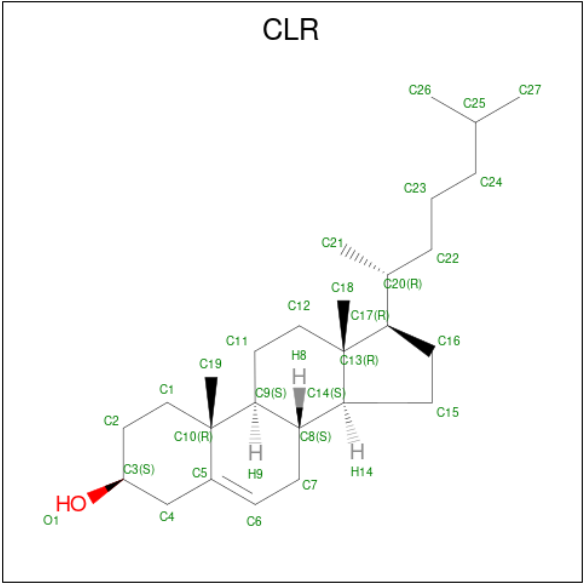


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	2	Total	C	O	0	0	0
			23	12	11			
5	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Mg	0	0
			3	3		
6	C	3	Total	Mg	0	0
			3	3		

- Molecule 7 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



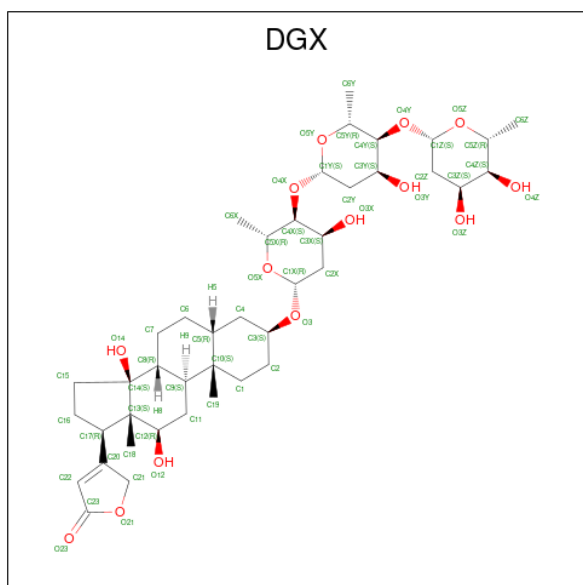
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		
7	G	1	Total	C	O	0	0
			28	27	1		

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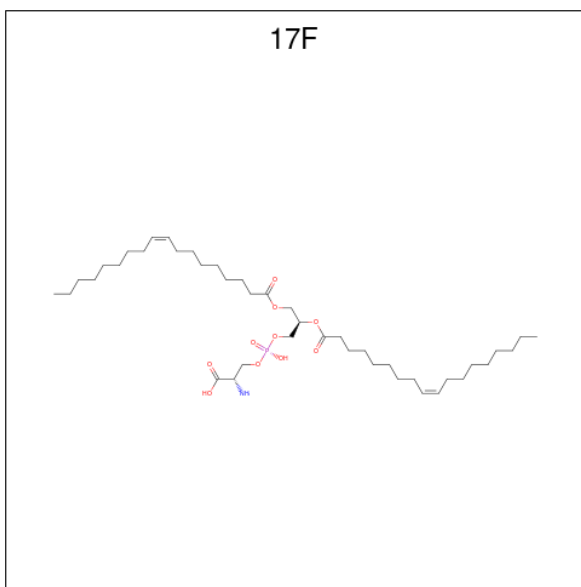
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			28	27	1		
7	C	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is DIGOXIN (CCD ID: DGX) (formula: $C_{41}H_{64}O_{14}$).



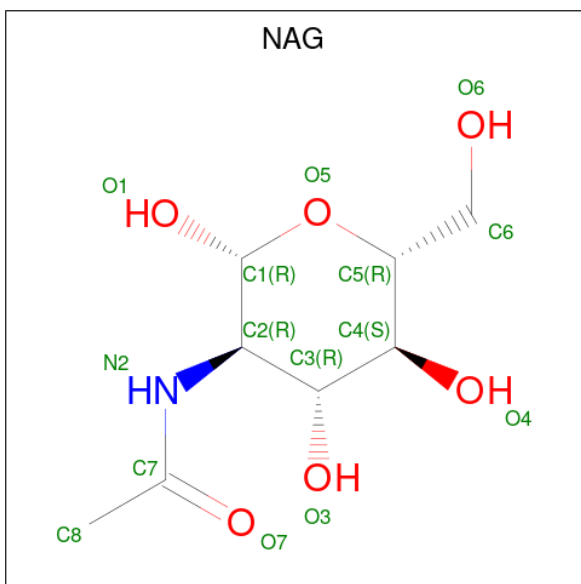
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			55	41	14		
8	C	1	Total	C	O	0	0
			55	41	14		

- Molecule 9 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: $C_{42}H_{78}NO_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			15	6	1	7	1		
9	B	1	Total	C	N	O	P	0	0
			24	13	1	9	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

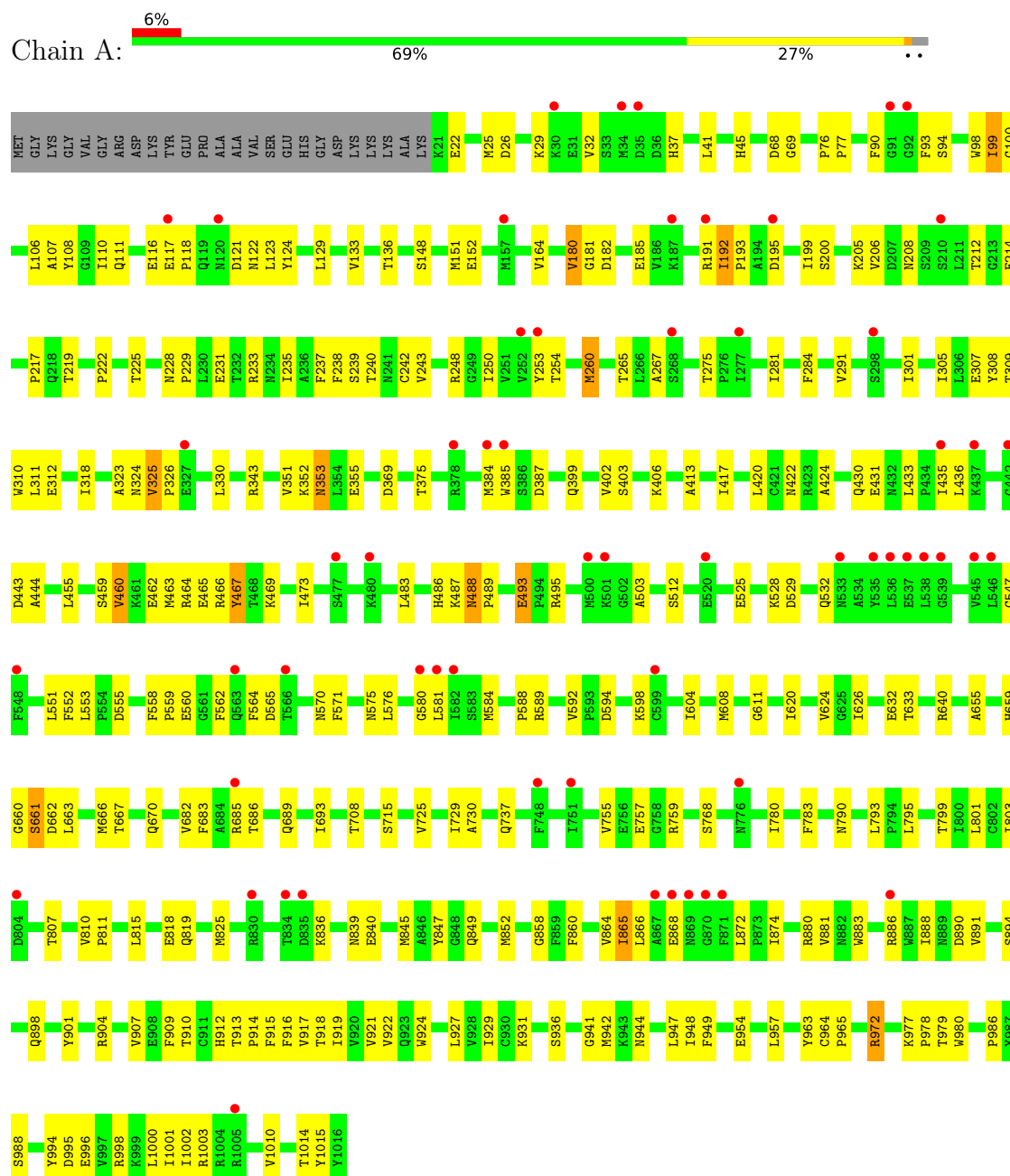
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	3	Total	O	0	0
			3	3		
11	C	3	Total	O	0	0
			3	3		

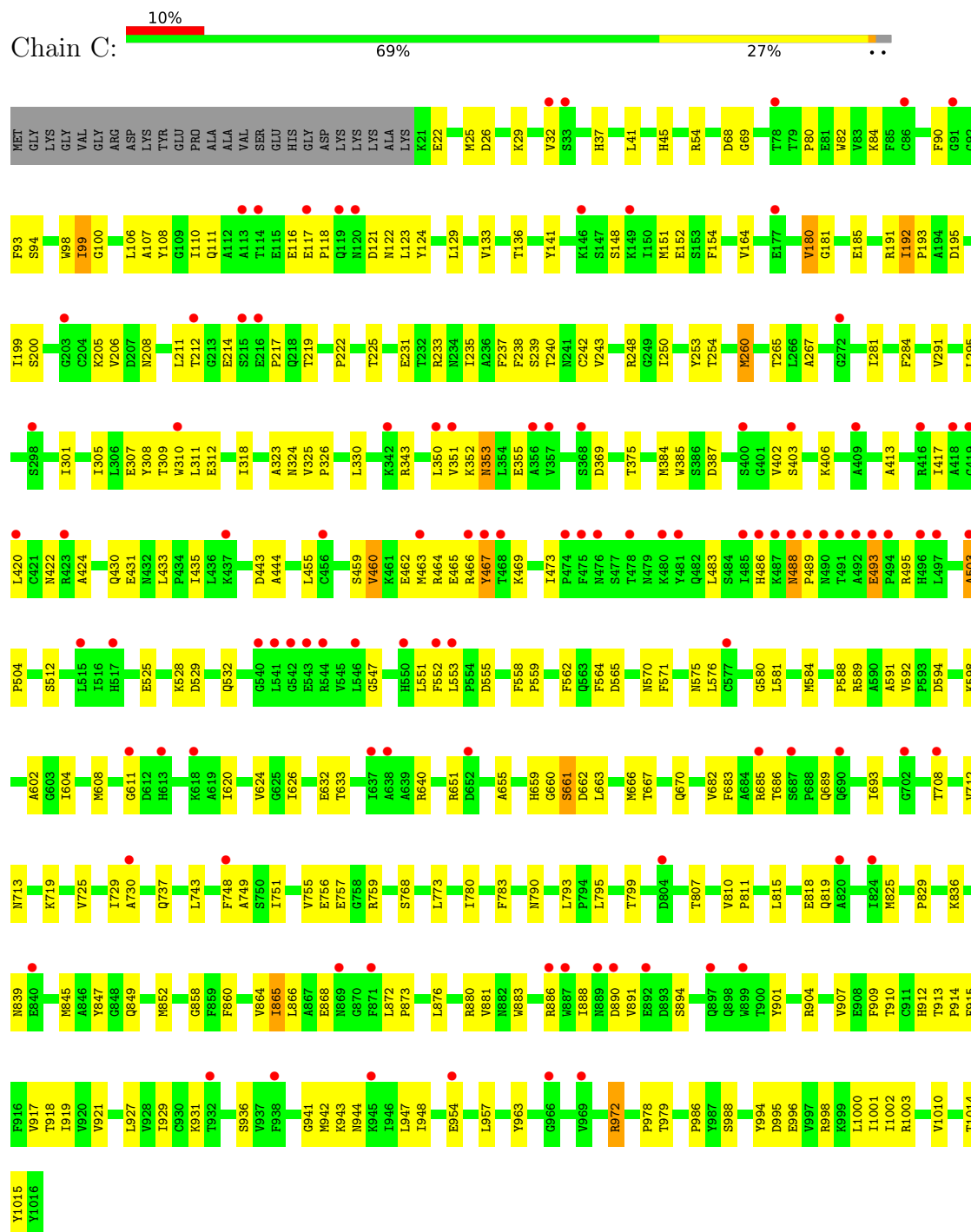
3 Residue-property plots [i](#)

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.

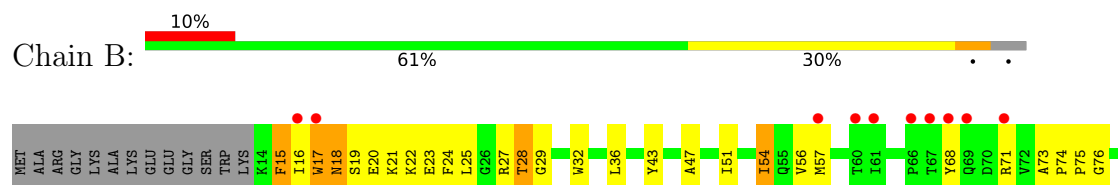
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

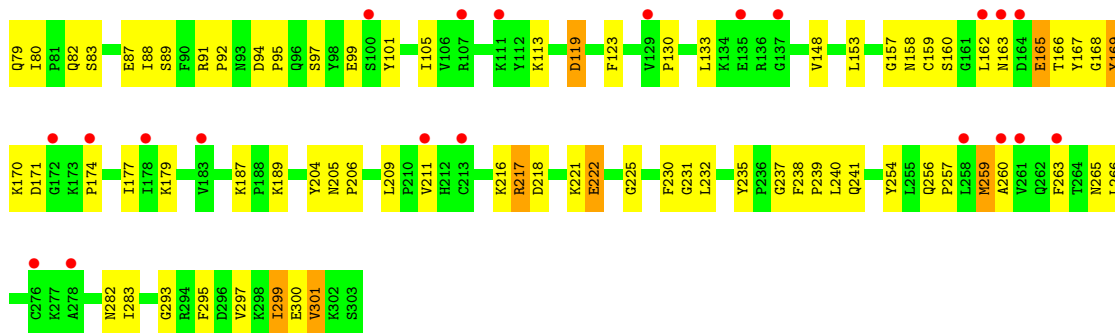


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

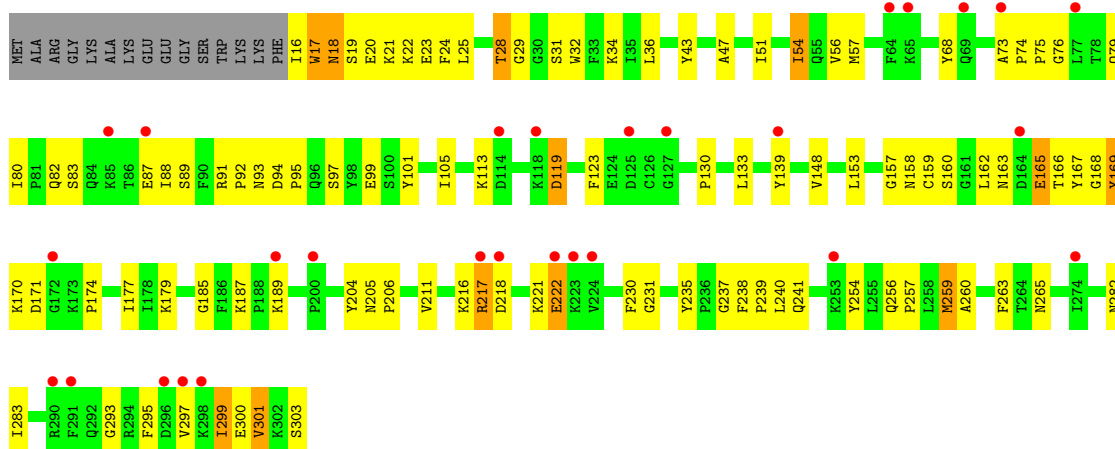


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

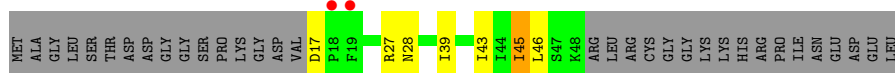
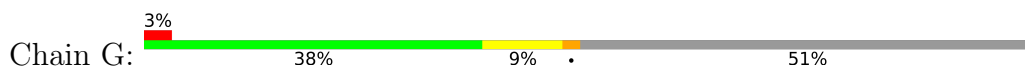




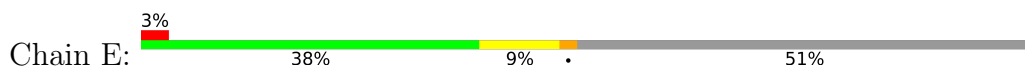
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain H:  50% 50%



- Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain I:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.24Å 118.35Å 494.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 4.00 49.41 – 4.00	Depositor EDS
% Data completeness (in resolution range)	72.2 (49.41-4.00) 74.2 (49.41-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, R_{free}	0.221 , 0.253 0.233 , 0.256	Depositor DCC
R_{free} test set	2209 reflections (2.31%)	wwPDB-VP
Wilson B-factor (Å ²)	153.1	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 146.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21123	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: GLC, CLR, PHD, NAG, FRU, MG, 17F, DGX

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	0.37	2/7867 (0.0%)	0.80	11/10674 (0.1%)
1	C	0.37	2/7867 (0.0%)	0.80	10/10674 (0.1%)
2	B	0.37	0/2440	0.85	5/3290 (0.2%)
2	D	0.36	0/2419	0.84	3/3263 (0.1%)
3	E	0.32	0/261	0.87	0/354
3	G	0.33	0/261	0.88	2/354 (0.6%)
All	All	0.37	4/21115 (0.0%)	0.81	31/28609 (0.1%)

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	3
2	D	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	737	GLN	CD-NE2	-7.83	1.16	1.33
1	A	737	GLN	CD-NE2	-7.46	1.17	1.33
1	A	737	GLN	CD-OE1	-6.17	1.11	1.23
1	C	737	GLN	CD-OE1	-5.73	1.12	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	ILE	CA-C-N	7.20	126.70	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	192	ILE	C-N-CA	7.20	126.70	118.85
1	A	192	ILE	CA-C-N	7.12	126.62	118.85
1	A	192	ILE	C-N-CA	7.12	126.62	118.85
2	D	205	ASN	CA-C-N	-7.02	111.67	118.97
2	D	205	ASN	C-N-CA	-7.02	111.67	118.97
2	B	205	ASN	CA-C-N	-6.93	111.77	118.97
2	B	205	ASN	C-N-CA	-6.93	111.77	118.97
1	A	503	ALA	CA-C-N	5.62	125.72	119.32
1	A	503	ALA	C-N-CA	5.62	125.72	119.32
1	A	493	GLU	CA-C-N	-5.59	116.01	121.65
1	A	493	GLU	C-N-CA	-5.59	116.01	121.65
1	C	488	ASN	CA-C-N	5.55	125.07	119.19
1	C	488	ASN	C-N-CA	5.55	125.07	119.19
1	A	488	ASN	CA-C-N	5.44	124.96	119.19
1	A	488	ASN	C-N-CA	5.44	124.96	119.19
1	C	503	ALA	CA-C-N	5.44	125.52	119.32
1	C	503	ALA	C-N-CA	5.44	125.52	119.32
1	C	793	LEU	CA-C-N	5.42	124.75	118.85
1	C	793	LEU	C-N-CA	5.42	124.75	118.85
1	C	493	GLU	CA-C-N	-5.40	116.20	121.65
1	C	493	GLU	C-N-CA	-5.40	116.20	121.65
1	A	793	LEU	CA-C-N	5.34	124.67	118.85
1	A	793	LEU	C-N-CA	5.34	124.67	118.85
3	G	17	ASP	CA-C-N	5.21	124.93	119.82
3	G	17	ASP	C-N-CA	5.21	124.93	119.82
2	B	222	GLU	N-CA-C	-5.17	106.82	113.02
2	D	222	GLU	N-CA-C	-5.17	106.82	113.02
1	A	325	VAL	N-CA-C	5.08	112.89	107.76
2	B	209	LEU	CA-C-N	5.04	125.49	120.14
2	B	209	LEU	C-N-CA	5.04	125.49	120.14

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	15	PHE	Peptide
2	B	165	GLU	Peptide
2	B	222	GLU	Peptide
2	D	165	GLU	Peptide
2	D	222	GLU	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	7730	0	7776	199	0
1	C	7730	0	7776	192	0
2	B	2377	0	2349	80	0
2	D	2357	0	2326	78	0
3	E	255	0	259	5	0
3	G	255	0	259	4	0
4	F	28	0	25	0	0
5	H	23	0	21	11	0
5	I	23	0	21	5	0
6	A	3	0	0	0	0
6	C	3	0	0	0	0
7	A	28	0	46	4	0
7	C	56	0	92	7	0
7	G	28	0	46	5	0
8	A	55	0	64	2	0
8	C	55	0	64	2	0
9	A	31	0	18	5	0
9	B	24	0	20	2	0
10	B	14	0	13	0	0
10	D	42	0	39	1	0
11	A	3	0	0	0	0
11	C	3	0	0	0	0
All	All	21123	0	21214	553	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 13.

All (553) 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)
2:D:170:LYS:HB2	2:D:174:PRO:HA	1.57	0.86
2:B:170:LYS:HB2	2:B:174:PRO:HA	1.57	0.86
1:C:488:ASN:ND2	1:C:493:GLU:O	2.09	0.86
1:A:488:ASN:ND2	1:A:493:GLU:O	2.09	0.84
1:A:977:LYS:HB3	5:H:1:GLC:H62	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.65	0.78
1:A:978:PRO:HB3	7:G:1001:CLR:H192	1.66	0.78
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.65	0.78
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.66	0.78
1:A:659:HIS:HB3	1:A:685:ARG:HH22	1.49	0.77
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.65	0.77
1:C:659:HIS:HB3	1:C:685:ARG:HH22	1.48	0.76
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.66	0.76
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.68	0.74
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.68	0.74
1:A:385:TRP:HB3	1:A:581:LEU:H	1.53	0.73
1:C:385:TRP:HB3	1:C:581:LEU:H	1.53	0.71
2:D:216:LYS:HB2	2:D:221:LYS:HG2	1.73	0.70
1:A:375:THR:HA	1:A:588:PRO:HA	1.74	0.70
1:A:565:ASP:O	1:A:570:ASN:ND2	2.25	0.70
2:B:80:ILE:HD11	2:B:177:ILE:HD12	1.73	0.70
2:B:216:LYS:HB2	2:B:221:LYS:HG2	1.73	0.70
1:A:979:THR:H	5:H:1:GLC:H61	1.56	0.69
1:C:565:ASP:O	1:C:570:ASN:ND2	2.25	0.69
1:C:22:GLU:HA	1:C:25:MET:HG3	1.75	0.69
2:D:80:ILE:HD11	2:D:177:ILE:HD12	1.73	0.69
1:C:111:GLN:HB3	1:C:116:GLU:HG2	1.75	0.68
1:A:22:GLU:HA	1:A:25:MET:HG3	1.75	0.68
2:B:29:GLY:HA2	2:B:32:TRP:CD1	2.30	0.67
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.60	0.67
1:A:111:GLN:HB3	1:A:116:GLU:HG2	1.75	0.67
1:A:493:GLU:OE1	1:A:495:ARG:NH2	2.29	0.66
2:D:29:GLY:HA2	2:D:32:TRP:CD1	2.30	0.66
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.60	0.66
1:C:493:GLU:OE1	1:C:495:ARG:NH2	2.28	0.65
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.78	0.65
1:C:865:ILE:HD12	1:C:914:PRO:HG3	1.78	0.65
2:D:160:SER:HB2	2:D:169:TYR:HE1	1.62	0.65
1:C:430:GLN:HG3	1:C:433:LEU:HD12	1.79	0.64
1:A:611:GLY:HA2	1:A:686:THR:H	1.63	0.64
1:C:267:ALA:O	1:C:719:LYS:NZ	2.31	0.63
1:C:611:GLY:HA2	1:C:686:THR:H	1.63	0.63
1:C:117:GLU:HG3	1:C:118:PRO:HD3	1.81	0.63
1:C:978:PRO:HB2	5:I:2:FRU:C1	2.28	0.63
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.80	0.63
1:A:430:GLN:HG3	1:A:433:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:SER:HB2	2:B:169:TYR:CE1	2.34	0.63
2:B:160:SER:HB2	2:B:169:TYR:HE1	1.62	0.63
2:D:160:SER:HB2	2:D:169:TYR:CE1	2.34	0.63
1:A:979:THR:HG22	7:A:1104:CLR:H41	1.81	0.62
1:C:200:SER:HA	1:C:222:PRO:HG3	1.81	0.62
2:D:189:LYS:H	2:D:282:ASN:HB2	1.64	0.62
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.80	0.62
2:D:165:GLU:HB3	2:D:166:THR:HA	1.81	0.62
1:C:941:GLY:HA3	5:H:2:FRU:H4	1.80	0.62
2:B:189:LYS:H	2:B:282:ASN:HB2	1.65	0.62
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.82	0.62
2:B:158:ASN:O	2:B:166:THR:OG1	2.17	0.61
1:A:117:GLU:HG3	1:A:118:PRO:HD3	1.82	0.61
1:A:907:VAL:HA	1:A:910:THR:HG22	1.82	0.61
1:C:868:GLU:OE1	7:C:2004:CLR:O1	2.17	0.61
2:D:158:ASN:O	2:D:166:THR:OG1	2.18	0.61
1:A:1010:VAL:O	1:A:1014:THR:OG1	2.14	0.61
2:B:165:GLU:HB3	2:B:166:THR:HA	1.81	0.61
1:A:208:ASN:HB3	1:A:212:THR:HG22	1.83	0.61
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.36	0.61
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.81	0.61
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.82	0.61
1:C:29:LYS:HE2	1:C:265:THR:HB	1.83	0.61
1:C:931:LYS:NZ	1:C:941:GLY:O	2.32	0.61
1:A:205:LYS:HG2	1:A:219:THR:HG22	1.82	0.60
1:C:907:VAL:HA	1:C:910:THR:HG22	1.83	0.60
1:A:29:LYS:HE2	1:A:265:THR:HB	1.83	0.60
1:A:931:LYS:NZ	1:A:941:GLY:O	2.32	0.60
1:C:807:THR:HG22	1:C:957:LEU:HD23	1.83	0.60
1:A:200:SER:HA	1:A:222:PRO:HG3	1.81	0.60
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.36	0.60
1:A:807:THR:HG22	1:A:957:LEU:HD23	1.84	0.60
1:C:205:LYS:HG2	1:C:219:THR:HG22	1.83	0.60
1:C:979:THR:HG22	7:C:2004:CLR:H41	1.82	0.60
2:B:16:ILE:C	2:B:18:ASN:H	2.09	0.60
2:D:265:ASN:HD22	10:D:2003:NAG:H83	1.67	0.60
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.83	0.59
1:A:529:ASP:HA	1:A:532:GLN:HB2	1.84	0.59
1:C:111:GLN:OE1	1:C:122:ASN:ND2	2.36	0.59
1:A:931:LYS:HE2	1:A:947:LEU:HD13	1.85	0.59
1:C:208:ASN:HB3	1:C:212:THR:HG22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:529:ASP:HA	1:C:532:GLN:HB2	1.84	0.59
2:D:204:TYR:C	2:D:206:PRO:HD2	2.28	0.59
2:D:130:PRO:HB2	2:D:204:TYR:CE1	2.38	0.58
1:A:180:VAL:HG23	1:A:254:THR:HG22	1.85	0.58
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.86	0.58
2:B:130:PRO:HB2	2:B:204:TYR:CE1	2.39	0.58
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.83	0.58
1:A:551:LEU:HD22	1:A:576:LEU:HD23	1.85	0.58
2:B:79:GLN:HE21	2:B:82:GLN:HA	1.68	0.58
1:C:180:VAL:HG23	1:C:254:THR:HG22	1.85	0.58
1:C:260:MET:HE2	1:C:712:VAL:HG11	1.84	0.58
1:C:608:MET:HE3	1:C:626:ILE:HD12	1.85	0.58
1:C:901:TYR:HA	1:C:904:ARG:HE	1.69	0.58
2:B:204:TYR:C	2:B:206:PRO:HD2	2.28	0.58
1:C:116:GLU:HG3	1:C:118:PRO:HD2	1.85	0.58
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.86	0.57
1:C:118:PRO:HB3	1:C:122:ASN:HB2	1.85	0.57
1:C:592:VAL:HG22	1:C:748:PHE:HD2	1.69	0.57
1:C:807:THR:HB	1:C:954:GLU:HG3	1.86	0.57
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.86	0.57
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.86	0.57
1:A:807:THR:HB	1:A:954:GLU:HG3	1.86	0.57
2:D:79:GLN:HE21	2:D:82:GLN:HA	1.67	0.57
1:A:901:TYR:HA	1:A:904:ARG:HE	1.69	0.57
2:B:25:LEU:H	2:B:29:GLY:HA3	1.70	0.57
1:A:118:PRO:HB3	1:A:122:ASN:HB2	1.85	0.57
1:A:608:MET:HE3	1:A:626:ILE:HD12	1.85	0.57
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.86	0.57
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.87	0.57
1:A:116:GLU:HG3	1:A:118:PRO:HD2	1.86	0.57
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.87	0.57
1:A:111:GLN:OE1	1:A:122:ASN:ND2	2.37	0.57
1:C:986:PRO:HG3	7:C:2004:CLR:H181	1.85	0.56
2:B:119:ASP:O	2:B:123:PHE:HB2	2.06	0.56
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.86	0.56
1:C:931:LYS:HE2	1:C:947:LEU:HD13	1.86	0.56
1:C:551:LEU:HD22	1:C:576:LEU:HD23	1.86	0.56
2:D:73:ALA:O	2:D:75:PRO:HD3	2.06	0.56
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.87	0.56
2:B:101:TYR:O	2:B:105:ILE:HG13	2.06	0.56
2:D:101:TYR:O	2:D:105:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:ILE:C	2:D:18:ASN:H	2.13	0.55
1:A:661:SER:HB3	1:A:685:ARG:HH21	1.71	0.55
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.87	0.55
1:C:978:PRO:HB3	7:C:2006:CLR:H192	1.87	0.55
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.88	0.55
2:B:73:ALA:O	2:B:75:PRO:HD3	2.06	0.55
1:A:888:ILE:O	1:A:904:ARG:NH2	2.40	0.55
2:B:16:ILE:O	2:B:18:ASN:N	2.40	0.55
1:C:1010:VAL:O	1:C:1014:THR:OG1	2.15	0.55
1:A:512:SER:HB3	1:A:575:ASN:HA	1.89	0.55
1:C:998:ARG:HE	1:C:1014:THR:HB	1.72	0.54
1:A:977:LYS:HB3	5:H:1:GLC:C6	2.33	0.54
1:C:551:LEU:HD13	1:C:576:LEU:HA	1.90	0.54
1:C:888:ILE:O	1:C:904:ARG:NH2	2.41	0.54
2:D:166:THR:HG21	2:D:170:LYS:H	1.72	0.54
2:D:133:LEU:HG	2:D:240:LEU:HB3	1.88	0.54
2:B:133:LEU:HG	2:B:240:LEU:HB3	1.89	0.54
1:C:661:SER:HB3	1:C:685:ARG:HH21	1.71	0.54
2:D:119:ASP:O	2:D:123:PHE:HB2	2.07	0.54
1:C:890:ASP:OD1	2:D:82:GLN:NE2	2.41	0.54
1:A:998:ARG:HE	1:A:1014:THR:HB	1.72	0.54
1:C:301:ILE:O	1:C:305:ILE:HG12	2.08	0.54
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.88	0.54
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.90	0.53
1:C:632:GLU:OE1	1:C:640:ARG:NH1	2.42	0.53
2:D:25:LEU:H	2:D:29:GLY:HA3	1.72	0.53
1:C:591:ALA:HB1	1:C:749:ALA:HB2	1.91	0.53
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.90	0.53
1:A:301:ILE:O	1:A:305:ILE:HG12	2.08	0.53
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.91	0.53
2:B:166:THR:HG21	2:B:170:LYS:H	1.73	0.53
1:A:551:LEU:HD13	1:A:576:LEU:HA	1.90	0.53
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.91	0.53
2:B:80:ILE:HG21	2:B:105:ILE:HA	1.91	0.53
1:C:890:ASP:OD1	1:C:890:ASP:N	2.42	0.53
1:A:632:GLU:OE1	1:A:640:ARG:NH1	2.42	0.52
1:A:547:GLY:HA2	1:A:581:LEU:HD23	1.92	0.52
1:A:661:SER:H	1:A:685:ARG:HH21	1.57	0.52
1:A:890:ASP:OD1	1:A:890:ASP:N	2.42	0.52
2:B:231:GLY:HA3	2:B:235:TYR:O	2.09	0.52
1:C:512:SER:HB3	1:C:575:ASN:HA	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:GLU:HG3	9:A:1108:17F:HN1	1.75	0.52
1:C:443:ASP:OD1	1:C:444:ALA:N	2.41	0.52
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.75	0.52
1:A:460:VAL:HG13	1:A:463:MET:HE3	1.92	0.52
1:C:68:ASP:OD1	1:C:69:GLY:N	2.33	0.52
1:C:206:VAL:HA	1:C:242:CYS:HA	1.92	0.52
1:C:661:SER:H	1:C:685:ARG:HH21	1.58	0.52
1:C:825:MET:HE2	1:C:825:MET:HA	1.91	0.52
2:D:80:ILE:HG21	2:D:105:ILE:HA	1.91	0.52
2:D:166:THR:HB	2:D:169:TYR:H	1.74	0.52
1:A:148:SER:O	1:A:152:GLU:HG2	2.10	0.52
2:B:166:THR:HB	2:B:169:TYR:H	1.74	0.52
2:B:217:ARG:NH1	2:B:218:ASP:OD2	2.43	0.52
1:C:460:VAL:HG13	1:C:463:MET:HE3	1.91	0.52
1:A:68:ASP:OD1	1:A:69:GLY:N	2.33	0.51
1:A:136:THR:HG21	1:A:330:LEU:HG	1.92	0.51
9:A:1108:17F:H5	9:A:1109:17F:H5	1.90	0.51
1:C:729:ILE:HG13	1:C:730:ALA:H	1.75	0.51
2:D:217:ARG:NH1	2:D:218:ASP:OD2	2.43	0.51
2:D:231:GLY:HA3	2:D:235:TYR:O	2.09	0.51
1:A:308:TYR:HB3	1:A:312:GLU:HB2	1.92	0.51
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.75	0.51
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.91	0.51
1:C:420:LEU:HB3	1:C:486:HIS:HE1	1.76	0.51
1:C:818:GLU:OE2	1:C:931:LYS:NZ	2.43	0.51
1:A:890:ASP:OD1	2:B:82:GLN:NE2	2.44	0.51
1:A:979:THR:OG1	5:H:1:GLC:H5	2.11	0.51
1:C:136:THR:HG21	1:C:330:LEU:HG	1.93	0.51
1:C:291:VAL:HG21	1:C:847:TYR:HE2	1.76	0.51
1:C:435:ILE:HD12	1:C:455:LEU:HD12	1.92	0.51
1:C:768:SER:HA	1:C:815:LEU:HD23	1.93	0.51
1:A:825:MET:HA	1:A:825:MET:HE2	1.91	0.51
1:C:375:THR:HA	1:C:588:PRO:HA	1.92	0.51
1:C:1002:ILE:HD13	1:C:1015:TYR:HB2	1.93	0.51
2:D:170:LYS:HB2	2:D:174:PRO:CA	2.36	0.51
1:A:206:VAL:HA	1:A:242:CYS:HA	1.92	0.51
1:A:435:ILE:HD12	1:A:455:LEU:HD12	1.91	0.51
1:C:90:PHE:O	1:C:94:SER:HB2	2.11	0.51
1:A:99:ILE:HG13	1:A:100:GLY:N	2.26	0.51
1:A:1002:ILE:HD13	1:A:1015:TYR:HB2	1.93	0.51
1:C:683:PHE:HB3	1:C:686:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:O	1:A:94:SER:HB2	2.12	0.50
1:A:93:PHE:HE1	1:A:284:PHE:HE2	1.59	0.50
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.75	0.50
1:A:729:ILE:HG13	1:A:730:ALA:H	1.74	0.50
1:C:547:GLY:HA2	1:C:581:LEU:HD23	1.92	0.50
1:A:275:THR:OG1	1:A:355:GLU:OE2	2.27	0.50
1:A:689:GLN:O	1:A:693:ILE:HG12	2.11	0.50
1:A:936:SER:OG	1:A:996:GLU:OE2	2.24	0.50
1:A:238:PHE:HD2	1:A:260:MET:HG2	1.77	0.50
1:A:443:ASP:OD1	1:A:444:ALA:N	2.42	0.50
1:A:768:SER:HA	1:A:815:LEU:HD23	1.93	0.50
1:A:840:GLU:HB3	9:B:1004:17F:C3	2.41	0.50
1:C:25:MET:O	1:C:29:LYS:HG3	2.12	0.50
1:C:99:ILE:HG13	1:C:100:GLY:N	2.27	0.50
1:C:689:GLN:O	1:C:693:ILE:HG12	2.11	0.50
1:C:909:PHE:CG	1:C:972:ARG:HG3	2.47	0.50
1:A:462:GLU:HA	1:A:465:GLU:HG2	1.93	0.50
1:C:978:PRO:HD2	5:I:1:GLC:O2	2.12	0.50
2:D:153:LEU:H	2:D:153:LEU:HD12	1.77	0.50
1:A:25:MET:O	1:A:29:LYS:HG3	2.11	0.50
1:A:909:PHE:CG	1:A:972:ARG:HG3	2.47	0.50
1:C:116:GLU:HG3	1:C:118:PRO:CD	2.42	0.50
1:C:238:PHE:HD2	1:C:260:MET:HG2	1.76	0.50
1:C:151:MET:HA	1:C:151:MET:HE2	1.94	0.50
1:C:308:TYR:HB3	1:C:312:GLU:HB2	1.92	0.50
1:C:462:GLU:HA	1:C:465:GLU:HG2	1.94	0.50
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.77	0.50
1:A:291:VAL:HG21	1:A:847:TYR:HE2	1.76	0.50
1:C:151:MET:HE3	1:C:350:LEU:HD23	1.93	0.50
1:C:237:PHE:O	1:C:240:THR:OG1	2.25	0.50
1:C:660:GLY:HA2	1:C:663:LEU:HD12	1.94	0.50
1:C:790:ASN:OD1	1:C:880:ARG:NH1	2.41	0.49
1:C:979:THR:CG2	7:C:2004:CLR:H41	2.42	0.49
2:B:153:LEU:H	2:B:153:LEU:HD12	1.77	0.49
1:A:986:PRO:HG3	7:A:1104:CLR:H181	1.94	0.49
1:A:551:LEU:HG	1:A:552:PHE:O	2.12	0.49
1:C:41:LEU:H	1:C:41:LEU:HD12	1.77	0.49
1:C:211:LEU:O	1:C:713:ASN:HB3	2.12	0.49
1:C:310:TRP:H	1:C:310:TRP:CD1	2.29	0.49
1:C:343:ARG:NH2	1:C:757:GLU:OE1	2.45	0.49
1:A:151:MET:HE2	1:A:151:MET:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:HA2	1:A:250:ILE:HG23	1.95	0.49
1:A:106:LEU:O	1:A:110:ILE:HG12	2.12	0.49
1:A:343:ARG:NH2	1:A:757:GLU:OE1	2.45	0.49
1:A:979:THR:HB	5:H:1:GLC:O6	2.12	0.49
1:C:181:GLY:HA2	1:C:250:ILE:HG23	1.94	0.49
1:C:836:LYS:HB2	1:C:839:ASN:HB3	1.94	0.49
1:C:942:MET:HE1	1:C:947:LEU:HD22	1.94	0.49
1:A:41:LEU:HD12	1:A:41:LEU:H	1.77	0.49
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.77	0.49
2:B:170:LYS:HB2	2:B:174:PRO:CA	2.36	0.49
1:A:898:GLN:HE22	2:B:179:LYS:HE3	1.78	0.49
1:A:915:PHE:O	1:A:919:ILE:HG12	2.12	0.49
1:A:924:TRP:CH2	7:G:1001:CLR:H231	2.48	0.49
1:C:93:PHE:HE1	1:C:284:PHE:HE2	1.59	0.49
1:A:116:GLU:HG3	1:A:118:PRO:CD	2.42	0.49
1:A:310:TRP:H	1:A:310:TRP:CD1	2.29	0.49
1:C:915:PHE:O	1:C:919:ILE:HG12	2.13	0.49
2:D:21:LYS:HD2	2:D:21:LYS:HA	1.55	0.49
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.94	0.48
2:B:79:GLN:N	2:B:79:GLN:OE1	2.45	0.48
1:C:106:LEU:O	1:C:110:ILE:HG12	2.13	0.48
1:A:872:LEU:HD23	1:A:894:SER:HB2	1.95	0.48
1:A:942:MET:HE1	1:A:947:LEU:HD22	1.94	0.48
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.95	0.48
1:C:148:SER:O	1:C:152:GLU:HG2	2.12	0.48
1:C:551:LEU:HG	1:C:552:PHE:O	2.12	0.48
1:A:783:PHE:CE1	8:A:1107:DGX:H2	2.49	0.48
1:A:1000:LEU:HD23	1:A:1003:ARG:NH2	2.29	0.48
1:C:872:LEU:HD23	1:C:894:SER:HB2	1.96	0.48
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.47	0.48
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.48	0.48
2:D:79:GLN:OE1	2:D:79:GLN:N	2.46	0.48
3:E:39:ILE:O	3:E:43:ILE:HG12	2.14	0.48
1:C:467:TYR:CZ	1:C:489:PRO:HG3	2.49	0.48
1:C:978:PRO:HB2	5:I:2:FRU:O1	2.14	0.48
1:A:467:TYR:CZ	1:A:489:PRO:HG3	2.49	0.48
1:A:790:ASN:OD1	1:A:880:ARG:NH1	2.42	0.48
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.95	0.47
1:A:978:PRO:HB2	5:H:2:FRU:H12	1.96	0.47
9:A:1108:17F:C5	9:A:1109:17F:H5	2.44	0.47
2:B:24:PHE:HB3	2:B:28:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1000:LEU:HD23	1:C:1003:ARG:NH2	2.29	0.47
2:D:157:GLY:C	2:D:159:CYS:H	2.22	0.47
1:A:129:LEU:O	1:A:133:VAL:HG23	2.14	0.47
1:A:237:PHE:O	1:A:240:THR:OG1	2.24	0.47
1:A:660:GLY:HA2	1:A:663:LEU:HD12	1.95	0.47
2:B:211:VAL:CG2	2:B:259:MET:HE1	2.43	0.47
7:C:2004:CLR:H231	7:C:2004:CLR:H211	1.62	0.47
1:A:963:TYR:CE2	7:G:1001:CLR:H6	2.50	0.47
2:B:21:LYS:O	2:B:23:GLU:HA	2.14	0.47
1:C:212:THR:HG23	1:C:214:GLU:H	1.80	0.47
1:A:979:THR:H	5:H:1:GLC:C6	2.27	0.47
3:G:39:ILE:O	3:G:43:ILE:HG12	2.14	0.47
1:C:858:GLY:HA2	1:C:918:THR:HG21	1.96	0.47
1:A:98:TRP:CE2	1:A:133:VAL:HG11	2.49	0.47
1:A:212:THR:HG23	1:A:214:GLU:H	1.79	0.47
2:D:21:LYS:O	2:D:23:GLU:HA	2.14	0.47
2:D:51:ILE:O	2:D:54:ILE:HG22	2.14	0.47
1:A:661:SER:H	1:A:685:ARG:NH2	2.12	0.47
2:B:157:GLY:C	2:B:159:CYS:H	2.22	0.47
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.48	0.47
1:C:661:SER:H	1:C:685:ARG:NH2	2.13	0.47
2:D:24:PHE:HB3	2:D:28:THR:HA	1.96	0.47
2:B:51:ILE:O	2:B:54:ILE:HG22	2.15	0.47
2:B:166:THR:N	2:B:167:TYR:HA	2.30	0.47
1:A:118:PRO:C	1:A:121:ASP:H	2.23	0.46
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.96	0.46
2:D:167:TYR:C	2:D:169:TYR:N	2.73	0.46
2:D:22:LYS:HA	2:D:23:GLU:HA	1.62	0.46
1:A:977:LYS:HB2	1:A:980:TRP:NE1	2.31	0.46
1:C:129:LEU:O	1:C:133:VAL:HG23	2.15	0.46
2:D:94:ASP:HB3	2:D:97:SER:HB2	1.98	0.46
1:A:836:LYS:HB2	1:A:839:ASN:HB3	1.96	0.46
1:C:107:ALA:HB2	1:C:318:ILE:HG21	1.98	0.46
1:C:118:PRO:C	1:C:121:ASP:H	2.24	0.46
1:C:424:ALA:O	1:C:464:ARG:NH2	2.48	0.46
1:C:462:GLU:O	1:C:466:ARG:HB2	2.16	0.46
1:A:422:ASN:HB3	1:A:424:ALA:H	1.81	0.46
1:A:979:THR:CG2	7:A:1104:CLR:H41	2.45	0.46
2:B:237:GLY:HA2	2:B:259:MET:HE2	1.98	0.46
1:C:324:ASN:HA	1:C:780:ILE:HD11	1.97	0.46
1:A:868:GLU:OE2	2:B:68:TYR:HE2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:795:LEU:HD13	1:C:915:PHE:HB3	1.97	0.46
1:A:963:TYR:O	3:G:27:ARG:HG3	2.15	0.46
1:C:93:PHE:CE2	1:C:330:LEU:HB2	2.51	0.46
2:D:237:GLY:HA2	2:D:259:MET:HE2	1.98	0.46
1:A:462:GLU:O	1:A:466:ARG:HB2	2.16	0.45
2:B:94:ASP:HB3	2:B:97:SER:HB2	1.98	0.45
2:D:166:THR:N	2:D:167:TYR:HA	2.30	0.45
2:D:230:PHE:HB2	2:D:260:ALA:HB3	1.97	0.45
1:A:424:ALA:O	1:A:464:ARG:NH2	2.49	0.45
1:A:729:ILE:HG13	1:A:730:ALA:N	2.31	0.45
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.51	0.45
1:C:936:SER:OG	1:C:996:GLU:OE2	2.23	0.45
1:C:963:TYR:O	3:E:27:ARG:HG3	2.16	0.45
1:A:191:ARG:HE	1:A:239:SER:HA	1.82	0.45
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.51	0.45
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.52	0.45
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.56	0.45
1:C:469:LYS:HA	1:C:486:HIS:CD2	2.52	0.45
1:C:729:ILE:HG13	1:C:730:ALA:N	2.31	0.45
1:C:852:MET:HG2	2:D:43:TYR:CE2	2.52	0.45
2:B:168:GLY:HA3	2:B:171:ASP:HB2	1.99	0.45
1:C:662:ASP:O	1:C:666:MET:HG3	2.16	0.45
1:A:325:VAL:HA	1:A:326:PRO:HD3	1.72	0.45
2:B:167:TYR:C	2:B:169:TYR:N	2.73	0.45
1:C:384:MET:HE3	1:C:384:MET:HB2	1.91	0.45
1:C:422:ASN:HB3	1:C:424:ALA:H	1.80	0.45
1:A:941:GLY:HA3	5:I:2:FRU:H61	1.97	0.45
1:C:929:ILE:HB	1:C:995:ASP:OD2	2.17	0.45
1:A:666:MET:HE2	1:A:666:MET:HB3	1.88	0.45
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.52	0.45
2:D:162:LEU:HB3	2:D:163:ASN:H	1.51	0.45
1:A:852:MET:HG2	2:B:43:TYR:CE2	2.52	0.45
1:A:972:ARG:HD3	1:A:972:ARG:HA	1.62	0.45
1:C:594:ASP:O	1:C:598:LYS:HG2	2.17	0.45
3:E:45:ILE:H	3:E:45:ILE:HG13	1.54	0.45
2:B:15:PHE:HB2	2:B:16:ILE:HG12	1.98	0.45
1:A:662:ASP:O	1:A:666:MET:HG3	2.16	0.45
1:C:467:TYR:HB3	1:C:486:HIS:HB3	1.99	0.45
2:B:230:PHE:HB2	2:B:260:ALA:HB3	1.98	0.44
1:C:845:MET:HA	1:C:849:GLN:HE21	1.82	0.44
2:B:79:GLN:HB3	2:B:295:PHE:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:GLN:HB3	2:D:295:PHE:CE1	2.52	0.44
1:A:93:PHE:CE2	1:A:330:LEU:HB2	2.52	0.44
1:A:107:ALA:HB2	1:A:318:ILE:HG21	1.98	0.44
1:A:608:MET:HE1	1:A:620:ILE:HG22	1.98	0.44
2:B:21:LYS:HG3	2:B:22:LYS:H	1.82	0.44
9:B:1004:17F:H1	9:B:1004:17F:H4A	1.99	0.44
1:C:80:PRO:HB2	1:C:84:LYS:HD3	1.99	0.44
1:C:191:ARG:HE	1:C:239:SER:HA	1.81	0.44
1:A:324:ASN:HA	1:A:780:ILE:HD11	1.98	0.44
1:A:929:ILE:HB	1:A:995:ASP:OD2	2.17	0.44
1:A:118:PRO:HA	1:A:121:ASP:CB	2.46	0.44
9:A:1108:17F:H2	2:B:27:ARG:NH2	2.32	0.44
1:C:891:VAL:HG21	1:C:904:ARG:NH1	2.33	0.44
1:A:801:LEU:HD23	1:A:801:LEU:HA	1.82	0.44
2:D:80:ILE:HG13	2:D:177:ILE:HB	2.00	0.44
1:A:469:LYS:HA	1:A:486:HIS:CD2	2.52	0.44
1:C:118:PRO:HA	1:C:121:ASP:CB	2.47	0.44
1:C:944:ASN:O	1:C:948:ILE:HG12	2.17	0.44
2:D:168:GLY:HA3	2:D:171:ASP:HB2	1.99	0.44
1:A:467:TYR:HB3	1:A:486:HIS:HB3	1.99	0.44
1:C:913:THR:N	1:C:914:PRO:HD2	2.33	0.44
1:A:845:MET:HA	1:A:849:GLN:HE21	1.83	0.44
1:C:633:THR:HA	1:C:655:ALA:O	2.18	0.44
1:A:868:GLU:OE1	7:A:1104:CLR:O1	2.25	0.43
2:B:80:ILE:HG13	2:B:177:ILE:HB	2.00	0.43
2:B:91:ARG:HD2	2:B:94:ASP:H	1.83	0.43
1:C:608:MET:HE1	1:C:620:ILE:HG22	1.99	0.43
1:C:667:THR:N	1:C:670:GLN:OE1	2.44	0.43
2:D:47:ALA:O	2:D:51:ILE:HG13	2.17	0.43
2:D:89:SER:HA	2:D:300:GLU:O	2.18	0.43
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.98	0.43
2:D:76:GLY:HA2	2:D:293:GLY:H	1.83	0.43
2:B:89:SER:HA	2:B:300:GLU:O	2.18	0.43
2:B:216:LYS:H	2:B:221:LYS:HD2	1.83	0.43
1:C:584:MET:HE2	1:C:584:MET:HB3	1.91	0.43
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.82	0.43
2:D:91:ARG:HD2	2:D:94:ASP:H	1.83	0.43
1:A:185:GLU:HB2	1:A:248:ARG:HD3	2.01	0.43
1:A:323:ALA:HB1	1:A:780:ILE:HG12	2.01	0.43
1:A:413:ALA:O	1:A:417:ILE:HG13	2.19	0.43
1:A:594:ASP:O	1:A:598:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.76	0.43
1:A:880:ARG:HG3	1:A:881:VAL:N	2.34	0.43
1:A:944:ASN:O	1:A:948:ILE:HG12	2.17	0.43
1:C:473:ILE:HD12	1:C:483:LEU:HD21	2.01	0.43
2:D:216:LYS:H	2:D:221:LYS:HD2	1.83	0.43
2:D:239:PRO:HB3	2:D:241:GLN:HE21	1.84	0.43
1:A:860:PHE:O	1:A:864:VAL:HG23	2.19	0.43
2:D:174:PRO:O	2:D:263:PHE:N	2.48	0.43
2:D:187:LYS:O	2:D:282:ASN:ND2	2.52	0.43
2:D:211:VAL:CG2	2:D:259:MET:HE1	2.49	0.43
1:A:891:VAL:HG21	1:A:904:ARG:NH1	2.34	0.43
1:C:559:PRO:HG2	1:C:562:PHE:HB2	2.00	0.43
1:A:76:PRO:HA	1:A:77:PRO:HD3	1.84	0.43
1:A:559:PRO:HG2	1:A:562:PHE:HB2	2.00	0.43
1:A:633:THR:HA	1:A:655:ALA:O	2.19	0.43
1:C:217:PRO:HB3	1:C:243:VAL:HG21	2.01	0.43
2:D:68:TYR:HH	5:I:1:GLC:HO3	1.64	0.43
1:A:225:THR:HG21	1:A:233:ARG:HD2	2.01	0.43
1:A:525:GLU:HA	1:A:528:LYS:HB3	2.01	0.43
1:A:849:GLN:OE1	1:A:994:TYR:OH	2.37	0.43
1:C:323:ALA:HB1	1:C:780:ILE:HG12	2.00	0.43
1:C:413:ALA:O	1:C:417:ILE:HG13	2.19	0.43
1:C:860:PHE:O	1:C:864:VAL:HG23	2.19	0.43
1:C:943:LYS:HE3	5:H:2:FRU:O3	2.19	0.43
1:A:620:ILE:HD13	1:A:620:ILE:HA	1.94	0.42
1:A:913:THR:N	1:A:914:PRO:HD2	2.34	0.42
1:C:185:GLU:HB2	1:C:248:ARG:HD3	2.01	0.42
1:C:192:ILE:HA	1:C:193:PRO:HD3	1.69	0.42
1:C:592:VAL:HG22	1:C:748:PHE:CD2	2.51	0.42
1:C:611:GLY:HA2	1:C:686:THR:N	2.33	0.42
1:A:217:PRO:HB3	1:A:243:VAL:HG21	2.01	0.42
1:A:667:THR:N	1:A:670:GLN:OE1	2.44	0.42
1:C:608:MET:HB3	1:C:682:VAL:HG22	2.01	0.42
1:C:880:ARG:HG3	1:C:881:VAL:N	2.33	0.42
2:D:21:LYS:HG3	2:D:22:LYS:H	1.84	0.42
2:B:47:ALA:O	2:B:51:ILE:HG13	2.18	0.42
2:B:68:TYR:OH	5:H:1:GLC:H4	2.19	0.42
2:B:174:PRO:O	2:B:263:PHE:N	2.47	0.42
1:A:182:ASP:OD1	1:A:182:ASP:N	2.51	0.42
1:A:810:VAL:HB	1:A:811:PRO:HD3	2.02	0.42
2:B:22:LYS:HA	2:B:23:GLU:HA	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LYS:O	2:B:282:ASN:ND2	2.52	0.42
2:D:179:LYS:HE2	2:D:179:LYS:HB3	1.91	0.42
1:A:384:MET:HE3	1:A:384:MET:HB2	1.90	0.42
1:C:225:THR:HG21	1:C:233:ARG:HD2	2.01	0.42
1:A:267:ALA:HB2	1:A:715:SER:HB3	2.01	0.42
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.85	0.42
1:A:584:MET:HE2	1:A:584:MET:HB3	1.91	0.42
2:B:71:ARG:HD3	2:B:71:ARG:HA	1.83	0.42
1:C:353:ASN:HD21	1:C:355:GLU:HG2	1.85	0.42
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.70	0.42
1:A:403:SER:OG	1:A:406:LYS:NZ	2.53	0.42
9:A:1108:17F:H2	2:B:27:ARG:CZ	2.50	0.42
1:A:977:LYS:C	5:H:1:GLC:H61	2.45	0.42
1:A:978:PRO:HB3	7:G:1001:CLR:C19	2.43	0.42
2:B:76:GLY:HA2	2:B:293:GLY:H	1.84	0.42
2:B:162:LEU:HB3	2:B:163:ASN:H	1.51	0.42
2:B:179:LYS:HD2	2:B:256:GLN:HE21	1.85	0.42
2:D:179:LYS:HD2	2:D:256:GLN:HE21	1.84	0.42
1:A:487:LYS:NZ	1:A:560:GLU:O	2.48	0.42
1:A:803:ILE:HG12	1:A:916:PHE:HD1	1.85	0.42
1:C:525:GLU:HA	1:C:528:LYS:HB3	2.01	0.42
1:C:743:LEU:HD11	1:C:751:ILE:CD1	2.49	0.42
1:C:849:GLN:OE1	1:C:994:TYR:OH	2.37	0.42
1:C:921:VAL:HG12	1:C:988:SER:OG	2.20	0.42
1:A:708:THR:HG22	1:A:725:VAL:HB	2.02	0.41
2:B:95:PRO:O	2:B:99:GLU:HG2	2.20	0.41
2:B:239:PRO:HB3	2:B:241:GLN:HE21	1.85	0.41
1:C:620:ILE:HD13	1:C:620:ILE:HA	1.94	0.41
1:C:708:THR:HG22	1:C:725:VAL:HB	2.02	0.41
2:D:16:ILE:O	2:D:18:ASN:N	2.51	0.41
1:A:663:LEU:HD23	1:A:666:MET:SD	2.60	0.41
1:A:874:ILE:H	1:A:874:ILE:HD12	1.85	0.41
1:C:555:ASP:N	1:C:555:ASP:OD1	2.53	0.41
1:A:108:TYR:CD2	1:A:123:LEU:HB2	2.55	0.41
2:B:80:ILE:CG2	2:B:105:ILE:HA	2.51	0.41
1:C:651:ARG:HD3	1:C:651:ARG:HA	1.89	0.41
1:C:978:PRO:HG3	3:E:26:VAL:HG13	2.02	0.41
1:C:325:VAL:HA	1:C:326:PRO:HD3	1.73	0.41
1:A:323:ALA:HA	8:A:1107:DGX:C23	2.51	0.41
1:C:108:TYR:CD2	1:C:123:LEU:HB2	2.55	0.41
1:A:555:ASP:N	1:A:555:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:CYS:HA	1:A:965:PRO:HD3	1.95	0.41
2:B:24:PHE:HB3	2:B:29:GLY:H	1.86	0.41
7:G:1001:CLR:H191	7:G:1001:CLR:H8	1.73	0.41
1:C:94:SER:HB3	1:C:133:VAL:HG13	2.03	0.41
1:C:873:PRO:HA	1:C:876:LEU:HD12	2.03	0.41
2:D:91:ARG:HG2	2:D:93:ASN:H	1.86	0.41
2:D:238:PHE:HA	2:D:239:PRO:HD3	1.95	0.41
2:B:83:SER:HB3	2:B:87:GLU:H	1.85	0.41
2:B:225:GLY:HA2	2:B:266:LEU:HD23	2.03	0.41
2:D:17:TRP:C	2:D:19:SER:H	2.28	0.41
1:A:921:VAL:HG12	1:A:988:SER:OG	2.21	0.41
2:D:31:SER:HB2	2:D:34:LYS:HD2	2.03	0.41
2:D:92:PRO:HD2	2:D:303:SER:HB2	2.03	0.41
2:D:167:TYR:O	2:D:167:TYR:CG	2.73	0.41
1:A:473:ILE:HD12	1:A:483:LEU:HD21	2.01	0.41
1:A:553:LEU:HD13	1:A:558:PHE:CD2	2.56	0.41
1:A:755:VAL:O	1:A:759:ARG:HB2	2.20	0.41
1:A:818:GLU:OE2	1:A:931:LYS:NZ	2.42	0.41
2:B:17:TRP:C	2:B:19:SER:H	2.29	0.41
2:B:238:PHE:HA	2:B:239:PRO:HD3	1.96	0.41
1:C:54:ARG:HE	1:C:54:ARG:HB3	1.73	0.41
1:C:82:TRP:CD1	1:C:141:TYR:HH	2.39	0.41
1:C:403:SER:OG	1:C:406:LYS:NZ	2.54	0.41
2:D:95:PRO:O	2:D:99:GLU:HG2	2.20	0.41
1:A:883:TRP:HA	1:A:904:ARG:NH1	2.36	0.41
1:A:918:THR:O	1:A:922:VAL:HG22	2.21	0.41
1:C:199:ILE:HG13	1:C:200:SER:N	2.36	0.41
1:C:309:THR:HG23	1:C:311:LEU:HB3	2.02	0.41
1:C:553:LEU:HD13	1:C:558:PHE:CD2	2.56	0.41
1:C:755:VAL:O	1:C:759:ARG:HB2	2.21	0.41
1:C:756:GLU:HA	1:C:825:MET:HE3	2.03	0.41
1:A:228:ASN:HA	1:A:229:PRO:HD3	1.89	0.40
1:A:309:THR:HG23	1:A:311:LEU:HB3	2.03	0.40
1:A:608:MET:HB3	1:A:682:VAL:HG22	2.02	0.40
1:C:602:ALA:O	1:C:829:PRO:HD3	2.22	0.40
1:C:773:LEU:HD23	1:C:773:LEU:HA	1.90	0.40
1:C:810:VAL:HB	1:C:811:PRO:HD3	2.02	0.40
1:C:503:ALA:HA	1:C:504:PRO:HD3	1.89	0.40
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.76	0.40
1:A:199:ILE:HG13	1:A:200:SER:N	2.36	0.40
1:A:353:ASN:HD21	1:A:355:GLU:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LYS:HE3	1:A:469:LYS:HB2	1.83	0.40
2:B:80:ILE:HD11	2:B:177:ILE:HB	2.04	0.40
2:B:179:LYS:HE2	2:B:179:LYS:HB3	1.92	0.40
1:C:108:TYR:CD1	1:C:118:PRO:HB2	2.57	0.40
1:C:295:LEU:HD23	1:C:295:LEU:HA	1.85	0.40
2:D:80:ILE:HD11	2:D:177:ILE:HB	2.03	0.40
2:D:83:SER:OG	2:D:87:GLU:O	2.29	0.40
1:A:949:PHE:HB2	3:G:45:ILE:HG23	2.04	0.40
1:C:663:LEU:HD23	1:C:666:MET:SD	2.61	0.40
1:C:783:PHE:CE1	8:C:2005:DGX:H2	2.56	0.40
8:C:2005:DGX:H19B	8:C:2005:DGX:H11	1.91	0.40
2:D:80:ILE:CG2	2:D:105:ILE:HA	2.51	0.40
2:B:225:GLY:HA2	2:B:265:ASN:O	2.22	0.40
7:C:2006:CLR:H213	7:C:2006:CLR:H231	1.88	0.40
2:D:139:TYR:OH	2:D:185:GLY:HA2	2.22	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	993/1021 (97%)	941 (95%)	52 (5%)	0	100	100
1	C	993/1021 (97%)	942 (95%)	51 (5%)	0	100	100
2	B	288/303 (95%)	268 (93%)	17 (6%)	3 (1%)	12	45
2	D	286/303 (94%)	265 (93%)	18 (6%)	3 (1%)	12	45
3	E	30/65 (46%)	30 (100%)	0	0	100	100
3	G	30/65 (46%)	30 (100%)	0	0	100	100
All	All	2620/2778 (94%)	2476 (94%)	138 (5%)	6 (0%)	43	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	TRP
2	B	18	ASN
2	B	217	ARG
2	D	18	ASN
2	D	217	ARG
2	D	17	TRP

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	846/864 (98%)	819 (97%)	27 (3%)	34	56
1	C	846/864 (98%)	818 (97%)	28 (3%)	33	56
2	B	260/269 (97%)	247 (95%)	13 (5%)	22	45
2	D	258/269 (96%)	246 (95%)	12 (5%)	23	46
3	E	26/52 (50%)	24 (92%)	2 (8%)	12	35
3	G	26/52 (50%)	24 (92%)	2 (8%)	12	35
All	All	2262/2370 (95%)	2178 (96%)	84 (4%)	30	52

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	32	VAL
1	A	45	HIS
1	A	99	ILE
1	A	124	TYR
1	A	164	VAL
1	A	180	VAL
1	A	231	GLU
1	A	260	MET
1	A	281	ILE
1	A	307	GLU
1	A	351	VAL
1	A	352	LYS

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Mol	Chain	Res	Type
1	A	353	ASN
1	A	387	ASP
1	A	402	VAL
1	A	431	GLU
1	A	459	SER
1	A	460	VAL
1	A	467	TYR
1	A	564	PHE
1	A	571	PHE
1	A	661	SER
1	A	819	GLN
1	A	865	ILE
1	A	917	VAL
1	A	972	ARG
2	B	20	GLU
2	B	28	THR
2	B	36	LEU
2	B	54	ILE
2	B	56	VAL
2	B	119	ASP
2	B	169	TYR
2	B	232	LEU
2	B	259	MET
2	B	283	ILE
2	B	297	VAL
2	B	299	ILE
2	B	301	VAL
3	G	28	ASN
3	G	45	ILE
1	C	26	ASP
1	C	32	VAL
1	C	45	HIS
1	C	99	ILE
1	C	124	TYR
1	C	154	PHE
1	C	164	VAL
1	C	180	VAL
1	C	231	GLU
1	C	260	MET
1	C	281	ILE
1	C	307	GLU
1	C	351	VAL

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Mol	Chain	Res	Type
1	C	352	LYS
1	C	353	ASN
1	C	387	ASP
1	C	402	VAL
1	C	431	GLU
1	C	459	SER
1	C	460	VAL
1	C	467	TYR
1	C	564	PHE
1	C	571	PHE
1	C	661	SER
1	C	819	GLN
1	C	865	ILE
1	C	917	VAL
1	C	972	ARG
2	D	20	GLU
2	D	28	THR
2	D	36	LEU
2	D	54	ILE
2	D	56	VAL
2	D	119	ASP
2	D	169	TYR
2	D	259	MET
2	D	283	ILE
2	D	297	VAL
2	D	299	ILE
2	D	301	VAL
3	E	28	ASN
3	E	45	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	ASN
1	A	486	HIS
1	A	521	GLN
1	A	557	GLN
1	A	737	GLN
2	B	69	GLN
2	B	96	GLN
1	C	241	ASN
1	C	486	HIS

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Mol	Chain	Res	Type
1	C	521	GLN
1	C	557	GLN
2	D	69	GLN
2	D	96	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	PHD	A	369	6,1	9,11,12	1.35	2 (22%)	9,15,17	1.69	2 (22%)
1	PHD	C	369	6,1	9,11,12	1.39	2 (22%)	9,15,17	1.79	2 (22%)

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	PHD	A	369	6,1	-	0/8/11/13	-
1	PHD	C	369	6,1	-	0/8/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	CB-CA	-2.32	1.48	1.53
1	A	369	PHD	CB-CA	-2.14	1.49	1.53
1	C	369	PHD	P-OD1	-2.09	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	PHD	P-OD1	-2.09	1.55	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	OD1-CG-CB	3.79	119.85	110.95
1	A	369	PHD	OD1-CG-CB	3.60	119.40	110.95
1	C	369	PHD	OD2-CG-CB	-2.65	118.50	124.65
1	A	369	PHD	OD2-CG-CB	-2.38	119.12	124.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

6 monosaccharides are 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	$\# Z > 2$
4	NAG	F	1	4,2	14,14,15	1.90	1 (7%)	17,19,21	0.75	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.38	0
5	GLC	H	1	5	11,11,12	0.56	0	15,15,17	1.11	2 (13%)
5	FRU	H	2	5	11,12,12	0.46	0	10,18,18	1.02	0
5	GLC	I	1	5	11,11,12	0.46	0	15,15,17	0.71	0
5	FRU	I	2	5	11,12,12	0.77	1 (9%)	10,18,18	0.68	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
4	NAG	F	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	GLC	H	1	5	-	1/2/19/22	0/1/1/1
5	FRU	H	2	5	-	0/5/24/24	0/1/1/1
5	GLC	I	1	5	-	2/2/19/22	0/1/1/1
5	FRU	I	2	5	-	3/5/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	O5-C1	6.88	1.55	1.43
5	I	2	FRU	O5-C2	-2.08	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1	GLC	O5-C5-C6	2.11	111.76	107.66
5	H	1	GLC	C6-C5-C4	-2.01	108.08	113.02

There are no chirality outliers.

All (8) torsion outliers are listed below:

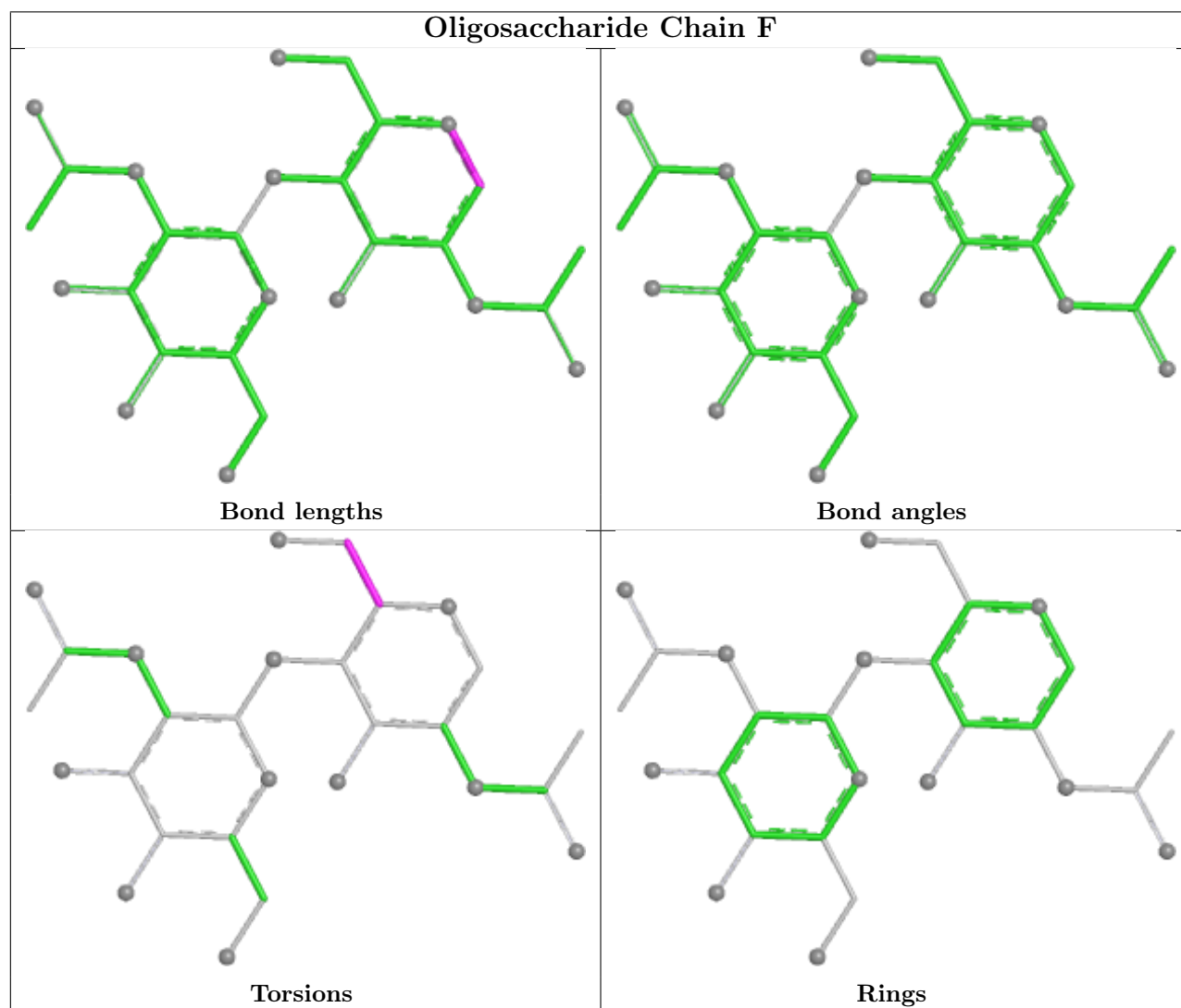
Mol	Chain	Res	Type	Atoms
5	I	2	FRU	O1-C1-C2-C3
5	I	2	FRU	O1-C1-C2-O2
5	I	2	FRU	O1-C1-C2-O5
4	F	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	I	1	GLC	O5-C5-C6-O6
5	I	1	GLC	C4-C5-C6-O6
5	H	1	GLC	O5-C5-C6-O6

There are no ring outliers.

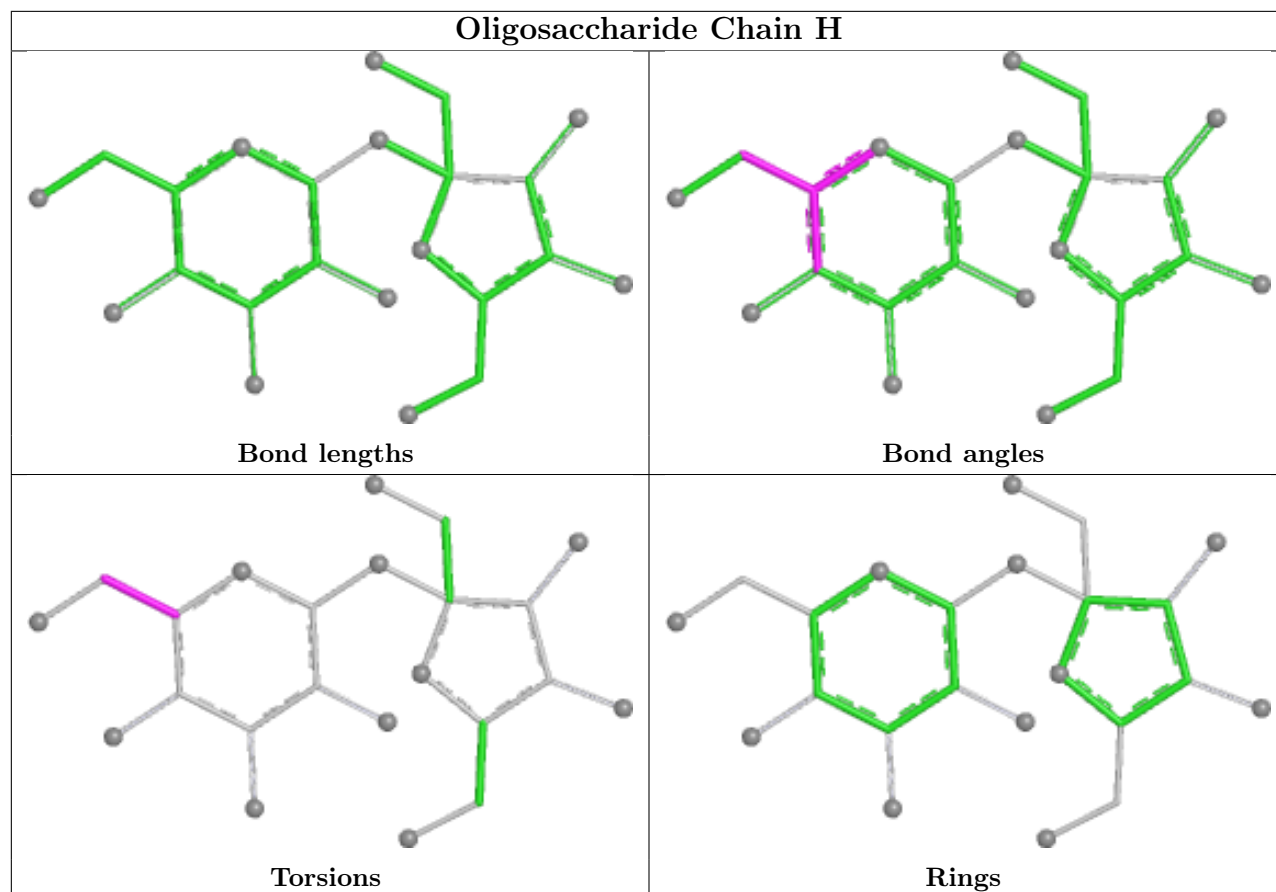
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	2	FRU	3	0
5	I	1	GLC	2	0
5	H	1	GLC	8	0
5	H	2	FRU	3	0

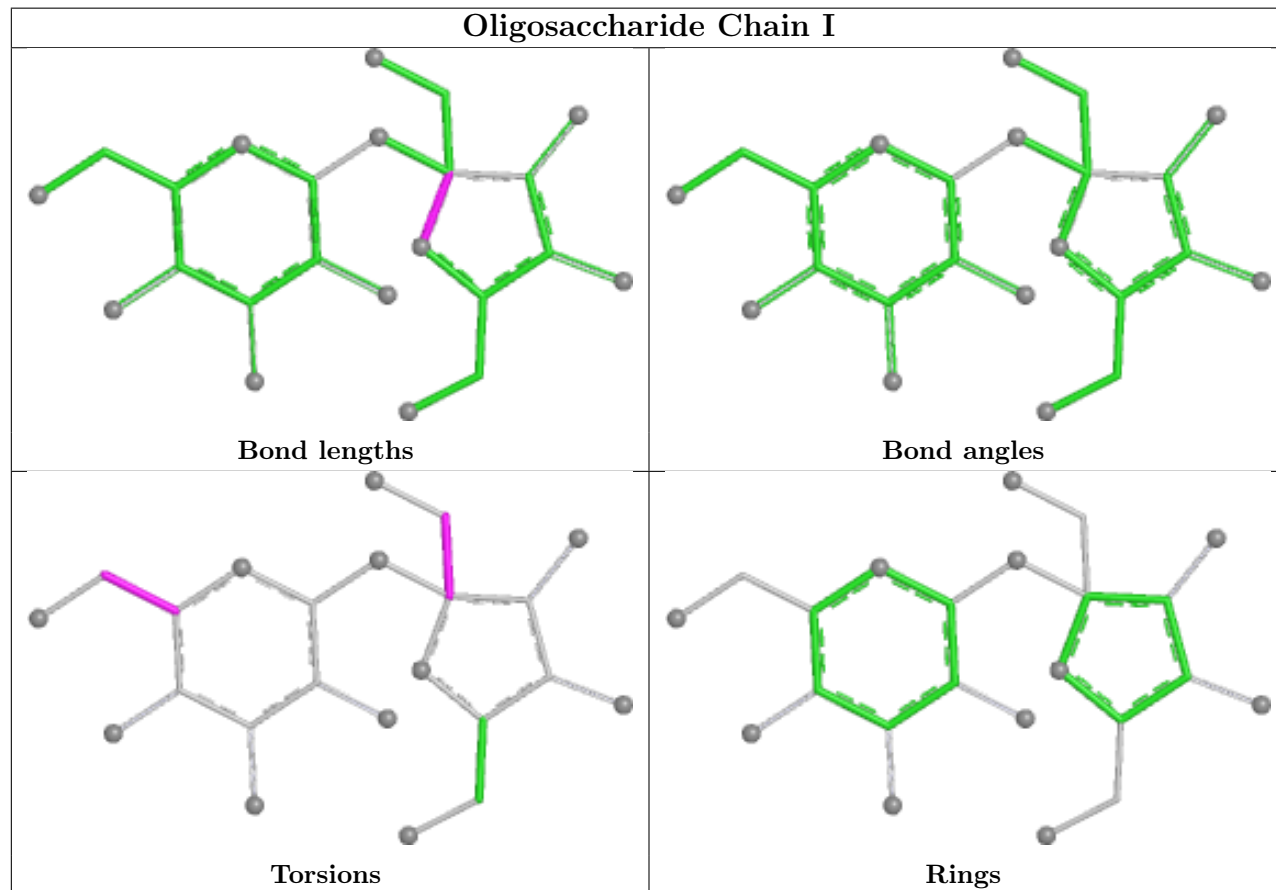
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



Oligosaccharide Chain H



Oligosaccharide Chain I



5.6 Ligand geometry

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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$
7	CLR	A	1104	-	31,31,31	2.49	9 (29%)	48,48,48	3.23	19 (39%)
10	NAG	D	2003	2	14,14,15	0.64	0	17,19,21	0.87	2 (11%)
7	CLR	G	1001	-	31,31,31	2.50	9 (29%)	48,48,48	3.17	19 (39%)
8	DGX	C	2005	-	62,62,62	1.19	3 (4%)	89,98,98	1.76	18 (20%)
7	CLR	C	2006	-	31,31,31	2.49	7 (22%)	48,48,48	2.93	17 (35%)
8	DGX	A	1107	-	62,62,62	1.22	5 (8%)	89,98,98	1.78	20 (22%)
10	NAG	B	1003	2	14,14,15	0.39	0	17,19,21	0.45	0
7	CLR	C	2004	-	31,31,31	2.51	9 (29%)	48,48,48	3.10	19 (39%)
10	NAG	D	2001	2	14,14,15	0.40	0	17,19,21	0.36	0
9	17F	A	1108	-	14,15,53	1.56	2 (14%)	14,20,60	1.95	2 (14%)
10	NAG	D	2002	2	14,14,15	0.30	0	17,19,21	0.44	0
9	17F	A	1109	-	13,14,53	1.85	2 (15%)	14,19,60	1.59	2 (14%)
9	17F	B	1004	-	22,23,53	1.65	3 (13%)	23,29,60	1.36	3 (13%)

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
7	CLR	A	1104	-	-	3/10/68/68	0/4/4/4
10	NAG	D	2003	2	-	4/6/23/26	0/1/1/1
7	CLR	G	1001	-	-	3/10/68/68	0/4/4/4
8	DGX	C	2005	-	-	3/16/141/141	0/8/8/8
7	CLR	C	2006	-	-	4/10/68/68	0/4/4/4
8	DGX	A	1107	-	-	3/16/141/141	0/8/8/8
10	NAG	B	1003	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLR	C	2004	-	-	4/10/68/68	0/4/4/4
10	NAG	D	2001	2	-	2/6/23/26	0/1/1/1
9	17F	A	1108	-	-	11/18/18/59	-
10	NAG	D	2002	2	-	4/6/23/26	0/1/1/1
9	17F	A	1109	-	-	11/16/16/59	-
9	17F	B	1004	-	-	10/28/28/59	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2004	CLR	C6-C5	9.72	1.53	1.33
7	G	1001	CLR	C6-C5	9.70	1.53	1.33
7	C	2006	CLR	C6-C5	9.65	1.52	1.33
7	A	1104	CLR	C6-C5	9.57	1.52	1.33
9	B	1004	17F	P1-O6	5.57	1.81	1.59
7	A	1104	CLR	C11-C9	5.17	1.62	1.53
7	C	2006	CLR	C11-C9	5.13	1.62	1.53
7	C	2004	CLR	C11-C9	5.05	1.62	1.53
9	A	1109	17F	P1-O6	4.95	1.78	1.59
7	G	1001	CLR	C11-C9	4.79	1.61	1.53
8	A	1107	DGX	C4X-C5X	4.14	1.59	1.52
8	C	2005	DGX	C4X-C5X	4.10	1.59	1.52
7	C	2004	CLR	C8-C14	3.67	1.60	1.53
7	C	2006	CLR	C8-C14	3.64	1.60	1.53
7	A	1104	CLR	C8-C14	3.57	1.60	1.53
9	A	1108	17F	P1-O6	3.49	1.73	1.59
7	G	1001	CLR	C8-C14	3.42	1.60	1.53
7	A	1104	CLR	C12-C13	3.36	1.60	1.54
7	C	2004	CLR	C12-C13	3.32	1.59	1.54
8	A	1107	DGX	C4Y-C5Y	3.28	1.58	1.52
7	G	1001	CLR	C12-C13	3.20	1.59	1.54
8	C	2005	DGX	C4Y-C5Y	3.19	1.58	1.52
7	C	2006	CLR	C12-C13	3.01	1.59	1.54
7	C	2006	CLR	C20-C17	-2.90	1.49	1.54
7	G	1001	CLR	C15-C14	-2.87	1.48	1.54
7	G	1001	CLR	C20-C17	-2.81	1.49	1.54
7	C	2006	CLR	C13-C17	-2.77	1.49	1.55
7	C	2006	CLR	C15-C14	-2.71	1.48	1.54
7	G	1001	CLR	C13-C17	-2.60	1.50	1.55
8	A	1107	DGX	O14-C14	-2.56	1.39	1.43
7	A	1104	CLR	C20-C17	-2.56	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1004	17F	C4-C5	2.54	1.58	1.50
7	C	2004	CLR	C15-C14	-2.53	1.49	1.54
7	A	1104	CLR	C15-C14	-2.52	1.49	1.54
9	A	1108	17F	P1-O3	2.50	1.69	1.59
7	C	2004	CLR	C20-C17	-2.40	1.50	1.54
7	C	2004	CLR	C4-C3	-2.37	1.48	1.52
8	C	2005	DGX	O14-C14	-2.33	1.40	1.43
7	A	1104	CLR	C4-C3	-2.33	1.48	1.52
7	G	1001	CLR	C19-C10	-2.26	1.50	1.54
7	A	1104	CLR	C16-C17	2.23	1.58	1.54
7	C	2004	CLR	C13-C17	-2.22	1.50	1.55
7	A	1104	CLR	C13-C17	-2.22	1.50	1.55
7	G	1001	CLR	C16-C17	2.21	1.58	1.54
9	A	1109	17F	C4-C5	2.12	1.60	1.51
7	C	2004	CLR	C16-C17	2.11	1.58	1.54
8	A	1107	DGX	C2Z-C1Z	2.07	1.56	1.50
9	B	1004	17F	P1-O3	2.03	1.67	1.59
8	A	1107	DGX	C4Z-C5Z	2.00	1.57	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1001	CLR	C19-C10-C9	-8.61	101.99	111.66
7	C	2006	CLR	C4-C5-C6	-8.60	108.91	120.57
7	C	2004	CLR	C4-C5-C6	-8.33	109.28	120.57
7	A	1104	CLR	C4-C5-C6	-8.30	109.32	120.57
7	A	1104	CLR	C7-C6-C5	-8.29	111.01	125.02
7	C	2004	CLR	C7-C6-C5	-8.23	111.12	125.02
7	G	1001	CLR	C7-C6-C5	-8.09	111.35	125.02
7	G	1001	CLR	C4-C5-C6	-7.82	109.97	120.57
7	A	1104	CLR	C12-C13-C17	-7.61	105.39	116.60
7	C	2006	CLR	C7-C6-C5	-6.96	113.26	125.02
7	C	2004	CLR	C12-C13-C17	-6.95	106.37	116.60
7	C	2006	CLR	C12-C13-C17	-6.90	106.44	116.60
7	G	1001	CLR	C12-C13-C17	-6.67	106.78	116.60
7	G	1001	CLR	C10-C5-C6	-6.36	113.64	122.93
7	C	2006	CLR	C1-C10-C9	6.28	117.04	108.74
7	A	1104	CLR	C1-C10-C9	6.24	116.99	108.74
7	A	1104	CLR	C7-C8-C9	6.23	116.92	109.72
7	G	1001	CLR	C1-C10-C9	6.08	116.78	108.74
7	C	2004	CLR	C19-C10-C9	-5.96	104.97	111.66
9	A	1108	17F	O3-C1-C2	5.91	113.21	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1104	CLR	C21-C20-C17	5.85	121.66	112.88
7	A	1104	CLR	C19-C10-C9	-5.80	105.16	111.66
7	C	2004	CLR	C1-C10-C9	5.78	116.39	108.74
7	C	2004	CLR	C7-C8-C9	5.72	116.33	109.72
7	A	1104	CLR	C7-C8-C14	5.64	118.91	110.93
7	C	2004	CLR	C7-C8-C14	5.54	118.78	110.93
7	G	1001	CLR	C21-C20-C17	5.31	120.86	112.88
7	C	2006	CLR	C10-C5-C6	-4.87	115.82	122.93
7	C	2006	CLR	C7-C8-C14	4.87	117.82	110.93
7	G	1001	CLR	C7-C8-C9	4.86	115.33	109.72
8	A	1107	DGX	C11-C9-C10	-4.69	108.94	113.70
8	C	2005	DGX	C4-C3-C2	-4.67	105.71	111.53
8	A	1107	DGX	C4-C3-C2	-4.59	105.81	111.53
7	C	2006	CLR	C19-C10-C9	-4.58	106.52	111.66
7	G	1001	CLR	C7-C8-C14	4.57	117.40	110.93
7	C	2006	CLR	C21-C20-C17	4.53	119.69	112.88
9	A	1109	17F	O3-C1-C2	4.51	111.99	108.06
7	C	2004	CLR	C21-C20-C17	4.51	119.65	112.88
7	A	1104	CLR	C10-C5-C6	-4.41	116.49	122.93
8	A	1107	DGX	O4X-C4X-C5X	4.40	117.98	106.77
8	A	1107	DGX	O4Y-C4Y-C5Y	4.37	117.92	106.77
9	B	1004	17F	O3-C1-C2	4.33	111.83	108.06
8	C	2005	DGX	O4X-C4X-C5X	4.33	117.81	106.77
8	C	2005	DGX	C7-C8-C14	4.26	115.45	111.38
7	C	2004	CLR	C10-C5-C6	-4.21	116.78	122.93
8	C	2005	DGX	C9-C10-C5	4.04	114.12	108.51
8	C	2005	DGX	O4Y-C4Y-C5Y	3.96	116.88	106.77
7	C	2004	CLR	C4-C5-C10	-3.95	111.36	116.42
7	A	1104	CLR	C4-C5-C10	-3.89	111.44	116.42
8	A	1107	DGX	C9-C10-C5	3.86	113.87	108.51
7	C	2006	CLR	C7-C8-C9	3.82	114.14	109.72
8	C	2005	DGX	C11-C9-C10	-3.82	109.83	113.70
8	A	1107	DGX	C7-C8-C14	3.78	114.99	111.38
8	A	1107	DGX	O3-C3-C4	3.78	118.48	108.79
8	C	2005	DGX	O3-C3-C4	3.68	118.22	108.79
7	C	2004	CLR	C17-C13-C14	3.64	104.28	100.10
8	C	2005	DGX	C16-C17-C20	3.62	120.36	113.62
8	A	1107	DGX	O5Y-C1Y-C2Y	-3.52	105.39	110.84
8	A	1107	DGX	C16-C17-C20	3.50	120.14	113.62
8	C	2005	DGX	C6Y-C5Y-C4Y	-3.48	108.22	113.39
8	A	1107	DGX	C6Y-C5Y-C4Y	-3.43	108.28	113.39
8	C	2005	DGX	C6Z-C5Z-C4Z	-3.40	106.85	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	2006	CLR	C11-C9-C10	3.38	117.25	113.08
7	A	1104	CLR	C12-C11-C9	3.36	118.85	113.14
7	C	2006	CLR	C11-C9-C8	3.33	116.42	111.78
8	C	2005	DGX	O5Y-C1Y-C2Y	-3.27	105.77	110.84
7	A	1104	CLR	C21-C20-C22	-3.19	105.41	110.34
7	C	2006	CLR	C17-C13-C14	3.14	103.70	100.10
8	C	2005	DGX	C6X-C5X-C4X	-3.13	108.73	113.39
9	A	1109	17F	O2-P1-O1	3.11	126.89	112.44
8	A	1107	DGX	C6Z-C5Z-C4Z	-3.10	107.40	113.08
7	C	2006	CLR	C21-C20-C22	-3.05	105.62	110.34
8	A	1107	DGX	O5X-C1X-C2X	-3.04	106.13	110.84
7	A	1104	CLR	C17-C13-C14	3.02	103.57	100.10
9	A	1108	17F	O2-P1-O1	3.01	126.45	112.44
8	C	2005	DGX	O5X-C1X-C2X	-2.91	106.33	110.84
7	C	2006	CLR	C19-C10-C1	-2.90	105.02	109.43
8	C	2005	DGX	C15-C16-C17	2.88	110.12	104.22
7	A	1104	CLR	C19-C10-C1	-2.88	105.05	109.43
9	B	1004	17F	O2-P1-O1	2.84	125.66	112.44
7	G	1001	CLR	C21-C20-C22	-2.84	105.95	110.34
7	C	2004	CLR	C21-C20-C22	-2.82	105.98	110.34
8	A	1107	DGX	C1-C2-C3	2.75	114.82	110.33
7	A	1104	CLR	C18-C13-C17	2.74	116.64	111.68
8	A	1107	DGX	C15-C16-C17	2.69	109.73	104.22
7	C	2006	CLR	C12-C11-C9	2.69	117.70	113.14
7	C	2004	CLR	C12-C11-C9	2.68	117.69	113.14
8	A	1107	DGX	C5-C4-C3	2.66	116.93	111.65
8	A	1107	DGX	C6X-C5X-C4X	-2.64	109.46	113.39
7	G	1001	CLR	C11-C9-C8	2.63	115.45	111.78
7	G	1001	CLR	C2-C1-C10	2.57	118.27	112.78
7	C	2004	CLR	C19-C10-C1	-2.57	105.52	109.43
7	C	2004	CLR	C1-C2-C3	2.55	113.86	110.48
10	D	2003	NAG	C1-O5-C5	2.52	115.57	112.19
7	A	1104	CLR	C2-C1-C10	2.49	118.09	112.78
8	C	2005	DGX	C5-C4-C3	2.49	116.58	111.65
8	A	1107	DGX	C19-C10-C9	-2.49	107.84	111.18
8	C	2005	DGX	C19-C10-C9	-2.46	107.87	111.18
9	B	1004	17F	O9-C17-C18	2.44	116.77	111.48
8	A	1107	DGX	O12-C12-C13	-2.44	105.67	110.88
7	A	1104	CLR	C3-C4-C5	-2.43	108.19	112.05
7	G	1001	CLR	C18-C13-C17	2.41	116.05	111.68
8	C	2005	DGX	O12-C12-C13	-2.34	105.87	110.88
7	C	2004	CLR	C11-C9-C8	2.34	115.04	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1104	CLR	C11-C9-C10	2.32	115.94	113.08
8	C	2005	DGX	C1Z-O4Y-C4Y	2.31	119.32	114.72
7	C	2004	CLR	C2-C1-C10	2.29	117.65	112.78
7	C	2006	CLR	C16-C17-C13	-2.27	101.17	103.84
7	G	1001	CLR	C11-C9-C10	2.27	115.88	113.08
7	A	1104	CLR	C13-C14-C8	-2.23	111.24	114.41
8	A	1107	DGX	C2-C1-C10	2.19	116.43	112.74
7	G	1001	CLR	C19-C10-C1	-2.16	106.15	109.43
7	C	2004	CLR	C11-C9-C10	2.12	115.70	113.08
7	C	2004	CLR	C3-C4-C5	-2.12	108.68	112.05
7	G	1001	CLR	C1-C10-C5	2.11	112.39	108.74
10	D	2003	NAG	O5-C1-C2	-2.11	108.03	111.29
7	G	1001	CLR	C11-C12-C13	-2.08	109.23	112.74
7	C	2006	CLR	C4-C5-C10	-2.06	113.79	116.42
7	G	1001	CLR	C1-C2-C3	2.04	113.18	110.48
7	G	1001	CLR	C16-C17-C13	-2.03	101.45	103.84
8	A	1107	DGX	C4-C5-C10	2.01	114.80	112.66

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1108	17F	O3-C1-C2-N1
9	A	1108	17F	O3-C1-C2-C3
9	A	1108	17F	C4-O6-P1-O1
9	A	1108	17F	C4-O6-P1-O2
9	A	1108	17F	C4-O6-P1-O3
9	A	1108	17F	C1-C2-C3-O4
9	A	1108	17F	C1-C2-C3-O5
9	A	1108	17F	O6-C4-C5-C6
9	A	1108	17F	C4-C5-C6-O7
9	A	1108	17F	O9-C5-C6-O7
9	A	1109	17F	O3-C1-C2-N1
9	A	1109	17F	O3-C1-C2-C3
9	A	1109	17F	C1-O3-P1-O2
9	A	1109	17F	C4-O6-P1-O1
9	A	1109	17F	C4-O6-P1-O2
9	A	1109	17F	C4-O6-P1-O3
9	A	1109	17F	N1-C2-C3-O4
9	A	1109	17F	O6-C4-C5-O9
9	B	1004	17F	C1-O3-P1-O6
9	B	1004	17F	C4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
9	B	1004	17F	O9-C5-C6-O7
9	B	1004	17F	C18-C17-O9-C5
9	B	1004	17F	O10-C17-O9-C5
10	B	1003	NAG	O5-C5-C6-O6
10	D	2003	NAG	O5-C5-C6-O6
10	D	2002	NAG	O5-C5-C6-O6
10	B	1003	NAG	C4-C5-C6-O6
10	D	2003	NAG	C4-C5-C6-O6
7	C	2004	CLR	C21-C20-C22-C23
10	D	2001	NAG	O5-C5-C6-O6
10	D	2001	NAG	C4-C5-C6-O6
10	B	1003	NAG	C8-C7-N2-C2
10	B	1003	NAG	O7-C7-N2-C2
10	D	2002	NAG	C8-C7-N2-C2
10	D	2002	NAG	O7-C7-N2-C2
10	D	2003	NAG	C8-C7-N2-C2
10	D	2003	NAG	O7-C7-N2-C2
9	A	1108	17F	O6-C4-C5-O9
7	C	2004	CLR	C20-C22-C23-C24
7	C	2004	CLR	C22-C23-C24-C25
10	D	2002	NAG	C4-C5-C6-O6
8	A	1107	DGX	C2Z-C1Z-O4Y-C4Y
8	C	2005	DGX	C2Z-C1Z-O4Y-C4Y
8	A	1107	DGX	O5Z-C1Z-O4Y-C4Y
8	C	2005	DGX	O5Z-C1Z-O4Y-C4Y
7	G	1001	CLR	C22-C23-C24-C25
7	A	1104	CLR	C23-C24-C25-C27
7	C	2006	CLR	C23-C24-C25-C27
7	C	2006	CLR	C23-C24-C25-C26
7	A	1104	CLR	C20-C22-C23-C24
9	A	1109	17F	O6-C4-C5-C6
9	A	1109	17F	N1-C2-C3-O5
7	A	1104	CLR	C23-C24-C25-C26
7	C	2006	CLR	C17-C20-C22-C23
9	B	1004	17F	O6-C4-C5-C6
9	B	1004	17F	O3-C1-C2-N1
7	G	1001	CLR	C23-C24-C25-C27
7	C	2004	CLR	C23-C24-C25-C26
9	B	1004	17F	C1Z-C1Y-C20-C19
9	B	1004	17F	O6-C4-C5-O9
8	C	2005	DGX	O5X-C1X-O3-C3
9	A	1109	17F	C1-O3-P1-O6

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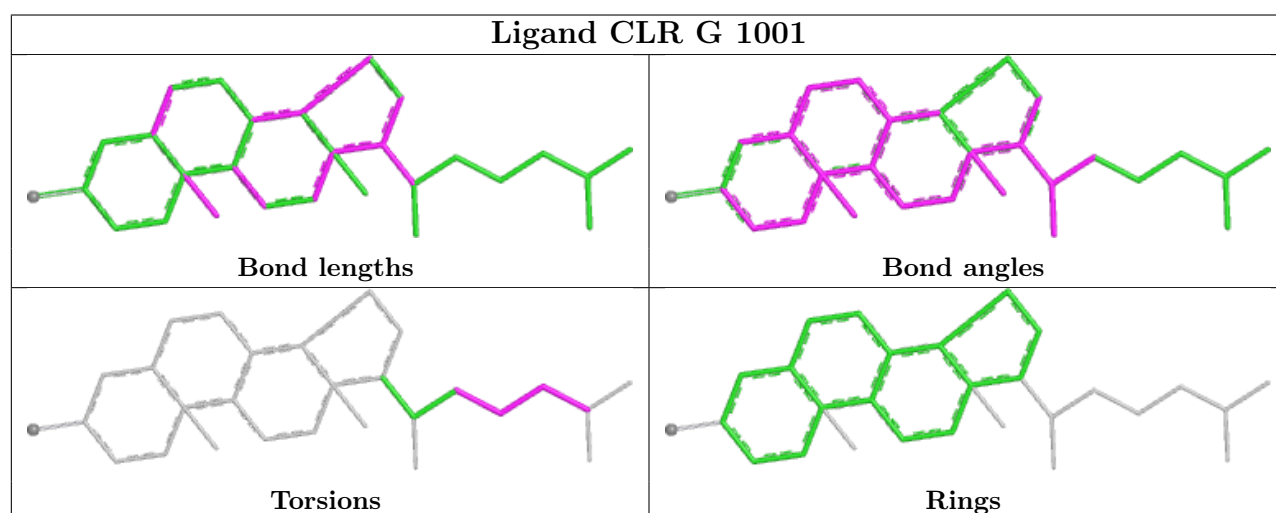
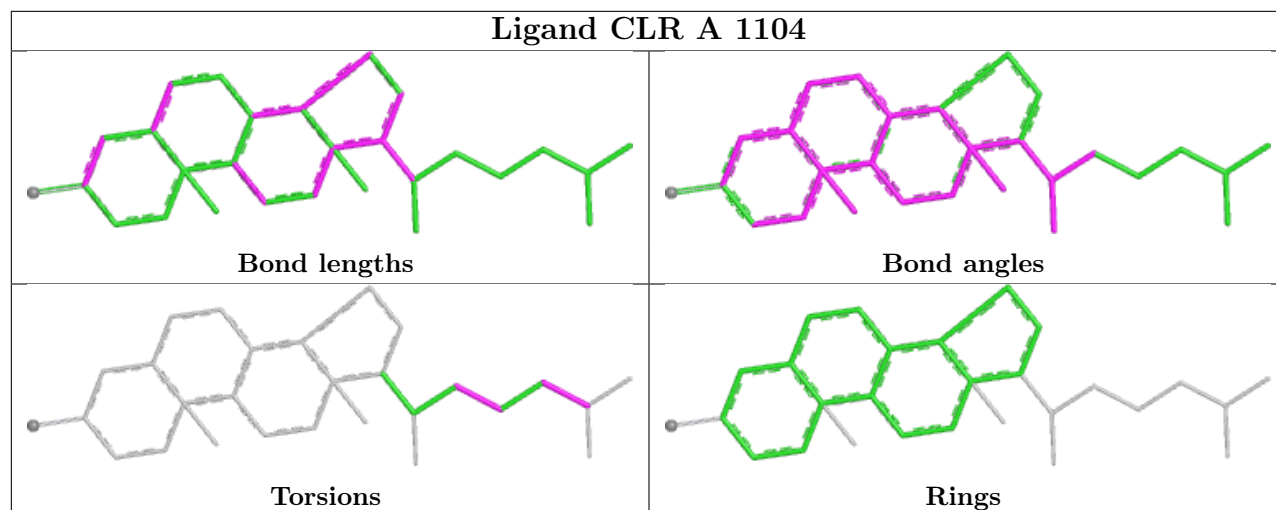
Mol	Chain	Res	Type	Atoms
7	C	2006	CLR	C13-C17-C20-C21
8	A	1107	DGX	O5X-C1X-O3-C3
7	G	1001	CLR	C20-C22-C23-C24
9	B	1004	17F	C2-C1-O3-P1

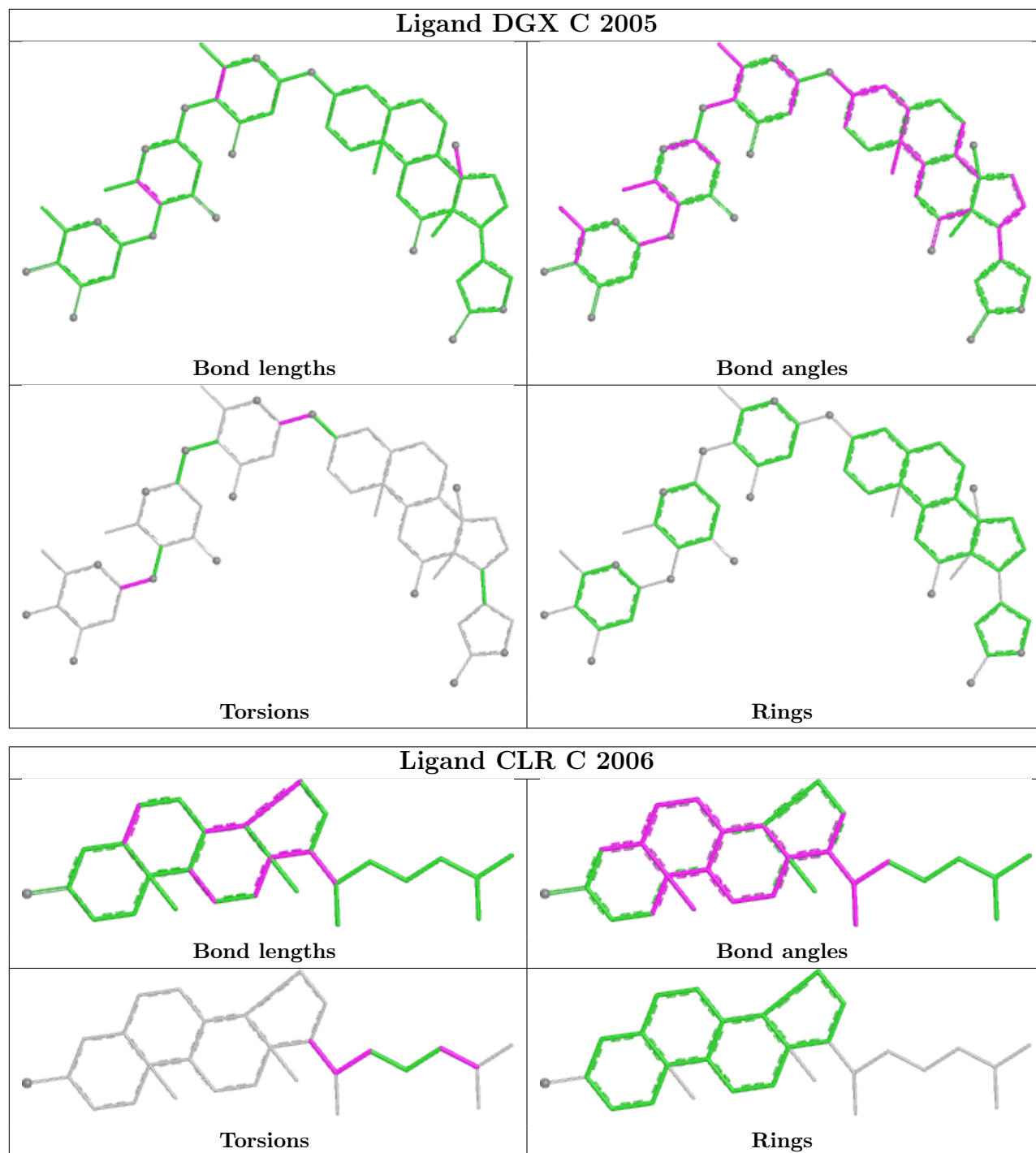
There are no ring outliers.

10 monomers are involved in 28 short contacts:

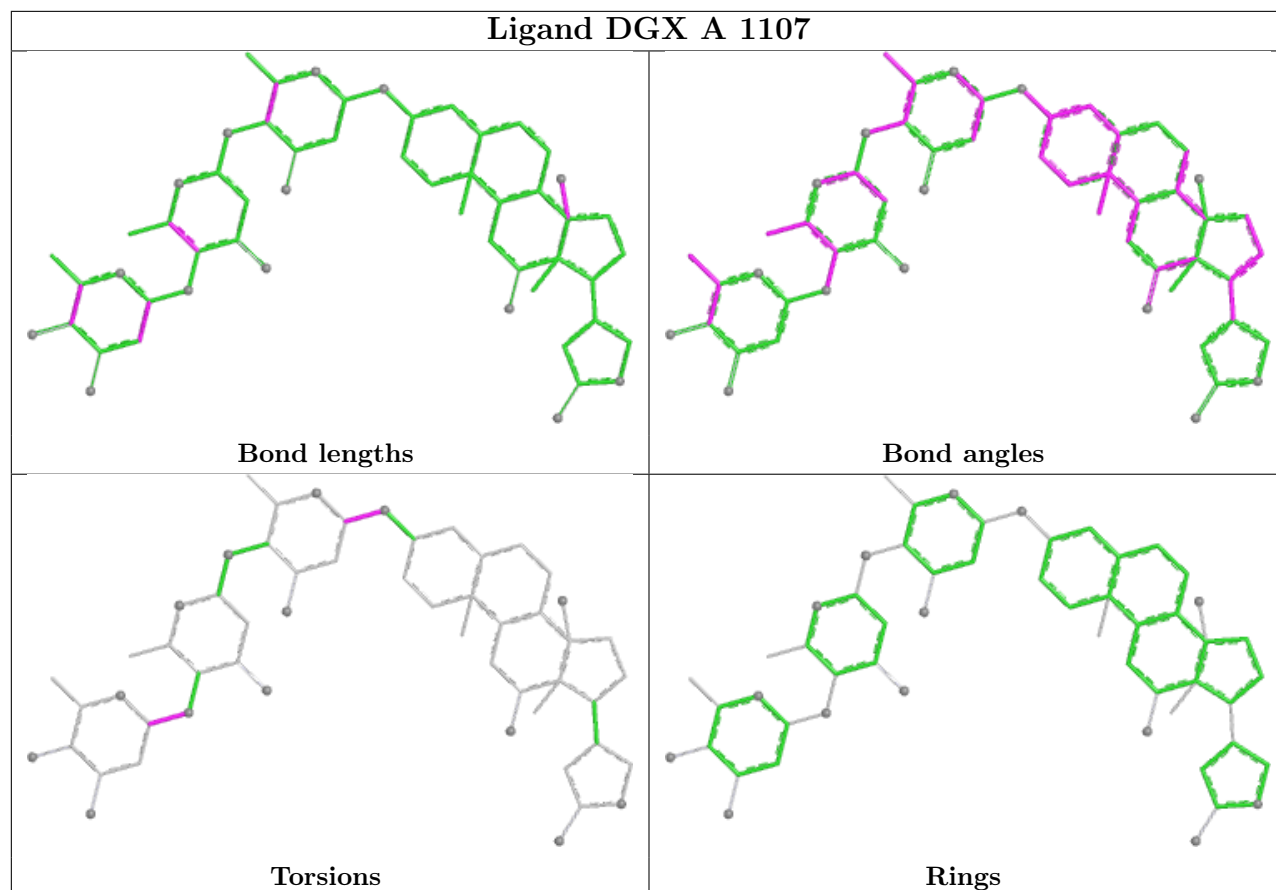
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1104	CLR	4	0
10	D	2003	NAG	1	0
7	G	1001	CLR	5	0
8	C	2005	DGX	2	0
7	C	2006	CLR	2	0
8	A	1107	DGX	2	0
7	C	2004	CLR	5	0
9	A	1108	17F	5	0
9	A	1109	17F	2	0
9	B	1004	17F	2	0

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

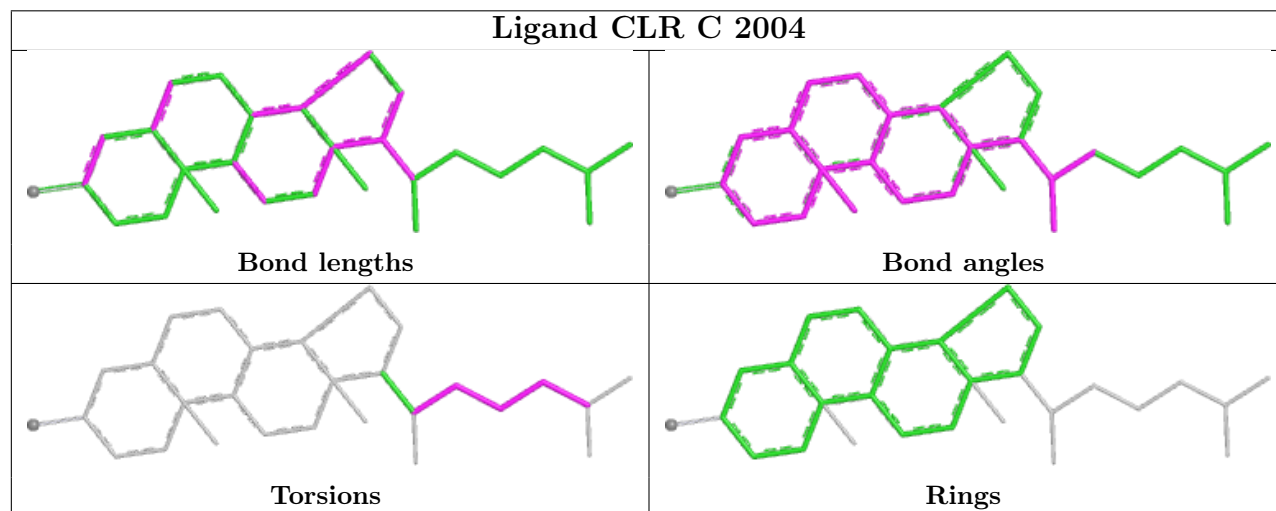


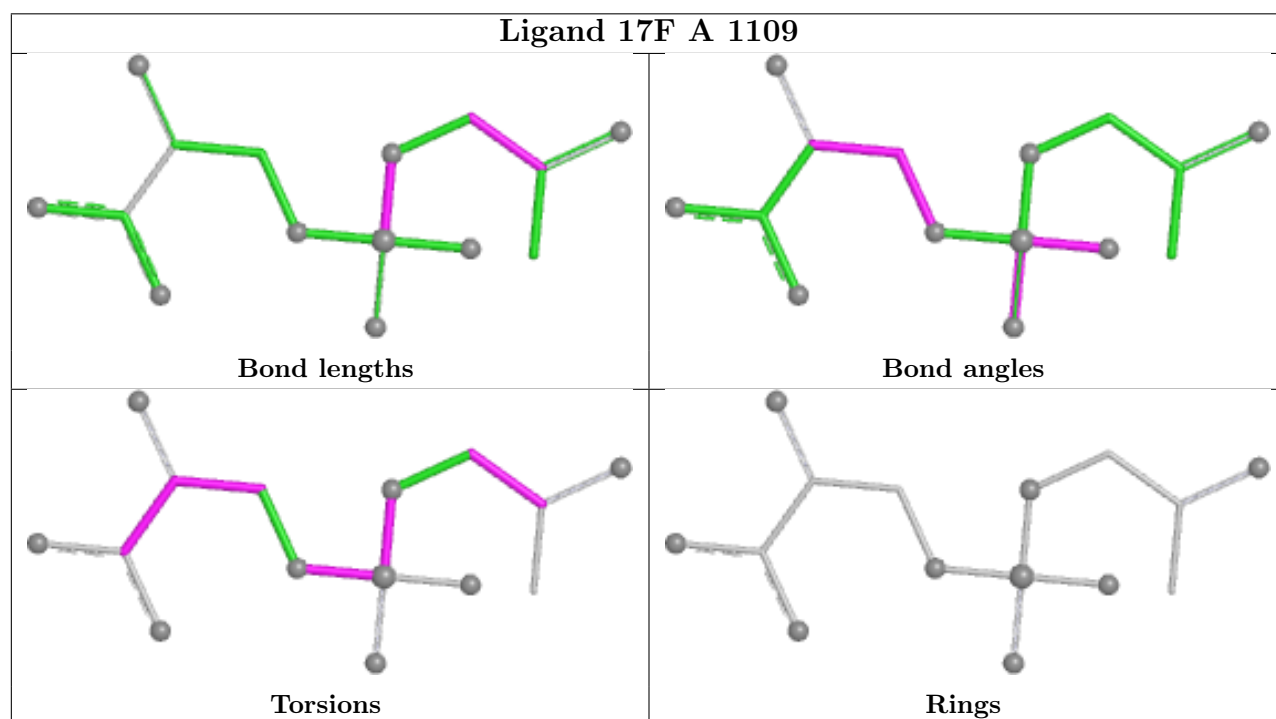
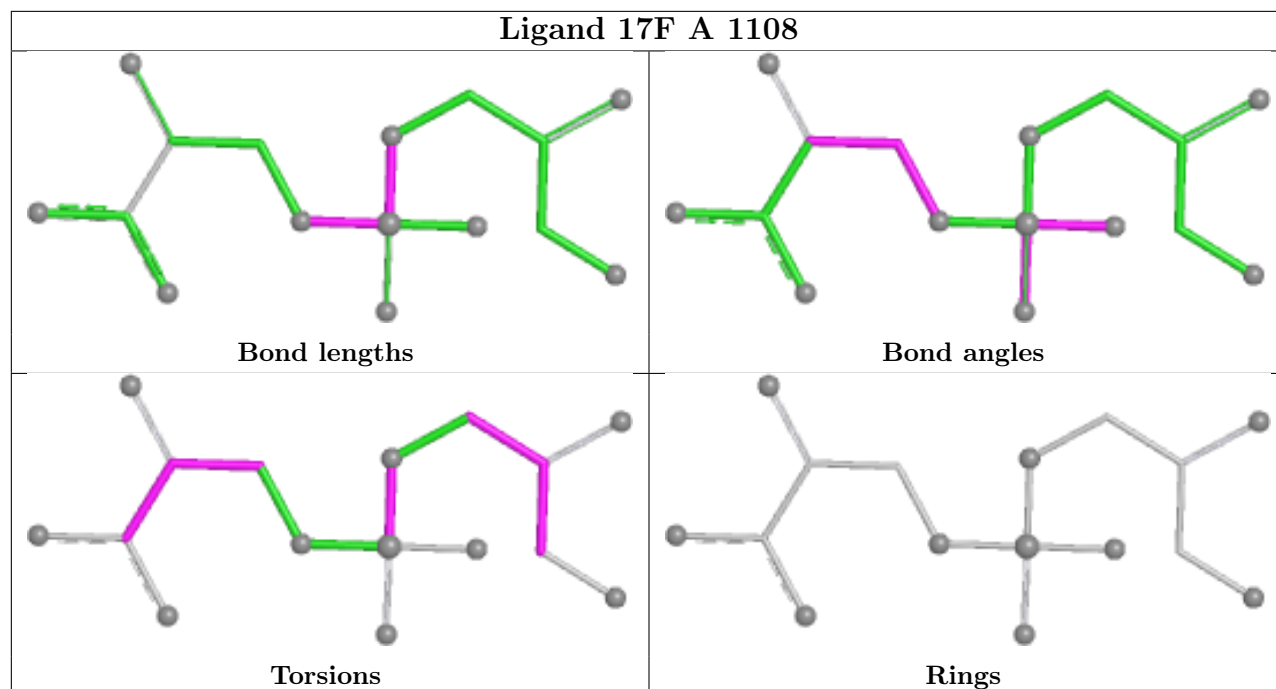


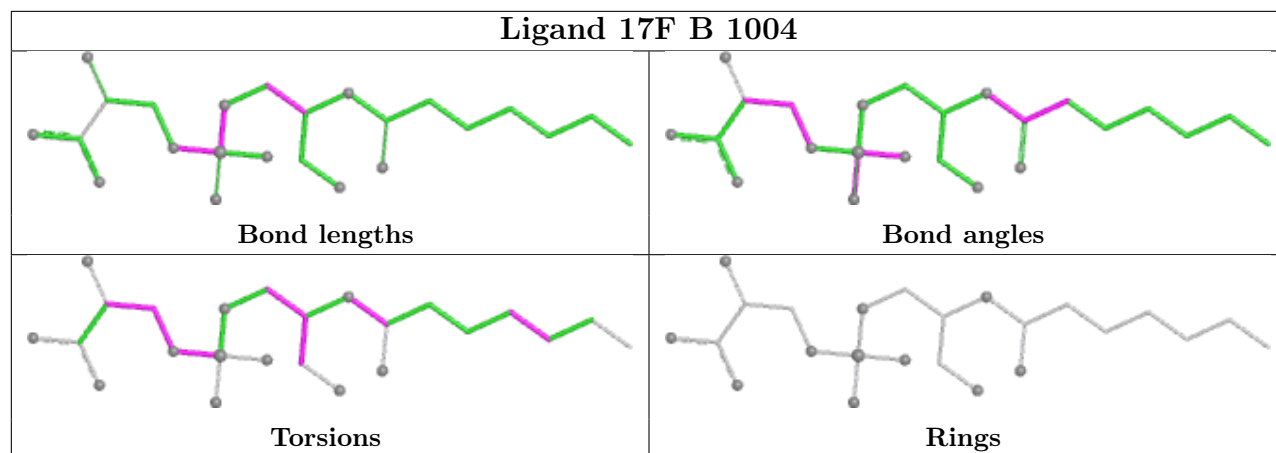
Ligand DGX A 1107



Ligand CLR C 2004







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	995/1021 (97%)	0.53	59 (5%)	28 25	109, 155, 307, 408	0
1	C	995/1021 (97%)	0.64	103 (10%)	11 14	116, 190, 348, 473	0
2	B	290/303 (95%)	0.73	31 (10%)	11 13	125, 222, 307, 421	0
2	D	288/303 (95%)	0.77	28 (9%)	13 15	120, 198, 300, 381	0
3	E	32/65 (49%)	0.40	2 (6%)	26 23	97, 148, 217, 297	0
3	G	32/65 (49%)	0.39	2 (6%)	26 23	128, 149, 228, 268	0
All	All	2632/2778 (94%)	0.62	225 (8%)	16 18	97, 181, 324, 473	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	480	LYS	7.7
2	D	218	ASP	7.2
1	C	467	TYR	7.2
2	B	67	THR	6.3
1	C	120	ASN	5.3
3	G	19	PHE	5.1
2	D	290	ARG	4.9
2	D	217	ARG	4.9
1	A	120	ASN	4.8
1	A	501	LYS	4.8
1	A	535	TYR	4.5
1	A	835	ASP	4.5
1	A	581	LEU	4.5
1	C	490	ASN	4.5
1	C	489	PRO	4.4
1	C	840	GLU	4.4
1	A	868	GLU	4.3
2	B	69	GLN	4.2
1	A	545	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	869	ASN	4.1
1	C	117	GLU	4.1
2	B	61	ILE	4.1
1	C	466	ARG	4.0
2	D	69	GLN	4.0
1	C	613	HIS	3.9
2	B	68	TYR	3.9
1	A	548	PHE	3.9
1	A	582	ILE	3.9
1	A	871	PHE	3.8
2	B	129	VAL	3.8
1	C	416	ARG	3.8
1	C	890	ASP	3.8
1	C	480	LYS	3.7
1	C	149	LYS	3.7
1	C	497	LEU	3.6
1	C	488	ASN	3.6
2	D	87	GLU	3.6
1	C	702	GLY	3.5
1	C	119	GLN	3.5
2	D	291	PHE	3.5
1	C	91	GLY	3.5
2	B	100	SER	3.5
2	B	60	THR	3.5
2	D	296	ASP	3.4
1	C	708	THR	3.4
1	C	542	GLY	3.4
1	C	541	LEU	3.4
1	C	889	ASN	3.4
1	C	685	ARG	3.4
1	C	420	LEU	3.3
1	A	35	ASP	3.3
1	A	1005	ARG	3.3
1	A	546	LEU	3.3
1	C	486	HIS	3.3
2	D	200	PRO	3.3
2	D	64	PHE	3.2
2	B	211	VAL	3.2
2	D	172	GLY	3.2
1	C	515	LEU	3.2
1	C	113	ALA	3.2
1	C	550	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	268	SER	3.1
2	D	125	ASP	3.1
1	A	91	GLY	3.1
1	C	86	CYS	3.1
1	C	203	GLY	3.1
1	C	368	SER	3.1
1	C	820	ALA	3.1
1	C	938	PHE	3.1
2	B	66	PRO	3.0
1	A	210	SER	3.0
3	E	19	PHE	3.0
1	C	272	GLY	3.0
1	A	252	VAL	3.0
1	A	870	GLY	3.0
1	A	533	ASN	3.0
1	C	543	GLU	2.9
2	B	261	VAL	2.9
2	D	73	ALA	2.9
1	A	538	LEU	2.9
1	C	897	GLN	2.9
1	A	477	SER	2.9
1	C	503	ALA	2.9
1	A	748	PHE	2.9
1	C	215	SER	2.8
2	B	278	ALA	2.8
2	B	71	ARG	2.8
1	C	216	GLU	2.8
1	C	403	SER	2.8
1	C	468	THR	2.8
1	C	687	SER	2.8
2	B	111	LYS	2.8
2	B	258	LEU	2.8
1	C	481	TYR	2.8
2	D	297	VAL	2.7
1	A	537	GLU	2.7
1	C	476	ASN	2.7
1	A	117	GLU	2.7
1	A	500	MET	2.7
1	A	539	GLY	2.7
1	C	748	PHE	2.7
1	C	730	ALA	2.6
1	A	191	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	869	ASN	2.6
2	B	263	PHE	2.6
1	A	751	ILE	2.6
3	E	44	ILE	2.6
1	A	195	ASP	2.6
1	A	834	THR	2.6
2	B	135	GLU	2.6
2	D	139	TYR	2.6
1	A	566	THR	2.6
1	C	517	HIS	2.6
2	D	164	ASP	2.6
2	B	183	VAL	2.6
2	B	16	ILE	2.5
1	C	456	CYS	2.5
3	G	18	PRO	2.5
1	C	637	ILE	2.5
2	D	223	LYS	2.5
2	D	274	ILE	2.5
2	D	189	LYS	2.5
1	A	277	ILE	2.5
2	B	178	ILE	2.5
1	C	544	ARG	2.5
1	C	652	ASP	2.5
1	A	157	MET	2.5
1	C	418	ALA	2.5
2	B	107	ARG	2.5
1	A	580	GLY	2.5
1	C	491	THR	2.4
1	C	32	VAL	2.4
1	A	442	GLY	2.4
2	B	162	LEU	2.4
1	C	932	THR	2.4
1	A	34	MET	2.4
1	C	546	LEU	2.4
1	C	475	PHE	2.4
1	C	496	HIS	2.4
2	B	260	ALA	2.4
1	C	887	TRP	2.4
2	B	164	ASP	2.4
2	B	57	MET	2.4
1	C	400	SER	2.4
1	C	177	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	137	GLY	2.3
1	A	253	TYR	2.3
1	A	536	LEU	2.3
1	C	690	GLN	2.3
1	C	437	LYS	2.3
1	C	409	ALA	2.3
1	C	871	PHE	2.3
1	A	563	GLN	2.3
1	C	886	ARG	2.3
1	C	78	THR	2.3
1	C	478	THR	2.3
2	D	77	LEU	2.3
1	C	474	PRO	2.3
1	A	804	ASP	2.3
1	C	892	GLU	2.3
1	C	356	ALA	2.3
1	C	804	ASP	2.3
1	C	493	GLU	2.3
1	C	33	SER	2.3
1	C	350	LEU	2.3
1	A	385	TRP	2.2
1	C	310	TRP	2.2
1	C	618	LYS	2.2
1	A	327	GLU	2.2
1	A	435	ILE	2.2
1	A	776	ASN	2.2
1	A	599	CYS	2.2
2	D	253	LYS	2.2
1	A	92	GLY	2.2
1	A	298	SER	2.2
1	C	357	VAL	2.2
1	C	494	PRO	2.2
1	C	552	PHE	2.2
2	D	65	LYS	2.2
1	C	492	ALA	2.2
1	C	966	GLY	2.2
2	D	127	GLY	2.2
1	C	342	LYS	2.2
1	C	419	GLY	2.2
1	C	485	ILE	2.2
2	D	298	LYS	2.2
1	C	969	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	520	GLU	2.2
1	C	954	GLU	2.2
1	C	638	ALA	2.2
1	C	146	LYS	2.2
1	C	553	LEU	2.1
2	B	172	GLY	2.1
2	B	174	PRO	2.1
2	D	114	ASP	2.1
1	A	685	ARG	2.1
1	C	423	ARG	2.1
1	A	187	LYS	2.1
1	A	384	MET	2.1
1	C	212	THR	2.1
1	C	487	LYS	2.1
1	C	899	TRP	2.1
1	C	351	VAL	2.1
2	D	224	VAL	2.1
1	A	378	ARG	2.1
2	D	85	LYS	2.1
1	C	298	SER	2.1
2	B	213	CYS	2.1
1	C	540	GLY	2.1
1	A	886	ARG	2.0
1	C	577	CYS	2.0
2	B	17	TRP	2.0
2	D	222	GLU	2.0
1	A	30	LYS	2.0
1	C	611	GLY	2.0
1	C	114	THR	2.0
2	B	276	CYS	2.0
1	A	830	ARG	2.0
1	C	463	MET	2.0
2	D	118	LYS	2.0
1	C	824	ILE	2.0
1	A	867	ALA	2.0
1	A	437	LYS	2.0
1	C	945	LYS	2.0
2	B	163	ASN	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	PHD	C	369	12/13	0.95	0.07	164,202,204,205	0
1	PHD	A	369	12/13	0.99	0.06	120,125,129,130	0

6.3 Carbohydrates [i](#)

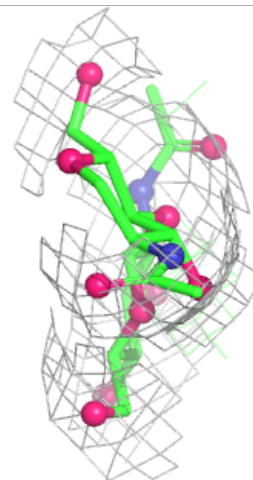
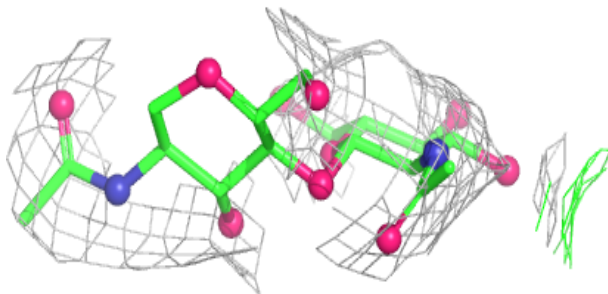
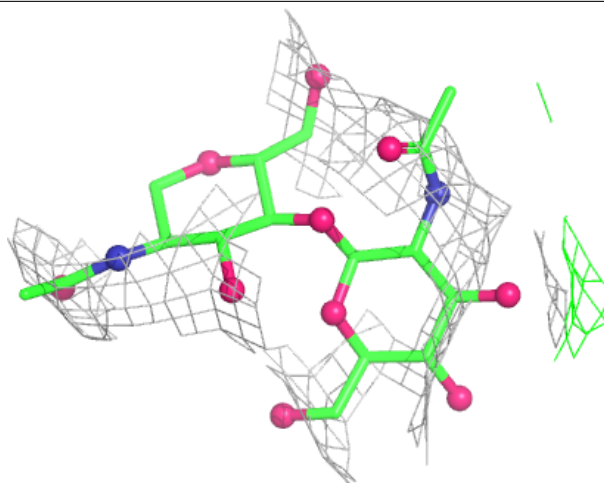
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	F	1	14/15	-	-	226,235,245,249	0
4	NAG	F	2	14/15	-	-	245,257,261,266	0
5	GLC	H	1	11/12	0.78	0.20	200,210,213,214	0
5	FRU	H	2	12/12	0.80	0.21	187,204,211,215	0
5	GLC	I	1	11/12	0.83	0.14	162,163,171,176	0
5	FRU	I	2	12/12	0.87	0.18	171,183,188,189	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

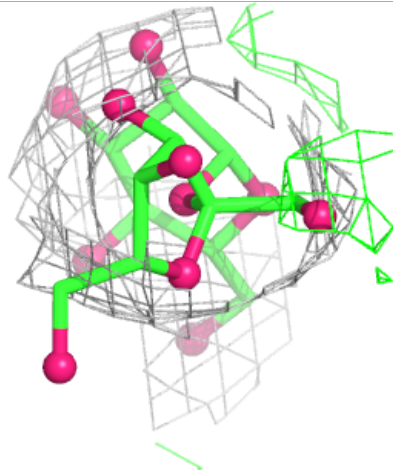
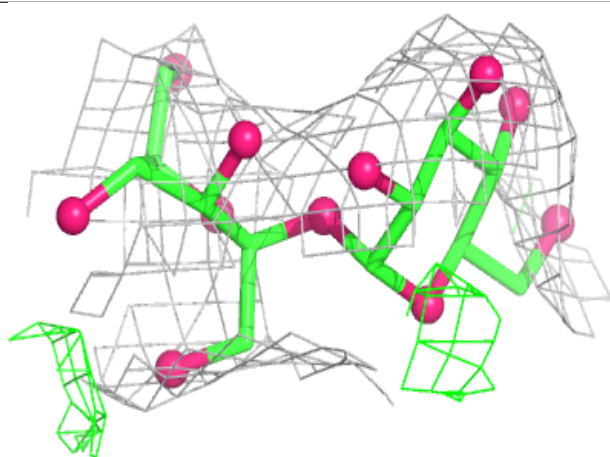
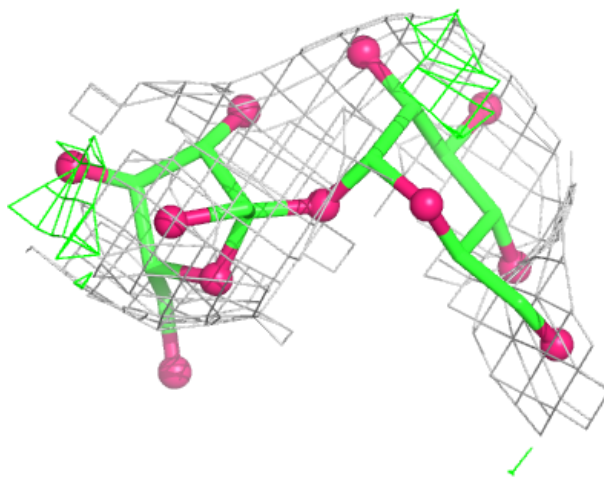
Electron density around Chain F:

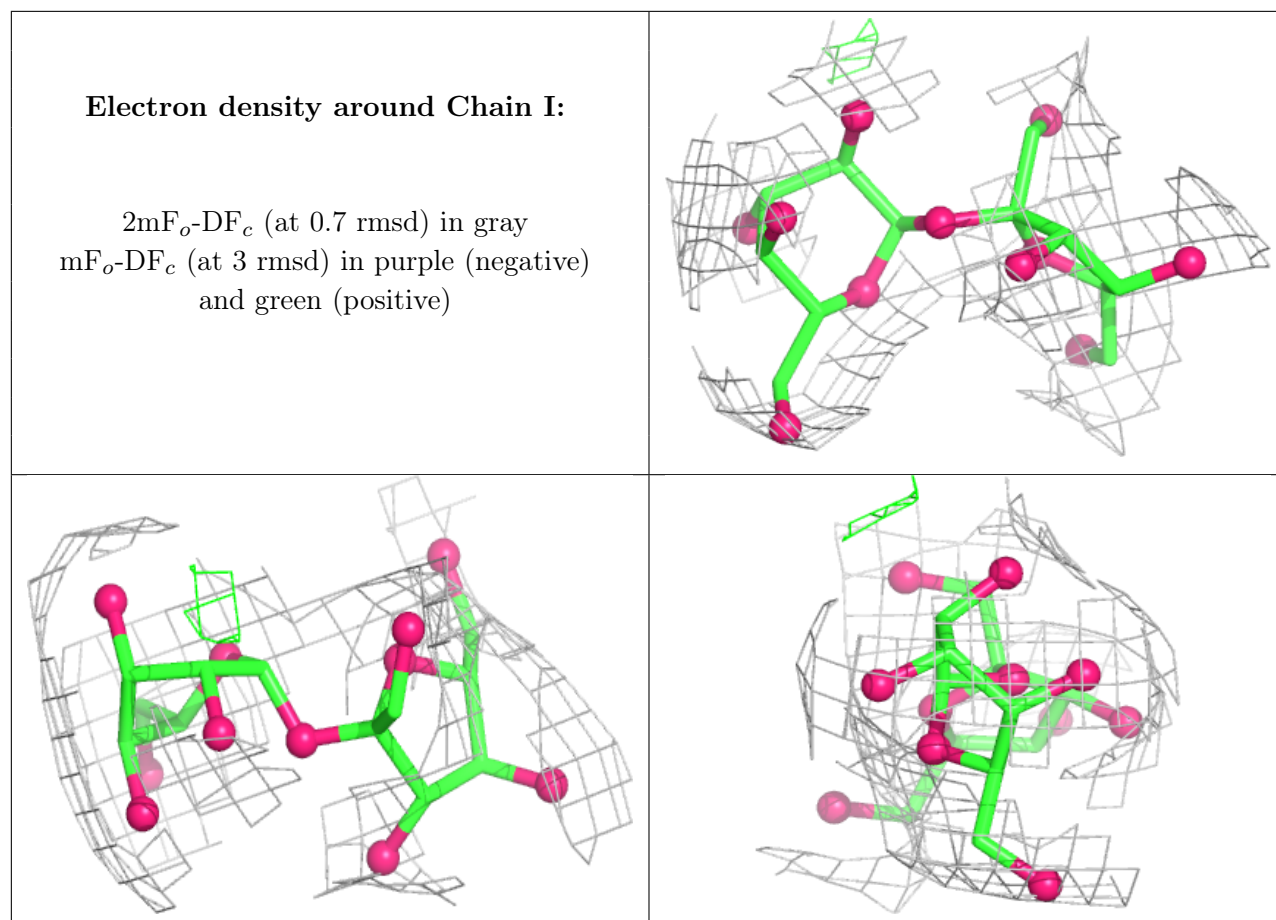
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





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.

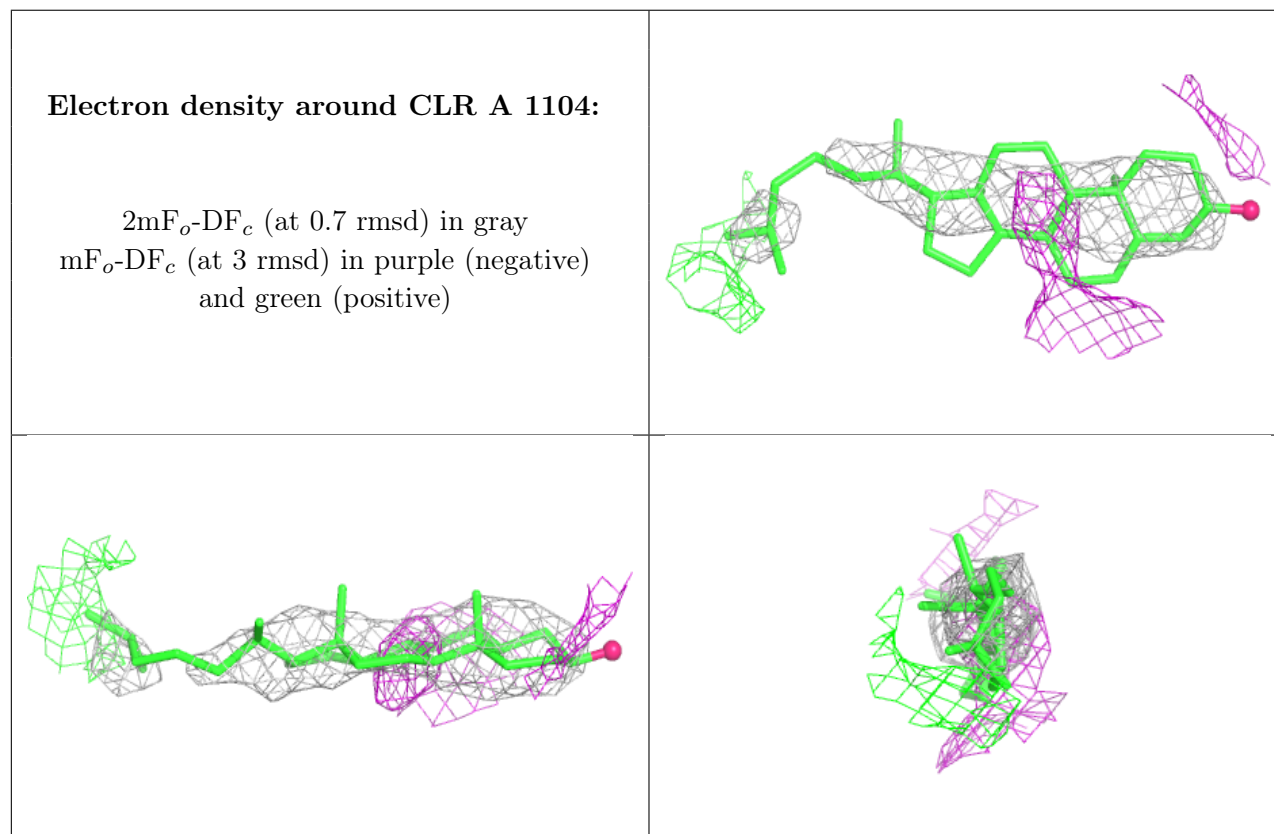
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	NAG	D	2001	14/15	0.37	0.16	201,213,221,222	0
10	NAG	D	2003	14/15	0.54	0.18	228,238,245,250	0
6	MG	A	1102	1/1	0.55	0.38	115,115,115,115	0
10	NAG	D	2002	14/15	0.66	0.15	179,191,200,204	0
10	NAG	B	1003	14/15	0.66	0.15	209,222,229,230	0
7	CLR	A	1104	28/28	0.67	0.41	128,137,188,190	0
9	17F	A	1109	15/54	0.72	0.25	143,217,306,306	0
9	17F	A	1108	16/54	0.76	0.21	196,222,271,271	0
9	17F	B	1004	24/54	0.76	0.24	128,215,240,263	0
7	CLR	C	2004	28/28	0.80	0.33	146,162,169,218	0
6	MG	C	2002	1/1	0.80	0.37	148,148,148,148	0
8	DGX	A	1107	55/55	0.89	0.20	128,187,256,259	0

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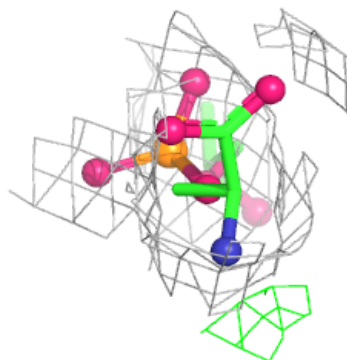
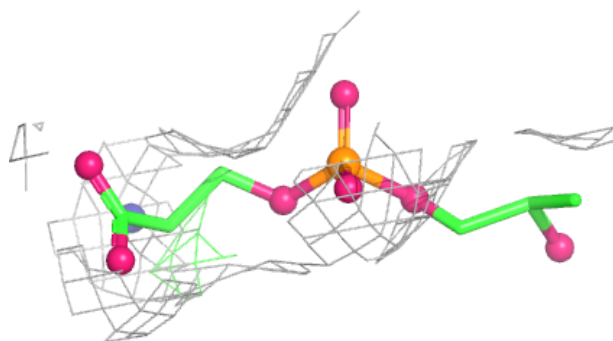
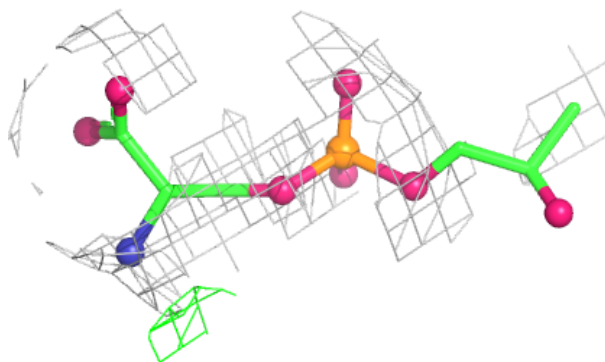
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	DGX	C	2005	55/55	0.90	0.15	153,182,232,234	0
7	CLR	C	2006	28/28	0.94	0.17	143,143,143,143	0
7	CLR	G	1001	28/28	0.95	0.22	143,143,143,143	0
6	MG	A	1103	1/1	0.98	0.05	112,112,112,112	0
6	MG	C	2003	1/1	0.98	0.06	130,130,130,130	0
6	MG	C	2001	1/1	0.98	0.04	147,147,147,147	0
6	MG	A	1101	1/1	0.99	0.03	123,123,123,123	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.

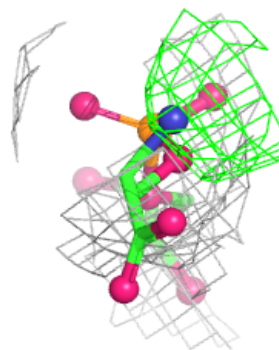
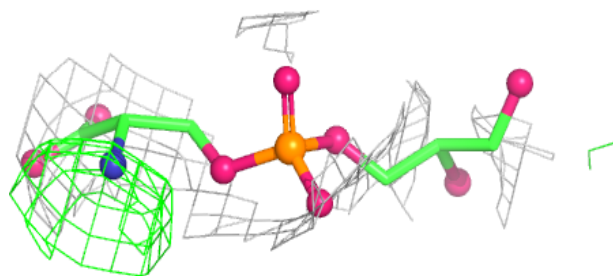
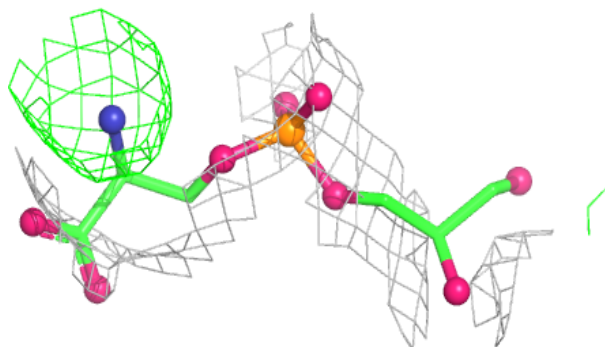


Electron density around 17F A 1109:

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

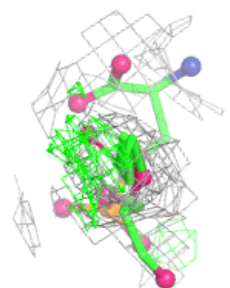
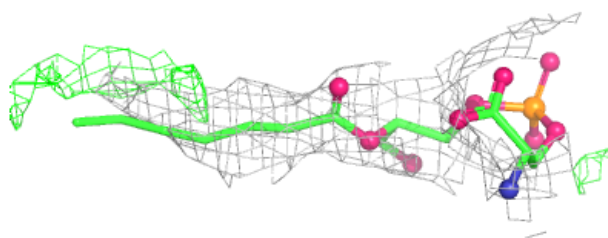
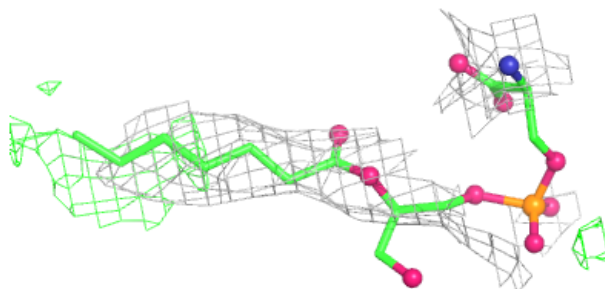
**Electron density around 17F A 1108:**

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

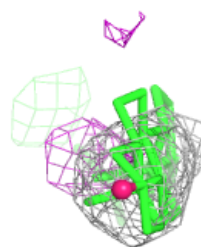
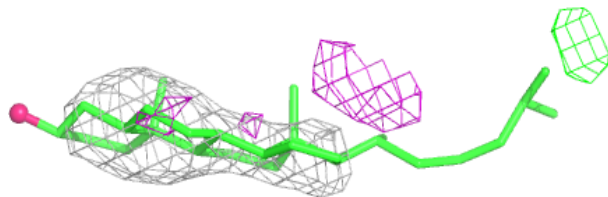
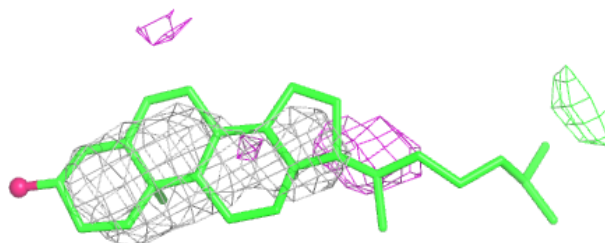


Electron density around 17F B 1004:

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

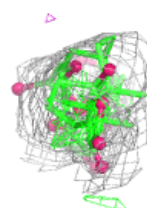
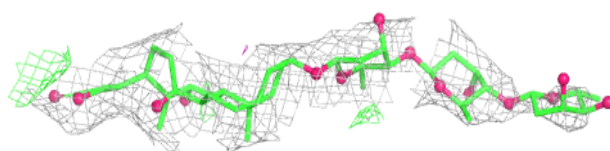
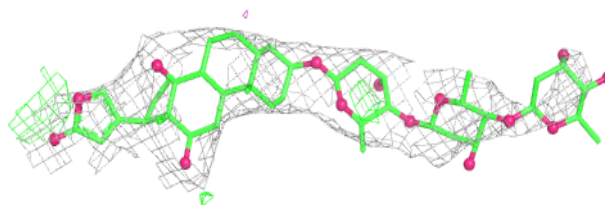
**Electron density around CLR C 2004:**

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

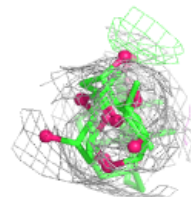
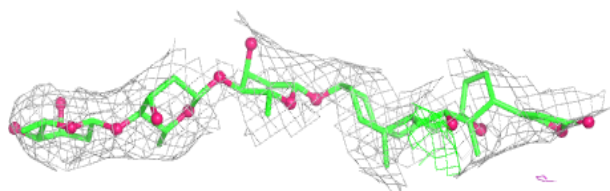
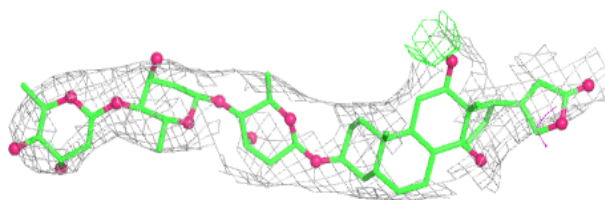


Electron density around DGX A 1107:

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

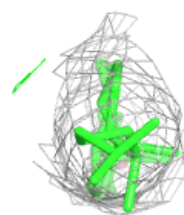
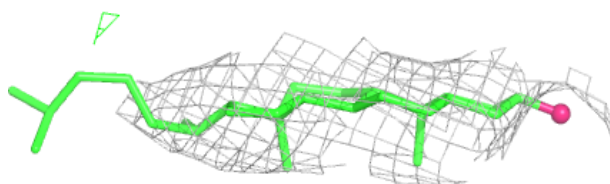
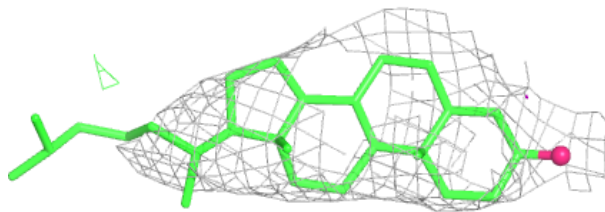
**Electron density around DGX C 2005:**

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and green (positive)

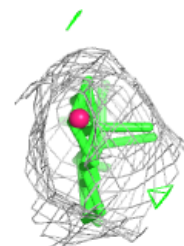
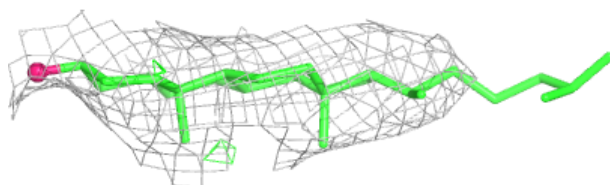
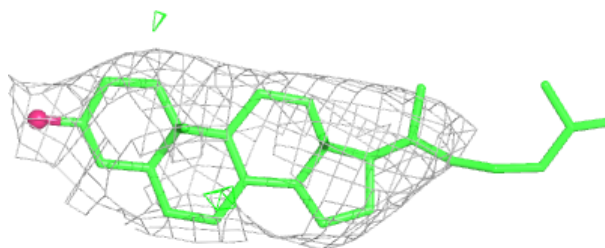


Electron density around CLR C 2006:

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

**Electron density around CLR G 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.