



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 07:14 AM BST

PDB ID : 4RES
Title : Crystal structure of the Na,K-ATPase E2P-bufalin complex with bound potassium
Authors : Laursen, M.; Yatime, L.; Gregersen, J.L.; Nissen, P.; Fedosova, N.U.
Deposited on : 2014-09-23
Resolution : 3.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

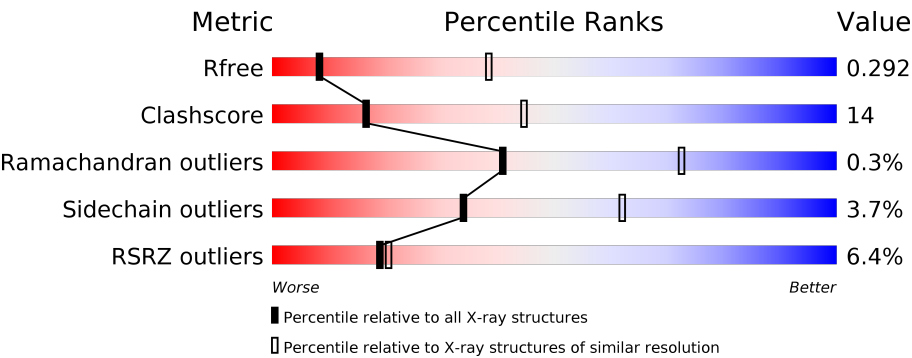
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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.





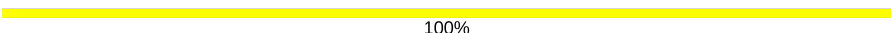
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	C	1021	
2	B	303	
2	D	303	
3	E	65	
3	G	65	

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Mol	Chain	Length	Quality of chain
4	F	2	 50%50%
5	H	2	 50%50%
5	I	2	 100%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20881 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	288	Total	C	N	O	S	0	0	0
			2357	1525	385	434	13			
2	D	285	Total	C	N	O	S	0	0	0
			2327	1504	380	430	13			

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

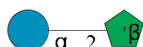
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

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



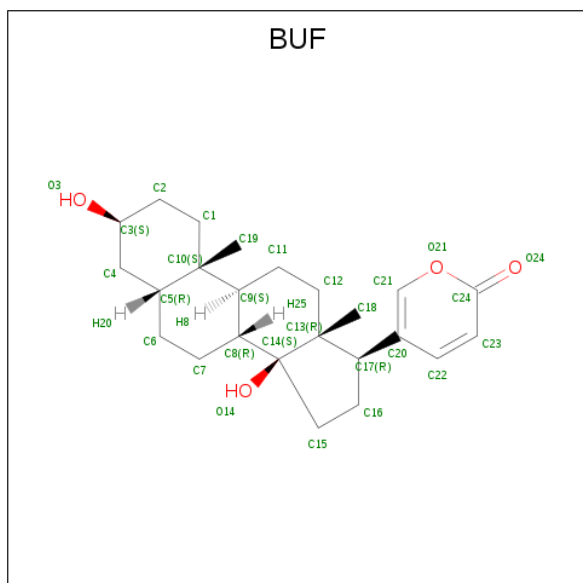
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



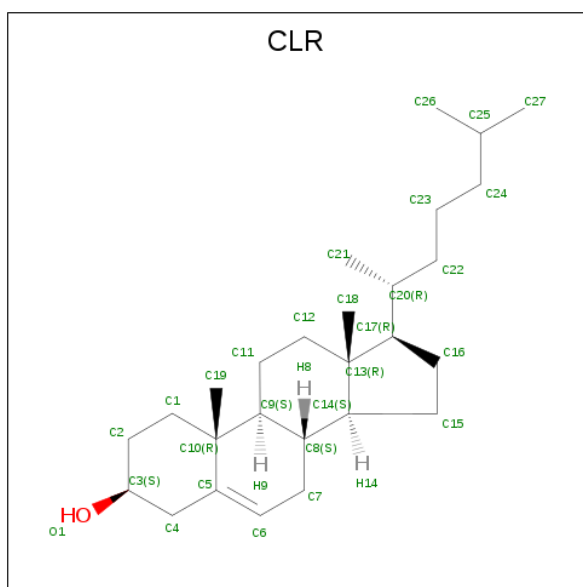
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	H	2	Total	C	O	0	0	0
			23	12	11			
5	I	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 6 is bufalin (three-letter code: BUF) (formula: $C_{24}H_{34}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			28	24	4		
6	C	1	Total	C	O	0	0
			28	24	4		

- Molecule 7 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



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

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	K	0	0
			3	3		
8	C	3	Total	K	0	0
			3	3		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

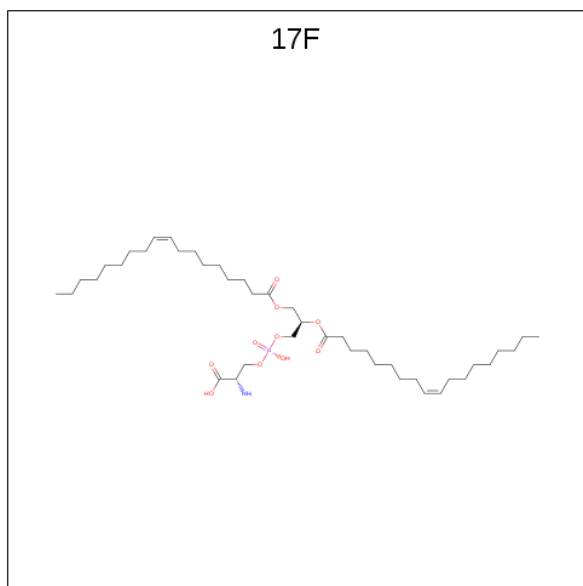
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Mg	0	0
			1	1		
9	C	1	Total	Mg	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 11 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (three-letter code: 17F) (formula: $C_{42}H_{78}NO_{10}P$).

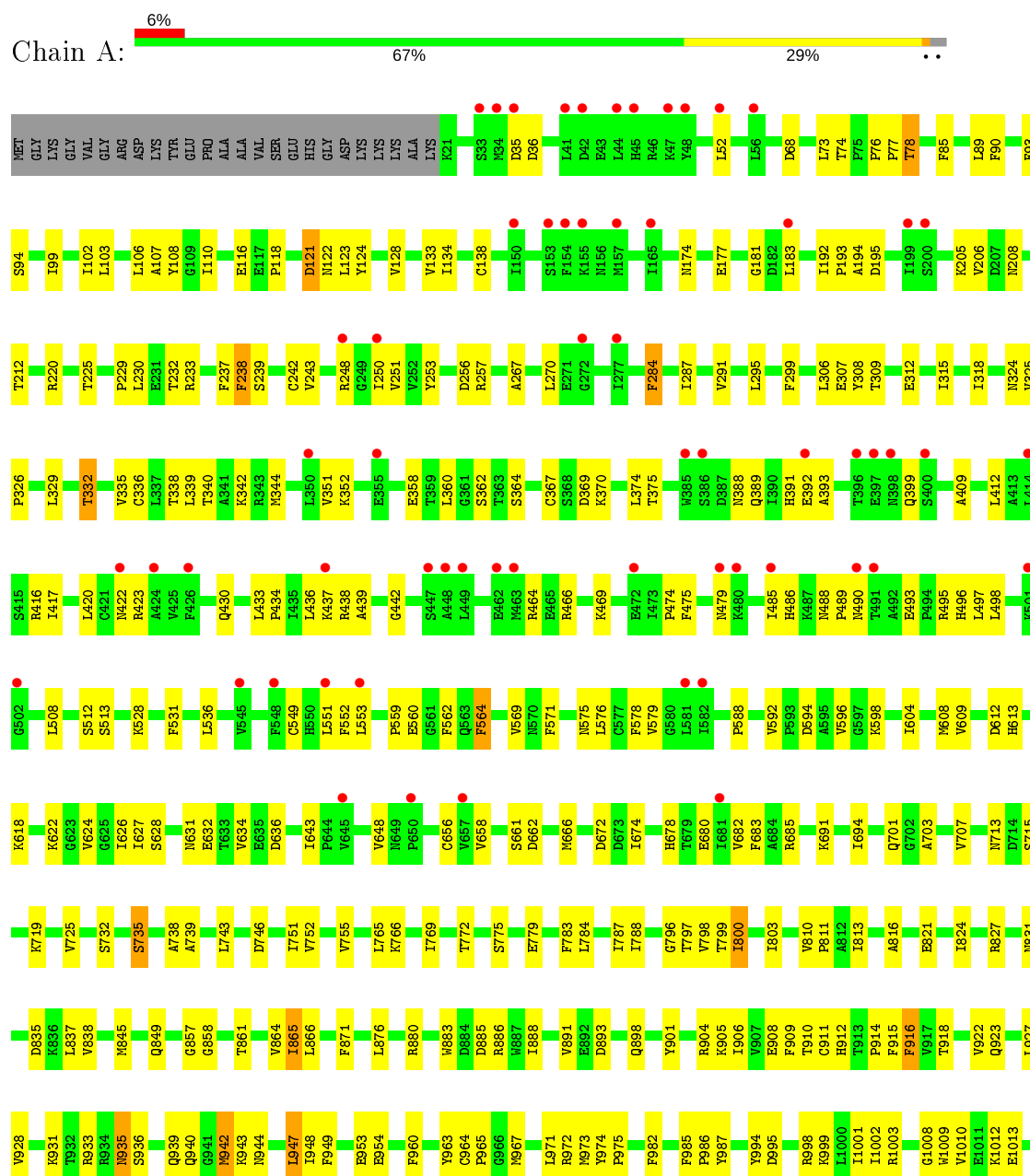


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	G	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

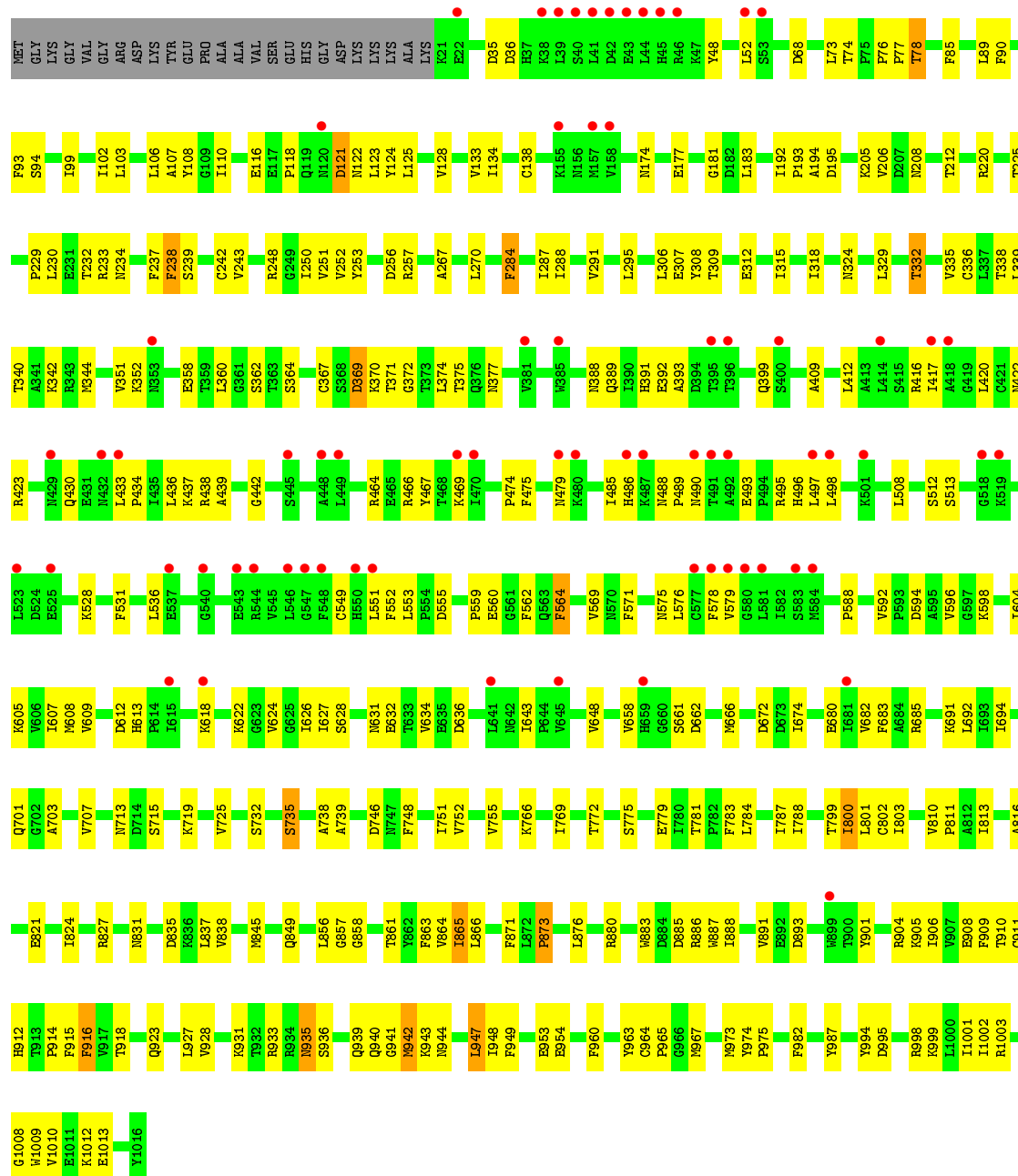
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



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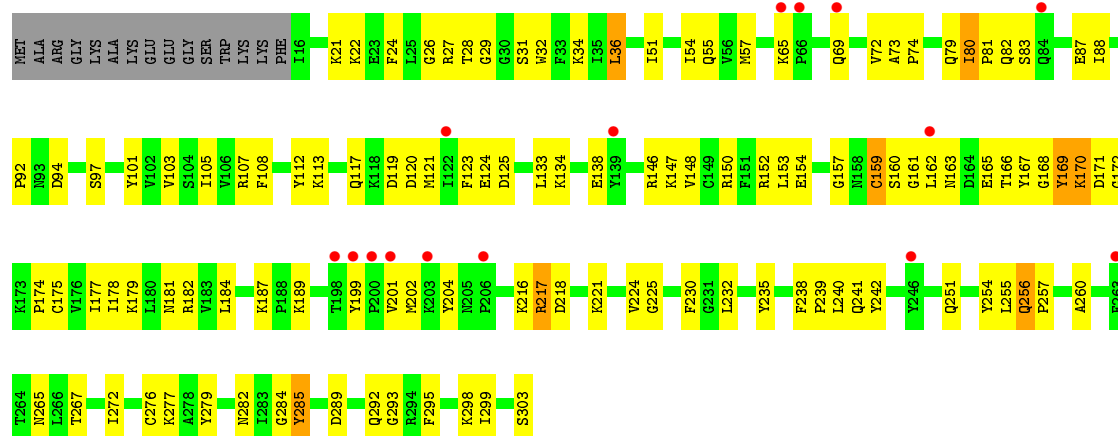
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain C:  7% 67% 29% ..

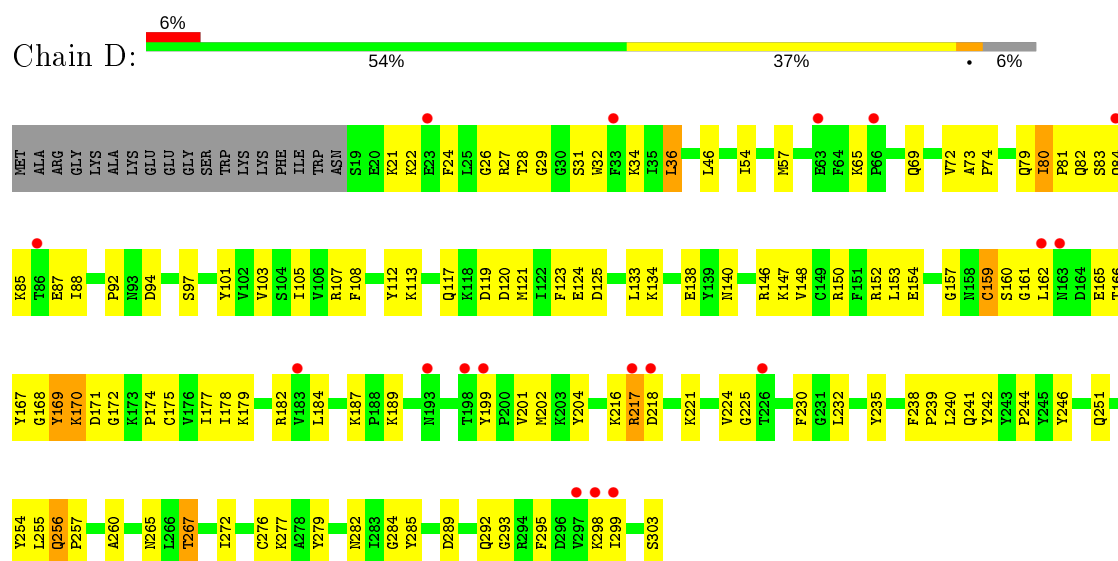


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

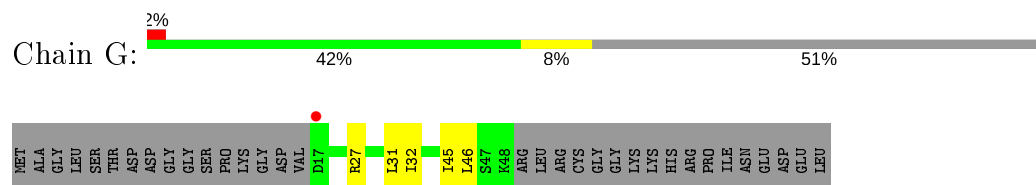
Chain B:  5% 56% 36% .. 5%



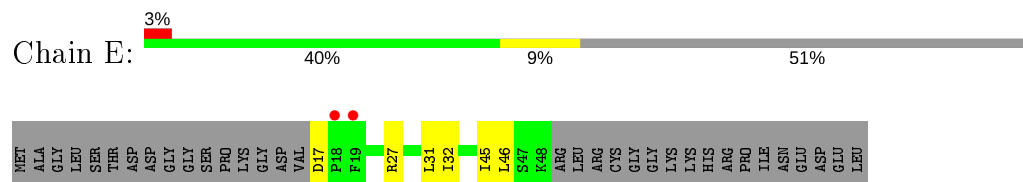
- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



- 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

Chain F:  50% 50%



- 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:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.91Å 240.27Å 152.70Å 90.00° 102.28° 90.00°	Depositor
Resolution (Å)	49.90 – 3.41 54.59 – 3.41	Depositor EDS
% Data completeness (in resolution range)	49.9 (49.90-3.41) 50.2 (54.59-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.245 , 0.288 0.248 , 0.292	Depositor DCC
R_{free} test set	1634 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20881	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, 17F, K, GLC, PHD, FRU, BUF, CLR

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	0.34	0/7867	0.54	0/10674
1	C	0.34	0/7867	0.54	0/10674
2	B	0.36	0/2419	0.59	0/3263
2	D	0.35	0/2387	0.59	0/3218
3	E	0.36	0/261	0.51	0/354
3	G	0.33	0/261	0.52	0/354
All	All	0.34	0/21062	0.55	0/28537

There are no bond length outliers.

There are no bond angle outliers.

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	7730	0	7776	211	0
1	C	7730	0	7776	219	0
2	B	2357	0	2328	83	0
2	D	2327	0	2301	83	0
3	E	255	0	259	5	0
3	G	255	0	259	4	0
4	F	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	23	0	21	3	0
5	I	23	0	21	2	0
6	A	28	0	34	2	0
6	C	28	0	34	4	0
7	A	28	0	46	4	0
7	E	28	0	46	4	0
8	A	3	0	0	0	0
8	C	3	0	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	B	14	0	13	1	0
11	G	19	0	10	0	0
All	All	20881	0	20949	595	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 14.

All (595) 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:B:80:ILE:HG13	2:B:81:PRO:HD3	1.44	0.97
2:D:80:ILE:HG13	2:D:81:PRO:HD3	1.45	0.97
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.33	0.93
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.34	0.91
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.52	0.91
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.52	0.91
1:A:910:THR:HG22	1:A:974:TYR:HB2	1.54	0.90
1:C:910:THR:HG22	1:C:974:TYR:HB2	1.55	0.88
2:B:165:GLU:HB3	2:B:166:THR:HA	1.60	0.84
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.59	0.83
2:D:165:GLU:HB3	2:D:166:THR:HA	1.60	0.83
1:C:375:THR:HA	1:C:588:PRO:HA	1.60	0.82
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.62	0.81
2:D:94:ASP:HB3	2:D:97:SER:HB2	1.62	0.81
2:B:94:ASP:HB3	2:B:97:SER:HB2	1.63	0.81
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.17	0.80
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.18	0.79
1:A:375:THR:HA	1:A:588:PRO:HA	1.68	0.76
1:A:612:ASP:OD1	1:A:613:HIS:N	2.18	0.76
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.68	0.76
1:C:612:ASP:OD1	1:C:613:HIS:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.68	0.76
1:A:800:ILE:HG21	6:A:2001:BUF:H33	1.69	0.75
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.67	0.75
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.70	0.73
1:C:800:ILE:HG21	6:C:1102:BUF:H33	1.70	0.73
2:D:80:ILE:HG12	2:D:177:ILE:HB	1.70	0.73
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.71	0.72
2:B:80:ILE:HG12	2:B:177:ILE:HB	1.72	0.71
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.72	0.71
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.71	0.71
2:D:166:THR:HB	2:D:169:TYR:H	1.55	0.71
1:C:901:TYR:HA	1:C:904:ARG:HE	1.55	0.70
1:C:672:ASP:OD1	1:C:701:GLN:NE2	2.24	0.70
2:B:166:THR:HB	2:B:169:TYR:H	1.56	0.70
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.56	0.70
1:A:672:ASP:OD1	1:A:701:GLN:NE2	2.25	0.69
2:B:170:LYS:HB2	2:B:174:PRO:HA	1.72	0.69
2:D:170:LYS:HB2	2:D:174:PRO:HA	1.72	0.69
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.74	0.69
1:A:901:TYR:HA	1:A:904:ARG:HE	1.56	0.69
2:D:171:ASP:OD1	2:D:172:GLY:N	2.24	0.69
1:C:434:PRO:HG2	1:C:437:LYS:HB2	1.74	0.69
1:A:399:GLN:HE21	1:A:436:LEU:HD11	1.56	0.69
1:C:399:GLN:HE21	1:C:436:LEU:HD11	1.57	0.69
2:B:171:ASP:OD1	2:B:172:GLY:N	2.24	0.69
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.75	0.68
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.58	0.68
1:A:849:GLN:OE1	1:A:994:TYR:OH	2.12	0.67
1:A:609:VAL:HG22	1:A:683:PHE:HD2	1.59	0.67
2:B:80:ILE:HD13	2:B:177:ILE:HD12	1.77	0.67
2:D:80:ILE:HD13	2:D:177:ILE:HD12	1.77	0.67
1:A:118:PRO:HA	1:A:121:ASP:HB2	1.75	0.66
1:C:118:PRO:HA	1:C:121:ASP:HB2	1.76	0.66
1:A:335:VAL:O	1:A:339:LEU:HG	1.96	0.66
1:C:609:VAL:HG22	1:C:683:PHE:HD2	1.61	0.65
2:B:124:GLU:OE2	2:B:134:LYS:NZ	2.29	0.65
1:C:225:THR:HG21	1:C:233:ARG:HD2	1.77	0.65
2:D:124:GLU:OE2	2:D:134:LYS:NZ	2.30	0.65
1:C:909:PHE:HA	1:C:912:HIS:HD2	1.62	0.65
1:A:909:PHE:HA	1:A:912:HIS:HD2	1.62	0.65
1:C:420:LEU:HB3	1:C:486:HIS:HE1	1.63	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:GLY:HA3	2:D:171:ASP:HB3	1.78	0.65
2:D:31:SER:HB2	2:D:34:LYS:HD2	1.77	0.64
1:C:849:GLN:OE1	1:C:994:TYR:OH	2.15	0.64
1:C:335:VAL:O	1:C:339:LEU:HG	1.97	0.64
2:D:79:GLN:HG2	2:D:82:GLN:HG2	1.80	0.64
1:A:225:THR:HG21	1:A:233:ARG:HD2	1.78	0.64
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.79	0.63
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.80	0.63
2:B:168:GLY:HA3	2:B:171:ASP:HB3	1.79	0.63
2:B:65:LYS:HG3	2:B:184:LEU:HD22	1.80	0.62
2:B:79:GLN:HG2	2:B:82:GLN:HG2	1.82	0.62
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.65	0.62
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.82	0.62
1:A:800:ILE:HD13	6:A:2001:BUF:H33	1.82	0.61
2:D:133:LEU:HG	2:D:240:LEU:HB3	1.82	0.61
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.81	0.61
1:A:845:MET:SD	1:A:849:GLN:NE2	2.74	0.61
2:B:31:SER:HB2	2:B:34:LYS:HD2	1.81	0.60
1:A:422:ASN:O	1:A:464:ARG:NH1	2.33	0.60
2:B:276:CYS:HB2	2:B:295:PHE:HB3	1.82	0.60
1:A:284:PHE:HB2	1:A:838:VAL:HB	1.84	0.60
1:C:338:THR:O	1:C:342:LYS:HG2	2.00	0.60
2:D:182:ARG:NH1	2:D:256:GLN:OE1	2.29	0.60
1:A:430:GLN:HG3	1:A:433:LEU:HD12	1.84	0.60
1:C:430:GLN:HG3	1:C:433:LEU:HD12	1.84	0.60
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.84	0.60
2:D:124:GLU:HB2	2:D:147:LYS:HD3	1.84	0.60
2:B:189:LYS:H	2:B:282:ASN:HB2	1.68	0.59
1:C:691:LYS:HA	1:C:694:ILE:HD12	1.85	0.59
1:C:422:ASN:O	1:C:464:ARG:NH1	2.34	0.59
2:D:202:MET:HB2	2:D:235:TYR:CD2	2.38	0.59
1:C:800:ILE:HD13	6:C:1102:BUF:H33	1.85	0.58
2:D:276:CYS:HB2	2:D:295:PHE:HB3	1.83	0.58
2:D:65:LYS:HG3	2:D:184:LEU:HD22	1.83	0.58
1:C:942:MET:H	5:H:2:FRU:H5	1.68	0.58
1:A:338:THR:O	1:A:342:LYS:HG2	2.03	0.58
2:B:153:LEU:HB2	2:B:162:LEU:HD23	1.84	0.58
1:C:364:SER:OG	1:C:703:ALA:HB1	2.04	0.58
2:B:202:MET:HB2	2:B:235:TYR:CD2	2.38	0.58
1:C:845:MET:SD	1:C:849:GLN:NE2	2.76	0.58
1:A:549:CYS:HA	1:A:579:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PHE:HB2	1:C:838:VAL:HB	1.86	0.58
2:D:189:LYS:H	2:D:282:ASN:HB2	1.69	0.58
1:C:116:GLU:HG3	1:C:118:PRO:HD3	1.86	0.58
2:D:153:LEU:HB2	2:D:162:LEU:HD23	1.85	0.58
1:A:116:GLU:HG3	1:A:118:PRO:HD3	1.86	0.58
1:A:943:LYS:HG3	5:I:2:FRU:H61	1.85	0.58
1:C:118:PRO:HB3	1:C:122:ASN:HB2	1.86	0.58
1:A:691:LYS:HA	1:A:694:ILE:HD12	1.86	0.57
1:A:909:PHE:HD1	1:A:912:HIS:CD2	2.22	0.57
1:A:118:PRO:HB3	1:A:122:ASN:HB2	1.86	0.57
2:B:133:LEU:HG	2:B:240:LEU:HB3	1.86	0.57
1:A:766:LYS:HG3	1:A:837:LEU:HD12	1.85	0.57
1:A:89:LEU:HD21	1:A:134:ILE:HA	1.85	0.57
1:A:942:MET:H	5:I:2:FRU:H5	1.70	0.57
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.87	0.57
1:A:928:VAL:O	1:A:931:LYS:HB3	2.04	0.57
1:A:909:PHE:HD1	1:A:912:HIS:HD2	1.52	0.56
1:A:364:SER:OG	1:A:703:ALA:HB1	2.05	0.56
2:D:230:PHE:HE1	4:F:1:NAG:H81	1.70	0.56
2:D:108:PHE:HZ	2:D:179:LYS:HD3	1.70	0.56
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.88	0.56
1:A:861:THR:HG21	1:A:914:PRO:HB2	1.87	0.56
1:C:89:LEU:HD21	1:C:134:ILE:HA	1.86	0.56
1:C:861:THR:HG21	1:C:914:PRO:HB2	1.87	0.56
2:D:138:GLU:O	2:D:146:ARG:NH2	2.39	0.56
1:C:909:PHE:HD1	1:C:912:HIS:CD2	2.24	0.56
1:C:928:VAL:O	1:C:931:LYS:HB3	2.05	0.56
1:A:775:SER:HB3	1:A:923:GLN:NE2	2.20	0.55
2:B:29:GLY:HA2	2:B:32:TRP:CD1	2.40	0.55
1:C:909:PHE:HD1	1:C:912:HIS:HD2	1.53	0.55
1:A:831:ASN:N	1:A:835:ASP:OD2	2.28	0.55
1:A:329:LEU:HD13	1:A:772:THR:HG21	1.87	0.55
1:C:866:LEU:HD13	1:C:876:LEU:HD21	1.89	0.55
1:C:230:LEU:HA	1:C:237:PHE:HZ	1.71	0.55
1:A:360:LEU:O	1:A:755:VAL:HG23	2.07	0.55
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.89	0.55
2:B:119:ASP:O	2:B:123:PHE:HB2	2.07	0.55
2:B:182:ARG:NH1	2:B:256:GLN:OE1	2.34	0.54
1:C:831:ASN:N	1:C:835:ASP:OD2	2.29	0.54
1:A:183:LEU:HD11	1:A:248:ARG:HB3	1.89	0.54
1:C:329:LEU:HD13	1:C:772:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:GLY:HA2	2:D:32:TRP:CD1	2.42	0.54
2:D:216:LYS:HB2	2:D:221:LYS:HG2	1.87	0.54
1:C:963:TYR:CE2	7:E:101:CLR:H6	2.43	0.54
1:C:183:LEU:HD11	1:C:248:ARG:HB3	1.89	0.54
1:C:909:PHE:HA	1:C:912:HIS:CD2	2.43	0.54
1:A:230:LEU:HA	1:A:237:PHE:HZ	1.72	0.54
1:A:909:PHE:HA	1:A:912:HIS:CD2	2.43	0.54
1:A:931:LYS:HE2	1:A:947:LEU:HD13	1.88	0.54
2:D:166:THR:N	2:D:167:TYR:HA	2.23	0.54
1:A:358:GLU:OE2	1:A:362:SER:OG	2.18	0.54
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.43	0.54
2:B:146:ARG:HB2	2:B:251:GLN:HG2	1.91	0.53
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.91	0.53
1:C:775:SER:HB3	1:C:923:GLN:NE2	2.23	0.53
2:D:146:ARG:HB2	2:D:251:GLN:HG2	1.91	0.53
2:D:119:ASP:O	2:D:123:PHE:HB2	2.09	0.53
1:A:608:MET:HB3	1:A:682:VAL:HG22	1.88	0.53
1:C:719:LYS:HB2	1:C:738:ALA:HB1	1.91	0.53
2:B:80:ILE:HD11	2:B:177:ILE:H	1.73	0.53
1:C:931:LYS:HE2	1:C:947:LEU:HD13	1.89	0.53
1:A:634:VAL:HG13	1:A:648:VAL:HB	1.91	0.53
2:B:138:GLU:O	2:B:146:ARG:NH2	2.42	0.53
1:C:811:PRO:HB3	1:C:927:LEU:HD13	1.91	0.53
2:B:108:PHE:HZ	2:B:179:LYS:HD3	1.73	0.53
2:B:166:THR:N	2:B:167:TYR:HA	2.24	0.52
1:A:883:TRP:NE1	1:A:908:GLU:OE1	2.43	0.52
2:B:216:LYS:HB2	2:B:221:LYS:HG2	1.89	0.52
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.91	0.52
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.91	0.52
1:A:108:TYR:CE2	1:A:123:LEU:HB2	2.45	0.52
1:A:430:GLN:HG2	1:A:438:ARG:HB2	1.91	0.52
2:D:24:PHE:HB3	2:D:28:THR:HA	1.90	0.52
1:C:963:TYR:HE2	7:E:101:CLR:H6	1.74	0.52
1:C:943:LYS:HG3	5:H:2:FRU:H61	1.91	0.52
2:D:103:VAL:HG12	2:D:107:ARG:HE	1.74	0.52
1:A:118:PRO:HB3	1:A:122:ASN:H	1.74	0.52
1:A:174:ASN:HB3	1:A:177:GLU:HG3	1.92	0.52
2:B:103:VAL:HG12	2:B:107:ARG:HE	1.74	0.52
1:C:766:LYS:HG3	1:C:837:LEU:HD12	1.90	0.52
1:C:887:TRP:CZ2	2:D:85:LYS:HB3	2.45	0.52
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.91	0.52
1:C:118:PRO:HB3	1:C:122:ASN:H	1.75	0.52
1:C:85:PHE:HE1	1:C:138:CYS:HA	1.75	0.52
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.91	0.52
1:A:238:PHE:O	1:A:239:SER:OG	2.24	0.52
1:A:488:ASN:ND2	1:A:490:ASN:HB2	2.25	0.52
1:A:963:TYR:CE2	7:A:2002:CLR:H6	2.45	0.52
1:C:108:TYR:CE2	1:C:123:LEU:HB2	2.45	0.52
2:B:24:PHE:HB3	2:B:28:THR:HA	1.91	0.51
1:C:99:ILE:HA	1:C:102:ILE:HD12	1.91	0.51
1:A:485:ILE:HB	1:A:498:LEU:HD13	1.92	0.51
1:A:866:LEU:HD13	1:A:876:LEU:HD21	1.93	0.51
1:A:811:PRO:HB3	1:A:927:LEU:HD13	1.93	0.51
1:A:799:THR:HA	1:A:973:MET:HE3	1.92	0.51
1:C:634:VAL:HG13	1:C:648:VAL:HB	1.93	0.51
1:A:85:PHE:HE1	1:A:138:CYS:HA	1.76	0.51
1:C:107:ALA:HB2	1:C:318:ILE:HG21	1.92	0.51
1:C:174:ASN:HB3	1:C:177:GLU:HG3	1.92	0.51
2:D:80:ILE:HD11	2:D:177:ILE:H	1.75	0.51
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.45	0.51
1:C:430:GLN:HG2	1:C:438:ARG:HB2	1.93	0.51
1:A:719:LYS:HB2	1:A:738:ALA:HB1	1.93	0.51
1:C:267:ALA:HB2	1:C:715:SER:HB3	1.91	0.51
1:C:485:ILE:HB	1:C:498:LEU:HD13	1.93	0.51
1:A:121:ASP:OD1	1:A:797:THR:OG1	2.26	0.51
2:B:284:GLY:O	2:B:293:GLY:HA3	2.10	0.51
1:C:551:LEU:HG	1:C:552:PHE:O	2.11	0.51
2:D:32:TRP:CE3	2:D:36:LEU:HD11	2.46	0.51
1:A:551:LEU:HG	1:A:552:PHE:O	2.11	0.51
1:A:594:ASP:O	1:A:598:LYS:HG2	2.10	0.51
2:D:284:GLY:O	2:D:293:GLY:HA3	2.10	0.51
2:B:224:VAL:HG11	2:B:267:THR:HG23	1.93	0.50
1:C:949:PHE:HB2	3:E:45:ILE:HG23	1.94	0.50
1:A:99:ILE:HA	1:A:102:ILE:HD12	1.93	0.50
1:C:206:VAL:HG23	1:C:242:CYS:HA	1.93	0.50
1:A:430:GLN:HG2	1:A:439:ALA:H	1.76	0.50
1:C:358:GLU:OE2	1:C:362:SER:OG	2.21	0.50
1:C:594:ASP:O	1:C:598:LYS:HG2	2.11	0.50
1:C:885:ASP:OD1	1:C:888:ILE:HG13	2.11	0.50
1:A:206:VAL:HG23	1:A:242:CYS:HA	1.93	0.50
1:C:352:LYS:NZ	1:C:739:ALA:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:PHE:O	1:C:964:CYS:HB2	2.11	0.50
1:C:799:THR:HA	1:C:973:MET:HE3	1.93	0.50
2:B:32:TRP:CE3	2:B:36:LEU:HD11	2.47	0.50
1:C:243:VAL:HG12	1:C:442:GLY:O	2.11	0.50
1:C:389:GLN:HB3	1:C:391:HIS:NE2	2.27	0.50
2:D:224:VAL:HG11	2:D:267:THR:HG23	1.93	0.50
1:A:107:ALA:HB2	1:A:318:ILE:HG21	1.93	0.50
1:A:779:GLU:HB3	1:A:800:ILE:HD11	1.94	0.49
1:C:999:LYS:O	1:C:1003:ARG:NE	2.45	0.49
1:C:360:LEU:O	1:C:755:VAL:HG23	2.12	0.49
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.47	0.49
1:A:417:ILE:HD13	1:A:579:VAL:HG21	1.95	0.49
1:C:416:ARG:HH12	1:C:497:LEU:HD21	1.76	0.49
1:C:608:MET:HB3	1:C:682:VAL:HG22	1.92	0.49
1:C:658:VAL:HB	1:C:683:PHE:HD1	1.77	0.49
2:D:167:TYR:C	2:D:169:TYR:N	2.64	0.49
1:C:488:ASN:ND2	1:C:490:ASN:HB2	2.28	0.49
2:D:177:ILE:HA	2:D:260:ALA:HA	1.94	0.49
2:B:167:TYR:C	2:B:169:TYR:N	2.65	0.49
1:A:935:ASN:HA	1:A:1003:ARG:HD3	1.94	0.49
1:A:389:GLN:HB3	1:A:391:HIS:NE2	2.28	0.49
1:A:949:PHE:HB2	3:G:45:ILE:HG23	1.95	0.49
1:C:76:PRO:HB2	1:C:78:THR:OG1	2.11	0.49
1:A:632:GLU:HB3	1:A:636:ASP:HB2	1.93	0.49
2:D:242:TYR:CD2	2:D:257:PRO:HG3	2.46	0.49
1:A:885:ASP:OD1	1:A:888:ILE:HG13	2.12	0.49
1:A:935:ASN:ND2	1:A:940:GLN:OE1	2.46	0.49
2:D:157:GLY:C	2:D:159:CYS:H	2.15	0.49
1:C:430:GLN:HG2	1:C:439:ALA:H	1.78	0.49
1:C:632:GLU:HB3	1:C:636:ASP:HB2	1.94	0.49
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.48	0.49
1:C:370:LYS:HA	1:C:374:LEU:HD12	1.95	0.49
1:A:370:LYS:HA	1:A:374:LEU:HD12	1.95	0.48
1:A:963:TYR:HE2	7:A:2002:CLR:H6	1.78	0.48
1:A:416:ARG:HH12	1:A:497:LEU:HD21	1.77	0.48
2:B:242:TYR:CD2	2:B:257:PRO:HG3	2.47	0.48
2:B:225:GLY:HA2	2:B:265:ASN:O	2.14	0.48
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.96	0.48
1:C:935:ASN:OD1	1:C:935:ASN:N	2.46	0.48
1:C:964:CYS:HB3	1:C:967:MET:CG	2.43	0.48
1:A:512:SER:HB3	1:A:575:ASN:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:PRO:HB2	1:A:78:THR:OG1	2.12	0.48
1:A:935:ASN:N	1:A:935:ASN:OD1	2.47	0.48
1:C:110:ILE:HB	1:C:315:ILE:HD11	1.95	0.48
1:C:306:LEU:HD12	1:C:308:TYR:HE2	1.79	0.48
2:B:119:ASP:OD2	2:B:121:MET:HB2	2.14	0.48
2:B:230:PHE:HE1	10:B:1001:NAG:H81	1.78	0.48
1:C:287:ILE:O	1:C:291:VAL:HG22	2.14	0.48
1:A:360:LEU:HD22	1:A:360:LEU:H	1.78	0.48
1:A:658:VAL:HB	1:A:683:PHE:HD1	1.78	0.48
1:A:964:CYS:HB3	1:A:967:MET:CG	2.44	0.48
1:C:329:LEU:HD11	1:C:769:ILE:HG12	1.94	0.48
1:C:935:ASN:ND2	1:C:940:GLN:OE1	2.47	0.48
1:C:417:ILE:HD13	1:C:579:VAL:HG21	1.96	0.48
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.49	0.48
2:D:92:PRO:HD2	2:D:303:SER:HB2	1.96	0.48
1:A:287:ILE:O	1:A:291:VAL:HG22	2.14	0.48
1:A:906:ILE:O	1:A:910:THR:HG23	2.13	0.48
1:C:732:SER:OG	1:C:735:SER:OG	2.30	0.48
1:C:941:GLY:HA2	5:H:2:FRU:H12	1.95	0.48
1:C:883:TRP:NE1	1:C:908:GLU:OE1	2.44	0.48
2:D:119:ASP:OD2	2:D:121:MET:HB2	2.14	0.48
2:B:177:ILE:HA	2:B:260:ALA:HA	1.96	0.47
1:C:512:SER:HB3	1:C:575:ASN:HA	1.94	0.47
1:C:784:LEU:O	1:C:788:ILE:HG12	2.14	0.47
2:D:225:GLY:HA2	2:D:265:ASN:O	2.14	0.47
1:A:332:THR:HA	1:A:813:ILE:HD11	1.96	0.47
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.95	0.47
1:A:732:SER:OG	1:A:735:SER:OG	2.31	0.47
1:C:559:PRO:HG2	1:C:562:PHE:HB2	1.96	0.47
1:A:423:ARG:NH1	1:A:474:PRO:HB3	2.29	0.47
1:A:559:PRO:HG2	1:A:562:PHE:HB2	1.96	0.47
1:C:76:PRO:HA	1:C:77:PRO:HD3	1.80	0.47
2:D:289:ASP:HB3	2:D:292:GLN:HB3	1.97	0.47
2:D:120:ASP:OD1	2:D:150:ARG:NH2	2.47	0.47
1:A:124:TYR:O	1:A:128:VAL:HG23	2.15	0.47
1:A:824:ILE:HG22	1:A:827:ARG:HH12	1.79	0.47
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.69	0.47
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.49	0.47
1:A:960:PHE:O	1:A:964:CYS:HB2	2.14	0.47
2:B:157:GLY:C	2:B:159:CYS:H	2.17	0.47
2:B:187:LYS:O	2:B:282:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:O	1:A:110:ILE:HG12	2.15	0.47
1:A:336:CYS:SG	1:A:816:ALA:HB2	2.54	0.47
1:C:1009:TRP:CH2	1:C:1013:GLU:HG3	2.50	0.47
1:C:332:THR:HA	1:C:813:ILE:HD11	1.97	0.47
1:C:779:GLU:HB3	1:C:800:ILE:HD11	1.97	0.47
2:D:239:PRO:HB2	2:D:241:GLN:HG2	1.97	0.47
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.97	0.47
2:B:87:GLU:HA	2:B:298:LYS:O	2.15	0.47
1:C:106:LEU:O	1:C:110:ILE:HG12	2.15	0.47
2:B:120:ASP:OD1	2:B:150:ARG:NH2	2.48	0.47
2:B:154:GLU:HG3	2:B:162:LEU:HG	1.97	0.47
2:B:74:PRO:O	2:B:292:GLN:HG3	2.14	0.47
2:D:88:ILE:HG23	2:D:101:TYR:CE1	2.50	0.47
1:A:181:GLY:N	1:A:251:VAL:O	2.42	0.47
1:A:871:PHE:CE1	1:A:893:ASP:HB3	2.51	0.47
1:A:352:LYS:NZ	1:A:739:ALA:O	2.47	0.46
1:A:466:ARG:HG2	1:A:489:PRO:HB3	1.97	0.46
1:C:423:ARG:NH1	1:C:474:PRO:HB3	2.29	0.46
1:A:118:PRO:C	1:A:121:ASP:H	2.18	0.46
1:A:306:LEU:HD12	1:A:308:TYR:HE2	1.80	0.46
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.96	0.46
1:C:508:LEU:HD21	1:C:528:LYS:HE2	1.97	0.46
1:C:551:LEU:HD13	1:C:576:LEU:HA	1.96	0.46
2:B:88:ILE:HG23	2:B:101:TYR:CE1	2.50	0.46
1:C:935:ASN:HA	1:C:1003:ARG:HD3	1.97	0.46
1:C:466:ARG:HG2	1:C:489:PRO:HB3	1.98	0.46
1:A:332:THR:HG22	1:A:813:ILE:HG12	1.96	0.46
1:A:871:PHE:CZ	1:A:893:ASP:HB3	2.50	0.46
2:B:160:SER:O	2:B:162:LEU:N	2.49	0.46
2:B:92:PRO:HD2	2:B:303:SER:HB2	1.98	0.46
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.97	0.46
2:D:160:SER:O	2:D:162:LEU:N	2.49	0.46
1:A:622:LYS:HA	1:A:627:ILE:O	2.16	0.46
1:A:76:PRO:HA	1:A:77:PRO:HD3	1.80	0.46
1:A:885:ASP:O	1:A:904:ARG:NH2	2.47	0.46
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.96	0.46
1:A:267:ALA:HB2	1:A:715:SER:HB3	1.97	0.46
1:A:643:ILE:HD11	1:A:648:VAL:HG22	1.97	0.46
2:B:153:LEU:H	2:B:153:LEU:HD12	1.81	0.46
1:C:118:PRO:C	1:C:121:ASP:H	2.18	0.46
1:C:622:LYS:HA	1:C:627:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:154:GLU:HG3	2:D:162:LEU:HG	1.98	0.46
1:A:592:VAL:O	1:A:596:VAL:HG23	2.16	0.46
1:C:360:LEU:HD22	1:C:360:LEU:H	1.80	0.46
1:C:871:PHE:CE1	1:C:893:ASP:HB3	2.51	0.46
1:A:508:LEU:HD21	1:A:528:LYS:HE2	1.98	0.46
1:A:230:LEU:HA	1:A:237:PHE:CZ	2.51	0.46
1:A:74:THR:HG23	1:A:256:ASP:OD1	2.16	0.46
1:A:713:ASN:N	1:A:713:ASN:OD1	2.49	0.46
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.98	0.46
2:D:87:GLU:HA	2:D:298:LYS:O	2.16	0.46
1:A:309:THR:HG22	1:A:312:GLU:OE1	2.16	0.45
1:A:551:LEU:HD13	1:A:576:LEU:HA	1.97	0.45
1:A:803:ILE:HD13	1:A:803:ILE:HA	1.81	0.45
1:C:238:PHE:O	1:C:239:SER:OG	2.25	0.45
1:A:628:SER:OG	1:A:631:ASN:OD1	2.34	0.45
1:C:824:ILE:HG22	1:C:827:ARG:HH12	1.81	0.45
1:C:891:VAL:HG21	1:C:904:ARG:NH1	2.31	0.45
1:A:110:ILE:HB	1:A:315:ILE:HD11	1.98	0.45
2:D:187:LYS:O	2:D:282:ASN:ND2	2.50	0.45
1:A:469:LYS:HA	1:A:486:HIS:CD2	2.52	0.45
1:C:488:ASN:ND2	1:C:493:GLU:O	2.49	0.45
1:C:90:PHE:O	1:C:94:SER:HB2	2.17	0.45
7:A:2002:CLR:H231	7:A:2002:CLR:H262	1.82	0.45
1:A:329:LEU:HD11	1:A:769:ILE:HG12	1.97	0.45
1:C:336:CYS:SG	1:C:816:ALA:HB2	2.56	0.45
1:C:372:GLY:CA	1:C:377:ASN:HB2	2.47	0.45
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.98	0.45
2:D:153:LEU:HD12	2:D:153:LEU:H	1.82	0.45
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.67	0.45
1:A:243:VAL:HG12	1:A:442:GLY:O	2.16	0.45
2:B:239:PRO:HB2	2:B:241:GLN:HG2	1.99	0.45
1:C:885:ASP:O	1:C:904:ARG:NH2	2.48	0.45
1:A:1009:TRP:CH2	1:A:1013:GLU:HG3	2.52	0.45
1:C:208:ASN:HB3	1:C:212:THR:OG1	2.17	0.45
1:C:628:SER:OG	1:C:631:ASN:OD1	2.34	0.45
1:A:295:LEU:HD12	1:A:324:ASN:ND2	2.31	0.45
2:D:83:SER:HB3	2:D:87:GLU:H	1.83	0.45
7:E:101:CLR:H262	7:E:101:CLR:H231	1.81	0.45
1:A:118:PRO:HA	1:A:121:ASP:CB	2.43	0.44
2:B:80:ILE:CD1	2:B:177:ILE:H	2.29	0.44
1:C:181:GLY:N	1:C:251:VAL:O	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.98	0.44
2:B:199:TYR:O	2:B:201:VAL:N	2.50	0.44
1:C:469:LYS:HA	1:C:486:HIS:CD2	2.53	0.44
1:C:965:PRO:HD3	3:E:31:LEU:HD11	1.99	0.44
2:D:199:TYR:O	2:D:201:VAL:N	2.50	0.44
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.99	0.44
1:C:121:ASP:OD1	6:C:1102:BUF:H11	2.18	0.44
1:A:666:MET:HE1	1:A:674:ILE:HD12	1.98	0.44
2:D:74:PRO:O	2:D:292:GLN:HG3	2.17	0.44
1:A:965:PRO:HD3	3:G:31:LEU:HD11	1.99	0.44
1:A:865:ILE:CD1	1:A:914:PRO:HG3	2.48	0.44
1:A:618:LYS:NZ	1:A:636:ASP:OD1	2.46	0.44
1:C:74:THR:HG23	1:C:256:ASP:OD1	2.18	0.44
1:C:309:THR:HG22	1:C:312:GLU:OE1	2.18	0.44
1:C:906:ILE:O	1:C:910:THR:HG23	2.17	0.44
2:D:166:THR:HB	2:D:169:TYR:N	2.27	0.44
2:D:277:LYS:HB3	2:D:279:TYR:CE1	2.53	0.44
1:A:409:ALA:HA	1:A:412:LEU:HD12	1.99	0.44
1:A:909:PHE:CD1	1:A:912:HIS:HD2	2.34	0.44
1:C:118:PRO:HA	1:C:121:ASP:CB	2.44	0.44
1:C:124:TYR:O	1:C:128:VAL:HG23	2.18	0.44
1:C:192:ILE:HA	1:C:193:PRO:HD3	1.67	0.44
1:C:332:THR:HG22	1:C:813:ILE:HG12	1.99	0.44
1:A:325:VAL:HA	1:A:326:PRO:HD3	1.66	0.43
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.87	0.43
2:B:289:ASP:HB3	2:B:292:GLN:HB3	2.00	0.43
1:C:234:ASN:N	1:C:234:ASN:OD1	2.50	0.43
1:C:779:GLU:HG2	1:C:800:ILE:HG12	2.01	0.43
1:A:52:LEU:O	1:A:183:LEU:HD22	2.18	0.43
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.82	0.43
1:C:1009:TRP:CZ2	1:C:1013:GLU:HG3	2.53	0.43
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.51	0.43
1:C:803:ILE:HA	1:C:803:ILE:HD13	1.82	0.43
1:A:662:ASP:O	1:A:666:MET:HG3	2.18	0.43
1:A:999:LYS:O	1:A:1003:ARG:NE	2.50	0.43
2:B:167:TYR:O	2:B:167:TYR:CG	2.72	0.43
2:B:26:GLY:HA2	2:B:27:ARG:HA	1.71	0.43
1:C:270:LEU:HD11	1:C:692:LEU:HD22	2.00	0.43
1:A:1009:TRP:CZ2	1:A:1013:GLU:HG3	2.53	0.43
1:A:340:THR:O	1:A:344:MET:HG2	2.19	0.43
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:O	1:A:94:SER:HB2	2.19	0.43
1:A:656:CYS:SG	1:A:678:HIS:ND1	2.87	0.43
2:B:166:THR:HB	2:B:169:TYR:N	2.28	0.43
1:C:52:LEU:O	1:C:183:LEU:HD22	2.18	0.43
1:C:423:ARG:NH2	1:C:474:PRO:HG3	2.34	0.43
1:C:666:MET:HE1	1:C:674:ILE:HD12	2.00	0.43
1:A:784:LEU:O	1:A:788:ILE:HG12	2.18	0.43
2:B:277:LYS:HB3	2:B:279:TYR:CE1	2.53	0.43
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.99	0.43
1:C:409:ALA:HA	1:C:412:LEU:HD12	2.00	0.43
1:C:865:ILE:CD1	1:C:914:PRO:HG3	2.49	0.43
2:D:167:TYR:O	2:D:167:TYR:CG	2.72	0.43
2:D:277:LYS:HE2	2:D:285:TYR:CE2	2.54	0.43
1:A:796:GLY:N	1:A:912:HIS:ND1	2.67	0.43
2:B:125:ASP:OD1	2:B:152:ARG:NH1	2.49	0.43
2:B:162:LEU:HB3	2:B:163:ASN:H	1.64	0.43
1:C:369:PHD:OP2	1:C:371:THR:OG1	2.31	0.43
1:A:985:PHE:N	1:A:986:PRO:HD2	2.34	0.43
2:B:69:GLN:O	2:B:72:VAL:HG22	2.19	0.43
1:C:205:LYS:HG3	1:C:475:PHE:CZ	2.54	0.43
1:C:871:PHE:CZ	1:C:893:ASP:HB3	2.54	0.43
1:C:125:LEU:HD22	6:C:1102:BUF:H3	1.99	0.42
1:C:953:GLU:OE1	1:C:954:GLU:N	2.52	0.42
2:D:244:PRO:HG2	2:D:246:TYR:CE1	2.54	0.42
1:A:488:ASN:ND2	1:A:493:GLU:O	2.52	0.42
2:B:277:LYS:HE2	2:B:285:TYR:CE2	2.54	0.42
1:C:564:PHE:HB2	1:C:571:PHE:CZ	2.54	0.42
1:C:618:LYS:NZ	1:C:636:ASP:OD1	2.47	0.42
1:C:865:ILE:HD12	1:C:914:PRO:HG3	1.99	0.42
1:C:821:GLU:OE1	1:C:933:ARG:HB2	2.19	0.42
1:A:208:ASN:HB3	1:A:212:THR:OG1	2.19	0.42
1:A:798:VAL:HG11	1:A:971:LEU:HD22	2.02	0.42
1:C:661:SER:OG	1:C:685:ARG:NH1	2.53	0.42
2:D:80:ILE:CD1	2:D:177:ILE:H	2.31	0.42
1:A:975:PRO:HG3	3:G:27:ARG:NH2	2.34	0.42
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.85	0.42
2:D:26:GLY:HA2	2:D:27:ARG:HA	1.72	0.42
1:A:430:GLN:NE2	1:A:439:ALA:HB3	2.34	0.42
1:A:512:SER:OG	1:A:513:SER:N	2.52	0.42
1:A:779:GLU:HG2	1:A:800:ILE:HG12	2.02	0.42
1:C:536:LEU:HA	1:C:536:LEU:HD23	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:856:LEU:HD11	2:D:46:LEU:HB3	2.00	0.42
2:D:69:GLN:O	2:D:72:VAL:HG22	2.19	0.42
2:D:83:SER:OG	2:D:87:GLU:O	2.22	0.42
1:A:103:LEU:HB3	1:A:318:ILE:HG23	2.01	0.42
1:A:982:PHE:HE1	7:A:2002:CLR:H183	1.84	0.42
1:C:430:GLN:HB3	1:C:438:ARG:HB2	2.02	0.42
1:A:898:GLN:NE2	2:B:181:ASN:OD1	2.52	0.42
1:C:810:VAL:HB	1:C:811:PRO:HD3	2.01	0.42
1:A:412:LEU:O	1:A:416:ARG:HG3	2.20	0.42
1:A:752:VAL:O	1:A:755:VAL:HG12	2.19	0.42
1:A:783:PHE:CZ	1:A:787:ILE:HD11	2.55	0.42
1:A:891:VAL:HG21	1:A:904:ARG:NH1	2.34	0.42
2:B:83:SER:OG	2:B:87:GLU:O	2.23	0.42
1:C:181:GLY:HA2	1:C:250:ILE:HG23	2.01	0.42
1:C:392:GLU:HG2	1:C:393:ALA:O	2.19	0.42
2:B:83:SER:HB3	2:B:87:GLU:H	1.85	0.42
1:C:605:LYS:HE2	1:C:607:ILE:HD11	2.01	0.42
1:C:935:ASN:HB3	1:C:939:GLN:OE1	2.20	0.42
1:C:982:PHE:HE1	7:E:101:CLR:H183	1.85	0.42
1:A:1008:GLY:O	1:A:1012:LYS:HG2	2.20	0.42
1:A:205:LYS:HG3	1:A:475:PHE:CZ	2.54	0.42
1:A:423:ARG:NH2	1:A:474:PRO:HG3	2.35	0.42
1:A:430:GLN:HB3	1:A:438:ARG:HB2	2.02	0.42
1:A:417:ILE:CD1	1:A:579:VAL:HG21	2.50	0.42
1:A:915:PHE:O	1:A:918:THR:HB	2.20	0.42
2:B:217:ARG:NH1	2:B:218:ASP:OD2	2.53	0.42
2:D:112:TYR:CE1	2:D:255:LEU:HB3	2.55	0.42
1:A:626:ILE:O	1:A:680:GLU:HB3	2.20	0.41
1:A:803:ILE:HG12	1:A:916:PHE:HD1	1.85	0.41
1:C:412:LEU:O	1:C:416:ARG:HG3	2.20	0.41
1:C:752:VAL:O	1:C:755:VAL:HG12	2.19	0.41
1:C:998:ARG:O	1:C:1002:ILE:HG13	2.20	0.41
1:A:936:SER:HB2	1:A:1003:ARG:NH2	2.34	0.41
1:A:564:PHE:HB2	1:A:571:PHE:CZ	2.55	0.41
1:A:810:VAL:HB	1:A:811:PRO:HD3	2.02	0.41
1:A:944:ASN:O	1:A:948:ILE:HG12	2.20	0.41
1:A:953:GLU:OE1	1:A:954:GLU:N	2.53	0.41
1:C:936:SER:HB2	1:C:1003:ARG:NH2	2.34	0.41
1:C:887:TRP:CD1	2:D:84:GLN:O	2.72	0.41
1:A:857:GLY:HA2	1:A:987:TYR:CD2	2.56	0.41
1:C:662:ASP:O	1:C:666:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:LEU:HA	1:C:73:LEU:HD23	1.83	0.41
1:C:909:PHE:CD1	1:C:912:HIS:HD2	2.37	0.41
1:C:857:GLY:HA2	1:C:987:TYR:CD2	2.55	0.41
1:A:392:GLU:HG2	1:A:393:ALA:O	2.20	0.41
1:C:430:GLN:NE2	1:C:439:ALA:HB3	2.35	0.41
1:A:496:HIS:HB2	1:A:553:LEU:HB2	2.03	0.41
2:B:80:ILE:CG1	2:B:177:ILE:H	2.33	0.41
1:C:496:HIS:HB2	1:C:553:LEU:HB2	2.02	0.41
1:C:592:VAL:O	1:C:596:VAL:HG23	2.21	0.41
1:C:783:PHE:CZ	1:C:787:ILE:HD11	2.56	0.41
1:C:801:LEU:HD23	1:C:801:LEU:HA	1.85	0.41
1:C:858:GLY:HA3	1:C:915:PHE:CZ	2.54	0.41
1:A:194:ALA:HB1	1:A:253:TYR:O	2.20	0.41
1:A:918:THR:O	1:A:922:VAL:HG22	2.21	0.41
1:A:972:ARG:NH2	1:A:974:TYR:OH	2.51	0.41
2:B:169:TYR:O	2:B:170:LYS:HB3	2.20	0.41
2:B:178:ILE:HG22	2:B:238:PHE:HZ	1.86	0.41
2:B:51:ILE:O	2:B:55:GLN:HG2	2.20	0.41
1:C:508:LEU:HD11	1:C:528:LYS:HE2	2.03	0.41
1:C:781:THR:HA	1:C:784:LEU:HD12	2.01	0.41
1:C:863:PHE:CD1	1:C:873:PRO:HB3	2.56	0.41
1:C:975:PRO:HG3	3:E:27:ARG:NH2	2.35	0.41
2:D:21:LYS:HG2	2:D:22:LYS:N	2.36	0.41
1:A:496:HIS:HE1	1:A:560:GLU:HA	1.85	0.41
1:A:508:LEU:HD11	1:A:528:LYS:HE2	2.02	0.41
1:A:936:SER:HB3	1:A:939:GLN:HG3	2.02	0.41
1:C:288:ILE:HA	1:C:288:ILE:HD13	1.85	0.41
1:C:340:THR:O	1:C:344:MET:HG2	2.21	0.41
1:C:496:HIS:HE1	1:C:560:GLU:HA	1.85	0.41
1:A:765:LEU:HA	1:A:765:LEU:HD23	1.82	0.41
2:B:238:PHE:HA	2:B:239:PRO:HD3	1.90	0.41
2:B:179:LYS:HD2	2:B:256:GLN:NE2	2.36	0.41
1:C:295:LEU:HD12	1:C:324:ASN:ND2	2.35	0.41
1:C:417:ILE:CD1	1:C:579:VAL:HG21	2.51	0.41
1:C:944:ASN:O	1:C:948:ILE:HG12	2.21	0.41
2:B:112:TYR:CE1	2:B:255:LEU:HB3	2.56	0.41
1:C:229:PRO:O	1:C:232:THR:HG22	2.21	0.41
1:C:488:ASN:HB2	1:C:495:ARG:O	2.20	0.41
2:D:140:ASN:O	2:D:146:ARG:NH2	2.53	0.41
1:A:229:PRO:O	1:A:232:THR:HG22	2.20	0.41
1:A:270:LEU:HB2	1:A:719:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:SER:OG	1:A:685:ARG:NH1	2.54	0.41
1:A:858:GLY:HA3	1:A:915:PHE:CZ	2.54	0.41
2:B:21:LYS:HG2	2:B:22:LYS:N	2.36	0.41
1:C:555:ASP:N	1:C:555:ASP:OD1	2.52	0.41
1:C:626:ILE:O	1:C:680:GLU:HB3	2.21	0.41
2:D:179:LYS:HD2	2:D:256:GLN:NE2	2.36	0.41
1:A:998:ARG:O	1:A:1002:ILE:HG13	2.21	0.41
1:C:103:LEU:HB3	1:C:318:ILE:HG23	2.03	0.41
1:C:549:CYS:HB3	1:C:578:PHE:HA	2.02	0.41
1:C:901:TYR:CZ	1:C:905:LYS:HE3	2.56	0.41
1:C:915:PHE:O	1:C:918:THR:HB	2.21	0.41
1:A:205:LYS:HG3	1:A:475:PHE:HZ	1.86	0.40
1:A:488:ASN:HA	1:A:489:PRO:HD2	1.94	0.40
1:C:194:ALA:HB1	1:C:253:TYR:O	2.20	0.40
1:C:512:SER:OG	1:C:513:SER:N	2.54	0.40
1:C:748:PHE:O	1:C:751:ILE:HB	2.21	0.40
2:D:167:TYR:C	2:D:169:TYR:H	2.22	0.40
2:D:169:TYR:O	2:D:170:LYS:HB3	2.21	0.40
1:A:821:GLU:OE1	1:A:933:ARG:HB2	2.21	0.40
1:A:901:TYR:CZ	1:A:905:LYS:HE3	2.57	0.40
1:C:866:LEU:HB3	1:C:876:LEU:HD11	2.02	0.40
1:A:181:GLY:HA2	1:A:250:ILE:HG23	2.03	0.40
1:C:1008:GLY:O	1:C:1012:LYS:HG2	2.21	0.40
1:C:467:TYR:HB3	1:C:486:HIS:CB	2.52	0.40
1:C:821:GLU:OE2	1:C:933:ARG:N	2.55	0.40
2:D:217:ARG:NH1	2:D:218:ASP:OD2	2.54	0.40
2:D:21:LYS:HG2	2:D:22:LYS:H	1.85	0.40
2:D:178:ILE:HG22	2:D:238:PHE:HZ	1.87	0.40
1:A:295:LEU:O	1:A:299:PHE:HB2	2.21	0.40
1:A:488:ASN:HB2	1:A:495:ARG:O	2.21	0.40
1:A:743:LEU:HD11	1:A:751:ILE:HD13	2.03	0.40
1:C:713:ASN:N	1:C:713:ASN:OD1	2.51	0.40
1:C:858:GLY:HA2	1:C:918:THR:HG21	2.04	0.40
1:C:803:ILE:HG12	1:C:916:PHE:HD1	1.86	0.40
1:A:549:CYS:HB3	1:A:578:PHE:HA	2.02	0.40
2:B:165:GLU:HB3	2:B:166:THR:CA	2.39	0.40
2:B:167:TYR:C	2:B:169:TYR:H	2.22	0.40
1:C:48:TYR:OH	1:C:252:VAL:HG13	2.21	0.40
1:C:799:THR:O	1:C:802:CYS:HB2	2.21	0.40
2:D:125:ASP:OD1	2:D:152:ARG:NH1	2.51	0.40
3:E:17:ASP:N	3:E:17:ASP:OD1	2.55	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	993/1021 (97%)	939 (95%)	53 (5%)	1 (0%)	51	82
1	C	993/1021 (97%)	937 (94%)	55 (6%)	1 (0%)	51	82
2	B	286/303 (94%)	265 (93%)	18 (6%)	3 (1%)	15	46
2	D	283/303 (93%)	263 (93%)	17 (6%)	3 (1%)	14	44
3	E	30/65 (46%)	30 (100%)	0	0	100	100
3	G	30/65 (46%)	30 (100%)	0	0	100	100
All	All	2615/2778 (94%)	2464 (94%)	143 (6%)	8 (0%)	41	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	170	LYS
2	B	217	ARG
2	D	170	LYS
2	D	217	ARG
1	A	78	THR
1	C	78	THR
2	B	161	GLY
2	D	161	GLY

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	846/864 (98%)	819 (97%)	27 (3%)	39	67
1	C	846/864 (98%)	818 (97%)	28 (3%)	38	66
2	B	258/269 (96%)	245 (95%)	13 (5%)	24	54
2	D	255/269 (95%)	242 (95%)	13 (5%)	24	54
3	E	26/52 (50%)	25 (96%)	1 (4%)	33	61
3	G	26/52 (50%)	25 (96%)	1 (4%)	33	61
All	All	2257/2370 (95%)	2174 (96%)	83 (4%)	34	62

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	36	ASP
1	A	68	ASP
1	A	93	PHE
1	A	121	ASP
1	A	220	ARG
1	A	238	PHE
1	A	257	ARG
1	A	284	PHE
1	A	307	GLU
1	A	332	THR
1	A	351	VAL
1	A	388	ASN
1	A	479	ASN
1	A	531	PHE
1	A	564	PHE
1	A	569	VAL
1	A	735	SER
1	A	746	ASP
1	A	800	ILE
1	A	865	ILE
1	A	911	CYS
1	A	916	PHE
1	A	935	ASN
1	A	942	MET
1	A	947	LEU
1	A	995	ASP
2	B	36	LEU
2	B	54	ILE
2	B	80	ILE

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Mol	Chain	Res	Type
2	B	117	GLN
2	B	159	CYS
2	B	169	TYR
2	B	175	CYS
2	B	204	TYR
2	B	232	LEU
2	B	256	GLN
2	B	272	ILE
2	B	285	TYR
2	B	299	ILE
3	G	32	ILE
1	C	35	ASP
1	C	36	ASP
1	C	68	ASP
1	C	93	PHE
1	C	121	ASP
1	C	220	ARG
1	C	238	PHE
1	C	257	ARG
1	C	284	PHE
1	C	307	GLU
1	C	332	THR
1	C	351	VAL
1	C	388	ASN
1	C	479	ASN
1	C	531	PHE
1	C	564	PHE
1	C	569	VAL
1	C	735	SER
1	C	746	ASP
1	C	800	ILE
1	C	865	ILE
1	C	873	PRO
1	C	911	CYS
1	C	916	PHE
1	C	935	ASN
1	C	942	MET
1	C	947	LEU
1	C	995	ASP
2	D	36	LEU
2	D	54	ILE
2	D	80	ILE

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Mol	Chain	Res	Type
2	D	117	GLN
2	D	159	CYS
2	D	169	TYR
2	D	175	CYS
2	D	204	TYR
2	D	232	LEU
2	D	256	GLN
2	D	267	THR
2	D	272	ILE
2	D	299	ILE
3	E	32	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	399	GLN
1	A	488	ASN
1	A	841	GLN
1	A	889	ASN
1	A	898	GLN
2	B	181	ASN
1	C	377	ASN
1	C	399	GLN
1	C	488	ASN
1	C	889	ASN
1	C	898	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1,9	9,11,12	1.37	1 (11%)	10,15,17	1.44	2 (20%)
1	PHD	C	369	1,9	9,11,12	1.38	1 (11%)	10,15,17	1.47	2 (20%)

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	1,9	-	1/8/11/13	-
1	PHD	C	369	1,9	-	1/8/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	PHD	CB-CA	-2.39	1.48	1.53
1	A	369	PHD	CB-CA	-2.30	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	OD2-CG-CB	-3.22	117.62	124.73
1	A	369	PHD	OD2-CG-CB	-3.20	117.66	124.73
1	A	369	PHD	OD1-CG-CB	2.28	117.39	111.11
1	C	369	PHD	OD1-CG-CB	2.21	117.19	111.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	369	PHD	CA-CB-CG-OD2
1	C	369	PHD	CA-CB-CG-OD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	369	PHD	1	0

5.5 Carbohydrates ⓘ

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	2,4	14,14,15	0.53	0	17,19,21	0.62	0
4	NAG	F	2	4	14,14,15	0.34	0	17,19,21	0.39	0
5	GLC	H	1	5	11,11,12	0.54	0	15,15,17	1.95	3 (20%)
5	FRU	H	2	5	11,12,12	0.72	1 (9%)	10,18,18	0.81	0
5	GLC	I	1	5	11,11,12	0.55	0	15,15,17	1.34	1 (6%)
5	FRU	I	2	5	11,12,12	0.65	0	10,18,18	1.08	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	2,4	-	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	-	0/2/19/22	0/1/1/1
5	FRU	H	2	5	-	2/5/24/24	0/1/1/1
5	GLC	I	1	5	-	1/2/19/22	0/1/1/1
5	FRU	I	2	5	-	2/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	2	FRU	O2-C2	2.05	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	H	1	GLC	C1-O5-C5	5.23	119.28	112.19
5	I	1	GLC	C1-O5-C5	3.38	116.77	112.19
5	H	1	GLC	C1-C2-C3	2.98	113.33	109.67
5	H	1	GLC	O5-C5-C6	2.09	110.49	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

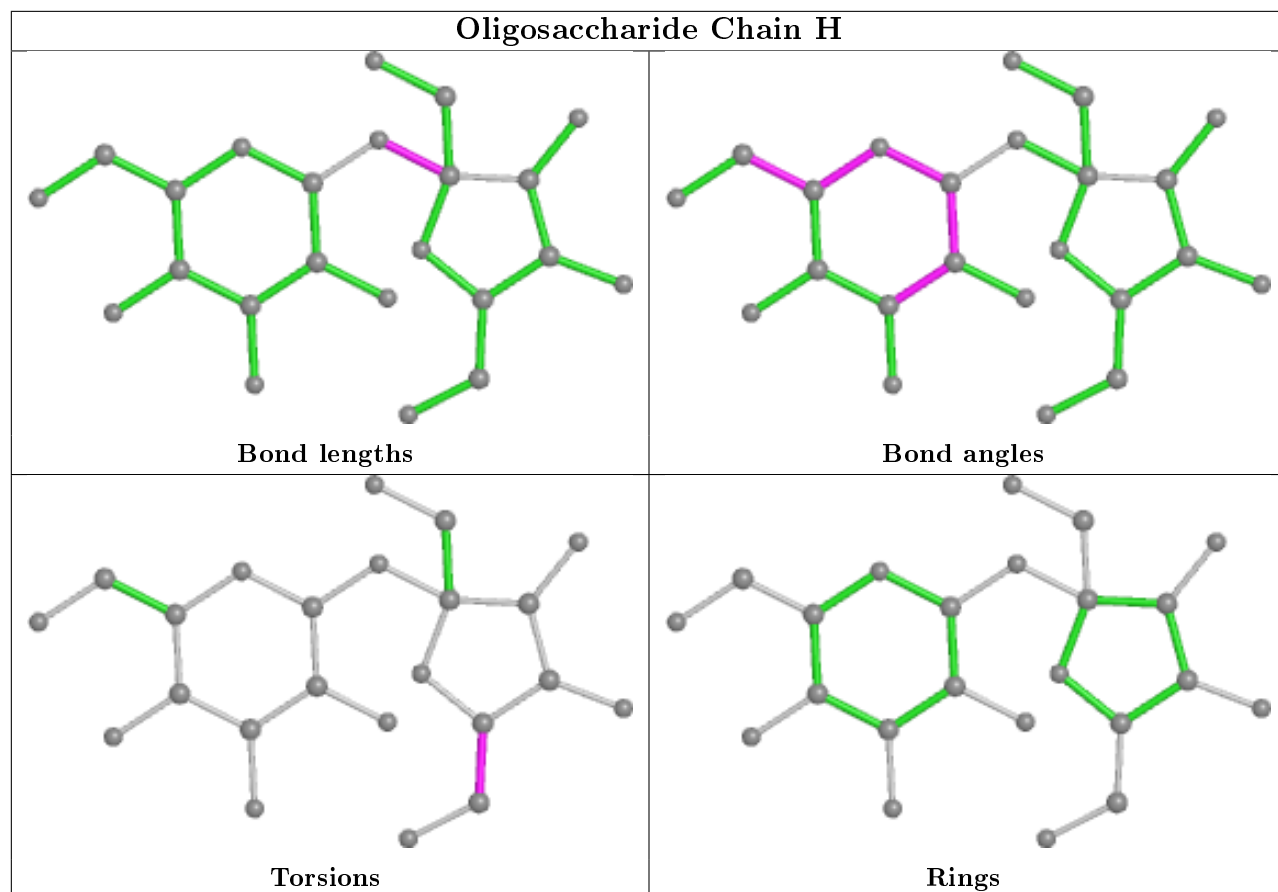
There are no ring outliers.

3 monomers are involved in 6 short contacts:

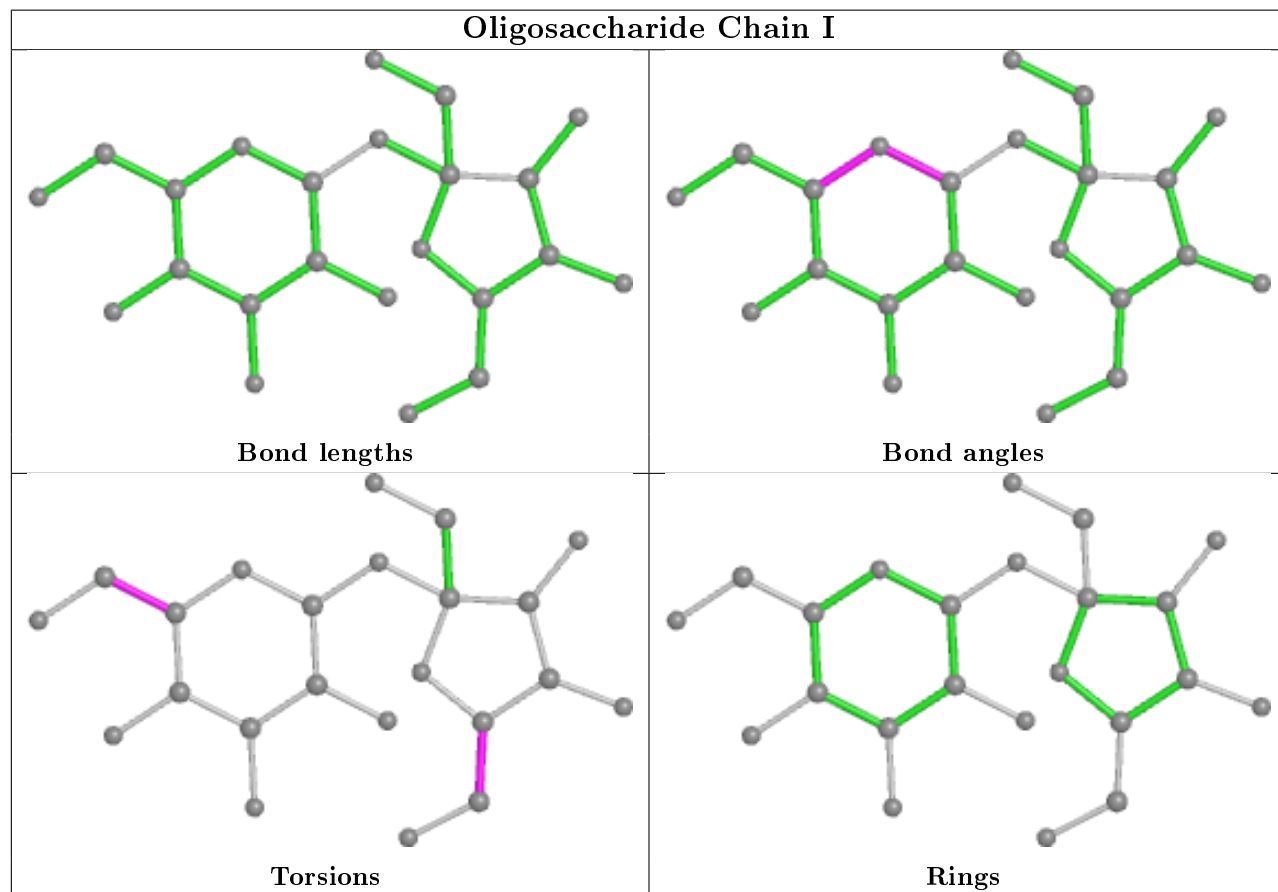
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	FRU	3	0
5	I	2	FRU	2	0
4	F	1	NAG	1	0

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 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BUF	C	1102	8	28,32,32	1.60	7 (25%)	46,52,52	1.71	7 (15%)
7	CLR	A	2002	-	31,31,31	2.52	12 (38%)	48,48,48	2.81	21 (43%)
7	CLR	E	101	-	31,31,31	2.49	9 (29%)	48,48,48	2.83	20 (41%)
11	17F	G	1001	-	15,18,53	1.79	3 (20%)	16,24,60	2.07	2 (12%)
10	NAG	B	1001	2	14,14,15	0.40	0	17,19,21	0.55	0
6	BUF	A	2001	8	28,32,32	1.54	6 (21%)	46,52,52	1.63	9 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BUF	C	1102	8	-	0/4/68/68	0/5/5/5
7	CLR	A	2002	-	-	3/10/68/68	0/4/4/4
7	CLR	E	101	-	-	3/10/68/68	0/4/4/4
11	17F	G	1001	-	-	12/17/21/59	-
10	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
6	BUF	A	2001	8	-	0/4/68/68	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2002	CLR	C6-C5	9.12	1.53	1.33
7	E	101	CLR	C6-C5	9.07	1.53	1.33
7	A	2002	CLR	C11-C9	4.74	1.61	1.53
7	E	101	CLR	C11-C9	4.65	1.61	1.53
11	G	1001	17F	P1-O6	4.50	1.77	1.59
6	A	2001	BUF	C23-C24	4.17	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1102	BUF	C23-C24	4.13	1.45	1.37
7	A	2002	CLR	C8-C14	3.97	1.61	1.53
7	E	101	CLR	C8-C14	3.70	1.60	1.53
6	C	1102	BUF	C13-C17	-3.59	1.53	1.58
7	E	101	CLR	C12-C13	3.58	1.60	1.54
7	A	2002	CLR	C13-C17	-3.54	1.48	1.55
6	A	2001	BUF	C22-C20	3.45	1.44	1.39
7	E	101	CLR	C13-C17	-3.34	1.48	1.55
7	E	101	CLR	C20-C17	-3.28	1.48	1.54
7	A	2002	CLR	C20-C17	-3.28	1.48	1.54
6	A	2001	BUF	C13-C17	-3.28	1.54	1.58
6	C	1102	BUF	C22-C20	3.13	1.44	1.39
7	A	2002	CLR	C12-C13	3.09	1.59	1.54
7	E	101	CLR	C15-C14	-2.93	1.48	1.54
6	C	1102	BUF	C14-C8	2.75	1.58	1.54
7	A	2002	CLR	C15-C14	-2.67	1.48	1.54
11	G	1001	17F	C1-C2	2.65	1.59	1.52
6	A	2001	BUF	C14-C8	2.50	1.57	1.54
11	G	1001	17F	P1-O3	2.47	1.69	1.59
7	E	101	CLR	C13-C14	-2.34	1.50	1.55
6	C	1102	BUF	O14-C14	-2.26	1.40	1.44
6	C	1102	BUF	C23-C22	-2.24	1.34	1.38
7	A	2002	CLR	C16-C17	2.19	1.58	1.54
7	A	2002	CLR	C13-C14	-2.19	1.50	1.55
6	A	2001	BUF	C23-C22	-2.17	1.34	1.38
6	C	1102	BUF	C4-C3	2.14	1.55	1.51
7	E	101	CLR	O1-C3	-2.11	1.37	1.43
7	A	2002	CLR	C19-C10	-2.05	1.51	1.54
7	A	2002	CLR	C4-C3	-2.05	1.48	1.52
7	A	2002	CLR	O1-C3	-2.04	1.37	1.43
6	A	2001	BUF	O14-C14	-2.00	1.40	1.44

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2002	CLR	C4-C5-C6	-7.59	109.67	120.61
7	E	101	CLR	C4-C5-C6	-7.45	109.87	120.61
7	E	101	CLR	C7-C6-C5	-7.14	111.89	125.06
11	G	1001	17F	O3-C1-C2	7.08	114.23	108.06
7	A	2002	CLR	C7-C6-C5	-6.82	112.48	125.06
7	E	101	CLR	C10-C5-C6	-5.82	114.00	122.90
7	A	2002	CLR	C12-C13-C17	-5.67	108.08	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	101	CLR	C12-C13-C17	-5.61	108.17	116.57
7	A	2002	CLR	C10-C5-C6	-5.52	114.46	122.90
7	E	101	CLR	C1-C10-C9	5.46	116.35	108.73
7	A	2002	CLR	C7-C8-C9	5.17	115.98	109.71
7	A	2002	CLR	C1-C10-C9	5.16	115.94	108.73
7	E	101	CLR	C21-C20-C17	5.03	120.62	112.92
6	C	1102	BUF	C15-C16-C17	4.84	108.78	103.17
7	A	2002	CLR	C21-C20-C17	4.82	120.30	112.92
6	A	2001	BUF	C15-C16-C17	4.77	108.70	103.17
7	E	101	CLR	C7-C8-C9	4.63	115.32	109.71
6	C	1102	BUF	C18-C13-C17	-4.29	111.41	115.99
6	A	2001	BUF	C18-C13-C17	-3.96	111.76	115.99
7	E	101	CLR	C19-C10-C1	-3.88	103.30	109.43
7	A	2002	CLR	C19-C10-C9	-3.79	107.16	111.68
7	E	101	CLR	C19-C10-C9	-3.65	107.33	111.68
7	E	101	CLR	C16-C17-C13	-3.57	99.54	103.84
7	E	101	CLR	C15-C14-C13	-3.45	99.68	103.84
7	A	2002	CLR	C11-C9-C10	3.43	117.60	113.08
7	A	2002	CLR	C19-C10-C1	-3.41	104.05	109.43
7	A	2002	CLR	C16-C17-C13	-3.37	99.78	103.84
7	A	2002	CLR	C7-C8-C14	3.26	115.64	110.91
7	E	101	CLR	C11-C9-C10	3.21	117.30	113.08
6	A	2001	BUF	C12-C13-C14	3.16	112.79	108.97
7	A	2002	CLR	C3-C4-C5	-3.13	106.72	112.03
6	C	1102	BUF	C18-C13-C12	3.10	114.12	109.73
7	E	101	CLR	C3-C4-C5	-3.07	106.82	112.03
7	A	2002	CLR	C11-C12-C13	-3.02	107.60	112.78
7	E	101	CLR	C7-C8-C14	2.89	115.10	110.91
6	C	1102	BUF	C14-C13-C17	2.86	106.84	103.56
6	A	2001	BUF	C18-C13-C12	2.81	113.71	109.73
7	A	2002	CLR	C15-C14-C13	-2.81	100.46	103.84
11	G	1001	17F	O2-P1-O1	2.80	126.10	112.24
6	C	1102	BUF	C9-C10-C5	2.79	112.50	108.58
7	E	101	CLR	C11-C12-C13	-2.69	108.17	112.78
6	C	1102	BUF	C12-C13-C14	2.62	112.14	108.97
7	E	101	CLR	C11-C9-C8	2.61	115.52	111.75
7	A	2002	CLR	C16-C17-C20	-2.51	108.26	112.15
7	A	2002	CLR	C11-C9-C8	2.45	115.29	111.75
7	A	2002	CLR	C21-C20-C22	-2.45	106.52	110.36
7	E	101	CLR	C17-C13-C14	2.44	102.96	100.07
7	E	101	CLR	C21-C20-C22	-2.41	106.58	110.36
6	A	2001	BUF	C14-C13-C17	2.32	106.22	103.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2001	BUF	C9-C10-C5	2.29	111.80	108.58
7	A	2002	CLR	C19-C10-C5	2.22	111.94	108.34
6	A	2001	BUF	C1-C2-C3	-2.15	107.71	110.47
7	E	101	CLR	C16-C17-C20	-2.15	108.82	112.15
6	C	1102	BUF	C1-C2-C3	-2.12	107.75	110.47
7	A	2002	CLR	C9-C10-C5	-2.10	106.36	109.65
6	A	2001	BUF	C22-C23-C24	2.08	121.03	118.45
6	A	2001	BUF	C7-C6-C5	2.06	115.97	111.84
7	E	101	CLR	C19-C10-C5	2.02	111.62	108.34
7	A	2002	CLR	C17-C13-C14	2.01	102.46	100.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	G	1001	17F	C4-O6-P1-O1
11	G	1001	17F	C4-O6-P1-O2
11	G	1001	17F	C4-O6-P1-O3
11	G	1001	17F	O6-C4-C5-C6
11	G	1001	17F	C4-C5-C6-O7
10	B	1001	NAG	O5-C5-C6-O6
11	G	1001	17F	O9-C5-C6-O7
10	B	1001	NAG	C4-C5-C6-O6
11	G	1001	17F	O6-C4-C5-O9
7	A	2002	CLR	C22-C23-C24-C25
7	E	101	CLR	C22-C23-C24-C25
11	G	1001	17F	C1-O3-P1-O6
11	G	1001	17F	C8-C7-O7-C6
7	E	101	CLR	C20-C22-C23-C24
7	A	2002	CLR	C20-C22-C23-C24
7	A	2002	CLR	C23-C24-C25-C26
7	E	101	CLR	C23-C24-C25-C26
11	G	1001	17F	O8-C7-O7-C6
11	G	1001	17F	C2-C1-O3-P1
11	G	1001	17F	C1-O3-P1-O1

There are no ring outliers.

5 monomers are involved in 15 short contacts:

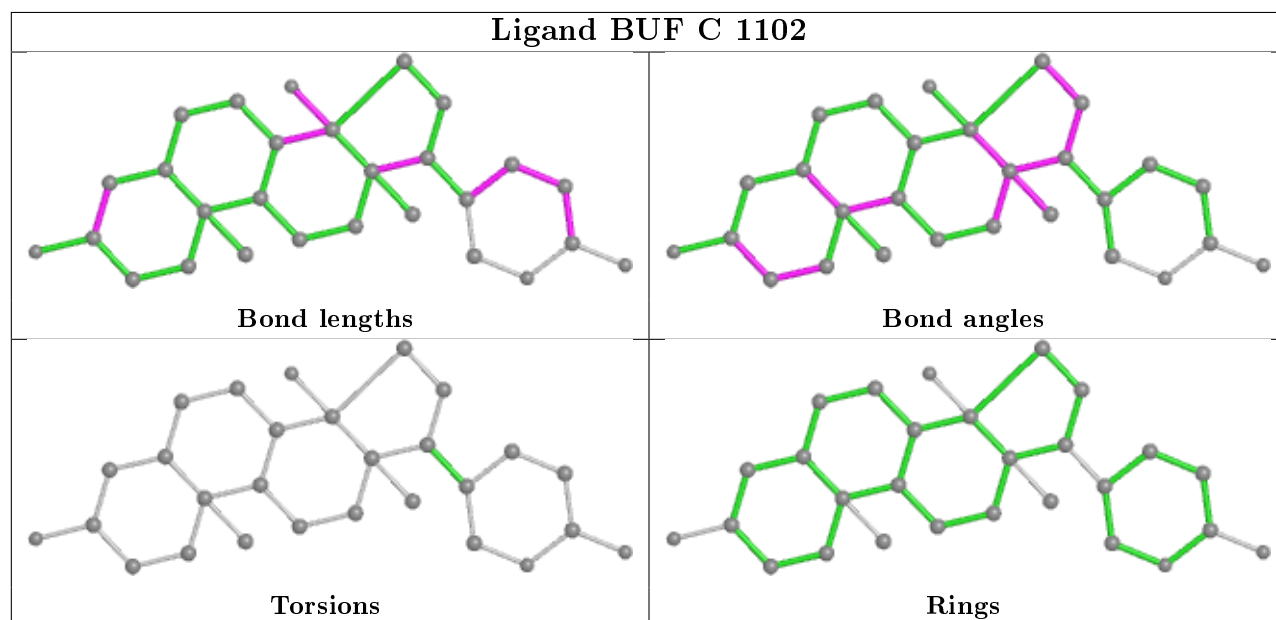
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1102	BUF	4	0

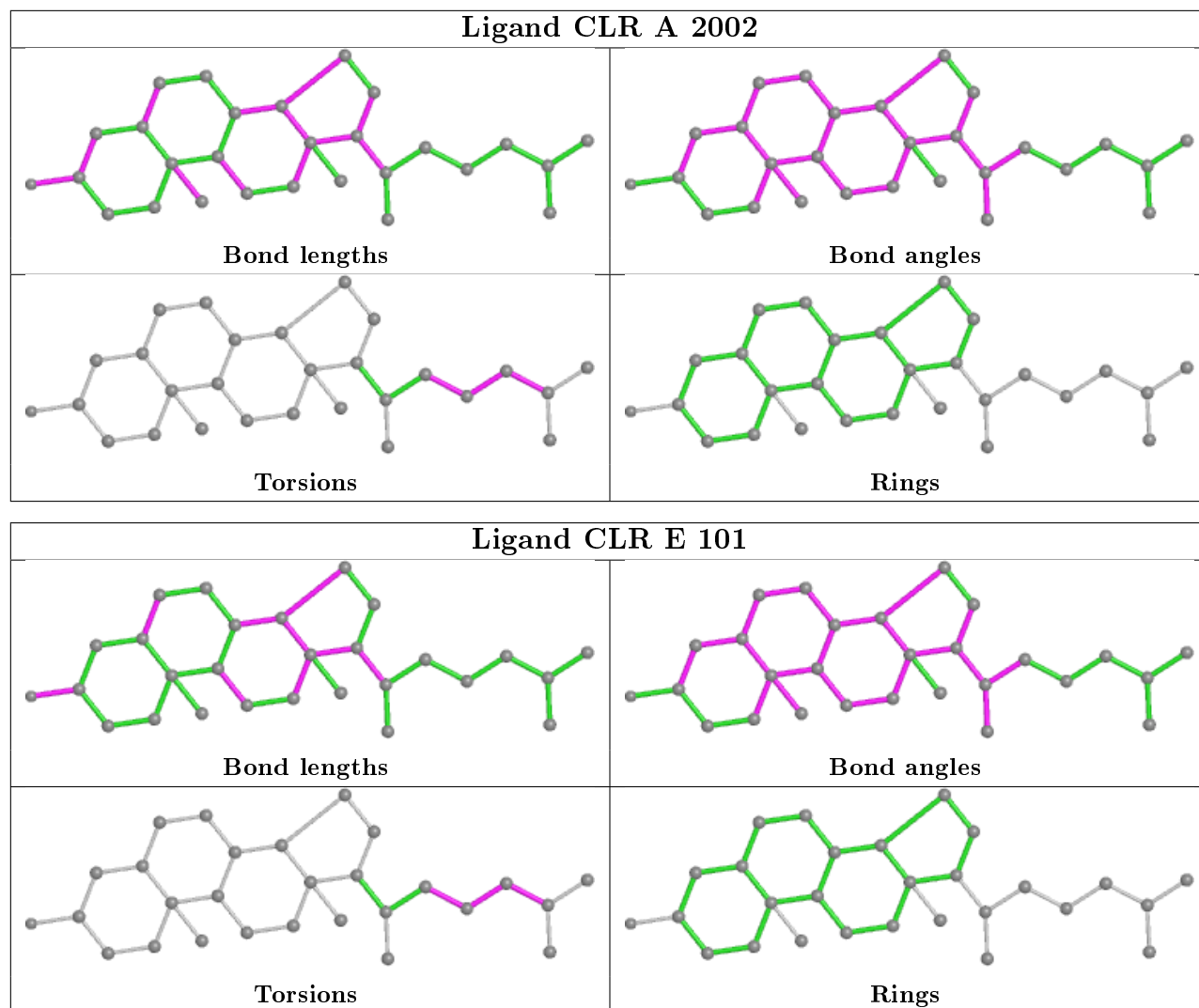
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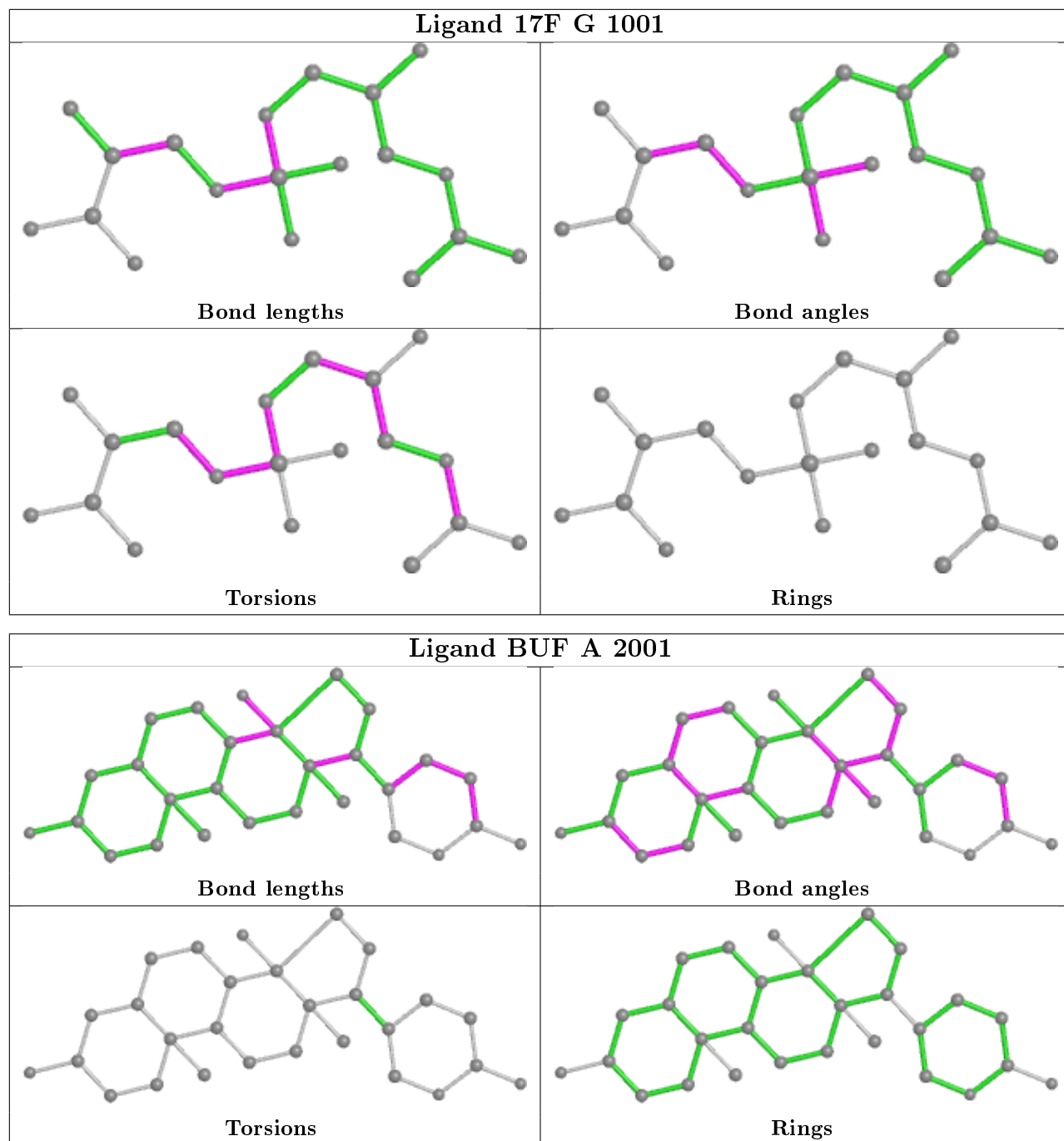
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2002	CLR	4	0
7	E	101	CLR	4	0
10	B	1001	NAG	1	0
6	A	2001	BUF	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.18	61 (6%)	21 22	40, 119, 201, 295	0
1	C	995/1021 (97%)	0.28	70 (7%)	16 18	41, 124, 212, 292	0
2	B	288/303 (95%)	0.25	15 (5%)	27 27	53, 124, 205, 248	0
2	D	285/303 (94%)	0.16	18 (6%)	20 21	56, 120, 199, 326	0
3	E	32/65 (49%)	0.13	2 (6%)	20 21	51, 80, 158, 178	0
3	G	32/65 (49%)	0.25	1 (3%)	49 48	56, 86, 144, 172	0
All	All	2627/2778 (94%)	0.23	167 (6%)	19 20	40, 121, 206, 326	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	547	GLY	11.6
2	B	198	THR	11.4
1	C	491	THR	9.0
2	B	199	TYR	8.7
1	C	550	HIS	7.3
1	A	397	GLU	6.4
1	A	645	VAL	6.3
1	A	545	VAL	6.1
1	A	42	ASP	5.8
1	C	518	GLY	5.8
1	C	41	LEU	5.7
2	D	198	THR	5.7
1	C	395	THR	5.5
1	C	480	LYS	5.4
2	D	199	TYR	5.4
1	A	183	LEU	5.3
1	C	45	HIS	5.3
2	B	139	TYR	5.2
1	C	52	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	193	ASN	5.1
1	C	580	GLY	5.1
1	C	497	LEU	5.0
1	A	396	THR	4.9
1	C	615	ILE	4.9
1	A	582	ILE	4.8
1	C	38	LYS	4.8
1	C	432	ASN	4.7
1	A	385	TRP	4.6
2	B	122	ILE	4.5
1	C	429	ASN	4.4
1	C	40	SER	4.3
1	A	153	SER	4.2
2	D	162	LEU	4.0
1	A	155	LYS	4.0
1	C	400	SER	4.0
1	C	519	LYS	4.0
1	A	150	ILE	3.9
1	C	548	PHE	3.9
1	A	44	LEU	3.9
2	D	33	PHE	3.9
1	A	33	SER	3.8
1	A	491	THR	3.8
1	A	272	GLY	3.7
1	C	39	LEU	3.7
1	A	548	PHE	3.6
1	C	584	MET	3.6
2	D	183	VAL	3.6
1	C	581	LEU	3.6
1	C	22	GLU	3.6
1	A	165	ILE	3.6
1	C	396	THR	3.5
1	C	681	ILE	3.5
1	A	462	GLU	3.5
1	A	392	GLU	3.5
1	A	398	ASN	3.4
2	D	84	GLN	3.4
1	C	540	GLY	3.4
1	C	486	HIS	3.3
1	C	155	LYS	3.3
1	C	46	ARG	3.3
2	D	218	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	579	VAL	3.2
1	C	544	ARG	3.2
1	C	53	SER	3.2
2	B	65	LYS	3.2
1	C	479	ASN	3.1
2	D	23	GLU	3.1
1	C	157	MET	3.0
1	A	250	ILE	3.0
2	D	298	LYS	2.9
1	A	472	GLU	2.9
1	C	44	LEU	2.9
1	A	437	LYS	2.9
1	A	657	VAL	2.8
1	C	618	LYS	2.8
1	C	385	TRP	2.8
2	D	297	VAL	2.8
3	G	17	ASP	2.8
1	C	42	ASP	2.8
1	A	400	SER	2.7
1	C	899	TRP	2.7
1	C	498	LEU	2.7
1	C	418	ALA	2.7
2	B	162	LEU	2.7
2	D	226	THR	2.7
1	A	501	LYS	2.7
1	A	41	LEU	2.7
1	C	469	LYS	2.7
1	C	490	ASN	2.7
1	C	445	SER	2.7
1	A	448	ALA	2.6
1	A	551	LEU	2.6
1	A	355	GLU	2.6
1	A	199	ILE	2.6
1	A	581	LEU	2.6
1	C	487	LYS	2.6
1	A	52	LEU	2.6
1	A	424	ALA	2.6
3	E	19	PHE	2.6
2	D	86	THR	2.6
1	C	492	ALA	2.5
1	A	485	ILE	2.5
1	C	537	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	553	LEU	2.5
1	A	447	SER	2.5
1	C	414	LEU	2.5
1	C	546	LEU	2.5
1	A	414	LEU	2.5
1	C	645	VAL	2.5
2	B	206	PRO	2.5
1	A	157	MET	2.4
1	A	502	GLY	2.4
1	C	448	ALA	2.4
2	B	201	VAL	2.4
1	A	463	MET	2.4
1	C	523	LEU	2.4
1	A	386	SER	2.4
1	A	48	TYR	2.4
2	B	246	TYR	2.4
1	C	417	ILE	2.4
1	C	433	LEU	2.4
2	D	217	ARG	2.4
1	C	501	LYS	2.4
1	C	449	LEU	2.3
1	C	43	GLU	2.3
2	B	84	GLN	2.3
1	A	154	PHE	2.3
1	A	35	ASP	2.3
1	C	641	LEU	2.3
2	B	263	PHE	2.3
1	A	47	LYS	2.3
1	C	659	HIS	2.3
1	A	426	PHE	2.3
1	C	353	ASN	2.3
1	A	449	LEU	2.2
1	A	200	SER	2.2
1	A	422	ASN	2.2
2	B	203	LYS	2.2
1	C	583	SER	2.2
1	A	277	ILE	2.2
1	C	120	ASN	2.2
1	C	578	PHE	2.2
1	A	480	LYS	2.2
1	C	470	ILE	2.2
1	C	158	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	490	ASN	2.2
2	B	66	PRO	2.2
1	C	543	GLU	2.2
2	D	299	ILE	2.2
1	A	248	ARG	2.1
1	C	577	CYS	2.1
1	A	650	PRO	2.1
1	A	479	ASN	2.1
3	E	18	PRO	2.1
1	A	34	MET	2.1
1	C	525	GLU	2.1
1	C	381	VAL	2.1
2	D	63	GLU	2.1
1	A	56	LEU	2.1
2	B	69	GLN	2.1
2	D	66	PRO	2.1
2	B	200	PRO	2.1
2	D	163	ASN	2.0
1	A	681	ILE	2.0
1	A	45	HIS	2.0
1	A	350	LEU	2.0
1	C	551	LEU	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.

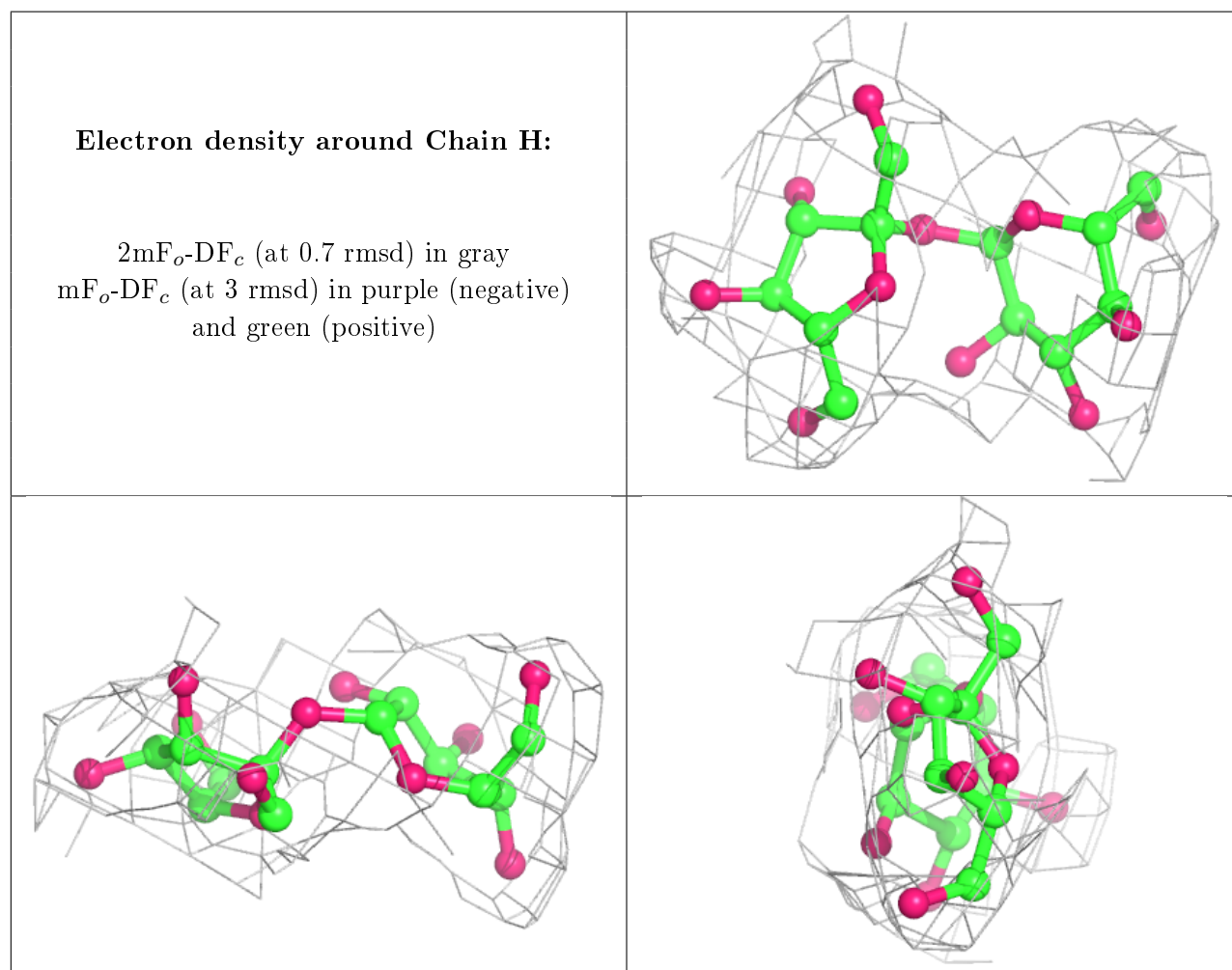
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PHD	C	369	12/13	0.97	0.23	102,103,105,105	0
1	PHD	A	369	12/13	0.98	0.18	116,118,121,121	0

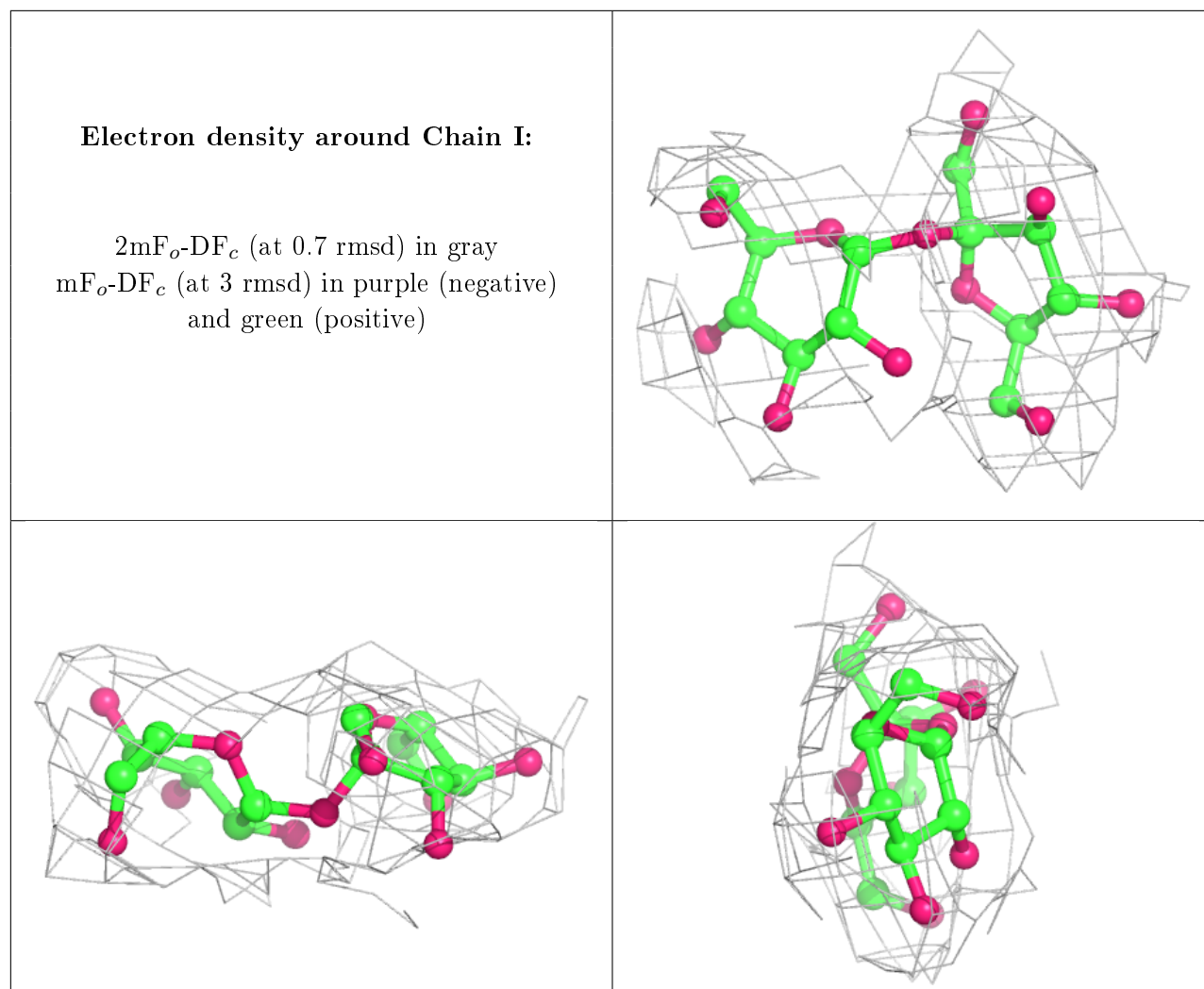
6.3 Carbohydrates [i](#)

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(\AA^2)	Q<0.9
4	NAG	F	1	14/15	0.78	0.33	157,166,174,177	0
4	NAG	F	2	14/15	0.84	0.38	168,173,183,184	0
5	GLC	H	1	11/12	0.95	0.17	113,115,118,120	0
5	FRU	I	2	12/12	0.96	0.20	101,104,105,106	0
5	GLC	I	1	11/12	0.96	0.15	104,105,108,109	0
5	FRU	H	2	12/12	0.98	0.18	110,113,115,116	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.





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.

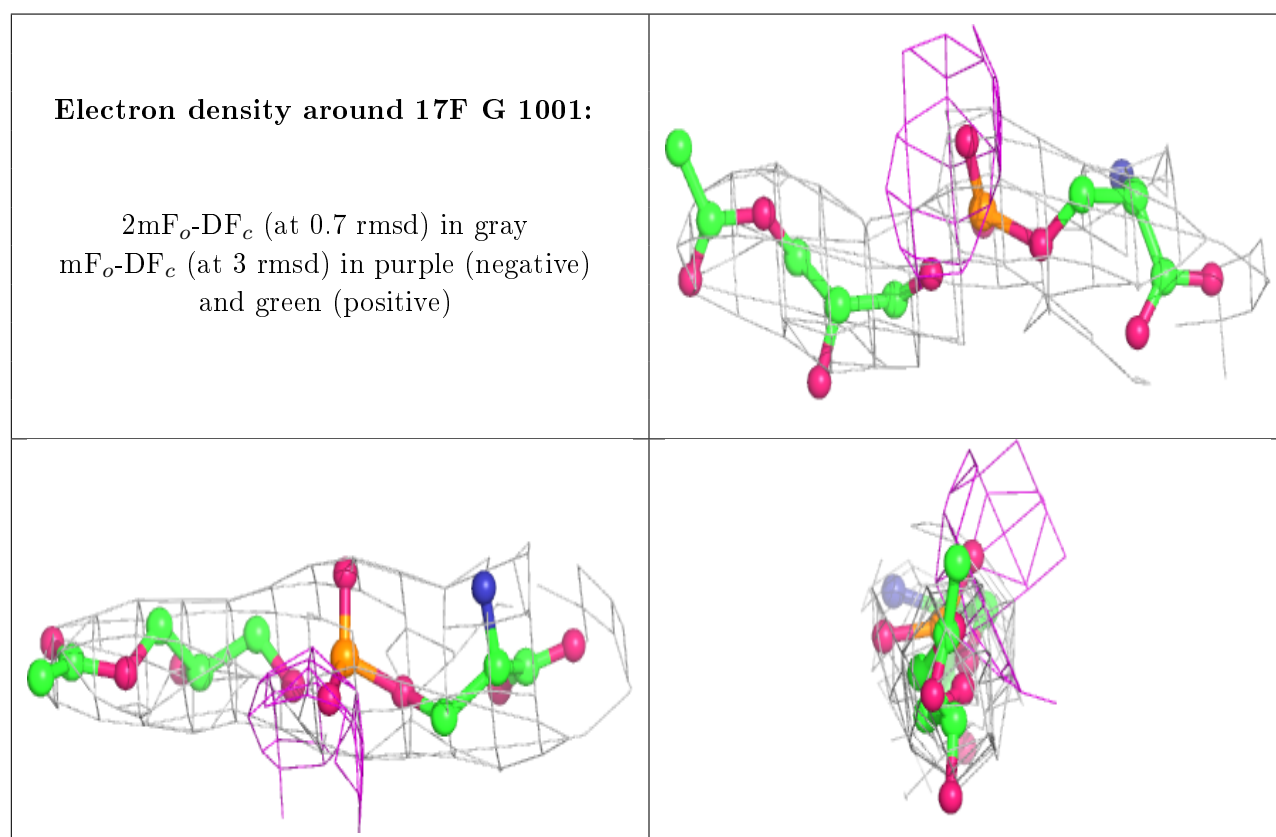
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	17F	G	1001	19/54	0.81	0.44	136,142,150,152	0
10	NAG	B	1001	14/15	0.87	0.16	138,146,152,154	0
8	K	A	2003	1/1	0.94	0.20	121,121,121,121	0
8	K	C	1104	1/1	0.96	0.18	92,92,92,92	0
6	BUF	A	2001	28/28	0.96	0.25	93,97,101,102	0
8	K	A	2005	1/1	0.96	0.28	121,121,121,121	0
6	BUF	C	1102	28/28	0.97	0.28	90,94,99,100	0
7	CLR	A	2002	28/28	0.98	0.36	40,44,51,53	0
7	CLR	E	101	28/28	0.98	0.31	56,60,65,67	0

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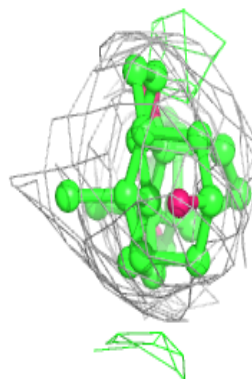
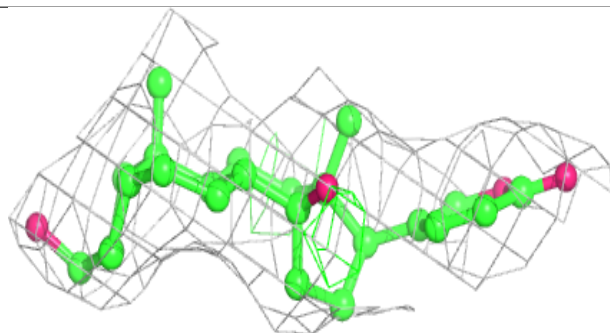
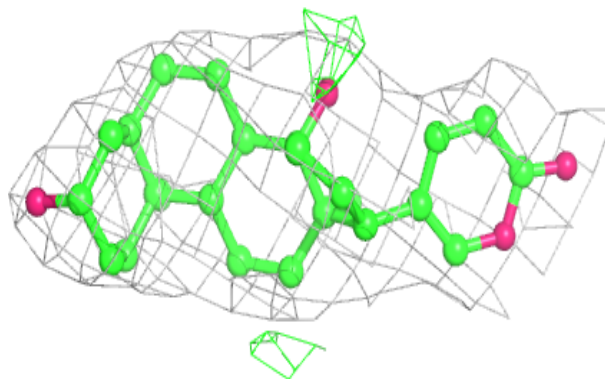
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	K	C	1105	1/1	0.98	0.13	60,60,60,60	0
8	K	C	1106	1/1	0.98	0.13	69,69,69,69	0
8	K	A	2004	1/1	0.99	0.14	54,54,54,54	0
9	MG	C	1107	1/1	0.99	0.18	106,106,106,106	0
9	MG	A	2006	1/1	1.00	0.20	71,71,71,71	0

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.

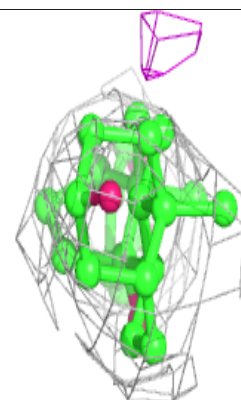
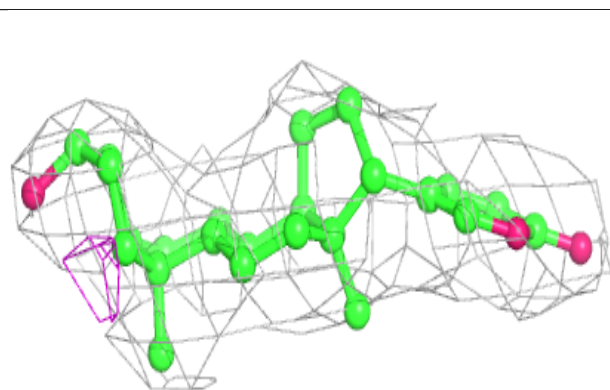
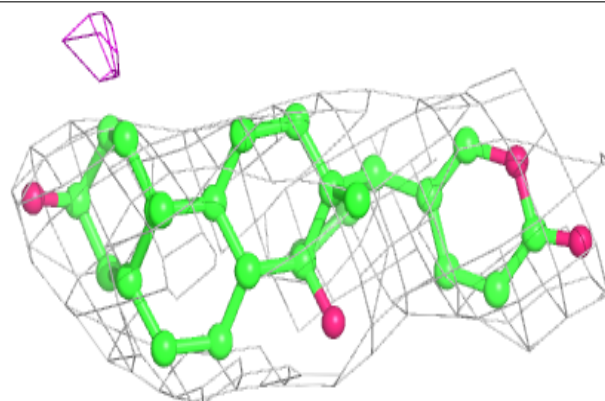


Electron density around BUF A 2001:

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

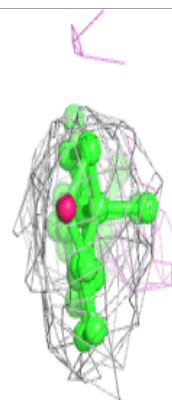
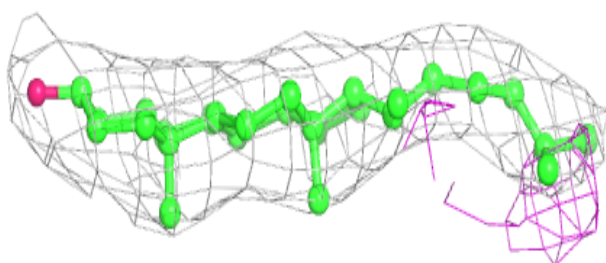
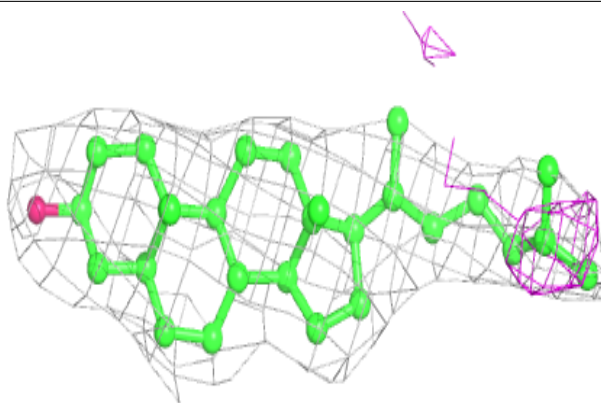
**Electron density around BUF C 1102:**

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

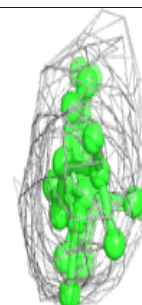
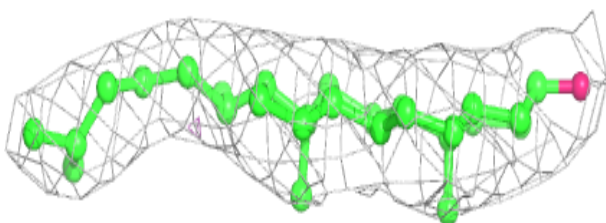
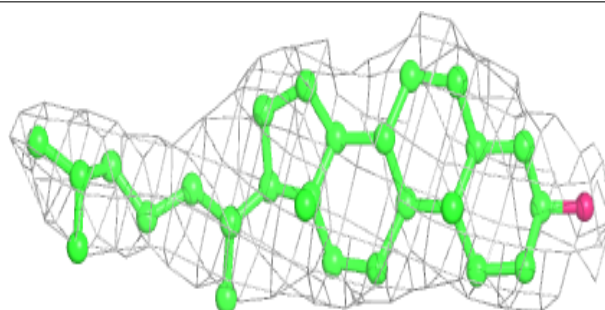


Electron density around CLR A 2002:

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

**Electron density around CLR E 101:**

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



6.5 Other polymers

There are no such residues in this entry.