



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:04 PM BST

PDB ID : 3WGV
Title : Crystal structure of a Na⁺-bound Na⁺,K⁺-ATPase preceding the E1P state with oligomycin
Authors : Kanai, R.; Ogawa, H.; Vilsen, B.; Cornelius, F.; Toyoshima, C.
Deposited on : 2013-08-09
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

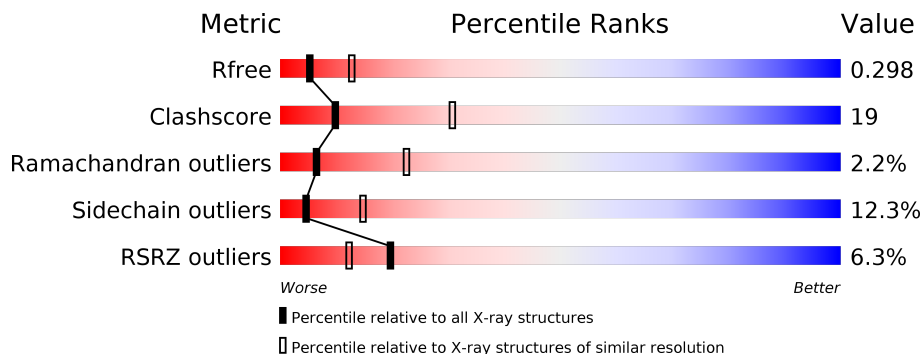
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1016	
1	C	1016	
2	B	303	
2	D	303	
3	E	65	
3	G	65	

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	EFO	C	2013	-	-	-	X
5	ALF	C	2002	-	-	X	-
7	NA	C	2006	-	-	-	X

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 21909 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
			Total	C	N	O	S			
1	A	994	7714	4918	1300	1449	47	0	0	0
1	C	994	7714	4918	1300	1449	47	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	303	2479	1603	408	454	14	0	0	0
2	D	303	2479	1603	408	454	14	0	0	0

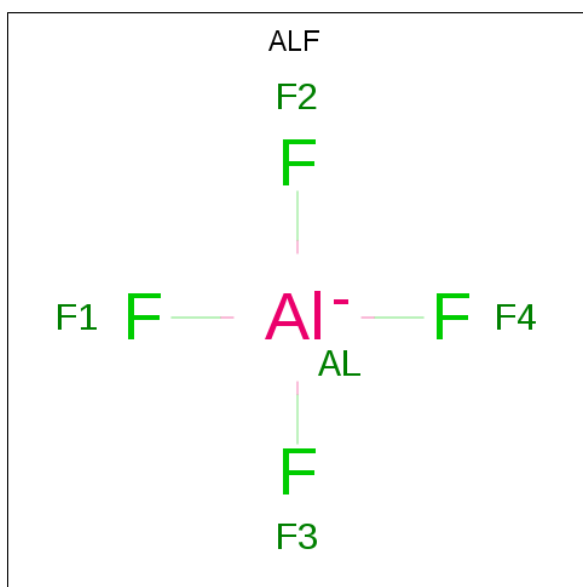
- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	G	34	270	183	39	48	0	0	0
3	E	35	281	189	43	49	0	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

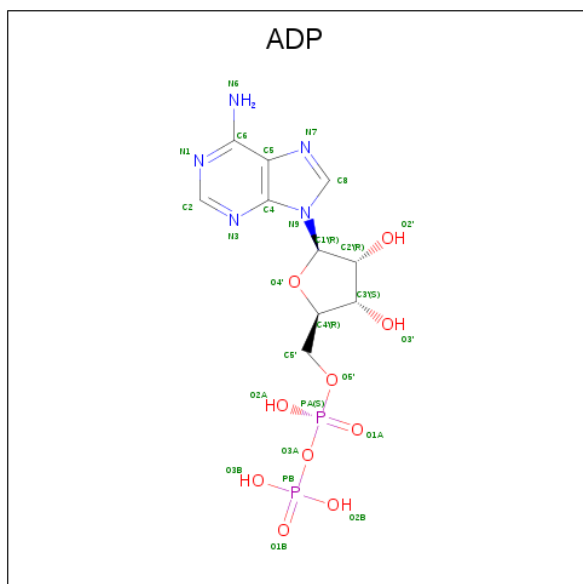
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0
4	C	2	2	2	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			5	1	4		
5	C	1	Total	Al	F	0	0
			5	1	4		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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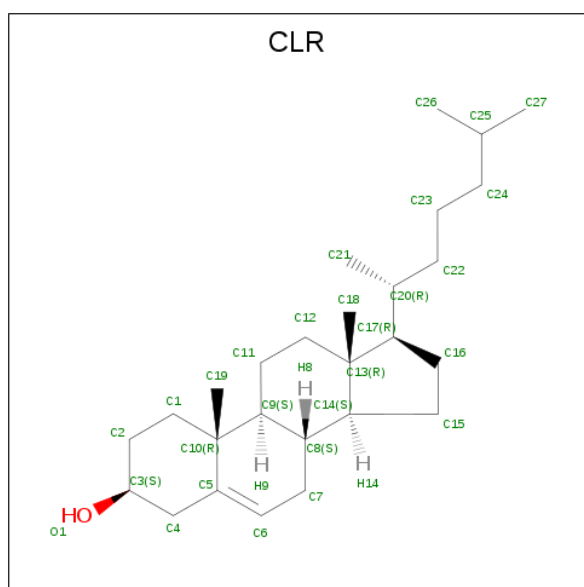
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	C	1	27	10	5	10	2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

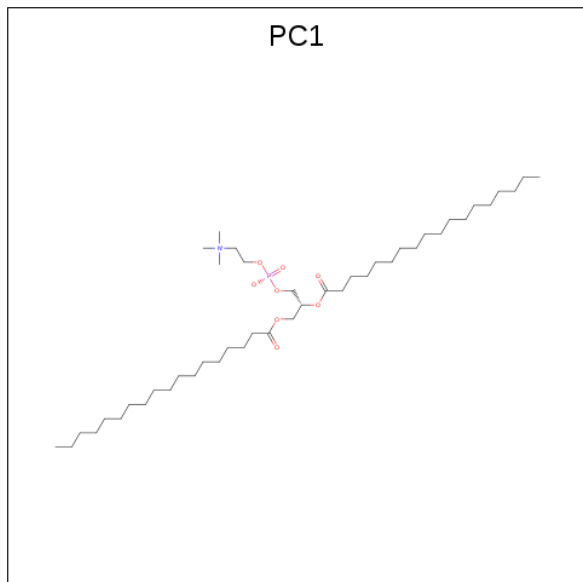
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	4	Total Na 4 4	0	0
7	C	4	Total Na 4 4	0	0

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



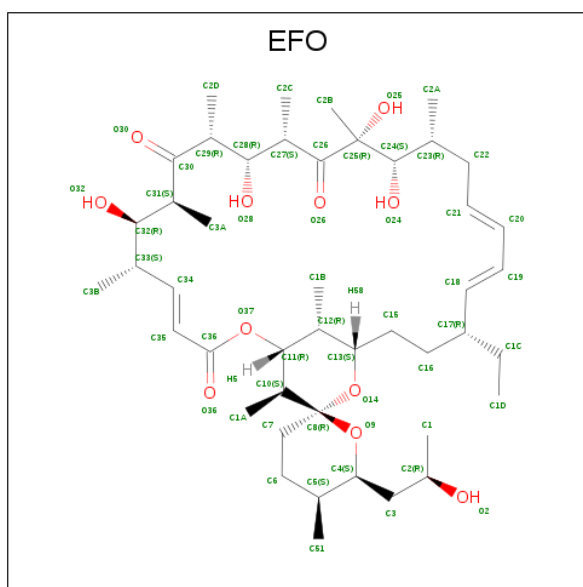
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 28 27 1	0	0
8	A	1	Total C O 28 27 1	0	0
8	G	1	Total C O 28 27 1	0	0
8	D	1	Total C O 28 27 1	0	0
8	D	1	Total C O 28 27 1	0	0
8	E	1	Total C O 28 27 1	0	0

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



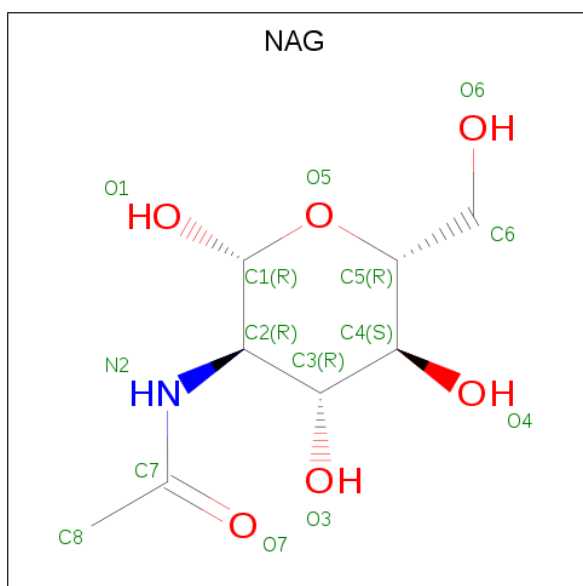
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	A	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
9	C	1	Total	C	N	O	P	0	0
			54	44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

- Molecule 10 is Oligomycin A (three-letter code: EFO) (formula: $C_{45}H_{74}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			56	45	11		
10	C	1	Total	C	O	0	0
			56	45	11		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

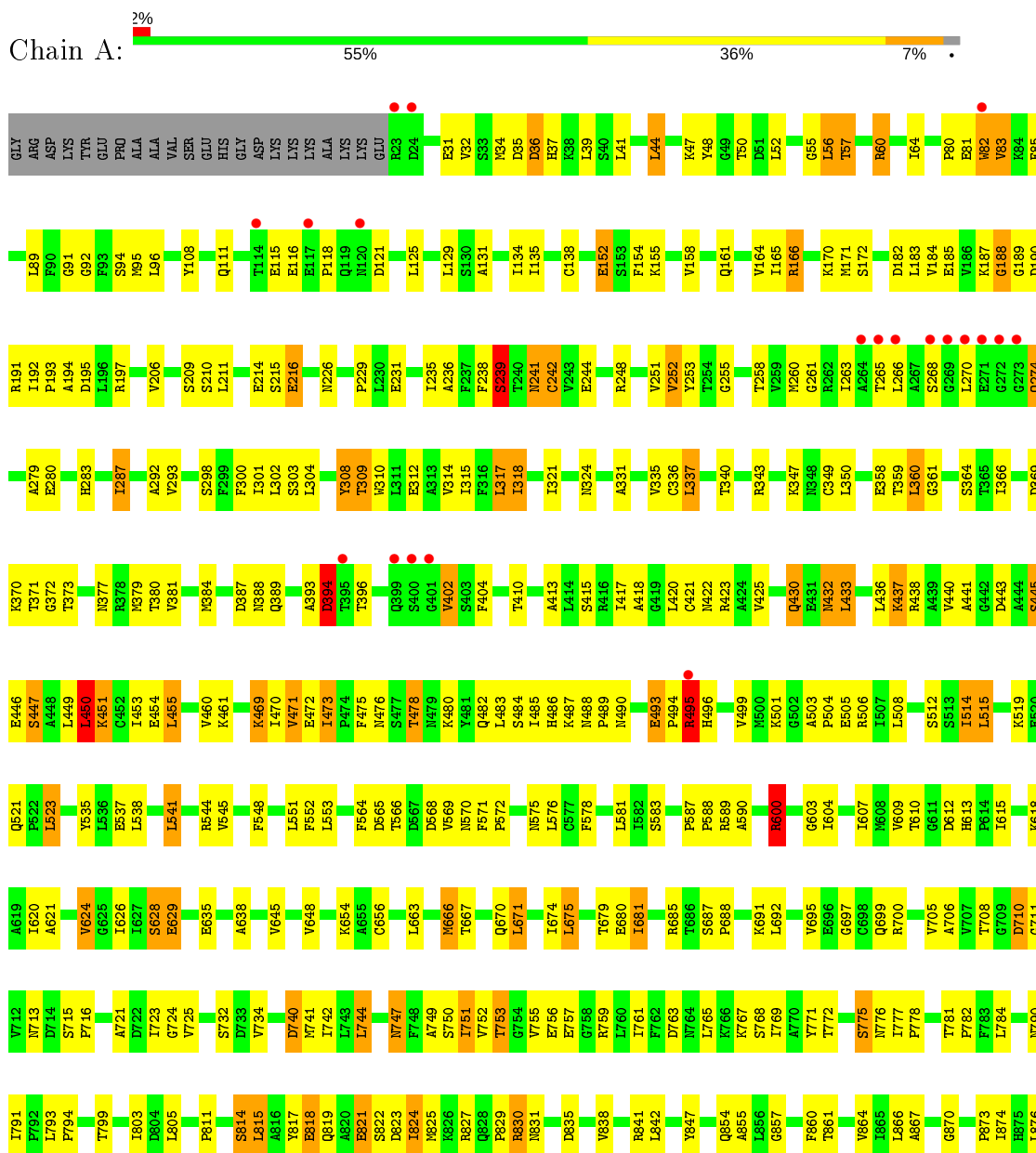
- Molecule 12 is water.

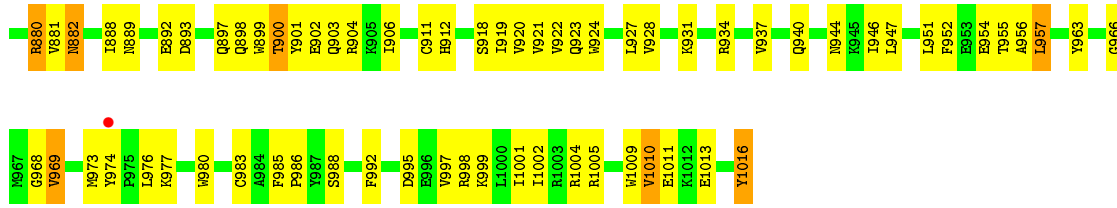
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	24	Total	O	0	0
			24	24		
12	B	2	Total	O	0	0
			2	2		
12	C	20	Total	O	0	0
			20	20		
12	D	2	Total	O	0	0
			2	2		

3 Residue-property plots

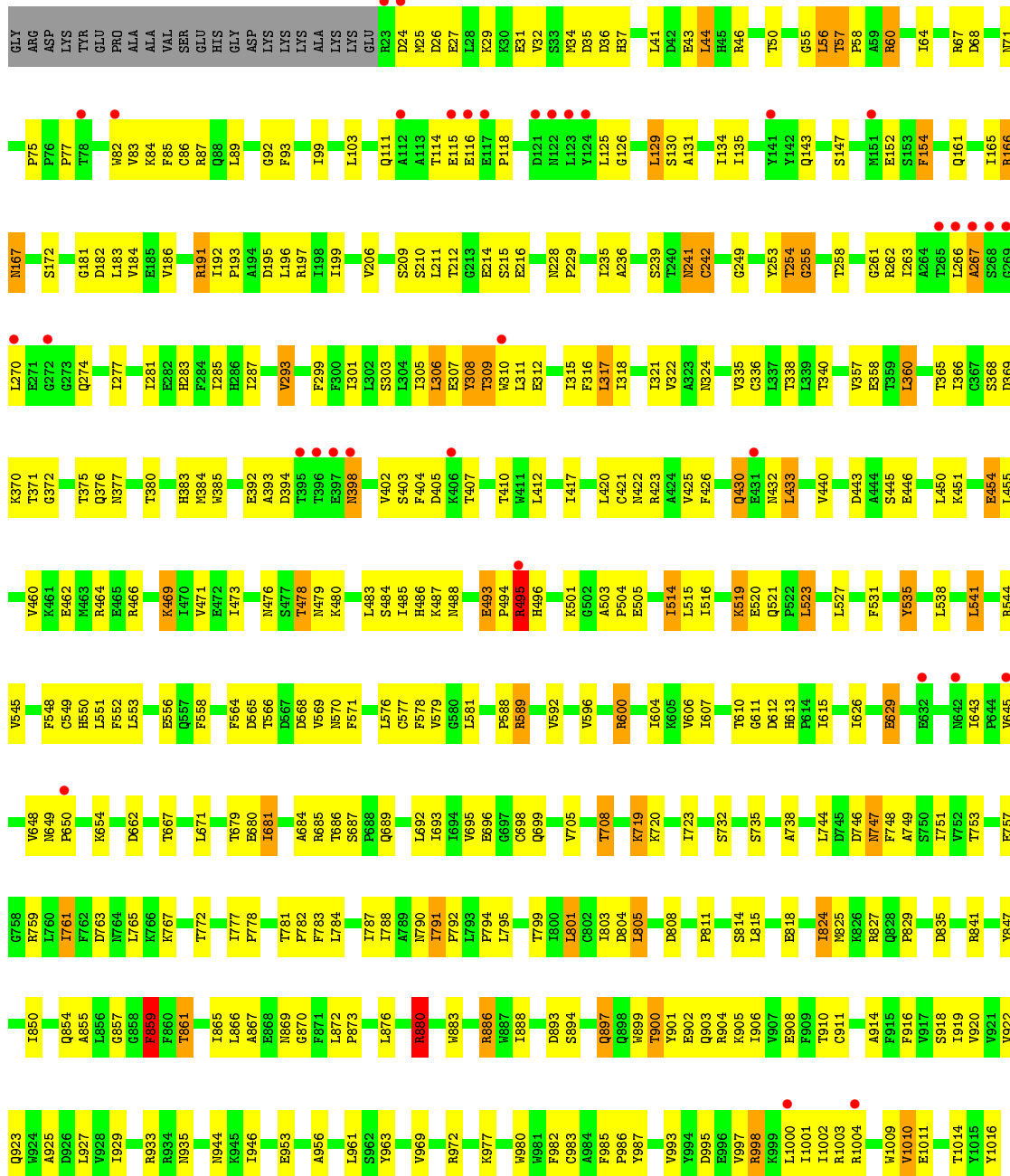
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

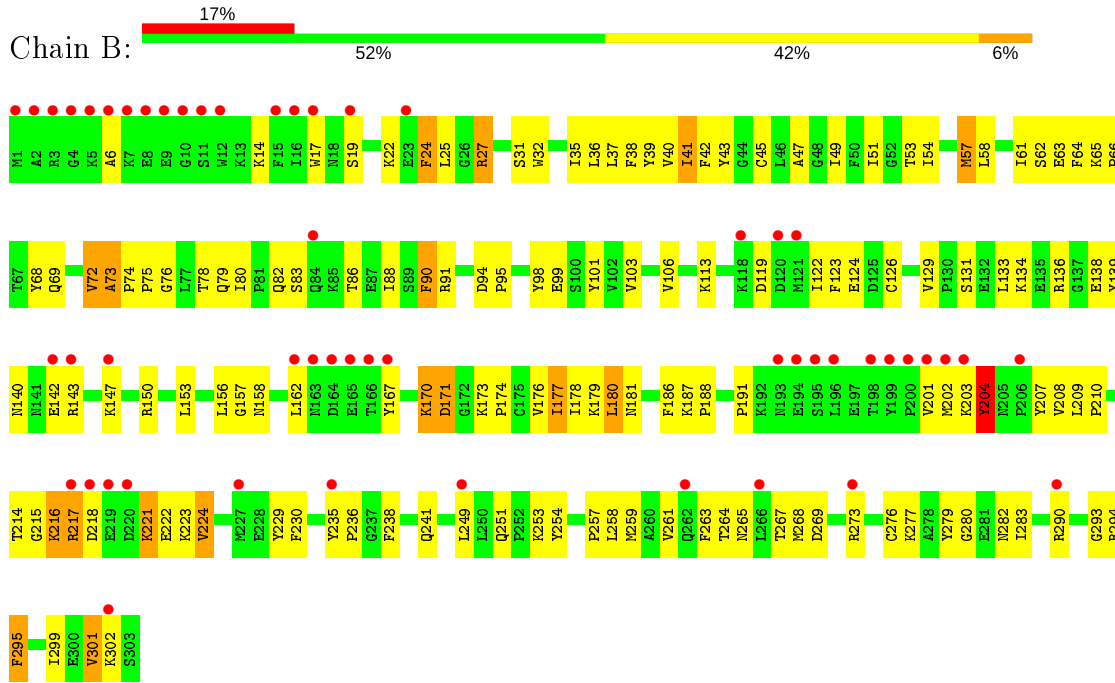




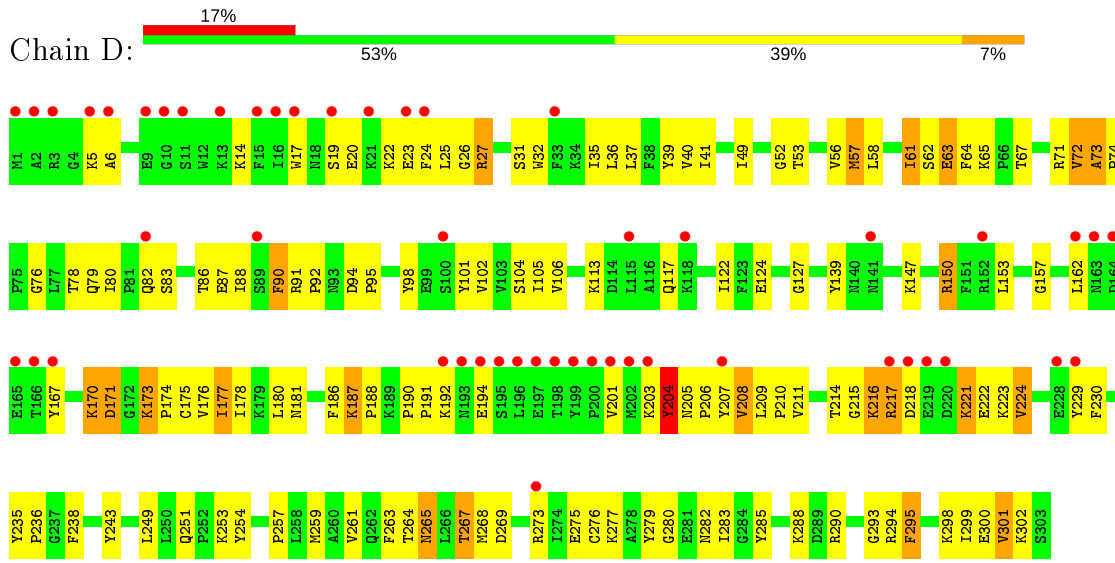
• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



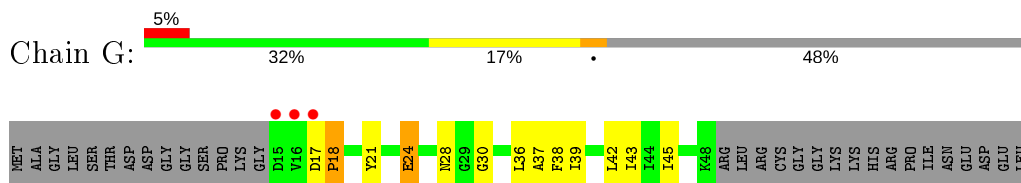
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



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

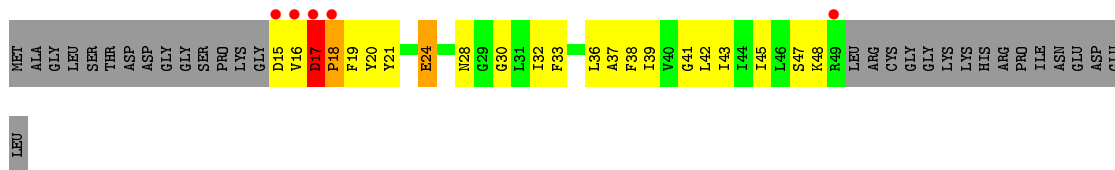


• Molecule 3: Na⁺/K⁺ ATPase gamma subunit transcript variant a



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.28Å 210.18Å 256.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (15.99-2.80) 94.4 (15.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.82Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.270 , 0.298 0.270 , 0.298	Depositor DCC
R_{free} test set	3965 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtrriage
Anisotropy	0.394	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	21909	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NAG, ADP, ALF, NA, PC1, EFO, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	1/7864 (0.0%)	0.66	7/10671 (0.1%)
1	C	0.39	0/7864	0.58	2/10671 (0.0%)
2	B	0.34	0/2544	0.53	1/3426 (0.0%)
2	D	0.34	0/2544	0.53	0/3426
3	E	0.35	0/287	0.56	0/389
3	G	0.38	0/276	0.54	0/375
All	All	0.41	1/21379 (0.0%)	0.60	10/28958 (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
3	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	656	CYS	CB-SG	-5.07	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	ARG	CB-CA-C	-9.36	91.69	110.40
1	A	600	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	600	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	239	SER	CB-CA-C	-6.59	97.57	110.10
1	C	239	SER	CB-CA-C	-6.45	97.85	110.10
1	C	495	ARG	CB-CA-C	-6.36	97.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	34	MET	N-CA-CB	-5.44	100.81	110.60
2	B	73	ALA	C-N-CD	5.16	139.24	128.40
1	A	508	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	17	ASP	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	7714	0	7770	303	0
1	C	7714	0	7769	264	0
2	B	2479	0	2458	103	0
2	D	2479	0	2458	98	0
3	E	281	0	285	14	0
3	G	270	0	272	12	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	A	5	0	0	1	0
5	C	5	0	0	2	0
6	A	27	0	12	3	0
6	C	27	0	12	6	0
7	A	4	0	0	0	0
7	C	4	0	0	0	0
8	A	56	0	92	27	0
8	D	56	0	92	29	0
8	E	28	0	45	13	0
8	G	28	0	45	9	0
9	A	216	0	352	14	0
9	B	54	0	88	2	0
9	C	216	0	352	15	0
9	D	54	0	88	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A	56	0	74	0	0
10	C	56	0	74	0	0
11	B	14	0	13	0	0
11	D	14	0	13	0	0
12	A	24	0	0	0	0
12	B	2	0	0	0	0
12	C	20	0	0	2	0
12	D	2	0	0	0	0
All	All	21909	0	22364	851	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 19.

All (851) 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)
8:A:2009:CLR:C11	8:A:2009:CLR:C9	1.77	1.62
8:D:3002:CLR:C11	8:D:3002:CLR:C12	1.74	1.60
8:A:2010:CLR:C9	8:A:2010:CLR:C11	1.76	1.59
8:D:3001:CLR:C9	8:D:3001:CLR:C11	1.78	1.57
8:E:101:CLR:C11	8:E:101:CLR:C9	1.78	1.56
8:D:3002:CLR:C11	8:D:3002:CLR:C9	1.78	1.55
8:G:101:CLR:C11	8:G:101:CLR:C9	1.79	1.54
1:C:495:ARG:HG3	1:C:495:ARG:O	1.42	1.11
1:C:493:GLU:HG2	1:C:495:ARG:H	1.24	1.03
1:A:600:ARG:HH11	1:A:600:ARG:HG2	1.33	0.94
2:D:221:LYS:HE3	2:D:223:LYS:HB2	1.49	0.93
1:A:417:ILE:HD11	1:A:548:PHE:HB3	1.48	0.93
1:A:493:GLU:HG2	1:A:495:ARG:H	1.35	0.91
8:A:2010:CLR:C10	8:A:2010:CLR:C11	2.50	0.90
2:B:76:GLY:HA2	2:B:293:GLY:H	1.37	0.90
1:C:44:LEU:HD11	1:C:197:ARG:HG2	1.54	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.52	0.90
1:A:790:ASN:HD22	1:A:880:ARG:HD2	1.38	0.88
1:C:166:ARG:NH1	1:C:182:ASP:OD1	2.06	0.88
1:A:57:THR:HG23	1:A:60:ARG:HB2	1.56	0.87
2:D:124:GLU:HB2	2:D:147:LYS:HD3	1.56	0.87
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.56	0.86
8:A:2009:CLR:C11	8:A:2009:CLR:C10	2.52	0.86
8:D:3002:CLR:C11	8:D:3002:CLR:C10	2.54	0.86
2:D:216:LYS:HG2	2:D:221:LYS:HB2	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ASP:HA	2:D:302:LYS:HA	1.56	0.85
1:A:480:LYS:HE3	6:A:2004:ADP:H5'2	1.57	0.85
1:A:443:ASP:HB2	1:A:446:GLU:HB2	1.60	0.84
8:D:3001:CLR:C11	8:D:3001:CLR:C10	2.55	0.84
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.59	0.83
8:E:101:CLR:C11	8:E:101:CLR:C10	2.56	0.82
1:A:679:THR:HG23	1:A:680:GLU:HG3	1.61	0.82
1:C:454:GLU:HG2	1:C:460:VAL:HG23	1.59	0.82
2:B:216:LYS:HG2	2:B:221:LYS:HB2	1.62	0.81
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.62	0.81
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.61	0.81
1:C:763:ASP:OD2	12:C:2114:HOH:O	1.97	0.81
1:A:495:ARG:HG3	1:A:495:ARG:O	1.77	0.81
1:C:495:ARG:O	1:C:495:ARG:CG	2.27	0.80
1:C:384:MET:HE1	1:C:393:ALA:HB2	1.62	0.80
1:C:165:ILE:HB	1:C:183:LEU:HD21	1.62	0.80
1:C:872:LEU:HD12	1:C:873:PRO:HD2	1.64	0.79
8:D:3001:CLR:H121	8:D:3001:CLR:H212	1.64	0.78
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.49	0.78
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.19	0.78
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.46	0.78
1:C:514:ILE:HG13	1:C:523:LEU:HG	1.66	0.77
1:C:565:ASP:H	1:C:570:ASN:HB2	1.51	0.76
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.21	0.75
1:C:57:THR:HG23	1:C:60:ARG:HB2	1.68	0.75
1:C:600:ARG:HB3	1:C:600:ARG:HH11	1.52	0.75
1:A:472:GLU:HB2	1:A:484:SER:HB3	1.68	0.75
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.69	0.75
1:A:165:ILE:HB	1:A:183:LEU:HD21	1.67	0.74
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.70	0.74
2:D:122:ILE:HG21	2:D:253:LYS:HE2	1.70	0.74
1:C:986:PRO:HG3	8:D:3002:CLR:H152	1.70	0.74
2:D:173:LYS:HG2	2:D:264:THR:HA	1.69	0.74
8:E:101:CLR:H121	8:E:101:CLR:H212	1.70	0.74
1:A:495:ARG:CG	1:A:495:ARG:O	2.35	0.73
1:C:309:THR:HG23	1:C:312:GLU:HB2	1.70	0.73
1:C:946:ILE:HG13	3:E:45:ILE:HD11	1.70	0.73
8:G:101:CLR:C11	8:G:101:CLR:C8	2.66	0.73
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.71	0.72
2:B:269:ASP:HA	2:B:302:LYS:HA	1.71	0.72
1:C:759:ARG:HH12	1:C:829:PRO:HA	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ILE:HG21	2:B:253:LYS:HE2	1.70	0.72
1:A:963:TYR:CE2	8:G:101:CLR:H21	2.24	0.71
1:C:56:LEU:HD11	1:C:182:ASP:HB3	1.72	0.71
2:D:187:LYS:O	2:D:282:ASN:ND2	2.22	0.71
8:G:101:CLR:C11	8:G:101:CLR:C10	2.63	0.71
1:A:44:LEU:HD11	1:A:197:ARG:HG2	1.72	0.71
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.72	0.71
1:C:685:ARG:NH2	6:C:2004:ADP:O3'	2.22	0.70
1:A:473:ILE:HD11	1:A:483:LEU:HD23	1.72	0.70
1:C:1003:ARG:HD2	9:C:2011:PC1:H122	1.72	0.70
8:D:3002:CLR:C11	8:D:3002:CLR:C8	2.68	0.70
8:A:2010:CLR:C11	8:A:2010:CLR:C8	2.64	0.70
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.73	0.70
1:A:255:GLY:O	1:A:258:THR:HG22	1.92	0.70
1:C:277:ILE:HD12	1:C:358:GLU:HG3	1.74	0.69
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.28	0.69
1:A:166:ARG:NH1	1:A:182:ASP:OD1	2.25	0.69
8:A:2009:CLR:H212	8:A:2009:CLR:H121	1.73	0.69
9:C:2012:PC1:H351	9:C:2012:PC1:H251	1.75	0.69
8:D:3001:CLR:C8	8:D:3001:CLR:C11	2.67	0.69
1:A:50:THR:HG22	1:A:56:LEU:HB3	1.75	0.69
1:A:551:LEU:HD22	1:A:553:LEU:HD23	1.75	0.69
1:C:50:THR:HG22	1:C:56:LEU:HD23	1.75	0.68
1:C:600:ARG:NH1	12:C:2120:HOH:O	2.25	0.68
2:B:14:LYS:HA	2:B:17:TRP:HB3	1.75	0.68
1:C:696:GLU:HG3	1:C:720:LYS:HE2	1.75	0.68
8:A:2010:CLR:H121	8:A:2010:CLR:H212	1.73	0.68
1:C:241:ASN:OD1	1:C:241:ASN:N	2.24	0.68
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	1.76	0.68
9:A:2013:PC1:H3B2	9:A:2013:PC1:H292	1.74	0.68
1:A:239:SER:OG	1:A:239:SER:O	2.11	0.68
3:G:17:ASP:HB3	3:G:18:PRO:HD2	1.76	0.68
1:A:493:GLU:HG2	1:A:495:ARG:N	2.09	0.67
3:G:24:GLU:O	3:G:28:ASN:ND2	2.26	0.67
1:C:867:ALA:HB2	1:C:873:PRO:HD3	1.76	0.67
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.77	0.67
2:D:191:PRO:HG3	2:D:280:GLY:HA2	1.77	0.67
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.76	0.67
1:C:488:ASN:HB3	1:C:493:GLU:HG3	1.75	0.66
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.75	0.66
2:D:216:LYS:HB3	2:D:273:ARG:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PHE:CD2	2:B:98:TYR:HB3	2.31	0.66
2:D:14:LYS:HA	2:D:17:TRP:HB3	1.77	0.66
1:A:108:TYR:HA	1:A:111:GLN:HE21	1.60	0.66
1:A:394:ASP:N	1:A:394:ASP:OD1	2.28	0.66
1:C:445:SER:OG	1:C:544:ARG:NH1	2.29	0.66
1:A:154:PHE:HB3	1:A:350:LEU:HD13	1.78	0.66
1:A:505:GLU:HG3	1:A:506:ARG:H	1.61	0.65
1:C:719:LYS:NZ	1:C:738:ALA:O	2.28	0.65
9:C:2009:PC1:H2D2	9:C:2012:PC1:H3F2	1.78	0.65
1:A:759:ARG:HH12	1:A:829:PRO:HA	1.60	0.65
8:D:3002:CLR:C11	8:D:3002:CLR:C13	2.68	0.65
2:D:229:TYR:HD1	2:D:261:VAL:HG12	1.60	0.65
9:C:2009:PC1:H2I3	9:C:2009:PC1:H3I1	1.78	0.65
1:A:842:LEU:HD12	1:A:1016:TYR:HD2	1.61	0.65
1:A:514:ILE:HG12	1:A:578:PHE:HB3	1.77	0.65
1:A:258:THR:HG23	1:A:261:GLY:H	1.60	0.65
1:C:777:ILE:HD11	1:C:847:TYR:HA	1.79	0.64
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.79	0.64
1:C:679:THR:HG23	1:C:680:GLU:HG3	1.79	0.64
8:A:2010:CLR:H193	8:A:2010:CLR:H111	1.79	0.64
1:A:790:ASN:ND2	1:A:880:ARG:HD2	2.11	0.64
1:A:274:GLN:HE22	1:A:279:ALA:HB2	1.62	0.64
2:D:217:ARG:HD2	2:D:218:ASP:H	1.62	0.64
2:B:27:ARG:HD3	2:B:32:TRP:HE3	1.62	0.64
1:A:1009:TRP:HZ2	2:B:35:ILE:HG22	1.63	0.64
1:C:211:LEU:HD23	1:C:212:THR:HG23	1.80	0.64
1:A:613:HIS:CD2	1:A:615:ILE:HG12	2.33	0.63
1:A:613:HIS:NE2	1:A:615:ILE:HG12	2.14	0.63
8:A:2009:CLR:C8	8:A:2009:CLR:C11	2.65	0.63
1:C:299:PHE:HB3	1:C:316:PHE:HE2	1.64	0.63
2:B:173:LYS:HG2	2:B:264:THR:HA	1.81	0.63
1:C:426:PHE:HE2	1:C:454:GLU:HG3	1.63	0.63
3:E:33:PHE:CE1	8:E:101:CLR:H183	2.34	0.63
2:B:224:VAL:HB	2:B:267:THR:HG21	1.81	0.62
1:A:36:ASP:OD1	1:A:47:LYS:NZ	2.32	0.62
1:C:963:TYR:CE2	8:E:101:CLR:H21	2.33	0.62
9:C:2011:PC1:H2H2	8:D:3002:CLR:H272	1.80	0.62
2:B:216:LYS:H	2:B:216:LYS:HD2	1.63	0.62
1:A:152:GLU:HA	1:A:155:LYS:HG2	1.82	0.62
1:A:209:SER:HB3	1:A:215:SER:HA	1.82	0.62
1:C:998:ARG:HE	1:C:1014:THR:HB	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:229:TYR:HD1	2:B:261:VAL:HG12	1.64	0.62
1:C:854:GLN:HG2	1:C:922:VAL:HB	1.81	0.62
1:C:266:LEU:HD22	1:C:270:LEU:HA	1.82	0.62
1:A:324:ASN:HA	1:A:776:ASN:OD1	2.00	0.61
1:A:708:THR:HG22	1:A:725:VAL:HB	1.81	0.61
2:D:83:SER:HB3	2:D:86:THR:HA	1.80	0.61
1:C:258:THR:HG23	1:C:261:GLY:H	1.64	0.61
1:A:483:LEU:HD21	1:A:571:PHE:HE2	1.65	0.61
1:A:946:ILE:HG13	3:G:45:ILE:HD11	1.81	0.61
1:C:777:ILE:HD12	1:C:777:ILE:H	1.65	0.61
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.81	0.61
1:C:480:LYS:HG2	6:C:2004:ADP:H5'1	1.83	0.61
1:A:1016:TYR:H	1:A:1016:TYR:HD1	1.48	0.61
1:C:956:ALA:HB2	3:E:37:ALA:HB3	1.83	0.61
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.82	0.60
1:C:471:VAL:HG21	1:C:564:PHE:HB2	1.83	0.60
1:C:982:PHE:HA	1:C:985:PHE:CD1	2.36	0.60
8:A:2009:CLR:H111	8:A:2009:CLR:H193	1.82	0.60
1:C:732:SER:HG	1:C:735:SER:HG	1.49	0.60
2:D:106:VAL:HG22	2:D:167:TYR:HB2	1.83	0.60
2:D:91:ARG:HG3	2:D:302:LYS:O	2.01	0.60
3:E:17:ASP:HB3	3:E:18:PRO:HD2	1.81	0.60
2:D:87:GLU:HA	2:D:298:LYS:O	2.02	0.60
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.83	0.60
1:A:360:LEU:HA	1:A:723:ILE:HD13	1.83	0.60
1:A:343:ARG:HD2	1:A:757:GLU:OE2	2.02	0.60
1:C:125:LEU:O	1:C:129:LEU:HB2	2.01	0.60
1:A:35:ASP:HB2	1:A:37:HIS:ND1	2.16	0.60
1:A:818:GLU:HG2	1:A:944:ASN:HD22	1.66	0.60
1:C:469:LYS:HA	1:C:486:HIS:HA	1.83	0.60
1:C:494:PRO:HG2	1:C:552:PHE:HB3	1.82	0.60
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.83	0.60
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.82	0.60
1:A:514:ILE:HG13	1:A:523:LEU:HG	1.84	0.59
1:A:80:PRO:HG2	1:A:83:VAL:HB	1.83	0.59
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.84	0.59
1:C:398:ASN:HB2	1:C:455:LEU:HD13	1.84	0.59
1:C:31:GLU:HG3	1:C:32:VAL:H	1.68	0.59
8:D:3002:CLR:H111	8:D:3002:CLR:H193	1.84	0.59
1:C:827:ARG:HH12	1:C:933:ARG:HH21	1.50	0.59
1:A:433:LEU:HD12	1:A:437:LYS:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:GLY:HA2	2:D:293:GLY:H	1.66	0.59
1:A:372:GLY:HA2	1:A:377:ASN:HB2	1.85	0.59
1:C:365:THR:HB	1:C:705:VAL:HG12	1.84	0.59
1:C:191:ARG:HA	1:C:241:ASN:HB3	1.85	0.58
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.84	0.58
5:A:2002:ALF:F1	6:A:2004:ADP:O3B	2.11	0.58
1:A:986:PRO:CG	8:A:2010:CLR:H181	2.33	0.58
1:A:874:ILE:HD12	1:A:874:ILE:H	1.68	0.58
2:B:214:THR:OG1	2:B:215:GLY:N	2.35	0.58
1:A:496:HIS:HB2	1:A:553:LEU:HB2	1.84	0.58
2:B:216:LYS:HB3	2:B:273:ARG:HB2	1.85	0.58
1:C:281:ILE:HD11	1:C:765:LEU:HD13	1.85	0.58
8:D:3002:CLR:H212	8:D:3002:CLR:H121	1.85	0.58
1:A:831:ASN:HD21	2:B:6:ALA:HB2	1.69	0.58
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.84	0.58
1:A:824:ILE:HD12	1:A:825:MET:H	1.68	0.58
1:A:889:ASN:HD22	1:A:900:THR:HB	1.69	0.58
1:C:902:GLU:O	1:C:906:ILE:HG12	2.03	0.58
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.86	0.58
8:A:2010:CLR:C11	8:A:2010:CLR:C19	2.82	0.57
1:A:927:LEU:HG	1:A:947:LEU:HD21	1.87	0.57
1:C:553:LEU:HD22	1:C:558:PHE:CE2	2.39	0.57
8:A:2010:CLR:C9	8:A:2010:CLR:C12	2.79	0.57
1:C:551:LEU:HD12	1:C:576:LEU:HA	1.87	0.57
1:C:303:SER:O	1:C:308:TYR:HB2	2.04	0.57
2:D:186:PHE:CZ	2:D:282:ASN:HB3	2.40	0.57
1:A:340:THR:HG22	1:A:757:GLU:OE1	2.04	0.57
1:A:857:GLY:O	1:A:861:THR:HG23	2.04	0.57
1:A:300:PHE:HB2	1:A:317:LEU:HB2	1.86	0.57
1:A:628:SER:OG	1:A:680:GLU:OE2	2.21	0.57
1:A:263:ILE:HG13	1:A:263:ILE:O	2.05	0.56
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.39	0.56
2:D:14:LYS:HZ3	2:D:17:TRP:HE3	1.53	0.56
1:C:126:GLY:O	1:C:130:SER:OG	2.17	0.56
1:C:60:ARG:O	1:C:64:ILE:HG13	2.05	0.56
1:A:370:LYS:NZ	1:A:612:ASP:OD2	2.37	0.56
1:A:671:LEU:O	1:A:675:LEU:HD22	2.06	0.56
1:A:420:LEU:HD13	1:A:486:HIS:ND1	2.20	0.56
1:A:638:ALA:HB2	1:A:648:VAL:HG21	1.87	0.56
1:A:902:GLU:O	1:A:906:ILE:HG12	2.05	0.56
1:C:206:VAL:HA	1:C:242:CYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:LEU:HA	1:C:541:LEU:HD22	1.88	0.56
1:C:987:TYR:OH	2:D:53:THR:HG21	2.06	0.56
9:C:2012:PC1:H361	9:C:2012:PC1:H3B2	1.88	0.56
1:C:99:ILE:O	1:C:103:LEU:HG	2.06	0.56
2:D:268:MET:HA	2:D:301:VAL:HG23	1.87	0.56
1:A:963:TYR:HE1	1:A:976:LEU:H	1.54	0.56
1:A:777:ILE:HD11	1:A:847:TYR:CG	2.41	0.55
1:A:892:GLU:HA	1:A:897:GLN:O	2.06	0.55
1:C:369:ASP:OD1	5:C:2002:ALF:F1	2.14	0.55
1:C:985:PHE:HZ	8:E:101:CLR:H221	1.72	0.55
2:B:217:ARG:HD2	2:B:218:ASP:H	1.71	0.55
1:C:565:ASP:H	1:C:570:ASN:CB	2.19	0.55
1:A:469:LYS:HB2	1:A:486:HIS:CD2	2.42	0.55
2:B:27:ARG:HD3	2:B:32:TRP:CE3	2.41	0.55
1:C:67:ARG:NH1	1:C:68:ASP:OD2	2.39	0.55
2:D:61:ILE:HG23	2:D:67:THR:HG23	1.87	0.55
1:A:350:LEU:HD23	1:A:742:ILE:HD12	1.88	0.55
1:A:768:SER:HA	1:A:815:LEU:HD23	1.89	0.55
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.41	0.55
2:B:178:ILE:HD11	2:B:276:CYS:SG	2.47	0.55
1:C:469:LYS:HB3	1:C:486:HIS:CE1	2.40	0.55
2:D:27:ARG:HD3	2:D:32:TRP:HE3	1.71	0.55
8:E:101:CLR:H111	8:E:101:CLR:H193	1.88	0.55
1:A:607:ILE:HG12	1:A:681:ILE:HG13	1.88	0.55
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.72	0.55
1:A:55:GLY:HA3	1:A:165:ILE:O	2.07	0.55
1:C:152:GLU:C	1:C:154:PHE:H	2.09	0.55
1:C:460:VAL:HG11	1:C:464:ARG:HH21	1.71	0.55
1:A:706:ALA:HA	1:A:723:ILE:HG13	1.88	0.55
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.88	0.55
9:C:2012:PC1:H3B1	9:C:2012:PC1:H282	1.87	0.55
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.89	0.55
1:A:183:LEU:HD23	1:A:183:LEU:H	1.73	0.54
1:A:475:PHE:H	1:A:482:GLN:HG3	1.72	0.54
1:A:777:ILE:HD11	1:A:847:TYR:HA	1.90	0.54
2:B:138:GLU:O	2:B:140:ASN:N	2.39	0.54
1:C:255:GLY:O	1:C:258:THR:HG22	2.07	0.54
1:A:60:ARG:O	1:A:64:ILE:HG13	2.07	0.54
1:C:861:THR:HG21	1:C:918:SER:OG	2.07	0.54
1:A:666:MET:HG3	1:A:670:GLN:HB3	1.90	0.54
1:C:747:ASN:HD21	1:C:749:ALA:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2014:PC1:H122	2:B:25:LEU:HD11	1.89	0.54
1:C:306:LEU:HD12	1:C:880:ARG:HE	1.73	0.54
8:D:3001:CLR:C9	8:D:3001:CLR:C12	2.84	0.54
1:A:977:LYS:HD3	2:B:68:TYR:CE1	2.43	0.54
3:G:17:ASP:CB	3:G:18:PRO:HD2	2.38	0.54
2:B:90:PHE:HD2	2:B:98:TYR:HB3	1.72	0.54
1:C:801:LEU:O	1:C:805:LEU:HG	2.07	0.54
1:A:336:CYS:O	1:A:340:THR:HG23	2.08	0.54
1:A:888:ILE:O	1:A:904:ARG:NH2	2.41	0.54
1:A:854:GLN:HE22	1:A:923:GLN:HE21	1.55	0.54
1:C:143:GLN:HE21	1:C:335:VAL:HG22	1.73	0.54
1:C:613:HIS:HD2	1:C:615:ILE:HB	1.72	0.54
1:A:472:GLU:CB	1:A:484:SER:HB3	2.36	0.53
1:C:814:SER:HB3	1:C:946:ILE:HG22	1.89	0.53
1:A:131:ALA:O	1:A:135:ILE:HG12	2.09	0.53
1:A:440:VAL:HG12	1:A:441:ALA:H	1.74	0.53
1:A:603:GLY:HA3	1:A:829:PRO:HD3	1.90	0.53
1:A:899:TRP:CE3	2:B:72:VAL:HG13	2.43	0.53
1:C:854:GLN:HE22	1:C:923:GLN:HE21	1.57	0.53
1:A:476:ASN:OD1	1:A:478:THR:HG23	2.08	0.53
1:C:906:ILE:O	1:C:910:THR:OG1	2.22	0.53
8:A:2009:CLR:C19	8:A:2009:CLR:C11	2.87	0.53
9:A:2013:PC1:H292	9:A:2013:PC1:C3B	2.39	0.53
2:B:83:SER:HB3	2:B:86:THR:HA	1.89	0.53
1:C:317:LEU:O	1:C:321:ILE:HG12	2.09	0.53
1:A:861:THR:HG21	1:A:918:SER:OG	2.08	0.53
2:B:106:VAL:HG22	2:B:167:TYR:HB2	1.91	0.53
1:A:505:GLU:OE2	1:A:613:HIS:ND1	2.34	0.53
1:A:951:LEU:O	1:A:955:THR:HG23	2.08	0.53
2:B:176:VAL:HB	2:B:261:VAL:HG23	1.90	0.53
1:C:440:VAL:HG21	1:C:451:LYS:HE3	1.90	0.53
1:A:1001:ILE:CG2	1:A:1010:VAL:HG21	2.39	0.53
1:A:609:VAL:HG12	1:A:691:LYS:HE2	1.89	0.53
1:A:335:VAL:HG11	1:A:817:TYR:CE2	2.43	0.53
8:E:101:CLR:C11	8:E:101:CLR:C8	2.69	0.53
1:A:421:CYS:O	1:A:482:GLN:NE2	2.42	0.52
1:C:184:VAL:HG11	1:C:193:PRO:HG3	1.91	0.52
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.91	0.52
1:C:916:PHE:O	1:C:920:VAL:HG23	2.10	0.52
2:D:176:VAL:HB	2:D:261:VAL:HG23	1.90	0.52
8:E:101:CLR:C12	8:E:101:CLR:C9	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2010:CLR:H121	8:A:2010:CLR:C21	2.39	0.52
2:D:224:VAL:HB	2:D:267:THR:HG21	1.91	0.52
1:A:997:VAL:O	1:A:1001:ILE:HG13	2.09	0.52
1:A:184:VAL:HG11	1:A:193:PRO:HG2	1.91	0.52
1:A:393:ALA:HA	1:A:402:VAL:HA	1.91	0.52
1:A:771:TYR:CE1	1:A:927:LEU:HB2	2.44	0.52
1:A:1009:TRP:CZ2	2:B:35:ILE:HG22	2.43	0.52
9:C:2009:PC1:H291	9:C:2009:PC1:H3A1	1.92	0.52
1:A:89:LEU:HD21	1:A:134:ILE:HA	1.91	0.52
1:A:422:ASN:OD1	1:A:423:ARG:N	2.42	0.52
1:A:921:VAL:HG22	1:A:924:TRP:CH2	2.45	0.52
2:D:90:PHE:CD2	2:D:98:TYR:HB3	2.44	0.52
1:C:421:CYS:O	1:C:501:LYS:NZ	2.23	0.52
1:C:986:PRO:CG	8:D:3002:CLR:H152	2.39	0.52
8:A:2010:CLR:H193	8:A:2010:CLR:C11	2.40	0.52
1:C:801:LEU:HD12	1:C:805:LEU:HD11	1.92	0.52
1:A:56:LEU:HG	1:A:182:ASP:HB3	1.91	0.52
1:A:777:ILE:H	1:A:777:ILE:HD12	1.74	0.52
1:C:493:GLU:HG2	1:C:495:ARG:N	2.08	0.52
1:C:514:ILE:HD12	1:C:527:LEU:HD13	1.90	0.52
1:A:501:LYS:HE3	6:A:2004:ADP:N1	2.24	0.52
2:B:76:GLY:H	2:B:181:ASN:HD22	1.56	0.52
1:A:258:THR:HG23	1:A:261:GLY:N	2.24	0.51
1:C:893:ASP:OD2	1:C:897:GLN:HG3	2.10	0.51
9:D:3003:PC1:H242	8:E:101:CLR:H6	1.92	0.51
2:B:251:GLN:HB3	2:B:254:TYR:HB2	1.92	0.51
1:C:115:GLU:HG2	1:C:116:GLU:H	1.74	0.51
1:C:283:HIS:NE2	1:C:287:ILE:HD11	2.25	0.51
1:C:531:PHE:HE2	1:C:581:LEU:HD21	1.75	0.51
1:A:986:PRO:HG3	8:A:2010:CLR:H181	1.92	0.51
1:A:347:LYS:HG3	1:A:753:THR:HG21	1.92	0.51
1:A:818:GLU:OE2	1:A:931:LYS:NZ	2.39	0.51
2:B:202:MET:SD	2:B:236:PRO:HG2	2.50	0.51
1:C:43:GLU:O	1:C:46:ARG:HG2	2.10	0.51
1:C:551:LEU:HD13	1:C:576:LEU:HD23	1.92	0.51
1:C:600:ARG:HH21	1:C:680:GLU:HG2	1.76	0.51
1:C:196:LEU:HB2	1:C:236:ALA:HB3	1.93	0.51
1:C:340:THR:HG21	1:C:357:VAL:HG11	1.91	0.51
1:C:997:VAL:O	1:C:1001:ILE:HG13	2.11	0.51
1:A:263:ILE:HD12	1:A:265:THR:OG1	2.10	0.51
1:A:889:ASN:ND2	1:A:901:TYR:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD11	1:A:197:ARG:CG	2.38	0.51
1:A:986:PRO:HG3	8:A:2010:CLR:H152	1.91	0.51
1:C:827:ARG:NH1	1:C:933:ARG:HH21	2.08	0.51
3:E:24:GLU:O	3:E:28:ASN:ND2	2.43	0.51
1:C:375:THR:HA	1:C:588:PRO:HA	1.92	0.51
1:C:698:CYS:HB2	1:C:705:VAL:HG11	1.93	0.51
1:A:31:GLU:HG3	1:A:32:VAL:H	1.76	0.51
1:A:443:ASP:O	1:A:447:SER:OG	2.29	0.51
2:D:192:LYS:HZ1	2:D:205:ASN:HB3	1.75	0.51
2:B:136:ARG:HD2	2:B:143:ARG:HH12	1.76	0.50
1:C:689:GLN:O	1:C:693:ILE:HG12	2.10	0.50
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.93	0.50
1:C:972:ARG:HH12	2:D:288:LYS:HZ1	1.59	0.50
1:C:782:PRO:HG3	1:C:795:LEU:HD23	1.94	0.50
1:C:376:GLN:HG3	1:C:589:ARG:HA	1.93	0.50
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.73	0.50
1:A:185:GLU:HG3	1:A:248:ARG:HG2	1.93	0.50
1:A:211:LEU:HD12	1:A:260:MET:SD	2.52	0.50
1:A:298:SER:HB2	9:A:2014:PC1:H3F1	1.93	0.50
2:B:90:PHE:CZ	2:B:174:PRO:HG3	2.46	0.50
1:C:824:ILE:HD12	1:C:825:MET:H	1.77	0.50
2:D:117:GLN:HB3	2:D:150:ARG:HD3	1.93	0.50
1:A:769:ILE:HA	1:A:772:THR:HG22	1.94	0.50
2:B:280:GLY:HA3	2:B:283:ILE:HD13	1.94	0.50
1:C:757:GLU:O	1:C:761:ILE:HG22	2.11	0.50
1:A:620:ILE:O	1:A:624:VAL:HG13	2.12	0.49
8:D:3002:CLR:C11	8:D:3002:CLR:C14	2.89	0.49
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.93	0.49
1:A:759:ARG:HH22	1:A:829:PRO:HG3	1.76	0.49
1:A:781:THR:HG22	8:A:2009:CLR:C27	2.41	0.49
1:C:131:ALA:O	1:C:135:ILE:HG12	2.12	0.49
2:D:56:VAL:HG11	8:D:3002:CLR:H122	1.92	0.49
8:A:2009:CLR:H191	2:B:39:TYR:CZ	2.46	0.49
1:A:928:VAL:O	1:A:931:LYS:HB3	2.12	0.49
1:A:998:ARG:HA	1:A:1001:ILE:HD12	1.94	0.49
2:B:191:PRO:HG3	2:B:280:GLY:HA2	1.93	0.49
2:B:35:ILE:HG13	2:B:36:LEU:N	2.26	0.49
9:C:2009:PC1:H391	9:C:2009:PC1:H291	1.94	0.49
1:C:503:ALA:HB1	1:C:685:ARG:NH1	2.26	0.49
2:D:178:ILE:HD11	2:D:276:CYS:SG	2.52	0.49
2:D:251:GLN:HB3	2:D:254:TYR:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:VAL:HG22	1:A:583:SER:HB3	1.94	0.49
2:B:138:GLU:HG3	2:B:140:ASN:ND2	2.27	0.49
2:B:42:PHE:HD2	2:B:43:TYR:CD1	2.30	0.49
1:C:861:THR:O	1:C:865:ILE:HD12	2.12	0.49
1:C:430:GLN:HA	1:C:430:GLN:HE21	1.76	0.49
1:C:93:PHE:CZ	1:C:285:ILE:HG23	2.48	0.49
1:A:192:ILE:HD12	1:A:236:ALA:HB1	1.95	0.49
1:A:413:ALA:O	1:A:417:ILE:HG23	2.12	0.49
1:A:454:GLU:HG2	1:A:460:VAL:HG23	1.94	0.49
2:B:37:LEU:O	2:B:41:ILE:HG23	2.13	0.49
1:C:777:ILE:CD1	1:C:847:TYR:HA	2.43	0.49
2:D:57:MET:HA	8:D:3002:CLR:H11	1.93	0.49
8:E:101:CLR:C11	8:E:101:CLR:C19	2.90	0.49
8:G:101:CLR:H183	8:G:101:CLR:H212	1.94	0.49
1:A:688:PRO:HG3	1:A:713:ASN:HB2	1.94	0.49
8:D:3002:CLR:C11	8:D:3002:CLR:C19	2.91	0.49
2:D:36:LEU:O	2:D:40:VAL:HG23	2.13	0.49
1:A:191:ARG:HA	1:A:241:ASN:HB3	1.95	0.49
1:A:283:HIS:O	1:A:287:ILE:HG12	2.12	0.49
1:A:317:LEU:O	1:A:321:ILE:HG12	2.13	0.49
1:A:710:ASP:OD1	1:A:711:GLY:N	2.44	0.49
1:A:861:THR:HG22	1:A:983:CYS:HB3	1.95	0.49
1:A:777:ILE:CD1	1:A:847:TYR:HA	2.42	0.49
1:A:882:ASN:HB3	1:A:888:ILE:HD12	1.95	0.49
2:B:157:GLY:H	2:B:230:PHE:HB3	1.78	0.49
1:C:607:ILE:HG23	1:C:681:ILE:HG13	1.93	0.49
2:D:90:PHE:CZ	2:D:174:PRO:HG3	2.48	0.49
1:C:1009:TRP:HZ2	2:D:35:ILE:HG22	1.78	0.48
1:C:426:PHE:CE2	1:C:454:GLU:HG3	2.47	0.48
1:C:763:ASP:O	1:C:767:LYS:HG3	2.13	0.48
2:D:214:THR:OG1	2:D:215:GLY:N	2.45	0.48
2:B:91:ARG:NH2	2:D:94:ASP:OD1	2.45	0.48
1:C:50:THR:HG21	1:C:181:GLY:C	2.33	0.48
1:C:611:GLY:O	6:C:2004:ADP:H5'2	2.12	0.48
8:D:3001:CLR:H121	8:D:3001:CLR:C21	2.40	0.48
1:A:944:ASN:ND2	1:A:947:LEU:HB2	2.29	0.48
2:B:14:LYS:HZ3	2:B:17:TRP:HE3	1.61	0.48
1:A:182:ASP:O	1:A:251:VAL:HG23	2.13	0.48
2:B:268:MET:HA	2:B:301:VAL:HG23	1.95	0.48
1:A:752:VAL:O	1:A:755:VAL:HG12	2.13	0.48
1:C:1001:ILE:CG2	1:C:1010:VAL:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2010:CLR:H111	8:A:2010:CLR:C19	2.44	0.48
1:A:340:THR:HG21	1:A:761:ILE:CD1	2.43	0.48
1:A:937:VAL:HG21	1:A:992:PHE:CE1	2.49	0.48
2:B:209:LEU:HD12	2:B:210:PRO:HD2	1.96	0.48
1:A:185:GLU:HG3	1:A:248:ARG:CG	2.43	0.48
1:A:838:VAL:HG13	1:A:842:LEU:HD22	1.95	0.48
2:B:36:LEU:O	2:B:40:VAL:HG23	2.14	0.48
1:C:565:ASP:CB	1:C:570:ASN:HD22	2.26	0.48
3:G:38:PHE:O	3:G:42:LEU:HG	2.12	0.48
1:A:565:ASP:HB3	1:A:570:ASN:HB2	1.95	0.48
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.49	0.48
2:D:192:LYS:NZ	2:D:205:ASN:HB3	2.29	0.48
2:D:216:LYS:HD2	2:D:216:LYS:H	1.77	0.48
1:C:899:TRP:CE3	2:D:72:VAL:HG13	2.49	0.48
8:E:101:CLR:C21	8:E:101:CLR:H121	2.43	0.48
1:A:387:ASP:O	1:A:389:GLN:N	2.46	0.48
1:A:777:ILE:N	1:A:777:ILE:HD12	2.29	0.48
1:A:793:LEU:O	1:A:912:HIS:NE2	2.43	0.48
1:C:147:SER:HB2	1:C:338:THR:HG23	1.96	0.48
1:C:556:GLU:N	1:C:556:GLU:OE1	2.43	0.48
1:C:613:HIS:CD2	1:C:615:ILE:HB	2.48	0.48
1:C:692:LEU:O	1:C:696:GLU:HB2	2.14	0.48
8:A:2009:CLR:H111	8:A:2009:CLR:C19	2.44	0.47
9:A:2013:PC1:H261	9:A:2013:PC1:H291	1.68	0.47
1:A:303:SER:O	1:A:308:TYR:HB2	2.14	0.47
1:A:37:HIS:CE1	1:A:229:PRO:HG3	2.49	0.47
2:D:204:TYR:CE2	2:D:207:TYR:HB2	2.48	0.47
2:D:52:GLY:O	2:D:56:VAL:HG23	2.13	0.47
1:A:1009:TRP:CE2	1:A:1013:GLU:HG3	2.48	0.47
2:B:277:LYS:HD2	2:B:279:TYR:CE2	2.49	0.47
2:B:38:PHE:HD2	2:B:39:TYR:CD1	2.32	0.47
1:A:956:ALA:HB2	3:G:37:ALA:HB3	1.95	0.47
1:A:815:LEU:HA	1:A:815:LEU:HD12	1.71	0.47
8:D:3001:CLR:H111	8:D:3001:CLR:H193	1.96	0.47
2:D:17:TRP:CZ2	2:D:19:SER:HB3	2.49	0.47
1:A:402:VAL:HG21	1:A:404:PHE:CZ	2.49	0.47
2:B:99:GLU:O	2:B:103:VAL:HG23	2.14	0.47
1:C:103:LEU:HD12	1:C:318:ILE:HD11	1.95	0.47
9:D:3003:PC1:H282	9:D:3003:PC1:H2B2	1.60	0.47
2:B:204:TYR:HB3	2:B:208:VAL:HB	1.97	0.47
1:A:512:SER:OG	1:A:575:ASN:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:CYS:SG	1:A:741:MET:HG2	2.55	0.47
1:A:790:ASN:C	1:A:880:ARG:HB2	2.35	0.47
1:A:803:ILE:HG23	1:A:919:ILE:HG21	1.96	0.47
2:B:131:SER:HB2	2:B:241:GLN:HB3	1.97	0.47
2:B:186:PHE:CZ	2:B:282:ASN:HB3	2.50	0.47
1:C:25:MET:O	1:C:29:LYS:HG3	2.15	0.47
1:C:804:ASP:O	1:C:808:ASP:HB2	2.15	0.47
2:D:98:TYR:CZ	2:D:171:ASP:HB3	2.50	0.47
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.71	0.47
2:B:170:LYS:N	2:B:170:LYS:HD2	2.30	0.47
2:B:173:LYS:HA	2:B:174:PRO:HD3	1.79	0.47
2:D:102:VAL:HA	2:D:105:ILE:HG22	1.95	0.47
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.78	0.47
2:D:49:ILE:O	2:D:53:THR:HG22	2.14	0.47
1:A:814:SER:HB2	1:A:946:ILE:HG22	1.97	0.47
1:A:861:THR:HG22	1:A:983:CYS:CB	2.45	0.47
1:A:864:VAL:HG22	2:B:57:MET:SD	2.54	0.47
1:C:613:HIS:CD2	1:C:615:ILE:H	2.32	0.47
1:A:188:GLY:HA2	1:A:244:GLU:HA	1.97	0.46
1:A:920:VAL:HG13	1:A:954:GLU:HG2	1.97	0.46
1:C:972:ARG:HH12	2:D:288:LYS:NZ	2.12	0.46
1:A:504:PRO:HB3	1:A:581:LEU:CD2	2.45	0.46
1:C:544:ARG:NH2	6:C:2004:ADP:O1B	2.48	0.46
2:D:277:LYS:HD2	2:D:279:TYR:CE2	2.51	0.46
3:E:39:ILE:O	3:E:43:ILE:HG12	2.15	0.46
1:C:778:PRO:HB3	1:C:855:ALA:HA	1.97	0.46
1:C:901:TYR:OH	1:C:905:LYS:HE3	2.15	0.46
3:E:47:SER:OG	3:E:47:SER:O	2.29	0.46
1:A:670:GLN:O	1:A:674:ILE:HG13	2.15	0.46
1:C:83:VAL:O	1:C:87:ARG:HG2	2.15	0.46
1:A:280:GLU:OE1	1:A:830:ARG:NH2	2.48	0.46
1:C:370:LYS:HB2	1:C:610:THR:HB	1.97	0.46
1:C:430:GLN:O	1:C:432:ASN:N	2.41	0.46
1:C:914:ALA:O	1:C:918:SER:N	2.44	0.46
2:D:101:TYR:O	2:D:104:SER:OG	2.33	0.46
1:A:985:PHE:HZ	8:G:101:CLR:H221	1.80	0.46
1:A:301:ILE:HD11	9:A:2014:PC1:H311	1.98	0.46
1:C:324:ASN:N	1:C:324:ASN:HD22	2.13	0.46
1:A:488:ASN:OD1	1:A:490:ASN:ND2	2.49	0.46
1:A:827:ARG:NH2	1:A:934:ARG:HD3	2.30	0.46
1:A:85:PHE:CZ	1:A:138:CYS:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:LYS:HD3	2:B:68:TYR:CZ	2.50	0.46
2:B:49:ILE:O	2:B:53:THR:HG22	2.16	0.46
2:D:23:GLU:HG2	2:D:24:PHE:H	1.81	0.46
1:A:36:ASP:HB3	1:A:39:LEU:HD12	1.97	0.46
1:A:410:THR:HG23	1:A:515:LEU:HD22	1.98	0.46
1:A:551:LEU:HD12	1:A:576:LEU:HD23	1.97	0.46
1:A:847:TYR:CD2	9:A:2011:PC1:H381	2.51	0.46
1:C:1002:ILE:HG23	1:C:1011:GLU:HB2	1.98	0.46
1:C:781:THR:N	1:C:782:PRO:HD2	2.31	0.46
1:A:473:ILE:HG12	1:A:473:ILE:H	1.64	0.46
1:A:898:GLN:OE1	2:B:181:ASN:HA	2.16	0.46
1:A:968:GLY:HA2	1:A:973:MET:N	2.30	0.46
1:C:935:ASN:HA	1:C:1003:ARG:HD3	1.98	0.46
1:C:383:HIS:CD2	1:C:392:GLU:HG2	2.51	0.46
1:C:883:TRP:HZ2	1:C:908:GLU:HB2	1.81	0.46
1:C:901:TYR:HA	1:C:904:ARG:CZ	2.46	0.46
1:A:781:THR:HG22	8:A:2009:CLR:H273	1.98	0.45
1:C:75:PRO:O	1:C:77:PRO:HD3	2.16	0.45
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.97	0.45
2:D:76:GLY:H	2:D:181:ASN:HD22	1.62	0.45
1:A:977:LYS:HG2	3:G:21:TYR:CE2	2.52	0.45
1:A:1016:TYR:N	1:A:1016:TYR:CD1	2.84	0.45
1:A:226:ASN:HB3	1:A:231:GLU:HB2	1.99	0.45
1:C:589:ARG:NH1	1:C:746:ASP:HB3	2.32	0.45
1:C:360:LEU:HA	1:C:723:ILE:HD13	1.98	0.45
2:D:180:LEU:HD13	2:D:181:ASN:N	2.30	0.45
2:D:275:GLU:HA	2:D:295:PHE:O	2.15	0.45
1:A:747:ASN:HD21	1:A:749:ALA:HB3	1.80	0.45
1:A:860:PHE:CE1	2:B:53:THR:HG23	2.51	0.45
9:A:2014:PC1:H361	9:A:2014:PC1:H2B2	1.98	0.45
1:A:318:ILE:HD13	1:A:318:ILE:HA	1.81	0.45
1:A:436:LEU:HG	1:A:455:LEU:HD11	1.97	0.45
1:C:183:LEU:HB2	1:C:249:GLY:O	2.16	0.45
1:C:483:LEU:HD21	1:C:571:PHE:HE2	1.81	0.45
1:C:71:ASN:OD1	1:C:254:THR:HG22	2.17	0.45
1:C:753:THR:O	1:C:757:GLU:HG2	2.17	0.45
2:D:27:ARG:HD3	2:D:32:TRP:CE3	2.51	0.45
8:D:3001:CLR:C19	8:D:3001:CLR:C11	2.94	0.45
8:D:3002:CLR:H111	8:D:3002:CLR:C19	2.47	0.45
2:B:203:LYS:HB2	2:B:235:TYR:HE2	1.82	0.45
1:C:993:VAL:O	1:C:997:VAL:HG13	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ALA:HA	1:A:238:PHE:HB2	1.99	0.45
1:A:475:PHE:N	1:A:482:GLN:HG3	2.32	0.45
1:A:968:GLY:HA3	1:A:974:TYR:CE2	2.52	0.45
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.97	0.45
1:A:50:THR:CG2	1:A:56:LEU:HD23	2.47	0.45
1:A:445:SER:OG	1:A:544:ARG:NH1	2.50	0.45
2:B:157:GLY:N	2:B:230:PHE:HB3	2.32	0.45
1:C:886:ARG:HA	1:C:901:TYR:CD1	2.51	0.45
2:D:24:PHE:C	2:D:26:GLY:H	2.20	0.45
1:A:1001:ILE:HG21	1:A:1010:VAL:HG21	1.99	0.45
1:A:977:LYS:N	1:A:980:TRP:CD1	2.80	0.45
2:B:134:LYS:HB2	2:B:136:ARG:HH12	1.82	0.45
2:B:91:ARG:HH21	2:B:94:ASP:HB2	1.82	0.45
2:B:95:PRO:HA	2:B:98:TYR:CE1	2.51	0.45
1:C:425:VAL:HG12	1:C:426:PHE:O	2.16	0.45
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.47	0.45
2:D:95:PRO:HA	2:D:98:TYR:CE1	2.52	0.45
1:A:214:GLU:HB2	1:A:216:GLU:HG3	1.99	0.45
2:B:98:TYR:HA	2:B:101:TYR:HD1	1.81	0.45
1:C:55:GLY:HA2	1:C:183:LEU:HD22	1.98	0.45
1:C:565:ASP:OD2	1:C:568:ASP:HB2	2.16	0.45
1:C:977:LYS:HG2	3:E:21:TYR:HE2	1.82	0.45
1:C:565:ASP:HB2	1:C:570:ASN:HD22	1.82	0.45
1:C:611:GLY:HA2	1:C:686:THR:H	1.82	0.45
1:A:654:LYS:HD3	1:A:654:LYS:HA	1.75	0.44
1:A:927:LEU:HD11	1:A:947:LEU:HG	1.99	0.44
1:C:695:VAL:O	1:C:699:GLN:HG3	2.18	0.44
8:A:2009:CLR:H193	8:A:2009:CLR:C11	2.47	0.44
1:A:238:PHE:CD2	1:A:258:THR:HG21	2.52	0.44
2:B:203:LYS:HB3	2:B:203:LYS:HE2	1.82	0.44
2:B:42:PHE:HD2	2:B:43:TYR:HD1	1.63	0.44
9:C:2009:PC1:H3H2	9:C:2012:PC1:H2H1	1.99	0.44
2:D:37:LEU:O	2:D:41:ILE:HG23	2.16	0.44
9:A:2012:PC1:H2A2	9:A:2012:PC1:H2E2	1.99	0.44
1:A:450:LEU:HD23	1:A:460:VAL:HG21	1.99	0.44
1:A:81:GLU:HG3	1:A:82:TRP:H	1.83	0.44
1:A:900:THR:HG23	1:A:903:GLN:NE2	2.33	0.44
2:D:204:TYR:HD2	2:D:207:TYR:H	1.65	0.44
3:G:45:ILE:HA	3:G:45:ILE:HD12	1.71	0.44
1:A:756:GLU:HB2	1:A:825:MET:SD	2.57	0.44
1:C:199:ILE:HA	1:C:199:ILE:HD13	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:GLY:O	1:C:893:ASP:HB2	2.18	0.44
1:C:929:ILE:HB	1:C:995:ASP:OD2	2.16	0.44
8:D:3001:CLR:H212	8:D:3001:CLR:C12	2.42	0.44
2:D:88:ILE:HG23	2:D:101:TYR:CE2	2.52	0.44
1:A:350:LEU:HB2	1:A:744:LEU:HD21	1.98	0.44
1:A:695:VAL:O	1:A:699:GLN:HG3	2.17	0.44
1:C:460:VAL:HG12	1:C:464:ARG:HE	1.82	0.44
1:C:487:LYS:HB3	1:C:487:LYS:HE2	1.85	0.44
1:C:592:VAL:O	1:C:596:VAL:HG13	2.18	0.44
3:E:28:ASN:O	3:E:32:ILE:HG12	2.17	0.44
1:A:315:ILE:HA	1:A:315:ILE:HD13	1.88	0.44
1:A:763:ASP:O	1:A:767:LYS:HG3	2.18	0.44
1:A:821:GLU:HA	1:A:940:GLN:OE1	2.17	0.44
2:B:204:TYR:CE2	2:B:207:TYR:HB2	2.52	0.44
1:C:305:ILE:C	1:C:307:GLU:H	2.21	0.44
2:D:31:SER:O	2:D:35:ILE:HG23	2.17	0.44
1:A:1001:ILE:O	1:A:1005:ARG:HB2	2.17	0.44
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.98	0.44
1:C:613:HIS:NE2	1:C:615:ILE:HD13	2.32	0.44
2:D:98:TYR:OH	2:D:171:ASP:HB3	2.18	0.44
1:A:618:LYS:O	1:A:621:ALA:HB3	2.17	0.44
2:B:17:TRP:CZ2	2:B:19:SER:HB3	2.52	0.44
9:A:2013:PC1:H2C2	9:B:401:PC1:H3I1	1.99	0.44
1:C:228:ASN:HA	1:C:229:PRO:HD3	1.86	0.44
1:C:759:ARG:HE	1:C:825:MET:CE	2.30	0.44
1:A:303:SER:HB2	1:A:308:TYR:CD2	2.52	0.44
1:A:488:ASN:O	1:A:493:GLU:HG3	2.17	0.44
1:A:724:GLY:N	1:A:740:ASP:OD2	2.41	0.44
9:A:2013:PC1:H3F1	9:B:401:PC1:H3H2	2.00	0.44
1:C:1001:ILE:HG21	1:C:1010:VAL:HG21	1.99	0.44
1:C:841:ARG:HB2	1:C:1016:TYR:HA	2.00	0.44
1:C:925:ALA:O	1:C:929:ILE:HG12	2.18	0.44
8:A:2010:CLR:C11	8:A:2010:CLR:C1	2.95	0.43
9:A:2013:PC1:H122	9:A:2013:PC1:H11	1.99	0.43
1:A:300:PHE:HE1	1:A:314:VAL:HG12	1.83	0.43
1:A:609:VAL:O	1:A:691:LYS:HE2	2.18	0.43
1:C:50:THR:CG2	1:C:56:LEU:HD23	2.44	0.43
1:C:794:PRO:HG2	1:C:859:PHE:HE2	1.83	0.43
2:D:157:GLY:H	2:D:230:PHE:HB3	1.83	0.43
1:A:781:THR:HA	1:A:784:LEU:HD12	2.00	0.43
2:B:88:ILE:HG23	2:B:101:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ILE:HG13	1:C:604:ILE:HG21	2.00	0.43
1:C:505:GLU:OE2	1:C:613:HIS:ND1	2.49	0.43
2:D:62:SER:C	2:D:64:PHE:H	2.22	0.43
8:A:2009:CLR:H121	8:A:2009:CLR:C21	2.46	0.43
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.84	0.43
1:C:258:THR:HG23	1:C:261:GLY:N	2.31	0.43
1:C:430:GLN:HE21	1:C:433:LEU:HD21	1.83	0.43
1:C:503:ALA:HA	1:C:504:PRO:HD3	1.88	0.43
2:D:209:LEU:HD12	2:D:210:PRO:HD2	2.00	0.43
1:A:115:GLU:HG2	1:A:116:GLU:N	2.34	0.43
1:A:206:VAL:HA	1:A:242:CYS:HA	2.00	0.43
1:A:35:ASP:HB2	1:A:37:HIS:CE1	2.53	0.43
1:A:418:ALA:O	1:A:422:ASN:HB2	2.18	0.43
1:A:471:VAL:HG21	1:A:564:PHE:HB2	2.00	0.43
1:A:624:VAL:CG2	1:A:626:ILE:HG12	2.49	0.43
1:A:697:GLY:HA2	1:A:700:ARG:NH2	2.34	0.43
1:C:483:LEU:HD12	1:C:484:SER:N	2.33	0.43
1:C:514:ILE:HG22	1:C:516:ILE:HG12	2.01	0.43
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.99	0.43
2:D:178:ILE:HD13	2:D:211:VAL:HG11	2.01	0.43
2:D:203:LYS:HE2	2:D:203:LYS:HB3	1.79	0.43
3:G:39:ILE:O	3:G:43:ILE:HG12	2.19	0.43
1:A:292:ALA:O	1:A:321:ILE:HD13	2.18	0.43
1:A:621:ALA:O	1:A:626:ILE:N	2.49	0.43
1:A:815:LEU:O	1:A:818:GLU:HB2	2.18	0.43
1:A:977:LYS:HG2	3:G:21:TYR:HE2	1.83	0.43
2:B:186:PHE:HZ	2:B:282:ASN:HB3	1.84	0.43
1:A:864:VAL:HA	2:B:57:MET:SD	2.58	0.43
2:B:98:TYR:CZ	2:B:171:ASP:HB3	2.54	0.43
1:C:372:GLY:O	1:C:589:ARG:NH2	2.52	0.43
1:C:612:ASP:O	1:C:684:ALA:HB1	2.19	0.43
1:C:654:LYS:HB3	1:C:679:THR:HG22	2.00	0.43
2:D:113:LYS:HA	2:D:153:LEU:HD11	2.01	0.43
1:C:963:TYR:CZ	8:E:101:CLR:H21	2.53	0.43
1:A:1009:TRP:CZ2	1:A:1013:GLU:HG3	2.54	0.43
1:A:752:VAL:HA	1:A:755:VAL:HG12	2.01	0.43
1:A:781:THR:N	1:A:782:PRO:HD2	2.34	0.43
2:B:123:PHE:HB3	2:B:150:ARG:HG3	2.00	0.43
2:B:62:SER:OG	2:B:65:LYS:HG2	2.19	0.43
1:C:263:ILE:HG13	1:C:267:ALA:HA	1.99	0.43
1:C:549:CYS:HB2	1:C:577:CYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:900:THR:H	1:C:903:GLN:HE21	1.67	0.43
2:D:277:LYS:HG2	2:D:285:TYR:CE2	2.54	0.43
2:B:88:ILE:HG23	2:B:101:TYR:CD2	2.54	0.43
1:C:462:GLU:O	1:C:466:ARG:HG3	2.18	0.43
1:A:358:GLU:O	1:A:361:GLY:N	2.45	0.43
1:A:654:LYS:O	1:A:679:THR:HG22	2.19	0.43
1:A:692:LEU:HD12	1:A:716:PRO:HB2	2.01	0.43
1:A:901:TYR:HA	1:A:904:ARG:CZ	2.49	0.43
1:A:957:LEU:HD22	1:A:957:LEU:HA	1.87	0.43
1:C:89:LEU:HD22	1:C:134:ILE:HD13	2.01	0.43
2:D:204:TYR:HB3	2:D:208:VAL:HB	2.00	0.43
2:D:39:TYR:CE2	8:D:3001:CLR:H182	2.54	0.43
2:D:90:PHE:O	2:D:92:PRO:HD3	2.19	0.43
1:A:571:PHE:HB2	1:A:572:PRO:HD2	2.00	0.42
1:C:410:THR:HG23	1:C:515:LEU:HD22	2.00	0.42
1:C:483:LEU:HD12	1:C:484:SER:H	1.84	0.42
2:D:62:SER:OG	2:D:65:LYS:HG2	2.19	0.42
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.53	0.42
1:A:366:ILE:HG13	1:A:604:ILE:HG21	2.01	0.42
1:A:841:ARG:HH11	1:A:841:ARG:HG3	1.82	0.42
1:C:55:GLY:HA3	1:C:165:ILE:O	2.19	0.42
1:C:340:THR:CG2	1:C:357:VAL:HG11	2.48	0.42
1:C:360:LEU:HG	1:C:723:ILE:HD13	2.00	0.42
1:C:514:ILE:HG12	1:C:578:PHE:HB3	2.00	0.42
1:C:982:PHE:O	1:C:985:PHE:HB2	2.19	0.42
1:A:483:LEU:HD12	1:A:499:VAL:O	2.18	0.42
1:A:565:ASP:OD2	1:A:568:ASP:HB2	2.17	0.42
1:A:765:LEU:O	1:A:769:ILE:HG13	2.19	0.42
2:B:47:ALA:O	2:B:51:ILE:HG13	2.19	0.42
2:D:238:PHE:CD1	2:D:257:PRO:HB2	2.54	0.42
1:A:430:GLN:HB3	1:A:438:ARG:HB3	2.01	0.42
1:A:503:ALA:HB3	1:A:506:ARG:HB2	2.02	0.42
1:A:450:LEU:HB3	1:A:451:LYS:H	1.73	0.42
1:A:600:ARG:NH1	1:A:600:ARG:HG2	2.11	0.42
1:C:31:GLU:HG3	1:C:32:VAL:N	2.31	0.42
1:A:293:VAL:HA	1:A:321:ILE:CD1	2.50	0.42
1:A:470:ILE:H	1:A:470:ILE:HG13	1.70	0.42
1:A:503:ALA:HA	1:A:504:PRO:HD3	1.78	0.42
1:A:538:LEU:HA	1:A:538:LEU:HD23	1.76	0.42
2:B:177:ILE:HD11	2:B:258:LEU:HD13	2.00	0.42
2:B:180:LEU:HD13	2:B:181:ASN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:ARG:HG3	2:B:31:SER:HB3	2.02	0.42
9:C:2011:PC1:H272	9:C:2011:PC1:H2A1	1.70	0.42
1:C:209:SER:HB3	1:C:215:SER:HA	2.02	0.42
1:C:479:ASN:O	1:C:480:LYS:HB2	2.20	0.42
1:C:899:TRP:CH2	2:D:72:VAL:HG22	2.55	0.42
3:E:18:PRO:HB2	3:E:19:PHE:H	1.52	0.42
1:A:778:PRO:HB3	1:A:855:ALA:HA	2.00	0.42
1:A:867:ALA:HB2	1:A:873:PRO:HD3	2.02	0.42
9:C:2012:PC1:H221	9:C:2012:PC1:H2	1.78	0.42
1:C:311:LEU:O	1:C:315:ILE:HG12	2.20	0.42
1:A:952:PHE:HD2	3:G:37:ALA:HA	1.84	0.42
1:A:187:LYS:HG2	1:A:190:ASP:OD2	2.20	0.42
1:A:331:ALA:O	1:A:335:VAL:HG23	2.20	0.42
1:A:360:LEU:HD23	1:A:723:ILE:CD1	2.50	0.42
1:A:968:GLY:HA2	1:A:973:MET:H	1.85	0.42
1:C:165:ILE:HB	1:C:183:LEU:CD2	2.44	0.42
5:C:2002:ALF:F1	6:C:2004:ADP:O3B	2.28	0.42
1:C:27:GLU:C	1:C:29:LYS:H	2.23	0.42
1:C:565:ASP:HB3	1:C:570:ASN:HB2	2.00	0.42
1:C:649:ASN:HA	1:C:650:PRO:HD3	1.91	0.42
3:E:38:PHE:CZ	3:E:42:LEU:HD11	2.55	0.42
1:A:192:ILE:CD1	1:A:236:ALA:HB1	2.50	0.42
1:A:587:PRO:HA	1:A:588:PRO:HD3	1.92	0.42
9:C:2009:PC1:H132	9:C:2009:PC1:H112	1.80	0.42
1:C:24:ASP:OD2	1:C:26:ASP:HB2	2.20	0.42
1:C:422:ASN:OD1	1:C:446:GLU:HB3	2.20	0.42
1:C:535:TYR:CE2	1:C:545:VAL:HB	2.55	0.42
2:D:190:PRO:HA	2:D:191:PRO:HD3	1.85	0.42
2:D:277:LYS:HB3	2:D:279:TYR:CE1	2.55	0.42
8:G:101:CLR:C12	8:G:101:CLR:C9	2.89	0.42
1:A:609:VAL:CG1	1:A:691:LYS:HG2	2.49	0.41
1:A:638:ALA:HB2	1:A:648:VAL:CG2	2.49	0.41
1:A:854:GLN:NE2	1:A:923:GLN:HE21	2.16	0.41
1:C:606:VAL:HG11	1:C:626:ILE:HD12	2.00	0.41
1:A:48:TYR:OH	1:A:252:VAL:HB	2.20	0.41
1:A:864:VAL:HG13	2:B:57:MET:HG3	2.01	0.41
2:B:57:MET:HE3	2:B:58:LEU:HA	2.02	0.41
1:C:791:ILE:HG12	1:C:792:PRO:O	2.20	0.41
8:D:3002:CLR:H212	8:D:3002:CLR:C12	2.49	0.41
1:A:471:VAL:HG11	1:A:566:THR:HB	2.02	0.41
1:A:827:ARG:HH21	1:A:934:ARG:HD3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:GLU:O	1:C:911:CYS:HB2	2.19	0.41
1:A:301:ILE:HG13	1:A:302:LEU:N	2.36	0.41
1:A:387:ASP:C	1:A:389:GLN:H	2.23	0.41
1:C:368:SER:HB2	1:C:708:THR:OG1	2.20	0.41
1:C:519:LYS:HG2	1:C:519:LYS:H	1.69	0.41
1:C:883:TRP:O	1:C:904:ARG:HD2	2.21	0.41
2:D:300:GLU:HG2	2:D:302:LYS:HB2	2.01	0.41
2:D:71:ARG:HA	2:D:71:ARG:HE	1.85	0.41
1:C:293:VAL:HA	1:C:321:ILE:HD12	2.02	0.41
1:C:460:VAL:CG1	1:C:464:ARG:HH21	2.32	0.41
1:C:803:ILE:HD12	1:C:919:ILE:HG21	2.03	0.41
2:D:216:LYS:HE2	2:D:273:ARG:O	2.21	0.41
2:D:277:LYS:HB3	2:D:279:TYR:CZ	2.54	0.41
1:C:1009:TRP:CZ2	2:D:35:ILE:HG22	2.55	0.41
2:D:57:MET:HE2	2:D:58:LEU:HA	2.03	0.41
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.89	0.41
1:A:966:GLY:O	1:A:969:VAL:HG22	2.21	0.41
2:B:179:LYS:HE2	2:B:179:LYS:HB3	1.80	0.41
2:B:24:PHE:HA	2:B:24:PHE:HD2	1.73	0.41
2:B:62:SER:C	2:B:64:PHE:H	2.23	0.41
6:C:2004:ADP:H3'	6:C:2004:ADP:O2B	2.19	0.41
1:C:32:VAL:O	1:C:262:ARG:NH1	2.54	0.41
2:D:35:ILE:HG13	2:D:36:LEU:N	2.36	0.41
1:A:370:LYS:HB2	1:A:610:THR:HB	2.02	0.41
1:A:430:GLN:C	1:A:432:ASN:H	2.24	0.41
1:A:866:LEU:HD13	1:A:876:LEU:HD21	2.02	0.41
2:B:216:LYS:HE2	2:B:273:ARG:HB2	2.02	0.41
1:C:763:ASP:HB3	1:C:767:LYS:HE3	2.03	0.41
1:C:861:THR:HG22	1:C:983:CYS:HB3	2.02	0.41
8:D:3001:CLR:C1	8:D:3001:CLR:C11	2.99	0.41
1:A:274:GLN:HB3	1:A:274:GLN:HE21	1.59	0.41
1:A:337:LEU:HD12	1:A:337:LEU:HA	1.90	0.41
1:A:369:ASP:HB3	1:A:373:THR:OG1	2.21	0.41
9:C:2009:PC1:H272	8:D:3001:CLR:H14	2.03	0.41
1:C:589:ARG:HD3	1:C:746:ASP:O	2.20	0.41
1:C:777:ILE:HD12	1:C:777:ILE:N	2.32	0.41
8:D:3002:CLR:C11	8:D:3002:CLR:C1	2.98	0.41
8:G:101:CLR:C21	8:G:101:CLR:H121	2.50	0.41
1:A:402:VAL:HG21	1:A:404:PHE:CE1	2.55	0.41
2:B:204:TYR:HD2	2:B:207:TYR:H	1.68	0.41
2:B:66:PRO:HG2	2:B:69:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:VAL:HG11	1:C:566:THR:HB	2.03	0.41
1:C:613:HIS:HD2	1:C:615:ILE:H	1.68	0.41
1:C:857:GLY:O	1:C:861:THR:HG23	2.20	0.41
1:A:505:GLU:CD	1:A:685:ARG:HH11	2.24	0.41
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.86	0.41
1:A:537:GLU:O	1:A:541:LEU:HD22	2.20	0.41
9:C:2009:PC1:H3C2	9:C:2009:PC1:H2A1	2.03	0.41
1:C:953:GLU:OE2	3:E:41:GLY:HA3	2.20	0.41
1:A:629:GLU:OE1	1:A:629:GLU:N	2.55	0.40
1:A:648:VAL:HG23	1:A:648:VAL:H	1.68	0.40
1:A:870:GLY:O	1:A:893:ASP:HB2	2.21	0.40
2:B:91:ARG:HG3	2:B:302:LYS:O	2.21	0.40
2:B:74:PRO:HA	2:B:75:PRO:HD3	1.86	0.40
1:C:565:ASP:N	1:C:570:ASN:HB2	2.28	0.40
1:C:900:THR:H	1:C:903:GLN:NE2	2.19	0.40
2:D:188:PRO:HG2	2:D:243:TYR:CD1	2.57	0.40
8:G:101:CLR:H121	8:G:101:CLR:H212	2.03	0.40
1:A:189:GLY:HA2	1:A:734:VAL:HG21	2.04	0.40
1:A:95:MET:HE3	1:A:96:LEU:N	2.36	0.40
1:A:998:ARG:NH1	1:A:999:LYS:HG3	2.37	0.40
1:C:318:ILE:O	1:C:322:VAL:HG23	2.20	0.40
1:C:476:ASN:O	1:C:478:THR:N	2.53	0.40
1:C:783:PHE:O	1:C:787:ILE:HG13	2.21	0.40
1:C:784:LEU:O	1:C:788:ILE:HG12	2.20	0.40
1:C:799:THR:O	1:C:803:ILE:HG12	2.21	0.40
2:D:170:LYS:N	2:D:170:LYS:HD2	2.36	0.40
2:D:5:LYS:HB3	2:D:6:ALA:H	1.73	0.40
3:E:15:ASP:HB3	3:E:16:VAL:H	1.64	0.40
9:A:2012:PC1:H152	9:A:2012:PC1:H112	1.88	0.40
1:A:309:THR:HG23	1:A:312:GLU:HB2	2.02	0.40
1:A:793:LEU:HD12	1:A:794:PRO:HD2	2.02	0.40
2:B:126:CYS:HB3	2:B:241:GLN:OE1	2.21	0.40
1:C:111:GLN:HB3	1:C:118:PRO:CB	2.51	0.40
1:C:84:LYS:HE2	1:C:84:LYS:HB3	1.93	0.40
1:C:850:ILE:O	1:C:854:GLN:HG3	2.21	0.40
2:D:235:TYR:HA	2:D:236:PRO:HD3	1.70	0.40
8:A:2010:CLR:H191	8:A:2010:CLR:H8	1.92	0.40
9:A:2013:PC1:H381	9:A:2013:PC1:H2C1	2.02	0.40
2:B:94:ASP:HA	2:B:95:PRO:HD3	1.84	0.40
1:C:214:GLU:HB2	1:C:216:GLU:HG3	2.03	0.40
1:C:301:ILE:O	1:C:305:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ASP:C	1:C:407:THR:H	2.23	0.40
1:C:748:PHE:O	1:C:751:ILE:HD12	2.21	0.40
1:C:854:GLN:NE2	1:C:923:GLN:HE21	2.17	0.40
2:D:265:ASN:HD22	2:D:267:THR:HG23	1.87	0.40
1:A:921:VAL:HG12	1:A:988:SER:HB2	2.03	0.40
1:C:790:ASN:C	1:C:880:ARG:HB2	2.42	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	992/1016 (98%)	859 (87%)	114 (12%)	19 (2%)	8	26
1	C	992/1016 (98%)	884 (89%)	91 (9%)	17 (2%)	9	29
2	B	301/303 (99%)	238 (79%)	55 (18%)	8 (3%)	5	17
2	D	301/303 (99%)	231 (77%)	59 (20%)	11 (4%)	3	11
3	E	33/65 (51%)	31 (94%)	1 (3%)	1 (3%)	4	15
3	G	32/65 (49%)	27 (84%)	4 (12%)	1 (3%)	4	14
All	All	2651/2768 (96%)	2270 (86%)	324 (12%)	57 (2%)	6	22

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	VAL
2	B	82	GLN
2	B	139	TYR
3	G	18	PRO
1	C	267	ALA

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Mol	Chain	Res	Type
1	C	398	ASN
1	C	880	ARG
3	E	18	PRO
1	A	381	VAL
1	A	710	ASP
2	B	201	VAL
2	B	204	TYR
2	B	265	ASN
1	C	34	MET
1	C	92	GLY
1	C	629	GLU
1	C	961	LEU
2	D	82	GLN
2	D	201	VAL
2	D	204	TYR
2	D	265	ASN
1	A	450	LEU
1	A	721	ALA
1	A	775	SER
1	A	821	GLU
2	B	133	LEU
2	B	156	LEU
1	C	167	ASN
1	C	210	SER
1	C	404	PHE
1	C	569	VAL
1	C	859	PHE
2	D	63	GLU
1	A	359	THR
1	A	451	LYS
1	A	590	ALA
2	B	142	GLU
1	C	944	ASN
2	D	194	GLU
2	D	206	PRO
1	A	92	GLY
1	A	118	PRO
1	A	394	ASP
1	C	306	LEU
1	C	835	ASP
2	D	139	TYR
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	569	VAL
2	D	25	LEU
1	C	255	GLY
2	D	73	ALA
1	A	188	GLY
1	C	402	VAL
2	D	127	GLY
1	A	91	GLY
1	A	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	844/861 (98%)	725 (86%)	119 (14%)	3 10
1	C	844/861 (98%)	755 (90%)	89 (10%)	7 20
2	B	269/269 (100%)	235 (87%)	34 (13%)	4 14
2	D	269/269 (100%)	237 (88%)	32 (12%)	5 16
3	E	29/52 (56%)	24 (83%)	5 (17%)	2 6
3	G	28/52 (54%)	26 (93%)	2 (7%)	14 39
All	All	2283/2364 (97%)	2002 (88%)	281 (12%)	4 15

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	41	LEU
1	A	44	LEU
1	A	57	THR
1	A	60	ARG
1	A	82	TRP
1	A	83	VAL
1	A	94	SER
1	A	121	ASP

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Mol	Chain	Res	Type
1	A	125	LEU
1	A	129	LEU
1	A	152	GLU
1	A	158	VAL
1	A	161	GLN
1	A	164	VAL
1	A	166	ARG
1	A	170	LYS
1	A	171	MET
1	A	172	SER
1	A	210	SER
1	A	216	GLU
1	A	239	SER
1	A	241	ASN
1	A	242	CYS
1	A	252	VAL
1	A	266	LEU
1	A	268	SER
1	A	270	LEU
1	A	274	GLN
1	A	287	ILE
1	A	308	TYR
1	A	309	THR
1	A	310	TRP
1	A	317	LEU
1	A	318	ILE
1	A	337	LEU
1	A	360	LEU
1	A	364	SER
1	A	371	THR
1	A	379	MET
1	A	380	THR
1	A	384	MET
1	A	394	ASP
1	A	396	THR
1	A	415	SER
1	A	425	VAL
1	A	430	GLN
1	A	432	ASN
1	A	433	LEU
1	A	437	LYS
1	A	445	SER

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Mol	Chain	Res	Type
1	A	447	SER
1	A	449	LEU
1	A	450	LEU
1	A	453	ILE
1	A	455	LEU
1	A	461	LYS
1	A	469	LYS
1	A	471	VAL
1	A	473	ILE
1	A	478	THR
1	A	485	ILE
1	A	487	LYS
1	A	493	GLU
1	A	495	ARG
1	A	514	ILE
1	A	515	LEU
1	A	519	LYS
1	A	521	GLN
1	A	523	LEU
1	A	535	TYR
1	A	541	LEU
1	A	589	ARG
1	A	600	ARG
1	A	624	VAL
1	A	628	SER
1	A	629	GLU
1	A	635	GLU
1	A	645	VAL
1	A	663	LEU
1	A	666	MET
1	A	667	THR
1	A	671	LEU
1	A	675	LEU
1	A	681	ILE
1	A	687	SER
1	A	705	VAL
1	A	715	SER
1	A	732	SER
1	A	740	ASP
1	A	744	LEU
1	A	747	ASN
1	A	750	SER

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Mol	Chain	Res	Type
1	A	751	ILE
1	A	753	THR
1	A	775	SER
1	A	791	ILE
1	A	805	LEU
1	A	814	SER
1	A	815	LEU
1	A	818	GLU
1	A	819	GLN
1	A	822	SER
1	A	823	ASP
1	A	824	ILE
1	A	830	ARG
1	A	835	ASP
1	A	880	ARG
1	A	881	VAL
1	A	882	ASN
1	A	900	THR
1	A	911	CYS
1	A	922	VAL
1	A	957	LEU
1	A	969	VAL
1	A	995	ASP
1	A	1004	ARG
1	A	1010	VAL
1	A	1016	TYR
2	B	22	LYS
2	B	24	PHE
2	B	27	ARG
2	B	41	ILE
2	B	45	CYS
2	B	54	ILE
2	B	57	MET
2	B	61	ILE
2	B	63	GLU
2	B	72	VAL
2	B	78	THR
2	B	90	PHE
2	B	119	ASP
2	B	129	VAL
2	B	158	ASN
2	B	162	LEU

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Mol	Chain	Res	Type
2	B	170	LYS
2	B	171	ASP
2	B	177	ILE
2	B	180	LEU
2	B	187	LYS
2	B	204	TYR
2	B	216	LYS
2	B	217	ARG
2	B	221	LYS
2	B	222	GLU
2	B	224	VAL
2	B	249	LEU
2	B	259	MET
2	B	263	PHE
2	B	290	ARG
2	B	294	ARG
2	B	295	PHE
2	B	301	VAL
3	G	24	GLU
3	G	36	LEU
1	C	35	ASP
1	C	36	ASP
1	C	41	LEU
1	C	44	LEU
1	C	56	LEU
1	C	57	THR
1	C	60	ARG
1	C	82	TRP
1	C	85	PHE
1	C	86	CYS
1	C	114	THR
1	C	129	LEU
1	C	154	PHE
1	C	161	GLN
1	C	166	ARG
1	C	172	SER
1	C	191	ARG
1	C	241	ASN
1	C	242	CYS
1	C	254	THR
1	C	274	GLN
1	C	293	VAL

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Mol	Chain	Res	Type
1	C	308	TYR
1	C	309	THR
1	C	310	TRP
1	C	317	LEU
1	C	336	CYS
1	C	360	LEU
1	C	371	THR
1	C	380	THR
1	C	394	ASP
1	C	403	SER
1	C	412	LEU
1	C	423	ARG
1	C	430	GLN
1	C	433	LEU
1	C	443	ASP
1	C	450	LEU
1	C	454	GLU
1	C	469	LYS
1	C	473	ILE
1	C	478	THR
1	C	485	ILE
1	C	493	GLU
1	C	495	ARG
1	C	514	ILE
1	C	519	LYS
1	C	520	GLU
1	C	521	GLN
1	C	523	LEU
1	C	535	TYR
1	C	541	LEU
1	C	550	HIS
1	C	589	ARG
1	C	600	ARG
1	C	629	GLU
1	C	645	VAL
1	C	662	ASP
1	C	667	THR
1	C	671	LEU
1	C	681	ILE
1	C	687	SER
1	C	708	THR
1	C	719	LYS

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Mol	Chain	Res	Type
1	C	744	LEU
1	C	747	ASN
1	C	761	ILE
1	C	772	THR
1	C	791	ILE
1	C	801	LEU
1	C	805	LEU
1	C	815	LEU
1	C	818	GLU
1	C	824	ILE
1	C	859	PHE
1	C	861	THR
1	C	869	ASN
1	C	880	ARG
1	C	886	ARG
1	C	888	ILE
1	C	894	SER
1	C	897	GLN
1	C	900	THR
1	C	969	VAL
1	C	980	TRP
1	C	998	ARG
1	C	1000	LEU
1	C	1004	ARG
1	C	1010	VAL
2	D	20	GLU
2	D	22	LYS
2	D	27	ARG
2	D	57	MET
2	D	61	ILE
2	D	63	GLU
2	D	72	VAL
2	D	78	THR
2	D	90	PHE
2	D	150	ARG
2	D	162	LEU
2	D	170	LYS
2	D	171	ASP
2	D	173	LYS
2	D	175	CYS
2	D	177	ILE
2	D	187	LYS

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Mol	Chain	Res	Type
2	D	204	TYR
2	D	208	VAL
2	D	216	LYS
2	D	217	ARG
2	D	221	LYS
2	D	222	GLU
2	D	224	VAL
2	D	249	LEU
2	D	259	MET
2	D	263	PHE
2	D	267	THR
2	D	290	ARG
2	D	294	ARG
2	D	295	PHE
2	D	301	VAL
3	E	17	ASP
3	E	20	TYR
3	E	24	GLU
3	E	36	LEU
3	E	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	156	ASN
1	A	161	GLN
1	A	274	GLN
1	A	324	ASN
1	A	388	ASN
1	A	430	GLN
1	A	479	ASN
1	A	550	HIS
1	A	699	GLN
1	A	701	GLN
1	A	747	ASN
1	A	790	ASN
1	A	854	GLN
1	A	882	ASN
1	A	889	ASN
1	A	903	GLN
1	A	923	GLN

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Mol	Chain	Res	Type
1	A	935	ASN
1	A	944	ASN
2	B	181	ASN
2	B	262	GLN
2	B	292	GLN
3	G	28	ASN
1	C	111	GLN
1	C	119	GLN
1	C	120	ASN
1	C	143	GLN
1	C	156	ASN
1	C	161	GLN
1	C	274	GLN
1	C	324	ASN
1	C	388	ASN
1	C	399	GLN
1	C	430	GLN
1	C	550	HIS
1	C	570	ASN
1	C	790	ASN
1	C	819	GLN
1	C	889	ASN
1	C	903	GLN
1	C	923	GLN
2	D	140	ASN
2	D	158	ASN
2	D	181	ASN
2	D	262	GLN
3	E	28	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLR	A	2010	-	31,31,31	4.42	11 (35%)	48,48,48	2.23	14 (29%)
8	CLR	D	3001	-	31,31,31	4.46	12 (38%)	48,48,48	2.15	15 (31%)
10	EFO	C	2013	-	57,58,58	2.26	21 (36%)	73,85,85	5.17	25 (34%)
9	PC1	C	2010	-	53,53,53	0.89	3 (5%)	59,61,61	1.37	5 (8%)
9	PC1	C	2011	-	53,53,53	0.93	5 (9%)	59,61,61	1.31	5 (8%)
9	PC1	A	2014	-	53,53,53	0.90	3 (5%)	59,61,61	1.33	4 (6%)
10	EFO	A	2015	-	57,58,58	2.18	20 (35%)	73,85,85	5.27	26 (35%)
5	ALF	C	2002	-	0,4,4	0.00	-	-	-	-
9	PC1	C	2012	-	53,53,53	0.90	3 (5%)	59,61,61	1.27	4 (6%)
11	NAG	D	3004	-	14,14,15	0.24	0	17,19,21	0.49	0
5	ALF	A	2002	-	0,4,4	0.00	-	-	-	-
9	PC1	A	2012	-	53,53,53	0.92	2 (3%)	59,61,61	1.41	7 (11%)
9	PC1	A	2013	-	53,53,53	0.88	3 (5%)	59,61,61	1.18	4 (6%)
6	ADP	A	2004	4	24,29,29	1.12	3 (12%)	29,45,45	1.50	3 (10%)
6	ADP	C	2004	-	24,29,29	0.88	0	29,45,45	1.24	3 (10%)
8	CLR	A	2009	-	31,31,31	4.44	11 (35%)	48,48,48	2.16	15 (31%)
9	PC1	A	2011	-	53,53,53	0.90	4 (7%)	59,61,61	1.31	6 (10%)
11	NAG	B	402	-	14,14,15	0.22	0	17,19,21	0.42	0
8	CLR	D	3002	-	31,31,31	4.51	12 (38%)	48,48,48	1.93	15 (31%)
9	PC1	C	2009	-	53,53,53	0.91	4 (7%)	59,61,61	1.28	5 (8%)
9	PC1	B	401	-	53,53,53	0.89	4 (7%)	59,61,61	1.30	5 (8%)
8	CLR	E	101	-	31,31,31	4.62	13 (41%)	48,48,48	2.42	14 (29%)
9	PC1	D	3003	-	53,53,53	0.90	4 (7%)	59,61,61	1.20	4 (6%)
8	CLR	G	101	-	31,31,31	4.63	13 (41%)	48,48,48	2.66	13 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLR	A	2010	-	-	1/10/68/68	0/4/4/4
8	CLR	D	3001	-	-	0/10/68/68	0/4/4/4
10	EFO	C	2013	-	-	10/72/110/110	0/2/3/3
9	PC1	C	2010	-	-	35/57/57/57	-
9	PC1	C	2011	-	-	33/57/57/57	-
9	PC1	A	2014	-	-	30/57/57/57	-
10	EFO	A	2015	-	-	9/72/110/110	0/2/3/3
9	PC1	C	2012	-	-	26/57/57/57	-
11	NAG	D	3004	-	-	1/6/23/26	0/1/1/1
9	PC1	A	2012	-	-	30/57/57/57	-
9	PC1	A	2013	-	-	30/57/57/57	-
6	ADP	A	2004	4	-	6/12/32/32	0/3/3/3
6	ADP	C	2004	-	-	1/12/32/32	0/3/3/3
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4
9	PC1	A	2011	-	-	24/57/57/57	-
11	NAG	B	402	-	-	0/6/23/26	0/1/1/1
8	CLR	D	3002	-	-	1/10/68/68	0/4/4/4
9	PC1	C	2009	-	-	27/57/57/57	-
9	PC1	B	401	-	-	32/57/57/57	-
8	CLR	E	101	-	-	0/10/68/68	0/4/4/4
9	PC1	D	3003	-	-	29/57/57/57	-
8	CLR	G	101	-	-	1/10/68/68	0/4/4/4

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	CLR	C11-C9	15.42	1.79	1.53
8	D	3002	CLR	C11-C9	14.84	1.78	1.53
8	E	101	CLR	C11-C9	14.69	1.78	1.53
8	D	3001	CLR	C11-C9	14.57	1.78	1.53
8	A	2009	CLR	C11-C9	14.11	1.77	1.53
8	A	2010	CLR	C11-C9	13.72	1.76	1.53
8	A	2010	CLR	C10-C9	-12.15	1.35	1.56
8	E	101	CLR	C10-C9	-12.12	1.35	1.56
8	A	2009	CLR	C10-C9	-12.03	1.35	1.56
8	G	101	CLR	C10-C9	-12.02	1.35	1.56
8	D	3002	CLR	C10-C9	-11.92	1.36	1.56
8	D	3001	CLR	C10-C9	-11.68	1.36	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	3002	CLR	C12-C11	10.06	1.74	1.53
8	G	101	CLR	C12-C11	9.67	1.74	1.53
8	D	3001	CLR	C12-C11	9.36	1.73	1.53
8	A	2009	CLR	C12-C11	9.13	1.72	1.53
8	E	101	CLR	C12-C11	9.07	1.72	1.53
8	A	2010	CLR	C12-C11	8.63	1.71	1.53
10	C	2013	EFO	C15-C13	-7.33	1.36	1.52
10	A	2015	EFO	C15-C13	-7.04	1.37	1.52
8	E	101	CLR	C6-C5	6.94	1.48	1.33
8	A	2009	CLR	C6-C5	6.85	1.48	1.33
8	D	3002	CLR	C6-C5	6.74	1.47	1.33
8	D	3001	CLR	C6-C5	6.71	1.47	1.33
8	A	2010	CLR	C6-C5	6.68	1.47	1.33
8	G	101	CLR	C6-C5	6.51	1.47	1.33
8	E	101	CLR	C8-C14	-6.38	1.41	1.53
8	A	2010	CLR	C13-C14	-6.20	1.43	1.55
8	E	101	CLR	C13-C14	-6.11	1.43	1.55
8	D	3001	CLR	C13-C14	-5.92	1.43	1.55
8	D	3002	CLR	C13-C14	-5.78	1.44	1.55
8	A	2009	CLR	C13-C14	-5.64	1.44	1.55
8	A	2010	CLR	C8-C14	-5.51	1.43	1.53
8	G	101	CLR	C13-C14	-5.32	1.44	1.55
8	D	3001	CLR	C8-C14	-5.10	1.43	1.53
8	G	101	CLR	C8-C14	-5.09	1.43	1.53
8	A	2009	CLR	C8-C14	-5.02	1.44	1.53
8	G	101	CLR	C12-C13	-4.92	1.45	1.54
8	A	2010	CLR	C12-C13	-4.72	1.45	1.54
8	E	101	CLR	C12-C13	-4.55	1.46	1.54
10	C	2013	EFO	C6-C5	-4.52	1.43	1.53
8	D	3002	CLR	C8-C14	-4.49	1.45	1.53
10	C	2013	EFO	O37-C11	4.45	1.51	1.44
10	A	2015	EFO	C6-C5	-4.42	1.43	1.53
8	A	2009	CLR	C16-C15	4.41	1.66	1.54
10	A	2015	EFO	O37-C11	4.41	1.51	1.44
8	A	2009	CLR	C12-C13	-4.41	1.46	1.54
8	D	3002	CLR	C16-C15	4.21	1.65	1.54
8	D	3001	CLR	C12-C13	-4.17	1.46	1.54
8	D	3002	CLR	C12-C13	-4.16	1.46	1.54
10	A	2015	EFO	C10-C11	-4.07	1.43	1.53
10	C	2013	EFO	C10-C11	-4.05	1.43	1.53
8	E	101	CLR	C16-C15	4.03	1.65	1.54
8	G	101	CLR	C16-C15	4.00	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	3001	CLR	C16-C15	3.98	1.64	1.54
8	A	2010	CLR	C16-C15	3.91	1.64	1.54
10	C	2013	EFO	C35-C34	3.76	1.41	1.32
10	C	2013	EFO	O14-C13	3.67	1.52	1.44
10	A	2015	EFO	O14-C13	3.66	1.51	1.44
10	A	2015	EFO	C35-C34	3.54	1.40	1.32
10	C	2013	EFO	C1A-C10	3.47	1.60	1.53
9	A	2012	PC1	O31-C31	3.45	1.43	1.33
9	C	2010	PC1	O31-C31	3.45	1.43	1.33
9	A	2014	PC1	O31-C31	3.43	1.43	1.33
10	C	2013	EFO	C7-C6	-3.41	1.46	1.53
10	A	2015	EFO	C1A-C10	3.41	1.60	1.53
10	A	2015	EFO	C7-C6	-3.39	1.46	1.53
10	C	2013	EFO	C23-C24	3.30	1.59	1.53
8	G	101	CLR	C20-C17	-3.29	1.48	1.54
8	E	101	CLR	C20-C17	-3.25	1.48	1.54
9	D	3003	PC1	O31-C31	3.18	1.42	1.33
9	C	2009	PC1	O31-C31	3.18	1.42	1.33
9	C	2011	PC1	O31-C31	3.18	1.42	1.33
8	G	101	CLR	C10-C5	3.17	1.59	1.52
10	C	2013	EFO	C19-C18	3.14	1.45	1.33
9	C	2012	PC1	O31-C31	3.14	1.42	1.33
8	D	3001	CLR	C20-C17	-3.12	1.48	1.54
10	C	2013	EFO	C17-C18	3.11	1.57	1.50
9	B	401	PC1	O31-C31	3.08	1.42	1.33
10	A	2015	EFO	C23-C24	3.08	1.59	1.53
10	A	2015	EFO	C19-C18	3.06	1.45	1.33
10	A	2015	EFO	C17-C18	3.05	1.56	1.50
10	A	2015	EFO	C2D-C29	-3.03	1.46	1.53
8	G	101	CLR	C15-C14	2.98	1.60	1.54
10	C	2013	EFO	C2D-C29	-2.96	1.46	1.53
8	A	2009	CLR	C10-C5	2.95	1.58	1.52
10	A	2015	EFO	C12-C11	-2.94	1.47	1.53
8	A	2010	CLR	C10-C5	2.92	1.58	1.52
8	A	2010	CLR	C15-C14	2.88	1.60	1.54
9	A	2011	PC1	O31-C31	2.87	1.41	1.33
9	A	2013	PC1	O31-C31	2.85	1.41	1.33
8	A	2009	CLR	C15-C14	2.81	1.60	1.54
8	A	2010	CLR	C20-C17	-2.80	1.49	1.54
10	C	2013	EFO	C8-C10	-2.80	1.50	1.53
10	C	2013	EFO	C12-C11	-2.77	1.47	1.53
10	A	2015	EFO	C20-C21	2.69	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	2013	EFO	C27-C28	2.67	1.59	1.53
6	A	2004	ADP	O4'-C1'	2.67	1.44	1.41
8	E	101	CLR	O1-C3	-2.66	1.35	1.43
10	C	2013	EFO	C20-C21	2.63	1.42	1.33
10	C	2013	EFO	O37-C36	2.61	1.40	1.34
8	D	3002	CLR	C10-C5	2.58	1.58	1.52
10	A	2015	EFO	O37-C36	2.58	1.40	1.34
8	D	3001	CLR	C10-C5	2.57	1.58	1.52
8	E	101	CLR	C10-C5	2.57	1.57	1.52
10	A	2015	EFO	C19-C20	2.57	1.51	1.44
10	C	2013	EFO	C19-C20	2.55	1.51	1.44
10	C	2013	EFO	O26-C26	2.49	1.25	1.21
9	A	2013	PC1	O21-C2	-2.48	1.40	1.46
10	C	2013	EFO	O30-C30	2.45	1.25	1.21
9	A	2011	PC1	O21-C21	2.44	1.41	1.34
10	A	2015	EFO	C8-C10	-2.39	1.50	1.53
8	D	3001	CLR	C15-C14	2.38	1.59	1.54
9	C	2009	PC1	O21-C2	-2.37	1.40	1.46
10	A	2015	EFO	O30-C30	2.35	1.25	1.21
8	E	101	CLR	C4-C3	-2.34	1.48	1.52
9	A	2014	PC1	O21-C21	2.33	1.40	1.34
9	C	2011	PC1	C2A-C29	-2.33	1.38	1.51
8	D	3002	CLR	C15-C14	2.33	1.59	1.54
10	A	2015	EFO	O26-C26	2.31	1.25	1.21
9	C	2012	PC1	O21-C21	2.29	1.40	1.34
8	G	101	CLR	O1-C3	-2.29	1.36	1.43
9	A	2011	PC1	C3A-C39	-2.27	1.38	1.51
9	D	3003	PC1	O21-C2	-2.27	1.40	1.46
8	E	101	CLR	C15-C14	2.27	1.59	1.54
9	C	2011	PC1	C3A-C39	-2.25	1.38	1.51
9	B	401	PC1	O21-C2	-2.25	1.41	1.46
9	C	2010	PC1	O21-C21	2.25	1.40	1.34
9	A	2013	PC1	C3A-C39	-2.24	1.39	1.51
9	C	2011	PC1	O21-C21	2.23	1.40	1.34
9	B	401	PC1	C3A-C39	-2.22	1.39	1.51
6	A	2004	ADP	C5-C4	2.21	1.46	1.40
9	C	2012	PC1	C3A-C39	-2.20	1.39	1.51
9	A	2011	PC1	O21-C2	-2.20	1.41	1.46
8	A	2009	CLR	C20-C17	-2.19	1.50	1.54
9	C	2009	PC1	C3A-C39	-2.18	1.39	1.51
9	B	401	PC1	O21-C21	2.18	1.40	1.34
9	D	3003	PC1	C3A-C39	-2.18	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	101	CLR	C16-C17	-2.14	1.49	1.54
9	C	2010	PC1	C3A-C39	-2.14	1.39	1.51
8	D	3001	CLR	O1-C3	-2.13	1.37	1.43
9	A	2014	PC1	C3A-C39	-2.12	1.39	1.51
10	A	2015	EFO	C27-C28	2.09	1.58	1.53
8	D	3002	CLR	O1-C3	-2.08	1.37	1.43
9	C	2009	PC1	O21-C21	2.08	1.40	1.34
9	D	3003	PC1	O21-C21	2.07	1.40	1.34
9	A	2012	PC1	C3A-C39	-2.04	1.40	1.51
10	C	2013	EFO	C3-C2	2.02	1.56	1.51
8	D	3002	CLR	C7-C6	2.02	1.54	1.50
9	C	2011	PC1	O21-C2	-2.02	1.41	1.46
6	A	2004	ADP	C2-N3	2.01	1.35	1.32

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2015	EFO	O9-C8-C10	-31.61	83.23	106.28
10	C	2013	EFO	O9-C8-C10	-30.78	83.85	106.28
10	A	2015	EFO	O9-C8-O14	20.84	161.70	109.68
10	C	2013	EFO	O9-C8-O14	20.26	160.24	109.68
10	A	2015	EFO	O14-C8-C7	-12.43	63.03	107.43
10	C	2013	EFO	O14-C8-C7	-11.96	64.72	107.43
10	C	2013	EFO	O9-C4-C3	9.76	118.41	105.95
8	G	101	CLR	C7-C8-C14	-9.36	97.33	110.91
10	C	2013	EFO	C31-C32-C33	8.25	124.67	114.87
8	E	101	CLR	C15-C14-C8	-8.08	105.77	119.08
10	A	2015	EFO	O9-C4-C3	7.98	116.14	105.95
8	G	101	CLR	C15-C14-C8	-7.84	106.18	119.08
8	E	101	CLR	C7-C8-C14	-7.37	100.23	110.91
10	A	2015	EFO	C31-C32-C33	7.25	123.48	114.87
10	A	2015	EFO	O14-C13-C15	6.67	113.78	106.07
10	A	2015	EFO	O14-C13-C12	-6.53	102.23	109.92
10	C	2013	EFO	O14-C13-C15	6.03	113.04	106.07
8	G	101	CLR	C12-C13-C17	-5.83	107.85	116.57
8	A	2009	CLR	C12-C13-C17	-5.68	108.08	116.57
8	A	2010	CLR	C7-C8-C14	-5.61	102.78	110.91
8	A	2010	CLR	C11-C9-C10	-5.41	105.96	113.08
8	D	3001	CLR	C7-C8-C14	-5.31	103.22	110.91
8	A	2010	CLR	C12-C13-C17	-5.26	108.70	116.57
8	A	2009	CLR	C7-C8-C14	-5.18	103.40	110.91
8	A	2009	CLR	C11-C9-C10	-4.91	106.61	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	2015	EFO	C1A-C10-C8	4.72	119.40	111.92
10	C	2013	EFO	O14-C13-C12	-4.71	104.37	109.92
9	A	2011	PC1	O21-C21-C22	4.61	121.44	111.50
8	D	3001	CLR	C15-C14-C8	-4.60	111.51	119.08
8	D	3001	CLR	C12-C13-C17	-4.56	109.75	116.57
8	D	3002	CLR	C11-C9-C10	-4.55	107.08	113.08
8	G	101	CLR	C16-C15-C14	-4.47	96.26	105.13
9	B	401	PC1	O21-C21-C22	4.46	121.12	111.50
10	C	2013	EFO	O37-C36-C35	4.46	121.50	111.38
10	C	2013	EFO	C8-O14-C13	-4.46	105.35	114.83
9	C	2011	PC1	O21-C21-C22	4.38	120.95	111.50
8	D	3002	CLR	C15-C14-C8	-4.37	111.88	119.08
8	A	2009	CLR	C15-C14-C8	-4.36	111.89	119.08
10	A	2015	EFO	C8-O14-C13	-4.32	105.63	114.83
10	C	2013	EFO	C22-C21-C20	-4.30	119.86	125.41
9	C	2012	PC1	O21-C21-C22	4.29	120.75	111.50
8	E	101	CLR	C12-C13-C17	-4.27	110.18	116.57
10	C	2013	EFO	C8-O9-C4	-4.26	105.77	114.83
8	A	2010	CLR	C15-C14-C8	-4.22	112.13	119.08
10	A	2015	EFO	C8-O9-C4	-4.19	105.92	114.83
9	B	401	PC1	C15-N-C13	4.17	119.70	108.97
9	A	2014	PC1	O31-C3-C2	4.15	120.52	108.43
8	G	101	CLR	C11-C12-C13	-4.12	105.71	112.78
6	A	2004	ADP	PA-O3A-PB	-4.11	118.73	132.83
9	C	2010	PC1	C15-N-C13	4.11	119.53	108.97
9	A	2014	PC1	O21-C21-C22	4.09	120.32	111.50
10	C	2013	EFO	C15-C16-C17	4.08	120.22	114.00
9	A	2013	PC1	O21-C21-C22	4.01	120.15	111.50
9	C	2009	PC1	C15-N-C13	4.00	119.25	108.97
9	C	2009	PC1	O21-C21-C22	3.98	120.07	111.50
9	C	2010	PC1	O31-C3-C2	3.97	119.99	108.43
8	E	101	CLR	C11-C12-C13	-3.97	105.97	112.78
9	A	2012	PC1	C15-N-C13	3.92	119.06	108.97
9	D	3003	PC1	O31-C3-C2	3.91	119.80	108.43
8	G	101	CLR	C21-C20-C17	3.90	118.89	112.92
8	E	101	CLR	C8-C7-C6	-3.89	107.15	112.73
9	A	2011	PC1	C15-N-C13	3.88	118.96	108.97
10	A	2015	EFO	O37-C36-C35	3.87	120.17	111.38
8	A	2010	CLR	C11-C9-C8	-3.80	106.29	111.75
8	G	101	CLR	C11-C9-C8	-3.78	106.31	111.75
10	A	2015	EFO	C15-C16-C17	3.75	119.72	114.00
9	C	2011	PC1	C15-N-C13	3.72	118.53	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	3001	CLR	C17-C13-C14	3.71	104.47	100.07
9	A	2014	PC1	C15-N-C13	3.71	118.52	108.97
8	A	2009	CLR	C17-C13-C14	3.71	104.47	100.07
9	A	2013	PC1	C15-N-C13	3.69	118.47	108.97
8	D	3002	CLR	C7-C8-C14	-3.67	105.58	110.91
9	A	2012	PC1	O31-C3-C2	3.65	119.07	108.43
9	C	2012	PC1	O31-C3-C2	3.65	119.06	108.43
8	D	3001	CLR	C11-C9-C10	-3.65	108.27	113.08
8	A	2010	CLR	C22-C20-C17	-3.65	102.75	110.28
8	A	2010	CLR	C12-C11-C9	-3.65	106.79	113.11
8	A	2010	CLR	C11-C12-C13	-3.61	106.59	112.78
8	D	3002	CLR	C13-C14-C8	3.60	119.71	114.38
8	A	2009	CLR	C11-C9-C8	-3.60	106.57	111.75
10	C	2013	EFO	C1A-C10-C8	3.58	117.59	111.92
9	D	3003	PC1	C15-N-C13	3.57	118.15	108.97
8	E	101	CLR	C22-C20-C17	-3.49	103.07	110.28
8	D	3002	CLR	C12-C13-C17	-3.49	111.35	116.57
9	C	2012	PC1	C15-N-C13	3.48	117.92	108.97
8	A	2010	CLR	C4-C5-C10	3.47	121.03	116.42
10	A	2015	EFO	C17-C18-C19	-3.46	117.68	126.48
10	A	2015	EFO	C22-C21-C20	-3.43	120.98	125.41
6	C	2004	ADP	N3-C2-N1	-3.41	123.35	128.68
8	E	101	CLR	C11-C9-C10	-3.38	108.62	113.08
8	G	101	CLR	C8-C7-C6	-3.38	107.88	112.73
9	A	2012	PC1	O21-C21-C22	3.36	118.75	111.50
8	D	3001	CLR	C16-C17-C20	-3.34	106.98	112.15
6	A	2004	ADP	C4-C5-N7	-3.31	105.94	109.40
9	C	2010	PC1	O21-C21-C22	3.25	118.51	111.50
8	A	2009	CLR	C10-C5-C6	-3.23	117.97	122.90
8	D	3002	CLR	C19-C10-C9	3.21	115.51	111.68
9	C	2009	PC1	O31-C3-C2	3.19	117.72	108.43
10	A	2015	EFO	O25-C25-C26	-3.18	105.34	108.86
8	D	3002	CLR	C11-C9-C8	-3.17	107.18	111.75
8	E	101	CLR	C12-C13-C14	3.13	112.12	107.27
8	G	101	CLR	C19-C10-C9	3.09	115.36	111.68
10	C	2013	EFO	O37-C36-O36	-3.07	118.35	123.35
8	D	3001	CLR	C10-C5-C6	-3.06	118.22	122.90
10	C	2013	EFO	C23-C22-C21	3.05	118.67	113.98
6	A	2004	ADP	N3-C2-N1	-3.03	123.95	128.68
8	D	3001	CLR	C11-C9-C8	-3.02	107.40	111.75
8	E	101	CLR	C12-C11-C9	-3.02	107.89	113.11
8	E	101	CLR	C16-C15-C14	-2.98	99.22	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	2010	PC1	C2-O21-C21	2.97	125.09	117.79
9	A	2011	PC1	O31-C31-O32	-2.93	116.19	123.59
8	D	3001	CLR	C12-C11-C9	-2.90	108.08	113.11
8	A	2009	CLR	C22-C20-C17	-2.90	104.30	110.28
9	C	2011	PC1	O31-C31-C32	2.89	120.98	111.91
8	D	3002	CLR	C2-C3-C4	-2.85	106.39	110.31
8	A	2009	CLR	C11-C12-C13	-2.85	107.90	112.78
9	C	2010	PC1	O31-C31-C32	2.85	120.84	111.91
10	A	2015	EFO	C27-C28-C29	-2.84	111.49	114.87
10	C	2013	EFO	C33-C34-C35	-2.84	118.69	126.44
8	D	3002	CLR	C12-C13-C14	2.84	111.67	107.27
9	A	2014	PC1	O31-C31-C32	2.83	120.78	111.91
8	D	3001	CLR	C4-C5-C10	2.80	120.14	116.42
8	A	2009	CLR	C4-C5-C10	2.80	120.13	116.42
8	A	2010	CLR	C2-C3-C4	-2.79	106.48	110.31
10	A	2015	EFO	C33-C34-C35	-2.78	118.84	126.44
9	B	401	PC1	O31-C3-C2	2.78	116.53	108.43
8	A	2010	CLR	C10-C5-C6	-2.74	118.71	122.90
8	G	101	CLR	C4-C5-C10	2.74	120.06	116.42
8	D	3002	CLR	C10-C5-C6	-2.71	118.75	122.90
10	A	2015	EFO	C6-C7-C8	2.70	116.60	111.93
8	D	3001	CLR	C11-C12-C13	-2.70	108.16	112.78
8	D	3001	CLR	C22-C20-C17	-2.70	104.72	110.28
8	E	101	CLR	C16-C17-C20	-2.69	107.98	112.15
10	C	2013	EFO	C17-C18-C19	-2.67	119.69	126.48
9	A	2011	PC1	O31-C3-C2	2.67	116.20	108.43
8	E	101	CLR	C10-C5-C6	-2.67	118.82	122.90
10	A	2015	EFO	C12-C11-C10	2.64	117.39	112.40
10	C	2013	EFO	O9-C4-C5	-2.62	106.91	110.50
8	G	101	CLR	C2-C3-C4	-2.62	106.71	110.31
9	D	3003	PC1	O31-C31-C32	2.61	120.11	111.91
8	D	3001	CLR	C19-C10-C9	2.60	114.78	111.68
10	C	2013	EFO	C51-C5-C4	-2.58	109.24	112.65
8	D	3002	CLR	C8-C7-C6	-2.56	109.06	112.73
9	A	2011	PC1	O31-C31-C32	2.55	119.90	111.91
10	C	2013	EFO	C1D-C1C-C17	2.54	119.20	113.72
10	A	2015	EFO	C32-C31-C30	2.53	114.94	110.36
9	A	2013	PC1	O31-C3-C2	2.52	115.76	108.43
9	A	2012	PC1	O31-C31-C32	2.51	119.79	111.91
9	A	2012	PC1	C2-O21-C21	2.51	123.97	117.79
8	D	3001	CLR	C12-C13-C14	2.50	111.16	107.27
9	D	3003	PC1	O21-C21-C22	2.44	116.77	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2004	ADP	C3'-C2'-C1'	2.43	104.64	100.98
9	C	2011	PC1	O31-C31-O32	-2.39	117.56	123.59
8	D	3001	CLR	C18-C13-C17	-2.39	107.26	111.71
10	A	2015	EFO	C11-O37-C36	2.38	121.33	117.47
8	A	2009	CLR	C8-C7-C6	-2.37	109.33	112.73
8	A	2009	CLR	C7-C8-C9	-2.36	106.85	109.71
8	E	101	CLR	C17-C13-C14	2.36	102.86	100.07
8	D	3002	CLR	C1-C2-C3	-2.35	107.44	110.47
8	D	3002	CLR	C2-C1-C10	-2.34	107.67	112.74
9	C	2012	PC1	O31-C31-C32	2.31	119.15	111.91
10	C	2013	EFO	O25-C25-C26	-2.30	106.32	108.86
8	A	2009	CLR	C7-C6-C5	-2.30	120.83	125.06
9	C	2009	PC1	O31-C31-C32	2.28	119.06	111.91
8	A	2010	CLR	C17-C13-C14	2.26	102.75	100.07
9	B	401	PC1	O31-C31-C32	2.26	119.00	111.91
9	A	2012	PC1	O21-C21-O22	-2.24	118.29	123.70
10	A	2015	EFO	O28-C28-C29	2.24	114.02	108.82
10	C	2013	EFO	O28-C28-C29	2.23	113.99	108.82
10	A	2015	EFO	C23-C22-C21	2.23	117.40	113.98
10	C	2013	EFO	C2C-C27-C28	-2.21	108.68	112.37
8	E	101	CLR	C15-C14-C13	2.21	106.50	103.84
10	C	2013	EFO	C11-C12-C13	2.20	112.87	108.23
8	G	101	CLR	C7-C6-C5	-2.19	121.02	125.06
9	C	2011	PC1	O31-C3-C2	2.18	114.77	108.43
10	A	2015	EFO	C11-C12-C13	2.17	112.81	108.23
8	A	2009	CLR	C2-C3-C4	-2.15	107.36	110.31
9	A	2012	PC1	C34-C33-C32	2.13	120.86	113.19
8	D	3002	CLR	C23-C22-C20	-2.13	108.91	115.03
9	B	401	PC1	O13-C11-C12	2.11	120.28	109.16
8	A	2009	CLR	C12-C11-C9	-2.11	109.46	113.11
10	C	2013	EFO	C12-C11-C10	2.11	116.38	112.40
8	G	101	CLR	C10-C5-C6	-2.10	119.69	122.90
10	A	2015	EFO	O37-C36-O36	-2.10	119.93	123.35
6	C	2004	ADP	C4-C5-N7	-2.10	107.21	109.40
8	D	3002	CLR	C4-C5-C10	2.10	119.21	116.42
8	A	2010	CLR	C16-C17-C20	-2.10	108.90	112.15
9	C	2009	PC1	O31-C31-O32	-2.06	118.38	123.59
9	A	2013	PC1	O31-C31-C32	2.06	118.36	111.91
8	A	2010	CLR	C8-C7-C6	-2.04	109.80	112.73
9	A	2011	PC1	O22-C21-C22	-2.04	115.79	123.73
10	A	2015	EFO	C2C-C27-C28	-2.01	109.01	112.37

There are no chirality outliers.

All (326) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	2013	EFO	C12-C13-C15-C16
10	C	2013	EFO	C1-C2-C3-C4
10	C	2013	EFO	O2-C2-C3-C4
9	C	2010	PC1	O13-C11-C12-N
9	C	2011	PC1	C11-O13-P-O14
9	C	2011	PC1	C11-O13-P-O11
9	C	2011	PC1	O13-C11-C12-N
9	A	2014	PC1	C22-C21-O21-C2
10	A	2015	EFO	C12-C13-C15-C16
10	A	2015	EFO	C2-C3-C4-O9
10	A	2015	EFO	C2-C3-C4-C5
9	C	2012	PC1	O22-C21-O21-C2
9	C	2012	PC1	C22-C21-O21-C2
9	A	2011	PC1	O13-C11-C12-N
9	A	2012	PC1	C11-O13-P-O12
9	A	2012	PC1	C11-O13-P-O14
9	A	2012	PC1	C11-O13-P-O11
9	A	2012	PC1	O13-C11-C12-N
6	A	2004	ADP	C5'-O5'-PA-O1A
6	A	2004	ADP	C5'-O5'-PA-O2A
6	A	2004	ADP	C5'-O5'-PA-O3A
6	A	2004	ADP	O4'-C4'-C5'-O5'
9	C	2009	PC1	C11-O13-P-O12
9	C	2009	PC1	O13-C11-C12-N
9	B	401	PC1	C1-O11-P-O14
9	B	401	PC1	O13-C11-C12-N
9	B	401	PC1	C22-C21-O21-C2
9	D	3003	PC1	O22-C21-O21-C2
9	D	3003	PC1	C22-C21-O21-C2
9	C	2010	PC1	O22-C21-O21-C2
9	A	2014	PC1	O22-C21-O21-C2
9	C	2011	PC1	C32-C31-O31-C3
9	C	2012	PC1	C38-C39-C3A-C3B
9	C	2009	PC1	C38-C39-C3A-C3B
9	D	3003	PC1	C28-C29-C2A-C2B
9	C	2012	PC1	C28-C29-C2A-C2B
9	A	2011	PC1	O22-C21-O21-C2
9	D	3003	PC1	C38-C39-C3A-C3B
9	C	2010	PC1	C32-C31-O31-C3
9	A	2013	PC1	C22-C21-O21-C2
9	B	401	PC1	C24-C25-C26-C27
9	A	2012	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
9	A	2013	PC1	C26-C27-C28-C29
9	A	2013	PC1	C38-C39-C3A-C3B
9	B	401	PC1	C38-C39-C3A-C3B
9	C	2010	PC1	C28-C29-C2A-C2B
9	A	2014	PC1	C24-C25-C26-C27
6	A	2004	ADP	C3'-C4'-C5'-O5'
9	A	2012	PC1	C2-C1-O11-P
9	C	2011	PC1	C27-C28-C29-C2A
9	C	2009	PC1	O22-C21-O21-C2
9	C	2010	PC1	O32-C31-O31-C3
9	C	2010	PC1	O11-C1-C2-O21
9	B	401	PC1	O22-C21-O21-C2
9	C	2009	PC1	C28-C29-C2A-C2B
9	A	2012	PC1	C21-C22-C23-C24
9	C	2011	PC1	O32-C31-O31-C3
9	D	3003	PC1	C21-C22-C23-C24
9	C	2011	PC1	C11-C12-N-C14
9	A	2011	PC1	C21-C22-C23-C24
9	C	2009	PC1	C21-C22-C23-C24
9	C	2009	PC1	C31-C32-C33-C34
9	C	2010	PC1	C22-C21-O21-C2
9	A	2012	PC1	O22-C21-O21-C2
9	A	2014	PC1	C32-C31-O31-C3
9	C	2012	PC1	O32-C31-O31-C3
9	C	2009	PC1	C11-O13-P-O11
9	C	2009	PC1	C1-O11-P-O13
9	C	2012	PC1	C32-C31-O31-C3
9	A	2011	PC1	C32-C31-O31-C3
9	A	2013	PC1	O22-C21-O21-C2
9	C	2010	PC1	C11-C12-N-C15
9	C	2012	PC1	C21-C22-C23-C24
9	C	2011	PC1	C35-C36-C37-C38
9	A	2013	PC1	C27-C28-C29-C2A
9	A	2014	PC1	C2D-C2E-C2F-C2G
9	A	2011	PC1	C24-C25-C26-C27
9	A	2013	PC1	C24-C25-C26-C27
9	A	2013	PC1	C36-C37-C38-C39
9	C	2009	PC1	C36-C37-C38-C39
9	C	2011	PC1	C22-C23-C24-C25
9	C	2011	PC1	C3C-C3D-C3E-C3F
9	C	2012	PC1	C23-C24-C25-C26
9	A	2013	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
9	C	2009	PC1	C35-C36-C37-C38
9	C	2009	PC1	C39-C3A-C3B-C3C
9	D	3003	PC1	C26-C27-C28-C29
9	C	2012	PC1	C24-C25-C26-C27
9	C	2009	PC1	C26-C27-C28-C29
9	A	2013	PC1	C29-C2A-C2B-C2C
9	A	2013	PC1	C2B-C2C-C2D-C2E
9	C	2009	PC1	C34-C35-C36-C37
9	C	2009	PC1	C3A-C3B-C3C-C3D
9	D	3003	PC1	C2B-C2C-C2D-C2E
9	C	2011	PC1	C21-C22-C23-C24
9	A	2011	PC1	C3A-C3B-C3C-C3D
9	B	401	PC1	C39-C3A-C3B-C3C
9	A	2014	PC1	C23-C24-C25-C26
9	A	2012	PC1	C2D-C2E-C2F-C2G
9	B	401	PC1	C2C-C2D-C2E-C2F
9	C	2010	PC1	C2A-C2B-C2C-C2D
9	C	2011	PC1	C29-C2A-C2B-C2C
9	A	2014	PC1	C2B-C2C-C2D-C2E
9	A	2014	PC1	C3D-C3E-C3F-C3G
9	C	2012	PC1	C34-C35-C36-C37
9	A	2011	PC1	C27-C28-C29-C2A
9	B	401	PC1	C33-C34-C35-C36
9	D	3003	PC1	C2C-C2D-C2E-C2F
9	A	2013	PC1	C2C-C2D-C2E-C2F
9	C	2010	PC1	C29-C2A-C2B-C2C
9	C	2011	PC1	C28-C29-C2A-C2B
9	A	2014	PC1	C29-C2A-C2B-C2C
9	A	2014	PC1	C36-C37-C38-C39
9	A	2012	PC1	C26-C27-C28-C29
9	C	2009	PC1	C2A-C2B-C2C-C2D
9	B	401	PC1	C3E-C3F-C3G-C3H
9	D	3003	PC1	C23-C24-C25-C26
9	C	2011	PC1	C11-C12-N-C13
9	C	2012	PC1	C27-C28-C29-C2A
9	C	2012	PC1	C36-C37-C38-C39
9	D	3003	PC1	C25-C26-C27-C28
9	D	3003	PC1	C3C-C3D-C3E-C3F
9	C	2010	PC1	C24-C25-C26-C27
9	C	2011	PC1	C26-C27-C28-C29
9	D	3003	PC1	C36-C37-C38-C39
9	C	2009	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
9	B	401	PC1	C2B-C2C-C2D-C2E
9	D	3003	PC1	C35-C36-C37-C38
9	C	2011	PC1	C24-C25-C26-C27
9	A	2011	PC1	C34-C35-C36-C37
9	C	2009	PC1	C22-C21-O21-C2
9	A	2013	PC1	C37-C38-C39-C3A
9	C	2011	PC1	C34-C35-C36-C37
9	A	2014	PC1	C35-C36-C37-C38
9	C	2009	PC1	C2B-C2C-C2D-C2E
9	C	2012	PC1	C2B-C2C-C2D-C2E
9	A	2011	PC1	C2D-C2E-C2F-C2G
9	A	2014	PC1	C27-C28-C29-C2A
9	A	2014	PC1	C3B-C3C-C3D-C3E
9	D	3003	PC1	C3B-C3C-C3D-C3E
9	B	401	PC1	C21-C22-C23-C24
9	A	2014	PC1	C33-C34-C35-C36
9	C	2010	PC1	C2B-C2C-C2D-C2E
9	B	401	PC1	C2A-C2B-C2C-C2D
9	D	3003	PC1	C27-C28-C29-C2A
9	C	2009	PC1	C29-C2A-C2B-C2C
9	D	3003	PC1	C29-C2A-C2B-C2C
9	A	2013	PC1	C32-C31-O31-C3
9	A	2013	PC1	C2D-C2E-C2F-C2G
9	B	401	PC1	C28-C29-C2A-C2B
9	D	3003	PC1	C31-C32-C33-C34
9	C	2010	PC1	C25-C26-C27-C28
9	C	2009	PC1	C23-C24-C25-C26
9	B	401	PC1	C32-C33-C34-C35
9	C	2011	PC1	C38-C39-C3A-C3B
9	B	401	PC1	C27-C28-C29-C2A
10	C	2013	EFO	O14-C13-C15-C16
10	A	2015	EFO	O14-C13-C15-C16
9	A	2011	PC1	C22-C21-O21-C2
9	A	2013	PC1	C32-C33-C34-C35
9	A	2014	PC1	C26-C27-C28-C29
9	B	401	PC1	C2D-C2E-C2F-C2G
9	C	2011	PC1	C2B-C2C-C2D-C2E
9	A	2012	PC1	C22-C23-C24-C25
9	C	2010	PC1	C34-C35-C36-C37
9	A	2013	PC1	C3B-C3C-C3D-C3E
9	B	401	PC1	C3C-C3D-C3E-C3F
9	C	2010	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
9	A	2012	PC1	C34-C35-C36-C37
9	C	2009	PC1	C3D-C3E-C3F-C3G
9	A	2012	PC1	C22-C21-O21-C2
9	A	2012	PC1	C2C-C2D-C2E-C2F
9	C	2012	PC1	O11-C1-C2-C3
9	B	401	PC1	O11-C1-C2-C3
9	A	2012	PC1	C35-C36-C37-C38
9	A	2012	PC1	C27-C28-C29-C2A
9	C	2009	PC1	C3E-C3F-C3G-C3H
9	C	2010	PC1	C3B-C3C-C3D-C3E
9	A	2013	PC1	C22-C23-C24-C25
9	A	2013	PC1	C34-C35-C36-C37
9	A	2011	PC1	C29-C2A-C2B-C2C
9	A	2012	PC1	C33-C34-C35-C36
9	A	2014	PC1	O32-C31-O31-C3
9	D	3003	PC1	C34-C35-C36-C37
10	C	2013	EFO	C34-C35-C36-O37
10	A	2015	EFO	C34-C35-C36-O37
9	D	3003	PC1	C1-C2-C3-O31
9	C	2011	PC1	C2D-C2E-C2F-C2G
9	C	2011	PC1	C2F-C2G-C2H-C2I
9	C	2011	PC1	C23-C24-C25-C26
9	C	2009	PC1	C3C-C3D-C3E-C3F
9	B	401	PC1	C26-C27-C28-C29
9	A	2014	PC1	C31-C32-C33-C34
9	C	2011	PC1	C3B-C3C-C3D-C3E
9	D	3003	PC1	C3A-C3B-C3C-C3D
9	B	401	PC1	C35-C36-C37-C38
9	A	2013	PC1	C21-C22-C23-C24
9	A	2011	PC1	C26-C27-C28-C29
9	A	2013	PC1	C23-C24-C25-C26
9	B	401	PC1	C34-C35-C36-C37
9	C	2012	PC1	C32-C33-C34-C35
9	A	2013	PC1	C2F-C2G-C2H-C2I
9	C	2012	PC1	C3A-C3B-C3C-C3D
9	C	2009	PC1	C2D-C2E-C2F-C2G
9	D	3003	PC1	C22-C23-C24-C25
9	A	2014	PC1	C3A-C3B-C3C-C3D
9	A	2011	PC1	C2F-C2G-C2H-C2I
9	A	2014	PC1	C28-C29-C2A-C2B
9	C	2010	PC1	C11-C12-N-C14
9	C	2010	PC1	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	C	2011	PC1	O11-C1-C2-C3
9	A	2012	PC1	O11-C1-C2-C3
9	D	3003	PC1	C24-C25-C26-C27
9	C	2012	PC1	C37-C38-C39-C3A
10	C	2013	EFO	C2-C3-C4-O9
9	C	2012	PC1	C3C-C3D-C3E-C3F
9	C	2012	PC1	C3F-C3G-C3H-C3I
9	C	2010	PC1	C2C-C2D-C2E-C2F
9	A	2013	PC1	C1-C2-C3-O31
9	A	2013	PC1	C3D-C3E-C3F-C3G
10	C	2013	EFO	C15-C16-C17-C18
10	A	2015	EFO	C15-C16-C17-C18
9	D	3003	PC1	C2A-C2B-C2C-C2D
9	B	401	PC1	O11-C1-C2-O21
9	D	3003	PC1	C3F-C3G-C3H-C3I
9	A	2014	PC1	C21-C22-C23-C24
9	A	2011	PC1	C37-C38-C39-C3A
9	B	401	PC1	C29-C2A-C2B-C2C
9	B	401	PC1	C31-C32-C33-C34
9	C	2011	PC1	C25-C26-C27-C28
9	A	2014	PC1	C3C-C3D-C3E-C3F
8	A	2010	CLR	C22-C23-C24-C25
9	C	2010	PC1	C3F-C3G-C3H-C3I
6	A	2004	ADP	PB-O3A-PA-O5'
6	C	2004	ADP	PB-O3A-PA-O5'
9	A	2011	PC1	O11-C1-C2-C3
9	C	2011	PC1	C2C-C2D-C2E-C2F
9	A	2012	PC1	C38-C39-C3A-C3B
9	C	2011	PC1	C32-C33-C34-C35
9	A	2012	PC1	O32-C31-O31-C3
9	A	2014	PC1	C3F-C3G-C3H-C3I
9	C	2010	PC1	C36-C37-C38-C39
9	C	2010	PC1	C39-C3A-C3B-C3C
9	D	3003	PC1	C39-C3A-C3B-C3C
9	A	2011	PC1	C2A-C2B-C2C-C2D
9	C	2010	PC1	C3-C2-O21-C21
9	C	2010	PC1	C1-C2-C3-O31
10	A	2015	EFO	C28-C29-C30-O30
9	A	2013	PC1	O32-C31-O31-C3
9	C	2011	PC1	O11-C1-C2-O21
9	A	2011	PC1	O11-C1-C2-O21
9	A	2012	PC1	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
9	A	2013	PC1	O11-C1-C2-O21
9	C	2011	PC1	C3F-C3G-C3H-C3I
10	C	2013	EFO	C2-C3-C4-C5
9	C	2011	PC1	C11-C12-N-C15
9	A	2011	PC1	C11-O13-P-O11
9	A	2014	PC1	C34-C35-C36-C37
9	D	3003	PC1	C3E-C3F-C3G-C3H
9	A	2012	PC1	C3E-C3F-C3G-C3H
9	C	2009	PC1	C1-O11-P-O12
9	A	2014	PC1	O11-C1-C2-C3
8	G	101	CLR	C21-C20-C22-C23
10	A	2015	EFO	C28-C29-C30-C31
9	A	2011	PC1	C12-C11-O13-P
9	B	401	PC1	C12-C11-O13-P
9	A	2014	PC1	O11-C1-C2-O21
9	A	2011	PC1	C36-C37-C38-C39
9	D	3003	PC1	C32-C33-C34-C35
9	B	401	PC1	O32-C31-O31-C3
9	C	2011	PC1	C31-C32-C33-C34
9	C	2010	PC1	C11-C12-N-C13
9	A	2013	PC1	O13-C11-C12-N
9	C	2010	PC1	O21-C2-C3-O31
9	D	3003	PC1	O21-C2-C3-O31
9	A	2011	PC1	C39-C3A-C3B-C3C
9	C	2012	PC1	C25-C26-C27-C28
9	A	2012	PC1	C3-C2-O21-C21
9	C	2010	PC1	C2-C1-O11-P
9	C	2011	PC1	C39-C3A-C3B-C3C
9	C	2012	PC1	O11-C1-C2-O21
9	A	2011	PC1	C23-C24-C25-C26
9	A	2014	PC1	C32-C33-C34-C35
9	C	2011	PC1	C1-O11-P-O13
9	A	2013	PC1	C2A-C2B-C2C-C2D
9	B	401	PC1	C23-C24-C25-C26
9	B	401	PC1	C32-C31-O31-C3
9	A	2012	PC1	C3A-C3B-C3C-C3D
9	C	2012	PC1	C31-C32-C33-C34
9	D	3003	PC1	O21-C21-C22-C23
9	A	2014	PC1	C3E-C3F-C3G-C3H
9	C	2012	PC1	C3D-C3E-C3F-C3G
9	A	2012	PC1	C29-C2A-C2B-C2C
11	D	3004	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	C	2010	PC1	C2D-C2E-C2F-C2G
9	A	2013	PC1	C35-C36-C37-C38
9	B	401	PC1	C3F-C3G-C3H-C3I
9	C	2010	PC1	C38-C39-C3A-C3B
9	A	2012	PC1	C2F-C2G-C2H-C2I
9	B	401	PC1	C2F-C2G-C2H-C2I
9	C	2010	PC1	C22-C23-C24-C25
9	A	2012	PC1	C3C-C3D-C3E-C3F
9	A	2011	PC1	O32-C31-O31-C3
9	A	2014	PC1	C38-C39-C3A-C3B
10	C	2013	EFO	C18-C19-C20-C21
9	C	2010	PC1	O21-C21-C22-C23
9	A	2014	PC1	O21-C21-C22-C23
9	C	2010	PC1	C37-C38-C39-C3A
9	A	2013	PC1	O11-C1-C2-C3
10	A	2015	EFO	O2-C2-C3-C4
9	B	401	PC1	C22-C23-C24-C25
8	D	3002	CLR	C23-C24-C25-C27
9	C	2009	PC1	O32-C31-O31-C3
9	A	2014	PC1	O22-C21-C22-C23
9	C	2010	PC1	C1-O11-P-O12
9	C	2012	PC1	C1-O11-P-O14
10	C	2013	EFO	C28-C29-C30-C31
9	A	2011	PC1	C3D-C3E-C3F-C3G
9	C	2010	PC1	C12-C11-O13-P
9	A	2013	PC1	C12-C11-O13-P
9	C	2012	PC1	O21-C21-C22-C23
9	A	2012	PC1	O31-C31-C32-C33
9	C	2010	PC1	C33-C34-C35-C36
9	A	2012	PC1	C2B-C2C-C2D-C2E
9	C	2012	PC1	O22-C21-C22-C23
9	A	2012	PC1	O22-C21-C22-C23

There are no ring outliers.

19 monomers are involved in 116 short contacts:

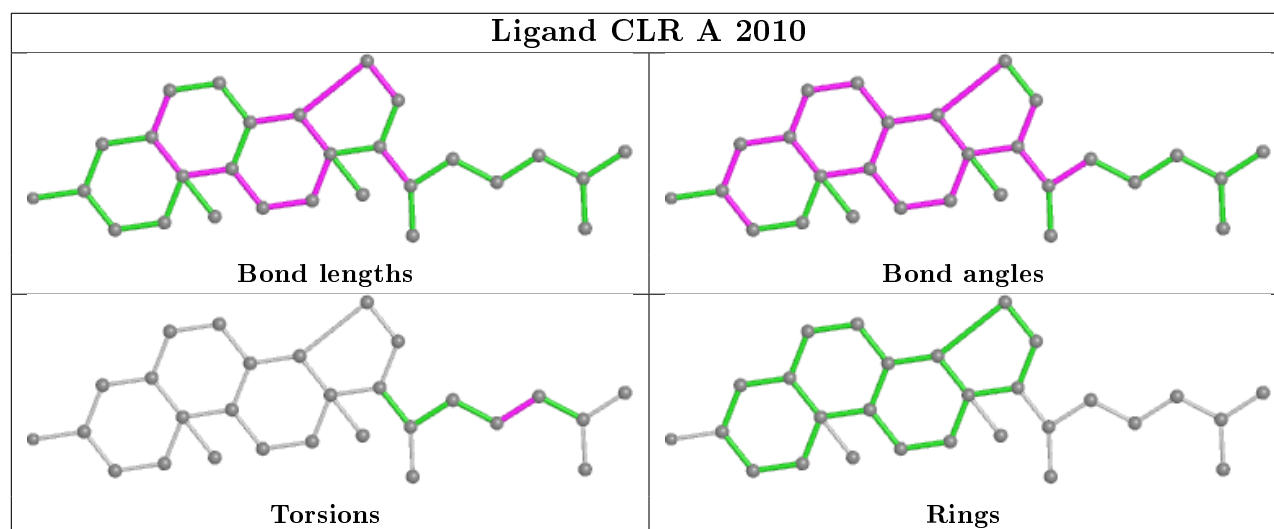
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	2010	CLR	15	0
8	D	3001	CLR	12	0
9	C	2011	PC1	3	0
9	A	2014	PC1	4	0
5	C	2002	ALF	2	0

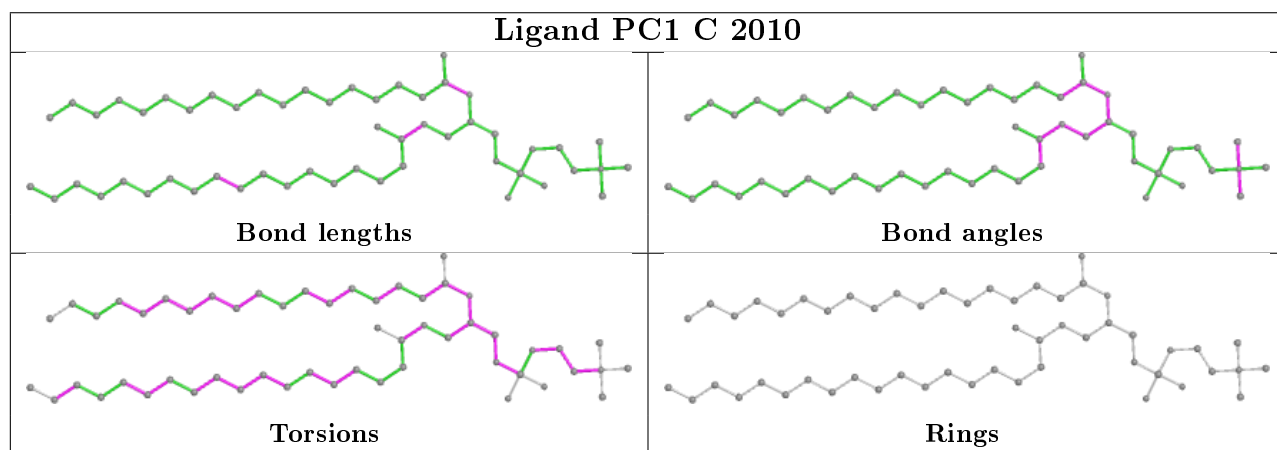
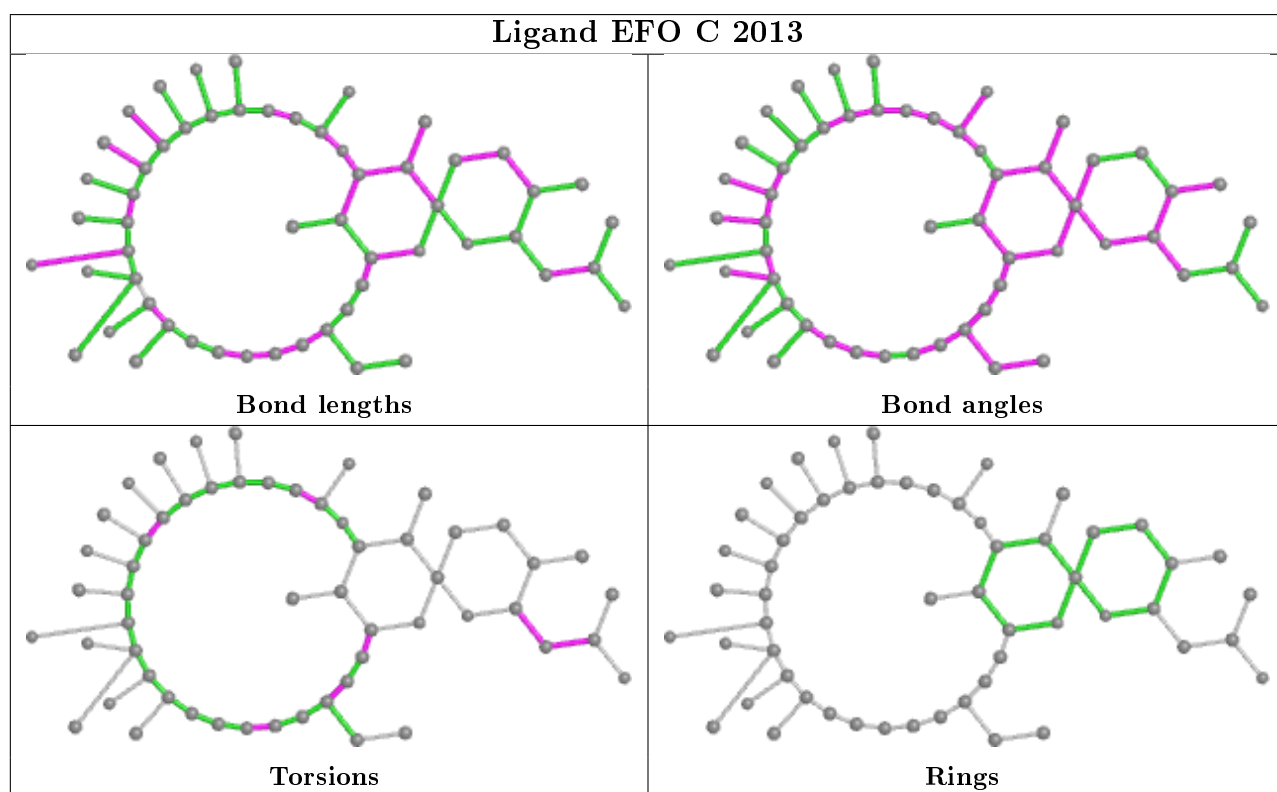
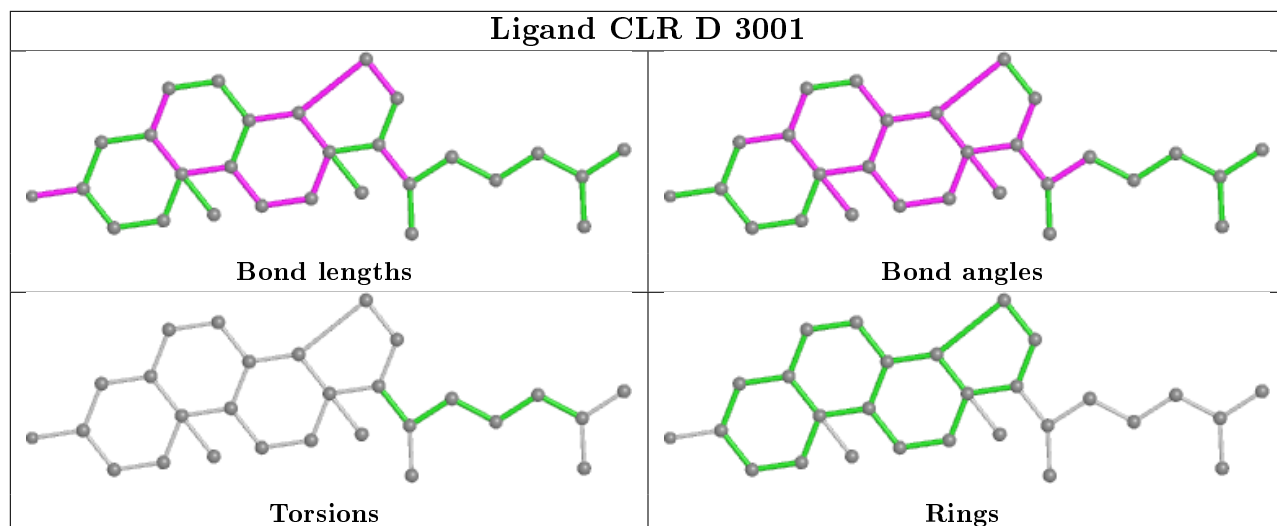
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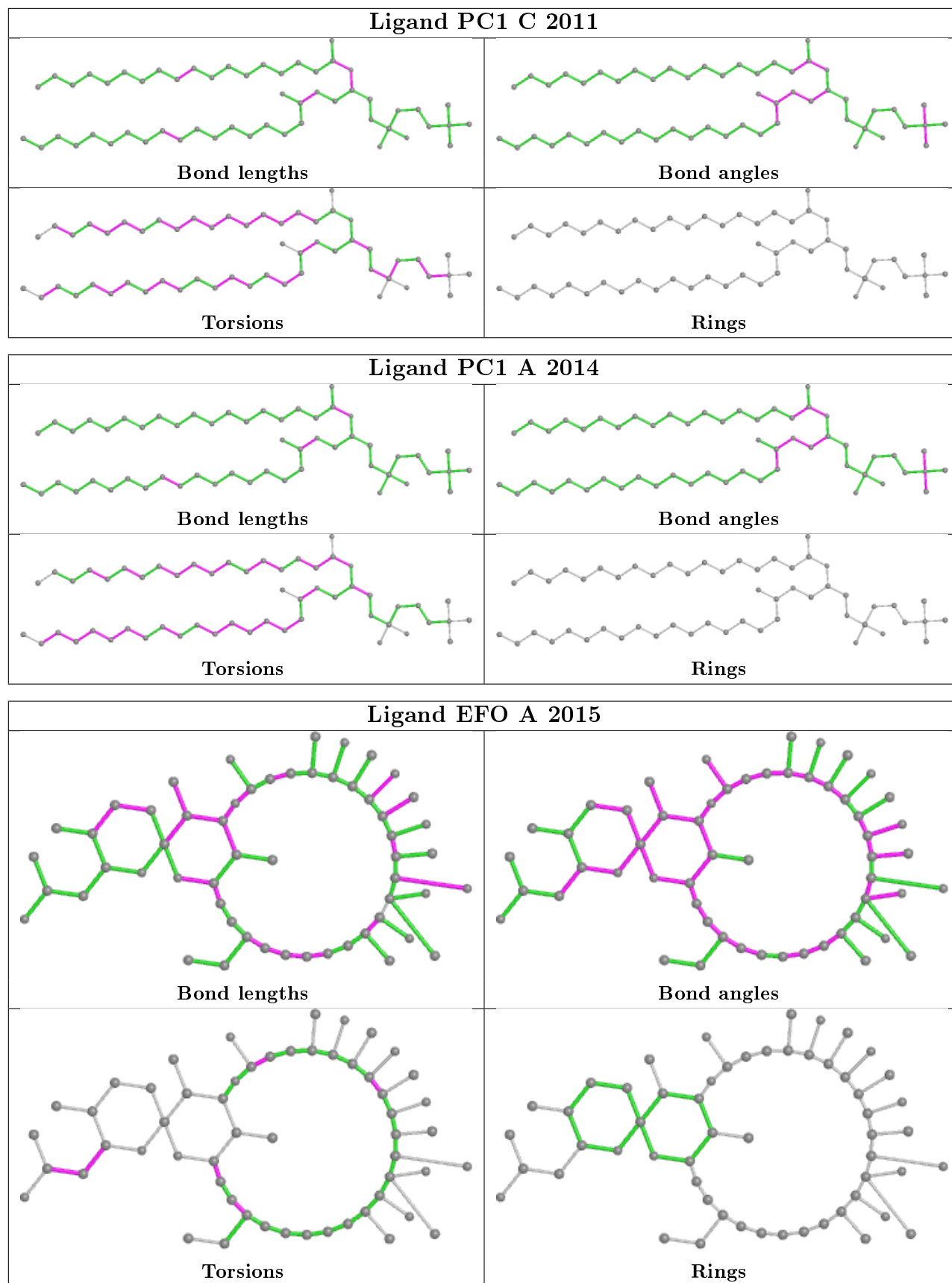
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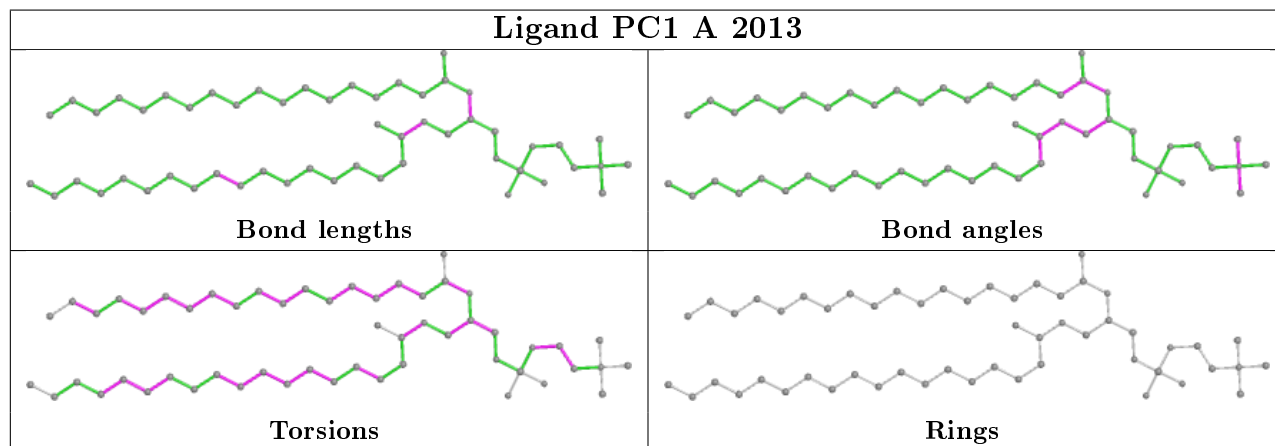
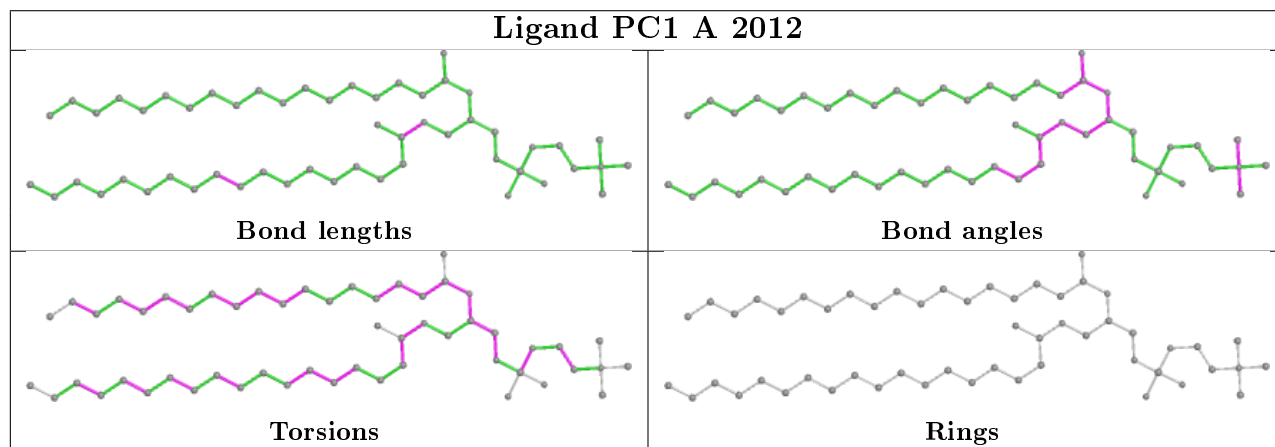
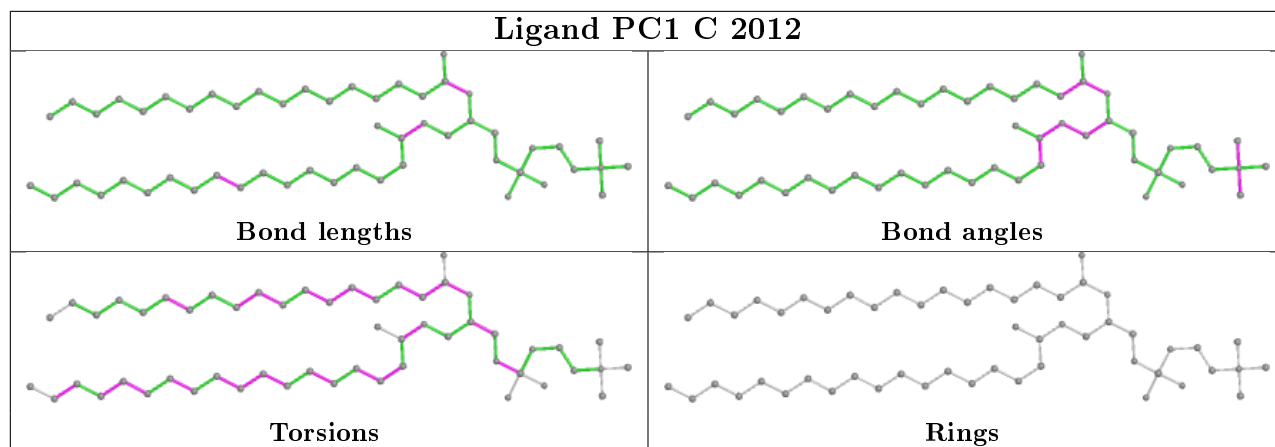
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2012	PC1	6	0
5	A	2002	ALF	1	0
9	A	2012	PC1	2	0
9	A	2013	PC1	7	0
6	A	2004	ADP	3	0
6	C	2004	ADP	6	0
8	A	2009	CLR	12	0
9	A	2011	PC1	1	0
8	D	3002	CLR	17	0
9	C	2009	PC1	8	0
9	B	401	PC1	2	0
8	E	101	CLR	13	0
9	D	3003	PC1	2	0
8	G	101	CLR	9	0

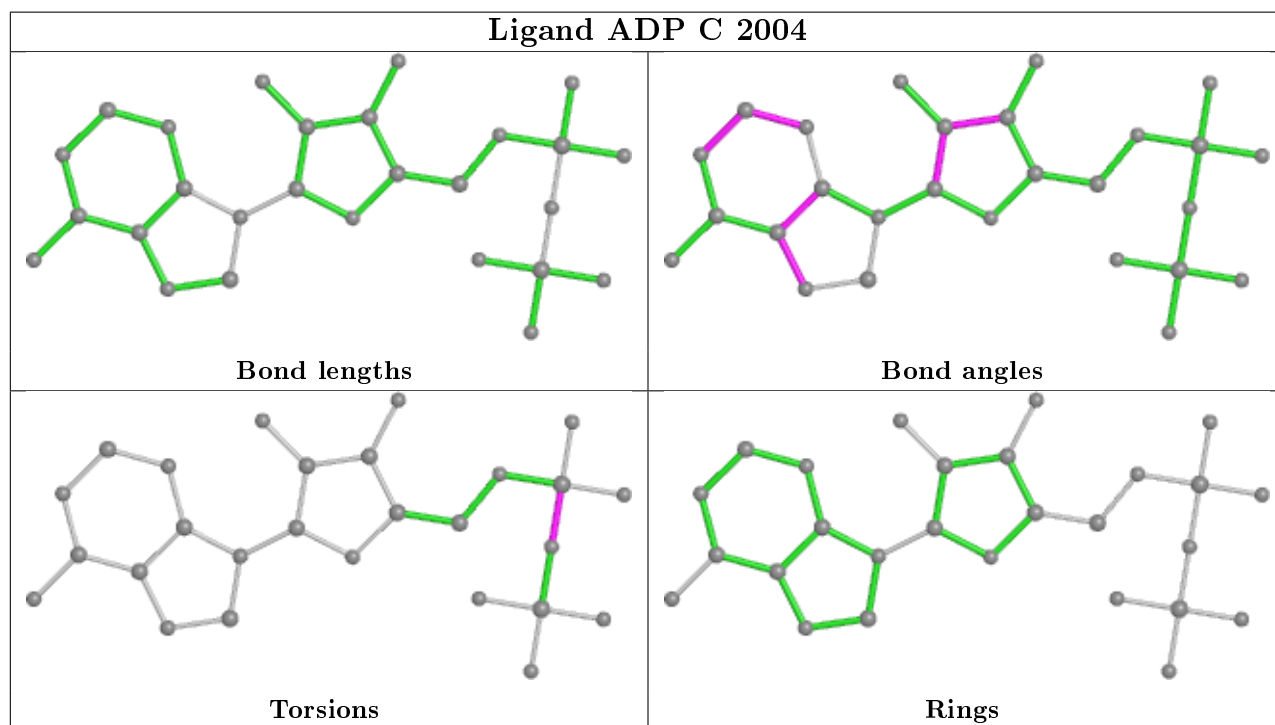
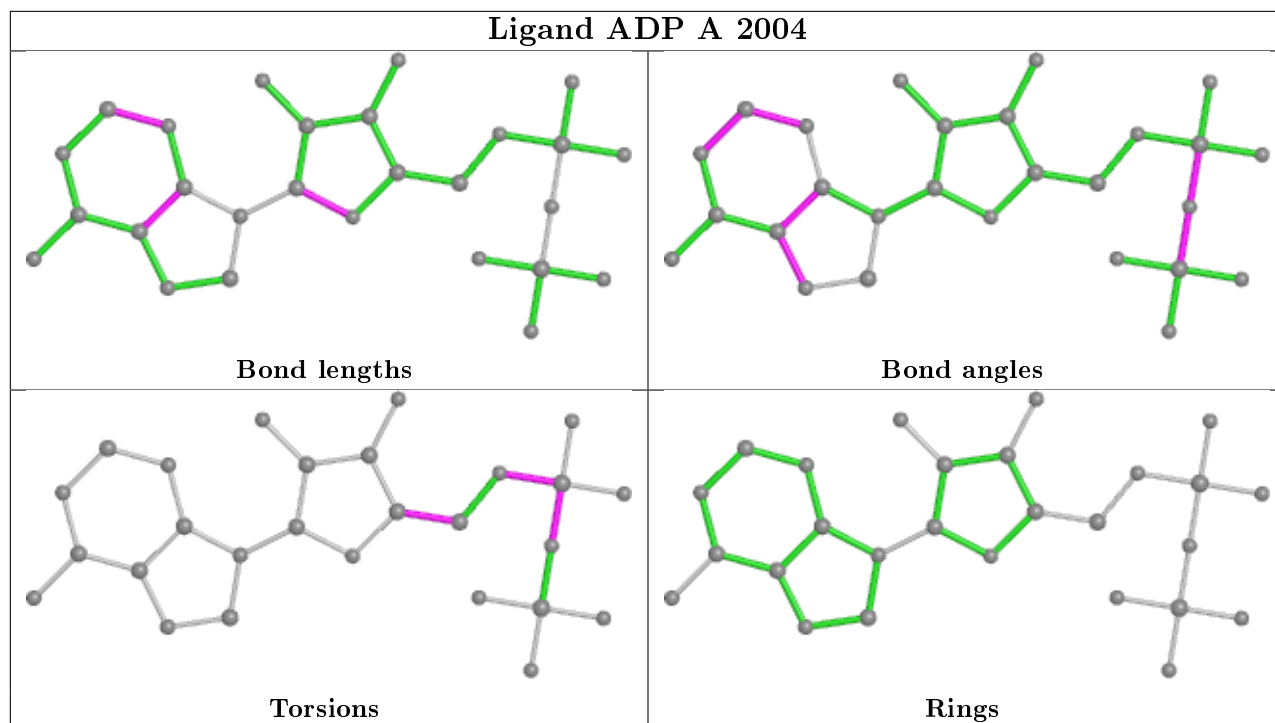
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

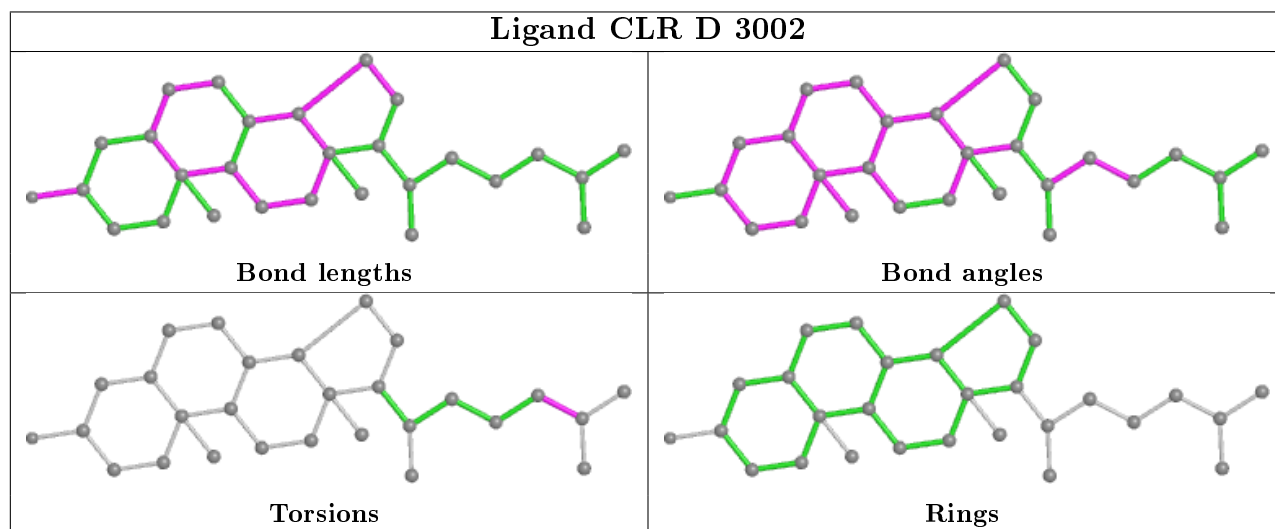
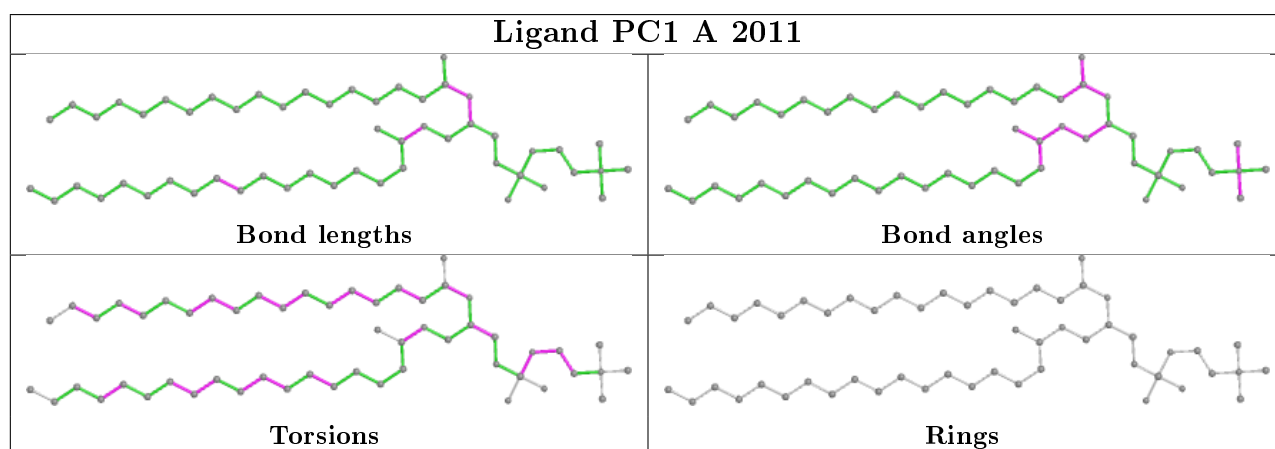
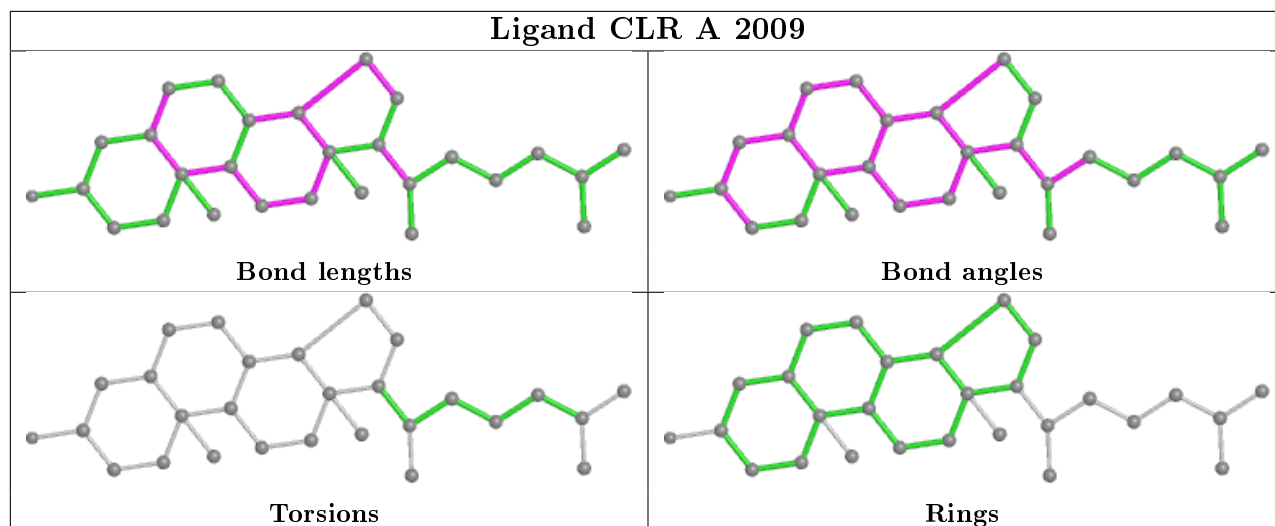


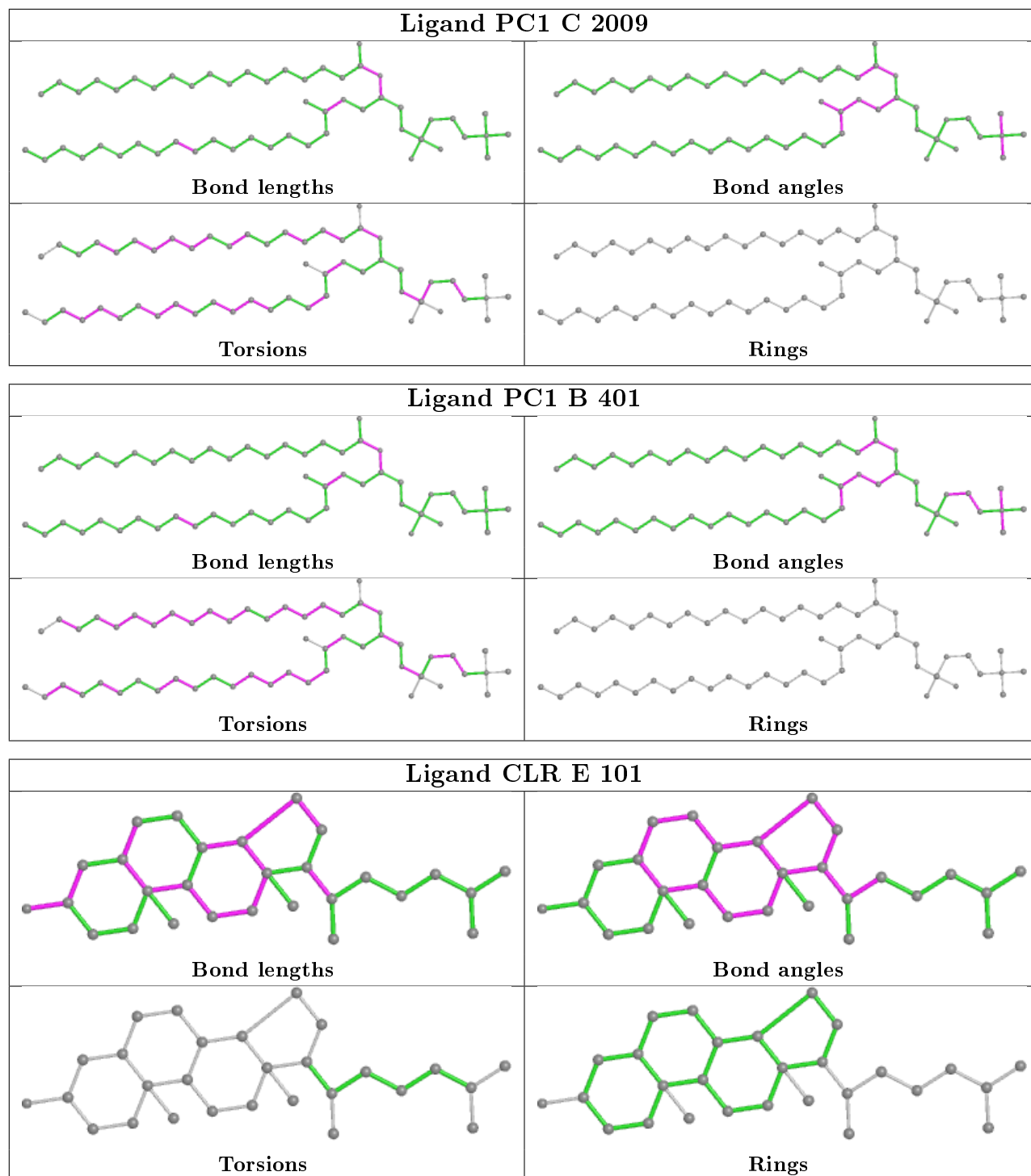


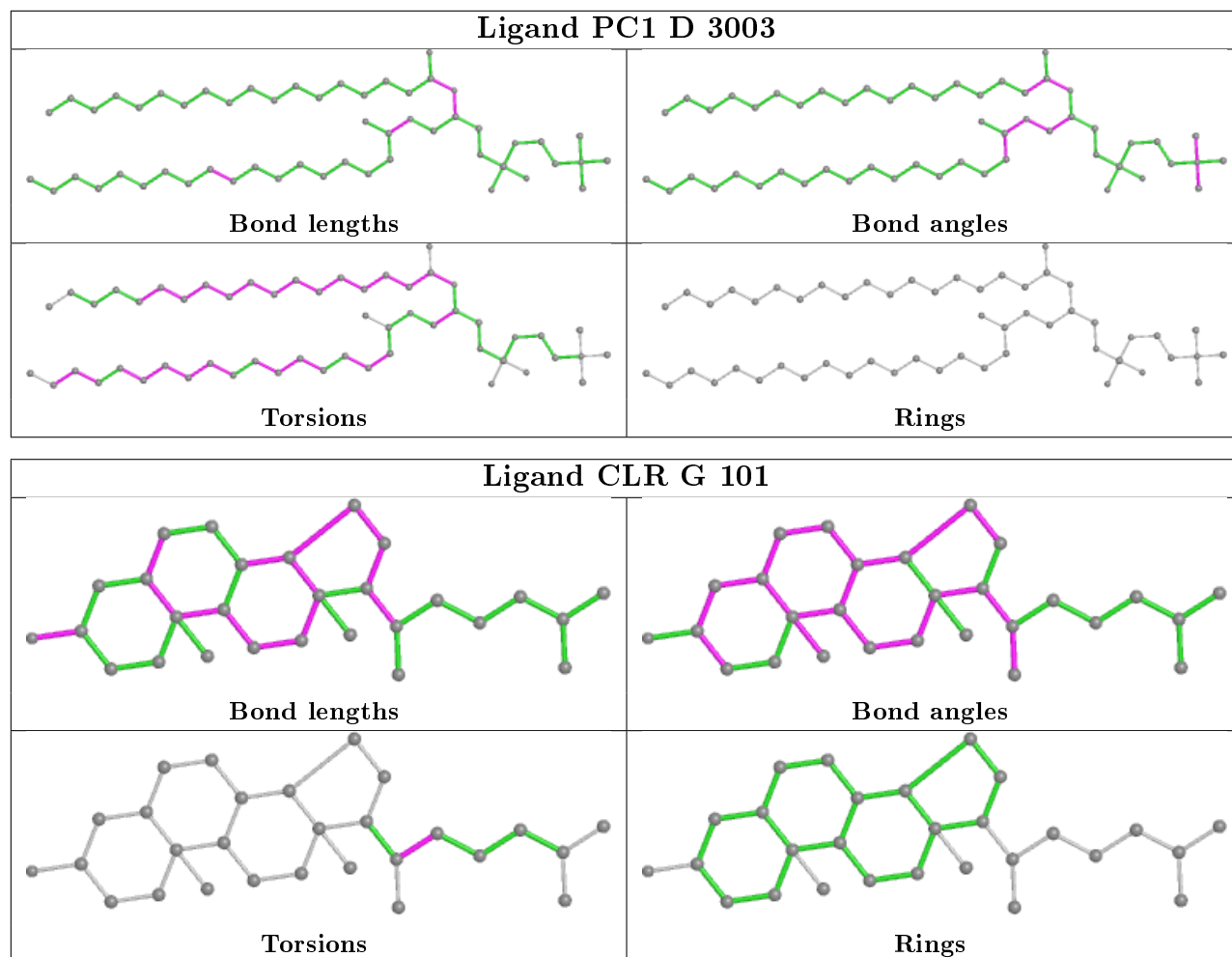












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	994/1016 (97%)	-0.29	21 (2%) 63 54	17, 57, 117, 181	0
1	C	994/1016 (97%)	0.01	35 (3%) 44 34	34, 74, 143, 199	0
2	B	303/303 (100%)	0.88	53 (17%) 1 1	59, 130, 199, 229	0
2	D	303/303 (100%)	0.90	50 (16%) 1 1	68, 127, 205, 239	0
3	E	35/65 (53%)	0.80	5 (14%) 2 1	70, 88, 165, 168	0
3	G	34/65 (52%)	0.50	3 (8%) 10 5	75, 91, 164, 175	0
All	All	2663/2768 (96%)	0.11	167 (6%) 20 12	17, 77, 161, 239	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	218	ASP	18.2
2	D	219	GLU	14.7
2	B	1	MET	9.8
3	E	16	VAL	9.6
3	E	15	ASP	9.3
2	D	167	TYR	9.3
2	D	166	THR	8.8
2	D	1	MET	8.6
1	C	396	THR	8.5
3	G	15	ASP	7.9
2	B	165	GLU	7.6
2	D	217	ARG	7.4
2	B	198	THR	7.3
1	C	268	SER	7.0
2	D	196	LEU	6.9
2	B	166	THR	6.8
1	A	272	GLY	6.7
2	D	195	SER	6.3
2	B	201	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
2	D	17	TRP	6.0
2	B	220	ASP	6.0
1	C	265	THR	5.8
2	B	164	ASP	5.8
2	D	162	LEU	5.8
2	B	15	PHE	5.8
2	B	163	ASN	5.6
2	B	217	ARG	5.6
2	D	16	ILE	5.5
2	D	2	ALA	5.4
2	B	218	ASP	5.4
3	E	17	ASP	5.3
3	G	16	VAL	5.2
2	D	228	GLU	5.2
1	C	397	GLU	5.1
2	B	219	GLU	4.9
1	A	400	SER	4.9
1	C	395	THR	4.9
2	D	198	THR	4.9
2	D	15	PHE	4.9
1	A	268	SER	4.8
2	D	203	LYS	4.8
2	D	197	GLU	4.8
1	A	23	ARG	4.8
3	E	18	PRO	4.8
2	B	7	LYS	4.7
2	D	201	VAL	4.7
2	D	163	ASN	4.5
1	A	271	GLU	4.5
1	C	269	GLY	4.4
2	D	11	SER	4.4
2	B	4	GLY	4.4
2	B	17	TRP	4.4
2	B	194	GLU	4.3
2	B	196	LEU	4.3
2	B	6	ALA	4.2
1	A	117	GLU	4.2
2	B	195	SER	4.2
2	D	164	ASP	4.2
2	D	9	GLU	4.1
1	C	82	TRP	4.1
2	B	302	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	200	PRO	4.0
2	B	227	MET	4.0
1	A	273	GLY	4.0
2	D	202	MET	3.9
2	D	165	GLU	3.9
1	A	270	LEU	3.9
3	G	17	ASP	3.8
2	D	220	ASP	3.8
2	B	167	TYR	3.8
1	C	24	ASP	3.6
2	B	3	ARG	3.6
1	C	642	ASN	3.6
2	D	23	GLU	3.6
2	B	9	GLU	3.5
1	A	395	THR	3.5
1	A	82	TRP	3.4
1	C	78	THR	3.4
2	D	118	LYS	3.4
1	C	650	PRO	3.3
1	C	398	ASN	3.3
1	A	265	THR	3.3
1	C	645	VAL	3.3
2	D	82	GLN	3.2
1	C	141	TYR	3.2
2	D	89	SER	3.2
1	C	270	LEU	3.1
1	A	114	THR	3.1
1	A	264	ALA	3.1
1	A	399	GLN	3.1
2	D	200	PRO	3.1
2	B	290	ARG	3.0
2	B	23	GLU	3.0
2	D	194	GLU	3.0
2	D	193	ASN	3.0
2	B	142	GLU	3.0
2	B	12	TRP	3.0
1	A	269	GLY	3.0
2	D	10	GLY	3.0
2	B	5	LYS	3.0
2	B	2	ALA	3.0
2	D	21	LYS	2.9
1	A	401	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	495	ARG	2.9
1	C	1004	ARG	2.9
2	B	273	ARG	2.9
1	C	121	ASP	2.9
1	C	267	ALA	2.9
1	C	151	MET	2.8
1	C	632	GLU	2.8
2	D	192	LYS	2.8
2	B	262	GLN	2.7
2	D	207	TYR	2.6
2	B	202	MET	2.6
2	B	147	LYS	2.6
2	B	11	SER	2.6
2	B	16	ILE	2.6
2	D	5	LYS	2.6
2	D	13	LYS	2.5
2	B	118	LYS	2.5
2	B	235	TYR	2.5
1	C	117	GLU	2.5
1	A	495	ARG	2.5
2	D	19	SER	2.5
2	D	273	ARG	2.5
2	B	203	LYS	2.5
1	C	124	TYR	2.5
2	D	3	ARG	2.4
2	B	206	PRO	2.4
1	C	266	LEU	2.4
1	C	1000	LEU	2.4
2	D	100	SER	2.4
2	B	121	MET	2.4
1	C	23	ARG	2.4
1	C	116	GLU	2.4
2	B	162	LEU	2.4
2	D	229	TYR	2.4
2	B	10	GLY	2.4
2	D	6	ALA	2.4
1	C	431	GLU	2.3
2	B	8	GLU	2.3
2	D	152	ARG	2.3
3	E	49	ARG	2.3
2	D	141	ASN	2.3
2	B	19	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	122	ASN	2.3
1	A	266	LEU	2.3
2	B	266	LEU	2.2
2	B	120	ASP	2.2
1	C	272	GLY	2.2
2	B	193	ASN	2.2
1	C	112	ALA	2.2
2	D	115	LEU	2.2
1	A	974	TYR	2.2
1	C	123	LEU	2.2
1	A	24	ASP	2.2
1	C	115	GLU	2.2
2	D	24	PHE	2.1
1	A	120	ASN	2.1
2	B	249	LEU	2.1
2	B	143	ARG	2.1
1	C	310	TRP	2.1
2	B	199	TYR	2.1
2	D	33	PHE	2.1
1	C	406	LYS	2.0
2	D	199	TYR	2.0
2	B	84	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NA	C	2006	1/1	0.18	0.44	83,83,83,83	0

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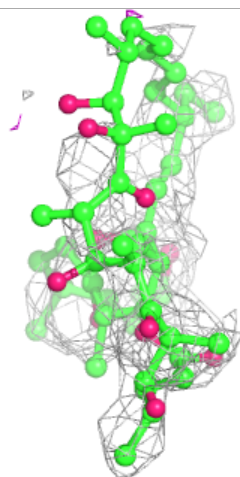
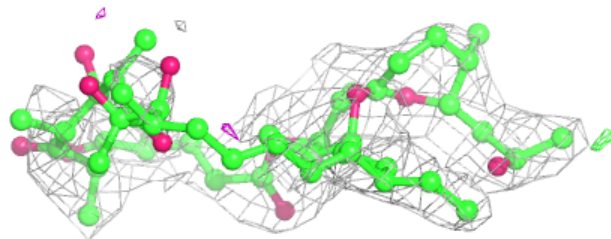
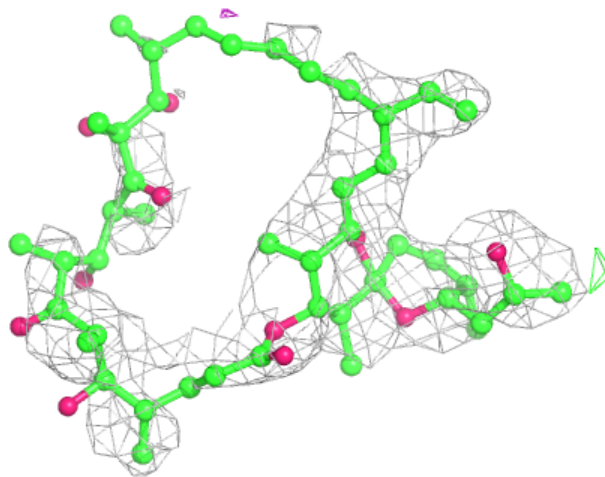
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NA	A	2008	1/1	0.71	0.18	59,59,59,59	0
10	EFO	C	2013	56/56	0.77	0.41	49,150,194,195	0
9	PC1	C	2012	54/54	0.77	0.35	79,133,162,185	0
9	PC1	A	2012	54/54	0.80	0.36	61,117,163,176	0
9	PC1	A	2014	54/54	0.81	0.36	86,123,160,189	0
9	PC1	C	2010	54/54	0.82	0.31	68,101,143,205	0
10	EFO	A	2015	56/56	0.82	0.33	91,134,150,160	0
9	PC1	B	401	54/54	0.82	0.26	61,90,146,170	0
9	PC1	C	2011	54/54	0.83	0.42	77,117,163,173	0
4	MG	C	2001	1/1	0.83	0.23	54,54,54,54	0
11	NAG	B	402	14/15	0.84	0.34	126,137,144,146	0
11	NAG	D	3004	14/15	0.84	0.31	96,123,132,133	0
8	CLR	D	3002	28/28	0.87	0.29	13,97,131,141	0
7	NA	C	2005	1/1	0.87	0.31	103,103,103,103	0
7	NA	A	2007	1/1	0.88	0.31	98,98,98,98	0
9	PC1	C	2009	54/54	0.88	0.26	59,107,140,145	0
9	PC1	A	2013	54/54	0.88	0.28	71,103,124,174	0
9	PC1	D	3003	54/54	0.88	0.23	44,80,121,142	0
8	CLR	A	2010	28/28	0.89	0.33	60,98,131,138	0
8	CLR	A	2009	28/28	0.89	0.22	62,93,107,147	0
9	PC1	A	2011	54/54	0.90	0.26	57,97,128,130	0
8	CLR	D	3001	28/28	0.91	0.18	35,83,89,92	0
8	CLR	G	101	28/28	0.91	0.18	54,91,100,131	0
7	NA	A	2005	1/1	0.92	0.19	95,95,95,95	0
8	CLR	E	101	28/28	0.92	0.16	37,77,109,172	0
7	NA	A	2006	1/1	0.93	0.16	65,65,65,65	0
4	MG	A	2001	1/1	0.94	0.38	61,61,61,61	0
7	NA	C	2007	1/1	0.95	0.26	77,77,77,77	0
7	NA	C	2008	1/1	0.95	0.16	46,46,46,46	0
6	ADP	C	2004	27/27	0.96	0.14	31,47,57,60	0
4	MG	C	2003	1/1	0.97	0.12	51,51,51,51	0
6	ADP	A	2004	27/27	0.97	0.11	10,23,38,47	0
5	ALF	A	2002	5/5	0.98	0.17	14,14,28,29	0
5	ALF	C	2002	5/5	0.99	0.16	20,24,71,106	0
4	MG	A	2003	1/1	1.00	0.11	15,15,15,15	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.

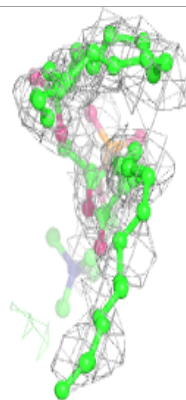
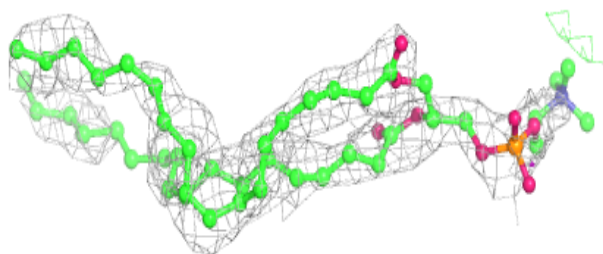
Electron density around EFO C 2013:

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

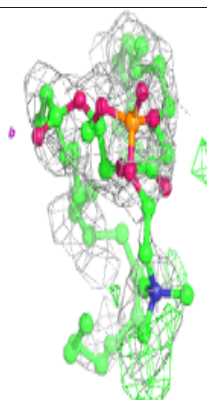
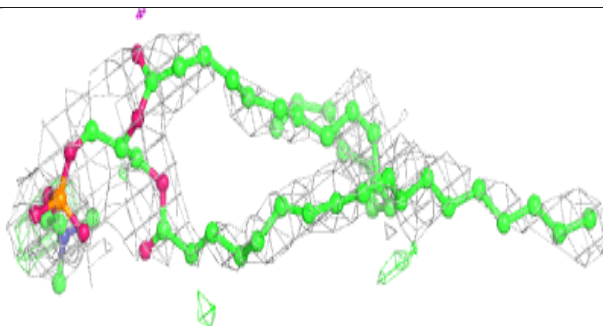
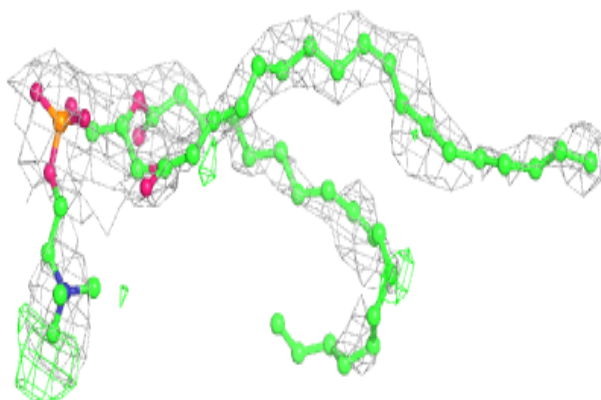


Electron density around PC1 C 2012:

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

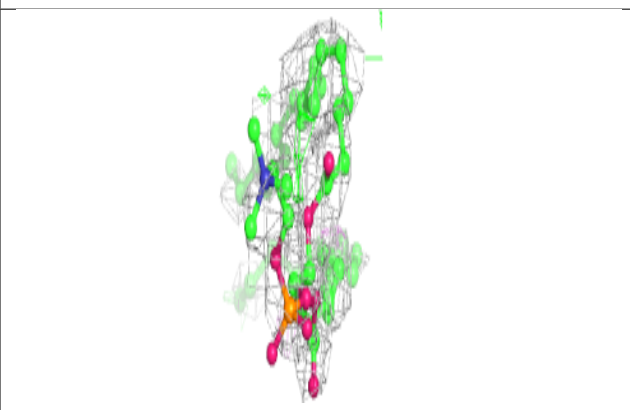
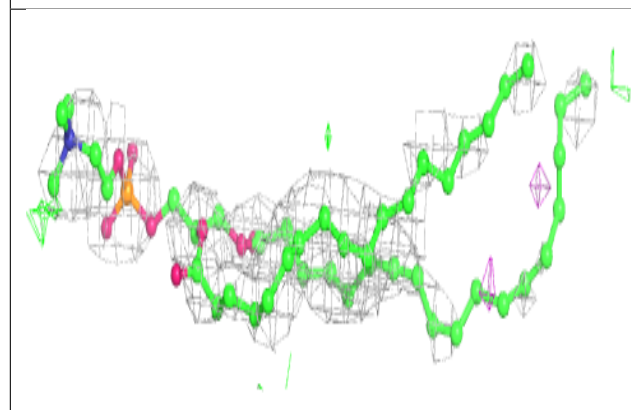
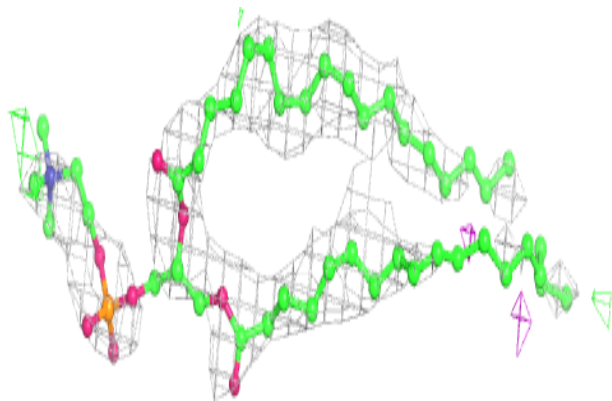
**Electron density around PC1 A 2012:**

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

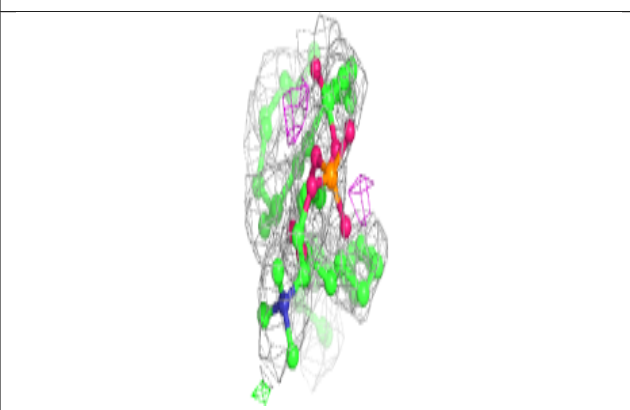
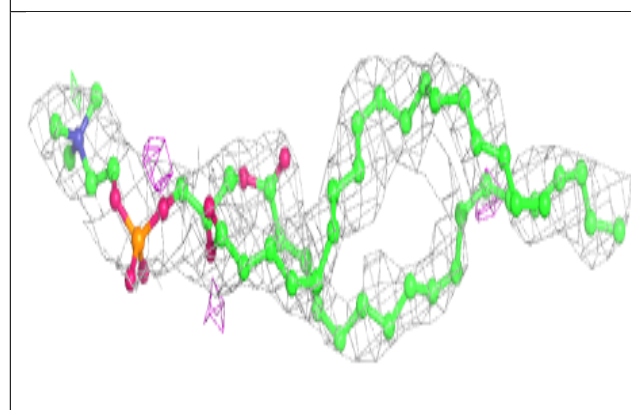
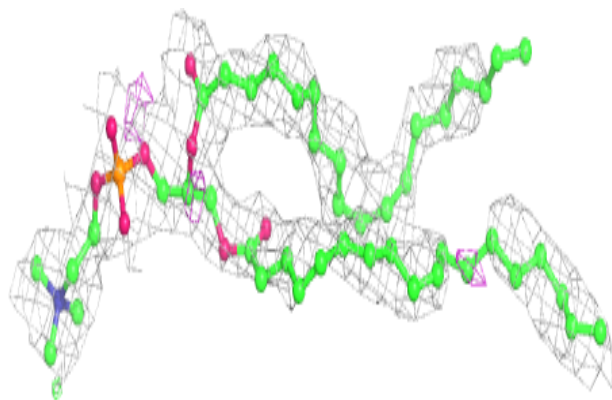


Electron density around PC1 A 2014:

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

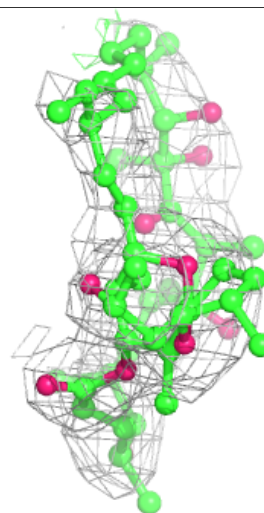
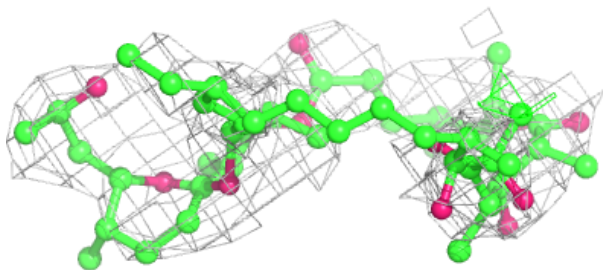
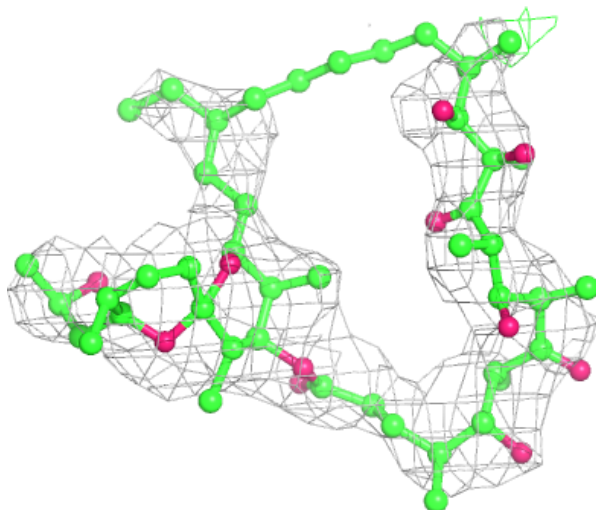
**Electron density around PC1 C 2010:**

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



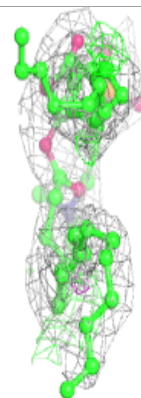
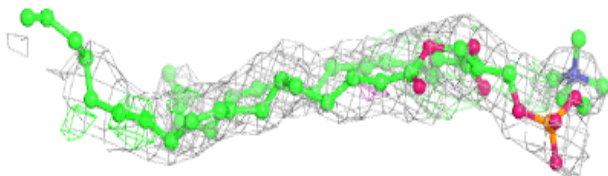
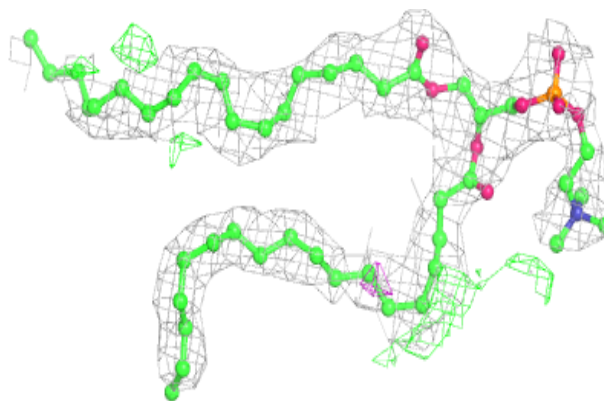
Electron density around EFO A 2015:

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

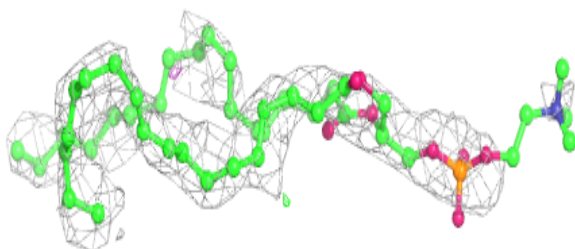
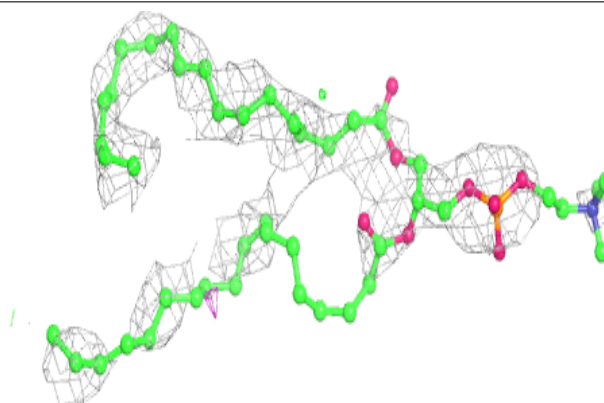


Electron density around PC1 B 401:

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

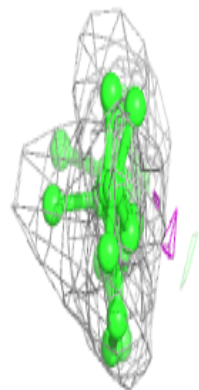
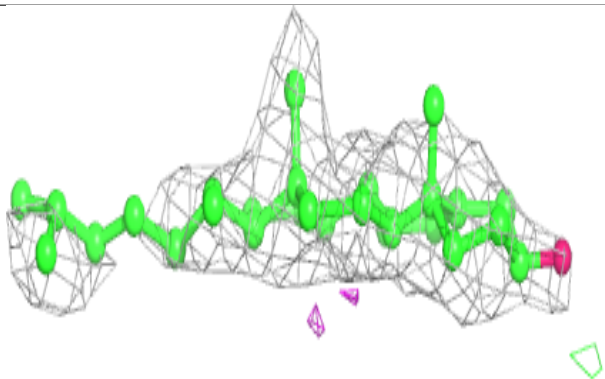
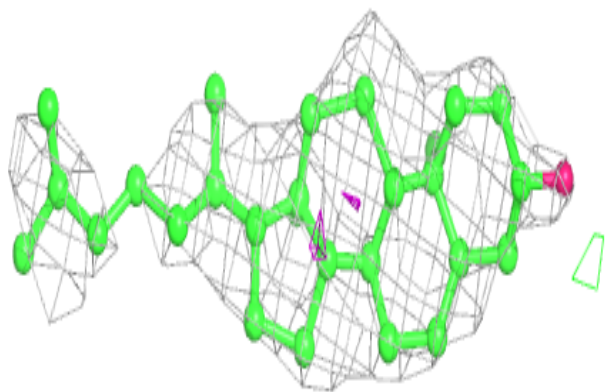
**Electron density around PC1 C 2011:**

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

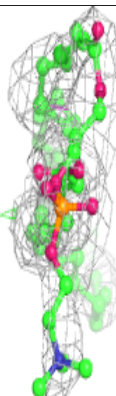
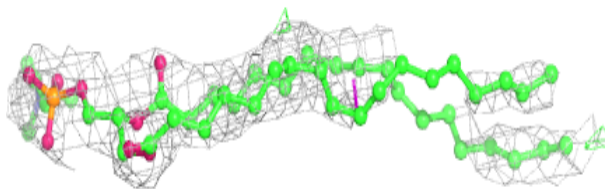
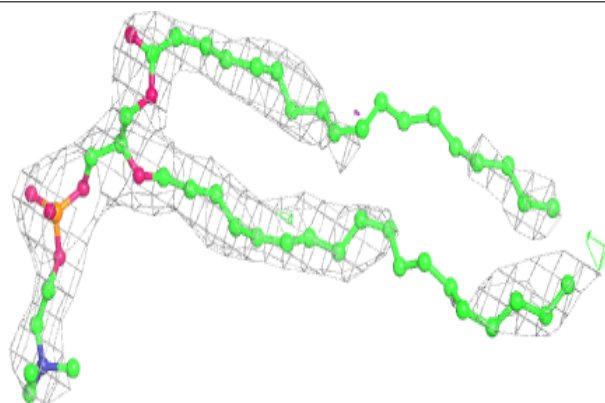


Electron density around CLR D 3002:

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

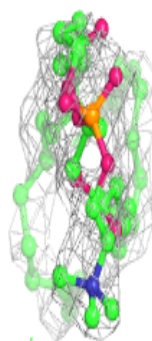
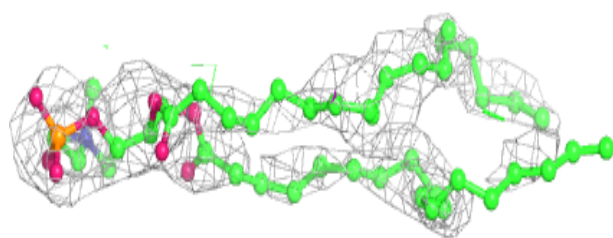
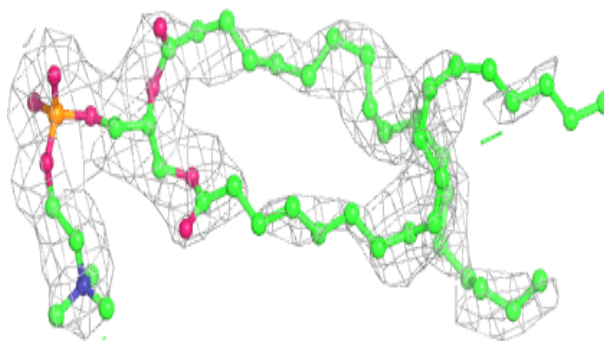
**Electron density around PC1 C 2009:**

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

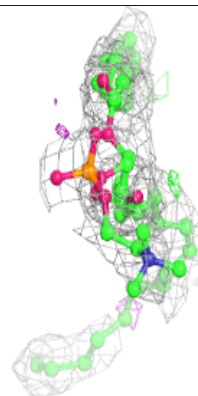
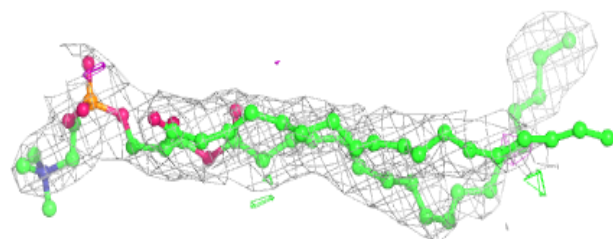
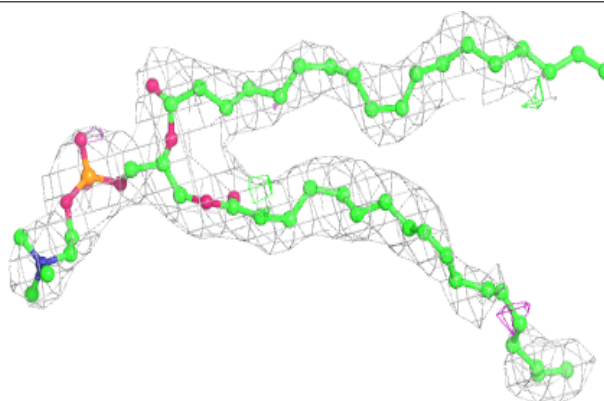


Electron density around PC1 A 2013:

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

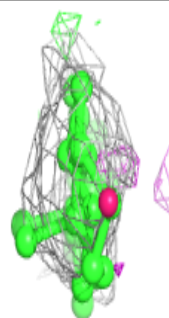
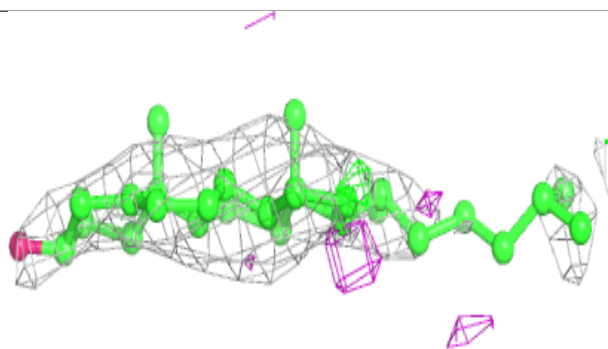
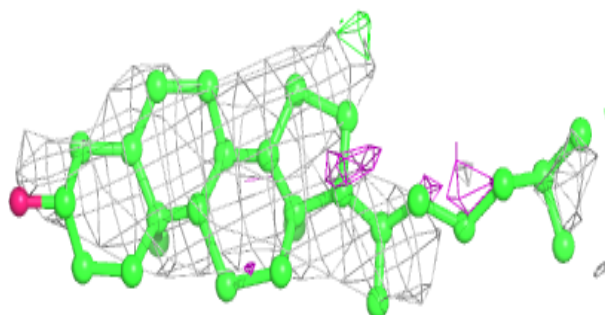
**Electron density around PC1 D 3003:**

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

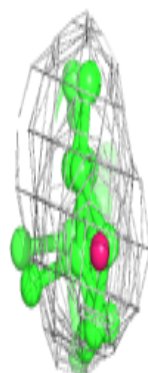
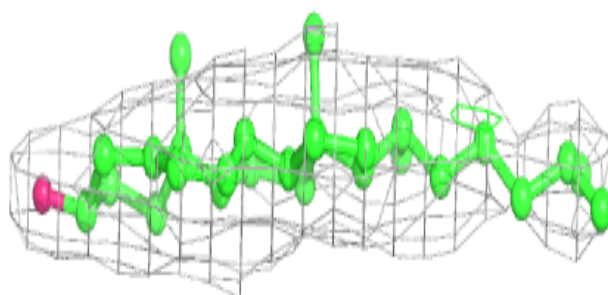
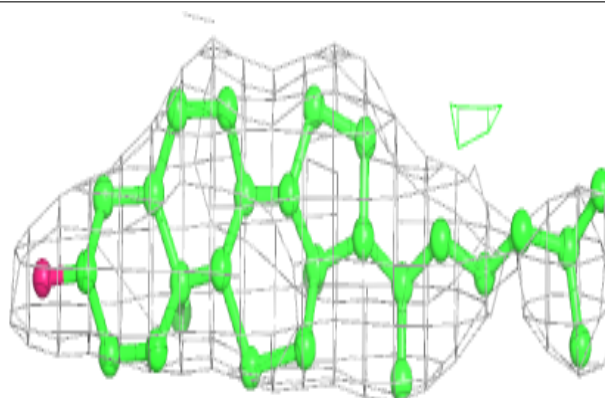


Electron density around CLR A 2010:

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

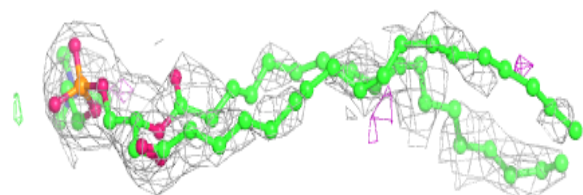
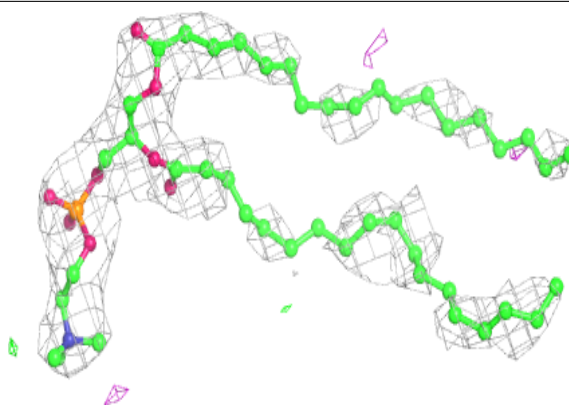
**Electron density around CLR A 2009:**

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

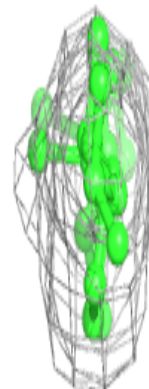
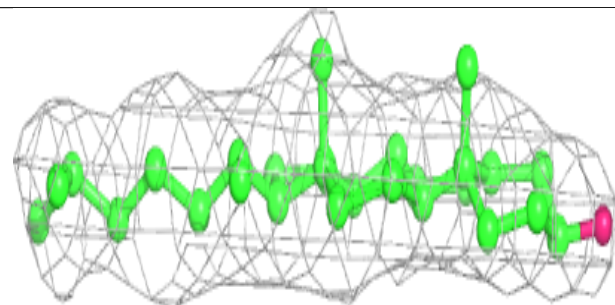
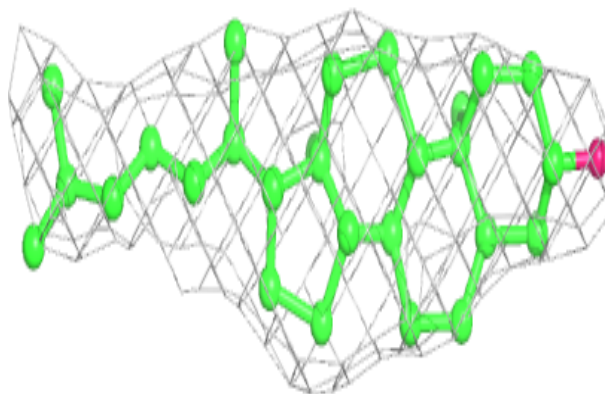


Electron density around PC1 A 2011:

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

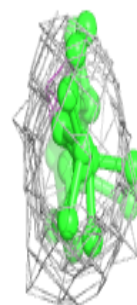
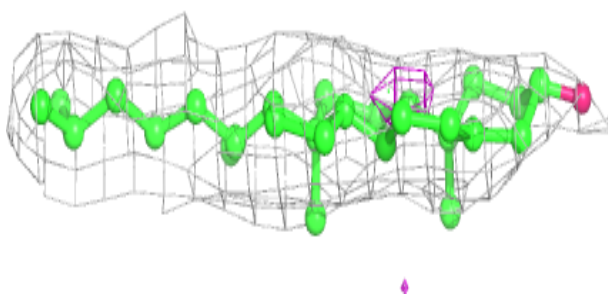
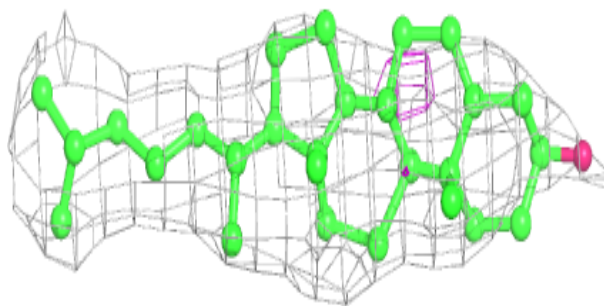
**Electron density around CLR D 3001:**

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

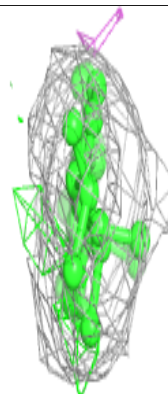
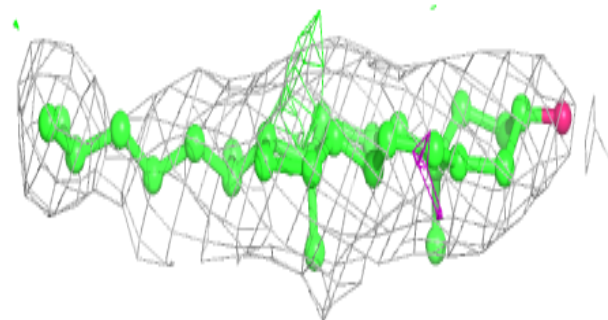
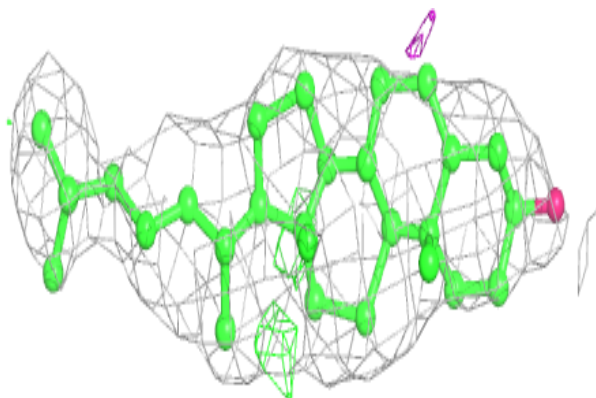


Electron density around CLR G 101:

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

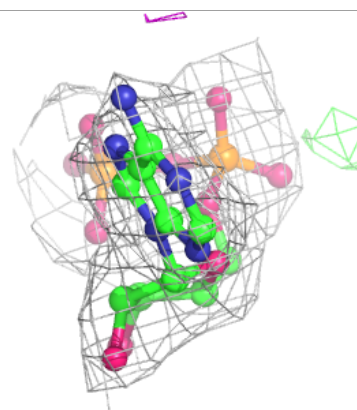
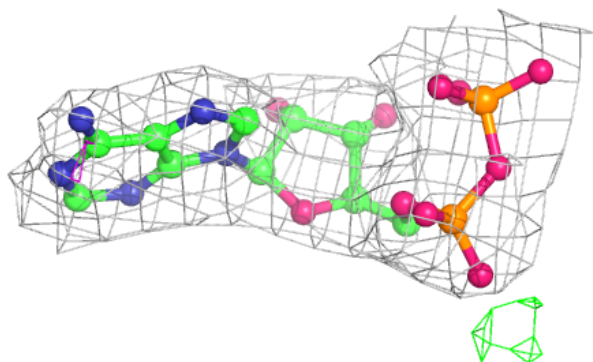
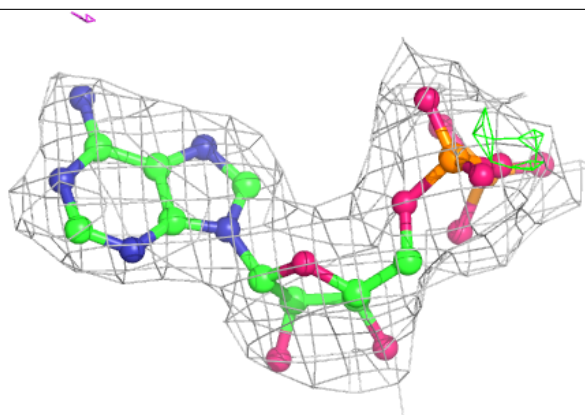
**Electron density around CLR E 101:**

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

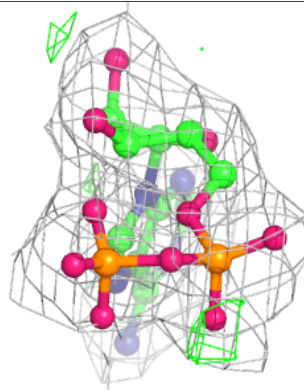
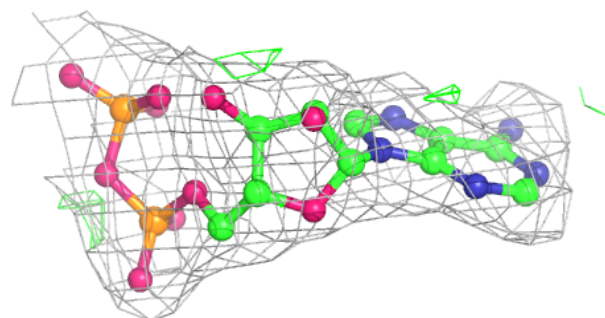
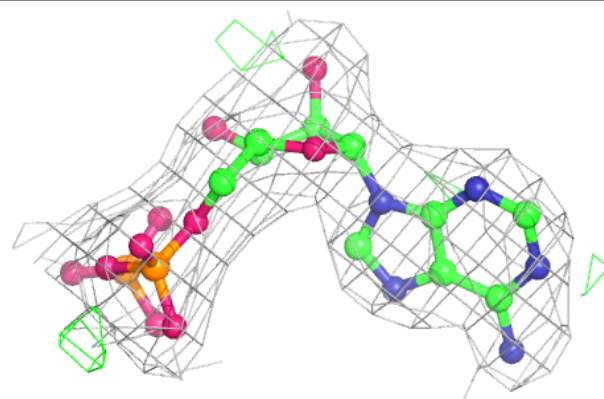


Electron density around ADP C 2004:

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

**Electron density around ADP A 2004:**

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



6.5 Other polymers

There are no such residues in this entry.