



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 3WGU / pdb_00003wgu
Title : Crystal structure of a Na⁺-bound Na⁺,K⁺-ATPase preceding the E1P state without 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

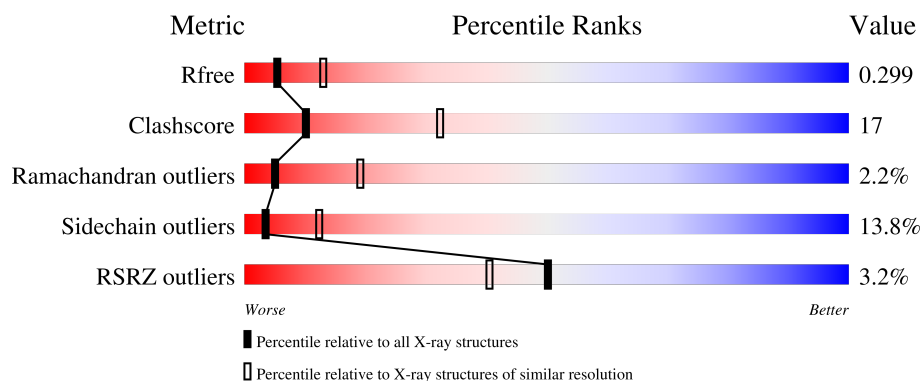
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



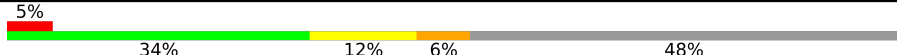
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1016	0% 55% 35% 7% .
1	C	1016	2% 58% 34% 6% .
2	B	303	7% 50% 42% 8% .
2	D	303	10% 55% 36% 7% .
3	E	65	3% 28% 22% 5% 46%

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Mol	Chain	Length	Quality of chain
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
5	ALF	C	2002	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21807 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			
1	C	994	Total	C	N	O	S	0	0	0
			7714	4918	1300	1449	47			

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

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

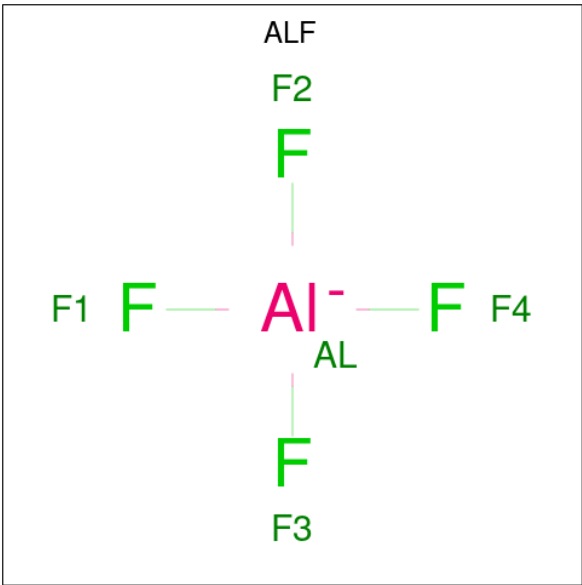
- Molecule 3 is a protein called Na⁺/K⁺ ATPase gamma subunit transcript variant a.

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

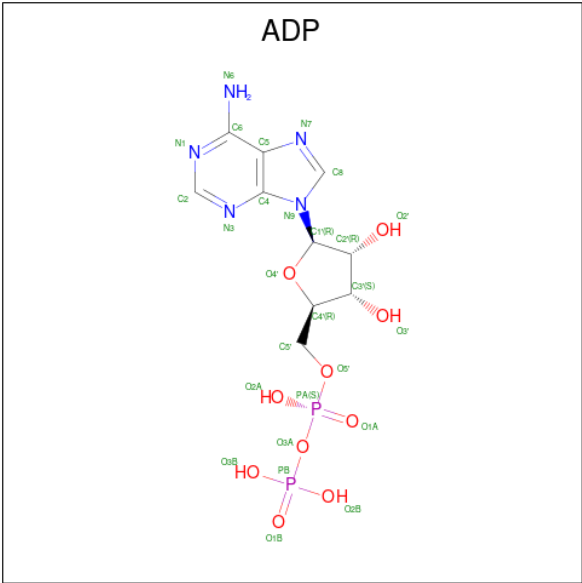
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: 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 (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

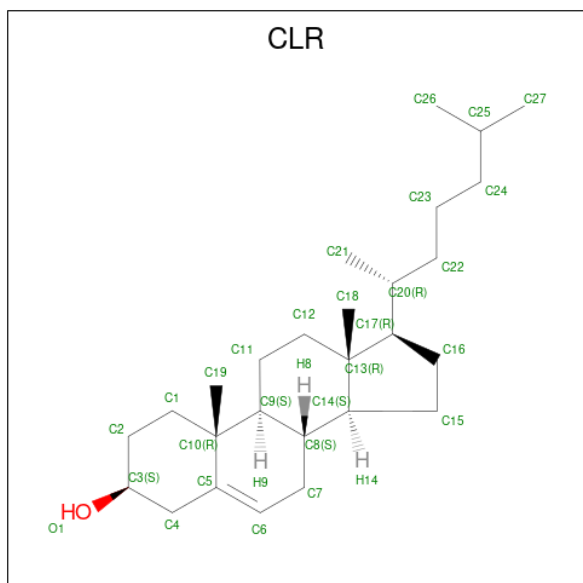


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

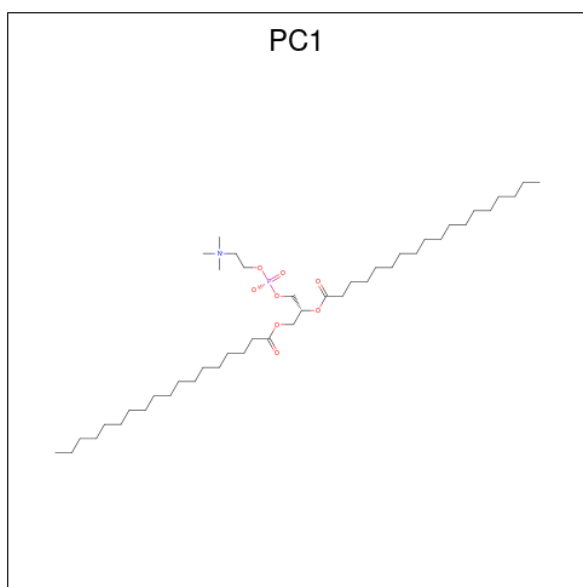
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	4	Total	Na	0	0
			4	4		
7	C	4	Total	Na	0	0
			4	4		

- Molecule 8 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



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

- Molecule 9 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



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

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



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

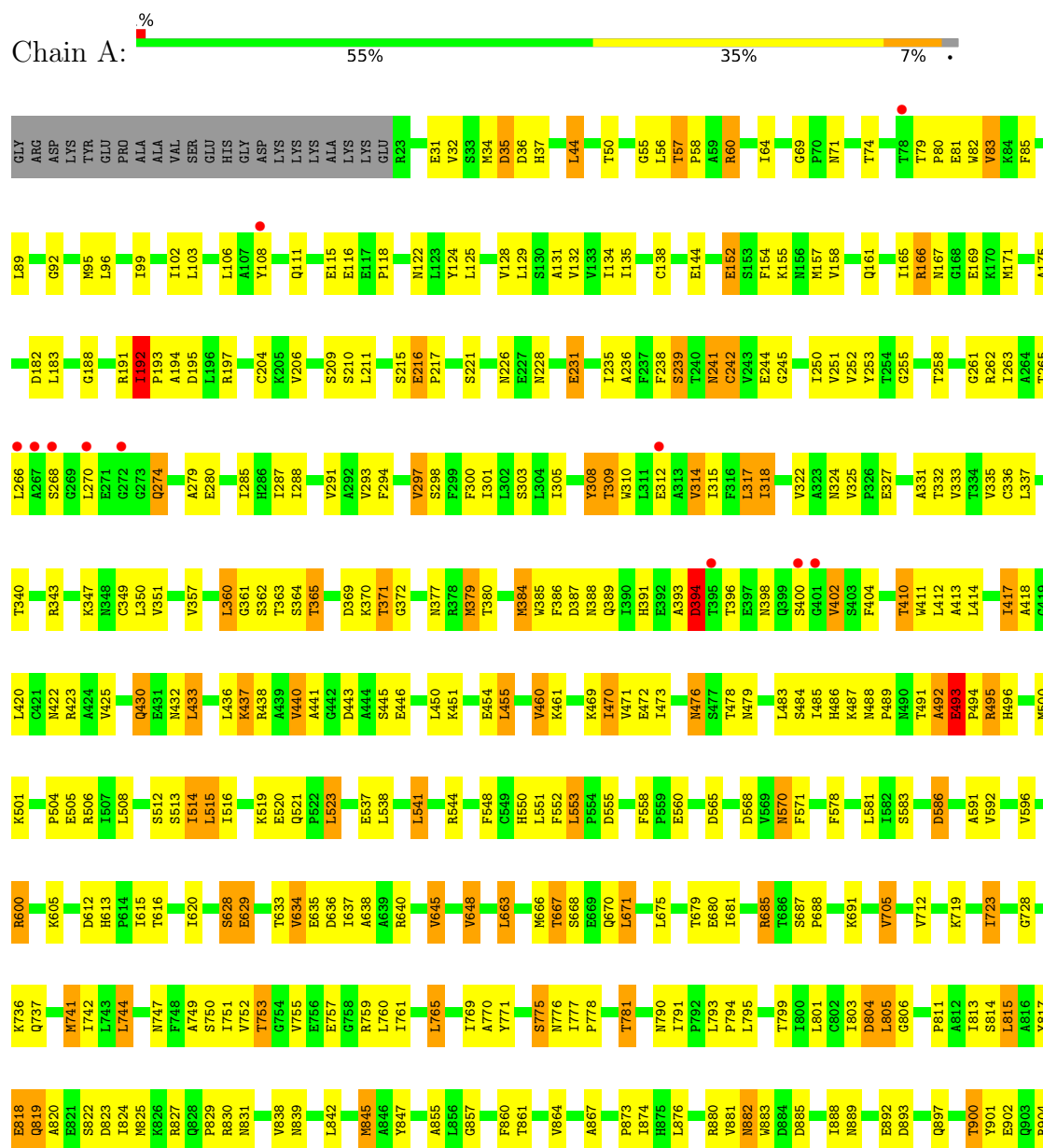
- Molecule 11 is water.

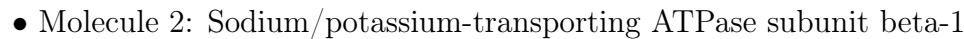
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	30	Total	O	0	0
			30	30		
11	B	2	Total	O	0	0
			2	2		
11	C	23	Total	O	0	0
			23	23		
11	D	3	Total	O	0	0
			3	3		

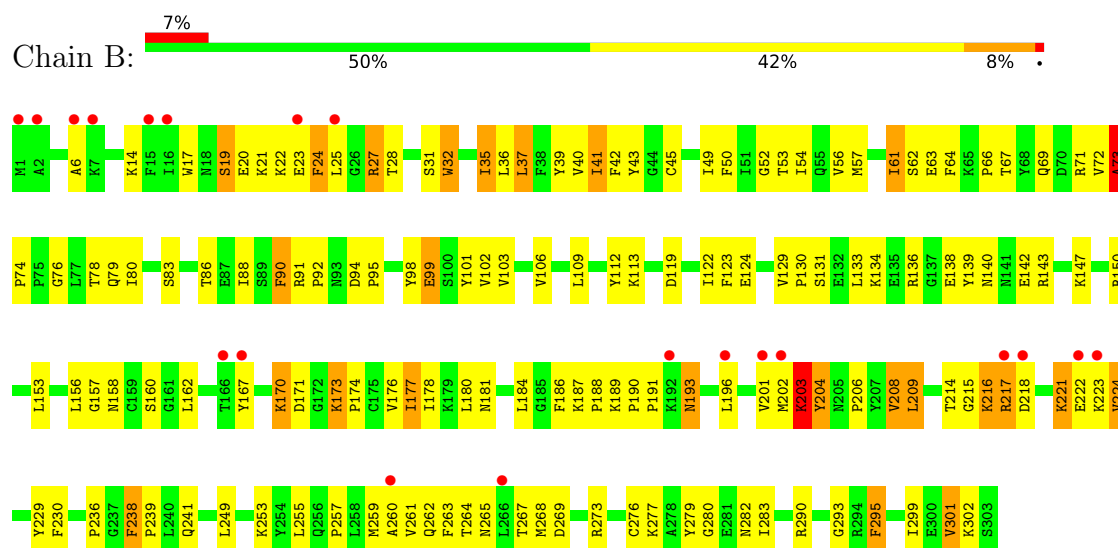
3 Residue-property plots

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

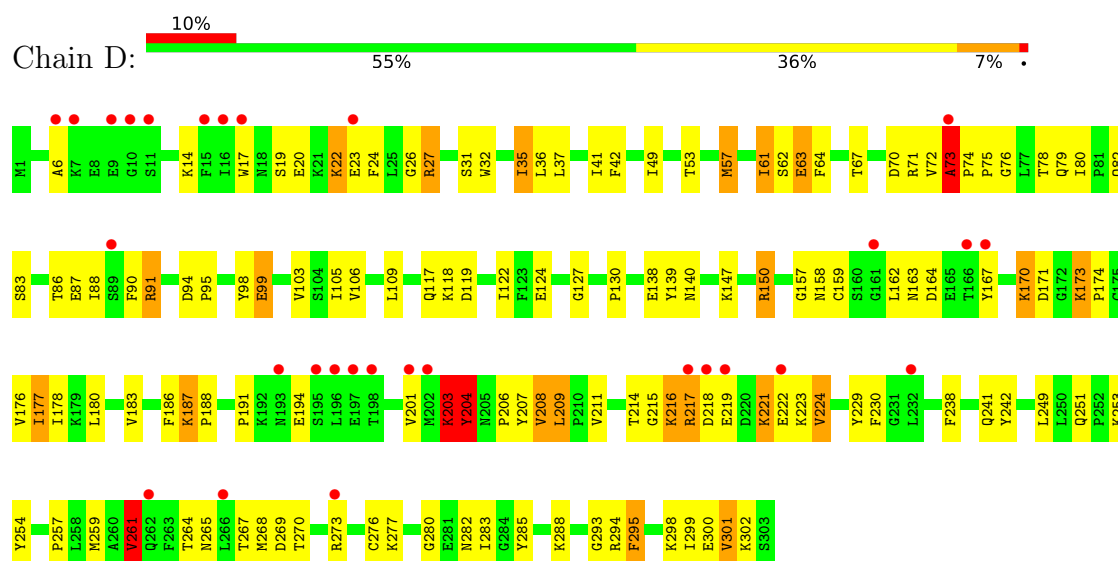
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1



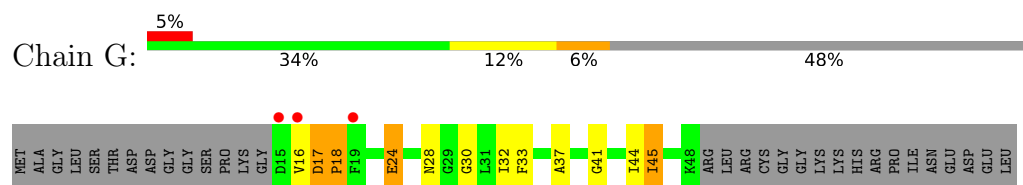




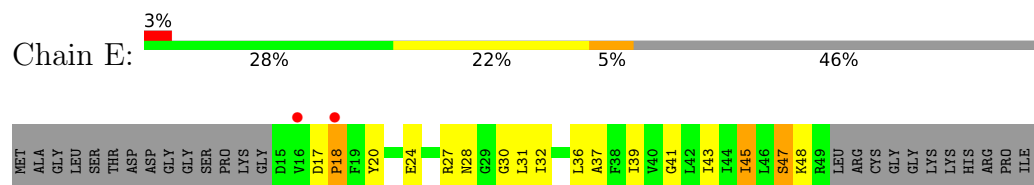
- Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1



- 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	106.38Å 211.60Å 257.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.99 – 2.80 15.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.9 (15.99-2.80) 88.3 (15.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.265 , 0.299 0.267 , 0.299	Depositor DCC
R_{free} test set	6460 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.15 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	21807	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: NAG, CLR, MG, ADP, NA, PC1, ALF

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	0.60	0/7864	0.99	23/10671 (0.2%)
1	C	0.51	0/7864	0.92	14/10671 (0.1%)
2	B	0.40	0/2544	0.94	11/3426 (0.3%)
2	D	0.40	0/2544	0.88	8/3426 (0.2%)
3	E	0.66	1/287 (0.3%)	1.12	3/389 (0.8%)
3	G	0.48	0/276	0.88	0/375
All	All	0.53	1/21379 (0.0%)	0.94	59/28958 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	18	PRO	N-CD	7.86	1.58	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	495	ARG	CB-CA-C	-15.90	94.09	109.83
2	B	73	ALA	CA-C-N	-10.73	109.33	120.38
2	B	73	ALA	C-N-CA	-10.73	109.33	120.38
2	D	73	ALA	CA-C-N	-10.32	109.75	120.38
2	D	73	ALA	C-N-CA	-10.32	109.75	120.38
1	A	495	ARG	CB-CA-C	-7.95	94.59	110.42
3	E	18	PRO	N-CA-CB	7.56	111.19	103.25
1	A	35	ASP	N-CA-C	7.17	117.73	108.34
2	B	173	LYS	CA-C-N	7.01	126.94	120.21
2	B	173	LYS	C-N-CA	7.01	126.94	120.21
3	E	18	PRO	CA-N-CD	-6.98	102.23	112.00
1	A	586	ASP	CA-C-N	6.95	124.66	119.66
1	A	586	ASP	C-N-CA	6.95	124.66	119.66
1	A	493	GLU	CA-C-N	-6.81	113.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	GLU	C-N-CA	-6.81	113.10	121.00
3	E	17	ASP	C-N-CD	-6.75	97.31	125.00
1	A	555	ASP	N-CA-C	6.36	117.88	111.07
1	C	705	VAL	N-CA-C	6.28	118.07	108.71
1	A	553	LEU	CA-C-N	6.07	125.83	119.76
1	A	553	LEU	C-N-CA	6.07	125.83	119.76
1	C	298	SER	N-CA-C	-6.00	104.66	111.14
1	A	192	ILE	CA-C-N	5.98	126.50	120.04
1	A	192	ILE	C-N-CA	5.98	126.50	120.04
1	A	931	LYS	N-CA-C	-5.95	106.57	113.88
1	A	74	THR	CA-C-N	5.86	126.41	120.38
1	A	74	THR	C-N-CA	5.86	126.41	120.38
2	B	209	LEU	CA-C-N	5.79	125.73	119.76
2	B	209	LEU	C-N-CA	5.79	125.73	119.76
1	C	734	VAL	N-CA-C	5.79	115.98	110.42
1	A	69	GLY	CA-C-N	5.70	125.71	119.89
1	A	69	GLY	C-N-CA	5.70	125.71	119.89
1	C	649	ASN	CA-C-N	5.54	125.21	119.56
1	C	649	ASN	C-N-CA	5.54	125.21	119.56
1	C	910	THR	N-CA-C	-5.54	106.48	113.18
1	C	964	CYS	CA-C-N	5.42	125.42	119.89
1	C	964	CYS	C-N-CA	5.42	125.42	119.89
1	C	793	LEU	CA-C-N	5.40	125.10	119.64
1	C	793	LEU	C-N-CA	5.40	125.10	119.64
1	A	977	LYS	CA-C-N	5.40	126.59	119.84
1	A	977	LYS	C-N-CA	5.40	126.59	119.84
1	A	492	ALA	N-CA-C	-5.38	106.57	113.02
2	B	238	PHE	CA-C-N	5.33	126.51	119.84
2	B	238	PHE	C-N-CA	5.33	126.51	119.84
1	A	770	ALA	N-CA-C	-5.24	105.48	111.14
1	A	221	SER	CA-C-N	-5.24	114.64	120.45
1	A	221	SER	C-N-CA	-5.24	114.64	120.45
2	D	173	LYS	CA-C-N	5.21	125.94	120.11
2	D	173	LYS	C-N-CA	5.21	125.94	120.11
2	D	91	ARG	CA-C-N	5.15	126.28	119.84
2	D	91	ARG	C-N-CA	5.15	126.28	119.84
1	C	740	ASP	N-CA-C	-5.14	106.69	113.17
1	A	705	VAL	N-CA-C	5.14	116.94	108.97
2	B	32	TRP	N-CA-C	-5.11	105.83	111.71
1	C	800	ILE	N-CA-C	-5.09	105.57	110.72
2	D	209	LEU	CA-C-N	5.06	124.97	119.76
2	D	209	LEU	C-N-CA	5.06	124.97	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	189	LYS	CA-C-N	5.05	125.58	120.38
2	B	189	LYS	C-N-CA	5.05	125.58	120.38
1	C	580	GLY	N-CA-C	5.03	117.38	110.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7714	0	7769	280	0
1	C	7714	0	7768	258	0
2	B	2479	0	2458	95	0
2	D	2479	0	2458	83	0
3	E	281	0	285	9	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	5	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	87	12	0
8	B	28	0	44	4	0
8	C	84	0	131	23	0
9	A	216	0	352	14	0
9	B	54	0	88	0	0
9	C	216	0	352	21	0
9	D	54	0	88	3	0
10	B	14	0	13	0	0
10	D	14	0	13	0	0
11	A	30	0	0	0	0
11	B	2	0	0	0	0
11	C	23	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D	3	0	0	1	0
All	All	21807	0	22202	757	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 17.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:ARG:HG3	1:C:495:ARG:O	1.61	0.97
1:C:57:THR:HG23	1:C:60:ARG:HB2	1.52	0.90
2:B:221:LYS:HE3	2:B:223:LYS:HB2	1.54	0.90
8:C:2010:CLR:H272	9:C:2014:PC1:H2I2	1.54	0.88
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.56	0.87
1:C:166:ARG:NH1	1:C:182:ASP:OD1	2.08	0.87
1:A:600:ARG:HG2	1:A:600:ARG:HH11	1.39	0.87
1:C:44:LEU:HD11	1:C:197:ARG:HG2	1.58	0.86
1:C:985:PHE:HZ	8:C:2011:CLR:H221	1.40	0.85
1:A:417:ILE:HD11	1:A:548:PHE:HB3	1.57	0.85
1:C:454:GLU:HG2	1:C:460:VAL:HG23	1.58	0.85
1:C:384:MET:HE1	1:C:393:ALA:HB2	1.60	0.84
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.41	0.83
2:D:124:GLU:HB2	2:D:147:LYS:HD3	1.60	0.83
1:A:44:LEU:HD11	1:A:197:ARG:HG2	1.61	0.82
2:D:221:LYS:HE3	2:D:223:LYS:HB2	1.60	0.82
2:D:269:ASP:HA	2:D:302:LYS:HA	1.60	0.82
1:C:493:GLU:HG2	1:C:495:ARG:H	1.43	0.82
2:B:216:LYS:HG2	2:B:221:LYS:HB2	1.62	0.81
1:A:369:ASP:OD2	5:A:2002:ALF:F4	1.88	0.81
1:A:274:GLN:HE22	1:A:279:ALA:HB2	1.42	0.80
1:A:493:GLU:HG2	1:A:495:ARG:H	1.44	0.79
1:A:369:ASP:OD1	1:A:691:LYS:NZ	2.15	0.79
2:B:76:GLY:HA2	2:B:293:GLY:H	1.47	0.79
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.65	0.78
2:D:216:LYS:HG2	2:D:221:LYS:HB2	1.65	0.78
2:B:188:PRO:HB3	2:B:209:LEU:HD22	1.65	0.78
1:A:790:ASN:HD22	1:A:880:ARG:HD2	1.48	0.78
1:A:370:LYS:NZ	1:A:612:ASP:OD2	2.17	0.77
1:C:946:ILE:HG13	3:E:45:ILE:HD11	1.67	0.77
1:A:759:ARG:HH12	1:A:829:PRO:HA	1.48	0.76
1:C:663:LEU:HA	1:C:666:MET:HE2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:HG3	1:A:495:ARG:O	1.83	0.76
1:A:565:ASP:H	1:A:570:ASN:HB2	1.49	0.76
8:C:2011:CLR:H121	8:C:2011:CLR:H212	1.65	0.76
1:A:443:ASP:HB2	1:A:446:GLU:HB2	1.68	0.76
1:C:565:ASP:H	1:C:570:ASN:HB2	1.47	0.76
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.68	0.75
9:A:2013:PC1:H292	9:A:2013:PC1:H3B2	1.68	0.75
1:C:495:ARG:O	1:C:495:ARG:CG	2.31	0.75
1:C:872:LEU:HD12	1:C:873:PRO:HD2	1.69	0.74
8:C:2009:CLR:H121	8:C:2009:CLR:H212	1.71	0.73
1:C:963:TYR:CE2	8:C:2011:CLR:H21	2.24	0.72
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.23	0.72
2:D:187:LYS:O	2:D:282:ASN:ND2	2.23	0.72
8:A:2009:CLR:H121	8:A:2009:CLR:H212	1.71	0.72
1:A:679:THR:HG23	1:A:680:GLU:HG3	1.72	0.72
1:C:801:LEU:HD13	1:C:805:LEU:HD21	1.71	0.72
2:B:269:ASP:HA	2:B:302:LYS:HA	1.72	0.72
1:C:195:ASP:HB2	1:C:253:TYR:HB2	1.71	0.72
8:C:2010:CLR:H121	8:C:2010:CLR:H212	1.71	0.72
1:C:986:PRO:HG3	8:C:2010:CLR:H152	1.70	0.71
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.55	0.71
1:A:50:THR:HG22	1:A:56:LEU:HB3	1.73	0.71
1:A:831:ASN:HD21	2:B:6:ALA:HB2	1.55	0.71
1:A:57:THR:HG23	1:A:60:ARG:HB2	1.72	0.70
1:C:763:ASP:OD2	11:C:2118:HOH:O	2.09	0.70
1:C:488:ASN:HB3	1:C:493:GLU:HG3	1.72	0.70
1:C:1003:ARG:HD2	9:C:2014:PC1:H122	1.73	0.70
1:A:166:ARG:NH1	1:A:182:ASP:OD1	2.23	0.70
1:A:445:SER:OG	1:A:544:ARG:NH1	2.25	0.70
8:B:3001:CLR:H121	8:B:3001:CLR:H212	1.71	0.70
1:C:365:THR:HB	1:C:705:VAL:HG12	1.73	0.69
2:B:14:LYS:HA	2:B:17:TRP:HB3	1.73	0.69
2:B:122:ILE:HG21	2:B:253:LYS:HE2	1.73	0.69
8:C:2010:CLR:H272	9:C:2014:PC1:C2I	2.22	0.69
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.73	0.69
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.28	0.68
9:C:2012:PC1:H3I1	9:C:2012:PC1:H2I3	1.75	0.68
9:C:2015:PC1:H351	9:C:2015:PC1:H251	1.76	0.68
1:A:544:ARG:NH2	6:A:2004:ADP:O2B	2.21	0.68
1:C:165:ILE:HB	1:C:183:LEU:HD21	1.75	0.68
1:C:696:GLU:HG3	1:C:720:LYS:HE2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:ILE:HG21	2:D:253:LYS:HE2	1.75	0.68
1:A:192:ILE:HD12	1:A:236:ALA:HB1	1.76	0.67
1:C:469:LYS:HA	1:C:486:HIS:HA	1.75	0.67
1:A:195:ASP:HB2	1:A:253:TYR:HB2	1.77	0.67
1:A:258:THR:HG23	1:A:261:GLY:H	1.59	0.67
1:A:986:PRO:HG3	8:A:2009:CLR:H181	1.78	0.66
1:A:495:ARG:O	1:A:495:ARG:CG	2.42	0.66
9:C:2012:PC1:H2D2	9:C:2015:PC1:H3F2	1.78	0.66
1:A:747:ASN:HD21	1:A:749:ALA:HB3	1.61	0.66
1:A:977:LYS:H	1:A:980:TRP:CD1	2.12	0.66
1:C:360:LEU:HG	1:C:723:ILE:HD13	1.76	0.66
2:D:188:PRO:HB3	2:D:209:LEU:HD22	1.76	0.66
2:B:88:ILE:HB	2:B:299:ILE:HG22	1.77	0.65
1:A:365:THR:HB	1:A:705:VAL:HG12	1.79	0.65
1:C:309:THR:HG23	1:C:312:GLU:HB2	1.78	0.65
1:A:946:ILE:HG13	3:G:45:ILE:HD11	1.78	0.65
1:C:471:VAL:HG21	1:C:564:PHE:HB2	1.78	0.65
1:C:372:GLY:O	1:C:589:ARG:NH2	2.28	0.65
1:C:771:TYR:OH	11:C:2113:HOH:O	2.13	0.65
1:A:799:THR:HG21	1:A:912:HIS:HB3	1.79	0.64
1:A:493:GLU:HG2	1:A:495:ARG:N	2.12	0.64
1:A:728:GLY:O	1:A:736:LYS:NZ	2.20	0.64
1:A:514:ILE:HG12	1:A:578:PHE:HB3	1.79	0.64
1:A:1009:TRP:HZ2	2:B:35:ILE:HG22	1.62	0.64
2:D:216:LYS:HB3	2:D:273:ARG:HB2	1.79	0.64
1:A:985:PHE:HZ	8:A:2010:CLR:H213	1.62	0.64
1:A:454:GLU:HG2	1:A:460:VAL:HG23	1.80	0.64
1:C:143:GLN:HE21	1:C:335:VAL:HG22	1.62	0.64
2:D:88:ILE:HB	2:D:299:ILE:HG22	1.79	0.64
2:D:14:LYS:HZ1	2:D:22:LYS:HG3	1.63	0.63
1:C:531:PHE:HE2	1:C:581:LEU:HD21	1.64	0.63
1:C:613:HIS:HD2	1:C:615:ILE:HB	1.63	0.63
1:C:643:ILE:HD11	1:C:648:VAL:HG22	1.80	0.63
1:A:777:ILE:HD11	1:A:847:TYR:HA	1.81	0.63
1:C:56:LEU:HD11	1:C:182:ASP:HB3	1.79	0.63
1:C:417:ILE:HD11	1:C:548:PHE:HB3	1.79	0.63
1:A:165:ILE:HB	1:A:183:LEU:HD21	1.79	0.63
8:C:2010:CLR:H272	9:C:2014:PC1:C2H	2.29	0.63
2:B:229:TYR:HD1	2:B:261:VAL:HG12	1.62	0.63
1:A:385:TRP:HB3	1:A:581:LEU:HB2	1.81	0.62
1:A:154:PHE:HB3	1:A:350:LEU:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:VAL:HB	2:B:267:THR:HG21	1.80	0.62
2:D:191:PRO:HG3	2:D:280:GLY:HA2	1.82	0.62
2:D:229:TYR:HD1	2:D:261:VAL:HG12	1.64	0.62
1:C:31:GLU:HG3	1:C:32:VAL:H	1.65	0.61
1:C:902:GLU:O	1:C:906:ILE:HG12	2.00	0.61
2:D:70:ASP:OD1	11:D:501:HOH:O	2.16	0.61
1:C:191:ARG:HA	1:C:241:ASN:HB3	1.83	0.61
2:D:91:ARG:HG3	2:D:302:LYS:O	2.01	0.61
1:C:299:PHE:HB3	1:C:316:PHE:HE2	1.65	0.61
1:A:838:VAL:HG13	1:A:842:LEU:HD22	1.81	0.61
1:C:505:GLU:OE2	1:C:613:HIS:ND1	2.32	0.61
1:C:398:ASN:HB2	1:C:455:LEU:HD13	1.83	0.60
2:D:14:LYS:HA	2:D:17:TRP:HB3	1.83	0.60
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.83	0.60
1:C:600:ARG:HH11	1:C:600:ARG:HB3	1.67	0.60
3:E:47:SER:O	3:E:47:SER:OG	2.18	0.60
1:A:309:THR:HG23	1:A:312:GLU:HB2	1.83	0.60
1:C:549:CYS:HA	1:C:579:VAL:HG23	1.83	0.60
1:C:446:GLU:OE2	1:C:482:GLN:NE2	2.34	0.60
2:D:224:VAL:HB	2:D:267:THR:HG21	1.83	0.60
1:A:360:LEU:HA	1:A:723:ILE:HD13	1.84	0.59
1:A:861:THR:HG21	1:A:918:SER:OG	2.02	0.59
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.83	0.59
1:C:553:LEU:HD22	1:C:558:PHE:CE2	2.37	0.59
1:A:300:PHE:HB2	1:A:317:LEU:HB2	1.85	0.59
1:A:340:THR:HG21	1:A:761:ILE:HD11	1.83	0.59
1:C:777:ILE:HD12	1:C:777:ILE:H	1.67	0.59
1:A:760:LEU:HD22	1:A:820:ALA:HB2	1.85	0.59
1:A:394:ASP:OD1	1:A:394:ASP:N	2.35	0.58
1:C:125:LEU:O	1:C:129:LEU:HB2	2.03	0.58
1:A:191:ARG:HA	1:A:241:ASN:HB3	1.85	0.58
1:A:777:ILE:HD11	1:A:847:TYR:CG	2.37	0.58
2:B:90:PHE:CD2	2:B:98:TYR:HB3	2.38	0.58
1:C:196:LEU:HB2	1:C:236:ALA:HB3	1.83	0.58
1:A:420:LEU:HB3	1:A:486:HIS:CE1	2.38	0.58
1:A:777:ILE:HD12	1:A:777:ILE:H	1.68	0.58
2:B:216:LYS:HB3	2:B:273:ARG:HB2	1.86	0.58
2:B:35:ILE:HG13	2:B:36:LEU:N	2.18	0.58
2:B:216:LYS:H	2:B:216:LYS:HD2	1.69	0.58
1:C:170:LYS:NZ	1:C:185:GLU:OE2	2.36	0.58
1:C:372:GLY:HA2	1:C:377:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1002:ILE:HG23	1:A:1011:GLU:HB2	1.84	0.58
2:D:106:VAL:HG22	2:D:167:TYR:HB2	1.86	0.58
1:A:258:THR:HG23	1:A:261:GLY:N	2.19	0.57
1:A:888:ILE:O	1:A:904:ARG:NH2	2.37	0.57
8:C:2010:CLR:H272	9:C:2014:PC1:H2G1	1.86	0.57
1:A:944:ASN:ND2	1:A:947:LEU:HB2	2.18	0.57
1:C:777:ILE:HD11	1:C:847:TYR:HA	1.86	0.57
1:A:422:ASN:OD1	1:A:423:ARG:N	2.37	0.57
1:A:752:VAL:HA	1:A:755:VAL:HG12	1.85	0.57
2:D:83:SER:HB3	2:D:86:THR:HA	1.85	0.57
1:A:902:GLU:O	1:A:906:ILE:HG12	2.04	0.57
8:C:2010:CLR:C27	9:C:2014:PC1:H2I2	2.31	0.57
2:D:35:ILE:HG13	2:D:36:LEU:N	2.18	0.57
3:G:17:ASP:HB3	3:G:18:PRO:HD2	1.86	0.57
1:A:298:SER:HB2	9:A:2014:PC1:H3F1	1.87	0.57
1:A:340:THR:HG22	1:A:757:GLU:OE1	2.04	0.57
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.39	0.57
2:D:80:ILE:HB	2:D:177:ILE:HG23	1.87	0.57
1:A:496:HIS:HB2	1:A:553:LEU:HB2	1.87	0.57
1:C:440:VAL:HG21	1:C:451:LYS:HE3	1.86	0.57
1:A:152:GLU:HA	1:A:155:LYS:HG2	1.87	0.56
1:A:294:PHE:HE2	9:A:2014:PC1:H3B2	1.70	0.56
1:A:324:ASN:HA	1:A:776:ASN:OD1	2.04	0.56
1:A:384:MET:HE1	1:A:393:ALA:HB2	1.87	0.56
1:A:483:LEU:HD21	1:A:571:PHE:HE2	1.71	0.56
1:C:238:PHE:O	1:C:260:MET:HG3	2.06	0.56
1:C:277:ILE:HD12	1:C:358:GLU:HG3	1.88	0.56
1:A:433:LEU:HD12	1:A:437:LYS:HB3	1.86	0.56
1:A:440:VAL:HG12	1:A:441:ALA:H	1.70	0.56
1:A:963:TYR:CD2	3:G:30:GLY:HA3	2.41	0.56
1:A:963:TYR:CE2	8:A:2010:CLR:H21	2.39	0.56
1:C:551:LEU:HD12	1:C:576:LEU:HA	1.88	0.56
1:C:867:ALA:HB2	1:C:873:PRO:HD3	1.88	0.56
1:C:998:ARG:HE	1:C:1014:THR:HB	1.71	0.56
2:D:173:LYS:HG2	2:D:264:THR:HA	1.86	0.56
1:A:857:GLY:O	1:A:861:THR:HG23	2.06	0.56
1:C:303:SER:O	1:C:308:TYR:HB2	2.05	0.56
1:C:956:ALA:HB2	3:E:37:ALA:HB3	1.88	0.55
1:A:790:ASN:ND2	1:A:880:ARG:HD2	2.19	0.55
1:A:551:LEU:HD22	1:A:553:LEU:HD23	1.88	0.55
1:A:889:ASN:ND2	1:A:901:TYR:H	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:O	1:A:258:THR:HG22	2.07	0.55
1:A:889:ASN:HD22	1:A:900:THR:HB	1.71	0.55
2:B:214:THR:OG1	2:B:215:GLY:N	2.35	0.55
2:D:176:VAL:HB	2:D:261:VAL:HG23	1.89	0.55
1:C:421:CYS:O	1:C:501:LYS:NZ	2.36	0.55
1:C:854:GLN:HB3	1:C:922:VAL:HG21	1.88	0.55
1:C:483:LEU:HD21	1:C:571:PHE:HE2	1.71	0.55
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.89	0.55
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.89	0.55
1:C:426:PHE:HE2	1:C:454:GLU:HG3	1.72	0.55
1:C:600:ARG:HH21	1:C:680:GLU:HG2	1.72	0.55
1:A:613:HIS:NE2	1:A:615:ILE:HG12	2.21	0.54
2:B:106:VAL:HG22	2:B:167:TYR:HB2	1.89	0.54
1:C:283:HIS:NE2	1:C:287:ILE:HD11	2.21	0.54
1:C:850:ILE:O	1:C:854:GLN:HG3	2.07	0.54
1:C:963:TYR:CZ	8:C:2011:CLR:H21	2.42	0.54
1:A:343:ARG:HD2	1:A:757:GLU:OE2	2.07	0.54
2:B:268:MET:HA	2:B:301:VAL:HG23	1.89	0.54
2:D:268:MET:HA	2:D:301:VAL:HG23	1.89	0.54
1:A:873:PRO:HA	1:A:876:LEU:HD12	1.90	0.54
1:A:613:HIS:CD2	1:A:615:ILE:HG12	2.43	0.54
1:A:372:GLY:HA2	1:A:377:ASN:HB2	1.88	0.54
1:C:778:PRO:HB3	1:C:855:ALA:HA	1.89	0.54
8:C:2011:CLR:H6	9:D:401:PC1:H242	1.90	0.54
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.72	0.54
1:A:864:VAL:HA	2:B:57:MET:SD	2.48	0.53
8:C:2010:CLR:H272	9:C:2014:PC1:C2G	2.38	0.53
1:A:892:GLU:HA	1:A:897:GLN:O	2.08	0.53
2:B:80:ILE:HB	2:B:177:ILE:HG23	1.91	0.53
1:C:50:THR:HG22	1:C:56:LEU:HD23	1.90	0.53
1:C:301:ILE:O	1:C:305:ILE:HG12	2.09	0.53
5:C:2002:ALF:F4	6:C:2004:ADP:O3B	2.15	0.53
2:D:204:TYR:HB3	2:D:208:VAL:HB	1.89	0.53
1:C:186:VAL:HG11	1:C:192:ILE:HD13	1.89	0.53
1:C:997:VAL:O	1:C:1001:ILE:HG13	2.08	0.53
1:C:1009:TRP:HZ2	2:D:35:ILE:HG22	1.73	0.53
1:C:496:HIS:HB2	1:C:553:LEU:HB2	1.91	0.53
1:C:933:ARG:HD2	1:C:1016:TYR:O	2.08	0.53
2:B:157:GLY:H	2:B:230:PHE:HB3	1.74	0.53
1:C:204:CYS:HA	1:C:245:GLY:HA3	1.91	0.53
2:B:130:PRO:O	2:B:204:TYR:OH	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ASN:HA	1:C:776:ASN:OD1	2.07	0.53
1:A:55:GLY:HA2	1:A:183:LEU:HD22	1.91	0.53
1:A:882:ASN:HB3	1:A:888:ILE:HD12	1.91	0.53
1:C:906:ILE:O	1:C:910:THR:OG1	2.22	0.53
1:A:303:SER:O	1:A:308:TYR:HB2	2.09	0.53
1:C:877:LEU:HD12	1:C:877:LEU:H	1.73	0.53
2:D:73:ALA:HB3	2:D:74:PRO:HD3	1.90	0.53
2:D:186:PHE:CZ	2:D:282:ASN:HB3	2.43	0.53
1:C:443:ASP:HB2	1:C:446:GLU:HB2	1.90	0.53
1:C:613:HIS:CD2	1:C:615:ILE:HB	2.44	0.52
1:A:387:ASP:O	1:A:389:GLN:N	2.42	0.52
1:C:759:ARG:HH12	1:C:829:PRO:HA	1.75	0.52
1:A:998:ARG:HH12	1:A:999:LYS:HG3	1.74	0.52
2:D:214:THR:OG1	2:D:215:GLY:N	2.43	0.52
2:B:191:PRO:HG3	2:B:280:GLY:HA2	1.92	0.52
1:C:99:ILE:O	1:C:103:LEU:HG	2.09	0.52
8:C:2010:CLR:C27	9:C:2014:PC1:H2G1	2.39	0.52
2:B:238:PHE:HD1	2:B:257:PRO:HB2	1.73	0.52
2:D:57:MET:HE3	2:D:61:ILE:HD11	1.91	0.52
1:A:80:PRO:HG2	1:A:83:VAL:HB	1.91	0.52
1:A:777:ILE:CD1	1:A:847:TYR:HA	2.39	0.52
1:C:670:GLN:O	1:C:674:ILE:HG13	2.10	0.52
1:A:58:PRO:HD3	1:A:167:ASN:HB2	1.91	0.52
1:A:913:THR:HG23	1:A:973:MET:HE2	1.91	0.52
2:B:176:VAL:HB	2:B:261:VAL:HG23	1.91	0.52
1:C:483:LEU:HB2	1:C:500:MET:HE2	1.91	0.52
1:A:387:ASP:C	1:A:389:GLN:H	2.17	0.52
1:A:628:SER:OG	1:A:680:GLU:OE2	2.28	0.52
1:A:384:MET:HE1	1:A:393:ALA:CB	2.40	0.52
1:A:413:ALA:HB1	1:A:550:HIS:HE1	1.74	0.51
1:C:544:ARG:NH2	6:C:2004:ADP:O1B	2.43	0.51
2:D:49:ILE:O	2:D:53:THR:HG22	2.10	0.51
2:B:193:ASN:OD1	2:B:193:ASN:N	2.43	0.51
1:C:305:ILE:C	1:C:307:GLU:H	2.18	0.51
2:D:216:LYS:H	2:D:216:LYS:HD2	1.74	0.51
1:A:347:LYS:HG3	1:A:753:THR:HG21	1.92	0.51
1:C:757:GLU:O	1:C:761:ILE:HG22	2.10	0.51
1:A:827:ARG:NH2	1:A:934:ARG:HD3	2.26	0.51
1:C:55:GLY:HA2	1:C:183:LEU:HD22	1.93	0.51
1:C:679:THR:HG23	1:C:680:GLU:HG3	1.93	0.51
1:C:689:GLN:O	1:C:693:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:THR:OG1	1:C:423:ARG:NH2	2.44	0.51
2:B:170:LYS:N	2:B:170:LYS:HD2	2.26	0.51
1:C:824:ILE:HD12	1:C:825:MET:H	1.76	0.51
1:A:1001:ILE:HG22	1:A:1010:VAL:HG21	1.93	0.51
1:A:928:VAL:O	1:A:931:LYS:HB3	2.10	0.51
1:A:997:VAL:O	1:A:1001:ILE:HG13	2.11	0.51
2:B:95:PRO:HA	2:B:98:TYR:CE1	2.46	0.50
1:C:39:LEU:HD22	1:C:43:GLU:HB3	1.93	0.50
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.93	0.50
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.93	0.50
1:C:254:THR:HB	1:C:257:ARG:HH21	1.76	0.50
1:C:322:VAL:HG12	1:C:804:ASP:OD2	2.11	0.50
2:D:90:PHE:CD2	2:D:98:TYR:HB3	2.46	0.50
1:A:241:ASN:ND2	1:A:737:GLN:OE1	2.45	0.50
1:C:306:LEU:HD12	1:C:880:ARG:HE	1.75	0.50
1:A:108:TYR:HA	1:A:111:GLN:HE21	1.74	0.50
1:A:1009:TRP:CE2	1:A:1013:GLU:HG3	2.46	0.50
3:G:24:GLU:O	3:G:28:ASN:ND2	2.44	0.50
1:C:781:THR:HG22	8:C:2009:CLR:H273	1.93	0.50
2:B:138:GLU:O	2:B:140:ASN:N	2.44	0.50
1:C:827:ARG:HH12	1:C:933:ARG:HH21	1.59	0.50
2:B:98:TYR:HA	2:B:101:TYR:HD1	1.77	0.50
1:C:152:GLU:C	1:C:154:PHE:H	2.20	0.50
1:C:255:GLY:O	1:C:258:THR:HG22	2.11	0.50
1:C:935:ASN:HA	1:C:1003:ARG:HD3	1.94	0.50
1:A:85:PHE:CZ	1:A:138:CYS:HB3	2.46	0.50
1:C:888:ILE:HG22	1:C:890:ASP:HB2	1.93	0.50
8:C:2011:CLR:H121	8:C:2011:CLR:C21	2.37	0.50
1:A:591:ALA:HB1	1:A:749:ALA:HB2	1.93	0.50
1:A:771:TYR:CE1	1:A:927:LEU:HB2	2.46	0.50
2:B:178:ILE:HD11	2:B:276:CYS:SG	2.51	0.50
1:C:28:LEU:C	1:C:31:GLU:HG2	2.37	0.50
1:C:50:THR:HG21	1:C:181:GLY:C	2.37	0.50
1:C:469:LYS:HB3	1:C:486:HIS:CE1	2.47	0.50
2:D:178:ILE:HD11	2:D:276:CYS:SG	2.52	0.50
1:A:206:VAL:HA	1:A:242:CYS:HA	1.94	0.49
1:A:420:LEU:HD13	1:A:486:HIS:ND1	2.27	0.49
2:B:37:LEU:O	2:B:41:ILE:HG23	2.12	0.49
1:A:803:ILE:HG23	1:A:919:ILE:HG21	1.94	0.49
1:C:876:LEU:HD23	1:C:879:LEU:HD12	1.93	0.49
1:A:96:LEU:HD12	1:A:99:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ILE:HD11	1:C:765:LEU:HD13	1.94	0.49
1:A:793:LEU:HD12	1:A:794:PRO:HD2	1.95	0.49
1:C:266:LEU:HD22	1:C:270:LEU:HA	1.93	0.49
1:A:55:GLY:HA3	1:A:165:ILE:O	2.11	0.49
1:A:89:LEU:HD21	1:A:134:ILE:HA	1.93	0.49
1:A:998:ARG:NH1	1:A:999:LYS:HG3	2.28	0.49
1:A:1001:ILE:CG2	1:A:1010:VAL:HG21	2.43	0.49
2:D:117:GLN:OE1	2:D:150:ARG:HG2	2.13	0.49
1:A:842:LEU:HD12	1:A:1016:TYR:HD2	1.77	0.49
2:B:91:ARG:HH21	2:B:94:ASP:HB2	1.77	0.49
1:C:502:GLY:HA2	6:C:2004:ADP:N3	2.28	0.49
1:C:861:THR:HG21	1:C:918:SER:OG	2.11	0.49
1:C:913:THR:HG23	1:C:973:MET:HE2	1.94	0.49
1:A:333:VAL:HG22	1:A:765:LEU:HD11	1.95	0.49
2:D:157:GLY:H	2:D:230:PHE:HB3	1.77	0.49
1:A:553:LEU:HD22	1:A:558:PHE:CE2	2.48	0.49
1:A:182:ASP:O	1:A:251:VAL:HG23	2.12	0.49
1:A:228:ASN:HB3	1:A:231:GLU:HG2	1.95	0.48
1:C:230:LEU:HA	1:C:237:PHE:CZ	2.48	0.48
1:C:985:PHE:CZ	8:C:2011:CLR:H221	2.32	0.48
1:A:335:VAL:HG11	1:A:817:TYR:CE2	2.47	0.48
2:B:27:ARG:HG3	2:B:31:SER:HB3	1.96	0.48
1:A:505:GLU:HG3	1:A:506:ARG:H	1.79	0.48
1:A:565:ASP:HB2	1:A:570:ASN:HD22	1.78	0.48
1:A:799:THR:O	1:A:803:ILE:HG12	2.14	0.48
2:B:202:MET:SD	2:B:236:PRO:HG2	2.54	0.48
1:C:51:ASP:N	1:C:55:GLY:O	2.46	0.48
1:C:781:THR:HG22	8:C:2009:CLR:C27	2.44	0.48
1:C:802:CYS:HB3	1:C:916:PHE:CE1	2.48	0.48
1:C:953:GLU:OE2	3:E:41:GLY:HA3	2.14	0.48
1:C:799:THR:O	1:C:803:ILE:HG12	2.13	0.48
1:A:874:ILE:H	1:A:874:ILE:HD12	1.77	0.48
1:A:953:GLU:OE2	3:G:41:GLY:HA3	2.13	0.48
2:B:83:SER:HB3	2:B:86:THR:HA	1.95	0.48
3:E:28:ASN:O	3:E:32:ILE:HG12	2.13	0.48
1:A:350:LEU:HB2	1:A:744:LEU:HD21	1.95	0.48
1:C:332:THR:HG21	1:C:768:SER:OG	2.14	0.48
9:C:2015:PC1:H3B1	9:C:2015:PC1:H282	1.94	0.48
2:D:62:SER:C	2:D:64:PHE:H	2.22	0.48
1:A:565:ASP:OD2	1:A:568:ASP:HB2	2.12	0.48
2:B:186:PHE:CZ	2:B:282:ASN:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:3001:CLR:H121	8:B:3001:CLR:C21	2.41	0.48
1:C:553:LEU:HB3	1:C:558:PHE:CD2	2.48	0.48
2:D:17:TRP:CZ2	2:D:19:SER:HB3	2.49	0.48
1:C:239:SER:OG	1:C:260:MET:HE2	2.14	0.48
1:C:768:SER:HA	1:C:815:LEU:HD23	1.96	0.48
2:D:23:GLU:HG2	2:D:24:PHE:H	1.78	0.48
2:D:76:GLY:HA2	2:D:293:GLY:H	1.78	0.48
1:A:488:ASN:HB3	1:A:493:GLU:HG3	1.95	0.47
1:C:209:SER:C	1:C:211:LEU:H	2.22	0.47
1:C:656:CYS:SG	1:C:681:ILE:HG22	2.54	0.47
1:C:773:LEU:HD22	1:C:847:TYR:HE1	1.79	0.47
1:C:777:ILE:CD1	1:C:847:TYR:HA	2.44	0.47
2:D:41:ILE:HG13	2:D:42:PHE:N	2.29	0.47
1:C:565:ASP:H	1:C:570:ASN:CB	2.20	0.47
2:D:24:PHE:C	2:D:26:GLY:H	2.22	0.47
1:A:194:ALA:HA	1:A:238:PHE:HB2	1.95	0.47
1:C:908:GLU:O	1:C:911:CYS:HB2	2.14	0.47
1:A:280:GLU:OE1	1:A:830:ARG:NH2	2.48	0.47
1:A:371:THR:OG1	6:A:2004:ADP:O3B	2.29	0.47
1:A:402:VAL:HG23	1:A:404:PHE:H	1.79	0.47
2:B:173:LYS:HB3	2:B:264:THR:HA	1.96	0.47
1:C:311:LEU:O	1:C:315:ILE:HG12	2.14	0.47
1:C:755:VAL:HG13	1:C:825:MET:HE1	1.97	0.47
1:A:393:ALA:HA	1:A:402:VAL:HA	1.95	0.47
1:A:436:LEU:HG	1:A:455:LEU:HD11	1.96	0.47
1:C:139:PHE:HD1	9:C:2013:PC1:H221	1.80	0.47
1:C:420:LEU:HB3	1:C:486:HIS:CE1	2.50	0.47
1:C:613:HIS:CD2	1:C:615:ILE:H	2.33	0.47
1:A:167:ASN:O	1:A:169:GLU:N	2.47	0.47
2:B:277:LYS:HD2	2:B:279:TYR:CE2	2.49	0.47
1:A:418:ALA:O	1:A:422:ASN:HB2	2.14	0.47
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.72	0.47
1:A:968:GLY:HA2	1:A:973:MET:N	2.29	0.47
1:C:27:GLU:C	1:C:29:LYS:H	2.22	0.47
1:C:606:VAL:HG11	1:C:626:ILE:HD12	1.97	0.47
1:C:841:ARG:HB2	1:C:1016:TYR:HA	1.95	0.47
1:C:1001:ILE:CG2	1:C:1010:VAL:HG21	2.44	0.47
2:D:80:ILE:HG22	2:D:105:ILE:HA	1.97	0.47
2:D:90:PHE:CE1	2:D:174:PRO:HG3	2.49	0.47
1:A:349:CYS:SG	1:A:741:MET:HG2	2.55	0.47
1:A:505:GLU:CD	1:A:685:ARG:HH11	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2009:CLR:H121	8:A:2009:CLR:C21	2.41	0.47
1:C:31:GLU:HG3	1:C:32:VAL:N	2.28	0.47
2:D:229:TYR:CD1	2:D:261:VAL:HG12	2.47	0.47
1:A:616:THR:O	1:A:620:ILE:HG12	2.14	0.47
1:A:755:VAL:HG13	1:A:825:MET:HE1	1.97	0.47
1:A:777:ILE:HD12	1:A:777:ILE:N	2.30	0.47
1:C:317:LEU:O	1:C:321:ILE:HG12	2.15	0.47
1:C:695:VAL:HG13	1:C:705:VAL:HG21	1.97	0.47
1:C:913:THR:O	1:C:917:VAL:HG23	2.15	0.47
1:A:300:PHE:HE1	1:A:314:VAL:HG12	1.80	0.47
1:A:379:MET:HE2	1:A:586:ASP:OD2	2.15	0.47
1:A:483:LEU:HD13	1:A:500:MET:HB3	1.96	0.47
1:A:951:LEU:O	1:A:955:THR:HG23	2.15	0.47
2:B:14:LYS:HZ3	2:B:17:TRP:HE3	1.62	0.47
2:B:203:LYS:HE2	2:B:203:LYS:HB3	1.77	0.47
1:C:493:GLU:HG2	1:C:495:ARG:N	2.22	0.47
1:A:131:ALA:O	1:A:135:ILE:HG12	2.14	0.46
1:A:633:THR:H	1:A:636:ASP:HB2	1.80	0.46
1:A:933:ARG:HD2	1:A:1016:TYR:O	2.15	0.46
9:A:2011:PC1:H112	9:A:2011:PC1:H132	1.68	0.46
1:C:420:LEU:C	1:C:422:ASN:H	2.23	0.46
2:D:27:ARG:HD3	2:D:32:TRP:HE3	1.79	0.46
1:A:327:GLU:H	1:A:327:GLU:CD	2.23	0.46
1:A:331:ALA:O	1:A:335:VAL:HG23	2.14	0.46
1:A:847:TYR:CD2	9:A:2011:PC1:H381	2.51	0.46
1:A:921:VAL:HG22	1:A:924:TRP:CH2	2.50	0.46
1:C:206:VAL:HA	1:C:242:CYS:HA	1.97	0.46
1:A:867:ALA:HB2	1:A:873:PRO:HD3	1.97	0.46
1:A:937:VAL:HG21	1:A:992:PHE:CE1	2.50	0.46
1:A:968:GLY:HA2	1:A:973:MET:H	1.80	0.46
1:C:888:ILE:O	1:C:904:ARG:NH2	2.41	0.46
9:C:2012:PC1:H3H2	9:C:2015:PC1:H2H1	1.97	0.46
2:D:87:GLU:HA	2:D:298:LYS:O	2.15	0.46
2:D:98:TYR:CZ	2:D:171:ASP:HB3	2.50	0.46
1:A:901:TYR:HA	1:A:904:ARG:CZ	2.45	0.46
1:C:801:LEU:O	1:C:805:LEU:HG	2.14	0.46
2:B:173:LYS:NZ	2:B:268:MET:HE3	2.30	0.46
1:C:383:HIS:CD2	1:C:392:GLU:HG2	2.50	0.46
2:D:277:LYS:HG2	2:D:285:TYR:CE2	2.50	0.46
1:A:861:THR:HG22	1:A:983:CYS:CB	2.45	0.46
1:A:942:MET:HE1	1:A:947:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:O	2:B:40:VAL:HG23	2.16	0.46
1:C:982:PHE:HA	1:C:985:PHE:CD1	2.50	0.46
1:A:122:ASN:ND2	1:A:315:ILE:HG13	2.31	0.46
1:A:592:VAL:O	1:A:596:VAL:HG22	2.16	0.46
2:B:173:LYS:HG2	2:B:264:THR:HA	1.98	0.46
3:G:17:ASP:CB	3:G:18:PRO:HD2	2.46	0.46
1:C:220:ARG:HD3	1:C:233:ARG:O	2.15	0.46
1:A:263:ILE:HG13	1:A:263:ILE:O	2.14	0.46
1:A:795:LEU:HD13	1:A:915:PHE:CD1	2.51	0.46
1:C:126:GLY:O	1:C:130:SER:OG	2.25	0.46
1:C:825:MET:HE2	1:C:825:MET:HA	1.97	0.46
1:C:889:ASN:ND2	1:C:901:TYR:H	2.13	0.46
1:C:924:TRP:HE1	1:C:955:THR:HG22	1.81	0.46
8:C:2010:CLR:H121	8:C:2010:CLR:C21	2.42	0.46
2:D:75:PRO:HG3	2:D:183:VAL:HG21	1.96	0.46
2:B:42:PHE:HD2	2:B:43:TYR:CD1	2.34	0.46
2:B:138:GLU:HG3	2:B:140:ASN:ND2	2.30	0.46
1:C:460:VAL:O	1:C:464:ARG:HB2	2.15	0.46
3:E:39:ILE:O	3:E:43:ILE:HG12	2.16	0.46
1:A:985:PHE:CZ	8:A:2010:CLR:H213	2.48	0.46
2:B:49:ILE:O	2:B:53:THR:HG22	2.16	0.46
2:B:131:SER:HB2	2:B:241:GLN:HB3	1.98	0.46
1:C:622:LYS:HA	1:C:627:ILE:O	2.16	0.46
1:A:921:VAL:HG13	1:A:924:TRP:CZ3	2.50	0.45
2:B:90:PHE:CZ	2:B:174:PRO:HG3	2.52	0.45
1:C:202:ASN:HB2	1:C:246:THR:HG22	1.97	0.45
1:C:366:ILE:HG12	1:C:706:ALA:HB3	1.98	0.45
1:C:950:GLY:O	1:C:954:GLU:HB2	2.16	0.45
1:A:402:VAL:HG21	1:A:404:PHE:CE1	2.51	0.45
1:A:818:GLU:HG2	1:A:944:ASN:HD22	1.80	0.45
1:C:535:TYR:CE2	1:C:545:VAL:HB	2.51	0.45
1:C:801:LEU:CD1	1:C:805:LEU:HD21	2.44	0.45
1:A:332:THR:OG1	1:A:813:ILE:HD13	2.17	0.45
1:A:741:MET:HE3	1:A:741:MET:HB2	1.88	0.45
1:C:460:VAL:HG11	1:C:464:ARG:HH21	1.80	0.45
1:C:827:ARG:NH1	1:C:933:ARG:HH21	2.15	0.45
1:C:987:TYR:OH	2:D:53:THR:HG21	2.17	0.45
1:A:303:SER:HB2	1:A:308:TYR:CD2	2.51	0.45
2:B:66:PRO:HG2	2:B:69:GLN:HG3	1.97	0.45
2:B:76:GLY:H	2:B:181:ASN:HD22	1.64	0.45
2:B:90:PHE:O	2:B:92:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ALA:O	1:C:335:VAL:HG23	2.16	0.45
1:C:685:ARG:NH2	6:C:2004:ADP:O3'	2.44	0.45
1:A:188:GLY:HA2	1:A:244:GLU:HA	1.99	0.45
1:A:860:PHE:CE1	2:B:53:THR:HG23	2.52	0.45
1:C:25:MET:O	1:C:29:LYS:HG3	2.16	0.45
1:C:99:ILE:HA	1:C:102:ILE:HD12	1.97	0.45
1:C:551:LEU:HD13	1:C:576:LEU:HD23	1.99	0.45
1:C:951:LEU:O	1:C:955:THR:HG23	2.17	0.45
2:B:66:PRO:HD2	2:B:184:LEU:HD22	1.98	0.45
2:B:153:LEU:O	2:B:160:SER:OG	2.27	0.45
8:C:2009:CLR:H121	8:C:2009:CLR:C21	2.43	0.45
1:A:336:CYS:O	1:A:340:THR:HG23	2.17	0.45
1:C:143:GLN:NE2	1:C:335:VAL:HG13	2.31	0.45
1:C:785:ILE:HG22	1:C:791:ILE:HD12	1.98	0.45
1:A:504:PRO:HB3	1:A:581:LEU:HD21	1.99	0.45
1:A:688:PRO:O	1:A:691:LYS:HB2	2.17	0.45
2:B:90:PHE:HD2	2:B:98:TYR:HB3	1.82	0.45
2:B:209:LEU:HB3	2:B:238:PHE:HB2	1.98	0.45
9:C:2015:PC1:H221	9:C:2015:PC1:H2	1.78	0.45
1:A:956:ALA:HB2	3:G:37:ALA:HB3	1.99	0.44
1:C:131:ALA:O	1:C:135:ILE:HG12	2.17	0.44
3:G:45:ILE:HD12	3:G:45:ILE:HA	1.73	0.44
1:C:589:ARG:NH1	1:C:746:ASP:HB3	2.33	0.44
1:A:60:ARG:O	1:A:64:ILE:HG13	2.17	0.44
8:A:2010:CLR:H121	8:A:2010:CLR:H212	1.99	0.44
1:C:209:SER:HB3	1:C:215:SER:HA	1.99	0.44
1:C:901:TYR:OH	1:C:905:LYS:HE3	2.18	0.44
2:D:163:ASN:HB3	2:D:164:ASP:H	1.62	0.44
1:A:192:ILE:HA	1:A:193:PRO:HD3	1.62	0.44
1:A:303:SER:C	1:A:308:TYR:HB2	2.43	0.44
1:A:968:GLY:HA3	1:A:974:TYR:CE2	2.52	0.44
1:C:230:LEU:HA	1:C:237:PHE:HZ	1.82	0.44
1:C:423:ARG:HD2	1:C:472:GLU:OE2	2.18	0.44
1:C:494:PRO:HG2	1:C:552:PHE:HB3	1.98	0.44
5:C:2002:ALF:F1	6:C:2004:ADP:O3B	2.25	0.44
1:A:300:PHE:CE1	1:A:314:VAL:HG12	2.53	0.44
2:B:17:TRP:CZ2	2:B:19:SER:HB3	2.52	0.44
3:G:28:ASN:O	3:G:32:ILE:HG12	2.18	0.44
3:E:45:ILE:HD12	3:E:45:ILE:HA	1.86	0.44
1:A:504:PRO:HB3	1:A:581:LEU:CD2	2.48	0.44
2:B:177:ILE:HA	2:B:260:ALA:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:TYR:HB3	2:B:208:VAL:HB	1.98	0.44
1:A:413:ALA:HB1	1:A:550:HIS:CE1	2.53	0.44
1:A:512:SER:O	1:A:523:LEU:HB2	2.18	0.44
1:C:480:LYS:HG2	6:C:2004:ADP:H5'1	1.99	0.44
1:A:204:CYS:HA	1:A:245:GLY:HA3	2.00	0.44
1:A:492:ALA:O	1:A:494:PRO:HD3	2.18	0.44
2:B:99:GLU:O	2:B:103:VAL:HG23	2.18	0.44
1:C:512:SER:O	1:C:523:LEU:HB2	2.18	0.44
1:C:531:PHE:CE2	1:C:581:LEU:HD21	2.48	0.44
9:C:2015:PC1:H3B2	9:C:2015:PC1:H361	2.00	0.44
9:D:401:PC1:H2B2	9:D:401:PC1:H282	1.65	0.44
1:A:483:LEU:HD22	1:A:500:MET:HE2	2.00	0.44
1:A:883:TRP:NE1	1:A:908:GLU:OE1	2.50	0.44
2:B:27:ARG:HD3	2:B:32:TRP:HE3	1.83	0.44
1:C:1016:TYR:H	1:C:1016:TYR:HD1	1.66	0.44
2:D:217:ARG:HD2	2:D:218:ASP:H	1.82	0.44
1:A:351:VAL:HG11	1:A:357:VAL:HG23	2.00	0.43
1:A:920:VAL:HG13	1:A:954:GLU:HG2	1.99	0.43
1:A:921:VAL:HG12	1:A:988:SER:HB2	2.00	0.43
1:C:258:THR:HG23	1:C:261:GLY:H	1.83	0.43
1:C:436:LEU:HG	1:C:455:LEU:HD11	2.00	0.43
1:C:857:GLY:O	1:C:861:THR:HG23	2.17	0.43
1:A:318:ILE:O	1:A:322:VAL:HG23	2.18	0.43
1:A:845:MET:HE3	1:A:845:MET:HB3	1.81	0.43
1:A:948:ILE:HG21	3:G:44:ILE:HD13	2.00	0.43
2:B:157:GLY:N	2:B:230:PHE:HB3	2.33	0.43
1:C:43:GLU:O	1:C:46:ARG:HG2	2.18	0.43
1:C:804:ASP:O	1:C:808:ASP:HB2	2.17	0.43
1:A:95:MET:HE3	1:A:95:MET:HB3	1.86	0.43
1:A:340:THR:HG21	1:A:761:ILE:CD1	2.48	0.43
2:B:193:ASN:HA	2:B:196:LEU:HD21	2.00	0.43
1:C:430:GLN:HE21	1:C:433:LEU:HD21	1.84	0.43
1:C:460:VAL:HG12	1:C:464:ARG:HE	1.82	0.43
1:C:790:ASN:C	1:C:880:ARG:HB2	2.43	0.43
2:B:217:ARG:HD2	2:B:218:ASP:H	1.83	0.43
1:A:103:LEU:HA	1:A:106:LEU:HB3	2.00	0.43
1:A:154:PHE:HD2	1:A:157:MET:HG3	1.82	0.43
1:C:91:GLY:O	1:C:93:PHE:N	2.51	0.43
9:C:2013:PC1:H331	9:C:2013:PC1:H272	1.99	0.43
2:D:203:LYS:HE2	2:D:203:LYS:HB3	1.79	0.43
1:A:32:VAL:O	1:A:262:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLN:C	1:A:432:ASN:H	2.26	0.43
1:C:185:GLU:HG3	1:C:248:ARG:HE	1.84	0.43
1:C:592:VAL:O	1:C:596:VAL:HG13	2.19	0.43
1:C:924:TRP:O	1:C:928:VAL:HG23	2.18	0.43
1:A:827:ARG:HH21	1:A:934:ARG:HD3	1.83	0.43
1:C:295:LEU:HD13	1:C:780:ILE:HD13	2.01	0.43
1:C:297:VAL:O	1:C:301:ILE:HG23	2.19	0.43
1:C:618:LYS:HB2	1:C:657:VAL:HG21	2.01	0.43
8:C:2010:CLR:C24	9:C:2014:PC1:H2I2	2.48	0.43
1:A:285:ILE:HA	1:A:288:ILE:HG22	1.99	0.43
1:A:514:ILE:HG22	1:A:516:ILE:HG12	2.01	0.43
2:D:251:GLN:HB3	2:D:254:TYR:HB2	2.00	0.43
1:A:667:THR:OG1	1:A:668:SER:N	2.51	0.43
2:B:94:ASP:HA	2:B:95:PRO:HD3	1.79	0.43
1:C:611:GLY:HA2	1:C:686:THR:H	1.83	0.43
1:C:707:VAL:HG23	1:C:721:ALA:HB2	2.00	0.43
2:D:138:GLU:HG3	2:D:140:ASN:ND2	2.34	0.43
2:D:178:ILE:HD13	2:D:211:VAL:HG11	2.01	0.43
1:A:544:ARG:O	1:A:583:SER:HA	2.19	0.42
1:A:667:THR:HG23	1:A:670:GLN:H	1.83	0.42
1:A:986:PRO:CG	8:A:2009:CLR:H181	2.48	0.42
9:A:2012:PC1:H152	9:A:2012:PC1:H112	1.85	0.42
2:B:136:ARG:HD2	2:B:143:ARG:HH12	1.84	0.42
1:C:84:LYS:HE2	1:C:84:LYS:HB3	1.88	0.42
1:C:777:ILE:HD12	1:C:777:ILE:N	2.31	0.42
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.99	0.42
1:C:1013:GLU:OE1	2:D:27:ARG:NH2	2.52	0.42
1:A:35:ASP:HB2	1:A:37:HIS:ND1	2.34	0.42
1:A:340:THR:HG21	1:A:761:ILE:CG1	2.49	0.42
1:C:379:MET:HE2	1:C:586:ASP:HB2	2.00	0.42
1:C:431:GLU:OE2	1:C:438:ARG:NH1	2.52	0.42
1:C:889:ASN:HD22	1:C:900:THR:HB	1.84	0.42
1:C:925:ALA:O	1:C:929:ILE:HG12	2.19	0.42
2:D:170:LYS:N	2:D:170:LYS:HD2	2.34	0.42
1:A:99:ILE:O	1:A:103:LEU:HG	2.19	0.42
1:A:231:GLU:HG2	1:A:231:GLU:H	1.66	0.42
1:A:819:GLN:H	1:A:819:GLN:HG3	1.42	0.42
2:B:123:PHE:HB3	2:B:150:ARG:HG3	2.00	0.42
2:B:230:PHE:HE2	2:B:262:GLN:HB3	1.84	0.42
1:C:831:ASN:HD21	2:D:6:ALA:HB2	1.84	0.42
1:C:115:GLU:HG2	1:C:116:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:LEU:O	2:D:41:ILE:HG23	2.18	0.42
3:E:27:ARG:O	3:E:31:LEU:HG	2.20	0.42
1:C:39:LEU:HA	1:C:39:LEU:HD23	1.85	0.42
1:A:365:THR:HG23	1:A:605:LYS:HB3	2.02	0.42
1:A:476:ASN:ND2	1:A:479:ASN:HB2	2.33	0.42
1:A:963:TYR:CZ	8:A:2010:CLR:H21	2.55	0.42
1:C:462:GLU:O	1:C:466:ARG:HG3	2.20	0.42
2:D:242:TYR:CG	2:D:257:PRO:HG3	2.54	0.42
1:A:501:LYS:HE3	6:A:2004:ADP:N1	2.35	0.42
1:C:430:GLN:HE21	1:C:430:GLN:HA	1.85	0.42
1:C:781:THR:N	1:C:782:PRO:HD2	2.35	0.42
1:C:815:LEU:HD12	1:C:815:LEU:HA	1.76	0.42
1:A:71:ASN:HB3	1:A:175:ALA:O	2.20	0.42
1:A:191:ARG:NH2	1:A:239:SER:HA	2.35	0.42
1:A:226:ASN:HB3	1:A:231:GLU:HB2	2.00	0.42
1:A:953:GLU:HB3	9:A:2012:PC1:H2D2	2.02	0.42
1:A:1001:ILE:O	1:A:1005:ARG:HB2	2.20	0.42
8:A:2010:CLR:H232	8:A:2010:CLR:H211	1.83	0.42
9:A:2012:PC1:H2E2	9:A:2012:PC1:H2A2	2.02	0.42
1:C:613:HIS:HD2	1:C:615:ILE:H	1.66	0.42
2:D:204:TYR:HD2	2:D:207:TYR:H	1.68	0.42
1:A:386:PHE:CE2	1:A:391:HIS:CD2	3.08	0.42
1:A:781:THR:HG22	8:B:3001:CLR:H271	2.02	0.42
1:C:180:VAL:HG23	11:C:2108:HOH:O	2.19	0.42
1:C:814:SER:HB3	1:C:946:ILE:HG22	2.02	0.42
1:A:411:TRP:CE3	1:A:414:LEU:HD23	2.55	0.42
9:A:2013:PC1:H381	9:A:2013:PC1:H2A2	2.02	0.42
1:C:154:PHE:HD2	1:C:154:PHE:HA	1.75	0.42
2:D:94:ASP:HA	2:D:95:PRO:HD3	1.90	0.42
1:A:216:GLU:HA	1:A:217:PRO:HD3	1.87	0.41
1:A:491:THR:C	1:A:493:GLU:H	2.28	0.41
1:A:638:ALA:HB2	1:A:648:VAL:HG21	2.00	0.41
1:A:882:ASN:HA	1:A:885:ASP:HB2	2.01	0.41
9:A:2011:PC1:H372	9:A:2014:PC1:H351	2.02	0.41
1:C:228:ASN:HA	1:C:229:PRO:HD3	1.90	0.41
1:C:375:THR:HA	1:C:588:PRO:HA	2.02	0.41
1:C:376:GLN:HG3	1:C:589:ARG:HA	2.01	0.41
2:D:157:GLY:N	2:D:230:PHE:HB3	2.35	0.41
9:D:401:PC1:H291	9:D:401:PC1:H351	2.02	0.41
1:A:31:GLU:HG3	1:A:32:VAL:H	1.84	0.41
1:A:398:ASN:ND2	1:A:400:SER:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:THR:HG23	1:A:515:LEU:HD22	2.01	0.41
1:A:537:GLU:O	1:A:541:LEU:HD22	2.19	0.41
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.86	0.41
1:A:637:ILE:HD13	1:A:640:ARG:NH1	2.35	0.41
1:C:41:LEU:O	1:C:52:LEU:HD11	2.20	0.41
1:C:587:PRO:HA	1:C:588:PRO:HD3	1.96	0.41
1:C:916:PHE:O	1:C:920:VAL:HG23	2.20	0.41
1:C:1009:TRP:CZ2	2:D:35:ILE:HG22	2.53	0.41
1:A:818:GLU:CD	1:A:931:LYS:HG3	2.46	0.41
2:B:25:LEU:O	2:B:25:LEU:HG	2.20	0.41
1:C:195:ASP:O	1:C:252:VAL:HG22	2.20	0.41
1:C:550:HIS:C	1:C:550:HIS:CD2	2.98	0.41
1:C:1013:GLU:CD	2:D:27:ARG:HH21	2.29	0.41
2:D:95:PRO:HA	2:D:98:TYR:CE1	2.56	0.41
1:A:778:PRO:HB3	1:A:855:ALA:HA	2.01	0.41
1:A:861:THR:HG22	1:A:983:CYS:HB3	2.02	0.41
2:B:238:PHE:HA	2:B:239:PRO:HD2	1.87	0.41
1:C:504:PRO:HA	1:C:547:GLY:HA3	2.02	0.41
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.91	0.41
1:A:384:MET:SD	1:A:384:MET:N	2.93	0.41
1:A:472:GLU:CB	1:A:484:SER:HB3	2.51	0.41
1:A:663:LEU:HD21	1:A:671:LEU:HG	2.02	0.41
1:C:199:ILE:HD13	1:C:199:ILE:HA	1.75	0.41
1:C:860:PHE:HZ	8:C:2010:CLR:H193	1.85	0.41
2:D:99:GLU:O	2:D:103:VAL:HG23	2.19	0.41
1:A:430:GLN:HE21	1:A:430:GLN:HA	1.86	0.41
1:A:505:GLU:OE2	1:A:613:HIS:ND1	2.38	0.41
8:A:2010:CLR:H183	3:G:33:PHE:CZ	2.56	0.41
2:B:24:PHE:HD2	2:B:24:PHE:HA	1.74	0.41
2:B:39:TYR:CZ	8:B:3001:CLR:H191	2.56	0.41
2:B:61:ILE:HG23	2:B:67:THR:HG23	2.02	0.41
2:D:27:ARG:HG3	2:D:31:SER:HB3	2.01	0.41
1:A:501:LYS:HG3	6:A:2004:ADP:H2	1.86	0.41
1:A:565:ASP:H	1:A:570:ASN:CB	2.27	0.41
1:A:839:ASN:HA	9:A:2011:PC1:O11	2.21	0.41
1:A:971:LEU:HB2	1:A:973:MET:HG3	2.03	0.41
2:B:27:ARG:HB2	2:B:28:THR:H	1.71	0.41
1:C:36:ASP:HB2	1:C:39:LEU:HD12	2.02	0.41
1:C:75:PRO:O	1:C:77:PRO:HD3	2.21	0.41
1:C:132:VAL:HG22	9:C:2013:PC1:H3A2	2.03	0.41
1:C:645:VAL:C	1:C:647:GLN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:842:LEU:HD12	1:C:1016:TYR:HD2	1.86	0.41
1:A:209:SER:HB3	1:A:215:SER:HA	2.03	0.41
1:A:228:ASN:HB3	1:A:231:GLU:CG	2.51	0.41
1:A:263:ILE:HD12	1:A:265:THR:OG1	2.20	0.41
1:A:301:ILE:HD11	9:A:2014:PC1:H3I1	2.03	0.41
1:A:350:LEU:HD23	1:A:742:ILE:HD12	2.03	0.41
1:A:451:LYS:O	1:A:455:LEU:HD12	2.21	0.41
1:A:637:ILE:HD13	1:A:640:ARG:HH12	1.86	0.41
1:A:765:LEU:O	1:A:769:ILE:HG13	2.21	0.41
1:A:860:PHE:HA	2:B:50:PHE:HE2	1.86	0.41
1:A:908:GLU:O	1:A:911:CYS:HB2	2.21	0.41
2:B:62:SER:C	2:B:64:PHE:H	2.28	0.41
2:B:112:TYR:CE2	2:B:255:LEU:HB3	2.55	0.41
2:B:190:PRO:HA	2:B:191:PRO:HD3	1.80	0.41
1:C:889:ASN:HD22	1:C:901:TYR:H	1.68	0.41
2:D:130:PRO:O	2:D:204:TYR:OH	2.37	0.41
2:D:216:LYS:HE2	2:D:273:ARG:O	2.21	0.41
2:D:270:THR:C	2:D:300:GLU:HG3	2.45	0.41
1:A:315:ILE:HD13	1:A:315:ILE:HA	1.85	0.41
8:A:2010:CLR:H212	8:A:2010:CLR:C12	2.51	0.41
2:B:27:ARG:HG3	2:B:31:SER:CB	2.51	0.41
2:B:91:ARG:NH2	2:D:94:ASP:OD1	2.54	0.41
2:B:134:LYS:HB2	2:B:136:ARG:HH12	1.86	0.41
2:B:186:PHE:HZ	2:B:282:ASN:HB3	1.84	0.41
1:C:122:ASN:OD1	1:C:315:ILE:HG13	2.21	0.41
1:C:228:ASN:OD1	1:C:230:LEU:N	2.53	0.41
1:C:445:SER:OG	1:C:544:ARG:NH1	2.54	0.41
1:C:889:ASN:HB3	1:C:900:THR:HA	2.03	0.41
2:D:157:GLY:C	2:D:159:CYS:H	2.30	0.41
1:A:124:TYR:O	1:A:128:VAL:HG23	2.21	0.40
1:A:470:ILE:H	1:A:470:ILE:HG13	1.51	0.40
9:A:2012:PC1:H281	9:A:2012:PC1:H2B1	1.91	0.40
2:B:23:GLU:HG2	2:B:24:PHE:H	1.86	0.40
2:B:27:ARG:CD	2:B:27:ARG:H	2.34	0.40
3:G:16:VAL:HG12	3:G:17:ASP:N	2.36	0.40
1:C:921:VAL:HG12	1:C:924:TRP:CZ2	2.56	0.40
1:C:964:CYS:HA	1:C:965:PRO:HD2	1.83	0.40
1:C:972:ARG:HH12	2:D:288:LYS:HZ1	1.69	0.40
1:C:995:ASP:OD1	1:C:998:ARG:NH1	2.54	0.40
2:D:27:ARG:HD3	2:D:32:TRP:CE3	2.56	0.40
2:D:79:GLN:HE21	2:D:83:SER:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD23	1:A:183:LEU:H	1.86	0.40
1:A:293:VAL:O	1:A:297:VAL:HG13	2.21	0.40
1:A:361:GLY:C	1:A:363:THR:H	2.28	0.40
1:A:1009:TRP:CZ2	2:B:35:ILE:HG22	2.49	0.40
9:A:2013:PC1:H292	9:A:2013:PC1:C3B	2.45	0.40
1:A:420:LEU:HB3	1:A:486:HIS:HE1	1.85	0.40
1:A:483:LEU:HD12	1:A:484:SER:N	2.37	0.40
1:A:801:LEU:O	1:A:805:LEU:HG	2.22	0.40
1:A:804:ASP:C	1:A:806:GLY:H	2.30	0.40
1:A:815:LEU:O	1:A:818:GLU:HB2	2.22	0.40
1:C:626:ILE:O	1:C:680:GLU:HB3	2.20	0.40
1:C:1000:LEU:HG	9:C:2014:PC1:H12	2.04	0.40
1:C:1002:ILE:HG23	1:C:1011:GLU:HB2	2.03	0.40
2:D:241:GLN:HG3	2:D:242:TYR:CD1	2.56	0.40
1:A:501:LYS:HG3	6:A:2004:ADP:C2	2.57	0.40
1:A:926:ASP:HA	1:A:929:ILE:HG12	2.02	0.40
2:B:52:GLY:O	2:B:56:VAL:HG23	2.22	0.40
2:B:238:PHE:CD1	2:B:257:PRO:HB2	2.56	0.40
1:C:287:ILE:H	1:C:287:ILE:HG13	1.57	0.40
1:C:783:PHE:CE2	1:C:787:ILE:HD11	2.57	0.40
2:D:61:ILE:HG23	2:D:67:THR:HG23	2.03	0.40
1:A:115:GLU:HG2	1:A:116:GLU:N	2.37	0.40
1:A:318:ILE:HD13	1:A:318:ILE:HA	1.89	0.40
1:A:379:MET:HE2	1:A:586:ASP:CG	2.46	0.40
1:A:634:VAL:HG23	1:A:645:VAL:HG12	2.03	0.40
1:C:410:THR:HA	1:C:515:LEU:HD22	2.02	0.40
1:C:879:LEU:O	1:C:880:ARG:C	2.64	0.40
9:C:2014:PC1:H272	9:C:2014:PC1:H2A1	1.71	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%)	882 (89%)	97 (10%)	13 (1%)	9	31
1	C	992/1016 (98%)	890 (90%)	88 (9%)	14 (1%)	9	30
2	B	301/303 (99%)	234 (78%)	55 (18%)	12 (4%)	2	8
2	D	301/303 (99%)	231 (77%)	55 (18%)	15 (5%)	1	5
3	E	33/65 (51%)	32 (97%)	0	1 (3%)	3	12
3	G	32/65 (49%)	27 (84%)	3 (9%)	2 (6%)	1	3
All	All	2651/2768 (96%)	2296 (87%)	298 (11%)	57 (2%)	5	19

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	402	VAL
2	B	139	TYR
3	G	17	ASP
3	G	18	PRO
1	C	267	ALA
1	C	398	ASN
1	C	880	ARG
3	E	18	PRO
2	B	19	SER
2	B	201	VAL
2	B	204	TYR
1	C	34	MET
1	C	92	GLY
1	C	629	GLU
2	D	82	GLN
2	D	201	VAL
2	D	204	TYR
1	A	362	SER
1	A	560	GLU
1	A	775	SER
1	A	804	ASP
2	B	142	GLU
2	B	265	ASN
1	C	775	SER
2	D	73	ALA
2	D	118	LYS
2	D	206	PRO
1	A	34	MET
1	A	394	ASP

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Mol	Chain	Res	Type
2	B	21	LYS
2	B	133	LEU
1	C	373	THR
1	C	432	ASN
1	C	804	ASP
2	D	139	TYR
2	D	158	ASN
2	D	265	ASN
1	A	118	PRO
2	B	73	ALA
2	B	156	LEU
1	C	306	LEU
2	D	63	GLU
2	D	194	GLU
2	D	203	LYS
1	A	629	GLU
1	A	893	ASP
2	B	203	LYS
2	B	206	PRO
1	C	210	SER
2	D	219	GLU
1	A	92	GLY
1	C	593	PRO
1	C	630	GLY
2	D	261	VAL
1	A	489	PRO
2	D	127	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	844/861 (98%)	711 (84%)	133 (16%)	2	9
1	C	844/861 (98%)	744 (88%)	100 (12%)	5	17
2	B	269/269 (100%)	228 (85%)	41 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	269/269 (100%)	236 (88%)	33 (12%)	4	16
3	E	29/52 (56%)	23 (79%)	6 (21%)	1	4
3	G	28/52 (54%)	26 (93%)	2 (7%)	13	39
All	All	2283/2364 (97%)	1968 (86%)	315 (14%)	3	12

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	44	LEU
1	A	57	THR
1	A	60	ARG
1	A	79	THR
1	A	81	GLU
1	A	82	TRP
1	A	83	VAL
1	A	102	ILE
1	A	125	LEU
1	A	129	LEU
1	A	132	VAL
1	A	144	GLU
1	A	152	GLU
1	A	158	VAL
1	A	161	GLN
1	A	166	ARG
1	A	171	MET
1	A	192	ILE
1	A	210	SER
1	A	211	LEU
1	A	216	GLU
1	A	231	GLU
1	A	239	SER
1	A	241	ASN
1	A	242	CYS
1	A	250	ILE
1	A	252	VAL
1	A	266	LEU
1	A	268	SER
1	A	270	LEU
1	A	274	GLN
1	A	287	ILE

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Mol	Chain	Res	Type
1	A	291	VAL
1	A	297	VAL
1	A	305	ILE
1	A	308	TYR
1	A	309	THR
1	A	310	TRP
1	A	314	VAL
1	A	317	LEU
1	A	318	ILE
1	A	325	VAL
1	A	337	LEU
1	A	360	LEU
1	A	364	SER
1	A	365	THR
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	410	THR
1	A	412	LEU
1	A	417	ILE
1	A	425	VAL
1	A	430	GLN
1	A	433	LEU
1	A	437	LYS
1	A	438	ARG
1	A	440	VAL
1	A	450	LEU
1	A	455	LEU
1	A	460	VAL
1	A	461	LYS
1	A	469	LYS
1	A	470	ILE
1	A	471	VAL
1	A	473	ILE
1	A	476	ASN
1	A	478	THR
1	A	485	ILE
1	A	487	LYS
1	A	493	GLU

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Mol	Chain	Res	Type
1	A	508	LEU
1	A	513	SER
1	A	514	ILE
1	A	515	LEU
1	A	519	LYS
1	A	520	GLU
1	A	521	GLN
1	A	523	LEU
1	A	541	LEU
1	A	570	ASN
1	A	600	ARG
1	A	628	SER
1	A	629	GLU
1	A	634	VAL
1	A	635	GLU
1	A	645	VAL
1	A	648	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	685	ARG
1	A	687	SER
1	A	712	VAL
1	A	719	LYS
1	A	723	ILE
1	A	741	MET
1	A	744	LEU
1	A	750	SER
1	A	751	ILE
1	A	753	THR
1	A	765	LEU
1	A	775	SER
1	A	781	THR
1	A	791	ILE
1	A	805	LEU
1	A	814	SER
1	A	815	LEU
1	A	818	GLU
1	A	819	GLN

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Mol	Chain	Res	Type
1	A	822	SER
1	A	823	ASP
1	A	824	ILE
1	A	845	MET
1	A	881	VAL
1	A	882	ASN
1	A	900	THR
1	A	917	VAL
1	A	928	VAL
1	A	936	SER
1	A	957	LEU
1	A	969	VAL
1	A	989	LEU
1	A	1004	ARG
1	A	1010	VAL
1	A	1014	THR
2	B	20	GLU
2	B	22	LYS
2	B	24	PHE
2	B	27	ARG
2	B	35	ILE
2	B	37	LEU
2	B	41	ILE
2	B	45	CYS
2	B	54	ILE
2	B	61	ILE
2	B	63	GLU
2	B	71	ARG
2	B	72	VAL
2	B	78	THR
2	B	90	PHE
2	B	99	GLU
2	B	102	VAL
2	B	109	LEU
2	B	119	ASP
2	B	129	VAL
2	B	158	ASN
2	B	162	LEU
2	B	170	LYS
2	B	171	ASP
2	B	177	ILE
2	B	180	LEU

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Mol	Chain	Res	Type
2	B	187	LYS
2	B	193	ASN
2	B	203	LYS
2	B	208	VAL
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	295	PHE
2	B	301	VAL
3	G	24	GLU
3	G	45	ILE
1	C	28	LEU
1	C	36	ASP
1	C	44	LEU
1	C	56	LEU
1	C	57	THR
1	C	60	ARG
1	C	82	TRP
1	C	86	CYS
1	C	114	THR
1	C	125	LEU
1	C	129	LEU
1	C	136	THR
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	244	GLU
1	C	254	THR
1	C	274	GLN
1	C	277	ILE
1	C	287	ILE
1	C	293	VAL

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Mol	Chain	Res	Type
1	C	301	ILE
1	C	302	LEU
1	C	308	TYR
1	C	309	THR
1	C	310	TRP
1	C	317	LEU
1	C	336	CYS
1	C	347	LYS
1	C	360	LEU
1	C	371	THR
1	C	379	MET
1	C	380	THR
1	C	394	ASP
1	C	403	SER
1	C	412	LEU
1	C	417	ILE
1	C	423	ARG
1	C	430	GLN
1	C	450	LEU
1	C	461	LYS
1	C	469	LYS
1	C	473	ILE
1	C	476	ASN
1	C	478	THR
1	C	485	ILE
1	C	491	THR
1	C	493	GLU
1	C	495	ARG
1	C	500	MET
1	C	514	ILE
1	C	515	LEU
1	C	519	LYS
1	C	520	GLU
1	C	521	GLN
1	C	523	LEU
1	C	541	LEU
1	C	569	VAL
1	C	596	VAL
1	C	600	ARG
1	C	612	ASP
1	C	629	GLU
1	C	645	VAL

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Mol	Chain	Res	Type
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
1	C	723	ILE
1	C	741	MET
1	C	744	LEU
1	C	750	SER
1	C	761	ILE
1	C	772	THR
1	C	785	ILE
1	C	791	ILE
1	C	805	LEU
1	C	815	LEU
1	C	818	GLU
1	C	824	ILE
1	C	825	MET
1	C	861	THR
1	C	872	LEU
1	C	881	VAL
1	C	886	ARG
1	C	888	ILE
1	C	894	SER
1	C	900	THR
1	C	903	GLN
1	C	969	VAL
1	C	980	TRP
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	35	ILE
2	D	57	MET
2	D	61	ILE
2	D	63	GLU
2	D	71	ARG
2	D	72	VAL

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Mol	Chain	Res	Type
2	D	78	THR
2	D	99	GLU
2	D	109	LEU
2	D	119	ASP
2	D	150	ARG
2	D	162	LEU
2	D	170	LYS
2	D	177	ILE
2	D	180	LEU
2	D	187	LYS
2	D	203	LYS
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	261	VAL
2	D	294	ARG
2	D	295	PHE
2	D	301	VAL
3	E	20	TYR
3	E	24	GLU
3	E	36	LEU
3	E	45	ILE
3	E	47	SER
3	E	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	119	GLN
1	A	143	GLN
1	A	161	GLN
1	A	274	GLN
1	A	432	ASN
1	A	550	HIS
1	A	570	ASN

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Mol	Chain	Res	Type
1	A	699	GLN
1	A	747	ASN
1	A	790	ASN
1	A	889	ASN
1	A	903	GLN
1	A	944	ASN
2	B	93	ASN
2	B	140	ASN
2	B	205	ASN
2	B	262	GLN
2	B	292	GLN
3	G	28	ASN
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	533	ASN
1	C	550	HIS
1	C	699	GLN
1	C	790	ASN
1	C	819	GLN
1	C	854	GLN
1	C	889	ASN
1	C	903	GLN
1	C	923	GLN
2	D	128	ASN
2	D	140	ASN
2	D	205	ASN
2	D	212	HIS
2	D	262	GLN
2	D	282	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
9	PC1	C	2013	-	53,53,53	0.94	4 (7%)	59,61,61	1.32	6 (10%)
5	ALF	C	2002	-	4,4,4	1.32	0	-		
10	NAG	D	402	-	14,14,15	0.46	0	17,19,21	0.68	0
8	CLR	C	2009	-	31,31,31	4.78	18 (58%)	48,48,48	2.61	19 (39%)
8	CLR	C	2010	-	31,31,31	4.87	16 (51%)	48,48,48	2.67	21 (43%)
9	PC1	A	2014	-	53,53,53	0.93	4 (7%)	59,61,61	1.31	4 (6%)
9	PC1	D	401	-	53,53,53	0.95	5 (9%)	59,61,61	1.24	6 (10%)
9	PC1	A	2013	-	53,53,53	0.93	4 (7%)	59,61,61	1.19	5 (8%)
9	PC1	A	2012	-	53,53,53	0.94	4 (7%)	59,61,61	1.32	6 (10%)
9	PC1	C	2012	-	53,53,53	0.93	5 (9%)	59,61,61	1.27	5 (8%)
10	NAG	B	3003	-	14,14,15	0.41	0	17,19,21	0.74	0
9	PC1	C	2014	-	53,53,53	0.98	4 (7%)	59,61,61	1.31	7 (11%)
5	ALF	A	2002	-	4,4,4	1.38	0	-		
6	ADP	A	2004	4	28,29,29	1.72	4 (14%)	43,45,45	1.89	10 (23%)
8	CLR	B	3001	-	31,31,31	4.86	17 (54%)	48,48,48	2.57	19 (39%)
9	PC1	C	2015	-	53,53,53	0.92	5 (9%)	59,61,61	1.28	5 (8%)
6	ADP	C	2004	-	28,29,29	1.54	6 (21%)	43,45,45	1.89	11 (25%)
9	PC1	A	2011	-	53,53,53	0.92	4 (7%)	59,61,61	1.21	5 (8%)
8	CLR	A	2010	-	31,31,31	4.90	15 (48%)	48,48,48	3.22	25 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLR	C	2011	-	31,31,31	4.98	14 (45%)	48,48,48	2.72	22 (45%)
9	PC1	B	3002	-	53,53,53	0.91	3 (5%)	59,61,61	1.20	5 (8%)
8	CLR	A	2009	-	31,31,31	4.86	16 (51%)	48,48,48	2.66	19 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PC1	C	2013	-	-	32/57/57/57	-
10	NAG	D	402	-	-	1/6/23/26	0/1/1/1
8	CLR	C	2009	-	-	0/10/68/68	0/4/4/4
8	CLR	C	2010	-	-	1/10/68/68	0/4/4/4
9	PC1	D	401	-	-	33/57/57/57	-
9	PC1	A	2014	-	-	30/57/57/57	-
9	PC1	A	2013	-	-	32/57/57/57	-
9	PC1	A	2012	-	-	32/57/57/57	-
9	PC1	C	2012	-	-	27/57/57/57	-
10	NAG	B	3003	-	-	1/6/23/26	0/1/1/1
9	PC1	C	2014	-	-	36/57/57/57	-
6	ADP	A	2004	4	-	5/16/32/32	0/3/3/3
8	CLR	B	3001	-	-	0/10/68/68	0/4/4/4
9	PC1	C	2015	-	-	24/57/57/57	-
6	ADP	C	2004	-	-	1/16/32/32	0/3/3/3
9	PC1	A	2011	-	-	25/57/57/57	-
8	CLR	A	2010	-	-	2/10/68/68	0/4/4/4
8	CLR	C	2011	-	-	0/10/68/68	0/4/4/4
9	PC1	B	3002	-	-	32/57/57/57	-
8	CLR	A	2009	-	-	0/10/68/68	0/4/4/4

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2011	CLR	C10-C9	-14.19	1.33	1.56
8	A	2010	CLR	C10-C9	-14.09	1.33	1.56
8	A	2009	CLR	C10-C9	-13.85	1.34	1.56
8	C	2010	CLR	C10-C9	-13.57	1.34	1.56
8	B	3001	CLR	C10-C9	-13.55	1.34	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	2009	CLR	C10-C9	-13.55	1.34	1.56
8	A	2010	CLR	C11-C9	12.48	1.74	1.53
8	C	2011	CLR	C11-C9	12.32	1.74	1.53
8	C	2010	CLR	C11-C9	12.25	1.73	1.53
8	C	2009	CLR	C11-C9	12.18	1.73	1.53
8	A	2009	CLR	C11-C9	12.12	1.73	1.53
8	B	3001	CLR	C11-C9	11.95	1.73	1.53
8	B	3001	CLR	C12-C13	-10.53	1.35	1.54
8	C	2011	CLR	C12-C13	-10.45	1.35	1.54
8	C	2010	CLR	C12-C13	-10.17	1.36	1.54
8	C	2009	CLR	C12-C13	-9.90	1.36	1.54
8	A	2009	CLR	C12-C13	-9.89	1.36	1.54
8	A	2010	CLR	C13-C14	-9.73	1.37	1.55
8	A	2010	CLR	C12-C13	-9.60	1.37	1.54
8	B	3001	CLR	C13-C14	-9.42	1.37	1.55
8	C	2011	CLR	C13-C14	-9.39	1.37	1.55
8	C	2010	CLR	C13-C14	-9.21	1.38	1.55
8	C	2009	CLR	C13-C14	-8.98	1.38	1.55
8	A	2009	CLR	C13-C14	-8.89	1.38	1.55
8	A	2010	CLR	C12-C11	6.96	1.67	1.53
8	A	2009	CLR	C12-C11	6.46	1.66	1.53
8	C	2011	CLR	C12-C11	6.38	1.66	1.53
8	C	2010	CLR	C12-C11	6.15	1.65	1.53
8	C	2011	CLR	C18-C13	-6.05	1.44	1.54
8	B	3001	CLR	C12-C11	5.90	1.65	1.53
8	B	3001	CLR	C18-C13	-5.87	1.44	1.54
8	C	2009	CLR	C12-C11	5.80	1.65	1.53
8	A	2010	CLR	C18-C13	-5.70	1.44	1.54
8	C	2010	CLR	C18-C13	-5.69	1.44	1.54
8	C	2011	CLR	C8-C14	-5.46	1.43	1.53
8	C	2009	CLR	C18-C13	-5.41	1.45	1.54
6	A	2004	ADP	C5-C4	5.28	1.48	1.39
8	C	2010	CLR	C8-C14	-5.17	1.43	1.53
8	A	2009	CLR	C18-C13	-5.15	1.45	1.54
8	B	3001	CLR	C8-C14	-5.12	1.44	1.53
8	A	2009	CLR	C8-C14	-5.03	1.44	1.53
8	A	2010	CLR	C8-C14	-4.97	1.44	1.53
8	C	2009	CLR	C8-C14	-4.95	1.44	1.53
8	C	2010	CLR	C20-C17	-4.68	1.46	1.54
8	C	2011	CLR	C19-C10	-4.65	1.47	1.54
8	C	2011	CLR	C20-C17	-4.63	1.46	1.54
8	A	2010	CLR	C19-C10	-4.57	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	2009	CLR	C19-C10	-4.55	1.47	1.54
8	B	3001	CLR	C20-C17	-4.49	1.46	1.54
8	C	2009	CLR	C6-C5	4.44	1.42	1.33
8	A	2009	CLR	C20-C17	-4.39	1.46	1.54
8	C	2009	CLR	C20-C17	-4.24	1.47	1.54
8	B	3001	CLR	C6-C5	4.23	1.41	1.33
8	C	2010	CLR	C19-C10	-4.20	1.47	1.54
6	C	2004	ADP	C5-C4	4.14	1.46	1.39
8	A	2009	CLR	C6-C5	4.12	1.41	1.33
6	A	2004	ADP	PA-O3A	4.12	1.63	1.59
6	C	2004	ADP	PA-O3A	4.01	1.63	1.59
8	B	3001	CLR	C19-C10	-3.93	1.48	1.54
8	A	2010	CLR	C6-C5	3.92	1.41	1.33
8	C	2011	CLR	C16-C17	-3.81	1.46	1.54
8	C	2010	CLR	C6-C5	3.76	1.40	1.33
8	C	2011	CLR	C6-C5	3.74	1.40	1.33
8	C	2009	CLR	C19-C10	-3.67	1.48	1.54
9	C	2013	PC1	O31-C31	3.51	1.43	1.33
8	A	2010	CLR	C16-C17	-3.50	1.47	1.54
9	D	401	PC1	O31-C31	3.39	1.43	1.33
8	C	2009	CLR	C16-C15	3.39	1.63	1.54
9	A	2012	PC1	O31-C31	3.38	1.43	1.33
9	C	2012	PC1	O31-C31	3.35	1.43	1.33
9	A	2014	PC1	O31-C31	3.34	1.43	1.33
6	A	2004	ADP	C5-C6	3.30	1.50	1.41
8	A	2009	CLR	C4-C3	-3.24	1.46	1.52
8	C	2010	CLR	C16-C15	3.23	1.62	1.54
8	A	2009	CLR	C16-C17	-3.18	1.47	1.54
8	B	3001	CLR	C16-C17	-3.09	1.48	1.54
9	C	2015	PC1	O31-C31	3.07	1.42	1.33
9	A	2011	PC1	O31-C31	3.06	1.42	1.33
8	C	2010	CLR	C16-C17	-3.05	1.48	1.54
9	C	2014	PC1	O31-C31	3.02	1.42	1.33
8	A	2010	CLR	C4-C3	-3.02	1.46	1.52
9	A	2013	PC1	O31-C31	3.02	1.42	1.33
8	A	2009	CLR	C16-C15	2.98	1.62	1.54
8	B	3001	CLR	C16-C15	2.95	1.62	1.54
8	C	2010	CLR	C4-C3	-2.91	1.47	1.52
8	C	2009	CLR	C16-C17	-2.88	1.48	1.54
8	A	2010	CLR	C20-C17	-2.85	1.49	1.54
8	B	3001	CLR	C4-C3	-2.83	1.47	1.52
6	A	2004	ADP	C8-N7	2.71	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2011	PC1	C3A-C39	-2.70	1.38	1.51
9	B	3002	PC1	O31-C31	2.69	1.41	1.33
9	A	2013	PC1	O21-C2	-2.69	1.40	1.46
8	A	2009	CLR	C1-C2	-2.65	1.48	1.53
8	C	2011	CLR	C4-C3	-2.65	1.47	1.52
8	A	2009	CLR	O1-C3	-2.61	1.35	1.43
9	C	2015	PC1	C3A-C39	-2.60	1.38	1.51
9	B	3002	PC1	C3A-C39	-2.60	1.38	1.51
9	B	3002	PC1	O21-C2	-2.59	1.40	1.46
6	C	2004	ADP	C5-C6	2.59	1.48	1.41
9	A	2013	PC1	C3A-C39	-2.59	1.38	1.51
6	C	2004	ADP	C8-N7	2.58	1.36	1.31
8	C	2009	CLR	C4-C3	-2.57	1.47	1.52
8	A	2010	CLR	C1-C2	-2.55	1.48	1.53
9	C	2013	PC1	C3A-C39	-2.54	1.39	1.51
9	C	2014	PC1	C3A-C39	-2.53	1.39	1.51
9	A	2011	PC1	O21-C2	-2.51	1.40	1.46
9	C	2012	PC1	C3A-C39	-2.51	1.39	1.51
6	C	2004	ADP	C5-N7	-2.49	1.34	1.39
8	C	2011	CLR	C16-C15	2.49	1.60	1.54
9	A	2012	PC1	C3A-C39	-2.49	1.39	1.51
9	A	2014	PC1	C3A-C39	-2.44	1.39	1.51
8	C	2009	CLR	C2-C3	-2.39	1.46	1.51
9	D	401	PC1	C3A-C39	-2.38	1.40	1.51
8	C	2010	CLR	O1-C3	-2.37	1.36	1.43
9	C	2015	PC1	O21-C2	-2.34	1.41	1.46
9	A	2012	PC1	O21-C2	-2.33	1.41	1.46
9	C	2012	PC1	O21-C2	-2.29	1.41	1.46
9	D	401	PC1	O21-C2	-2.28	1.41	1.46
9	A	2014	PC1	O21-C2	-2.28	1.41	1.46
8	C	2009	CLR	C1-C2	-2.26	1.48	1.53
9	C	2014	PC1	O21-C2	-2.26	1.41	1.46
6	C	2004	ADP	C4-N9	-2.25	1.33	1.37
8	A	2010	CLR	C16-C15	2.25	1.60	1.54
8	C	2011	CLR	C1-C2	-2.24	1.48	1.53
8	B	3001	CLR	C2-C3	-2.23	1.46	1.51
8	B	3001	CLR	C15-C14	2.23	1.58	1.54
9	C	2012	PC1	O21-C21	2.21	1.40	1.34
9	C	2013	PC1	O21-C21	2.19	1.40	1.34
8	B	3001	CLR	O1-C3	-2.19	1.37	1.43
9	C	2014	PC1	O21-C21	2.17	1.40	1.34
8	C	2009	CLR	O1-C3	-2.17	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2014	PC1	O21-C21	2.17	1.40	1.34
8	A	2009	CLR	C2-C3	-2.15	1.46	1.51
8	C	2009	CLR	C15-C14	2.15	1.58	1.54
9	A	2013	PC1	C2A-C29	-2.12	1.41	1.51
8	B	3001	CLR	C1-C2	-2.12	1.49	1.53
8	A	2010	CLR	O1-C3	-2.12	1.37	1.43
9	A	2012	PC1	O21-C21	2.12	1.40	1.34
8	C	2010	CLR	C15-C14	2.10	1.58	1.54
8	C	2010	CLR	C1-C2	-2.05	1.49	1.53
9	D	401	PC1	C2A-C29	-2.05	1.41	1.51
9	C	2013	PC1	O21-C2	-2.04	1.41	1.46
9	C	2015	PC1	O21-C21	2.03	1.40	1.34
9	C	2015	PC1	C2A-C29	-2.03	1.41	1.51
9	A	2011	PC1	C2A-C29	-2.03	1.41	1.51
9	D	401	PC1	O21-C21	2.02	1.40	1.34
8	C	2009	CLR	C21-C20	-2.01	1.47	1.53
9	C	2012	PC1	C2A-C29	-2.00	1.41	1.51

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2010	CLR	C21-C20-C22	-10.84	93.56	110.34
8	A	2010	CLR	C21-C20-C17	-8.54	100.07	112.88
8	C	2009	CLR	C17-C13-C14	7.28	108.45	100.10
8	C	2010	CLR	C17-C13-C14	7.19	108.35	100.10
8	A	2009	CLR	C17-C13-C14	7.02	108.16	100.10
8	C	2011	CLR	C17-C13-C14	6.73	107.83	100.10
8	B	3001	CLR	C17-C13-C14	6.58	107.65	100.10
6	C	2004	ADP	C5-C4-N3	-6.22	118.15	126.72
6	A	2004	ADP	C5-C4-N3	-5.94	118.54	126.72
8	A	2010	CLR	C13-C14-C8	5.93	122.83	114.41
8	A	2010	CLR	C17-C13-C14	5.85	106.81	100.10
8	C	2010	CLR	C10-C5-C6	-5.77	114.50	122.93
8	C	2009	CLR	C13-C14-C8	5.76	122.59	114.41
8	A	2009	CLR	C13-C14-C8	5.67	122.47	114.41
8	C	2011	CLR	C13-C14-C8	5.67	122.46	114.41
8	A	2010	CLR	C11-C9-C10	5.61	120.01	113.08
8	B	3001	CLR	C10-C5-C6	-5.51	114.88	122.93
8	C	2011	CLR	C10-C5-C6	-5.46	114.95	122.93
8	B	3001	CLR	C13-C14-C8	5.39	122.07	114.41
8	C	2009	CLR	C10-C5-C6	-5.37	115.09	122.93
8	C	2010	CLR	C11-C9-C10	5.35	119.68	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2009	CLR	C11-C9-C10	5.33	119.66	113.08
8	A	2009	CLR	C11-C9-C10	5.14	119.42	113.08
8	B	3001	CLR	C11-C9-C10	5.06	119.33	113.08
8	C	2011	CLR	C11-C9-C10	5.00	119.25	113.08
8	C	2011	CLR	C9-C10-C5	4.98	116.95	109.65
8	A	2009	CLR	C19-C10-C9	-4.98	106.07	111.66
8	A	2010	CLR	C14-C8-C9	4.70	115.22	109.09
8	C	2010	CLR	C13-C14-C8	4.65	121.02	114.41
8	C	2010	CLR	C9-C10-C5	4.61	116.41	109.65
8	C	2011	CLR	C11-C9-C8	-4.60	105.36	111.78
8	A	2010	CLR	C11-C9-C8	-4.60	105.36	111.78
8	A	2009	CLR	C14-C8-C9	4.57	115.06	109.09
8	A	2010	CLR	C10-C5-C6	-4.56	116.28	122.93
8	C	2010	CLR	C11-C9-C8	-4.55	105.43	111.78
9	C	2015	PC1	O21-C21-C22	4.50	121.21	111.48
8	A	2009	CLR	C10-C5-C6	-4.45	116.43	122.93
8	B	3001	CLR	C14-C8-C9	4.34	114.76	109.09
6	C	2004	ADP	N3-C4-N9	4.33	134.52	127.17
8	A	2009	CLR	C11-C9-C8	-4.28	105.80	111.78
8	B	3001	CLR	C19-C10-C9	-4.24	106.90	111.66
8	A	2009	CLR	C10-C9-C8	4.22	118.88	112.71
6	A	2004	ADP	N3-C4-N9	4.21	134.33	127.17
8	C	2010	CLR	C12-C13-C17	-4.19	110.43	116.60
6	A	2004	ADP	O2A-PA-O3A	4.18	118.57	107.27
9	C	2012	PC1	C15-N-C13	4.15	119.86	108.98
9	A	2014	PC1	O21-C21-C22	4.11	120.37	111.48
8	C	2011	CLR	C4-C5-C10	4.10	121.68	116.42
8	B	3001	CLR	C9-C10-C5	4.10	115.65	109.65
8	B	3001	CLR	C12-C13-C17	-4.10	110.57	116.60
9	C	2014	PC1	O21-C21-C22	4.09	120.32	111.48
8	B	3001	CLR	C11-C9-C8	-4.08	106.08	111.78
8	C	2009	CLR	C4-C5-C6	4.07	126.09	120.57
9	A	2011	PC1	C15-N-C13	4.05	119.63	108.98
9	C	2013	PC1	C15-N-C13	3.97	119.41	108.98
9	A	2014	PC1	O31-C3-C2	3.94	119.75	108.40
9	B	3002	PC1	O21-C21-C22	3.92	119.97	111.48
6	C	2004	ADP	C2-N3-C4	3.92	121.41	111.83
6	C	2004	ADP	C4-C5-N7	-3.90	106.12	110.58
8	A	2010	CLR	C9-C10-C5	3.89	115.36	109.65
9	A	2013	PC1	O21-C21-C22	3.89	119.90	111.48
8	A	2009	CLR	C18-C13-C12	-3.89	104.87	110.61
8	C	2009	CLR	C12-C13-C17	-3.89	110.88	116.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2009	CLR	C19-C10-C9	-3.88	107.31	111.66
8	C	2011	CLR	C14-C8-C9	3.86	114.13	109.09
8	C	2010	CLR	C19-C10-C9	-3.85	107.34	111.66
9	A	2011	PC1	O21-C21-C22	3.84	119.78	111.48
8	C	2011	CLR	C19-C10-C9	-3.83	107.37	111.66
8	C	2009	CLR	C11-C9-C8	-3.82	106.45	111.78
9	A	2012	PC1	C15-N-C13	3.82	119.01	108.98
9	B	3002	PC1	C15-N-C13	3.80	118.96	108.98
8	C	2009	CLR	C9-C10-C5	3.80	115.21	109.65
8	C	2009	CLR	C10-C9-C8	3.79	118.25	112.71
6	A	2004	ADP	C4-C5-N7	-3.76	106.28	110.58
9	A	2013	PC1	C15-N-C13	3.72	118.75	108.98
8	B	3001	CLR	C4-C5-C6	3.71	125.59	120.57
8	A	2009	CLR	C12-C13-C14	3.71	112.79	107.25
8	B	3001	CLR	C10-C9-C8	3.64	118.03	112.71
9	C	2012	PC1	O21-C21-C22	3.62	119.31	111.48
9	D	401	PC1	O31-C3-C2	3.60	118.77	108.40
6	A	2004	ADP	C2-N3-C4	3.59	120.59	111.83
8	A	2009	CLR	C12-C13-C17	-3.58	111.33	116.60
9	C	2013	PC1	O31-C3-C2	3.57	118.68	108.40
9	C	2014	PC1	C15-N-C13	3.56	118.32	108.98
9	C	2015	PC1	C15-N-C13	3.56	118.31	108.98
8	C	2009	CLR	C14-C8-C9	3.55	113.73	109.09
9	C	2012	PC1	O31-C3-C2	3.53	118.58	108.40
9	A	2014	PC1	C15-N-C13	3.52	118.23	108.98
8	C	2010	CLR	C12-C13-C14	3.50	112.48	107.25
9	A	2012	PC1	O31-C3-C2	3.47	118.40	108.40
8	C	2011	CLR	C12-C13-C14	3.45	112.41	107.25
9	C	2015	PC1	O31-C3-C2	3.45	118.33	108.40
9	C	2013	PC1	O21-C21-C22	3.43	118.91	111.48
8	C	2010	CLR	C4-C5-C6	3.41	125.19	120.57
9	D	401	PC1	C15-N-C13	3.40	117.91	108.98
8	C	2011	CLR	C12-C13-C17	-3.35	111.67	116.60
8	C	2010	CLR	C14-C8-C9	3.33	113.43	109.09
8	A	2010	CLR	C19-C10-C9	-3.31	107.95	111.66
9	D	401	PC1	O21-C21-C22	3.31	118.63	111.48
8	C	2011	CLR	C3-C4-C5	-3.29	106.81	112.05
8	A	2009	CLR	C4-C5-C6	3.28	125.02	120.57
8	C	2009	CLR	C12-C13-C14	3.22	112.07	107.25
8	C	2010	CLR	C23-C24-C25	-3.22	101.57	115.94
8	B	3001	CLR	C12-C13-C14	3.19	112.01	107.25
9	A	2013	PC1	O31-C3-C2	3.14	117.44	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2010	CLR	C18-C13-C12	-3.08	106.06	110.61
8	A	2009	CLR	C9-C10-C5	3.08	114.16	109.65
8	C	2011	CLR	C16-C17-C20	-3.06	107.55	112.18
8	C	2010	CLR	C10-C9-C8	3.01	117.11	112.71
9	C	2013	PC1	O31-C31-C32	2.99	120.96	111.83
8	C	2010	CLR	C4-C5-C10	2.99	120.25	116.42
8	C	2011	CLR	C18-C13-C12	-2.98	106.21	110.61
9	A	2012	PC1	O21-C21-C22	2.96	117.89	111.48
8	C	2009	CLR	C16-C17-C20	-2.95	107.71	112.18
8	C	2010	CLR	C7-C8-C14	-2.92	106.80	110.93
9	A	2011	PC1	O31-C31-C32	2.92	120.73	111.83
8	C	2011	CLR	C2-C3-C4	-2.91	106.20	110.29
8	A	2010	CLR	C10-C9-C8	2.90	116.95	112.71
8	C	2011	CLR	C10-C9-C8	2.86	116.89	112.71
8	C	2010	CLR	C22-C20-C17	-2.84	104.43	110.33
9	A	2014	PC1	O31-C31-C32	2.82	120.42	111.83
6	C	2004	ADP	N3-C2-N1	-2.81	124.32	128.58
8	A	2010	CLR	C4-C5-C10	2.72	119.90	116.42
8	A	2010	CLR	C12-C13-C14	2.71	111.29	107.25
9	C	2014	PC1	O31-C3-C2	2.70	116.17	108.40
9	C	2015	PC1	O31-C31-C32	2.69	120.03	111.83
8	A	2009	CLR	C19-C10-C1	-2.68	105.35	109.43
6	C	2004	ADP	C5-N7-C8	2.66	107.63	103.45
8	C	2011	CLR	C27-C25-C26	-2.66	98.67	110.53
9	C	2014	PC1	O31-C31-C32	2.65	119.92	111.83
9	A	2012	PC1	O31-C31-C32	2.64	119.90	111.83
6	A	2004	ADP	N3-C2-N1	-2.62	124.61	128.58
9	C	2012	PC1	O31-C31-C32	2.61	119.80	111.83
8	A	2009	CLR	C3-C4-C5	-2.58	107.94	112.05
9	B	3002	PC1	O31-C3-C2	2.57	115.81	108.40
9	A	2011	PC1	O31-C3-C2	2.57	115.80	108.40
8	A	2010	CLR	C2-C3-C4	-2.56	106.69	110.29
9	C	2014	PC1	O31-C31-O32	-2.54	117.28	123.63
8	A	2010	CLR	C18-C13-C12	-2.53	106.88	110.61
9	B	3002	PC1	O31-C31-C32	2.50	119.47	111.83
8	A	2010	CLR	C7-C8-C14	-2.50	107.40	110.93
8	A	2010	CLR	C23-C22-C20	-2.49	108.12	115.08
9	D	401	PC1	O31-C31-C32	2.47	119.37	111.83
9	A	2012	PC1	O21-C21-O22	-2.46	117.94	123.70
8	A	2010	CLR	C18-C13-C17	-2.43	107.26	111.68
8	B	3001	CLR	C4-C5-C10	2.42	119.53	116.42
8	C	2009	CLR	C21-C20-C22	-2.41	106.61	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	2010	CLR	C19-C10-C1	-2.41	105.77	109.43
8	C	2011	CLR	C18-C13-C17	-2.40	107.33	111.68
6	A	2004	ADP	C5-N7-C8	2.39	107.21	103.45
8	A	2010	CLR	C4-C5-C6	2.38	123.79	120.57
9	A	2011	PC1	O31-C31-O32	-2.37	117.69	123.63
8	A	2010	CLR	C15-C14-C8	-2.36	115.33	119.10
6	C	2004	ADP	O2A-PA-O3A	2.36	113.65	107.27
6	C	2004	ADP	O4'-C1'-N9	2.35	112.60	108.09
8	C	2009	CLR	C18-C13-C12	-2.34	107.15	110.61
8	A	2010	CLR	C3-C4-C5	-2.34	108.32	112.05
8	B	3001	CLR	C16-C17-C20	-2.34	108.64	112.18
9	C	2015	PC1	O21-C21-O22	-2.33	118.26	123.70
6	A	2004	ADP	C6-C5-N7	2.32	136.56	132.09
8	C	2010	CLR	C3-C4-C5	-2.31	108.38	112.05
9	A	2012	PC1	C2-O21-C21	2.29	123.28	117.80
8	C	2011	CLR	O1-C3-C4	-2.28	104.56	109.71
8	B	3001	CLR	C19-C10-C1	-2.27	105.97	109.43
6	C	2004	ADP	C6-C5-N7	2.27	136.47	132.09
6	C	2004	ADP	C4-N9-C8	2.27	108.12	105.74
8	A	2009	CLR	C8-C7-C6	-2.26	109.63	112.76
8	C	2010	CLR	C1-C10-C9	2.25	111.72	108.74
8	C	2011	CLR	C21-C20-C22	-2.25	106.86	110.34
8	A	2010	CLR	C1-C2-C3	2.22	113.42	110.48
8	A	2009	CLR	C23-C24-C25	-2.21	106.06	115.94
6	C	2004	ADP	N9-C8-N7	-2.21	110.81	113.94
8	B	3001	CLR	C21-C20-C22	-2.20	106.93	110.34
9	C	2013	PC1	C2-O21-C21	2.20	123.05	117.80
8	C	2009	CLR	C7-C8-C14	-2.18	107.85	110.93
6	A	2004	ADP	O4'-C1'-N9	2.17	112.26	108.09
9	A	2013	PC1	O31-C31-C32	2.17	118.45	111.83
8	A	2009	CLR	C13-C17-C20	2.17	122.84	119.50
8	C	2010	CLR	C19-C10-C1	-2.16	106.14	109.43
9	C	2014	PC1	C2G-C2F-C2E	2.16	125.28	114.37
8	C	2009	CLR	C18-C13-C17	-2.14	107.79	111.68
9	C	2012	PC1	O31-C31-O32	-2.12	118.32	123.63
9	D	401	PC1	C2I-C2H-C2G	2.12	127.65	113.36
8	C	2009	CLR	C8-C7-C6	-2.11	109.83	112.76
8	C	2010	CLR	C27-C25-C26	2.10	119.89	110.53
8	B	3001	CLR	C18-C13-C12	-2.09	107.53	110.61
8	B	3001	CLR	C13-C17-C20	2.09	122.72	119.50
9	A	2013	PC1	O31-C31-O32	-2.07	118.46	123.63
8	B	3001	CLR	C1-C10-C9	2.07	111.47	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	2014	PC1	C2B-C2A-C29	2.06	124.81	114.37
9	B	3002	PC1	C2F-C2E-C2D	2.06	124.80	114.37
8	C	2011	CLR	C4-C5-C6	2.06	123.36	120.57
8	A	2010	CLR	C18-C13-C14	-2.06	107.94	111.68
9	D	401	PC1	O21-C21-O22	-2.05	118.91	123.70
8	A	2009	CLR	C18-C13-C17	-2.04	107.98	111.68
9	C	2013	PC1	O21-C21-O22	-2.03	118.95	123.70
8	A	2010	CLR	C24-C23-C22	-2.02	104.24	113.28
8	C	2011	CLR	C22-C20-C17	-2.01	106.16	110.33
8	C	2009	CLR	C1-C10-C9	2.01	111.39	108.74
6	A	2004	ADP	O3B-PB-O2B	2.01	115.33	107.80

There are no chirality outliers.

All (314) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2004	ADP	C5'-O5'-PA-O2A
6	A	2004	ADP	C5'-O5'-PA-O3A
9	A	2011	PC1	C11-O13-P-O11
9	A	2011	PC1	C12-C11-O13-P
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
9	A	2014	PC1	C22-C21-O21-C2
9	B	3002	PC1	C1-O11-P-O14
9	B	3002	PC1	O13-C11-C12-N
9	B	3002	PC1	C22-C21-O21-C2
9	C	2012	PC1	C11-O13-P-O12
9	C	2012	PC1	C11-O13-P-O11
9	C	2012	PC1	C1-O11-P-O12
9	C	2012	PC1	C1-O11-P-O13
9	C	2012	PC1	O13-C11-C12-N
9	C	2013	PC1	O13-C11-C12-N
9	C	2014	PC1	C11-O13-P-O14
9	C	2014	PC1	O13-C11-C12-N
9	C	2015	PC1	O22-C21-O21-C2
9	C	2015	PC1	C22-C21-O21-C2
9	D	401	PC1	C22-C21-O21-C2
9	A	2014	PC1	O22-C21-O21-C2
9	B	3002	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
9	C	2013	PC1	O22-C21-O21-C2
9	D	401	PC1	O22-C21-O21-C2
9	C	2014	PC1	C32-C31-O31-C3
9	C	2015	PC1	C28-C29-C2A-C2B
9	A	2012	PC1	C28-C29-C2A-C2B
9	B	3002	PC1	C38-C39-C3A-C3B
9	A	2013	PC1	C22-C21-O21-C2
9	A	2014	PC1	C24-C25-C26-C27
9	C	2015	PC1	C38-C39-C3A-C3B
9	D	401	PC1	C28-C29-C2A-C2B
9	C	2013	PC1	C32-C31-O31-C3
9	C	2012	PC1	C38-C39-C3A-C3B
9	D	401	PC1	C38-C39-C3A-C3B
9	A	2012	PC1	O22-C21-O21-C2
9	A	2014	PC1	C32-C31-O31-C3
9	A	2013	PC1	C26-C27-C28-C29
9	C	2014	PC1	C11-C12-N-C14
9	B	3002	PC1	C24-C25-C26-C27
9	C	2013	PC1	O32-C31-O31-C3
9	C	2014	PC1	O32-C31-O31-C3
9	D	401	PC1	C21-C22-C23-C24
9	C	2014	PC1	C27-C28-C29-C2A
9	C	2013	PC1	C28-C29-C2A-C2B
9	A	2011	PC1	C21-C22-C23-C24
9	A	2012	PC1	C2-C1-O11-P
9	A	2012	PC1	C21-C22-C23-C24
9	A	2014	PC1	C26-C27-C28-C29
9	C	2012	PC1	C21-C22-C23-C24
9	C	2012	PC1	C31-C32-C33-C34
9	C	2015	PC1	C21-C22-C23-C24
9	C	2014	PC1	C21-C22-C23-C24
9	A	2011	PC1	O22-C21-O21-C2
9	A	2013	PC1	O22-C21-O21-C2
9	C	2012	PC1	O22-C21-O21-C2
9	A	2011	PC1	C32-C31-O31-C3
9	C	2013	PC1	C11-C12-N-C15
9	B	3002	PC1	C31-C32-C33-C34
9	C	2012	PC1	C32-C31-O31-C3
9	C	2013	PC1	C22-C21-O21-C2
8	A	2010	CLR	C16-C17-C20-C21
9	A	2013	PC1	C38-C39-C3A-C3B
9	D	401	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
9	A	2013	PC1	C32-C31-O31-C3
10	D	402	NAG	O5-C5-C6-O6
9	B	3002	PC1	C3E-C3F-C3G-C3H
9	C	2012	PC1	C39-C3A-C3B-C3C
9	C	2013	PC1	C2A-C2B-C2C-C2D
9	A	2013	PC1	C3C-C3D-C3E-C3F
9	A	2014	PC1	C29-C2A-C2B-C2C
9	A	2014	PC1	C3D-C3E-C3F-C3G
9	A	2011	PC1	C24-C25-C26-C27
9	C	2013	PC1	C24-C25-C26-C27
9	C	2014	PC1	C22-C23-C24-C25
9	A	2014	PC1	C2D-C2E-C2F-C2G
9	C	2014	PC1	C29-C2A-C2B-C2C
9	A	2013	PC1	C36-C37-C38-C39
9	B	3002	PC1	C39-C3A-C3B-C3C
9	C	2012	PC1	C26-C27-C28-C29
9	B	3002	PC1	C21-C22-C23-C24
9	C	2015	PC1	C23-C24-C25-C26
9	C	2015	PC1	C27-C28-C29-C2A
9	D	401	PC1	C26-C27-C28-C29
9	A	2014	PC1	C2B-C2C-C2D-C2E
9	A	2011	PC1	C27-C28-C29-C2A
9	C	2014	PC1	C35-C36-C37-C38
9	C	2015	PC1	C24-C25-C26-C27
9	A	2013	PC1	C2B-C2C-C2D-C2E
9	A	2014	PC1	C27-C28-C29-C2A
9	B	3002	PC1	C28-C29-C2A-C2B
9	B	3002	PC1	C33-C34-C35-C36
9	C	2012	PC1	C36-C37-C38-C39
9	D	401	PC1	C25-C26-C27-C28
9	C	2014	PC1	C11-C12-N-C13
9	A	2013	PC1	C37-C38-C39-C3A
9	C	2012	PC1	C35-C36-C37-C38
9	C	2014	PC1	C34-C35-C36-C37
9	C	2015	PC1	C36-C37-C38-C39
9	A	2013	PC1	C24-C25-C26-C27
9	A	2013	PC1	C3B-C3C-C3D-C3E
9	A	2014	PC1	C36-C37-C38-C39
9	D	401	PC1	C23-C24-C25-C26
9	A	2013	PC1	C32-C33-C34-C35
9	C	2014	PC1	C28-C29-C2A-C2B
9	D	401	PC1	C2B-C2C-C2D-C2E

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Mol	Chain	Res	Type	Atoms
9	C	2014	PC1	C24-C25-C26-C27
9	B	3002	PC1	C32-C33-C34-C35
9	A	2012	PC1	C2D-C2E-C2F-C2G
9	A	2013	PC1	C27-C28-C29-C2A
9	A	2011	PC1	C3A-C3B-C3C-C3D
9	C	2012	PC1	C2A-C2B-C2C-C2D
9	C	2015	PC1	C34-C35-C36-C37
9	A	2014	PC1	C21-C22-C23-C24
9	A	2014	PC1	C23-C24-C25-C26
9	C	2013	PC1	C34-C35-C36-C37
9	A	2013	PC1	C34-C35-C36-C37
9	C	2012	PC1	C29-C2A-C2B-C2C
9	D	401	PC1	C27-C28-C29-C2A
9	C	2015	PC1	C32-C31-O31-C3
9	A	2011	PC1	C22-C21-O21-C2
9	C	2012	PC1	C22-C21-O21-C2
9	A	2011	PC1	C36-C37-C38-C39
9	C	2014	PC1	C3B-C3C-C3D-C3E
9	C	2012	PC1	C3A-C3B-C3C-C3D
6	A	2004	ADP	O4'-C4'-C5'-O5'
9	B	3002	PC1	C23-C24-C25-C26
9	C	2012	PC1	C34-C35-C36-C37
9	C	2014	PC1	C3C-C3D-C3E-C3F
9	C	2014	PC1	C11-C12-N-C15
9	A	2013	PC1	C29-C2A-C2B-C2C
9	A	2013	PC1	C2C-C2D-C2E-C2F
9	B	3002	PC1	C34-C35-C36-C37
9	B	3002	PC1	C2D-C2E-C2F-C2G
9	C	2013	PC1	O11-C1-C2-O21
9	C	2015	PC1	C3C-C3D-C3E-C3F
9	D	401	PC1	C3B-C3C-C3D-C3E
9	A	2012	PC1	C22-C23-C24-C25
9	B	3002	PC1	C35-C36-C37-C38
9	C	2012	PC1	C23-C24-C25-C26
9	A	2013	PC1	C21-C22-C23-C24
9	A	2012	PC1	C26-C27-C28-C29
9	D	401	PC1	C2E-C2F-C2G-C2H
9	A	2013	PC1	C23-C24-C25-C26
9	B	3002	PC1	O32-C31-O31-C3
9	B	3002	PC1	C27-C28-C29-C2A
9	C	2014	PC1	C26-C27-C28-C29
9	C	2013	PC1	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
9	C	2014	PC1	C2B-C2C-C2D-C2E
9	A	2014	PC1	O32-C31-O31-C3
9	C	2015	PC1	O32-C31-O31-C3
9	C	2012	PC1	C2D-C2E-C2F-C2G
9	A	2013	PC1	C11-C12-N-C15
9	A	2012	PC1	C33-C34-C35-C36
9	B	3002	PC1	O11-C1-C2-C3
9	C	2013	PC1	O11-C1-C2-C3
9	C	2014	PC1	O11-C1-C2-C3
9	A	2014	PC1	C35-C36-C37-C38
9	C	2013	PC1	C2B-C2C-C2D-C2E
9	C	2013	PC1	C1-C2-C3-O31
9	D	401	PC1	C2C-C2D-C2E-C2F
9	C	2013	PC1	C25-C26-C27-C28
9	C	2014	PC1	C3A-C3B-C3C-C3D
9	C	2012	PC1	C2B-C2C-C2D-C2E
9	C	2013	PC1	C11-C12-N-C14
9	C	2014	PC1	C31-C32-C33-C34
9	C	2014	PC1	C38-C39-C3A-C3B
9	A	2014	PC1	C3B-C3C-C3D-C3E
9	B	3002	PC1	C3C-C3D-C3E-C3F
9	C	2015	PC1	C37-C38-C39-C3A
8	A	2010	CLR	C13-C17-C20-C21
9	A	2012	PC1	C3-C2-O21-C21
9	C	2013	PC1	C3C-C3D-C3E-C3F
9	C	2015	PC1	C32-C33-C34-C35
9	D	401	PC1	C35-C36-C37-C38
9	C	2014	PC1	C3F-C3G-C3H-C3I
6	A	2004	ADP	C3'-C4'-C5'-O5'
9	C	2015	PC1	C2B-C2C-C2D-C2E
9	A	2011	PC1	C29-C2A-C2B-C2C
9	A	2014	PC1	C33-C34-C35-C36
9	A	2012	PC1	C29-C2A-C2B-C2C
9	B	3002	PC1	C26-C27-C28-C29
9	A	2014	PC1	C34-C35-C36-C37
9	C	2013	PC1	C3E-C3F-C3G-C3H
9	A	2012	PC1	C2C-C2D-C2E-C2F
9	C	2012	PC1	C3D-C3E-C3F-C3G
9	C	2013	PC1	C39-C3A-C3B-C3C
9	C	2014	PC1	C39-C3A-C3B-C3C
9	C	2013	PC1	C2C-C2D-C2E-C2F
9	A	2012	PC1	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
9	A	2013	PC1	C22-C23-C24-C25
9	A	2011	PC1	C2F-C2G-C2H-C2I
9	C	2014	PC1	C23-C24-C25-C26
9	C	2015	PC1	C3A-C3B-C3C-C3D
9	A	2011	PC1	C37-C38-C39-C3A
9	A	2013	PC1	C2F-C2G-C2H-C2I
9	A	2014	PC1	C3A-C3B-C3C-C3D
9	D	401	PC1	C32-C33-C34-C35
9	A	2011	PC1	C26-C27-C28-C29
9	D	401	PC1	C1-C2-C3-O31
9	D	401	PC1	C31-C32-C33-C34
9	A	2012	PC1	C34-C35-C36-C37
9	B	3002	PC1	O11-C1-C2-O21
9	C	2014	PC1	O11-C1-C2-O21
9	A	2013	PC1	C2D-C2E-C2F-C2G
9	D	401	PC1	C29-C2A-C2B-C2C
9	A	2011	PC1	C39-C3A-C3B-C3C
8	C	2010	CLR	C23-C24-C25-C27
9	D	401	PC1	O21-C21-C22-C23
9	C	2013	PC1	O21-C2-C3-O31
9	D	401	PC1	C3A-C3B-C3C-C3D
9	C	2013	PC1	C3B-C3C-C3D-C3E
9	B	3002	PC1	C2B-C2C-C2D-C2E
9	A	2011	PC1	C34-C35-C36-C37
9	D	401	PC1	C39-C3A-C3B-C3C
9	D	401	PC1	C34-C35-C36-C37
6	C	2004	ADP	PB-O3A-PA-O5'
9	A	2011	PC1	C2A-C2B-C2C-C2D
9	D	401	PC1	C3C-C3D-C3E-C3F
9	A	2013	PC1	C35-C36-C37-C38
9	C	2012	PC1	C3C-C3D-C3E-C3F
9	C	2013	PC1	C36-C37-C38-C39
9	A	2012	PC1	O11-C1-C2-C3
9	A	2014	PC1	O11-C1-C2-C3
9	C	2015	PC1	O11-C1-C2-C3
9	A	2012	PC1	C3E-C3F-C3G-C3H
9	C	2014	PC1	C2D-C2E-C2F-C2G
9	A	2012	PC1	C3A-C3B-C3C-C3D
9	A	2012	PC1	C35-C36-C37-C38
9	A	2014	PC1	C38-C39-C3A-C3B
9	C	2013	PC1	C3-C2-O21-C21
9	A	2011	PC1	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
9	A	2011	PC1	C38-C39-C3A-C3B
9	C	2014	PC1	C3D-C3E-C3F-C3G
9	A	2012	PC1	O11-C1-C2-O21
9	A	2014	PC1	O11-C1-C2-O21
9	C	2015	PC1	O11-C1-C2-O21
9	C	2014	PC1	C2C-C2D-C2E-C2F
9	A	2012	PC1	O32-C31-O31-C3
9	B	3002	PC1	C12-C11-O13-P
9	C	2012	PC1	C3E-C3F-C3G-C3H
9	A	2011	PC1	C2D-C2E-C2F-C2G
9	D	401	PC1	C2A-C2B-C2C-C2D
9	C	2014	PC1	C25-C26-C27-C28
9	A	2014	PC1	C3F-C3G-C3H-C3I
9	A	2013	PC1	O13-C11-C12-N
9	C	2013	PC1	C11-C12-N-C13
9	A	2013	PC1	C3A-C3B-C3C-C3D
9	B	3002	PC1	C3D-C3E-C3F-C3G
9	D	401	PC1	C24-C25-C26-C27
9	B	3002	PC1	C2A-C2B-C2C-C2D
9	B	3002	PC1	C2C-C2D-C2E-C2F
9	A	2014	PC1	C31-C32-C33-C34
9	B	3002	PC1	C3F-C3G-C3H-C3I
9	C	2013	PC1	C3F-C3G-C3H-C3I
9	D	401	PC1	O21-C2-C3-O31
9	D	401	PC1	C3D-C3E-C3F-C3G
9	B	3002	PC1	C37-C38-C39-C3A
6	A	2004	ADP	C5'-O5'-PA-O1A
9	B	3002	PC1	C1-O11-P-O13
9	C	2015	PC1	C1-O11-P-O14
9	D	401	PC1	C1-O11-P-O12
9	A	2013	PC1	C2A-C2B-C2C-C2D
9	C	2014	PC1	C36-C37-C38-C39
9	A	2011	PC1	C11-C12-N-C13
9	A	2011	PC1	C23-C24-C25-C26
9	A	2013	PC1	O32-C31-O31-C3
9	D	401	PC1	C3F-C3G-C3H-C3I
9	A	2014	PC1	C3C-C3D-C3E-C3F
9	A	2012	PC1	C3B-C3C-C3D-C3E
9	A	2014	PC1	C32-C33-C34-C35
9	A	2012	PC1	C2F-C2G-C2H-C2I
9	C	2013	PC1	C2-C1-O11-P
9	B	3002	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
9	D	401	PC1	C36-C37-C38-C39
9	C	2012	PC1	C28-C29-C2A-C2B
9	C	2013	PC1	C2D-C2E-C2F-C2G
9	C	2015	PC1	C33-C34-C35-C36
9	C	2014	PC1	C32-C33-C34-C35
9	C	2015	PC1	C25-C26-C27-C28
9	A	2014	PC1	C3E-C3F-C3G-C3H
9	A	2011	PC1	C32-C33-C34-C35
9	A	2013	PC1	C11-C12-N-C14
9	A	2013	PC1	C3D-C3E-C3F-C3G
9	A	2012	PC1	O31-C31-C32-C33
9	A	2013	PC1	C1-C2-C3-O31
10	B	3003	NAG	O5-C5-C6-O6
9	A	2011	PC1	O11-C1-C2-C3
9	C	2013	PC1	C33-C34-C35-C36
9	A	2012	PC1	C38-C39-C3A-C3B
9	C	2013	PC1	C22-C23-C24-C25
9	C	2012	PC1	O32-C31-O31-C3
9	C	2014	PC1	C3E-C3F-C3G-C3H
9	C	2015	PC1	C3D-C3E-C3F-C3G
9	C	2014	PC1	C2F-C2G-C2H-C2I
9	A	2012	PC1	C27-C28-C29-C2A
9	D	401	PC1	C22-C23-C24-C25
9	A	2012	PC1	C11-C12-N-C13
9	D	401	PC1	C11-C12-N-C13
9	A	2012	PC1	C2B-C2C-C2D-C2E
9	A	2014	PC1	O21-C21-C22-C23
9	C	2013	PC1	O21-C21-C22-C23
9	A	2014	PC1	O22-C21-C22-C23
9	A	2013	PC1	C25-C26-C27-C28
9	A	2013	PC1	C11-C12-N-C13
9	C	2014	PC1	C33-C34-C35-C36
9	A	2012	PC1	C24-C25-C26-C27
9	C	2015	PC1	O22-C21-C22-C23
9	A	2012	PC1	O32-C31-C32-C33
9	A	2014	PC1	O31-C31-C32-C33

There are no ring outliers.

19 monomers are involved in 80 short contacts:

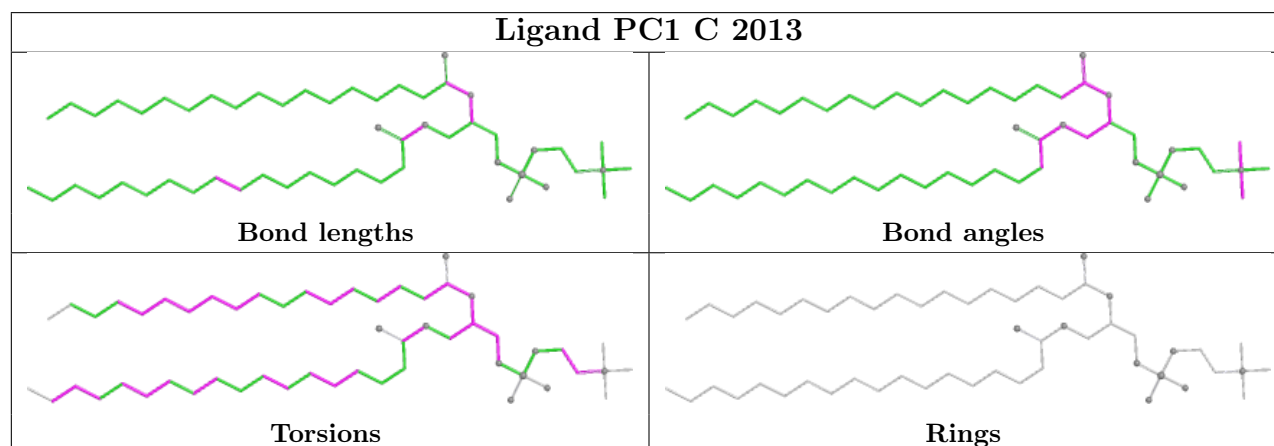
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2013	PC1	3	0

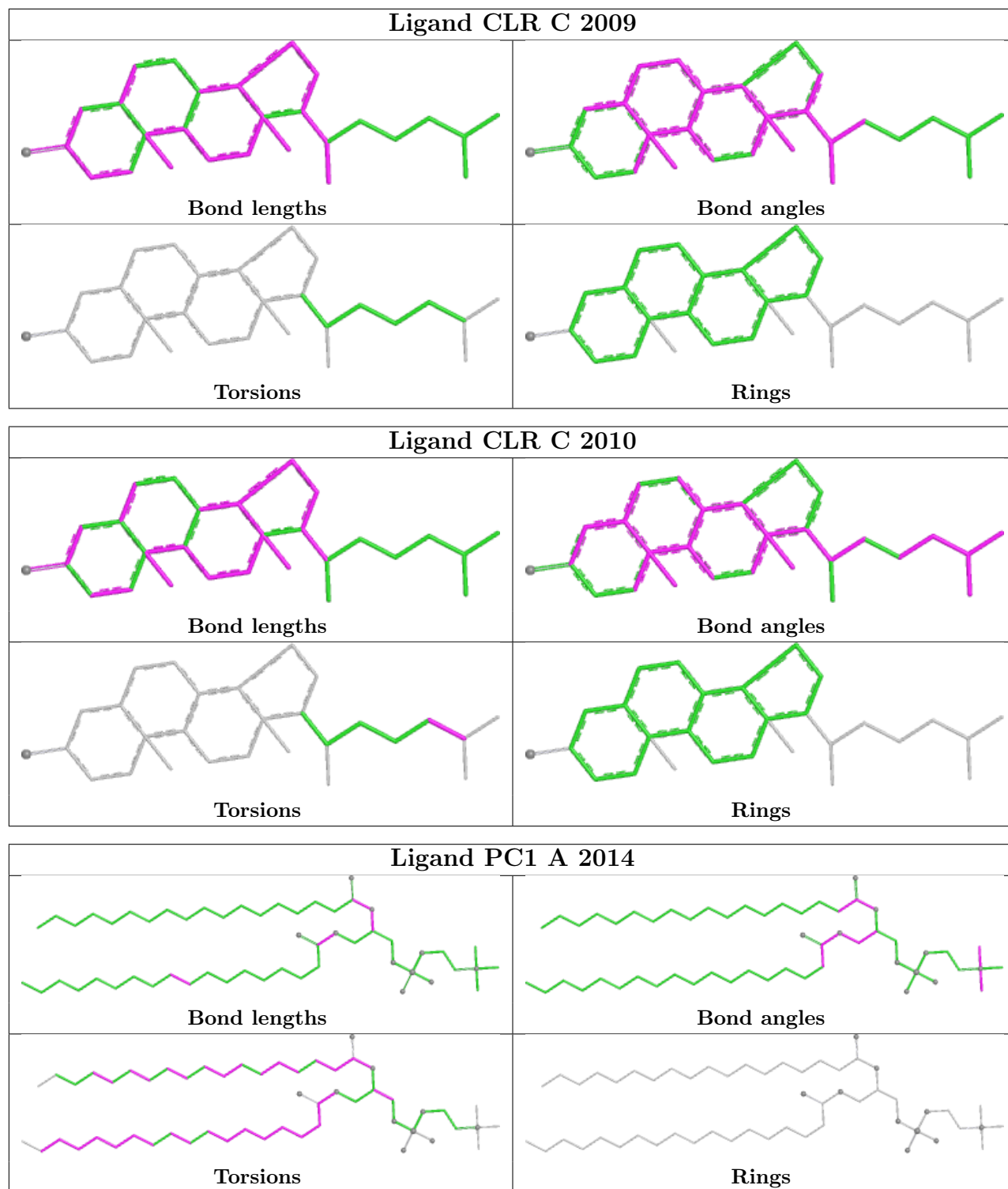
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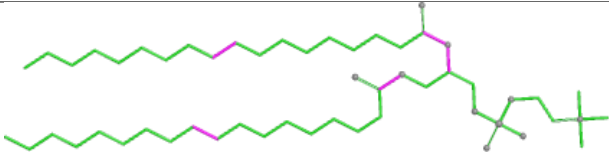
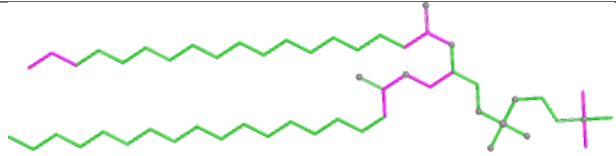
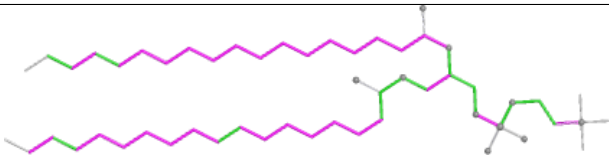
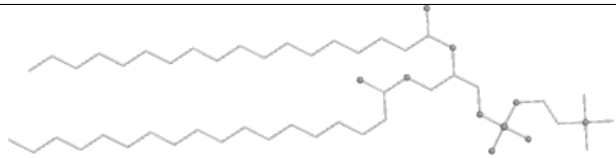
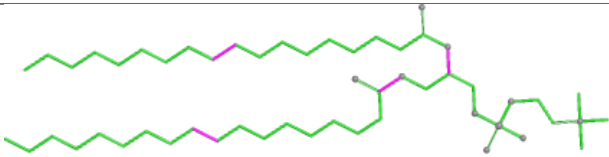
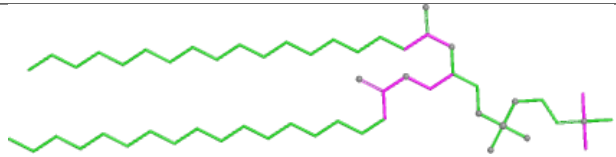
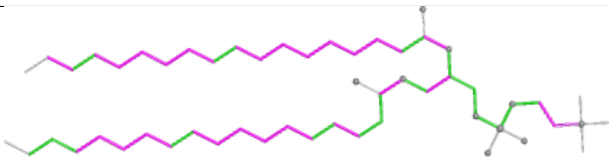
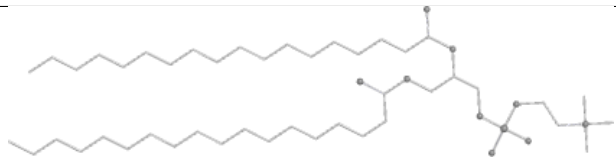
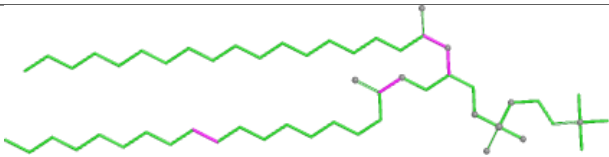
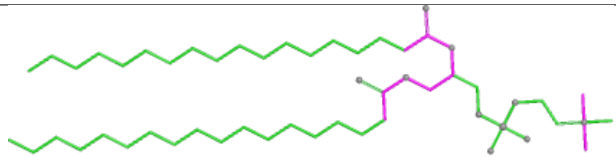
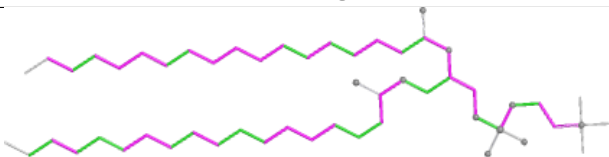
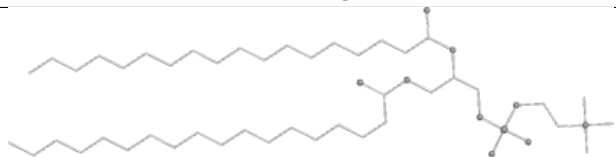
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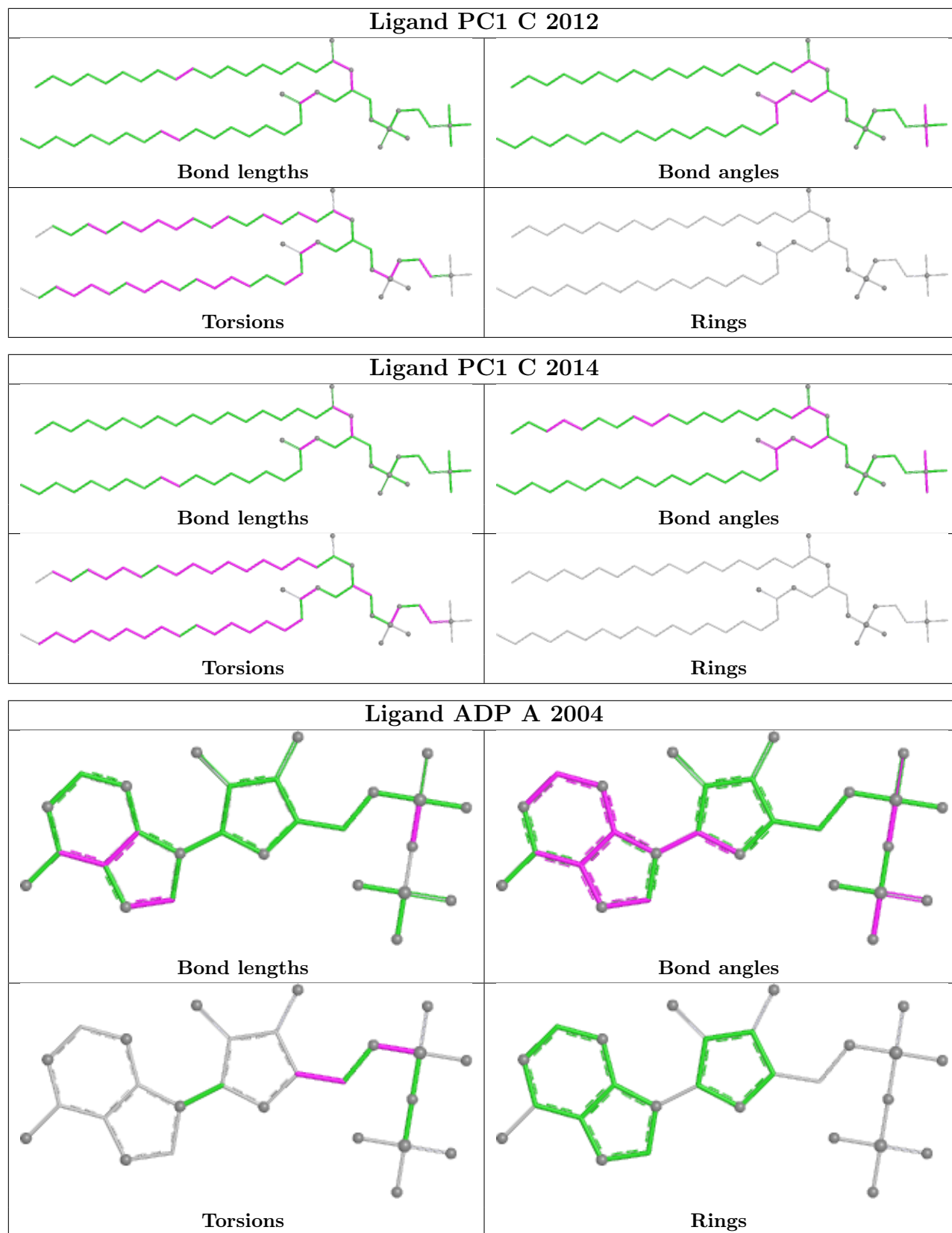
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2002	ALF	2	0
8	C	2009	CLR	4	0
8	C	2010	CLR	12	0
9	A	2014	PC1	4	0
9	D	401	PC1	3	0
9	A	2013	PC1	3	0
9	A	2012	PC1	4	0
9	C	2012	PC1	3	0
9	C	2014	PC1	11	0
5	A	2002	ALF	1	0
6	A	2004	ADP	5	0
8	B	3001	CLR	4	0
9	C	2015	PC1	6	0
6	C	2004	ADP	6	0
9	A	2011	PC1	4	0
8	A	2010	CLR	8	0
8	C	2011	CLR	7	0
8	A	2009	CLR	4	0

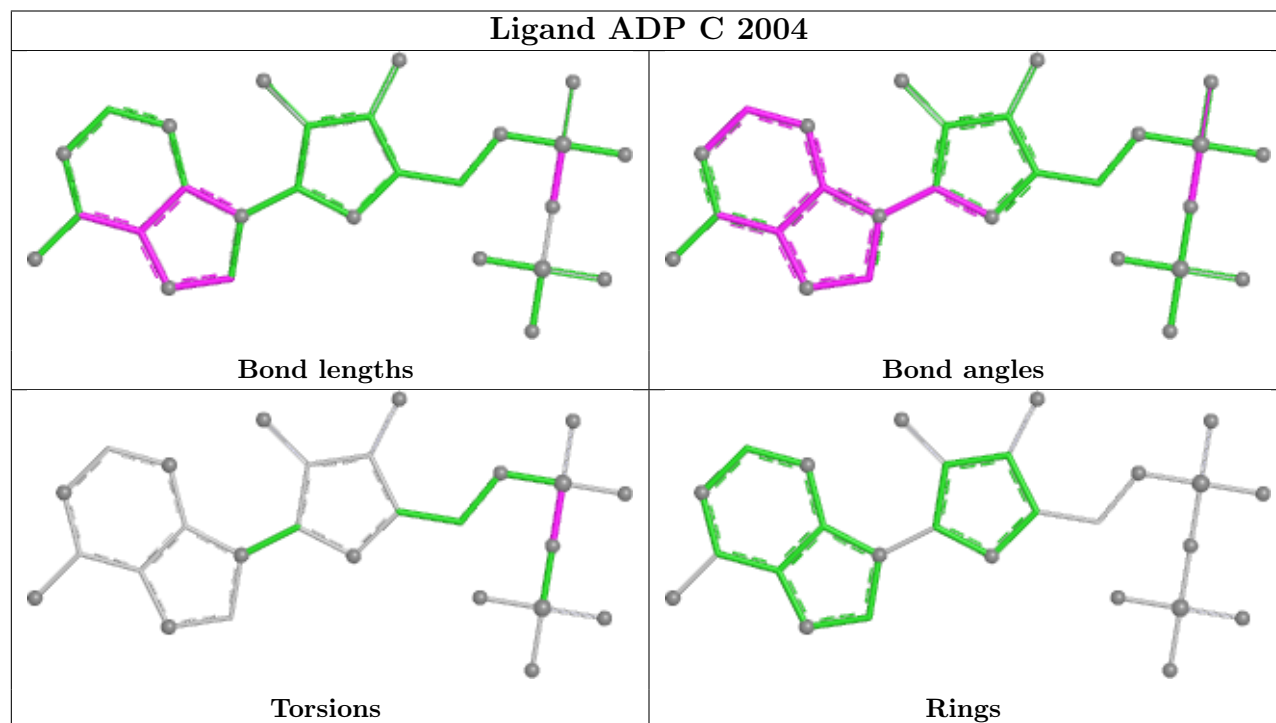
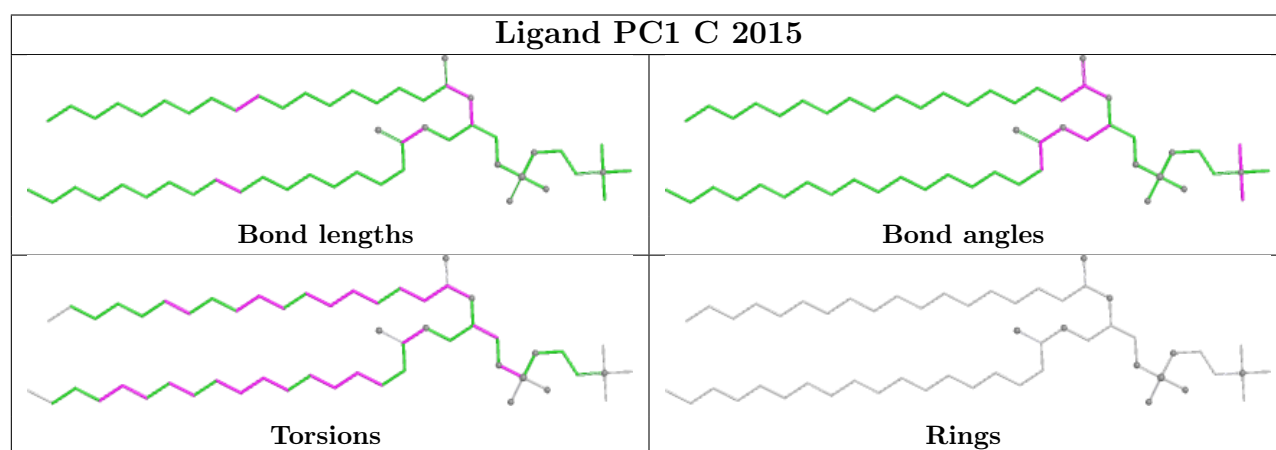
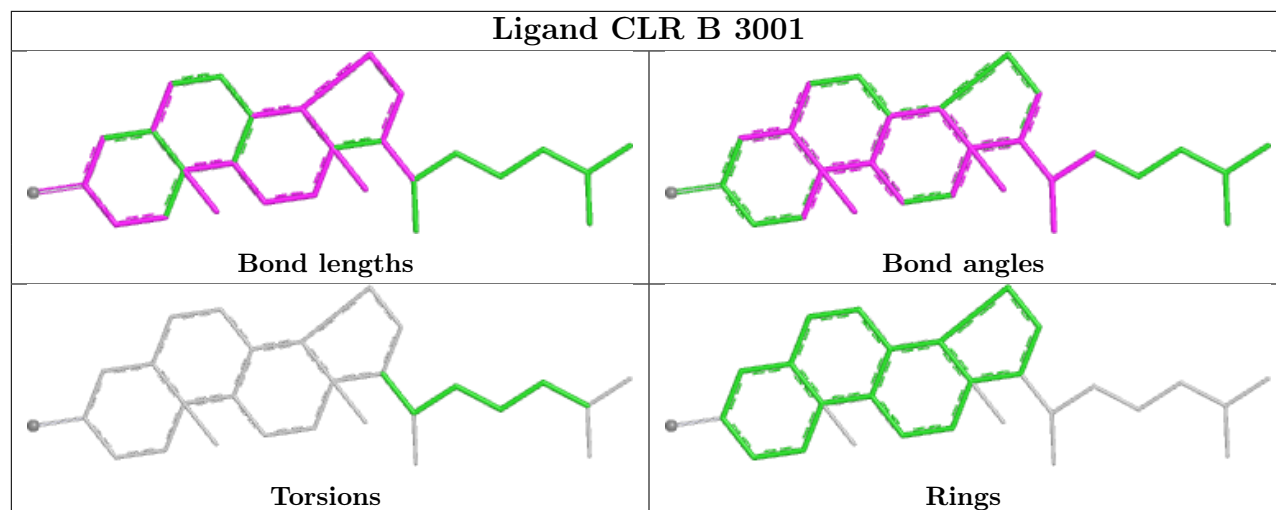
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

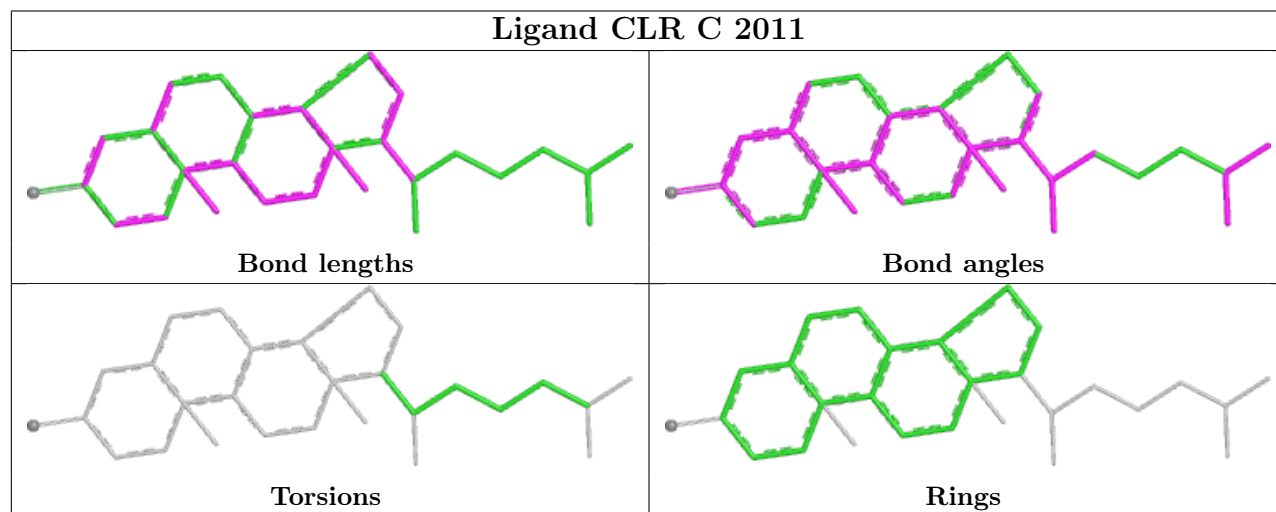
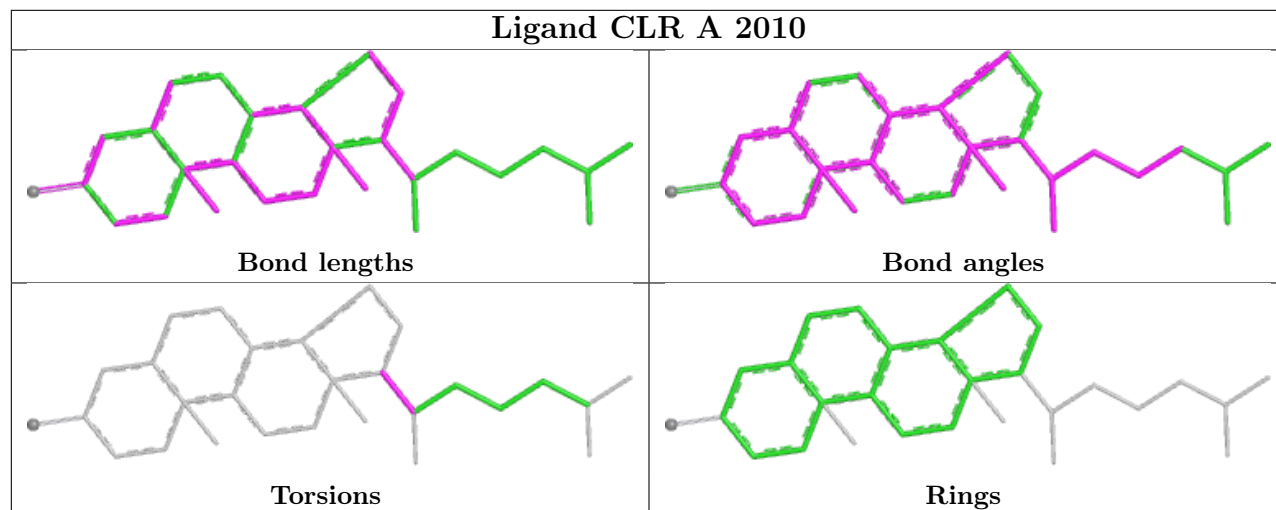
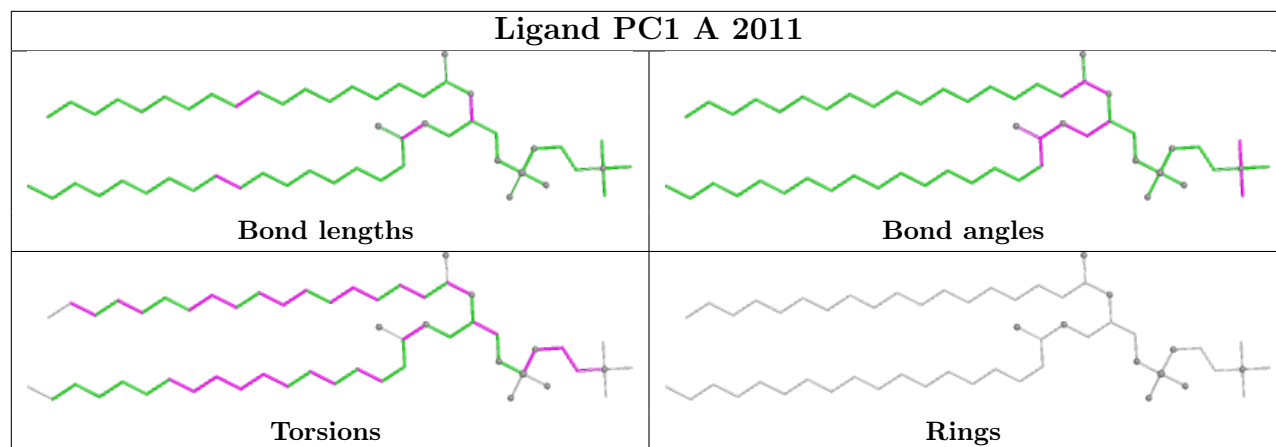


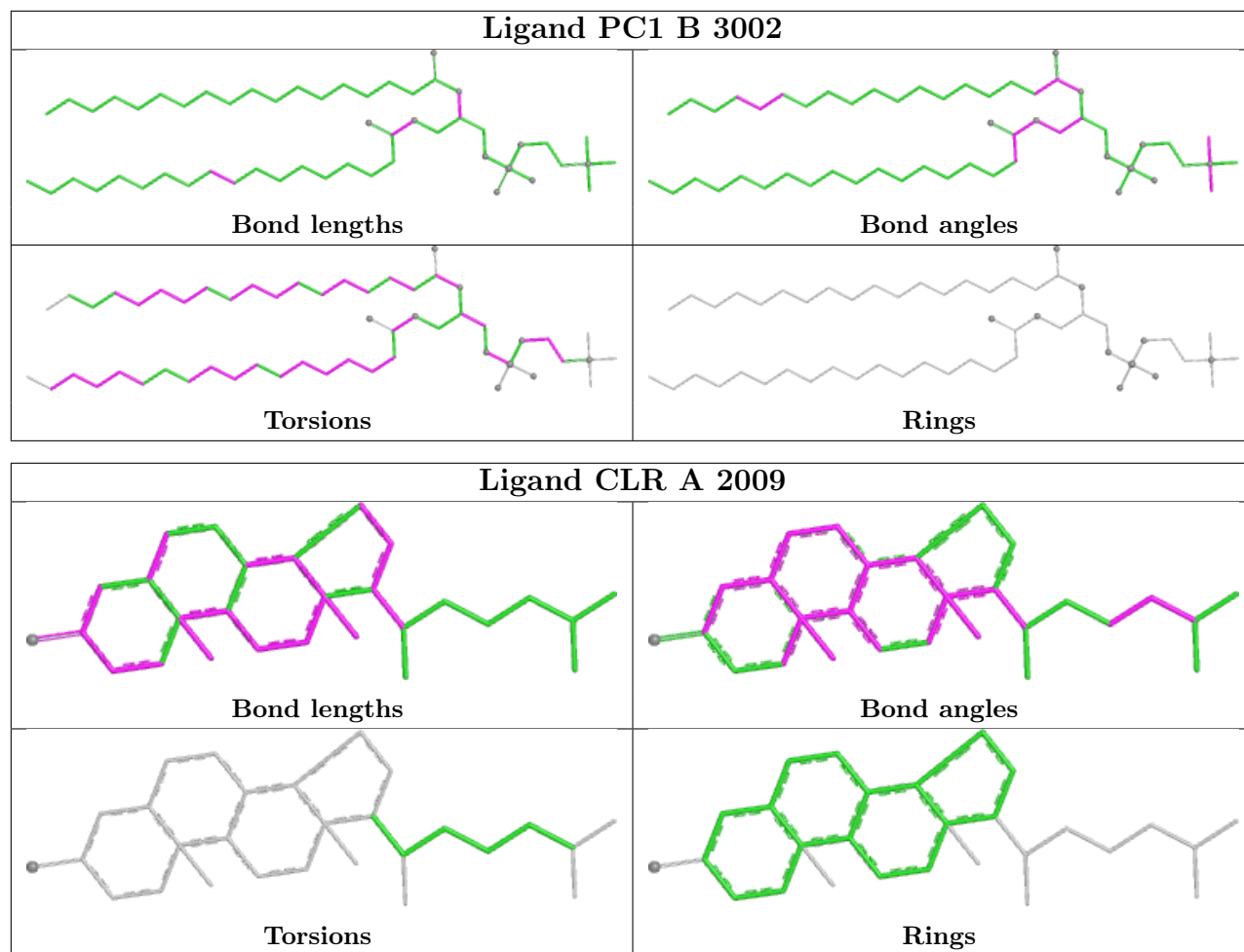


Ligand PC1 D 401	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 2013	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 2012	
 Bond lengths	 Bond angles
 Torsions	 Rings









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%)	-0.51	11 (1%)	78 70	25, 73, 140, 201	0
1	C	994/1016 (97%)	-0.31	20 (2%)	65 56	47, 84, 159, 204	0
2	B	303/303 (100%)	0.35	20 (6%)	24 18	71, 147, 222, 240	0
2	D	303/303 (100%)	0.34	29 (9%)	13 10	71, 136, 214, 240	0
3	E	35/65 (53%)	0.01	2 (5%)	29 22	76, 95, 189, 199	0
3	G	34/65 (52%)	-0.06	3 (8%)	15 11	78, 101, 174, 199	0
All	All	2663/2768 (96%)	-0.23	85 (3%)	50 40	25, 89, 176, 240	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	167	TYR	6.2
2	D	16	ILE	5.6
1	C	396	THR	5.4
2	D	166	THR	4.8
1	C	267	ALA	4.7
2	D	218	ASP	4.6
2	D	266	LEU	4.6
1	C	395	THR	4.5
1	C	398	ASN	4.5
2	D	196	LEU	4.4
3	E	16	VAL	4.3
1	A	270	LEU	4.1
3	G	16	VAL	4.1
2	B	266	LEU	4.0
1	A	401	GLY	4.0
2	B	201	VAL	4.0
2	B	1	MET	3.9
2	D	273	ARG	3.7
1	C	402	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	2	ALA	3.7
1	C	28	LEU	3.6
2	D	201	VAL	3.6
1	A	268	SER	3.5
1	C	266	LEU	3.5
2	B	15	PHE	3.4
2	B	202	MET	3.3
2	D	23	GLU	3.2
1	A	78	THR	3.2
2	B	167	TYR	3.2
2	D	9	GLU	3.2
1	A	272	GLY	3.2
1	A	395	THR	3.2
2	D	217	ARG	3.2
1	A	267	ALA	3.2
2	D	198	THR	3.1
2	D	15	PHE	3.0
2	D	7	LYS	3.0
2	B	166	THR	3.0
1	C	121	ASP	2.9
2	D	202	MET	2.8
1	A	108	TYR	2.8
2	D	17	TRP	2.8
2	D	193	ASN	2.8
2	D	232	LEU	2.7
1	C	648	VAL	2.7
1	C	265	THR	2.7
2	D	195	SER	2.6
1	C	495	ARG	2.6
1	A	266	LEU	2.6
2	B	23	GLU	2.6
2	B	217	ARG	2.5
2	D	89	SER	2.5
1	C	268	SER	2.5
1	C	270	LEU	2.5
2	D	6	ALA	2.4
2	B	218	ASP	2.4
3	G	15	ASP	2.4
2	B	192	LYS	2.4
2	B	196	LEU	2.4
2	B	7	LYS	2.4
1	C	111	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	222	GLU	2.3
2	D	73	ALA	2.3
1	C	80	PRO	2.3
2	D	11	SER	2.3
1	C	77	PRO	2.3
2	B	16	ILE	2.2
2	D	161	GLY	2.2
2	B	6	ALA	2.2
2	D	10	GLY	2.2
2	B	25	LEU	2.2
1	C	393	ALA	2.2
2	D	219	GLU	2.2
2	D	262	GLN	2.2
1	A	312	GLU	2.2
2	D	197	GLU	2.2
3	G	19	PHE	2.1
1	A	400	SER	2.1
1	C	105	PHE	2.1
1	C	119	GLN	2.1
2	D	222	GLU	2.1
3	E	18	PRO	2.0
2	B	260	ALA	2.0
2	B	223	LYS	2.0
1	C	78	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

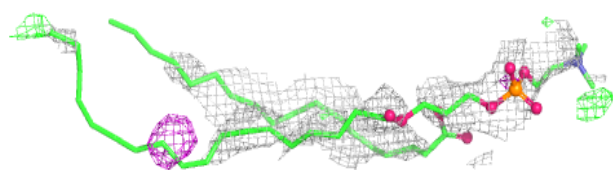
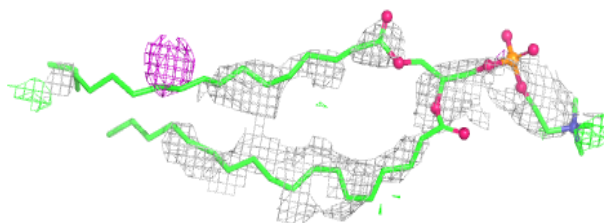
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	NAG	B	3003	14/15	0.51	0.14	145,151,160,164	0
9	PC1	A	2014	54/54	0.70	0.17	105,138,172,233	0
9	PC1	C	2015	54/54	0.71	0.16	119,145,185,228	0
7	NA	A	2007	1/1	0.76	0.12	127,127,127,127	0
7	NA	A	2008	1/1	0.78	0.13	100,100,100,100	0
9	PC1	C	2014	54/54	0.78	0.19	93,138,188,199	0
9	PC1	A	2013	54/54	0.80	0.18	88,124,142,168	0
9	PC1	A	2012	54/54	0.80	0.17	70,138,173,177	0
9	PC1	B	3002	54/54	0.80	0.15	76,116,145,193	0
10	NAG	D	402	14/15	0.81	0.12	114,138,143,143	0
9	PC1	C	2013	54/54	0.82	0.15	76,124,159,196	0
9	PC1	D	401	54/54	0.82	0.12	68,94,169,191	0
7	NA	A	2006	1/1	0.83	0.10	86,86,86,86	0
8	CLR	A	2009	28/28	0.83	0.17	115,125,157,163	0
8	CLR	A	2010	28/28	0.86	0.10	91,115,123,156	0
7	NA	C	2006	1/1	0.87	0.07	113,113,113,113	0
9	PC1	C	2012	54/54	0.87	0.13	93,118,156,159	0
8	CLR	C	2011	28/28	0.88	0.10	45,98,125,139	0
8	CLR	C	2010	28/28	0.88	0.12	42,104,166,180	0
8	CLR	B	3001	28/28	0.89	0.11	55,124,129,156	0
9	PC1	A	2011	54/54	0.92	0.13	81,119,150,155	0
7	NA	C	2008	1/1	0.92	0.08	62,62,62,62	0
7	NA	C	2007	1/1	0.93	0.21	179,179,179,179	0
8	CLR	C	2009	28/28	0.93	0.10	56,113,136,137	0
4	MG	A	2001	1/1	0.95	0.12	67,67,67,67	0
4	MG	C	2001	1/1	0.95	0.09	96,96,96,96	0
7	NA	A	2005	1/1	0.96	0.04	159,159,159,159	0
7	NA	C	2005	1/1	0.97	0.04	84,84,84,84	0
6	ADP	C	2004	27/27	0.97	0.06	8,62,69,86	0
5	ALF	C	2002	5/5	0.98	0.06	38,48,56,67	0
5	ALF	A	2002	5/5	0.99	0.07	9,16,42,141	0
4	MG	A	2003	1/1	0.99	0.06	24,24,24,24	0
6	ADP	A	2004	27/27	0.99	0.04	6,35,51,60	0
4	MG	C	2003	1/1	1.00	0.05	48,48,48,48	0

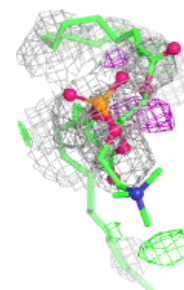
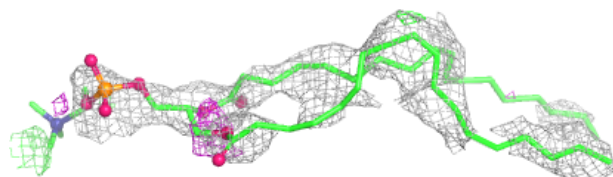
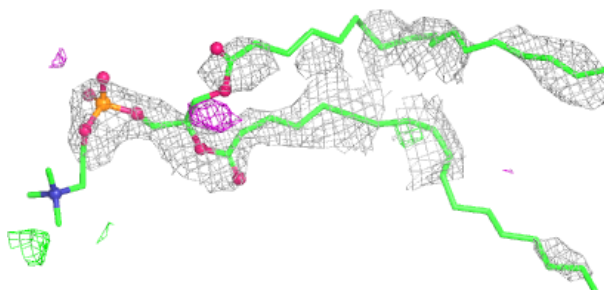
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

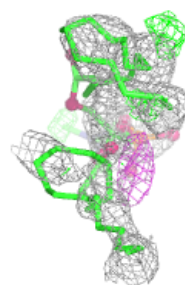
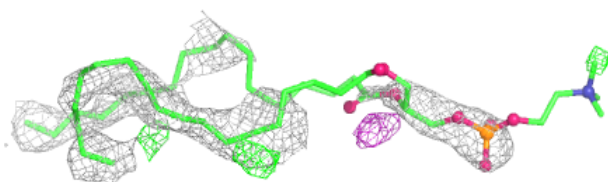
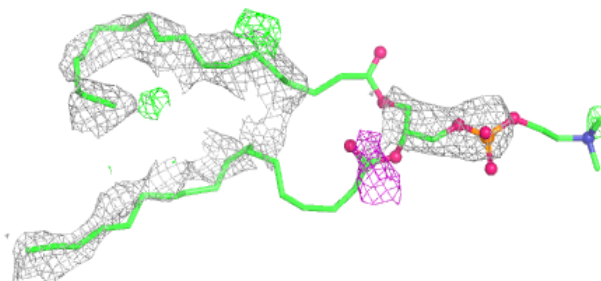
**Electron density around PC1 C 2015:**

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

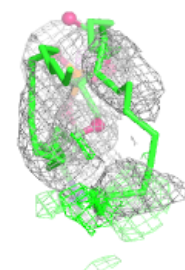
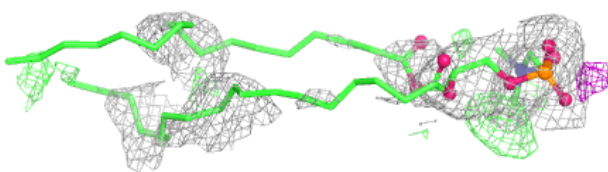
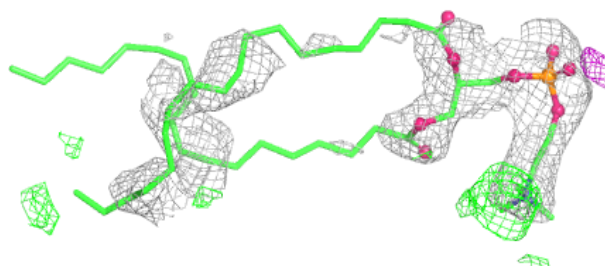


Electron density around PC1 C 2014:

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

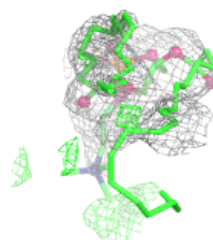
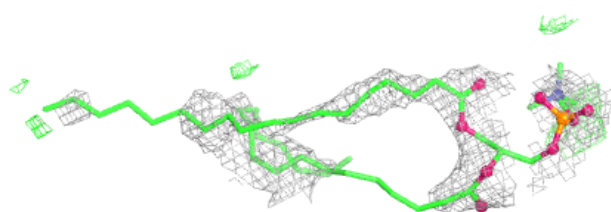
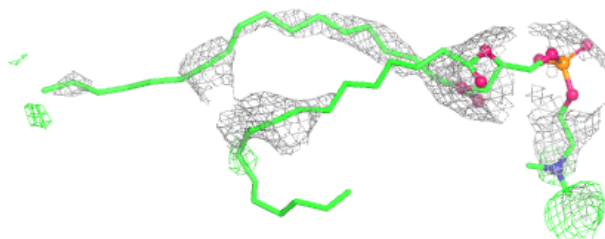
**Electron density around PC1 A 2013:**

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

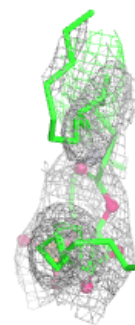
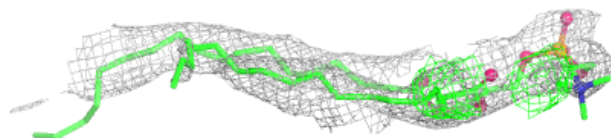
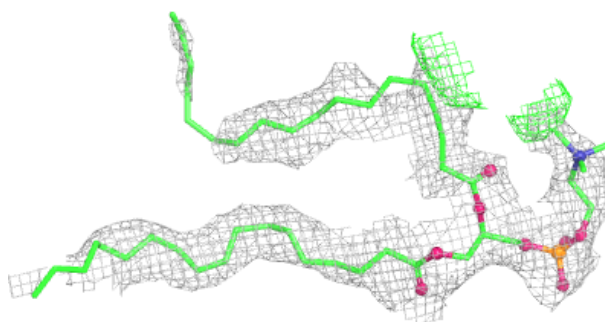


Electron density around PC1 A 2012:

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

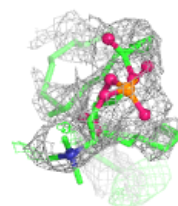
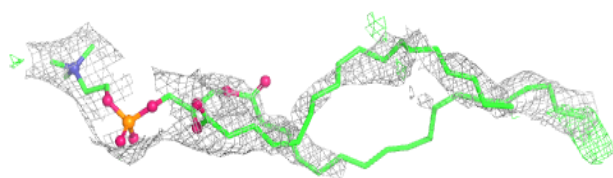
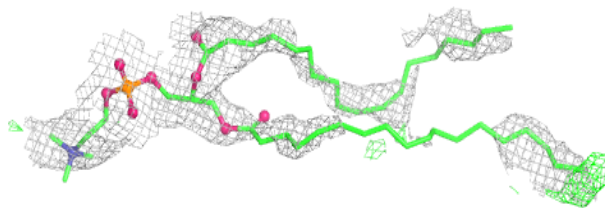
**Electron density around PC1 B 3002:**

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

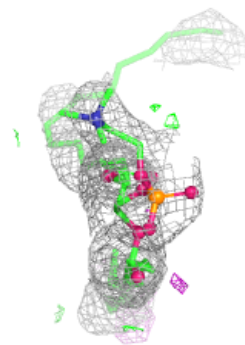
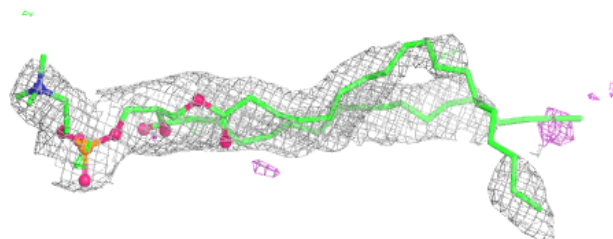
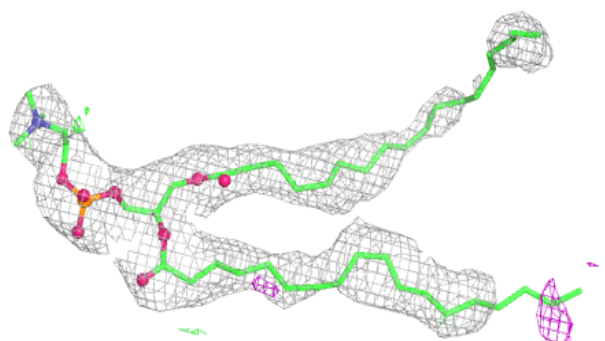


Electron density around PC1 C 2013:

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

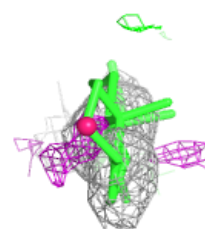
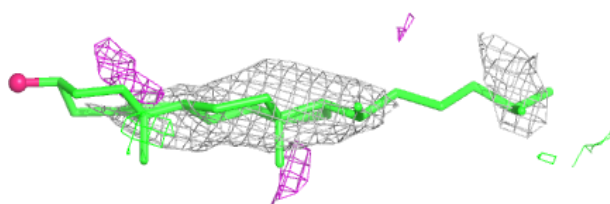
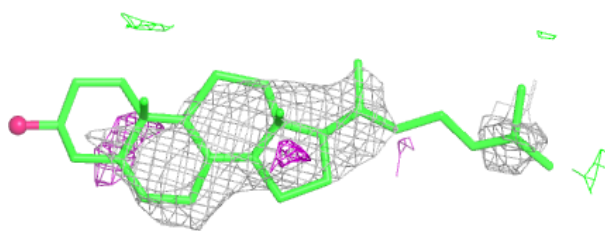
**Electron density around PC1 D 401:**

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

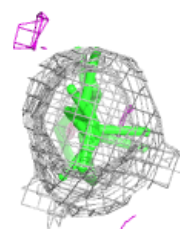
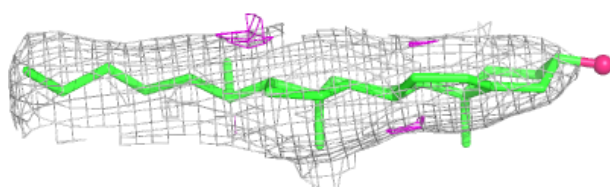
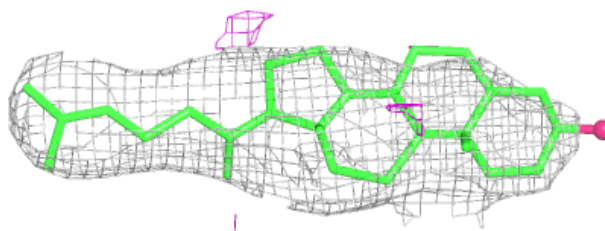


Electron density around CLR A 2009:

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

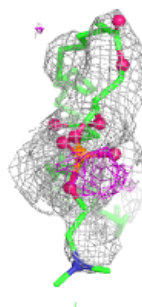
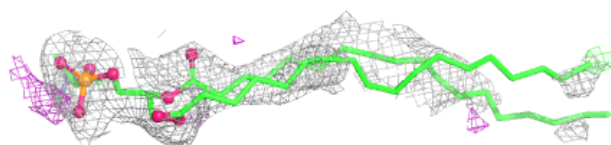
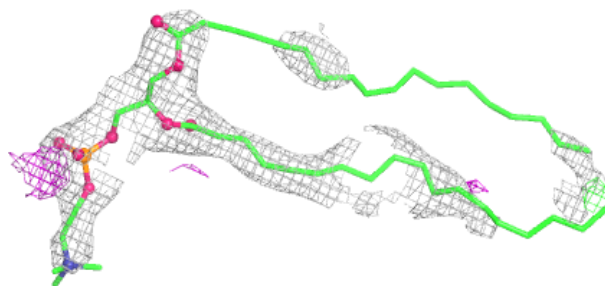
**Electron density around CLR A 2010:**

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

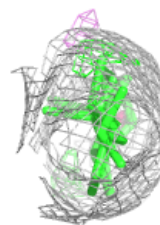
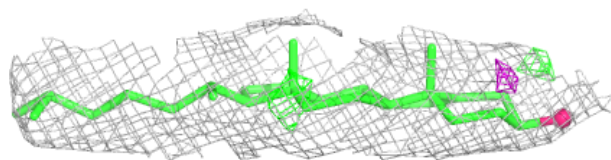
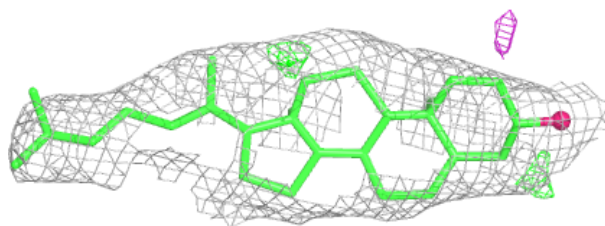


Electron density around PC1 C 2012:

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

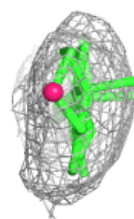
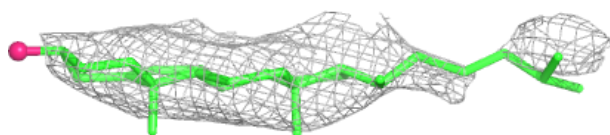
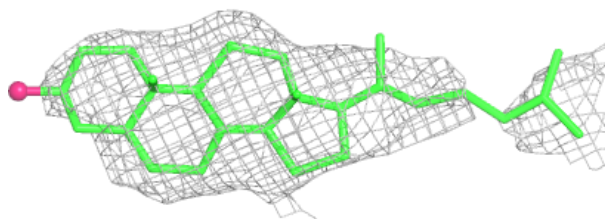
**Electron density around CLR C 2011:**

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

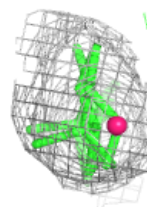
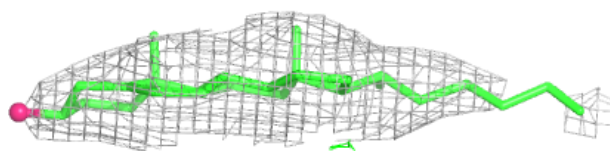


Electron density around CLR C 2010:

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

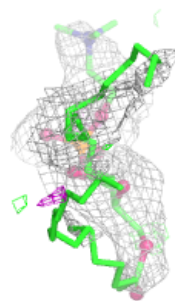
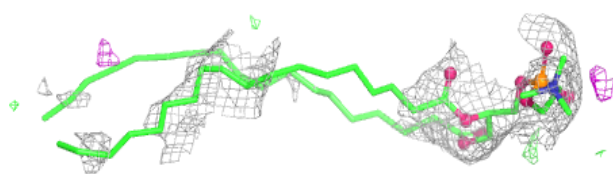
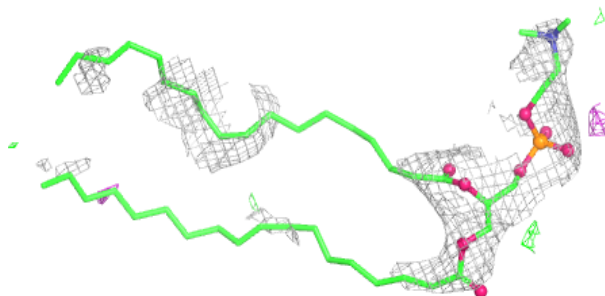
**Electron density around CLR B 3001:**

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

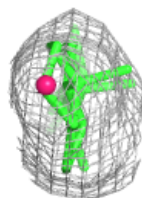
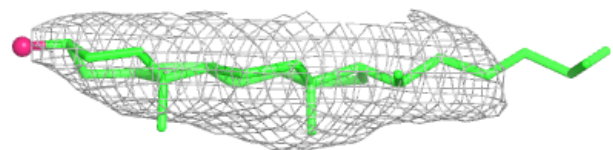
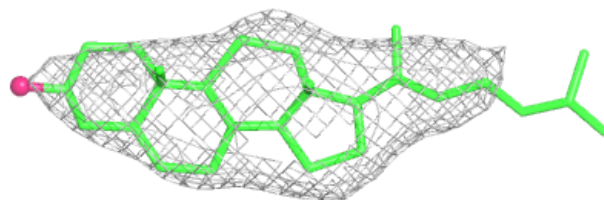


Electron density around PC1 A 2011:

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

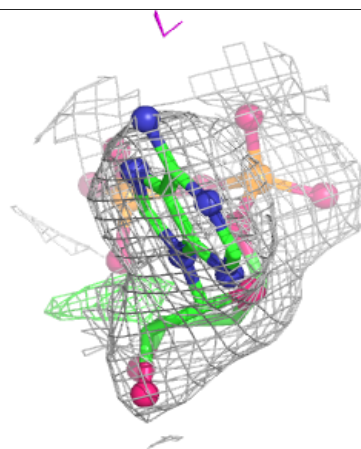
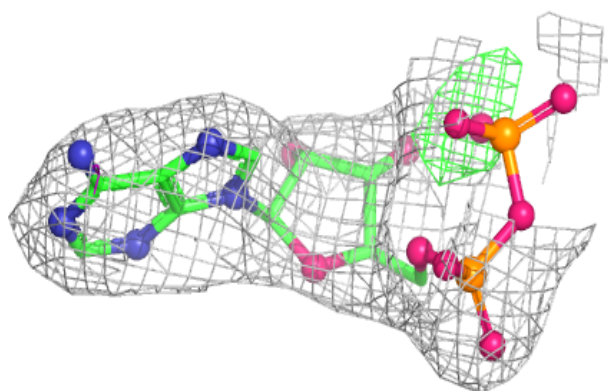
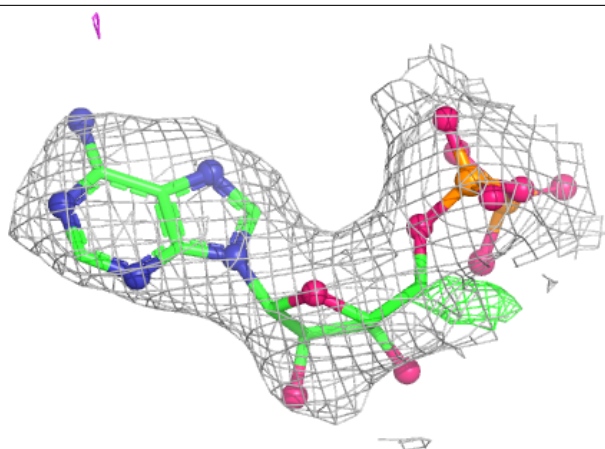
**Electron density around CLR C 2009:**

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



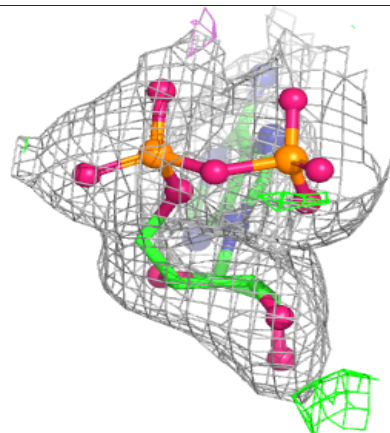
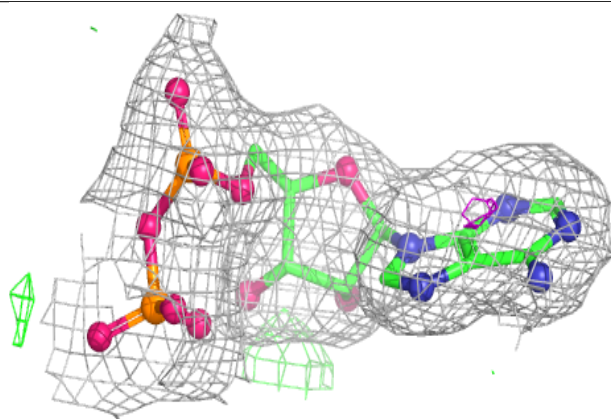
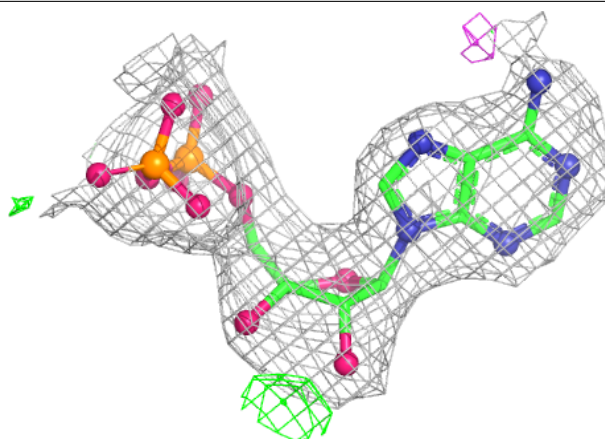
Electron density around ADP C 2004:

$2mF_o - DF_c$ (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 [i](#)

There are no such residues in this entry.