



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:12 AM UTC

PDB ID : 4HYT / pdb_00004hyt
Title : Na,K-ATPase in the E2P state with bound ouabain and Mg²⁺ in the cation-binding site
Authors : Laursen, M.; Yatime, L.; Nissen, P.; Fedosova, N.U.
Deposited on : 2012-11-14
Resolution : 3.40 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

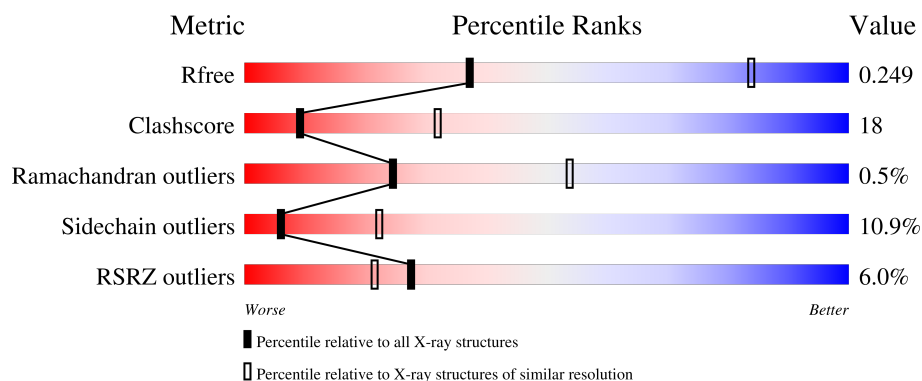
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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.



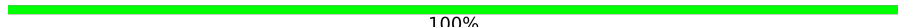
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	3% 63% 31% • •
1	C	1021	7% 64% 29% • •
2	B	303	8% 50% 36% 9% • 5%
2	D	303	8% 48% 37% 9% 5%
3	E	65	29% 18% • 51%

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Mol	Chain	Length	Quality of chain
3	G	65	 2% 26% 20% 51%
4	F	2	 100%

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
10	17F	A	1109	-	X	-	-
10	17F	B	1005	-	X	-	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 21220 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	289	Total	C	N	O	S	0	0	0
			2368	1534	386	435	13			
2	D	287	Total	C	N	O	S	0	0	0
			2349	1519	384	433	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.

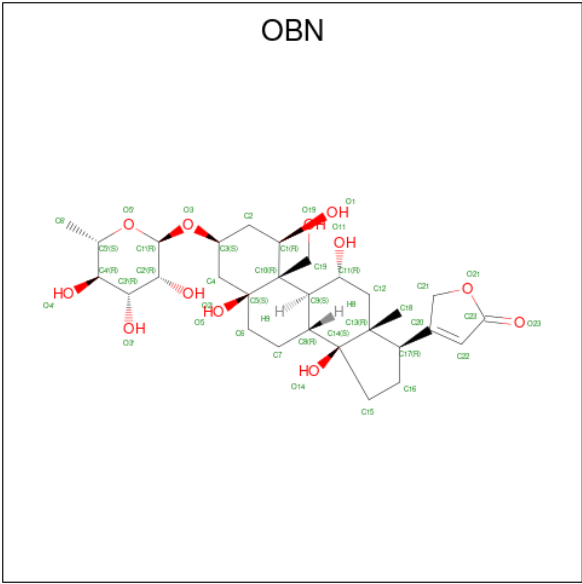


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

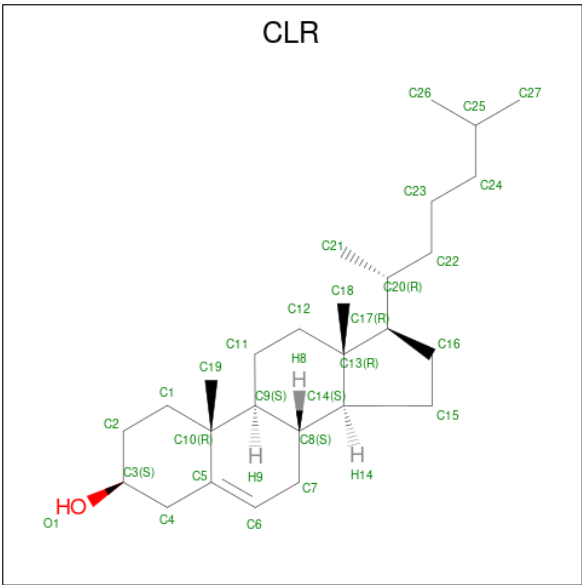
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		
5	C	3	Total	Mg	0	0
			3	3		

- Molecule 6 is OUABAIN (CCD ID: OBN) (formula: C₂₉H₄₄O₁₂).



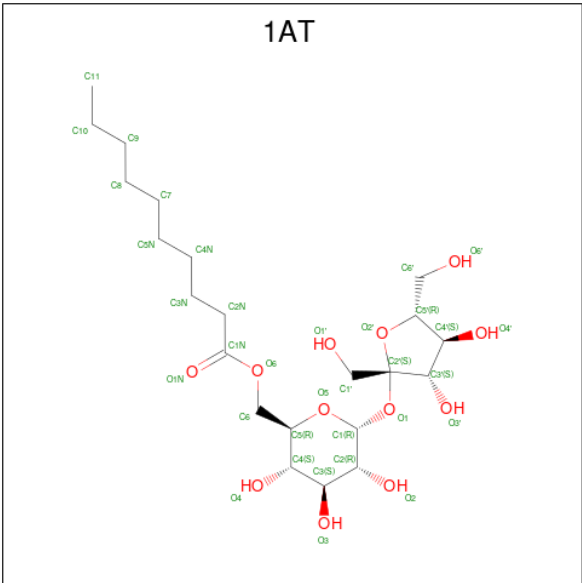
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			41	29	12		
6	C	1	Total	C	O	0	0
			41	29	12		

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



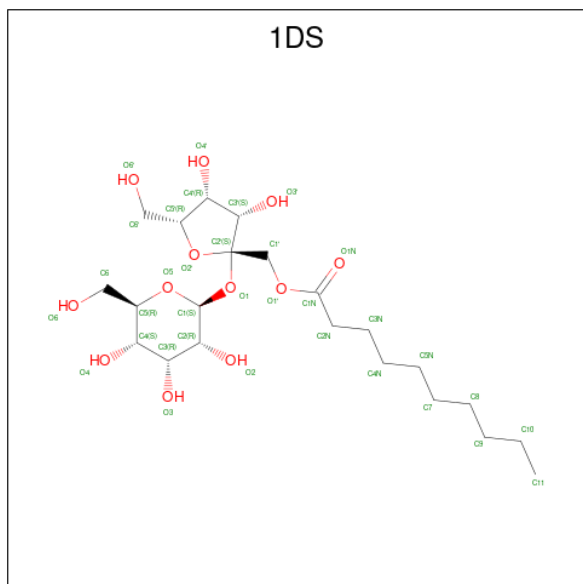
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			28	27	1		
7	G	1	Total	C	O	0	0
			28	27	1		
7	C	1	Total	C	O	0	0
			28	27	1		
7	E	1	Total	C	O	0	0
			28	27	1		

- Molecule 8 is beta-D-fructofuranosyl 6-O-decanoyl-alpha-D-glucopyranoside (CCD ID: 1AT) (formula: C₂₂H₄₀O₁₂).



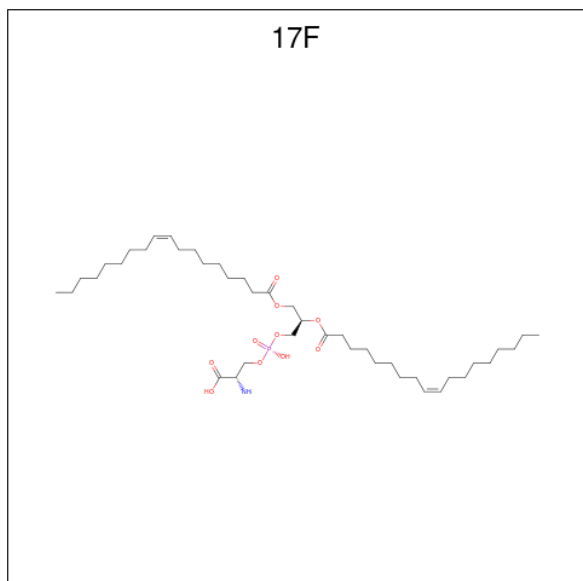
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			29	17	12		

- Molecule 9 is 1-O-decanoyl-beta-D-tagatofuranosyl beta-D-allopyranoside (CCD ID: 1DS) (formula: C₂₂H₄₀O₁₂).



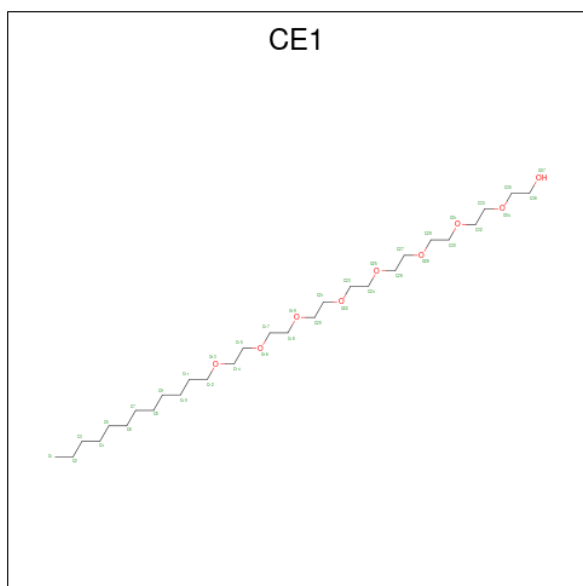
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			29	17	12		

- Molecule 10 is O-[(S)-({(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propyl}oxy)(hydroxy)phosphoryl]-L-serine (CCD ID: 17F) (formula: C₄₂H₇₈NO₁₀P).



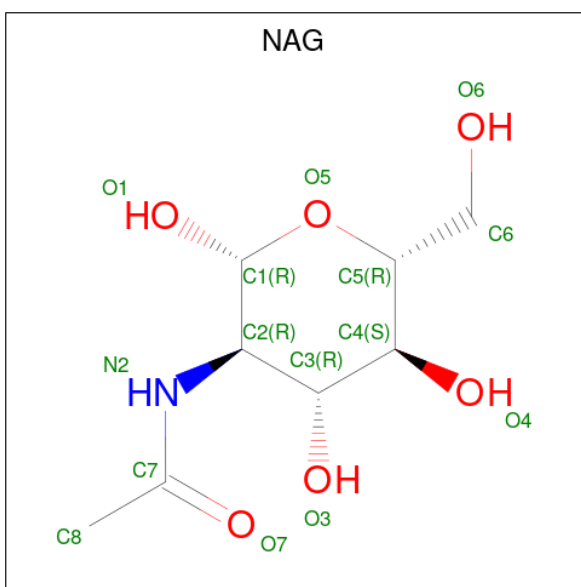
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	N	O	P	0	0
			18	8	1	8	1		
10	A	1	Total	C	N	O	P	0	0
			18	8	1	8	1		
10	B	1	Total	C	N	O	P	0	0
			24	14	1	8	1		
10	G	1	Total	C	N	O	P	0	0
			27	15	1	10	1		
10	D	1	Total	C	N	O	P	0	0
			28	16	1	10	1		

- Molecule 11 is O-DODECANYL OCTAETHYLENE GLYCOL (CCD ID: CE1) (formula: $C_{28}H_{58}O_9$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	C O	0	0
			34 26 8			
11	E	1	Total	C O	0	0
			22 18 4			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

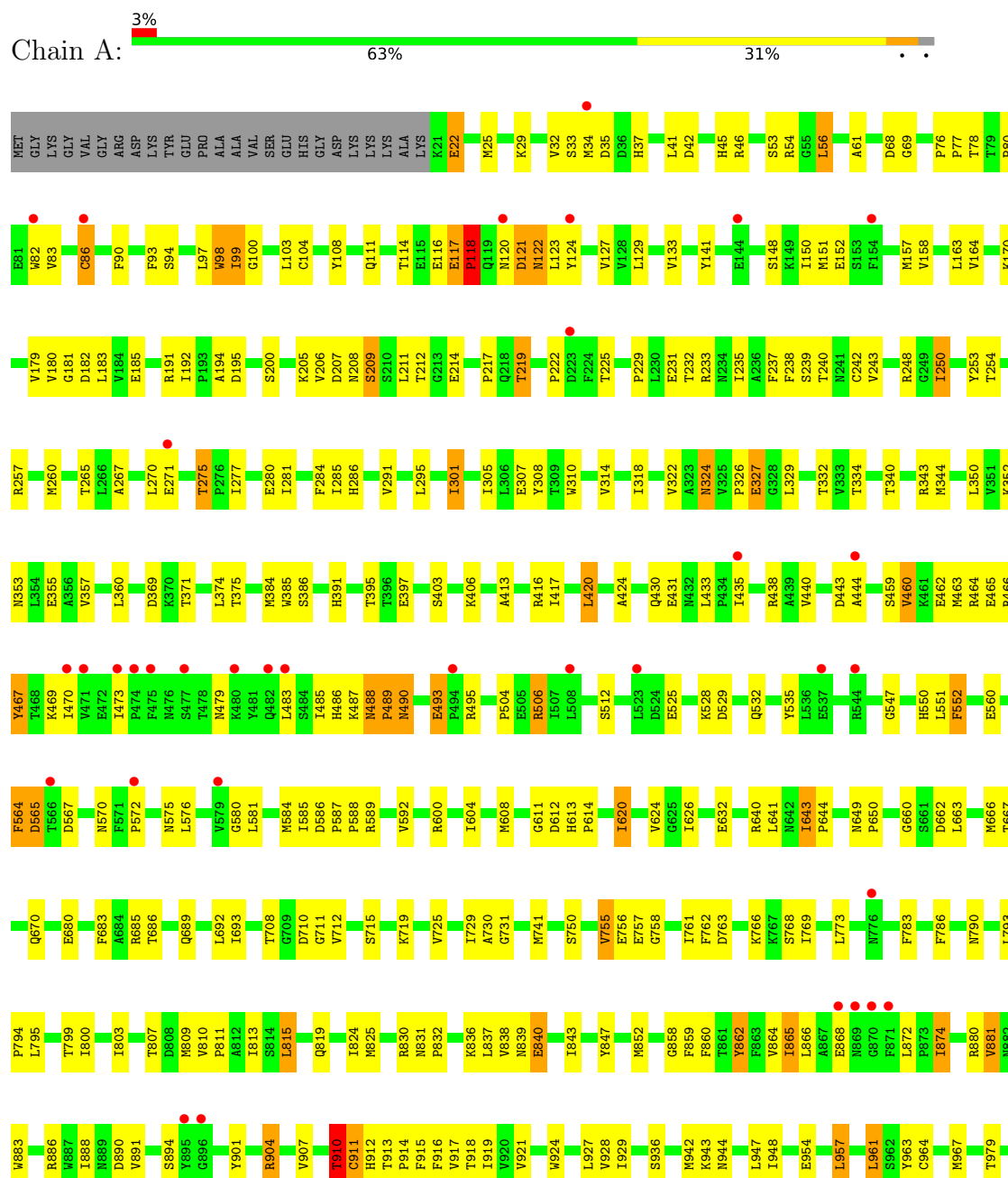
- Molecule 13 is water.

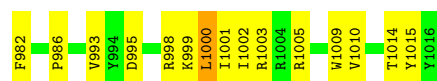
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	3	Total	O	0	0
			3	3		
13	C	3	Total	O	0	0
			3	3		

3 Residue-property plots

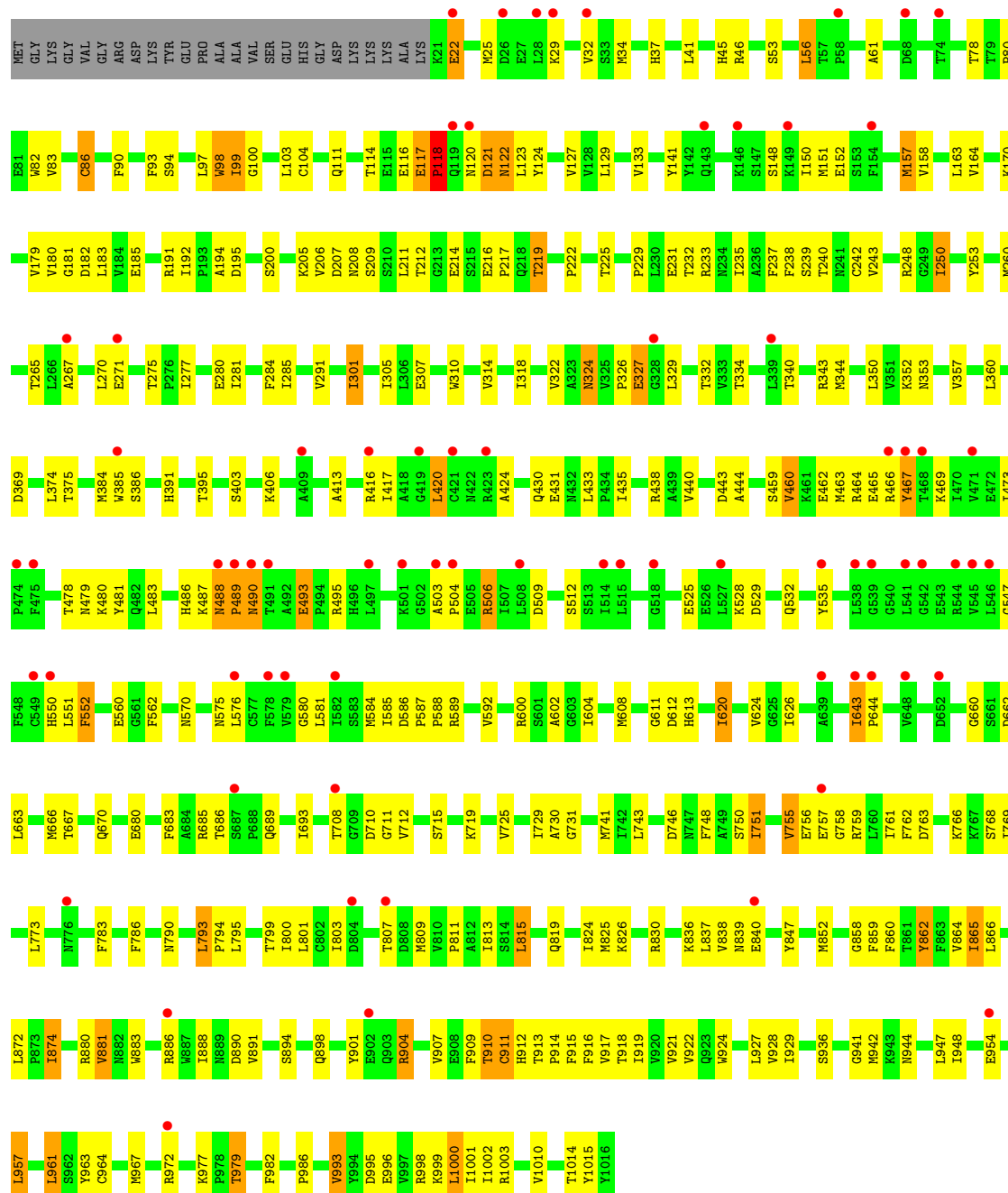
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



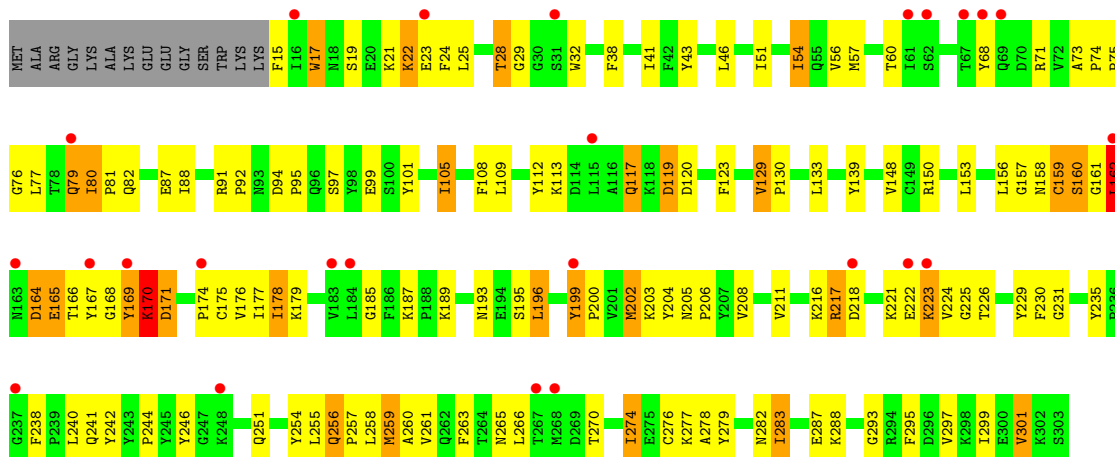


- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

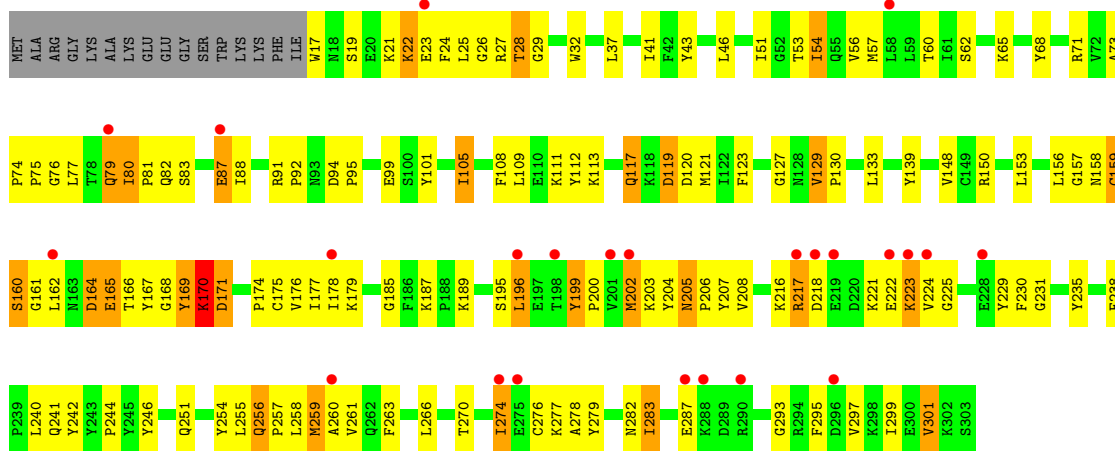


- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

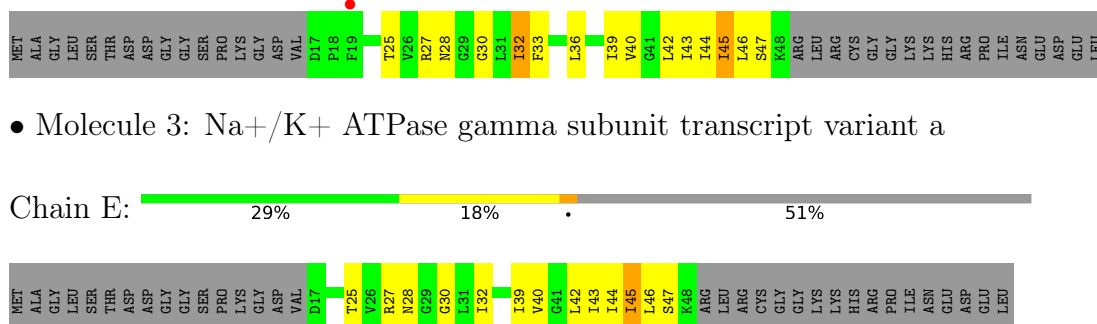
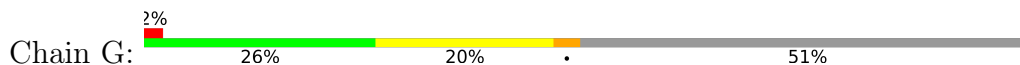




• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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



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

Chain F:

100%

3AG1
3AG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.47Å 118.08Å 494.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.40 49.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.83-3.40) 75.7 (49.83-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.226 , 0.244 0.229 , 0.249	Depositor DCC
R_{free} test set	3603 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	111.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 91.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21220	wwPDB-VP
Average B, all atoms (Å ²)	130.0	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: 1DS, CE1, CLR, 1AT, OBN, 17F, NAG, MG, PHD

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	0.39	0/7867	0.85	3/10674 (0.0%)
1	C	0.38	0/7867	0.85	2/10674 (0.0%)
2	B	0.39	0/2431	0.90	3/3279 (0.1%)
2	D	0.42	0/2411	0.91	5/3252 (0.2%)
3	E	0.47	0/261	0.86	0/354
3	G	0.48	0/261	0.89	0/354
All	All	0.39	0/21098	0.87	13/28587 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	LEU	CB-CA-C	-5.72	109.96	116.54
1	C	793	LEU	CA-C-N	5.71	125.07	118.85
1	C	793	LEU	C-N-CA	5.71	125.07	118.85
2	D	87	GLU	N-CA-C	5.44	117.26	108.34
2	B	87	GLU	N-CA-C	5.37	117.14	108.34
2	D	129	VAL	N-CA-C	-5.16	104.96	109.19
2	D	205	ASN	CA-C-N	5.14	124.59	119.24
2	D	205	ASN	C-N-CA	5.14	124.59	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	910	THR	N-CA-C	-5.10	107.03	113.20
2	D	127	GLY	N-CA-C	5.09	117.79	111.93
1	A	493	GLU	CA-CB-CG	-5.08	103.95	114.10
1	A	33	SER	N-CA-C	5.06	117.33	110.35
2	B	129	VAL	N-CA-C	-5.05	105.05	109.19

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	160	SER	Peptide
2	B	165	GLU	Peptide
2	D	160	SER	Peptide
2	D	165	GLU	Peptide

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	7777	261	0
1	C	7730	0	7777	245	0
2	B	2368	0	2335	121	0
2	D	2349	0	2315	124	0
3	E	255	0	259	7	0
3	G	255	0	259	9	0
4	F	28	0	25	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	41	0	44	10	0
6	C	41	0	44	6	0
7	A	28	0	46	5	0
7	C	28	0	46	2	0
7	E	28	0	46	4	0
7	G	28	0	46	4	0
8	A	29	0	27	6	0
9	A	29	0	27	6	0
10	A	36	0	16	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	24	0	20	2	0
10	D	28	0	22	0	0
10	G	27	0	20	4	0
11	A	34	0	53	18	0
11	E	22	0	37	1	0
12	B	28	0	26	0	0
12	D	42	0	39	0	0
13	A	3	0	0	1	0
13	C	3	0	0	0	0
All	All	21220	0	21306	772	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 18.

All (772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:OD1	1:A:69:GLY:N	1.78	1.15
1:A:794:PRO:HG3	1:A:862:TYR:HE2	1.15	1.07
1:C:794:PRO:HG3	1:C:862:TYR:HE2	1.17	1.07
1:C:794:PRO:HG3	1:C:862:TYR:CE2	1.95	1.00
1:A:794:PRO:HG3	1:A:862:TYR:CE2	1.95	1.00
2:B:199:TYR:HB3	2:B:200:PRO:CD	1.93	0.99
2:B:204:TYR:C	2:B:206:PRO:HD2	1.88	0.97
2:D:199:TYR:HB3	2:D:200:PRO:CD	1.95	0.96
1:A:22:GLU:HA	1:A:25:MET:HG3	1.49	0.94
2:D:170:LYS:HB2	2:D:174:PRO:HA	1.51	0.93
10:B:1005:17F:H4A	10:B:1005:17F:HN1	1.35	0.92
1:C:22:GLU:HA	1:C:25:MET:HG3	1.50	0.92
2:B:170:LYS:HB2	2:B:174:PRO:HA	1.51	0.91
2:D:199:TYR:HB3	2:D:200:PRO:HD2	1.54	0.89
2:B:199:TYR:HB3	2:B:200:PRO:HD2	1.52	0.89
1:A:794:PRO:HB3	1:A:862:TYR:CD2	2.09	0.86
8:A:1106:1AT:H9	1:C:982:PHE:CE2	2.10	0.86
2:D:204:TYR:C	2:D:206:PRO:HD2	2.01	0.84
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.61	0.81
2:D:205:ASN:N	2:D:206:PRO:HD2	1.97	0.80
1:A:1009:TRP:H	11:A:1110:CE1:H271	1.47	0.80
2:D:80:ILE:HG13	2:D:81:PRO:HD3	1.62	0.79
1:A:111:GLN:HB3	1:A:116:GLU:HG2	1.65	0.79
2:D:204:TYR:O	2:D:208:VAL:HG12	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:VAL:HG22	2:D:57:MET:HG3	1.64	0.78
1:C:111:GLN:HB3	1:C:116:GLU:HG2	1.65	0.78
2:B:204:TYR:O	2:B:208:VAL:HG12	1.84	0.77
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.65	0.77
2:B:217:ARG:HG2	2:B:217:ARG:HH11	1.50	0.76
2:B:216:LYS:HB2	2:B:221:LYS:HG2	1.67	0.76
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.67	0.76
2:D:216:LYS:HB2	2:D:221:LYS:HG2	1.66	0.76
1:A:116:GLU:HG3	1:A:118:PRO:HD2	1.66	0.75
2:D:217:ARG:HG2	2:D:217:ARG:HH11	1.51	0.75
2:D:129:VAL:HG22	2:D:204:TYR:OH	1.87	0.75
2:B:148:VAL:HG11	2:B:254:TYR:HA	1.67	0.75
11:A:1110:CE1:H212	11:A:1110:CE1:H272	1.68	0.75
2:B:205:ASN:N	2:B:206:PRO:HD2	2.01	0.75
11:A:1110:CE1:H211	11:A:1110:CE1:H152	1.67	0.75
1:C:116:GLU:HG3	1:C:118:PRO:HD2	1.66	0.75
1:C:862:TYR:HE1	1:C:866:LEU:HD12	1.52	0.74
10:A:1108:17F:O1	10:A:1109:17F:H4	1.88	0.74
1:A:1009:TRP:HB3	11:A:1110:CE1:H242	1.69	0.74
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.70	0.74
9:A:1107:1DS:H18	1:C:941:GLY:HA3	1.70	0.73
1:C:794:PRO:HB3	1:C:862:TYR:CD2	2.24	0.73
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.69	0.72
8:A:1106:1AT:H9	1:C:982:PHE:HE2	1.53	0.72
1:A:840:GLU:HA	10:A:1108:17F:H4A	1.70	0.72
2:B:168:GLY:HA3	2:B:171:ASP:HB3	1.72	0.72
1:A:862:TYR:HE1	1:A:866:LEU:HD12	1.54	0.72
2:B:130:PRO:HB2	2:B:204:TYR:CE1	2.26	0.71
2:D:204:TYR:HD2	2:D:235:TYR:CZ	2.08	0.71
1:C:865:ILE:HD12	1:C:914:PRO:HG3	1.73	0.71
1:A:865:ILE:HD12	1:A:914:PRO:HG3	1.73	0.70
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.73	0.70
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.73	0.70
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.73	0.70
2:D:204:TYR:CD2	2:D:235:TYR:CZ	2.79	0.70
2:D:168:GLY:HA3	2:D:171:ASP:HB3	1.72	0.69
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.75	0.69
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.73	0.69
1:C:385:TRP:HB3	1:C:581:LEU:H	1.58	0.69
1:A:385:TRP:HB3	1:A:581:LEU:H	1.58	0.68
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:786:PHE:CZ	6:C:2004:OBN:H6'1	2.29	0.68
1:C:890:ASP:OD1	2:D:82:GLN:NE2	2.26	0.68
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.75	0.67
1:A:907:VAL:HA	1:A:910:THR:HG22	1.77	0.67
2:B:165:GLU:HB3	2:B:166:THR:HA	1.76	0.67
1:A:565:ASP:O	1:A:570:ASN:ND2	2.26	0.67
11:A:1110:CE1:H92	2:B:38:PHE:HD1	1.59	0.67
2:D:80:ILE:HD11	2:D:176:VAL:HA	1.77	0.67
2:D:216:LYS:H	2:D:221:LYS:HD2	1.60	0.67
1:C:907:VAL:HA	1:C:910:THR:HG22	1.77	0.67
2:D:165:GLU:HB3	2:D:166:THR:HA	1.76	0.67
2:B:205:ASN:N	2:B:206:PRO:CD	2.59	0.66
3:G:45:ILE:HD12	3:G:46:LEU:HG	1.75	0.66
2:B:216:LYS:H	2:B:221:LYS:HD2	1.60	0.66
1:A:840:GLU:OE2	10:A:1108:17F:N1	2.28	0.66
1:A:794:PRO:HB3	1:A:862:TYR:HD2	1.59	0.65
2:B:80:ILE:HD11	2:B:176:VAL:HA	1.77	0.65
1:A:375:THR:HA	1:A:588:PRO:HA	1.79	0.65
2:B:29:GLY:HA2	2:B:32:TRP:CD1	2.31	0.65
1:C:550:HIS:HE2	1:C:552:PHE:HE1	1.44	0.65
1:A:212:THR:HG23	1:A:214:GLU:H	1.62	0.65
2:D:130:PRO:HB2	2:D:204:TYR:CE1	2.32	0.65
2:D:29:GLY:HA2	2:D:32:TRP:CD1	2.31	0.65
2:D:205:ASN:N	2:D:206:PRO:CD	2.61	0.64
1:C:592:VAL:HG22	1:C:748:PHE:HD2	1.62	0.64
2:D:24:PHE:HB3	2:D:28:THR:HA	1.80	0.64
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.62	0.64
2:D:189:LYS:H	2:D:282:ASN:HB2	1.63	0.64
1:A:275:THR:OG1	1:A:355:GLU:OE2	2.16	0.64
1:A:430:GLN:HG3	1:A:433:LEU:HD13	1.79	0.64
1:C:604:ILE:HD11	1:C:755:VAL:HG21	1.80	0.64
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.63	0.64
1:A:550:HIS:HE2	1:A:552:PHE:HE1	1.45	0.63
2:B:189:LYS:H	2:B:282:ASN:HB2	1.63	0.63
1:C:430:GLN:HG3	1:C:433:LEU:HD13	1.80	0.63
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.81	0.63
1:A:1009:TRP:H	11:A:1110:CE1:C27	2.11	0.63
1:C:624:VAL:HG23	1:C:626:ILE:HG13	1.81	0.63
2:B:24:PHE:HB3	2:B:28:THR:HA	1.79	0.62
1:C:208:ASN:HB3	1:C:212:THR:HG22	1.82	0.62
1:A:942:MET:HE1	1:A:947:LEU:HD22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:HG23	1:C:214:GLU:H	1.64	0.62
1:A:270:LEU:HB2	1:A:719:LYS:HG2	1.82	0.61
1:A:632:GLU:OE1	1:A:640:ARG:NH1	2.33	0.61
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.35	0.61
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.35	0.61
1:A:790:ASN:OD1	1:A:880:ARG:NH1	2.31	0.61
1:A:208:ASN:HB3	1:A:212:THR:HG22	1.82	0.60
1:C:790:ASN:OD1	1:C:880:ARG:NH1	2.31	0.60
1:C:375:THR:HA	1:C:588:PRO:HA	1.83	0.60
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.82	0.60
2:D:76:GLY:HA2	2:D:293:GLY:H	1.67	0.60
2:D:158:ASN:O	2:D:166:THR:OG1	2.19	0.60
1:A:624:VAL:HG23	1:A:626:ILE:HG13	1.82	0.60
2:D:21:LYS:O	2:D:23:GLU:HA	2.02	0.60
2:D:80:ILE:HD12	2:D:105:ILE:HD12	1.83	0.60
1:C:117:GLU:HG3	1:C:118:PRO:HD3	1.83	0.60
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.83	0.60
2:B:21:LYS:O	2:B:23:GLU:HA	2.02	0.60
1:A:604:ILE:HD11	1:A:755:VAL:HG21	1.83	0.60
3:G:36:LEU:HD12	10:G:1002:17F:C18	2.32	0.60
1:A:371:THR:O	1:A:710:ASP:OD2	2.20	0.60
2:B:80:ILE:HD12	2:B:105:ILE:HD12	1.83	0.60
1:A:529:ASP:HA	1:A:532:GLN:HB2	1.84	0.60
2:D:179:LYS:HD2	2:D:256:GLN:HE21	1.66	0.60
1:C:942:MET:HE1	1:C:947:LEU:HD22	1.83	0.59
2:B:166:THR:HB	2:B:169:TYR:H	1.68	0.59
1:C:786:PHE:HZ	6:C:2004:OBN:H6'1	1.67	0.59
2:B:130:PRO:HA	2:B:241:GLN:NE2	2.17	0.59
2:D:166:THR:HB	2:D:169:TYR:H	1.68	0.59
2:B:25:LEU:H	2:B:29:GLY:HA3	1.67	0.59
2:D:130:PRO:HA	2:D:241:GLN:NE2	2.17	0.59
1:C:163:LEU:HD23	1:C:185:GLU:HB3	1.84	0.59
2:D:25:LEU:H	2:D:29:GLY:HA3	1.67	0.59
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.85	0.59
1:C:529:ASP:HA	1:C:532:GLN:HB2	1.84	0.59
1:A:117:GLU:HG3	1:A:118:PRO:HD3	1.83	0.59
3:G:40:VAL:O	3:G:44:ILE:HG12	2.03	0.59
1:C:430:GLN:HB3	1:C:438:ARG:HD3	1.85	0.59
2:B:79:GLN:HB3	2:B:295:PHE:CE1	2.38	0.59
2:B:179:LYS:HD2	2:B:256:GLN:HE21	1.67	0.59
2:D:217:ARG:NH1	2:D:218:ASP:OD2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:TYR:CB	2:B:200:PRO:CD	2.71	0.58
2:B:217:ARG:NH1	2:B:218:ASP:OD2	2.36	0.58
2:D:222:GLU:OE1	2:D:222:GLU:N	2.26	0.58
2:B:204:TYR:HD2	2:B:235:TYR:CZ	2.21	0.58
1:C:794:PRO:CG	1:C:862:TYR:CE2	2.81	0.58
1:A:551:LEU:HD22	1:A:576:LEU:HD23	1.86	0.58
1:A:840:GLU:HG3	10:A:1108:17F:P1	2.43	0.58
2:B:119:ASP:O	2:B:123:PHE:HB2	2.03	0.58
1:A:163:LEU:HD23	1:A:185:GLU:HB3	1.84	0.58
2:D:22:LYS:HG2	2:D:23:GLU:HG3	1.85	0.58
1:A:794:PRO:CG	1:A:862:TYR:CE2	2.78	0.58
2:D:160:SER:O	2:D:162:LEU:N	2.37	0.58
1:A:512:SER:HB3	1:A:575:ASN:HA	1.86	0.58
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.86	0.57
2:B:158:ASN:O	2:B:166:THR:OG1	2.21	0.57
2:B:225:GLY:HA2	2:B:266:LEU:HD23	1.85	0.57
1:C:129:LEU:HD21	1:C:327:GLU:HG2	1.86	0.57
1:C:512:SER:HB3	1:C:575:ASN:HA	1.86	0.57
1:C:880:ARG:HA	1:C:883:TRP:HB3	1.85	0.57
1:C:551:LEU:HD22	1:C:576:LEU:HD23	1.86	0.57
1:C:825:MET:HE2	1:C:825:MET:HA	1.87	0.57
1:A:238:PHE:HD1	1:A:239:SER:N	2.03	0.57
1:A:807:THR:HB	1:A:954:GLU:HG3	1.86	0.57
1:C:343:ARG:NH2	1:C:757:GLU:OE1	2.38	0.57
1:A:943:LYS:HE3	8:A:1106:1AT:H25	1.87	0.57
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.86	0.57
2:B:76:GLY:HA2	2:B:293:GLY:H	1.68	0.57
2:D:225:GLY:HA2	2:D:266:LEU:HD23	1.86	0.57
1:A:200:SER:HA	1:A:222:PRO:HG3	1.87	0.57
1:C:807:THR:HB	1:C:954:GLU:HG3	1.86	0.57
2:D:79:GLN:HB3	2:D:295:PHE:CE1	2.39	0.57
6:A:1104:OBN:H3	6:A:1104:OBN:H5'	1.87	0.57
1:C:794:PRO:HB3	1:C:862:TYR:HD2	1.69	0.57
1:A:430:GLN:HB3	1:A:438:ARG:HD3	1.85	0.56
1:A:825:MET:HA	1:A:825:MET:HE2	1.87	0.56
1:C:478:THR:O	1:C:506:ARG:NH1	2.39	0.56
3:E:40:VAL:O	3:E:44:ILE:HG12	2.06	0.56
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.88	0.56
1:C:443:ASP:OD1	1:C:444:ALA:N	2.35	0.56
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.87	0.56
2:B:22:LYS:HG2	2:B:23:GLU:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:PHE:HD1	1:C:239:SER:N	2.03	0.56
1:C:329:LEU:HD11	1:C:769:ILE:HA	1.88	0.56
2:B:204:TYR:CD2	2:B:235:TYR:CZ	2.93	0.56
2:D:119:ASP:O	2:D:123:PHE:HB2	2.05	0.56
1:A:329:LEU:HD11	1:A:769:ILE:HA	1.87	0.56
1:A:118:PRO:HB3	1:A:122:ASN:H	1.71	0.55
1:A:860:PHE:HZ	7:A:1105:CLR:H191	1.70	0.55
1:A:608:MET:HE1	1:A:620:ILE:HG22	1.89	0.55
11:A:1110:CE1:H92	2:B:38:PHE:CD1	2.41	0.55
2:B:80:ILE:CG1	2:B:81:PRO:HD3	2.36	0.55
1:A:443:ASP:OD1	1:A:444:ALA:N	2.37	0.55
1:A:585:ILE:HG13	1:A:586:ASP:N	2.21	0.55
1:A:888:ILE:O	1:A:904:ARG:NH2	2.40	0.55
2:B:160:SER:O	2:B:162:LEU:N	2.39	0.55
1:A:683:PHE:HB3	1:A:686:THR:HG21	1.89	0.55
1:A:118:PRO:C	1:A:121:ASP:H	2.15	0.55
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.88	0.55
1:A:685:ARG:HB3	1:A:685:ARG:NH1	2.22	0.54
1:C:151:MET:HA	1:C:151:MET:HE2	1.89	0.54
1:A:488:ASN:ND2	1:A:493:GLU:O	2.40	0.54
1:C:469:LYS:HA	1:C:486:HIS:CD2	2.42	0.54
1:A:291:VAL:HG21	1:A:847:TYR:HE2	1.73	0.54
2:B:278:ALA:O	2:B:283:ILE:HG21	2.08	0.54
1:C:118:PRO:HB3	1:C:122:ASN:H	1.72	0.54
1:C:488:ASN:ND2	1:C:493:GLU:O	2.41	0.54
3:G:39:ILE:O	3:G:43:ILE:HG12	2.08	0.54
1:C:683:PHE:HB3	1:C:686:THR:HG21	1.89	0.54
1:C:999:LYS:O	1:C:1003:ARG:HG3	2.08	0.54
2:D:278:ALA:O	2:D:283:ILE:HG21	2.07	0.54
1:C:200:SER:HA	1:C:222:PRO:HG3	1.89	0.54
1:C:710:ASP:OD1	1:C:711:GLY:N	2.40	0.54
1:C:890:ASP:OD1	1:C:890:ASP:N	2.41	0.54
1:C:909:PHE:HE2	1:C:972:ARG:CZ	2.21	0.54
1:A:329:LEU:HA	1:A:332:THR:OG1	2.06	0.54
1:A:343:ARG:NH2	1:A:757:GLU:OE1	2.41	0.54
1:C:585:ILE:HG13	1:C:586:ASP:N	2.22	0.54
1:C:888:ILE:O	1:C:904:ARG:NH2	2.40	0.54
1:A:890:ASP:OD1	1:A:890:ASP:N	2.41	0.54
1:C:118:PRO:C	1:C:121:ASP:H	2.16	0.54
11:A:1110:CE1:H321	11:A:1110:CE1:H182	1.90	0.54
1:C:608:MET:HE1	1:C:620:ILE:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:2005:CLR:H212	2:D:53:THR:HA	1.90	0.54
2:D:170:LYS:HB2	2:D:174:PRO:CA	2.34	0.54
1:A:710:ASP:OD1	1:A:711:GLY:N	2.41	0.53
1:C:1000:LEU:HD23	1:C:1003:ARG:NH2	2.22	0.53
1:C:260:MET:HE2	1:C:712:VAL:HG11	1.88	0.53
1:A:151:MET:HE2	1:A:151:MET:HA	1.89	0.53
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.90	0.53
1:A:267:ALA:HB2	1:A:715:SER:HB3	1.91	0.53
1:A:469:LYS:HA	1:A:486:HIS:CD2	2.43	0.53
1:A:42:ASP:OD1	1:A:46:ARG:NH1	2.41	0.53
1:A:963:TYR:O	3:G:27:ARG:HG3	2.09	0.53
1:C:469:LYS:HA	1:C:486:HIS:HD2	1.73	0.53
2:D:101:TYR:O	2:D:105:ILE:HG12	2.09	0.53
1:A:662:ASP:O	1:A:666:MET:HG3	2.09	0.53
3:E:39:ILE:O	3:E:43:ILE:HG12	2.08	0.53
8:A:1106:1AT:H20	1:C:979:THR:H	1.74	0.53
1:C:662:ASP:O	1:C:666:MET:HG3	2.09	0.53
1:C:685:ARG:NH1	1:C:685:ARG:HB3	2.24	0.52
1:A:982:PHE:CE2	9:A:1107:1DS:H24	2.44	0.52
11:A:1110:CE1:H81	2:B:41:ILE:HG21	1.90	0.52
2:B:179:LYS:HD2	2:B:256:GLN:NE2	2.25	0.52
2:B:202:MET:HE3	2:B:202:MET:HA	1.92	0.52
1:C:395:THR:HB	1:C:587:PRO:HB3	1.92	0.52
1:A:1000:LEU:HD23	1:A:1003:ARG:NH2	2.24	0.52
2:B:101:TYR:O	2:B:105:ILE:HG12	2.09	0.52
1:C:386:SER:HB2	1:C:391:HIS:HE2	1.75	0.52
1:C:329:LEU:HA	1:C:332:THR:OG1	2.10	0.52
1:C:550:HIS:NE2	1:C:552:PHE:HE1	2.08	0.52
1:C:963:TYR:O	3:E:27:ARG:HG3	2.10	0.52
2:D:179:LYS:HD2	2:D:256:GLN:NE2	2.24	0.52
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.42	0.52
1:A:395:THR:HB	1:A:587:PRO:HB3	1.92	0.52
1:A:551:LEU:HG	1:A:552:PHE:O	2.10	0.51
1:A:999:LYS:O	1:A:1003:ARG:HG3	2.10	0.51
2:D:120:ASP:OD1	2:D:150:ARG:NH2	2.43	0.51
1:A:25:MET:O	1:A:29:LYS:HG3	2.11	0.51
2:B:120:ASP:OD1	2:B:150:ARG:NH2	2.44	0.51
2:B:242:TYR:CD2	2:B:257:PRO:HG3	2.45	0.51
1:C:977:LYS:HD3	2:D:68:TYR:CZ	2.45	0.51
2:B:166:THR:N	2:B:167:TYR:HA	2.25	0.51
10:G:1002:17F:H5	3:E:44:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:H	2:D:153:LEU:HD12	1.76	0.51
2:D:202:MET:HA	2:D:202:MET:HE3	1.91	0.51
1:C:104:CYS:SG	1:C:322:VAL:HG11	2.51	0.51
2:D:205:ASN:OD1	2:D:206:PRO:HD3	2.10	0.51
1:A:643:ILE:HG22	1:A:644:PRO:HD2	1.93	0.51
1:C:206:VAL:HA	1:C:242:CYS:HA	1.93	0.51
2:D:166:THR:N	2:D:167:TYR:HA	2.25	0.51
1:A:117:GLU:OE2	6:A:1104:OBN:O5	2.28	0.51
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.43	0.51
1:C:460:VAL:HG13	1:C:463:MET:HE3	1.92	0.51
1:A:467:TYR:CZ	1:A:489:PRO:HG3	2.46	0.51
1:A:469:LYS:HA	1:A:486:HIS:HD2	1.75	0.51
2:D:242:TYR:CD2	2:D:257:PRO:HG3	2.45	0.51
1:A:206:VAL:HA	1:A:242:CYS:HA	1.93	0.50
1:A:460:VAL:HG13	1:A:463:MET:HE3	1.93	0.50
1:C:467:TYR:CZ	1:C:489:PRO:HG3	2.46	0.50
1:A:284:PHE:HE1	1:A:773:LEU:HD11	1.76	0.50
1:A:386:SER:HB2	1:A:391:HIS:HE2	1.76	0.50
1:A:852:MET:HG2	2:B:43:TYR:CE2	2.45	0.50
2:B:216:LYS:HG3	2:B:221:LYS:HA	1.93	0.50
1:C:82:TRP:CD1	1:C:141:TYR:HH	2.29	0.50
1:C:103:LEU:HB3	1:C:318:ILE:HG23	1.93	0.50
1:C:551:LEU:HG	1:C:552:PHE:O	2.10	0.50
1:C:666:MET:HE3	1:C:670:GLN:HB3	1.93	0.50
1:C:852:MET:HG2	2:D:43:TYR:CE2	2.46	0.50
2:D:167:TYR:C	2:D:169:TYR:N	2.70	0.50
1:A:547:GLY:HA2	1:A:581:LEU:HD23	1.93	0.50
2:B:153:LEU:H	2:B:153:LEU:HD12	1.75	0.50
1:A:485:ILE:HD13	1:A:564:PHE:CZ	2.46	0.50
1:A:963:TYR:CE2	7:G:1001:CLR:H6	2.46	0.50
2:B:204:TYR:HB2	2:B:235:TYR:CE1	2.47	0.50
1:A:1010:VAL:HG13	11:A:1110:CE1:H241	1.92	0.50
1:C:181:GLY:HA2	1:C:250:ILE:HG23	1.93	0.50
1:C:862:TYR:CE1	1:C:866:LEU:HD12	2.40	0.50
1:A:192:ILE:HG12	1:A:240:THR:O	2.12	0.50
1:A:550:HIS:NE2	1:A:552:PHE:HE1	2.09	0.50
2:B:92:PRO:HG3	2:B:301:VAL:HG12	1.93	0.50
1:C:667:THR:N	1:C:670:GLN:OE1	2.43	0.50
1:A:551:LEU:HD13	1:A:576:LEU:HA	1.94	0.50
1:C:267:ALA:HB2	1:C:715:SER:HB3	1.93	0.50
2:D:133:LEU:HG	2:D:240:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:GLY:HA2	1:A:918:THR:HG21	1.94	0.50
2:B:222:GLU:OE1	2:B:222:GLU:N	2.27	0.50
1:C:270:LEU:HB2	1:C:719:LYS:HG2	1.93	0.50
1:C:551:LEU:HD13	1:C:576:LEU:HA	1.94	0.50
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.93	0.50
1:C:862:TYR:CD1	1:C:862:TYR:C	2.90	0.50
1:A:525:GLU:HA	1:A:528:LYS:HB3	1.94	0.50
1:A:862:TYR:CD1	1:A:862:TYR:C	2.90	0.50
1:A:880:ARG:NH2	6:A:1104:OBN:C6'	2.75	0.50
1:C:291:VAL:HG21	1:C:847:TYR:HE2	1.77	0.50
2:D:80:ILE:CG1	2:D:81:PRO:HD3	2.37	0.50
1:C:192:ILE:HG12	1:C:240:THR:O	2.12	0.49
1:C:301:ILE:O	1:C:305:ILE:HG12	2.12	0.49
1:C:547:GLY:HA2	1:C:581:LEU:HD23	1.94	0.49
1:C:592:VAL:HG22	1:C:748:PHE:CD2	2.46	0.49
1:C:963:TYR:CE2	7:E:2001:CLR:H6	2.47	0.49
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.93	0.49
1:A:840:GLU:H	1:A:840:GLU:CD	2.19	0.49
6:A:1104:OBN:O3	6:A:1104:OBN:O1	2.25	0.49
1:A:181:GLY:HA2	1:A:250:ILE:HG23	1.93	0.49
1:A:862:TYR:CE1	1:A:866:LEU:HD12	2.42	0.49
1:C:795:LEU:HD13	1:C:915:PHE:HB3	1.94	0.49
1:C:858:GLY:HA2	1:C:918:THR:HG21	1.93	0.49
2:D:276:CYS:HB2	2:D:295:PHE:HD2	1.76	0.49
9:A:1107:1DS:H21	2:B:68:TYR:HH	1.57	0.49
2:B:276:CYS:HB2	2:B:295:PHE:HD2	1.77	0.49
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.47	0.49
1:C:479:ASN:HB3	1:C:481:TYR:CE2	2.48	0.49
1:C:552:PHE:N	1:C:552:PHE:CD1	2.80	0.49
1:C:942:MET:HE3	1:C:948:ILE:HD13	1.94	0.49
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.93	0.49
1:A:552:PHE:N	1:A:552:PHE:CD1	2.81	0.49
1:A:874:ILE:H	1:A:874:ILE:HD12	1.77	0.49
2:B:51:ILE:O	2:B:54:ILE:HG22	2.12	0.49
1:C:643:ILE:HG22	1:C:644:PRO:HD2	1.93	0.49
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.47	0.49
1:C:237:PHE:O	1:C:240:THR:OG1	2.26	0.49
1:A:83:VAL:O	1:A:86:CYS:HB2	2.13	0.49
2:B:133:LEU:HG	2:B:240:LEU:HB3	1.95	0.49
6:C:2004:OBN:H3	6:C:2004:OBN:H5'	1.93	0.49
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:HB2	2:D:162:LEU:HD23	1.94	0.49
1:A:666:MET:HE3	1:A:670:GLN:HB3	1.94	0.49
2:B:80:ILE:HG12	2:B:177:ILE:H	1.78	0.49
2:B:167:TYR:C	2:B:169:TYR:N	2.69	0.49
1:C:763:ASP:O	1:C:766:LYS:HB2	2.13	0.49
2:D:199:TYR:CB	2:D:200:PRO:CD	2.70	0.49
1:A:68:ASP:CG	1:A:69:GLY:H	1.90	0.49
1:A:795:LEU:HD13	1:A:915:PHE:HB3	1.95	0.49
1:A:880:ARG:HH21	6:A:1104:OBN:H6'3	1.78	0.49
1:A:301:ILE:O	1:A:305:ILE:HG12	2.13	0.48
1:A:872:LEU:HD23	1:A:894:SER:HB2	1.94	0.48
2:D:204:TYR:CD2	2:D:235:TYR:CE2	3.01	0.48
1:C:799:THR:HG21	1:C:912:HIS:HB3	1.94	0.48
2:D:204:TYR:HB2	2:D:235:TYR:CE1	2.47	0.48
1:A:284:PHE:CD1	1:A:838:VAL:HG21	2.48	0.48
1:A:794:PRO:CB	1:A:862:TYR:CD2	2.89	0.48
1:A:809:MET:O	1:A:813:ILE:HG12	2.13	0.48
1:C:217:PRO:HB3	1:C:243:VAL:HG21	1.95	0.48
2:D:216:LYS:HG3	2:D:221:LYS:HA	1.95	0.48
1:A:98:TRP:CE2	1:A:133:VAL:HG11	2.48	0.48
1:A:891:VAL:HG21	1:A:904:ARG:NH1	2.29	0.48
1:C:840:GLU:H	1:C:840:GLU:CD	2.22	0.48
1:C:872:LEU:HD23	1:C:894:SER:HB2	1.94	0.48
2:B:170:LYS:HB2	2:B:174:PRO:CA	2.33	0.48
1:C:891:VAL:HG21	1:C:904:ARG:NH1	2.29	0.48
1:A:99:ILE:HG13	1:A:100:GLY:N	2.28	0.48
1:A:880:ARG:NH2	6:A:1104:OBN:H6'2	2.29	0.48
1:A:217:PRO:HB3	1:A:243:VAL:HG21	1.96	0.48
1:A:942:MET:HE3	1:A:948:ILE:HD13	1.95	0.48
1:C:29:LYS:HE2	1:C:265:THR:HB	1.96	0.48
1:C:403:SER:OG	1:C:406:LYS:NZ	2.47	0.48
1:A:291:VAL:HG21	1:A:847:TYR:CE2	2.48	0.48
1:A:794:PRO:HG2	1:A:859:PHE:HE1	1.78	0.48
1:A:915:PHE:O	1:A:919:ILE:HG12	2.14	0.48
2:B:95:PRO:O	2:B:99:GLU:HG2	2.14	0.48
1:A:116:GLU:HG3	1:A:118:PRO:CD	2.40	0.48
1:A:1009:TRP:H	11:A:1110:CE1:H262	1.78	0.48
1:C:525:GLU:HA	1:C:528:LYS:HB3	1.95	0.48
1:A:403:SER:OG	1:A:406:LYS:NZ	2.47	0.47
1:C:284:PHE:HE1	1:C:773:LEU:HD11	1.78	0.47
1:A:41:LEU:HD12	1:A:41:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:O	1:A:240:THR:OG1	2.24	0.47
1:A:929:ILE:HB	1:A:995:ASP:OD2	2.14	0.47
8:A:1106:1AT:O4	8:A:1106:1AT:O1N	2.32	0.47
2:B:73:ALA:O	2:B:75:PRO:HD3	2.15	0.47
1:C:836:LYS:HB2	1:C:839:ASN:HB3	1.96	0.47
1:C:874:ILE:HD12	1:C:874:ILE:H	1.78	0.47
2:D:80:ILE:HG12	2:D:177:ILE:H	1.79	0.47
1:A:667:THR:N	1:A:670:GLN:OE1	2.42	0.47
1:A:708:THR:HG22	1:A:725:VAL:HB	1.96	0.47
1:C:99:ILE:HG13	1:C:100:GLY:N	2.29	0.47
1:C:479:ASN:HB3	1:C:481:TYR:CD2	2.49	0.47
1:C:612:ASP:OD1	1:C:613:HIS:N	2.40	0.47
1:C:689:GLN:O	1:C:693:ILE:HG12	2.14	0.47
2:D:263:PHE:CE1	2:D:274:ILE:HG13	2.49	0.47
1:A:310:TRP:CD1	1:A:310:TRP:H	2.32	0.47
1:A:944:ASN:O	1:A:948:ILE:HG12	2.14	0.47
1:A:1009:TRP:N	11:A:1110:CE1:H262	2.29	0.47
1:C:83:VAL:O	1:C:86:CYS:HB2	2.13	0.47
1:C:386:SER:HB2	1:C:391:HIS:NE2	2.29	0.47
1:C:809:MET:O	1:C:813:ILE:HG12	2.14	0.47
1:C:862:TYR:C	1:C:862:TYR:HD1	2.23	0.47
2:D:73:ALA:O	2:D:75:PRO:HD3	2.15	0.47
2:D:244:PRO:HG2	2:D:246:TYR:CE1	2.50	0.47
1:A:416:ARG:NH1	1:A:467:TYR:OH	2.37	0.47
2:B:129:VAL:HG22	2:B:204:TYR:OH	2.15	0.47
3:G:32:ILE:HG22	10:G:1002:17F:O10	2.15	0.47
2:D:95:PRO:O	2:D:99:GLU:HG2	2.14	0.47
2:D:230:PHE:HD2	2:D:260:ALA:HB3	1.80	0.47
1:A:129:LEU:HD21	1:A:327:GLU:HG2	1.97	0.47
1:A:148:SER:O	1:A:152:GLU:HG2	2.15	0.47
1:A:689:GLN:O	1:A:693:ILE:HG12	2.14	0.47
2:B:263:PHE:CE1	2:B:274:ILE:HG13	2.49	0.47
1:C:562:PHE:HZ	1:C:570:ASN:HD22	1.62	0.47
1:C:602:ALA:HB1	1:C:759:ARG:HH12	1.79	0.47
2:D:204:TYR:HB2	2:D:235:TYR:CD1	2.50	0.47
1:A:386:SER:HB2	1:A:391:HIS:NE2	2.30	0.47
1:C:25:MET:O	1:C:29:LYS:HG3	2.15	0.47
1:C:755:VAL:HG22	1:C:825:MET:HE1	1.96	0.47
1:C:793:LEU:HD12	1:C:794:PRO:HD2	1.96	0.47
1:C:929:ILE:HB	1:C:995:ASP:OD2	2.15	0.47
1:A:29:LYS:HE2	1:A:265:THR:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:HA	1:A:98:TRP:CE3	2.50	0.47
1:A:763:ASP:O	1:A:766:LYS:HB2	2.14	0.47
1:A:768:SER:HA	1:A:815:LEU:HD23	1.97	0.47
1:A:836:LYS:HB2	1:A:839:ASN:HB3	1.96	0.47
1:A:868:GLU:OE2	2:B:68:TYR:HE2	1.98	0.47
2:D:51:ILE:O	2:D:54:ILE:HG22	2.15	0.47
7:A:1105:CLR:H25	1:C:993:VAL:HG21	1.98	0.46
2:B:160:SER:HB2	2:B:169:TYR:CE1	2.49	0.46
1:C:191:ARG:HE	1:C:239:SER:HA	1.81	0.46
1:C:768:SER:HA	1:C:815:LEU:HD23	1.98	0.46
2:B:217:ARG:HH11	2:B:217:ARG:CG	2.25	0.46
1:C:473:ILE:HD12	1:C:483:LEU:HD21	1.97	0.46
2:D:26:GLY:HA2	2:D:27:ARG:HA	1.62	0.46
1:A:762:PHE:CE1	1:A:837:LEU:HD13	2.51	0.46
1:C:944:ASN:O	1:C:948:ILE:HG12	2.16	0.46
1:C:998:ARG:HE	1:C:1014:THR:HB	1.81	0.46
1:A:360:LEU:HD21	1:A:741:MET:HE1	1.98	0.46
1:A:755:VAL:HG22	1:A:825:MET:HE1	1.96	0.46
1:A:860:PHE:CZ	7:A:1105:CLR:H191	2.50	0.46
1:A:883:TRP:HA	1:A:904:ARG:NH1	2.30	0.46
2:D:133:LEU:HD12	2:D:133:LEU:H	1.80	0.46
1:A:936:SER:HB2	1:A:1003:ARG:HH21	1.81	0.46
1:C:148:SER:O	1:C:152:GLU:HG2	2.15	0.46
1:C:98:TRP:HA	1:C:98:TRP:CE3	2.50	0.46
2:D:148:VAL:HG11	2:D:255:LEU:H	1.81	0.46
1:A:104:CYS:SG	1:A:322:VAL:HG11	2.56	0.46
1:A:118:PRO:HA	1:A:121:ASP:CB	2.46	0.46
1:A:862:TYR:C	1:A:862:TYR:HD1	2.23	0.46
2:B:277:LYS:HB3	2:B:279:TYR:CE1	2.51	0.46
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.81	0.46
1:C:883:TRP:HA	1:C:904:ARG:NH1	2.31	0.46
1:C:915:PHE:O	1:C:919:ILE:HG12	2.16	0.46
1:A:611:GLY:HA2	1:A:686:THR:H	1.81	0.46
1:A:998:ARG:HE	1:A:1014:THR:HB	1.81	0.46
2:B:21:LYS:HG3	2:B:22:LYS:H	1.81	0.46
1:A:191:ARG:HE	1:A:239:SER:HA	1.80	0.46
1:A:385:TRP:HE3	1:A:580:GLY:HA2	1.81	0.46
2:B:148:VAL:HG11	2:B:255:LEU:H	1.81	0.45
1:C:794:PRO:HG2	1:C:859:PHE:HE1	1.80	0.45
1:C:957:LEU:O	1:C:961:LEU:HD12	2.16	0.45
1:A:490:ASN:OD1	1:A:490:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LYS:CB	2:B:174:PRO:HA	2.36	0.45
1:A:182:ASP:OD1	1:A:182:ASP:N	2.49	0.45
2:B:112:TYR:CE2	2:B:258:LEU:HD11	2.51	0.45
1:C:660:GLY:HA2	1:C:663:LEU:HB2	1.98	0.45
1:A:883:TRP:HA	1:A:904:ARG:HH11	1.81	0.45
2:B:91:ARG:HD2	2:B:94:ASP:H	1.82	0.45
2:B:177:ILE:HA	2:B:260:ALA:HA	1.99	0.45
2:B:229:TYR:CD1	2:B:261:VAL:HG22	2.52	0.45
1:C:41:LEU:H	1:C:41:LEU:HD12	1.80	0.45
1:A:78:THR:OG1	1:A:80:PRO:HD3	2.16	0.45
2:B:105:ILE:HG22	2:B:109:LEU:HD13	1.98	0.45
2:B:244:PRO:HG2	2:B:246:TYR:CE1	2.51	0.45
2:D:112:TYR:CE2	2:D:258:LEU:HD11	2.51	0.45
1:A:840:GLU:CD	10:A:1108:17F:N1	2.75	0.45
1:A:901:TYR:HA	1:A:904:ARG:HE	1.81	0.45
1:A:1009:TRP:HB3	11:A:1110:CE1:C24	2.44	0.45
10:B:1005:17F:H18A	10:B:1005:17F:H32	1.67	0.45
1:C:182:ASP:N	1:C:182:ASP:OD1	2.48	0.45
1:C:708:THR:HG22	1:C:725:VAL:HB	1.98	0.45
1:C:773:LEU:HD23	1:C:773:LEU:HA	1.77	0.45
1:A:872:LEU:HD13	1:A:872:LEU:HA	1.86	0.45
1:A:880:ARG:HH21	6:A:1104:OBN:C6'	2.29	0.45
1:C:710:ASP:O	1:C:731:GLY:HA2	2.17	0.45
1:A:286:HIS:HB3	10:A:1109:17F:H1A	1.99	0.45
1:A:986:PRO:HG3	7:A:1105:CLR:H152	1.97	0.45
1:C:310:TRP:CD1	1:C:310:TRP:H	2.33	0.45
6:C:2004:OBN:O3	6:C:2004:OBN:O1	2.28	0.45
2:D:21:LYS:HG3	2:D:22:LYS:H	1.81	0.45
2:D:164:ASP:OD1	2:D:164:ASP:N	2.50	0.45
7:E:2001:CLR:H211	7:E:2001:CLR:H231	1.69	0.45
1:A:82:TRP:CD1	1:A:141:TYR:HH	2.34	0.45
1:A:911:CYS:C	1:A:914:PRO:HD2	2.42	0.45
2:B:230:PHE:HD2	2:B:260:ALA:HB3	1.81	0.45
2:B:241:GLN:H	2:B:241:GLN:HG2	1.63	0.45
1:A:786:PHE:CZ	6:A:1104:OBN:H6'1	2.52	0.45
1:A:340:THR:O	1:A:344:MET:HG2	2.17	0.44
1:A:430:GLN:CG	1:A:438:ARG:HB2	2.47	0.44
8:A:1106:1AT:H18	2:D:68:TYR:OH	2.17	0.44
2:B:133:LEU:HD12	2:B:133:LEU:H	1.81	0.44
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.99	0.44
2:D:108:PHE:HZ	2:D:179:LYS:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:LYS:HB3	2:D:279:TYR:CE1	2.52	0.44
1:A:689:GLN:OE1	1:A:689:GLN:N	2.38	0.44
1:A:957:LEU:O	1:A:961:LEU:HD12	2.16	0.44
1:C:118:PRO:HA	1:C:121:ASP:CB	2.47	0.44
2:D:216:LYS:HE3	2:D:222:GLU:OE1	2.17	0.44
2:D:241:GLN:H	2:D:241:GLN:HG2	1.61	0.44
2:D:251:GLN:HB3	2:D:254:TYR:HB2	1.99	0.44
1:A:473:ILE:HD12	1:A:483:LEU:HD21	1.99	0.44
1:A:793:LEU:HD12	1:A:794:PRO:HD2	1.99	0.44
1:A:880:ARG:HG3	1:A:881:VAL:N	2.33	0.44
1:C:280:GLU:OE2	1:C:830:ARG:NH2	2.51	0.44
1:C:385:TRP:HE3	1:C:580:GLY:HA2	1.81	0.44
1:C:490:ASN:OD1	1:C:490:ASN:N	2.48	0.44
1:C:710:ASP:CG	1:C:711:GLY:N	2.75	0.44
1:C:794:PRO:CB	1:C:862:TYR:CD2	3.00	0.44
2:D:71:ARG:HA	2:D:71:ARG:HD3	1.76	0.44
1:A:1009:TRP:H	11:A:1110:CE1:C26	2.30	0.44
1:C:911:CYS:C	1:C:914:PRO:HD2	2.42	0.44
2:D:221:LYS:HE3	2:D:223:LYS:HG3	2.00	0.44
1:A:424:ALA:O	1:A:464:ARG:NH2	2.50	0.44
1:A:487:LYS:NZ	1:A:560:GLU:O	2.46	0.44
1:A:729:ILE:HG13	1:A:730:ALA:N	2.33	0.44
2:B:164:ASP:OD1	2:B:164:ASP:N	2.50	0.44
1:C:430:GLN:CG	1:C:438:ARG:HB2	2.47	0.44
1:C:762:PHE:CE1	1:C:837:LEU:HD13	2.53	0.44
1:A:584:MET:HE2	1:A:584:MET:HB3	1.92	0.44
1:C:78:THR:OG1	1:C:80:PRO:HD3	2.18	0.44
1:C:360:LEU:HD21	1:C:741:MET:HE1	1.99	0.44
1:C:913:THR:N	1:C:914:PRO:HD2	2.33	0.44
2:D:80:ILE:HG12	2:D:177:ILE:HB	2.00	0.44
2:D:222:GLU:H	2:D:222:GLU:CD	2.20	0.44
1:A:982:PHE:CD2	9:A:1107:1DS:H24	2.53	0.44
2:B:221:LYS:HE3	2:B:223:LYS:HG3	2.00	0.44
1:C:756:GLU:HA	1:C:825:MET:HE3	1.99	0.44
1:C:1010:VAL:O	1:C:1014:THR:OG1	2.26	0.44
1:C:901:TYR:HA	1:C:904:ARG:HE	1.81	0.44
1:C:936:SER:HB2	1:C:1003:ARG:HH21	1.82	0.44
2:D:105:ILE:HG22	2:D:109:LEU:HD13	1.99	0.44
2:D:177:ILE:HA	2:D:260:ALA:HA	2.00	0.44
1:A:600:ARG:NH2	1:A:680:GLU:HG2	2.33	0.43
2:B:80:ILE:HG12	2:B:177:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:HG3	1:C:118:PRO:CD	2.40	0.43
2:B:71:ARG:HD3	2:B:71:ARG:HA	1.77	0.43
1:C:986:PRO:HB2	7:C:2005:CLR:H262	2.00	0.43
2:D:259:MET:HE2	2:D:259:MET:HB3	1.73	0.43
1:A:93:PHE:HA	1:A:285:ILE:HD11	2.01	0.43
1:A:229:PRO:O	1:A:232:THR:HG22	2.18	0.43
1:A:374:LEU:O	1:A:592:VAL:HG21	2.18	0.43
1:A:660:GLY:HA2	1:A:663:LEU:HB2	2.00	0.43
1:C:291:VAL:HG21	1:C:847:TYR:CE2	2.53	0.43
1:A:326:PRO:HA	13:A:1203:HOH:O	2.18	0.43
1:A:710:ASP:CG	1:A:711:GLY:N	2.77	0.43
1:A:1010:VAL:O	1:A:1014:THR:OG1	2.28	0.43
2:B:108:PHE:HZ	2:B:179:LYS:HD3	1.83	0.43
1:C:29:LYS:HE3	1:C:29:LYS:HB3	1.87	0.43
1:C:413:ALA:O	1:C:417:ILE:HG13	2.18	0.43
1:C:762:PHE:CE2	1:C:830:ARG:HD2	2.54	0.43
1:C:909:PHE:CE2	1:C:972:ARG:CZ	3.01	0.43
1:A:183:LEU:HD21	1:A:248:ARG:NH2	2.34	0.43
1:A:612:ASP:OD1	1:A:613:HIS:N	2.39	0.43
2:B:193:ASN:OD1	2:B:205:ASN:ND2	2.51	0.43
1:A:886:ARG:HA	1:A:901:TYR:CD1	2.54	0.43
1:C:503:ALA:HA	1:C:504:PRO:HD3	1.90	0.43
1:A:225:THR:HG21	1:A:233:ARG:HD2	2.01	0.43
1:A:758:GLY:HA2	1:A:761:ILE:HG22	2.01	0.43
1:C:324:ASN:O	1:C:326:PRO:HD3	2.18	0.43
1:C:374:LEU:O	1:C:592:VAL:HG21	2.18	0.43
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.54	0.43
2:D:62:SER:HB3	2:D:65:LYS:O	2.19	0.43
2:D:207:TYR:C	2:D:240:LEU:HD13	2.43	0.43
1:A:90:PHE:O	1:A:94:SER:HB2	2.19	0.43
1:A:260:MET:HE2	1:A:712:VAL:HG11	2.00	0.43
1:A:397:GLU:H	1:A:397:GLU:HG2	1.62	0.43
1:A:413:ALA:O	1:A:417:ILE:HG13	2.18	0.43
1:A:831:ASN:HA	1:A:832:PRO:HD2	1.90	0.43
1:C:90:PHE:O	1:C:94:SER:HB2	2.19	0.43
1:C:183:LEU:HD21	1:C:248:ARG:NH2	2.34	0.43
1:C:340:THR:O	1:C:344:MET:HG2	2.18	0.43
1:C:611:GLY:HA2	1:C:686:THR:H	1.83	0.43
2:D:80:ILE:HG21	2:D:177:ILE:HD12	2.00	0.43
2:D:91:ARG:HD2	2:D:94:ASP:H	1.82	0.43
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:LYS:HA	2:B:288:LYS:HD2	1.80	0.43
1:C:743:LEU:HD11	1:C:751:ILE:HD13	2.00	0.43
2:D:206:PRO:HB2	2:D:207:TYR:CD2	2.54	0.43
11:E:2002:CE1:H122	11:E:2002:CE1:H151	1.73	0.43
1:A:207:ASP:HB2	1:A:243:VAL:CG2	2.48	0.43
1:A:267:ALA:CB	1:A:715:SER:HB3	2.48	0.43
1:A:435:ILE:O	1:A:438:ARG:HG2	2.19	0.43
1:A:762:PHE:CE2	1:A:830:ARG:HD2	2.54	0.43
2:B:274:ILE:HD13	2:B:274:ILE:HA	1.78	0.43
1:C:424:ALA:O	1:C:464:ARG:NH2	2.51	0.43
1:C:964:CYS:HB3	1:C:967:MET:HG3	2.01	0.43
2:D:187:LYS:O	2:D:282:ASN:ND2	2.52	0.43
1:A:56:LEU:HD11	1:A:182:ASP:HB3	2.01	0.42
1:A:212:THR:HG21	1:A:214:GLU:OE1	2.18	0.42
1:A:295:LEU:HD23	1:A:295:LEU:HA	1.75	0.42
1:A:384:MET:HE3	1:A:384:MET:HB2	1.79	0.42
1:A:913:THR:N	1:A:914:PRO:HD2	2.33	0.42
1:C:384:MET:HE3	1:C:384:MET:HB2	1.78	0.42
1:C:416:ARG:HD2	1:C:467:TYR:OH	2.19	0.42
1:C:435:ILE:O	1:C:438:ARG:HG2	2.18	0.42
2:D:217:ARG:HH11	2:D:217:ARG:CG	2.26	0.42
1:A:205:LYS:HA	1:A:219:THR:HA	2.01	0.42
1:A:280:GLU:OE2	1:A:830:ARG:NH2	2.52	0.42
1:C:225:THR:HG21	1:C:233:ARG:HD2	2.01	0.42
1:A:803:ILE:HD13	1:A:803:ILE:HA	1.85	0.42
11:A:1110:CE1:H212	11:A:1110:CE1:C27	2.44	0.42
1:C:666:MET:HE2	1:C:666:MET:HB3	1.78	0.42
1:C:880:ARG:HG3	1:C:881:VAL:N	2.33	0.42
1:A:54:ARG:HE	1:A:54:ARG:HB3	1.54	0.42
1:A:843:ILE:HB	10:A:1108:17F:H5	2.02	0.42
9:A:1107:1DS:O4	2:B:68:TYR:OH	2.33	0.42
7:G:1001:CLR:H211	7:G:1001:CLR:H231	1.70	0.42
1:C:207:ASP:HB2	1:C:243:VAL:CG2	2.49	0.42
1:C:860:PHE:O	1:C:864:VAL:HG23	2.19	0.42
1:C:936:SER:OG	1:C:996:GLU:OE2	2.28	0.42
2:D:121:MET:HB3	2:D:121:MET:HE3	1.79	0.42
2:D:157:GLY:C	2:D:159:CYS:H	2.27	0.42
1:A:254:THR:O	1:A:257:ARG:NE	2.49	0.42
1:A:416:ARG:HD2	1:A:467:TYR:OH	2.19	0.42
2:B:117:GLN:HA	2:B:123:PHE:CE2	2.54	0.42
1:C:420:LEU:HB3	1:C:486:HIS:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:907:VAL:O	1:C:911:CYS:HB2	2.20	0.42
2:D:231:GLY:HA3	2:D:235:TYR:O	2.19	0.42
1:A:470:ILE:HD12	1:A:564:PHE:CE1	2.54	0.42
1:A:773:LEU:HD23	1:A:773:LEU:HA	1.78	0.42
1:A:890:ASP:OD1	2:B:82:GLN:NE2	2.53	0.42
1:C:462:GLU:HA	1:C:465:GLU:HG2	2.02	0.42
1:C:729:ILE:HG13	1:C:730:ALA:N	2.34	0.42
1:C:898:GLN:HE22	2:D:179:LYS:HE3	1.84	0.42
2:D:274:ILE:HD13	2:D:274:ILE:HA	1.78	0.42
1:A:479:ASN:OD1	1:A:506:ARG:NH1	2.53	0.42
2:B:204:TYR:HB2	2:B:235:TYR:CD1	2.54	0.42
1:C:157:MET:HE3	1:C:157:MET:HB3	1.80	0.42
1:C:866:LEU:HA	1:C:866:LEU:HD23	1.65	0.42
2:D:24:PHE:CD1	2:D:28:THR:HG22	2.54	0.42
1:A:76:PRO:HA	1:A:77:PRO:HD3	1.85	0.42
2:B:91:ARG:H	2:B:97:SER:HG	1.65	0.42
2:B:157:GLY:C	2:B:159:CYS:H	2.27	0.42
2:B:174:PRO:O	2:B:263:PHE:N	2.47	0.42
2:B:178:ILE:HD12	2:B:211:VAL:HG11	2.01	0.42
2:B:222:GLU:H	2:B:222:GLU:CD	2.22	0.42
2:D:117:GLN:HA	2:D:123:PHE:CE2	2.54	0.42
1:A:103:LEU:HB3	1:A:318:ILE:HG23	2.01	0.42
1:A:462:GLU:HA	1:A:465:GLU:HG2	2.02	0.42
1:A:504:PRO:HG2	1:A:535:TYR:CE1	2.55	0.42
1:A:710:ASP:O	1:A:731:GLY:HA2	2.20	0.42
2:B:259:MET:HB3	2:B:259:MET:HE2	1.72	0.42
1:C:194:ALA:HB1	1:C:253:TYR:O	2.20	0.42
1:C:600:ARG:NH2	1:C:680:GLU:HG2	2.34	0.42
2:D:229:TYR:CD1	2:D:261:VAL:HG22	2.54	0.42
2:D:244:PRO:HG2	2:D:246:TYR:HE1	1.84	0.42
1:A:467:TYR:HB3	1:A:486:HIS:HB3	2.02	0.42
1:A:964:CYS:HB3	1:A:967:MET:HG3	2.01	0.42
2:B:139:TYR:OH	2:B:185:GLY:HA2	2.20	0.42
2:B:231:GLY:HA3	2:B:235:TYR:O	2.20	0.42
1:C:467:TYR:HB3	1:C:486:HIS:HB3	2.02	0.42
1:C:880:ARG:NH2	6:C:2004:OBN:H6'2	2.35	0.42
3:E:42:LEU:HA	3:E:45:ILE:HD11	2.01	0.42
1:A:42:ASP:O	1:A:46:ARG:HB2	2.19	0.41
1:A:756:GLU:HA	1:A:825:MET:HE3	2.02	0.41
1:A:1002:ILE:HD13	1:A:1015:TYR:HB2	2.01	0.41
1:C:205:LYS:HA	1:C:219:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:LYS:HE3	1:C:506:ARG:HH11	1.85	0.41
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.55	0.41
1:C:982:PHE:CE1	7:E:2001:CLR:H183	2.55	0.41
2:D:139:TYR:OH	2:D:185:GLY:HA2	2.20	0.41
2:D:204:TYR:O	2:D:208:VAL:CG1	2.61	0.41
7:A:1105:CLR:H162	7:A:1105:CLR:H241	2.01	0.41
11:A:1110:CE1:H212	11:A:1110:CE1:H242	1.66	0.41
2:B:80:ILE:HG21	2:B:177:ILE:HD12	2.00	0.41
1:C:56:LEU:HD11	1:C:182:ASP:HB3	2.01	0.41
1:C:97:LEU:HB2	1:C:133:VAL:HG22	2.02	0.41
2:D:167:TYR:O	2:D:167:TYR:CG	2.73	0.41
1:A:469:LYS:HB2	1:A:469:LYS:HE3	1.82	0.41
11:A:1110:CE1:H101	2:B:38:PHE:HA	2.02	0.41
1:C:212:THR:HG21	1:C:214:GLU:OE1	2.20	0.41
1:C:487:LYS:NZ	1:C:560:GLU:O	2.45	0.41
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.84	0.41
1:A:982:PHE:CE1	7:G:1001:CLR:H183	2.54	0.41
9:A:1107:1DS:O6'	9:A:1107:1DS:O3'	2.29	0.41
1:C:192:ILE:HB	1:C:237:PHE:O	2.19	0.41
1:C:208:ASN:HB3	1:C:212:THR:CG2	2.49	0.41
1:C:872:LEU:HD13	1:C:872:LEU:HA	1.86	0.41
1:A:194:ALA:HB1	1:A:253:TYR:O	2.20	0.41
1:A:963:TYR:HE2	7:G:1001:CLR:H6	1.83	0.41
1:C:462:GLU:O	1:C:466:ARG:HB2	2.21	0.41
1:C:584:MET:HE2	1:C:584:MET:HB3	1.93	0.41
2:D:83:SER:OG	2:D:87:GLU:O	2.33	0.41
1:A:324:ASN:O	1:A:326:PRO:HD3	2.21	0.41
1:A:783:PHE:CD2	6:A:1104:OBN:H161	2.55	0.41
1:A:803:ILE:HG12	1:A:916:PHE:HD1	1.85	0.41
1:A:921:VAL:HG13	1:A:924:TRP:CZ3	2.56	0.41
2:B:187:LYS:O	2:B:282:ASN:ND2	2.54	0.41
2:B:244:PRO:HG2	2:B:246:TYR:HE1	1.85	0.41
3:G:42:LEU:HA	3:G:45:ILE:HD11	2.03	0.41
1:C:967:MET:HE3	1:C:967:MET:HB3	1.81	0.41
1:C:977:LYS:HE2	2:D:68:TYR:CD1	2.55	0.41
1:A:207:ASP:OD1	1:A:209:SER:HB3	2.21	0.41
2:B:166:THR:HG21	2:B:170:LYS:H	1.86	0.41
2:B:216:LYS:HE3	2:B:222:GLU:OE1	2.20	0.41
2:B:226:THR:HB	2:B:265:ASN:HB2	2.03	0.41
1:C:82:TRP:CD1	1:C:141:TYR:OH	2.74	0.41
1:C:921:VAL:HG13	1:C:924:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:963:TYR:HE2	7:E:2001:CLR:H6	1.84	0.41
1:A:614:PRO:HD3	1:A:685:ARG:HD2	2.02	0.41
1:C:216:GLU:H	1:C:216:GLU:HG2	1.64	0.41
1:C:504:PRO:HG2	1:C:535:TYR:CE1	2.56	0.41
1:C:783:PHE:CD2	6:C:2004:OBN:H161	2.55	0.41
1:C:803:ILE:HG12	1:C:916:PHE:HD1	1.86	0.41
1:C:1002:ILE:HD13	1:C:1015:TYR:HB2	2.01	0.41
2:D:22:LYS:HA	2:D:23:GLU:HA	1.77	0.41
2:D:111:LYS:H	2:D:111:LYS:HG3	1.71	0.41
1:A:97:LEU:HB2	1:A:133:VAL:HG22	2.03	0.41
1:A:462:GLU:O	1:A:466:ARG:HB2	2.21	0.41
1:A:907:VAL:O	1:A:911:CYS:HB2	2.21	0.41
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.56	0.41
2:B:204:TYR:CA	2:B:206:PRO:HD2	2.50	0.41
3:G:33:PHE:HA	10:G:1002:17F:C18	2.51	0.41
1:C:61:ALA:O	1:C:179:VAL:HG11	2.20	0.41
1:C:506:ARG:O	1:C:509:ASP:HB3	2.21	0.41
2:D:160:SER:HB2	2:D:169:TYR:CE1	2.55	0.41
2:D:174:PRO:O	2:D:263:PHE:N	2.46	0.41
1:C:93:PHE:HA	1:C:285:ILE:HD11	2.02	0.41
2:D:80:ILE:CD1	2:D:177:ILE:H	2.34	0.41
1:A:82:TRP:CD1	1:A:141:TYR:OH	2.73	0.40
1:A:551:LEU:CD2	1:A:572:PRO:HG2	2.51	0.40
1:A:1005:ARG:HH21	11:A:1110:CE1:H291	1.85	0.40
1:C:229:PRO:O	1:C:232:THR:HG22	2.20	0.40
1:C:267:ALA:CB	1:C:715:SER:HB3	2.51	0.40
1:C:416:ARG:NH1	1:C:467:TYR:OH	2.37	0.40
1:C:493:GLU:H	1:C:493:GLU:HG2	1.70	0.40
2:D:37:LEU:O	2:D:41:ILE:HG12	2.21	0.40
1:A:61:ALA:O	1:A:179:VAL:HG11	2.21	0.40
1:A:794:PRO:O	1:A:912:HIS:HD2	2.04	0.40
2:B:17:TRP:CE3	2:B:17:TRP:HA	2.55	0.40
2:B:170:LYS:HD3	2:B:175:CYS:H	1.85	0.40
1:C:129:LEU:CD2	1:C:327:GLU:HG2	2.51	0.40
1:C:758:GLY:HA2	1:C:761:ILE:HG22	2.02	0.40
1:C:826:LYS:HA	1:C:826:LYS:HD2	1.82	0.40
2:D:217:ARG:HG2	2:D:217:ARG:NH1	2.28	0.40
1:A:689:GLN:O	1:A:692:LEU:HB3	2.22	0.40
2:B:80:ILE:HG23	2:B:177:ILE:HB	2.04	0.40
2:B:167:TYR:O	2:B:167:TYR:CG	2.73	0.40
1:A:308:TYR:HE1	1:A:880:ARG:HH12	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:ASN:HA	1:A:650:PRO:HD3	1.89	0.40
1:A:810:VAL:HB	1:A:811:PRO:HD3	2.03	0.40
6:A:1104:OBN:H191	6:A:1104:OBN:H8	1.94	0.40
1:C:918:THR:O	1:C:922:VAL:HG22	2.21	0.40
1:A:108:TYR:HB2	1:A:122:ASN:HB3	2.03	0.40
2:B:80:ILE:HG12	2:B:177:ILE:N	2.36	0.40
1:C:493:GLU:O	1:C:493:GLU:HG2	2.22	0.40
1:C:801:LEU:HD23	1:C:801:LEU:HA	1.73	0.40
2:D:170:LYS:HD3	2:D:175:CYS:H	1.86	0.40
2:D:204:TYR:HD2	2:D:235:TYR:CE1	2.39	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%)	940 (95%)	51 (5%)	2 (0%)	43	71
1	C	993/1021 (97%)	947 (95%)	44 (4%)	2 (0%)	43	71
2	B	287/303 (95%)	255 (89%)	28 (10%)	4 (1%)	9	31
2	D	285/303 (94%)	255 (90%)	26 (9%)	4 (1%)	9	31
3	E	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
3	G	30/65 (46%)	28 (93%)	2 (7%)	0	100	100
All	All	2618/2778 (94%)	2453 (94%)	153 (6%)	12 (0%)	24	54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	199	TYR
2	D	199	TYR

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Mol	Chain	Res	Type
2	B	161	GLY
2	D	161	GLY
2	B	170	LYS
2	B	196	LEU
2	D	170	LYS
2	D	196	LEU
1	A	118	PRO
1	C	118	PRO
1	A	489	PRO
1	C	489	PRO

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%)	764 (90%)	82 (10%)	8	28
1	C	846/864 (98%)	766 (90%)	80 (10%)	8	29
2	B	259/269 (96%)	221 (85%)	38 (15%)	3	12
2	D	257/269 (96%)	221 (86%)	36 (14%)	3	13
3	E	26/52 (50%)	21 (81%)	5 (19%)	1	6
3	G	26/52 (50%)	21 (81%)	5 (19%)	1	6
All	All	2260/2370 (95%)	2014 (89%)	246 (11%)	6	22

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	32	VAL
1	A	34	MET
1	A	35	ASP
1	A	45	HIS
1	A	53	SER
1	A	56	LEU
1	A	86	CYS

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Mol	Chain	Res	Type
1	A	98	TRP
1	A	99	ILE
1	A	114	THR
1	A	117	GLU
1	A	118	PRO
1	A	120	ASN
1	A	121	ASP
1	A	122	ASN
1	A	123	LEU
1	A	124	TYR
1	A	127	VAL
1	A	150	ILE
1	A	157	MET
1	A	158	VAL
1	A	164	VAL
1	A	170	LYS
1	A	180	VAL
1	A	209	SER
1	A	211	LEU
1	A	219	THR
1	A	231	GLU
1	A	250	ILE
1	A	271	GLU
1	A	275	THR
1	A	277	ILE
1	A	281	ILE
1	A	301	ILE
1	A	307	GLU
1	A	314	VAL
1	A	324	ASN
1	A	327	GLU
1	A	334	THR
1	A	350	LEU
1	A	352	LYS
1	A	353	ASN
1	A	357	VAL
1	A	420	LEU
1	A	431	GLU
1	A	440	VAL
1	A	459	SER
1	A	460	VAL
1	A	467	TYR

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Mol	Chain	Res	Type
1	A	488	ASN
1	A	490	ASN
1	A	495	ARG
1	A	506	ARG
1	A	552	PHE
1	A	564	PHE
1	A	565	ASP
1	A	567	ASP
1	A	620	ILE
1	A	641	LEU
1	A	643	ILE
1	A	750	SER
1	A	755	VAL
1	A	800	ILE
1	A	815	LEU
1	A	819	GLN
1	A	824	ILE
1	A	840	GLU
1	A	862	TYR
1	A	865	ILE
1	A	874	ILE
1	A	881	VAL
1	A	904	ARG
1	A	910	THR
1	A	911	CYS
1	A	917	VAL
1	A	928	VAL
1	A	957	LEU
1	A	961	LEU
1	A	979	THR
1	A	993	VAL
1	A	1000	LEU
2	B	15	PHE
2	B	17	TRP
2	B	19	SER
2	B	22	LYS
2	B	28	THR
2	B	46	LEU
2	B	54	ILE
2	B	56	VAL
2	B	60	THR
2	B	77	LEU

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Mol	Chain	Res	Type
2	B	79	GLN
2	B	80	ILE
2	B	105	ILE
2	B	117	GLN
2	B	119	ASP
2	B	156	LEU
2	B	159	CYS
2	B	162	LEU
2	B	164	ASP
2	B	169	TYR
2	B	170	LYS
2	B	171	ASP
2	B	178	ILE
2	B	195	SER
2	B	196	LEU
2	B	202	MET
2	B	203	LYS
2	B	217	ARG
2	B	223	LYS
2	B	224	VAL
2	B	256	GLN
2	B	259	MET
2	B	270	THR
2	B	274	ILE
2	B	283	ILE
2	B	287	GLU
2	B	297	VAL
2	B	301	VAL
3	G	25	THR
3	G	28	ASN
3	G	32	ILE
3	G	45	ILE
3	G	47	SER
1	C	22	GLU
1	C	32	VAL
1	C	34	MET
1	C	45	HIS
1	C	46	ARG
1	C	53	SER
1	C	56	LEU
1	C	86	CYS
1	C	98	TRP

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Mol	Chain	Res	Type
1	C	99	ILE
1	C	114	THR
1	C	117	GLU
1	C	118	PRO
1	C	120	ASN
1	C	121	ASP
1	C	122	ASN
1	C	123	LEU
1	C	124	TYR
1	C	127	VAL
1	C	150	ILE
1	C	157	MET
1	C	158	VAL
1	C	164	VAL
1	C	170	LYS
1	C	180	VAL
1	C	209	SER
1	C	211	LEU
1	C	219	THR
1	C	231	GLU
1	C	250	ILE
1	C	271	GLU
1	C	275	THR
1	C	277	ILE
1	C	281	ILE
1	C	301	ILE
1	C	307	GLU
1	C	314	VAL
1	C	324	ASN
1	C	327	GLU
1	C	334	THR
1	C	350	LEU
1	C	352	LYS
1	C	353	ASN
1	C	357	VAL
1	C	420	LEU
1	C	431	GLU
1	C	440	VAL
1	C	459	SER
1	C	460	VAL
1	C	467	TYR
1	C	488	ASN

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Mol	Chain	Res	Type
1	C	490	ASN
1	C	493	GLU
1	C	495	ARG
1	C	506	ARG
1	C	552	PHE
1	C	620	ILE
1	C	643	ILE
1	C	746	ASP
1	C	750	SER
1	C	751	ILE
1	C	755	VAL
1	C	800	ILE
1	C	815	LEU
1	C	819	GLN
1	C	824	ILE
1	C	862	TYR
1	C	865	ILE
1	C	874	ILE
1	C	881	VAL
1	C	904	ARG
1	C	910	THR
1	C	911	CYS
1	C	917	VAL
1	C	928	VAL
1	C	957	LEU
1	C	961	LEU
1	C	979	THR
1	C	993	VAL
1	C	1000	LEU
2	D	17	TRP
2	D	19	SER
2	D	22	LYS
2	D	28	THR
2	D	46	LEU
2	D	54	ILE
2	D	56	VAL
2	D	60	THR
2	D	77	LEU
2	D	79	GLN
2	D	80	ILE
2	D	105	ILE
2	D	117	GLN

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Mol	Chain	Res	Type
2	D	119	ASP
2	D	156	LEU
2	D	159	CYS
2	D	164	ASP
2	D	169	TYR
2	D	170	LYS
2	D	171	ASP
2	D	178	ILE
2	D	195	SER
2	D	196	LEU
2	D	202	MET
2	D	203	LYS
2	D	217	ARG
2	D	223	LYS
2	D	224	VAL
2	D	256	GLN
2	D	259	MET
2	D	270	THR
2	D	274	ILE
2	D	283	ILE
2	D	287	GLU
2	D	297	VAL
2	D	301	VAL
3	E	25	THR
3	E	28	ASN
3	E	32	ILE
3	E	45	ILE
3	E	47	SER

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

Mol	Chain	Res	Type
1	A	120	ASN
1	A	324	ASN
1	A	521	GLN
1	A	659	HIS
2	B	69	GLN
2	B	241	GLN
1	C	120	ASN
1	C	324	ASN
1	C	570	ASN
2	D	69	GLN

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Mol	Chain	Res	Type
2	D	241	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	C	369	5,1	9,11,12	1.35	2 (22%)	9,15,17	1.70	2 (22%)
1	PHD	A	369	5,1	9,11,12	1.42	2 (22%)	9,15,17	1.73	3 (33%)

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	C	369	5,1	-	0/8/11/13	-
1	PHD	A	369	5,1	-	1/8/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	PHD	P-OD1	-2.48	1.55	1.59
1	C	369	PHD	CB-CA	-2.23	1.49	1.53
1	C	369	PHD	P-OD1	-2.14	1.55	1.59
1	A	369	PHD	CB-CA	-2.11	1.49	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PHD	OD1-CG-CB	3.43	118.99	110.95
1	A	369	PHD	OD1-CG-CB	3.38	118.89	110.95
1	A	369	PHD	OD2-CG-CB	-2.78	118.19	124.65
1	C	369	PHD	OD2-CG-CB	-2.53	118.77	124.65
1	A	369	PHD	CA-CB-CG	2.02	117.11	112.78

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	369	PHD	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

2 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	0.33	0	17,19,21	0.49	0
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.37	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	-	1/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

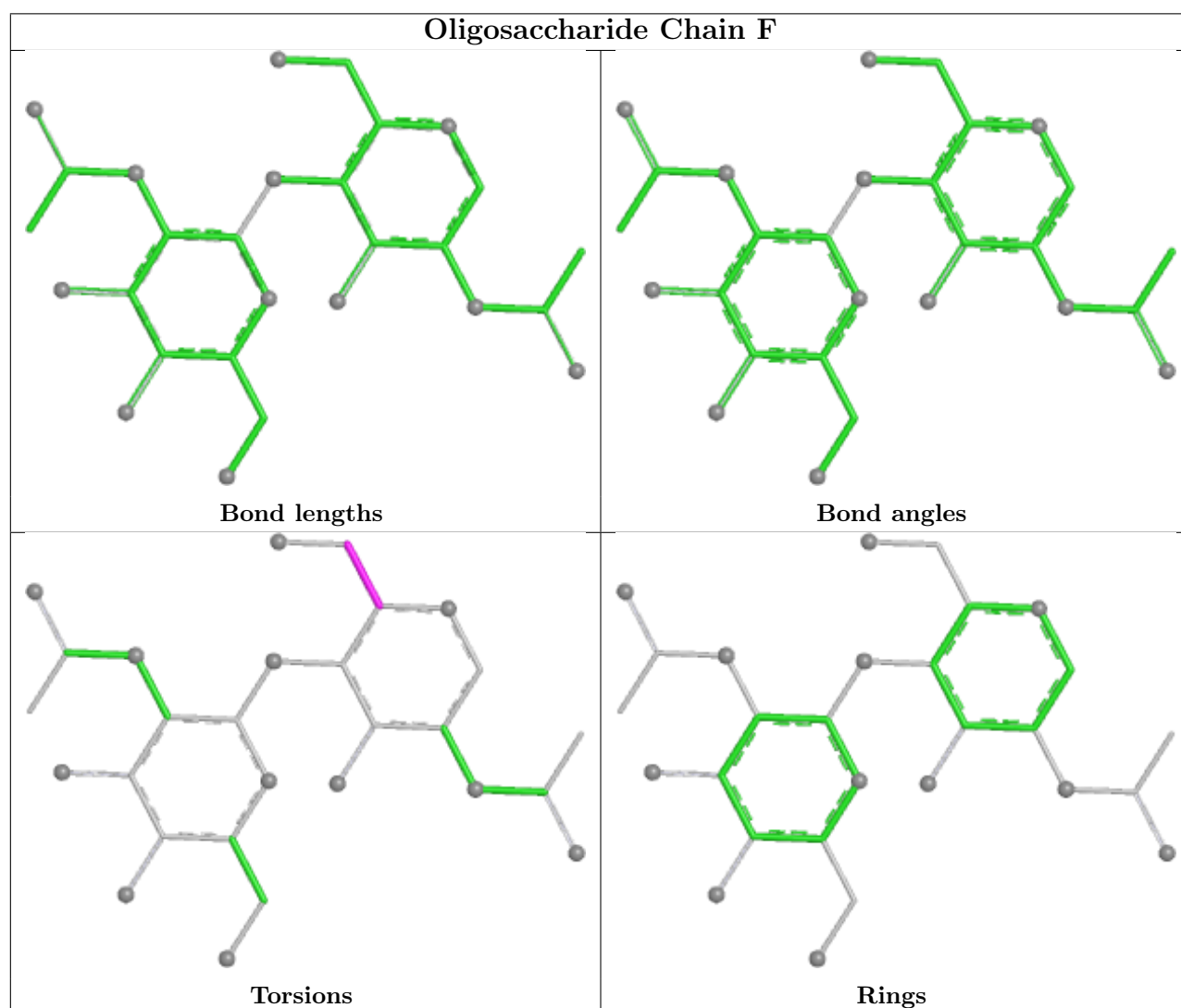
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	1	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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$
9	1DS	A	1107	-	30,30,35	1.31	5 (16%)	42,43,48	2.31	14 (33%)
12	NAG	B	1004	2	14,14,15	0.49	0	17,19,21	0.41	0
10	17F	G	1002	-	25,26,53	1.18	2 (8%)	27,33,60	2.64	8 (29%)
12	NAG	D	2001	2	14,14,15	0.37	0	17,19,21	0.46	0
10	17F	B	1005	-	22,23,53	1.33	3 (13%)	23,29,60	2.70	8 (34%)
8	1AT	A	1106	-	30,30,35	1.45	3 (10%)	43,43,48	2.46	15 (34%)
10	17F	D	2004	-	26,27,53	1.16	4 (15%)	28,34,60	1.96	8 (28%)
6	OBN	C	2004	-	44,46,46	0.81	1 (2%)	69,76,76	1.70	18 (26%)
12	NAG	D	2003	2	14,14,15	0.53	0	17,19,21	0.55	0
7	CLR	G	1001	-	31,31,31	2.56	10 (32%)	48,48,48	2.93	19 (39%)
7	CLR	C	2005	-	31,31,31	2.57	8 (25%)	48,48,48	2.97	18 (37%)
10	17F	A	1109	-	16,17,53	1.30	2 (12%)	17,23,60	3.47	6 (35%)
11	CE1	A	1110	-	33,33,36	0.58	0	32,32,35	0.94	1 (3%)
6	OBN	A	1104	-	44,46,46	0.86	1 (2%)	69,76,76	1.81	18 (26%)
12	NAG	B	1003	2	14,14,15	0.33	0	17,19,21	0.53	0
7	CLR	A	1105	-	31,31,31	2.60	10 (32%)	48,48,48	3.06	18 (37%)
10	17F	A	1108	-	16,17,53	1.46	2 (12%)	17,23,60	3.08	5 (29%)
7	CLR	E	2001	-	31,31,31	2.54	8 (25%)	48,48,48	2.92	20 (41%)
11	CE1	E	2002	-	21,21,36	0.75	0	20,20,35	1.13	2 (10%)
12	NAG	D	2002	2	14,14,15	0.61	0	17,19,21	0.57	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
9	1DS	A	1107	-	-	7/19/58/63	0/2/2/2
12	NAG	B	1004	2	-	4/6/23/26	0/1/1/1
10	17F	G	1002	-	-	9/31/31/59	-
12	NAG	D	2001	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	17F	B	1005	-	-	21/27/27/59	-
8	1AT	A	1106	-	-	8/19/58/63	0/2/2/2
10	17F	D	2004	-	-	17/33/33/59	-
6	OBN	C	2004	-	-	4/11/116/116	0/6/6/6
12	NAG	D	2003	2	-	4/6/23/26	0/1/1/1
7	CLR	G	1001	-	-	4/10/68/68	0/4/4/4
7	CLR	C	2005	-	-	7/10/68/68	0/4/4/4
10	17F	A	1109	-	-	16/20/20/59	-
11	CE1	A	1110	-	-	16/31/31/34	-
6	OBN	A	1104	-	-	4/11/116/116	0/6/6/6
12	NAG	B	1003	2	-	0/6/23/26	0/1/1/1
7	CLR	A	1105	-	-	9/10/68/68	0/4/4/4
10	17F	A	1108	-	-	12/20/20/59	-
7	CLR	E	2001	-	-	4/10/68/68	0/4/4/4
11	CE1	E	2002	-	-	15/19/19/34	-
12	NAG	D	2002	2	-	4/6/23/26	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	2005	CLR	C6-C5	10.05	1.53	1.33
7	A	1105	CLR	C6-C5	10.01	1.53	1.33
7	G	1001	CLR	C6-C5	9.84	1.53	1.33
7	E	2001	CLR	C6-C5	9.79	1.53	1.33
7	A	1105	CLR	C11-C9	5.35	1.62	1.53
7	C	2005	CLR	C11-C9	5.11	1.62	1.53
7	E	2001	CLR	C11-C9	4.73	1.61	1.53
7	G	1001	CLR	C11-C9	4.57	1.61	1.53
8	A	1106	1AT	O6-C1N	4.33	1.46	1.33
7	C	2005	CLR	C8-C14	4.32	1.61	1.53
7	A	1105	CLR	C8-C14	4.05	1.61	1.53
7	G	1001	CLR	C8-C14	3.98	1.61	1.53
7	E	2001	CLR	C8-C14	3.71	1.60	1.53
7	A	1105	CLR	C12-C13	3.68	1.60	1.54
6	A	1104	OBN	O21-C23	3.67	1.45	1.36
6	C	2004	OBN	O21-C23	3.65	1.45	1.36
10	G	1002	17F	O9-C5	-3.61	1.38	1.46
7	C	2005	CLR	C12-C13	3.60	1.60	1.54
10	B	1005	17F	O9-C5	-3.54	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1001	CLR	C12-C13	3.45	1.60	1.54
10	A	1108	17F	O9-C17	3.37	1.42	1.35
7	E	2001	CLR	C12-C13	3.30	1.59	1.54
10	A	1108	17F	O9-C5	-3.23	1.41	1.47
7	E	2001	CLR	C20-C17	-3.18	1.48	1.54
7	G	1001	CLR	C20-C17	-3.13	1.49	1.54
7	E	2001	CLR	C13-C17	-3.11	1.49	1.55
10	B	1005	17F	O9-C17	3.11	1.43	1.34
7	G	1001	CLR	C13-C17	-3.11	1.49	1.55
10	A	1109	17F	O9-C17	3.07	1.42	1.35
7	E	2001	CLR	C15-C14	-2.93	1.48	1.54
9	A	1107	1DS	O1'-C1N	2.90	1.41	1.33
10	D	2004	17F	O7-C6	-2.88	1.38	1.45
7	A	1105	CLR	C15-C14	-2.74	1.48	1.54
10	A	1109	17F	O9-C5	-2.72	1.42	1.47
7	G	1001	CLR	C15-C14	-2.70	1.48	1.54
8	A	1106	1AT	C4'-C5'	-2.66	1.46	1.53
9	A	1107	1DS	C1'-C2'	-2.65	1.48	1.52
7	A	1105	CLR	C16-C17	2.61	1.59	1.54
9	A	1107	1DS	C4'-C3'	-2.59	1.42	1.53
7	C	2005	CLR	C15-C14	-2.52	1.49	1.54
10	D	2004	17F	O9-C17	2.43	1.41	1.34
9	A	1107	1DS	C2N-C1N	2.43	1.57	1.50
10	G	1002	17F	O7-C7	2.41	1.40	1.33
8	A	1106	1AT	C4-C5	-2.36	1.48	1.53
7	C	2005	CLR	C20-C17	-2.36	1.50	1.54
7	G	1001	CLR	C16-C17	2.33	1.59	1.54
7	A	1105	CLR	C20-C17	-2.30	1.50	1.54
7	C	2005	CLR	C16-C17	2.30	1.59	1.54
7	E	2001	CLR	C16-C17	2.28	1.59	1.54
7	C	2005	CLR	C13-C17	-2.22	1.50	1.55
10	D	2004	17F	O9-C5	-2.15	1.41	1.46
7	A	1105	CLR	C19-C10	-2.12	1.51	1.54
7	A	1105	CLR	C22-C20	2.09	1.59	1.54
7	G	1001	CLR	C19-C10	-2.08	1.51	1.54
10	D	2004	17F	O7-C7	2.08	1.39	1.33
7	A	1105	CLR	C13-C17	-2.07	1.51	1.55
9	A	1107	1DS	O2'-C5'	2.06	1.48	1.43
7	G	1001	CLR	C13-C14	-2.06	1.51	1.55
10	B	1005	17F	O5-C3	-2.00	1.24	1.30

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1105	CLR	C4-C5-C6	-8.79	108.65	120.57
10	B	1005	17F	C5-O9-C17	8.57	130.15	117.78
10	A	1109	17F	C5-O9-C17	8.57	132.78	118.29
7	A	1105	CLR	C7-C6-C5	-8.31	110.99	125.02
7	G	1001	CLR	C7-C6-C5	-7.97	111.56	125.02
7	E	2001	CLR	C7-C6-C5	-7.81	111.82	125.02
10	G	1002	17F	O3-C1-C2	7.70	114.78	108.06
7	C	2005	CLR	C7-C6-C5	-7.68	112.05	125.02
10	A	1109	17F	O3-C1-C2	7.66	114.73	108.06
7	G	1001	CLR	C4-C5-C6	-7.52	110.37	120.57
7	C	2005	CLR	C4-C5-C6	-7.41	110.53	120.57
7	E	2001	CLR	C4-C5-C6	-7.27	110.72	120.57
10	G	1002	17F	C5-O9-C17	7.10	130.38	117.85
10	A	1108	17F	O9-C17-C18	7.01	123.60	111.09
7	A	1105	CLR	C12-C13-C17	-6.99	106.31	116.60
7	E	2001	CLR	C12-C13-C17	-6.85	106.51	116.60
10	A	1108	17F	O3-C1-C2	6.83	114.02	108.06
7	G	1001	CLR	C12-C13-C17	-6.78	106.61	116.60
7	A	1105	CLR	C7-C8-C9	6.70	117.47	109.72
8	A	1106	1AT	O2-C2-C3	-6.70	94.58	110.38
7	E	2001	CLR	C10-C5-C6	-6.34	113.67	122.93
7	C	2005	CLR	C7-C8-C9	6.30	117.00	109.72
9	A	1107	1DS	C1'-O1'-C1N	6.25	127.84	116.71
7	C	2005	CLR	C10-C5-C6	-6.18	113.91	122.93
6	A	1104	OBN	C6'-C5'-C4'	-6.17	101.79	113.08
10	A	1109	17F	O9-C17-C18	5.99	121.78	111.09
7	C	2005	CLR	C12-C13-C17	-5.96	107.83	116.60
7	G	1001	CLR	C7-C8-C9	5.91	116.55	109.72
7	G	1001	CLR	C10-C5-C6	-5.79	114.47	122.93
10	A	1108	17F	C5-O9-C17	5.73	127.99	118.29
8	A	1106	1AT	O1-C1-C2	5.67	124.20	108.42
7	E	2001	CLR	C7-C8-C9	5.62	116.22	109.72
8	A	1106	1AT	O2-C2-C1	5.56	123.32	110.08
7	A	1105	CLR	C10-C5-C6	-5.44	114.98	122.93
9	A	1107	1DS	O2-C2-C3	5.42	123.16	110.38
10	B	1005	17F	O9-C17-C18	5.29	122.92	111.48
8	A	1106	1AT	O1-C2'-C3'	5.23	124.10	108.20
7	C	2005	CLR	C7-C8-C14	5.17	118.26	110.93
7	A	1105	CLR	C19-C10-C9	-5.17	105.86	111.66
7	C	2005	CLR	C17-C13-C14	5.15	106.01	100.10
7	C	2005	CLR	C1-C10-C9	4.99	115.33	108.74
7	G	1001	CLR	C19-C10-C9	-4.95	106.10	111.66
10	D	2004	17F	C5-O9-C17	4.88	129.47	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1001	CLR	C21-C20-C17	4.83	120.13	112.88
7	E	2001	CLR	C21-C20-C17	4.67	119.90	112.88
7	E	2001	CLR	C19-C10-C9	-4.61	106.48	111.66
9	A	1107	1DS	C2'-O1-C1	4.60	129.52	117.29
10	D	2004	17F	O9-C17-C18	4.55	121.33	111.48
7	A	1105	CLR	C1-C10-C9	4.55	114.75	108.74
6	C	2004	OBN	O5'-C5'-C4'	4.51	117.68	109.55
7	E	2001	CLR	C1-C10-C9	4.40	114.56	108.74
7	E	2001	CLR	C7-C8-C14	4.27	116.98	110.93
7	G	1001	CLR	C7-C8-C14	4.25	116.95	110.93
7	G	1001	CLR	C1-C10-C9	4.22	114.33	108.74
9	A	1107	1DS	O1-C2'-C3'	4.22	121.04	108.20
8	A	1106	1AT	O6-C1N-C2N	4.18	124.58	111.83
7	A	1105	CLR	C19-C10-C1	-4.18	103.08	109.43
10	B	1005	17F	O3-C1-C2	4.09	111.62	108.06
8	A	1106	1AT	C1'-C2'-C3'	-4.01	103.04	114.83
10	G	1002	17F	C6-O7-C7	3.89	131.33	117.12
6	C	2004	OBN	C6-C5-C4	-3.80	107.20	111.15
7	A	1105	CLR	C7-C8-C14	3.77	116.27	110.93
7	C	2005	CLR	C19-C10-C1	-3.74	103.74	109.43
9	A	1107	1DS	O2'-C2'-C3'	-3.71	97.97	105.42
10	G	1002	17F	O9-C17-O10	-3.70	115.85	122.99
6	C	2004	OBN	C1'-O3-C3	3.68	122.14	114.84
6	A	1104	OBN	C1'-O3-C3	3.50	121.78	114.84
7	C	2005	CLR	C11-C9-C10	3.50	117.40	113.08
6	A	1104	OBN	C6-C5-C4	-3.49	107.52	111.15
7	C	2005	CLR	C21-C20-C22	-3.48	104.95	110.34
6	A	1104	OBN	C1'-O5'-C5'	3.47	119.55	113.63
7	E	2001	CLR	C17-C13-C14	3.47	104.08	100.10
6	C	2004	OBN	C1'-O5'-C5'	3.46	119.53	113.63
7	G	1001	CLR	C17-C13-C14	3.41	104.01	100.10
10	B	1005	17F	O9-C5-C4	3.39	114.02	106.21
10	G	1002	17F	O5-C3-O4	-3.39	116.38	124.08
6	A	1104	OBN	O5'-C5'-C4'	3.37	115.62	109.55
7	C	2005	CLR	C21-C20-C17	3.37	117.94	112.88
10	A	1108	17F	O10-C17-C18	-3.36	112.86	124.77
7	A	1105	CLR	C21-C20-C17	3.34	117.89	112.88
8	A	1106	1AT	O2'-C2'-C1'	3.29	115.95	107.94
10	A	1109	17F	O10-C17-C18	-3.28	113.16	124.77
8	A	1106	1AT	O5-C5-C6	3.24	113.12	106.69
9	A	1107	1DS	O5-C5-C6	3.24	114.46	106.44
10	A	1108	17F	O9-C5-C4	3.23	113.65	106.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	2004	17F	O10-C17-C18	-3.23	111.16	123.78
9	A	1107	1DS	O3'-C3'-C4'	-3.19	102.00	113.25
10	G	1002	17F	O9-C17-C18	3.17	116.75	111.09
6	A	1104	OBN	C15-C14-C13	3.17	105.74	103.37
7	E	2001	CLR	C21-C20-C22	-3.17	105.44	110.34
6	C	2004	OBN	C16-C17-C13	3.05	108.27	105.01
9	A	1107	1DS	C2'-C3'-C4'	3.01	108.89	102.19
7	A	1105	CLR	C3-C4-C5	3.00	116.83	112.05
10	A	1109	17F	O9-C5-C4	3.00	113.11	106.21
7	A	1105	CLR	C2-C3-C4	2.99	114.49	110.29
7	E	2001	CLR	C16-C17-C13	-2.98	100.33	103.84
8	A	1106	1AT	O4'-C4'-C3'	2.98	121.08	112.16
9	A	1107	1DS	O3-C3-C2	2.97	117.38	110.38
6	C	2004	OBN	C17-C20-C22	-2.96	121.03	128.83
6	A	1104	OBN	C6-C7-C8	-2.92	108.18	113.14
7	G	1001	CLR	C21-C20-C22	-2.91	105.83	110.34
6	A	1104	OBN	C17-C20-C22	-2.89	121.23	128.83
6	A	1104	OBN	O5'-C5'-C6'	2.88	113.12	106.74
6	A	1104	OBN	C16-C17-C13	2.85	108.06	105.01
6	C	2004	OBN	C15-C14-C13	2.84	105.49	103.37
6	C	2004	OBN	C7-C6-C5	-2.84	109.38	112.72
6	A	1104	OBN	C7-C6-C5	-2.83	109.39	112.72
7	G	1001	CLR	C1-C2-C3	2.81	114.21	110.48
9	A	1107	1DS	C1-C2-C3	-2.79	104.14	110.01
7	G	1001	CLR	C16-C17-C13	-2.74	100.61	103.84
6	A	1104	OBN	C5-C4-C3	-2.72	110.65	113.95
9	A	1107	1DS	O5-C1-O1	2.71	118.09	109.61
7	C	2005	CLR	C19-C10-C9	-2.71	108.62	111.66
10	D	2004	17F	O7-C7-O8	-2.70	116.89	123.63
9	A	1107	1DS	O2'-C5'-C6'	2.69	116.22	108.89
7	C	2005	CLR	C22-C20-C17	2.65	115.83	110.33
7	E	2001	CLR	C11-C12-C13	-2.65	108.27	112.74
9	A	1107	1DS	O4-C4-C5	2.65	115.85	109.32
10	D	2004	17F	O5-C3-O4	-2.64	118.10	124.08
6	A	1104	OBN	C18-C13-C12	-2.63	107.45	111.08
8	A	1106	1AT	C2'-C3'-C4'	2.62	108.04	102.19
8	A	1106	1AT	O1N-C1N-C2N	-2.62	113.53	123.78
6	C	2004	OBN	C6-C7-C8	-2.61	108.70	113.14
10	G	1002	17F	O7-C7-C8	2.61	119.79	111.83
7	A	1105	CLR	C11-C9-C10	2.58	116.27	113.08
10	G	1002	17F	O9-C5-C6	-2.56	99.15	108.34
10	B	1005	17F	C19-C18-C17	2.54	123.00	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	2004	17F	O7-C7-C8	2.51	119.50	111.83
6	C	2004	OBN	C6'-C5'-C4'	-2.51	108.49	113.08
7	E	2001	CLR	C2-C1-C10	2.50	118.11	112.78
7	G	1001	CLR	C11-C12-C13	-2.48	108.56	112.74
8	A	1106	1AT	O1-C2'-O2'	-2.47	103.21	110.47
7	G	1001	CLR	C2-C1-C10	2.47	118.04	112.78
11	E	2002	CE1	C17-O16-C15	2.46	124.03	113.26
6	C	2004	OBN	C21-C20-C22	2.42	113.68	108.48
6	C	2004	OBN	C18-C13-C12	-2.42	107.74	111.08
11	A	1110	CE1	C20-O19-C18	2.40	123.78	113.26
7	E	2001	CLR	C1-C2-C3	2.40	113.67	110.48
7	E	2001	CLR	C4-C5-C10	-2.38	113.37	116.42
10	A	1109	17F	O9-C5-C6	2.37	113.27	107.96
9	A	1107	1DS	O2'-C2'-C1'	2.36	112.71	107.78
7	A	1105	CLR	C18-C13-C17	2.35	115.94	111.68
7	A	1105	CLR	C17-C13-C14	2.34	102.79	100.10
6	C	2004	OBN	O11-C11-C9	2.34	116.61	111.29
6	A	1104	OBN	C21-C20-C22	2.34	113.49	108.48
10	B	1005	17F	C6-C5-C4	-2.31	106.19	112.69
7	G	1001	CLR	C11-C9-C8	2.30	114.99	111.78
7	A	1105	CLR	C12-C11-C9	2.28	117.02	113.14
6	A	1104	OBN	C6-C5-C10	2.25	113.80	111.16
7	C	2005	CLR	C12-C11-C9	2.24	116.94	113.14
11	E	2002	CE1	C20-O19-C18	2.22	122.99	113.26
7	A	1105	CLR	C4-C5-C10	2.22	119.26	116.42
6	C	2004	OBN	C5-C4-C3	-2.22	111.27	113.95
6	C	2004	OBN	C4-C5-C10	2.20	114.32	111.63
6	C	2004	OBN	C6-C5-C10	2.18	113.72	111.16
7	E	2001	CLR	C19-C10-C1	-2.18	106.12	109.43
8	A	1106	1AT	C1-O5-C5	-2.18	109.47	113.72
10	B	1005	17F	O9-C5-C6	2.17	112.83	107.96
10	D	2004	17F	O2-P1-O1	-2.17	102.34	112.44
6	A	1104	OBN	O11-C11-C9	2.17	116.23	111.29
10	B	1005	17F	O9-C17-O10	-2.15	118.68	123.70
7	C	2005	CLR	C2-C1-C10	2.15	117.36	112.78
7	C	2005	CLR	C15-C14-C8	2.15	122.53	119.10
7	G	1001	CLR	C19-C10-C1	-2.13	106.19	109.43
10	D	2004	17F	O7-C6-C5	2.13	114.54	108.40
7	E	2001	CLR	C11-C9-C8	2.13	114.75	111.78
7	C	2005	CLR	C3-C4-C5	-2.12	108.68	112.05
6	A	1104	OBN	O23-C23-C22	-2.11	126.66	130.80
7	E	2001	CLR	C15-C14-C13	-2.07	101.40	103.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1001	CLR	C3-C4-C5	-2.07	108.75	112.05
6	A	1104	OBN	O5-C5-C10	-2.07	106.42	109.60
6	C	2004	OBN	O23-C23-C22	-2.06	126.75	130.80
7	E	2001	CLR	C3-C4-C5	-2.04	108.80	112.05
8	A	1106	1AT	C2-C3-C4	-2.04	107.25	110.83
7	A	1105	CLR	C14-C8-C9	-2.03	106.43	109.09
8	A	1106	1AT	O6'-C6'-C5'	-2.02	104.45	111.33
6	C	2004	OBN	O5-C5-C10	-2.02	106.48	109.60
7	G	1001	CLR	C4-C5-C10	-2.01	113.85	116.42

There are no chirality outliers.

All (167) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1104	OBN	C1-C10-C19-O19
6	A	1104	OBN	C5-C10-C19-O19
6	A	1104	OBN	C9-C10-C19-O19
6	C	2004	OBN	C1-C10-C19-O19
6	C	2004	OBN	C5-C10-C19-O19
8	A	1106	1AT	O1'-C1'-C2'-O1
8	A	1106	1AT	O1'-C1'-C2'-C3'
9	A	1107	1DS	O1'-C1'-C2'-O1
9	A	1107	1DS	O1'-C1'-C2'-C3'
9	A	1107	1DS	O1'-C1'-C2'-O2'
10	A	1108	17F	O3-C1-C2-N1
10	A	1108	17F	C4-O6-P1-O1
10	A	1108	17F	C4-O6-P1-O2
10	A	1108	17F	C4-O6-P1-O3
10	A	1108	17F	C1-C2-C3-O4
10	A	1108	17F	C1-C2-C3-O5
10	A	1108	17F	O6-C4-C5-C6
10	A	1108	17F	O6-C4-C5-O9
10	A	1108	17F	O10-C17-O9-C5
10	A	1108	17F	C18-C17-O9-C5
10	A	1109	17F	O3-C1-C2-N1
10	A	1109	17F	O3-C1-C2-C3
10	A	1109	17F	C1-O3-P1-O1
10	A	1109	17F	C1-O3-P1-O2
10	A	1109	17F	C1-O3-P1-O6
10	A	1109	17F	C4-O6-P1-O2
10	A	1109	17F	C4-O6-P1-O3
10	A	1109	17F	N1-C2-C3-O4

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Mol	Chain	Res	Type	Atoms
10	A	1109	17F	O6-C4-C5-O9
10	A	1109	17F	C5-C4-O6-P1
10	A	1109	17F	C6-C5-O9-C17
10	A	1109	17F	O10-C17-O9-C5
10	A	1109	17F	C18-C17-O9-C5
10	B	1005	17F	O3-C1-C2-N1
10	B	1005	17F	O3-C1-C2-C3
10	B	1005	17F	C1-O3-P1-O1
10	B	1005	17F	C1-O3-P1-O2
10	B	1005	17F	C1-O3-P1-O6
10	B	1005	17F	C4-O6-P1-O1
10	B	1005	17F	C1-C2-C3-O4
10	B	1005	17F	C1-C2-C3-O5
10	B	1005	17F	N1-C2-C3-O4
10	B	1005	17F	O6-C4-C5-C6
10	B	1005	17F	C6-C5-O9-C17
10	B	1005	17F	C18-C17-O9-C5
10	G	1002	17F	C2-C1-O3-P1
10	G	1002	17F	C4-O6-P1-O2
10	G	1002	17F	C4-O6-P1-O3
10	D	2004	17F	C4-O6-P1-O1
10	D	2004	17F	C1-C2-C3-O4
10	D	2004	17F	C1-C2-C3-O5
10	D	2004	17F	N1-C2-C3-O4
10	G	1002	17F	O10-C17-O9-C5
10	G	1002	17F	C18-C17-O9-C5
6	A	1104	OBN	O5'-C1'-O3-C3
6	C	2004	OBN	O5'-C1'-O3-C3
10	B	1005	17F	O10-C17-O9-C5
11	E	2002	CE1	C15-C14-O13-C12
11	A	1110	CE1	C24-C23-O22-C21
7	A	1105	CLR	C21-C20-C22-C23
10	D	2004	17F	O10-C17-O9-C5
12	D	2001	NAG	O5-C5-C6-O6
12	D	2003	NAG	O5-C5-C6-O6
12	D	2001	NAG	C4-C5-C6-O6
12	B	1004	NAG	O5-C5-C6-O6
11	A	1110	CE1	O25-C26-C27-O28
8	A	1106	1AT	C4-C5-C6-O6
11	A	1110	CE1	O19-C20-C21-O22
10	D	2004	17F	N1-C2-C3-O5
7	A	1105	CLR	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
12	D	2003	NAG	C4-C5-C6-O6
8	A	1106	1AT	O5-C5-C6-O6
12	D	2002	NAG	O5-C5-C6-O6
7	A	1105	CLR	C13-C17-C20-C21
11	A	1110	CE1	C18-C17-O16-C15
7	A	1105	CLR	C17-C20-C22-C23
12	B	1004	NAG	C4-C5-C6-O6
7	G	1001	CLR	C21-C20-C22-C23
7	E	2001	CLR	C21-C20-C22-C23
12	B	1004	NAG	C8-C7-N2-C2
12	B	1004	NAG	O7-C7-N2-C2
12	D	2002	NAG	C8-C7-N2-C2
12	D	2002	NAG	O7-C7-N2-C2
12	D	2003	NAG	C8-C7-N2-C2
12	D	2003	NAG	O7-C7-N2-C2
7	A	1105	CLR	C13-C17-C20-C22
10	A	1109	17F	N1-C2-C3-O5
10	B	1005	17F	N1-C2-C3-O5
9	A	1107	1DS	C1N-C2N-C3N-C4N
7	A	1105	CLR	C16-C17-C20-C22
10	B	1005	17F	C17-C18-C19-C20
8	A	1106	1AT	O1'-C1'-C2'-O2'
7	C	2005	CLR	C22-C23-C24-C25
10	D	2004	17F	C18-C17-O9-C5
10	B	1005	17F	C18-C19-C20-C1Y
6	C	2004	OBN	C9-C10-C19-O19
8	A	1106	1AT	C2N-C3N-C4N-C5N
7	A	1105	CLR	C20-C22-C23-C24
7	G	1001	CLR	C20-C22-C23-C24
7	G	1001	CLR	C23-C24-C25-C26
7	E	2001	CLR	C20-C22-C23-C24
7	E	2001	CLR	C23-C24-C25-C26
9	A	1107	1DS	O1N-C1N-O1'-C1'
7	A	1105	CLR	C23-C24-C25-C27
11	E	2002	CE1	O19-C20-C21-O22
10	D	2004	17F	O8-C7-O7-C6
7	A	1105	CLR	C23-C24-C25-C26
11	A	1110	CE1	C5-C6-C7-C8
11	E	2002	CE1	O16-C17-C18-O19
10	A	1108	17F	O3-C1-C2-C3
10	D	2004	17F	O9-C5-C6-O7
11	E	2002	CE1	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
10	D	2004	17F	C11-C10-C9-C8
11	A	1110	CE1	C2-C3-C4-C5
10	D	2004	17F	C4-C5-C6-O7
11	A	1110	CE1	C9-C10-C11-C12
12	D	2002	NAG	C4-C5-C6-O6
9	A	1107	1DS	O5-C5-C6-O6
10	B	1005	17F	C20-C1Y-C1Z-C31
10	B	1005	17F	C1Y-C1Z-C31-C32
11	A	1110	CE1	C11-C10-C9-C8
9	A	1107	1DS	C2N-C1N-O1'-C1'
11	E	2002	CE1	C2-C3-C4-C5
11	E	2002	CE1	C1-C2-C3-C4
11	A	1110	CE1	O16-C17-C18-O19
10	G	1002	17F	O6-C4-C5-C6
10	A	1109	17F	O6-C4-C5-C6
11	A	1110	CE1	C1-C2-C3-C4
11	A	1110	CE1	C3-C4-C5-C6
10	B	1005	17F	O6-C4-C5-O9
11	A	1110	CE1	C21-C20-O19-C18
7	C	2005	CLR	C23-C24-C25-C26
7	C	2005	CLR	C23-C24-C25-C27
7	E	2001	CLR	C23-C24-C25-C27
7	G	1001	CLR	C23-C24-C25-C27
7	C	2005	CLR	C13-C17-C20-C22
11	E	2002	CE1	C21-C20-O19-C18
10	D	2004	17F	C6-C5-O9-C17
11	E	2002	CE1	C11-C10-C9-C8
7	C	2005	CLR	C21-C20-C22-C23
10	D	2004	17F	C2-C1-O3-P1
7	C	2005	CLR	C13-C17-C20-C21
10	G	1002	17F	O6-C4-C5-O9
10	D	2004	17F	O6-C4-C5-O9
8	A	1106	1AT	C4'-C5'-C6'-O6'
10	A	1109	17F	C4-O6-P1-O1
10	G	1002	17F	C1-C2-C3-O5
10	D	2004	17F	C1-O3-P1-O1
10	D	2004	17F	C4-O6-P1-O3
11	E	2002	CE1	C17-C18-O19-C20
11	A	1110	CE1	C27-C26-O25-C24
11	E	2002	CE1	C3-C4-C5-C6
11	E	2002	CE1	C11-C12-O13-C14
11	E	2002	CE1	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
7	C	2005	CLR	C16-C17-C20-C22
8	A	1106	1AT	O2'-C5'-C6'-O6'
11	A	1110	CE1	O28-C29-C30-O31
10	G	1002	17F	N1-C2-C3-O5
11	A	1110	CE1	C6-C7-C8-C9
10	B	1005	17F	O9-C17-C18-C19
11	E	2002	CE1	C6-C7-C8-C9
10	B	1005	17F	O10-C17-C18-C19
11	E	2002	CE1	O13-C14-C15-O16
10	D	2004	17F	O8-C7-C8-C9
11	A	1110	CE1	C23-C24-O25-C26
11	E	2002	CE1	C14-C15-O16-C17
10	A	1108	17F	N1-C2-C3-O5

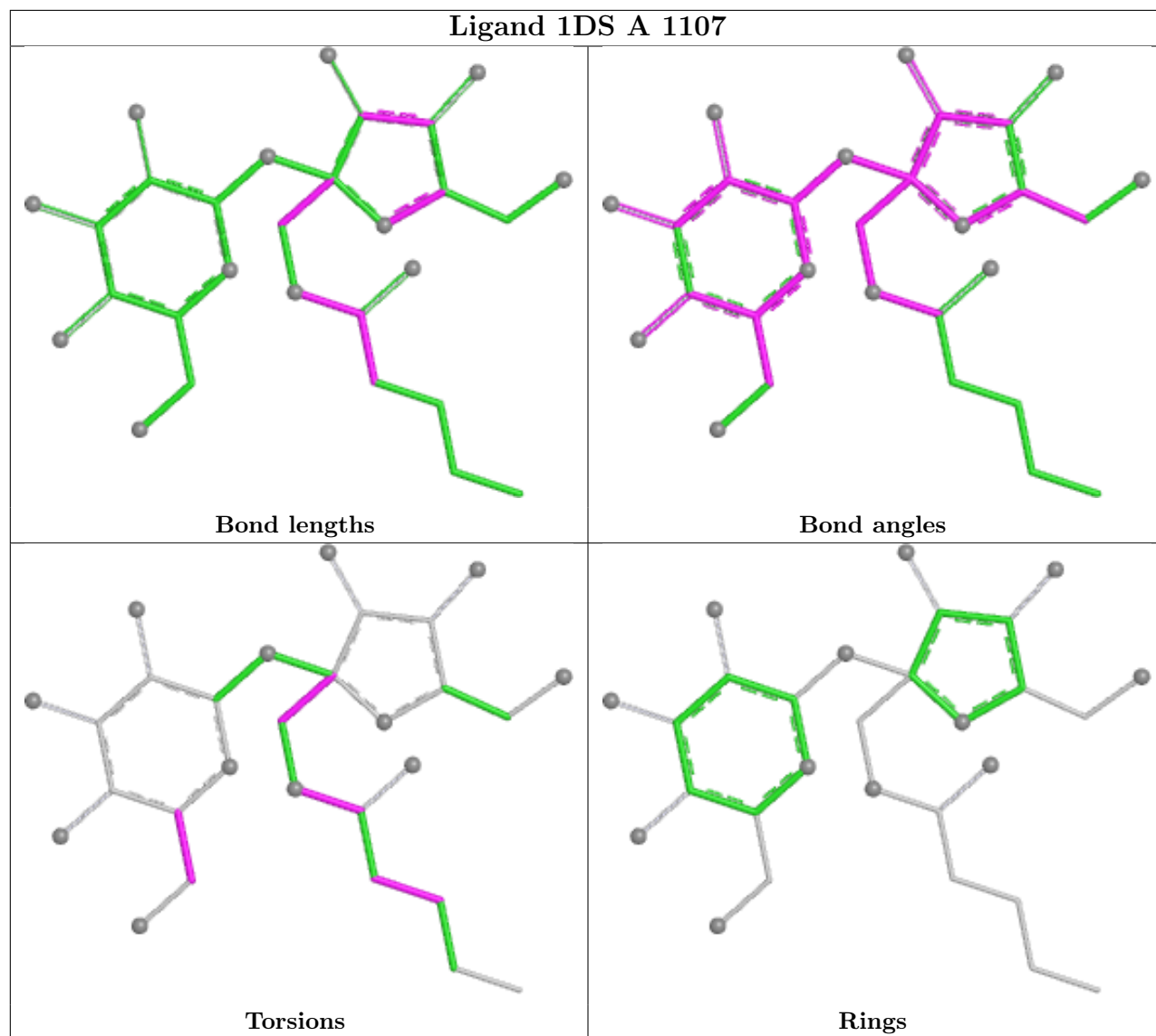
There are no ring outliers.

14 monomers are involved in 75 short contacts:

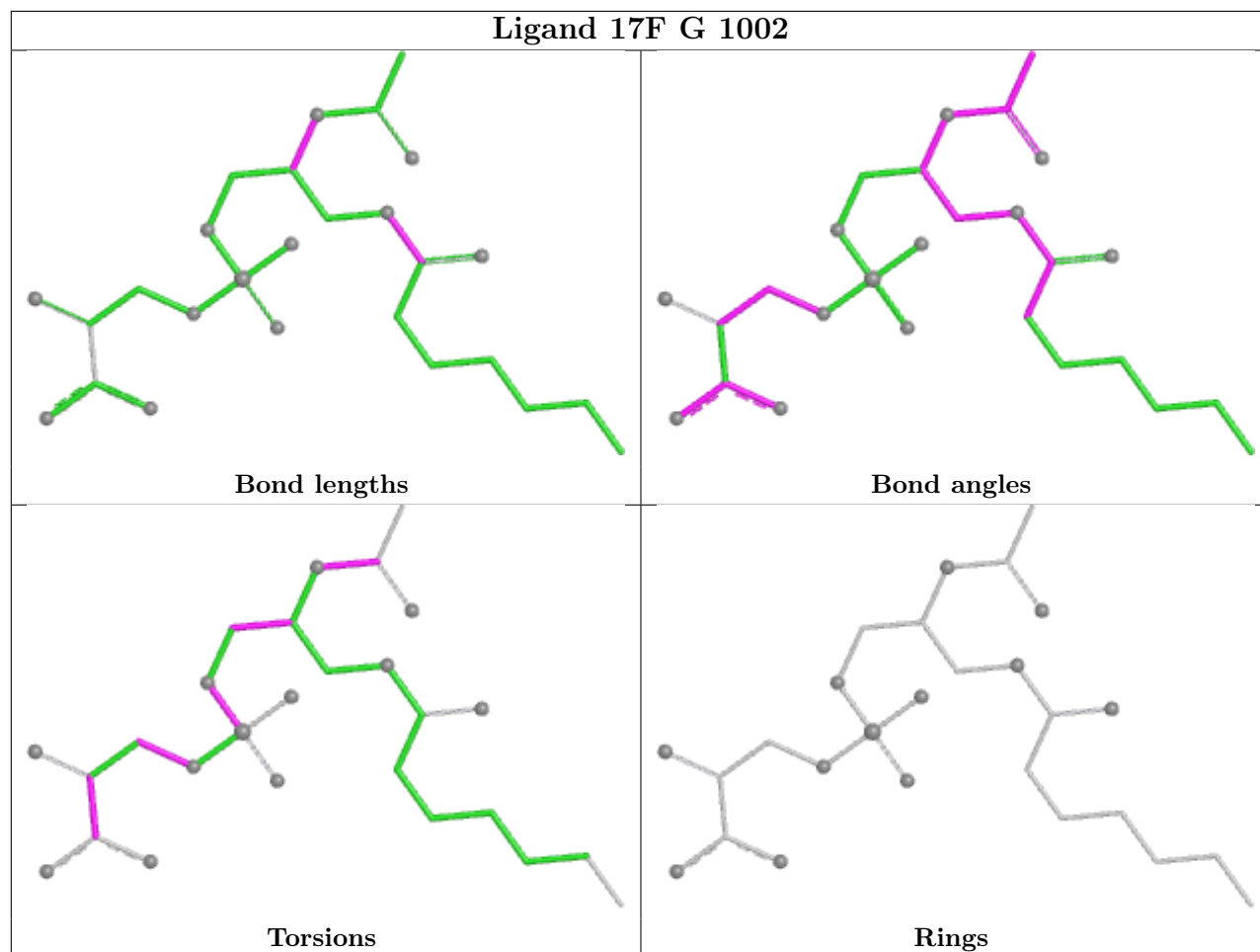
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1107	1DS	6	0
10	G	1002	17F	4	0
10	B	1005	17F	2	0
8	A	1106	1AT	6	0
6	C	2004	OBN	6	0
7	G	1001	CLR	4	0
7	C	2005	CLR	2	0
10	A	1109	17F	2	0
11	A	1110	CE1	18	0
6	A	1104	OBN	10	0
7	A	1105	CLR	5	0
10	A	1108	17F	6	0
7	E	2001	CLR	4	0
11	E	2002	CE1	1	0

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

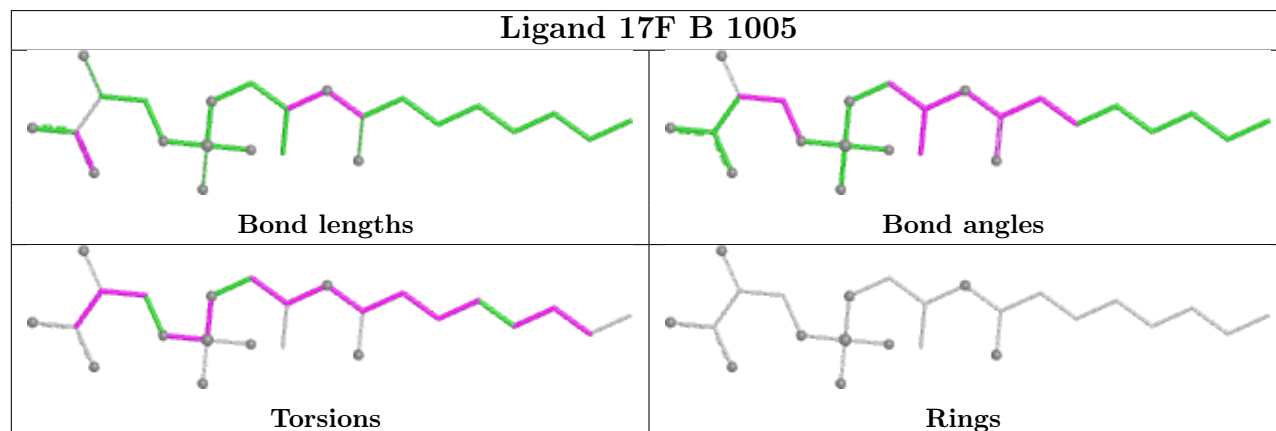
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

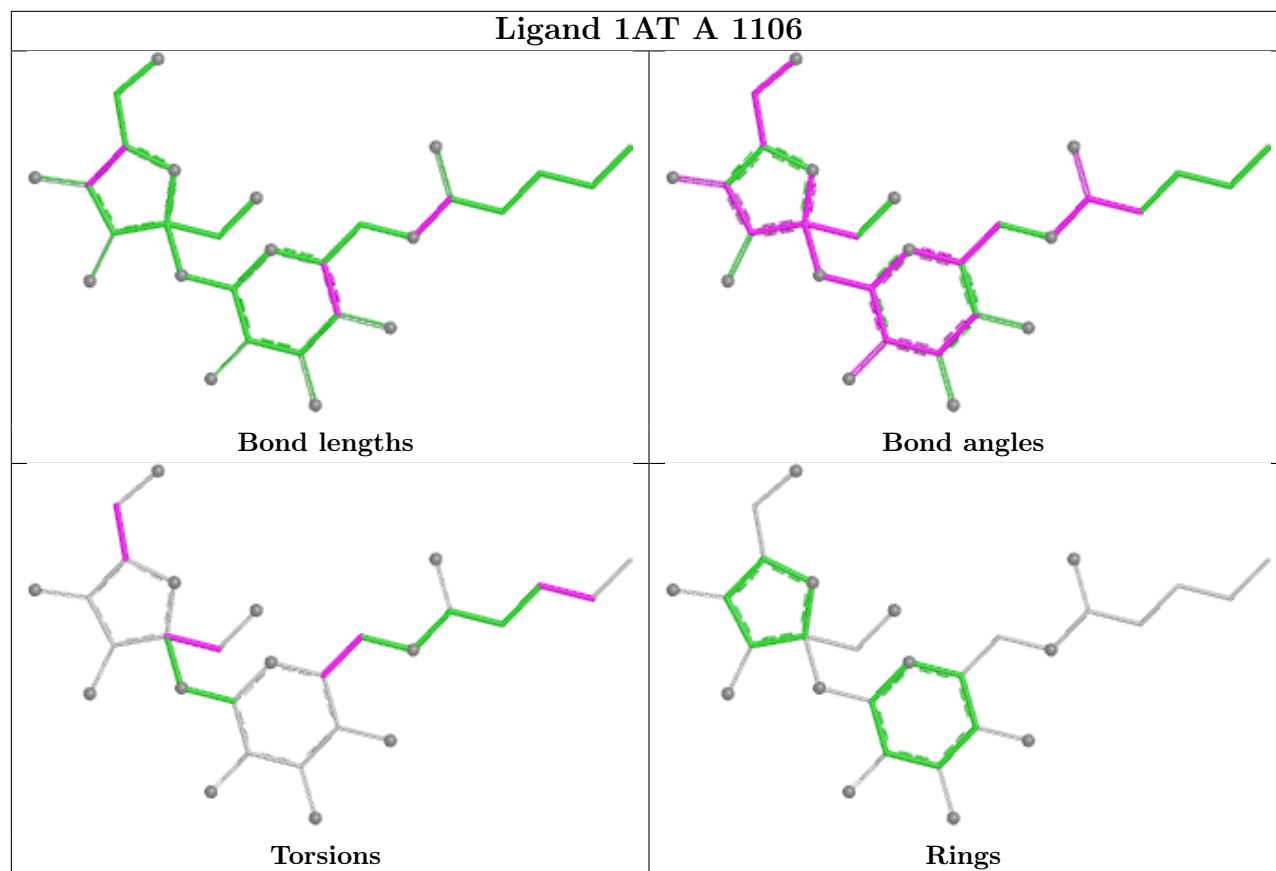


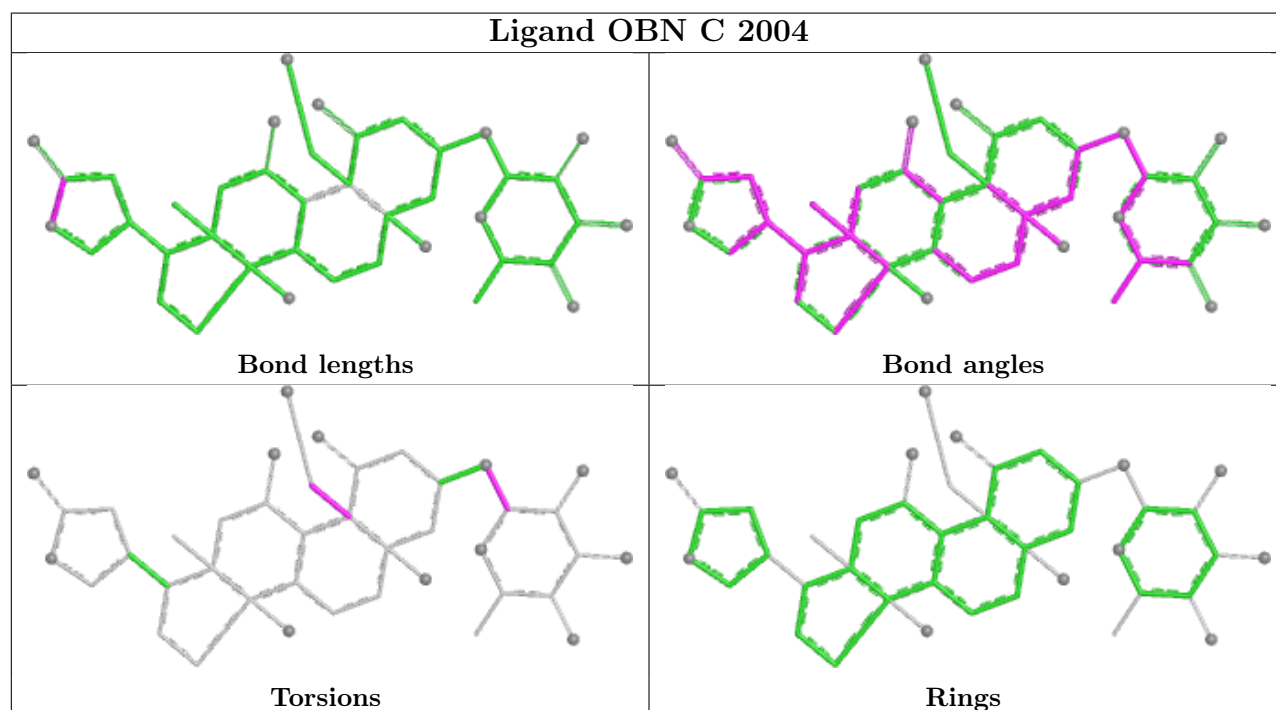
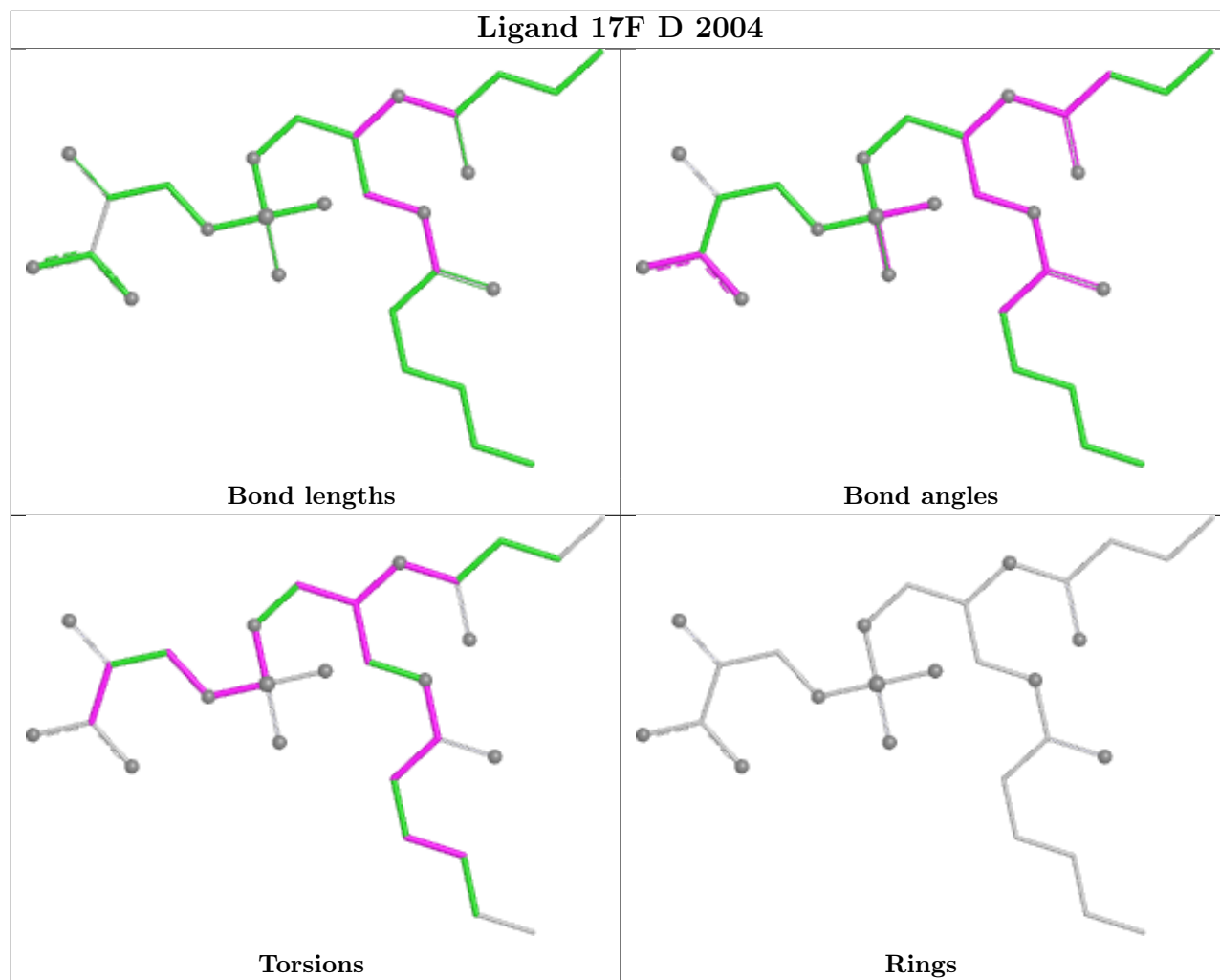
Ligand 17F G 1002

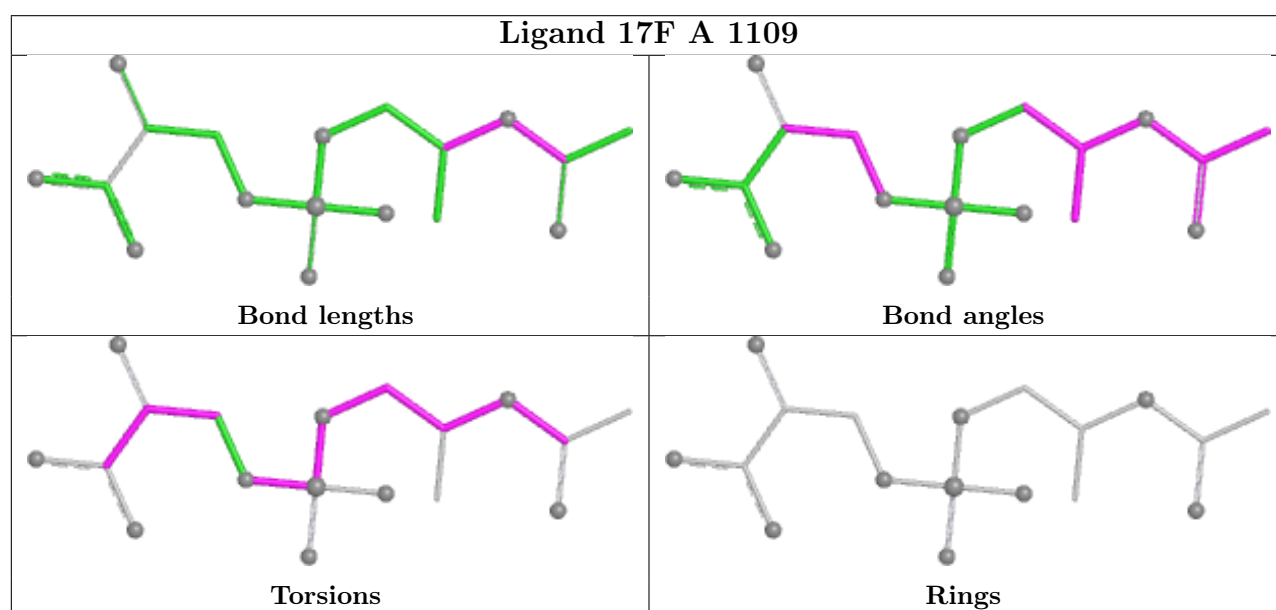
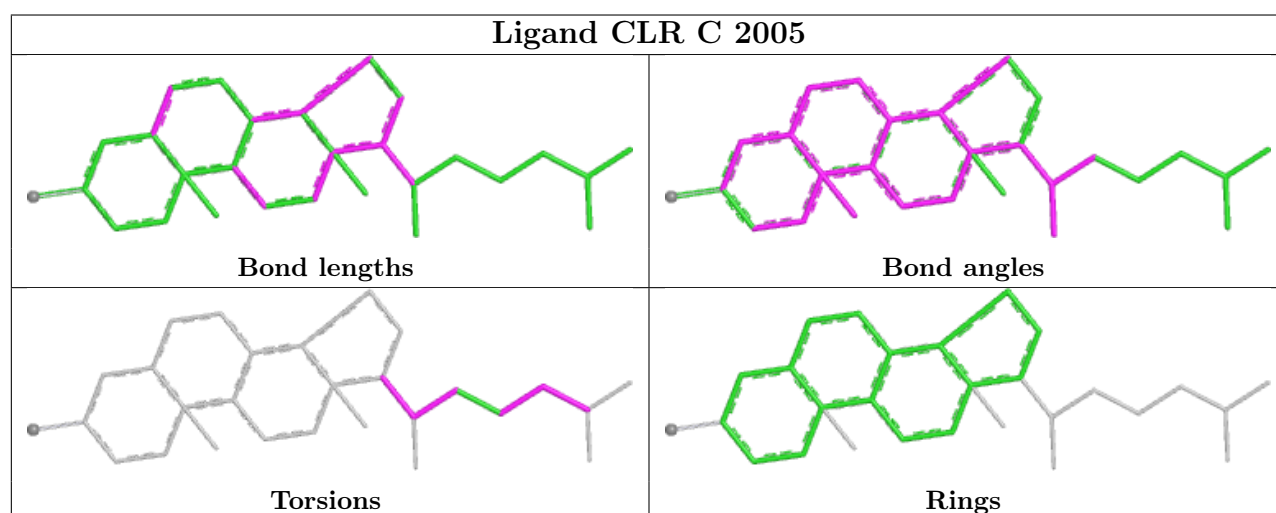
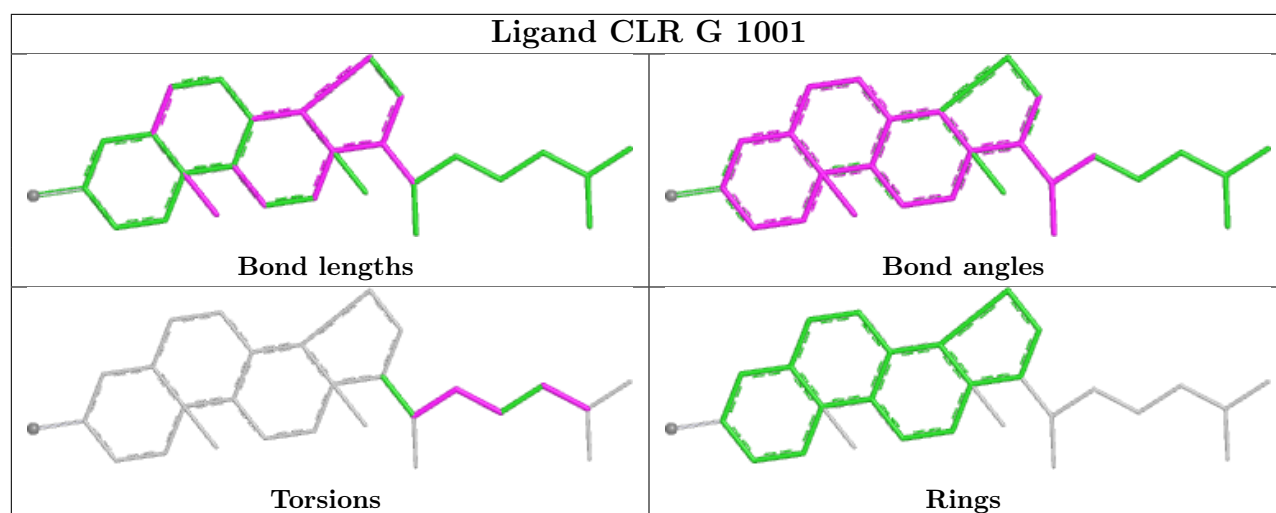


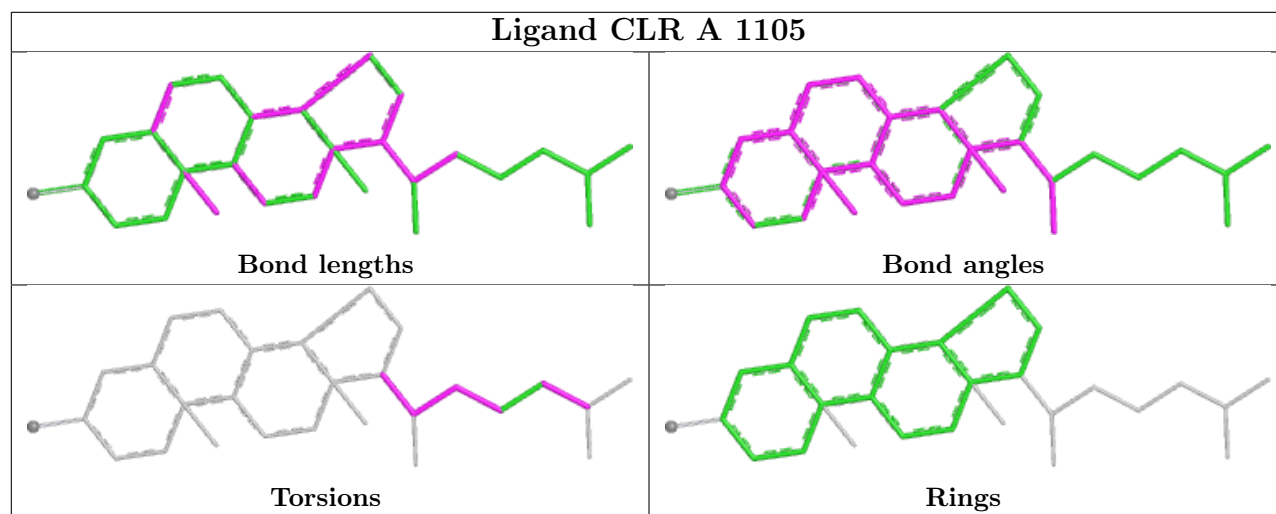
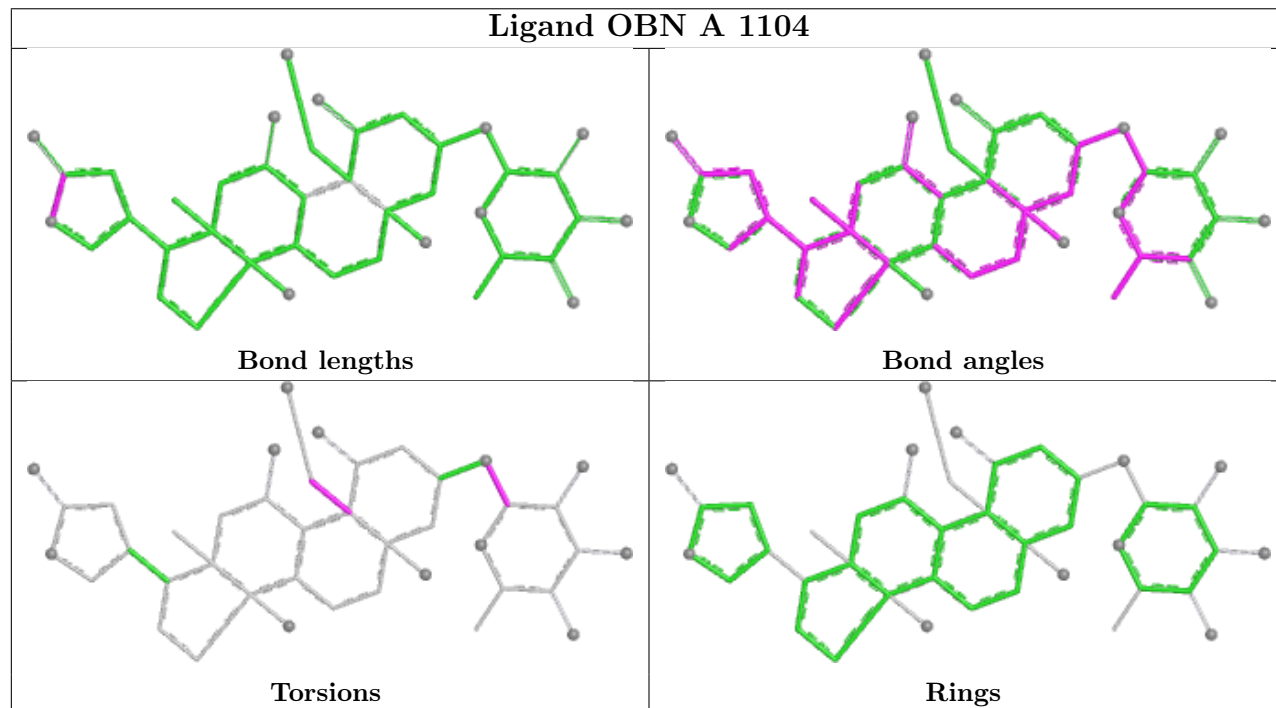
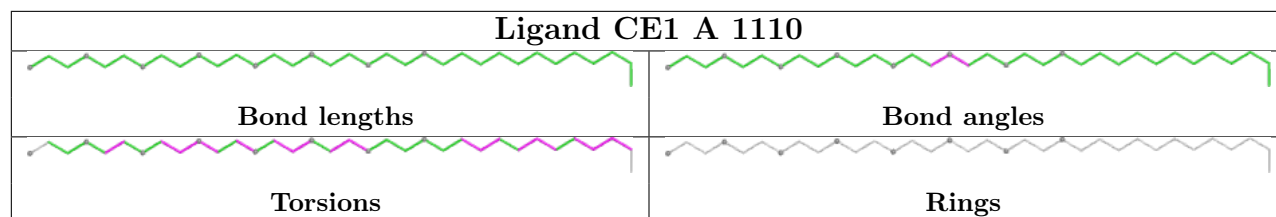
Ligand 17F B 1005

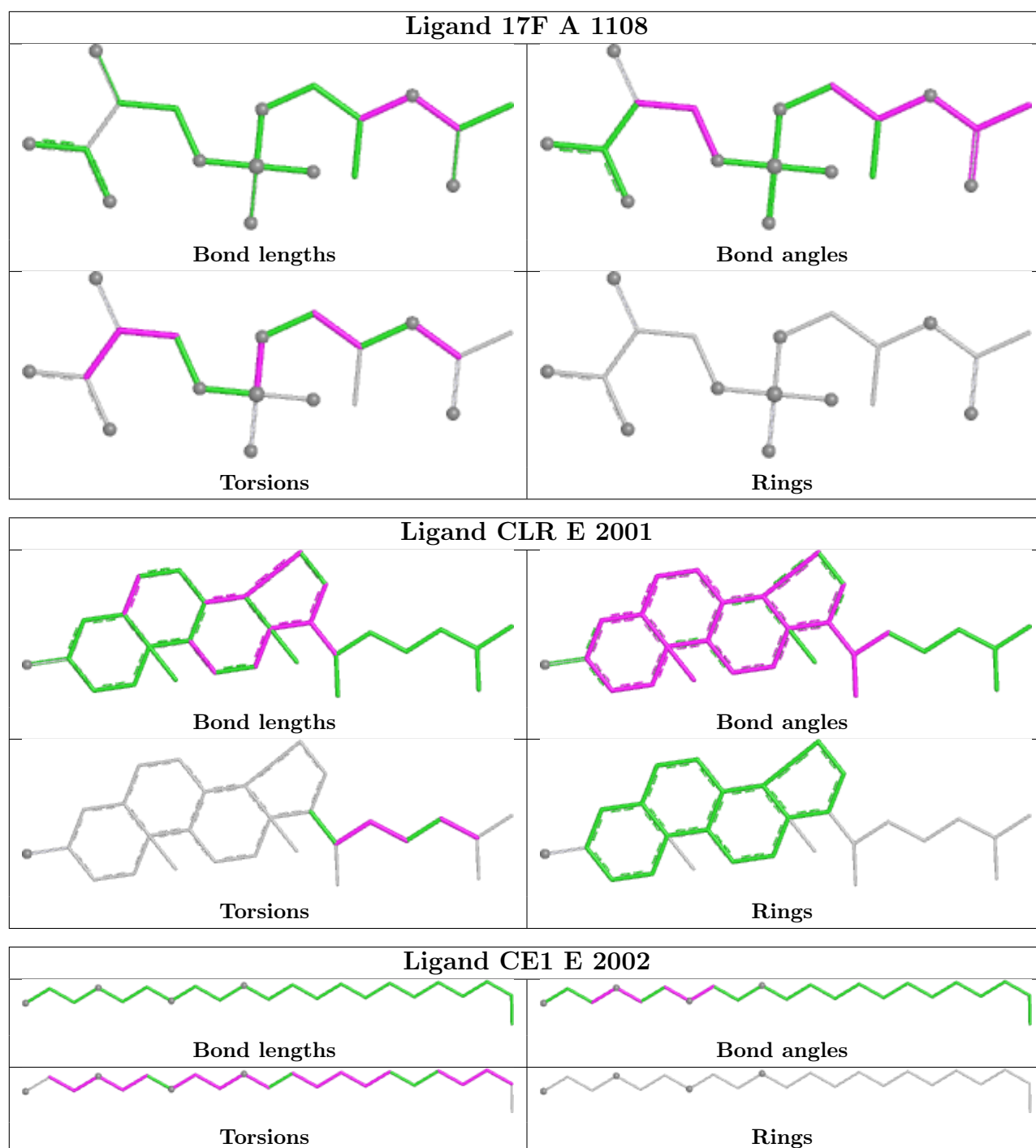












5.7 Other polymers [i](#)

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%)	0.08	35 (3%)	47	34	51, 91, 218, 288	0
1	C	995/1021 (97%)	0.37	73 (7%)	21	18	58, 126, 273, 342	0
2	B	289/303 (95%)	0.51	25 (8%)	16	14	67, 151, 221, 258	0
2	D	287/303 (94%)	0.63	24 (8%)	17	15	63, 136, 210, 241	0
3	E	32/65 (49%)	-0.45	0	100	100	72, 81, 120, 147	0
3	G	32/65 (49%)	-0.22	1 (3%)	51	38	64, 83, 134, 141	0
All	All	2630/2778 (94%)	0.29	158 (6%)	27	21	51, 116, 242, 342	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	218	ASP	10.1
2	D	217	ARG	9.7
1	A	480	LYS	7.0
1	C	539	GLY	6.9
1	C	489	PRO	6.6
1	C	491	THR	6.4
1	C	497	LEU	6.1
1	A	477	SER	5.6
1	C	468	THR	4.5
1	C	490	ASN	4.4
1	C	32	VAL	4.3
1	C	488	ASN	4.2
2	D	287	GLU	4.1
1	C	466	ARG	4.1
1	C	467	TYR	4.0
1	C	515	LEU	3.9
2	D	219	GLU	3.8
1	C	579	VAL	3.7
1	C	542	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	16	ILE	3.6
2	B	69	GLN	3.6
2	B	183	VAL	3.6
1	A	120	ASN	3.6
2	B	163	ASN	3.5
1	C	119	GLN	3.5
1	A	444	ALA	3.5
2	B	184	LEU	3.5
1	C	776	ASN	3.4
1	A	868	GLU	3.4
1	C	527	LEU	3.4
1	C	578	PHE	3.3
1	C	687	SER	3.3
1	C	22	GLU	3.3
1	C	68	ASP	3.3
1	C	541	LEU	3.3
2	D	23	GLU	3.3
2	B	61	ILE	3.2
2	D	288	LYS	3.2
1	A	537	GLU	3.2
1	A	566	THR	3.2
1	A	895	TYR	3.2
1	C	475	PHE	3.2
1	A	223	ASP	3.1
1	C	546	LEU	3.1
2	B	115	LEU	3.1
1	A	471	VAL	3.1
1	C	545	VAL	3.1
1	A	34	MET	3.1
1	C	416	ARG	3.1
2	D	87	GLU	3.1
2	B	267	THR	3.0
1	A	508	LEU	3.0
1	C	120	ASN	3.0
1	C	544	ARG	3.0
2	D	224	VAL	3.0
1	A	483	LEU	2.9
1	C	29	LYS	2.9
1	A	473	ILE	2.9
2	B	162	LEU	2.9
1	C	149	LYS	2.9
2	D	198	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	421	CYS	2.9
2	D	222	GLU	2.9
1	C	902	GLU	2.8
1	A	475	PHE	2.8
2	D	223	LYS	2.8
1	A	124	TYR	2.8
1	C	576	LEU	2.8
1	C	886	ARG	2.8
2	B	167	TYR	2.8
2	D	58	LEU	2.8
2	D	260	ALA	2.8
1	C	146	LYS	2.7
2	B	237	GLY	2.7
1	C	26	ASP	2.7
1	A	482	GLN	2.7
1	A	871	PHE	2.7
1	A	870	GLY	2.6
1	A	523	LEU	2.6
1	C	58	PRO	2.6
2	B	174	PRO	2.6
1	A	271	GLU	2.6
1	C	143	GLN	2.6
1	A	776	ASN	2.6
2	B	23	GLU	2.6
2	D	275	GLU	2.6
1	C	501	LYS	2.6
2	D	178	ILE	2.6
2	B	62	SER	2.6
1	C	549	CYS	2.5
1	C	644	PRO	2.5
1	C	423	ARG	2.5
1	C	28	LEU	2.5
1	C	550	HIS	2.5
2	B	218	ASP	2.5
2	D	196	LEU	2.5
2	B	68	TYR	2.5
2	B	268	MET	2.4
1	C	804	ASP	2.4
2	B	223	LYS	2.4
1	C	385	TRP	2.4
1	C	807	THR	2.4
2	D	296	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	896	GLY	2.4
1	A	470	ILE	2.4
1	A	572	PRO	2.4
2	B	169	TYR	2.4
1	A	435	ILE	2.4
2	B	79	GLN	2.4
1	C	954	GLU	2.4
1	A	82	TRP	2.4
1	C	74	THR	2.4
1	C	474	PRO	2.4
2	D	201	VAL	2.4
1	C	503	ALA	2.4
3	G	19	PHE	2.4
1	C	508	LEU	2.4
1	C	271	GLU	2.4
2	D	228	GLU	2.4
1	C	409	ALA	2.3
2	D	274	ILE	2.3
1	A	494	PRO	2.3
1	C	471	VAL	2.3
1	A	474	PRO	2.3
1	C	538	LEU	2.3
2	B	67	THR	2.3
2	D	162	LEU	2.3
1	C	514	ILE	2.2
1	C	518	GLY	2.2
2	D	202	MET	2.2
1	C	339	LEU	2.2
1	A	544	ARG	2.2
1	A	869	ASN	2.2
1	A	144	GLU	2.2
1	C	639	ALA	2.2
1	C	535	TYR	2.2
1	C	757	GLU	2.2
1	A	86	CYS	2.2
2	B	199	TYR	2.2
1	C	582	ILE	2.2
2	B	248	LYS	2.2
1	C	652	ASP	2.2
1	A	579	VAL	2.1
1	C	267	ALA	2.1
1	C	328	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	290	ARG	2.1
1	C	708	THR	2.1
1	C	972	ARG	2.1
1	A	154	PHE	2.1
2	B	31	SER	2.1
1	C	504	PRO	2.1
1	C	643	ILE	2.0
1	C	419	GLY	2.0
1	C	840	GLU	2.0
2	B	222	GLU	2.0
1	C	154	PHE	2.0
2	D	79	GLN	2.0
1	C	648	VAL	2.0

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

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

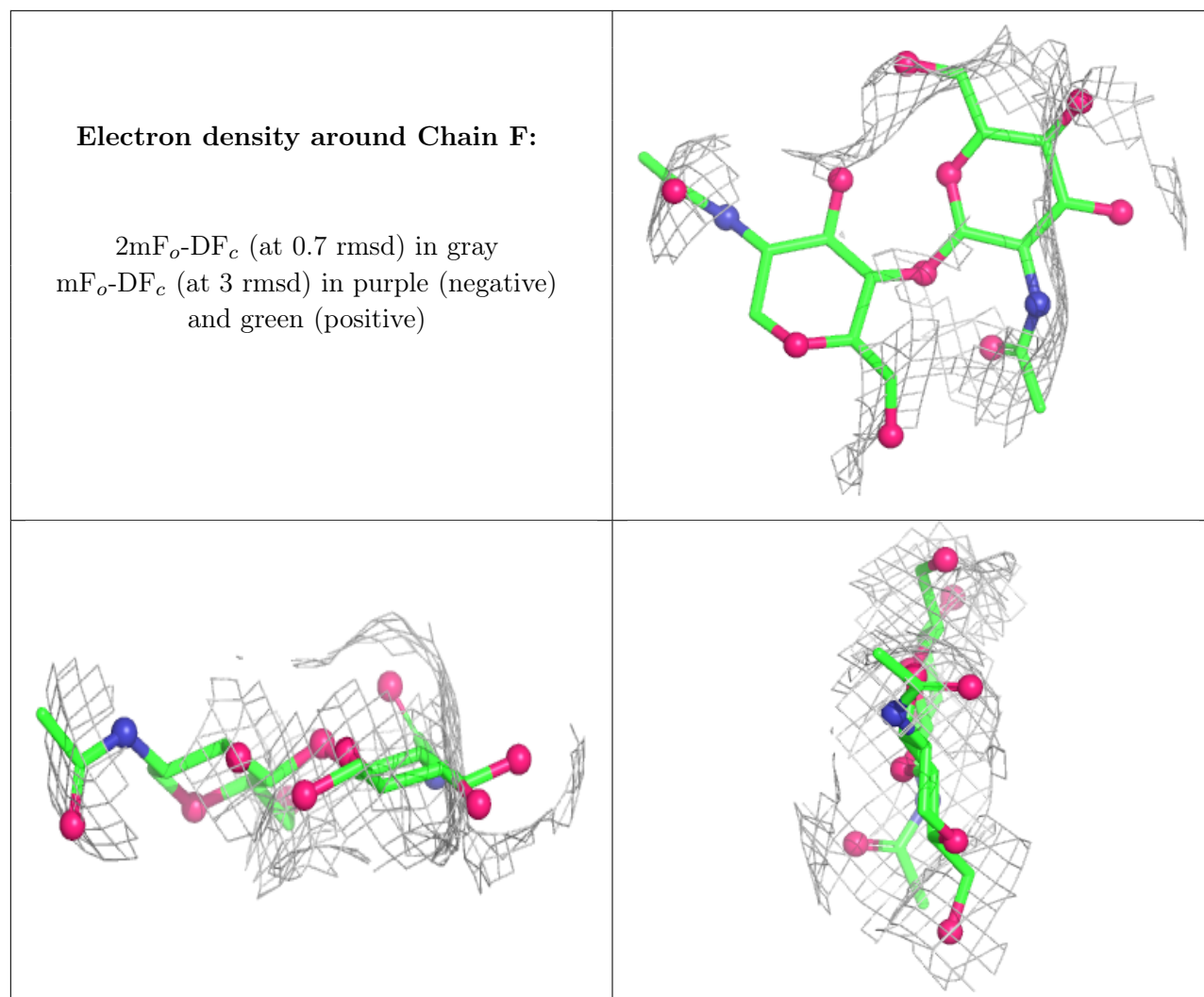
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PHD	C	369	12/13	0.97	0.05	107,112,123,124	0
1	PHD	A	369	12/13	0.98	0.05	66,71,74,75	0

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	-	-	179,192,203,207	0
4	NAG	F	2	14/15	-	-	205,218,224,229	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($\text{\AA}^2$)	Q<0.9
12	NAG	D	2003	14/15	0.44	0.12	191,198,211,218	0
12	NAG	B	1004	14/15	0.48	0.13	199,203,212,213	0
12	NAG	B	1003	14/15	0.54	0.12	197,209,221,225	0
12	NAG	D	2001	14/15	0.57	0.11	138,159,173,175	0
12	NAG	D	2002	14/15	0.69	0.10	142,150,163,169	0
10	17F	B	1005	24/54	0.76	0.18	74,128,199,208	0
10	17F	A	1108	18/54	0.77	0.23	80,155,188,197	0
10	17F	A	1109	18/54	0.77	0.18	96,114,166,169	0
10	17F	D	2004	28/54	0.79	0.21	154,172,243,246	0

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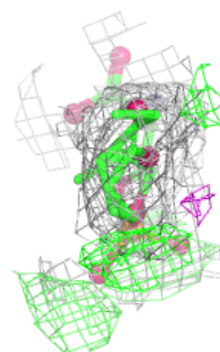
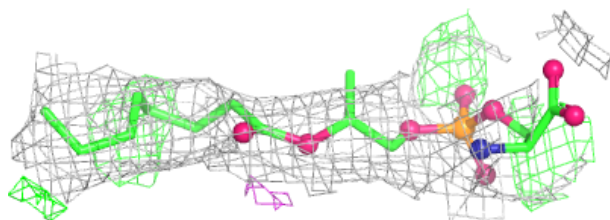
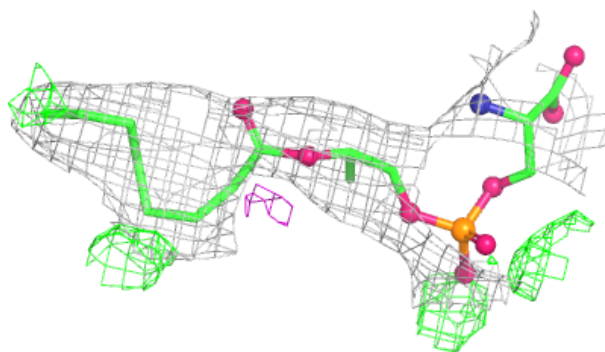
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	17F	G	1002	27/54	0.79	0.26	83,124,256,258	0
5	MG	C	2002	1/1	0.86	0.27	124,124,124,124	0
11	CE1	A	1110	34/37	0.87	0.14	79,110,144,146	0
7	CLR	C	2005	28/28	0.87	0.26	93,104,113,231	0
5	MG	A	1102	1/1	0.87	0.27	82,82,82,82	0
6	OBN	C	2004	41/41	0.91	0.11	84,92,99,104	0
11	CE1	E	2002	22/37	0.92	0.22	67,109,155,157	0
8	1AT	A	1106	29/34	0.92	0.11	85,99,116,118	0
9	1DS	A	1107	29/34	0.92	0.12	56,123,141,170	0
7	CLR	A	1105	28/28	0.94	0.21	74,112,143,159	0
6	OBN	A	1104	41/41	0.94	0.10	72,81,85,88	0
7	CLR	E	2001	28/28	0.98	0.11	64,71,73,73	0
5	MG	A	1101	1/1	0.98	0.04	113,113,113,113	0
5	MG	C	2003	1/1	0.98	0.06	81,81,81,81	0
7	CLR	G	1001	28/28	0.98	0.08	57,66,79,83	0
5	MG	C	2001	1/1	0.98	0.04	147,147,147,147	0
5	MG	A	1103	1/1	0.99	0.04	58,58,58,58	0

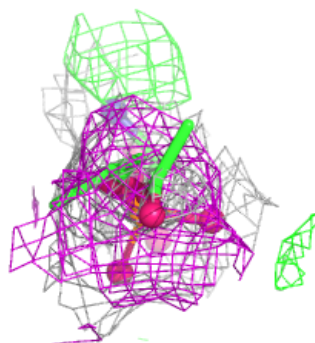
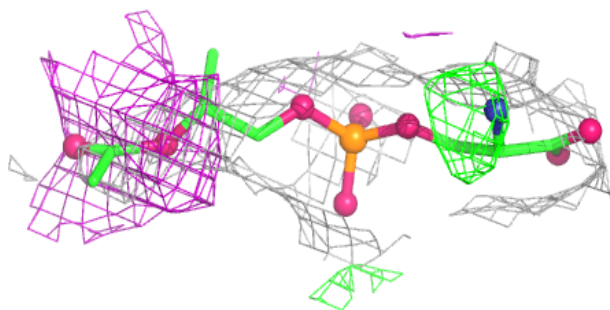
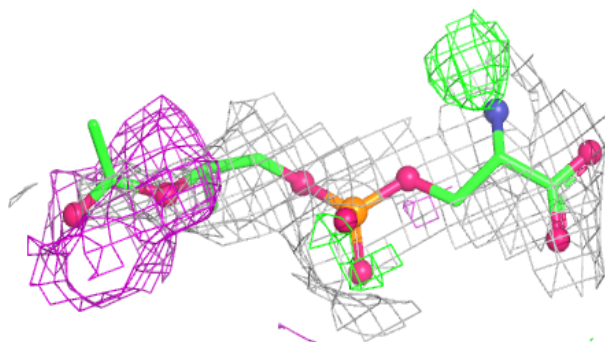
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 17F B 1005:

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

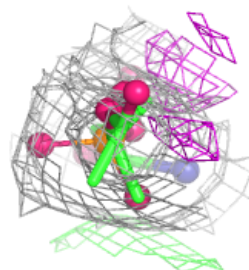
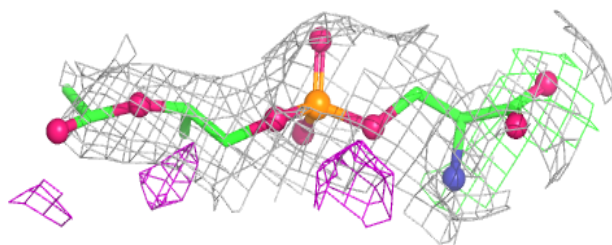
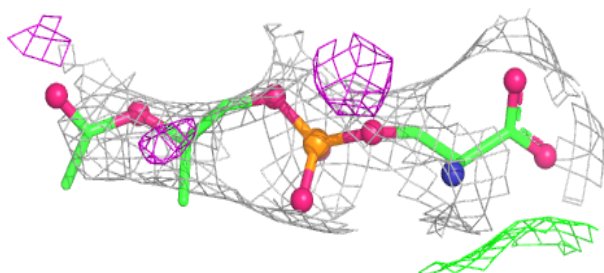
**Electron density around 17F A 1108:**

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

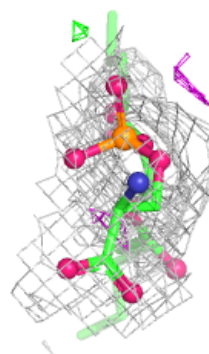
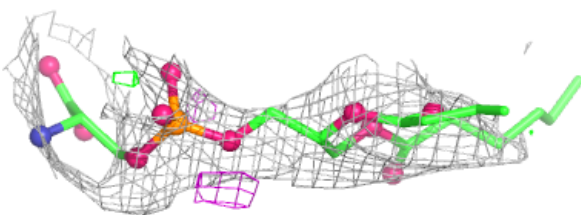
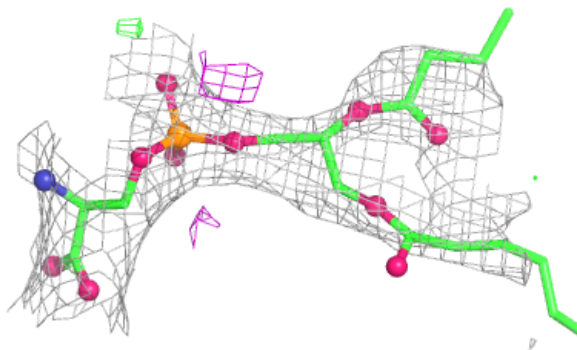


Electron density around 17F A 1109:

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

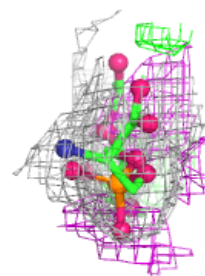
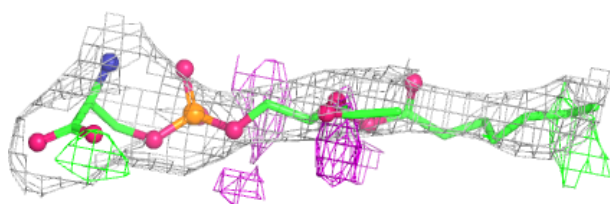
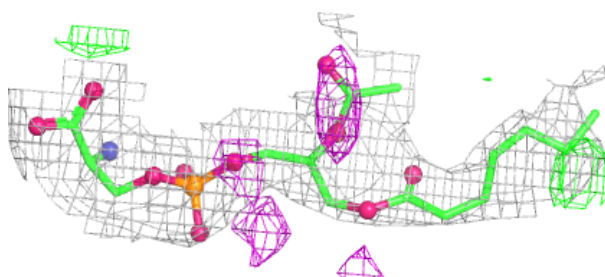
**Electron density around 17F D 2004:**

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

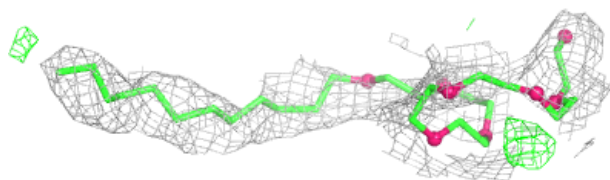
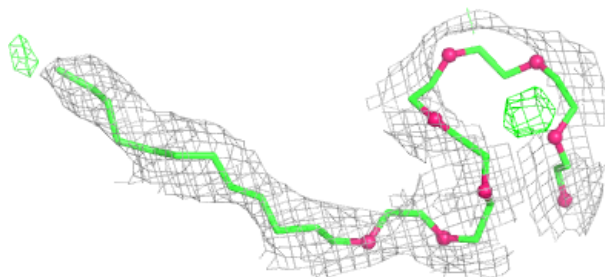


Electron density around 17F G 1002:

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

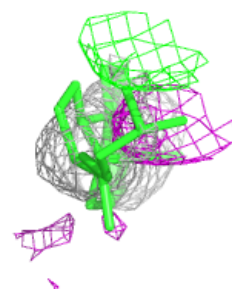
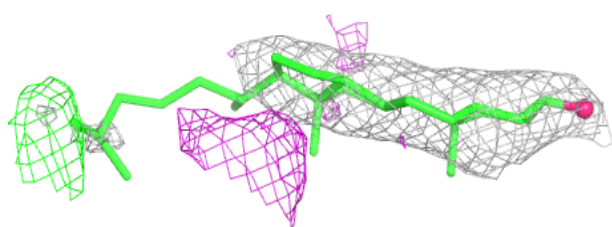
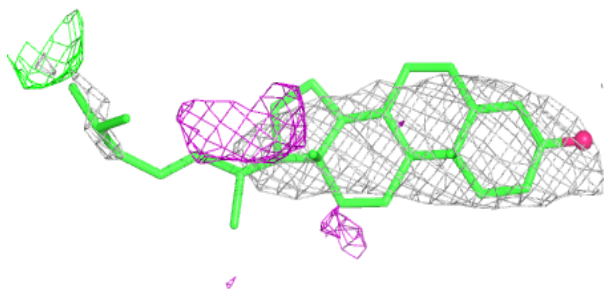
**Electron density around CE1 A 1110:**

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

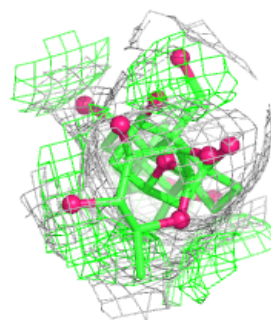
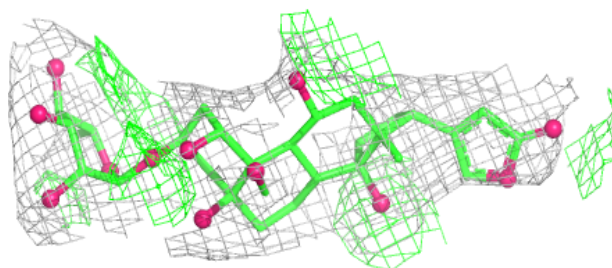
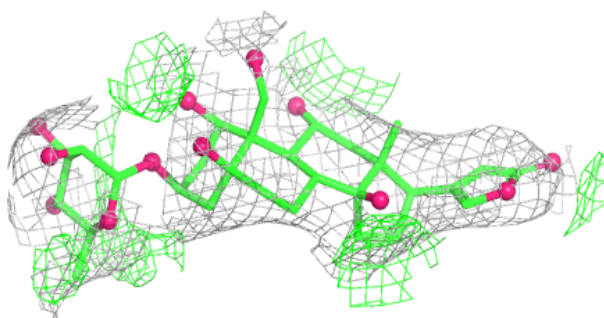


Electron density around CLR C 2005:

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

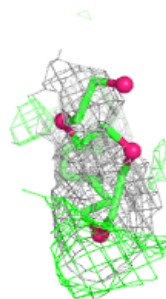
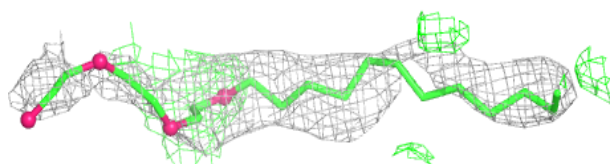
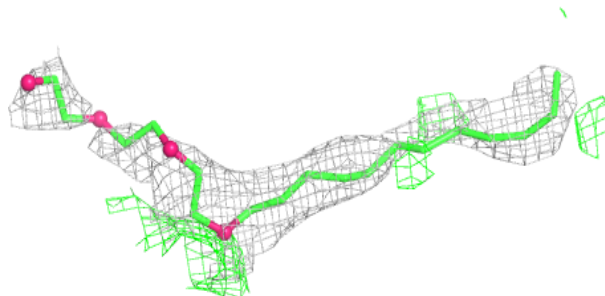
**Electron density around OBN C 2004:**

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

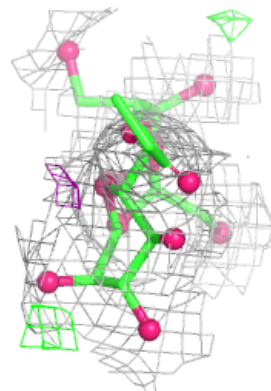
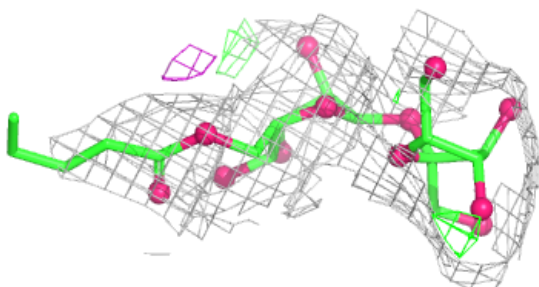
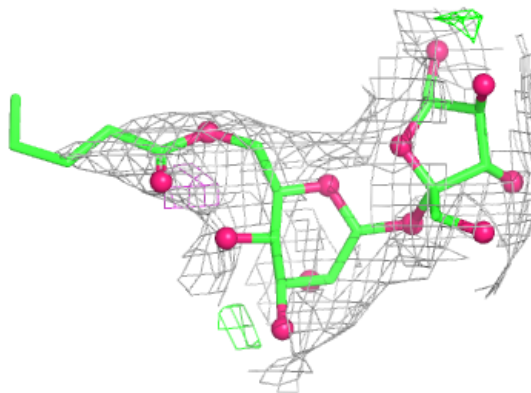


Electron density around CE1 E 2002:

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

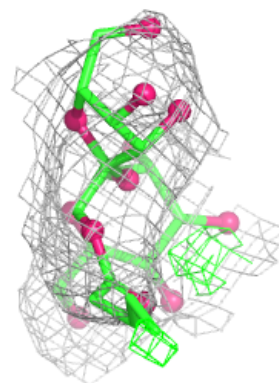
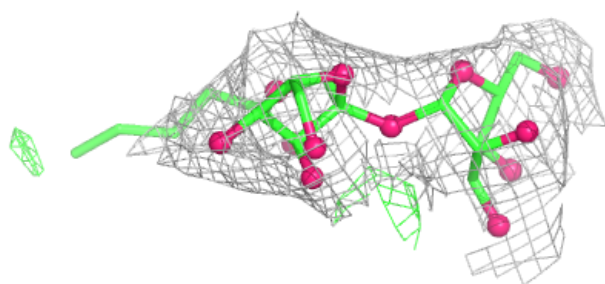
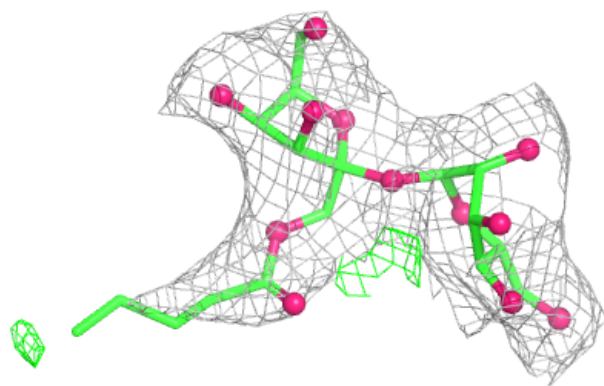
**Electron density around 1AT A 1106:**

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

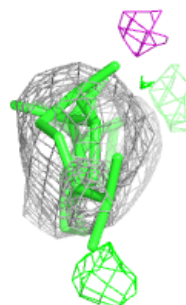
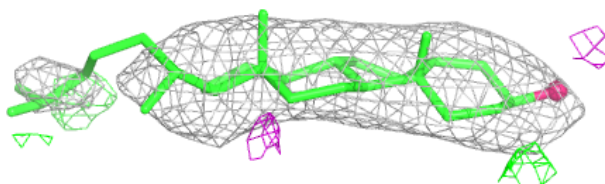
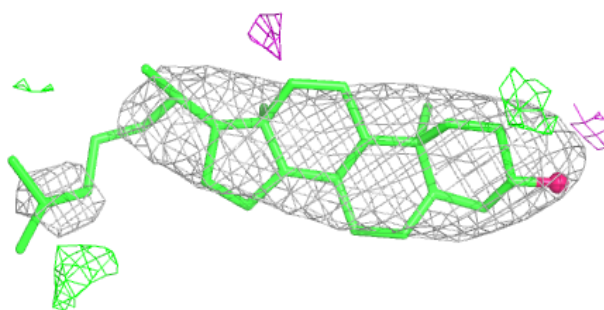


Electron density around 1DS A 1107:

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

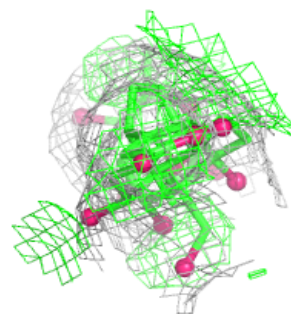
**Electron density around CLR A 1105:**

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

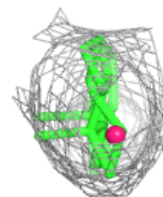
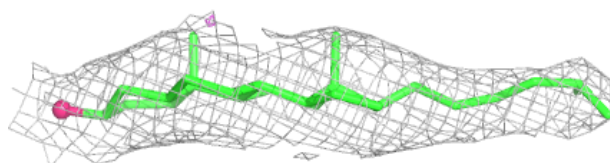
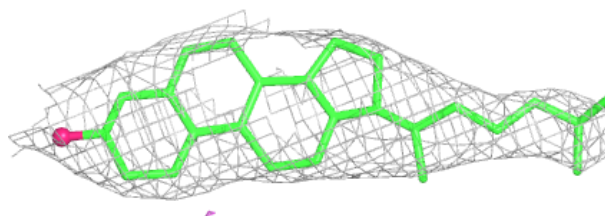


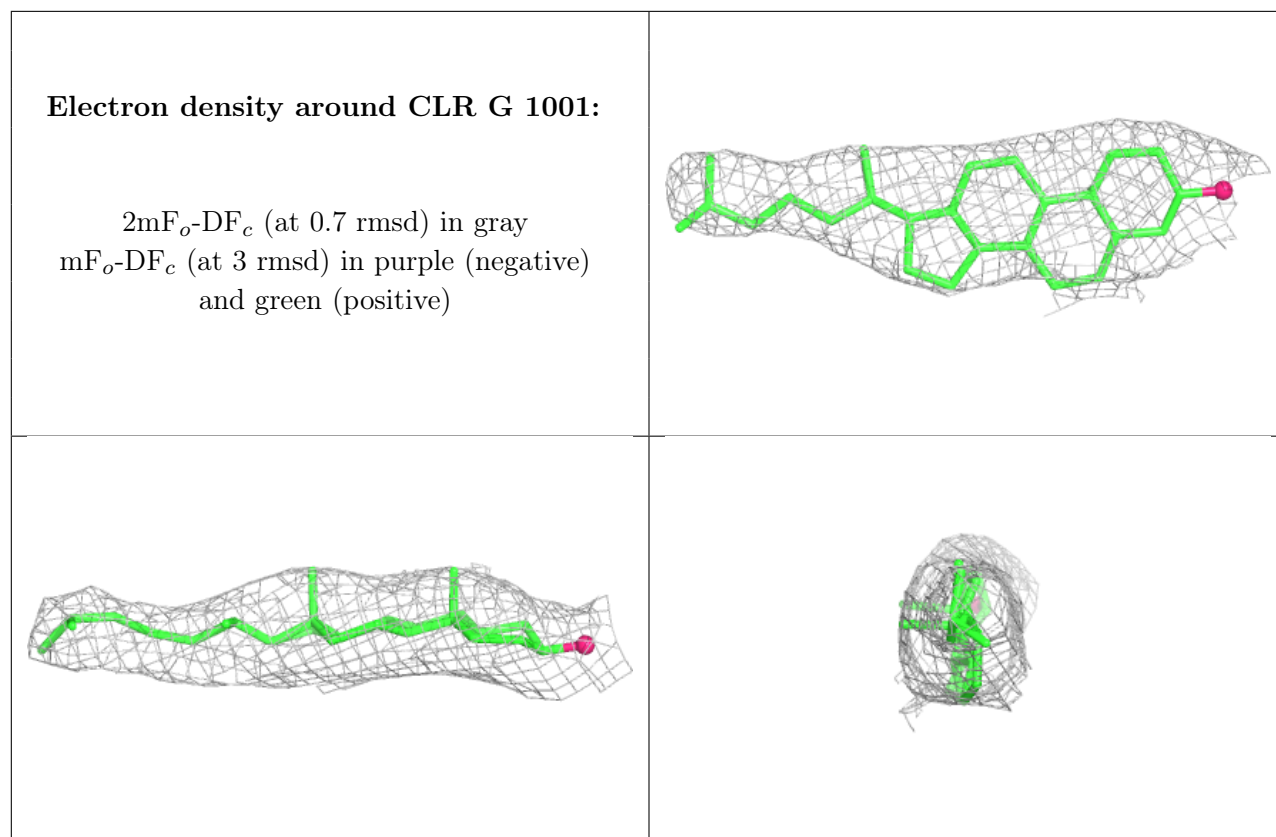
Electron density around OBN A 1104:

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

**Electron density around CLR E 2001:**

$2mF_o-DF_c$ (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.