



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 03:07 PM EDT

PDB ID : 1SEJ
Title : Crystal Structure of Dihydrofolate Reductase-Thymidylate Synthase from *Cryptosporidium hominis* Bound to 1843U89/NADPH/dUMP
Authors : Anderson, A.C.
Deposited on : 2004-02-17
Resolution : 2.87 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

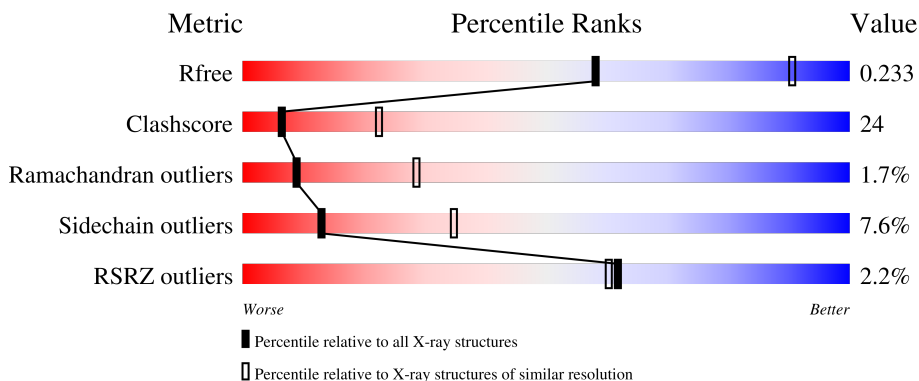
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	521	 2% 60% 33% 6%
1	B	521	 2% 60% 32% 7%
1	C	521	 2% 60% 32% 6%
1	D	521	 2% 61% 32% 6%
1	E	521	 3% 62% 31% 6%

2 Entry composition [i](#)

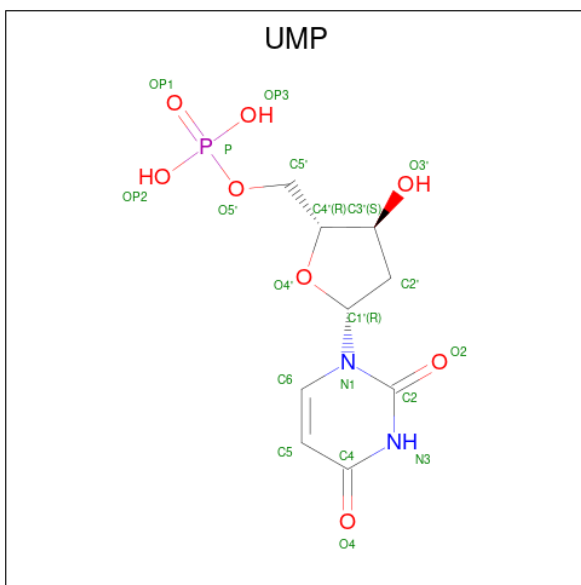
There are 5 unique types of molecules in this entry. The entry contains 22194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	Total 4223	C 2694	N 713	O 793	S 23	0	0	0
1	B	519	Total 4223	C 2694	N 713	O 793	S 23	0	0	0
1	C	519	Total 4223	C 2694	N 713	O 793	S 23	0	0	0
1	D	519	Total 4223	C 2694	N 713	O 793	S 23	0	0	0
1	E	519	Total 4223	C 2694	N 713	O 793	S 23	0	0	0

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



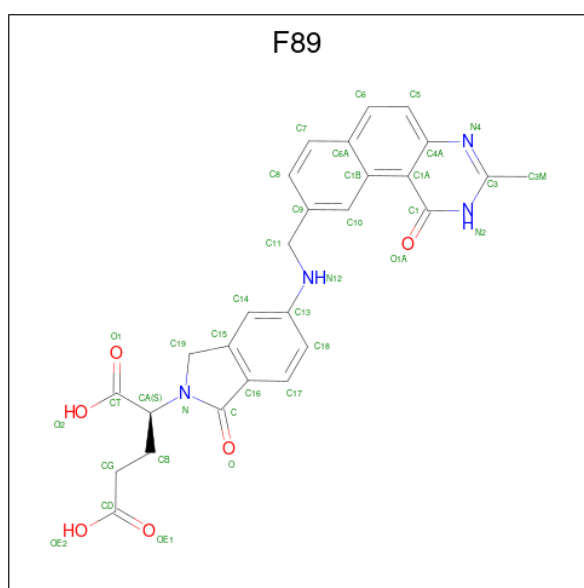
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 20	C 9	N 2	O 8	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	Total 20	C 9	N 2	O 8	P 1	0	0
2	C	1	Total 20	C 9	N 2	O 8	P 1	0	0
2	D	1	Total 20	C 9	N 2	O 8	P 1	0	0
2	E	1	Total 20	C 9	N 2	O 8	P 1	0	0

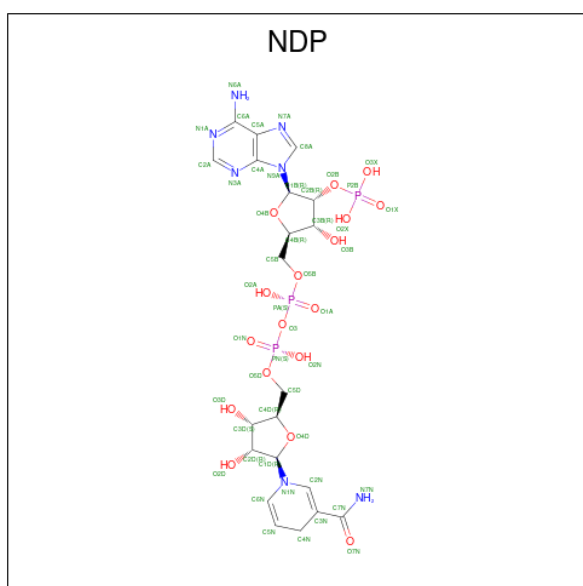
- Molecule 3 is S)-2-(5(((1,2-DIHYDRO-3-METHYL-1-OXOBENZO(F)QUINAZOLIN-9-YL)METHYL)AMINO)1-OXO-2-ISOINDOLINYL)GLUTARIC ACID (three-letter code: F89) (formula: C₂₇H₂₄N₄O₆).



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			37	27	4	6		
3	D	1	Total	C	N	O	0	0
			37	27	4	6		
3	E	1	Total	C	N	O	0	0
			37	27	4	6		
3	E	1	Total	C	N	O	0	0
			37	27	4	6		

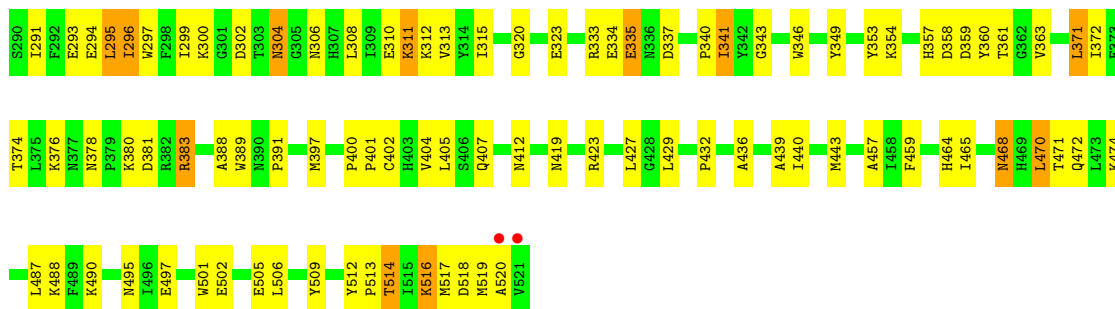
- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



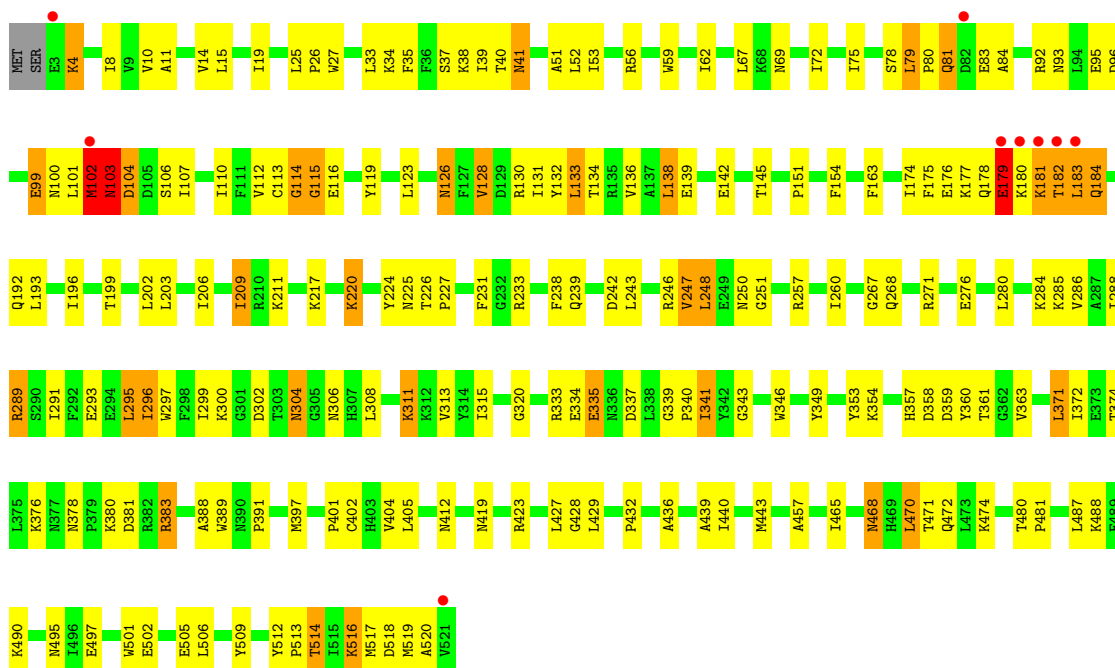
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is water.

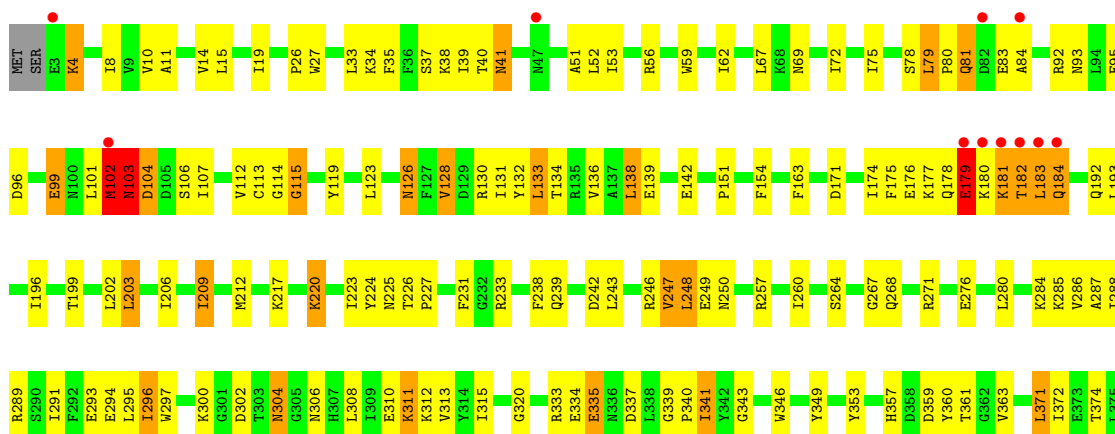
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	93	Total O 93 93	0	0
5	B	101	Total O 101 101	0	0
5	C	77	Total O 77 77	0	0
5	D	67	Total O 67 67	0	0
5	E	31	Total O 31 31	0	0

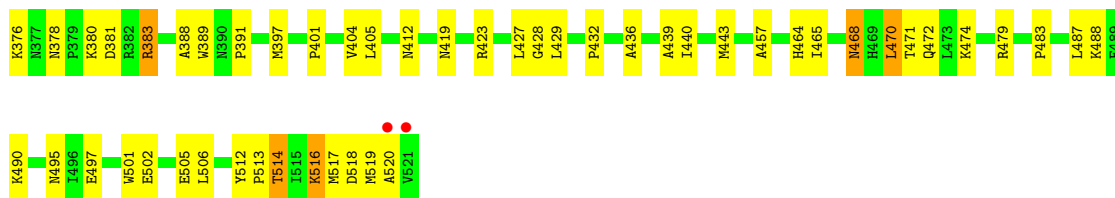


• Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase

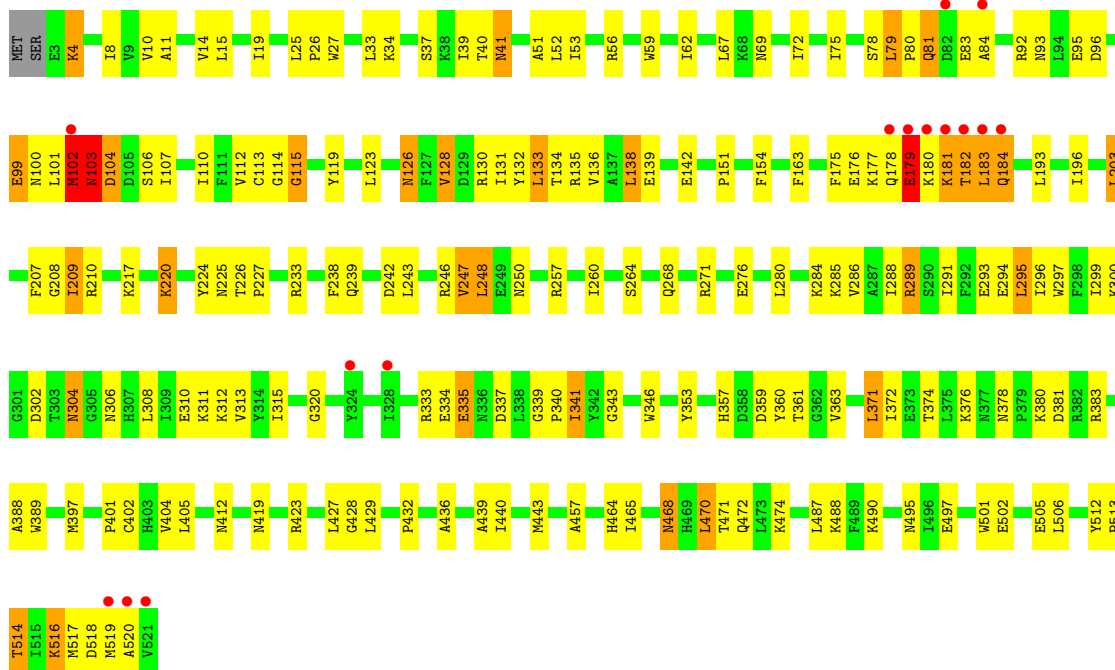


• Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase





● Molecule 1: bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.90Å 116.30Å 219.70Å 90.00° 95.23° 90.00°	Depositor
Resolution (Å)	45.15 – 2.87 45.15 – 2.87	Depositor EDS
% Data completeness (in resolution range)	90.4 (45.15-2.87) 90.5 (45.15-2.87)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.86Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.237 0.215 , 0.233	Depositor DCC
R_{free} test set	11185 reflections (9.40%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22194	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage'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: F89, UMP, NDP

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	0.40	0/4320	0.70	5/5838 (0.1%)
1	B	0.41	0/4320	0.73	6/5838 (0.1%)
1	C	0.40	0/4320	0.70	5/5838 (0.1%)
1	D	0.40	0/4320	0.70	4/5838 (0.1%)
1	E	0.42	0/4320	0.73	5/5838 (0.1%)
All	All	0.41	0/21600	0.71	25/29190 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	257	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	E	257	ARG	NE-CZ-NH1	13.77	127.18	120.30
1	B	257	ARG	NE-CZ-NH2	-13.71	113.44	120.30
1	B	257	ARG	NE-CZ-NH1	13.56	127.08	120.30
1	A	257	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	D	257	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	A	257	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	C	257	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	D	257	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	C	257	ARG	NE-CZ-NH2	7.90	124.25	120.30
1	E	257	ARG	CD-NE-CZ	6.67	132.94	123.60
1	B	257	ARG	CD-NE-CZ	6.47	132.66	123.60
1	A	115	GLY	N-CA-C	-5.40	99.61	113.10
1	E	115	GLY	N-CA-C	-5.37	99.67	113.10
1	C	115	GLY	N-CA-C	-5.30	99.86	113.10
1	D	115	GLY	N-CA-C	-5.26	99.96	113.10
1	B	115	GLY	N-CA-C	-5.24	100.00	113.10
1	A	114	GLY	N-CA-C	5.21	126.11	113.10
1	B	114	GLY	N-CA-C	5.17	126.02	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	LYS	N-CA-C	-5.12	97.17	111.00
1	E	180	LYS	N-CA-C	-5.11	97.22	111.00
1	C	114	GLY	N-CA-C	5.08	125.81	113.10
1	A	180	LYS	N-CA-C	-5.06	97.33	111.00
1	B	180	LYS	N-CA-C	-5.05	97.37	111.00
1	D	180	LYS	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4223	0	4159	218	0
1	B	4223	0	4159	211	0
1	C	4223	0	4159	207	0
1	D	4223	0	4159	206	0
1	E	4223	0	4159	197	0
2	A	20	0	11	2	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	2	0
2	E	20	0	11	2	0
3	A	74	0	44	16	0
3	B	74	0	44	13	0
3	C	74	0	44	15	0
3	D	74	0	44	17	0
3	E	74	0	44	17	0
4	A	48	0	26	10	0
4	B	48	0	26	8	0
4	C	48	0	26	8	0
4	D	48	0	26	8	0
4	E	48	0	26	8	0
5	A	93	0	0	2	0
5	B	101	0	0	3	0
5	C	77	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	67	0	0	4	0
5	E	31	0	0	1	0
All	All	22194	0	21200	1028	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 24.

All (1028) 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:E:341:ILE:HA	1:E:397:MET:HE3	1.32	1.10
1:C:341:ILE:HA	1:C:397:MET:HE3	1.35	1.09
1:A:341:ILE:HA	1:A:397:MET:HE3	1.34	1.07
1:D:341:ILE:HA	1:D:397:MET:HE3	1.34	1.06
1:B:341:ILE:HA	1:B:397:MET:HE3	1.34	1.04
1:D:209:ILE:HD12	1:D:209:ILE:H	1.25	1.02
1:B:209:ILE:HD12	1:B:209:ILE:H	1.24	1.01
1:A:209:ILE:HD12	1:A:209:ILE:H	1.23	1.00
1:E:209:ILE:H	1:E:209:ILE:HD12	1.23	1.00
1:C:209:ILE:H	1:C:209:ILE:HD12	1.24	0.99
1:B:178:GLN:O	1:B:179:GLU:HB2	1.70	0.91
1:D:178:GLN:O	1:D:179:GLU:HB2	1.70	0.91
1:E:178:GLN:O	1:E:179:GLU:HB2	1.70	0.91
1:C:178:GLN:O	1:C:179:GLU:HB2	1.70	0.91
1:D:33:LEU:HB3	3:D:617:F89:HG1	1.55	0.89
1:A:178:GLN:O	1:A:179:GLU:HB2	1.71	0.88
1:E:360:TYR:O	1:E:363:VAL:HG12	1.81	0.81
1:C:26:PRO:HG2	1:C:27:TRP:CE3	2.16	0.80
3:A:605:F89:H10	3:A:605:F89:O1A	1.81	0.80
1:E:209:ILE:H	1:E:209:ILE:CD1	1.95	0.80
1:A:209:ILE:H	1:A:209:ILE:CD1	1.94	0.80
1:A:289:ARG:HH11	1:A:289:ARG:HB3	1.47	0.79
3:D:617:F89:O1A	3:D:617:F89:H10	1.81	0.79
1:C:231:PHE:CD2	1:D:192:GLN:HG3	2.16	0.79
1:D:360:TYR:O	1:D:363:VAL:HG12	1.83	0.79
3:B:609:F89:H10	3:B:609:F89:O1A	1.81	0.79
3:A:604:F89:O1A	3:A:604:F89:H10	1.83	0.78
1:A:304:ASN:ND2	1:A:306:ASN:H	1.82	0.78
1:B:26:PRO:HG2	1:B:27:TRP:CE3	2.17	0.78
1:E:304:ASN:ND2	1:E:306:ASN:H	1.81	0.78
1:C:4:LYS:CB	1:C:101:LEU:HD23	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:613:F89:O1A	3:C:613:F89:H10	1.82	0.78
1:C:209:ILE:H	1:C:209:ILE:CD1	1.94	0.78
1:E:26:PRO:HG2	1:E:27:TRP:CE3	2.18	0.78
1:A:360:TYR:O	1:A:363:VAL:HG12	1.82	0.78
1:B:209:ILE:H	1:B:209:ILE:CD1	1.95	0.78
1:C:304:ASN:ND2	1:C:306:ASN:H	1.82	0.77
3:B:608:F89:O1A	3:B:608:F89:H10	1.83	0.77
1:E:4:LYS:CB	1:E:101:LEU:HD23	2.14	0.77
1:E:289:ARG:HH11	1:E:289:ARG:HB3	1.50	0.77
1:D:26:PRO:HG2	1:D:27:TRP:CE3	2.19	0.77
3:E:620:F89:H10	3:E:620:F89:O1A	1.84	0.77
1:A:192:GLN:HG3	1:B:231:PHE:CD2	2.20	0.77
1:C:193:LEU:HD21	1:C:196:ILE:HD12	1.66	0.77
1:C:289:ARG:HB3	1:C:289:ARG:HH11	1.50	0.77
3:C:612:F89:H10	3:C:612:F89:O1A	1.82	0.77
1:E:26:PRO:HG2	1:E:27:TRP:CZ3	2.19	0.77
1:D:209:ILE:H	1:D:209:ILE:CD1	1.96	0.76
1:C:304:ASN:C	1:C:304:ASN:HD22	1.88	0.76
1:B:289:ARG:HH11	1:B:289:ARG:HB3	1.50	0.76
1:C:192:GLN:HG3	1:D:231:PHE:CD2	2.21	0.76
3:E:621:F89:O1A	3:E:621:F89:H10	1.82	0.76
3:D:616:F89:O1A	3:D:616:F89:H10	1.83	0.76
1:B:304:ASN:ND2	1:B:306:ASN:H	1.81	0.76
1:B:360:TYR:O	1:B:363:VAL:HG12	1.86	0.76
1:B:4:LYS:CB	1:B:101:LEU:HD23	2.15	0.75
3:C:613:F89:C6	4:C:614:NDP:H42N	2.16	0.75
1:D:304:ASN:ND2	1:D:306:ASN:H	1.84	0.75
1:A:193:LEU:HD21	1:A:196:ILE:HD12	1.69	0.75
1:A:304:ASN:HD22	1:A:304:ASN:C	1.90	0.75
1:D:4:LYS:CB	1:D:101:LEU:HD23	2.15	0.75
1:A:4:LYS:CB	1:A:101:LEU:HD23	2.15	0.75
1:B:209:ILE:HD12	1:B:209:ILE:N	2.01	0.75
1:C:26:PRO:HG2	1:C:27:TRP:CZ3	2.21	0.75
1:D:26:PRO:HG2	1:D:27:TRP:CZ3	2.21	0.75
1:C:360:TYR:O	1:C:363:VAL:HG12	1.86	0.75
1:A:26:PRO:HG2	1:A:27:TRP:CE3	2.20	0.75
1:D:289:ARG:HH11	1:D:289:ARG:HB3	1.51	0.74
1:D:304:ASN:C	1:D:304:ASN:HD22	1.90	0.74
1:C:209:ILE:HD12	1:C:209:ILE:N	2.02	0.74
1:D:193:LEU:HD21	1:D:196:ILE:HD12	1.68	0.74
1:E:246:ARG:HH11	1:E:268:GLN:HE21	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:HH11	1:B:268:GLN:HE21	1.35	0.74
1:E:209:ILE:HD12	1:E:209:ILE:N	2.01	0.74
1:E:217:LYS:H	1:E:250:ASN:HD21	1.35	0.74
1:A:26:PRO:HG2	1:A:27:TRP:CZ3	2.22	0.74
1:C:56:ARG:HD3	4:C:614:NDP:O1X	1.87	0.74
1:B:304:ASN:C	1:B:304:ASN:HD22	1.91	0.74
1:A:209:ILE:HD12	1:A:209:ILE:N	2.01	0.73
1:B:26:PRO:HG2	1:B:27:TRP:CZ3	2.23	0.73
1:C:33:LEU:HB3	3:C:613:F89:HG1	1.70	0.73
1:C:246:ARG:HH11	1:C:268:GLN:HE21	1.34	0.73
1:A:359:ASP:OD2	1:A:361:THR:HG22	1.89	0.73
1:E:193:LEU:HD21	1:E:196:ILE:HD12	1.70	0.73
1:E:246:ARG:HH11	1:E:268:GLN:NE2	1.87	0.73
1:E:304:ASN:C	1:E:304:ASN:HD22	1.92	0.73
1:D:217:LYS:H	1:D:250:ASN:HD21	1.36	0.73
1:E:516:LYS:HE3	1:E:518:ASP:OD1	1.88	0.73
1:A:231:PHE:CD2	1:B:192:GLN:HG3	2.24	0.72
1:B:193:LEU:HD21	1:B:196:ILE:HD12	1.70	0.72
1:E:304:ASN:HD22	1:E:306:ASN:H	1.36	0.72
1:E:359:ASP:OD2	1:E:361:THR:HG22	1.89	0.72
1:E:151:PRO:HG2	1:E:154:PHE:HD2	1.54	0.72
1:A:38:LYS:HB3	1:B:202:LEU:HG	1.72	0.72
1:D:516:LYS:HE3	1:D:518:ASP:OD1	1.89	0.72
1:E:33:LEU:HB3	3:E:621:F89:HG1	1.70	0.72
1:A:271:ARG:NH2	1:B:267:GLY:O	2.23	0.71
1:B:217:LYS:H	1:B:250:ASN:HD21	1.38	0.71
1:C:246:ARG:HH11	1:C:268:GLN:NE2	1.87	0.71
1:D:209:ILE:HD12	1:D:209:ILE:N	2.02	0.71
1:D:246:ARG:HH11	1:D:268:GLN:HE21	1.37	0.71
1:C:217:LYS:H	1:C:250:ASN:HD21	1.38	0.71
1:D:34:LYS:HD3	5:D:678:HOH:O	1.90	0.71
1:A:217:LYS:H	1:A:250:ASN:HD21	1.38	0.71
1:C:304:ASN:HD22	1:C:306:ASN:H	1.39	0.70
1:A:516:LYS:HE3	1:A:518:ASP:OD1	1.91	0.70
1:D:151:PRO:HG2	1:D:154:PHE:HD2	1.56	0.70
1:C:349:TYR:CE2	1:D:391:PRO:HD2	2.27	0.70
1:C:4:LYS:HB2	1:C:101:LEU:HD23	1.72	0.70
1:D:359:ASP:OD2	1:D:361:THR:HG22	1.91	0.70
1:E:4:LYS:HB2	1:E:101:LEU:HD23	1.73	0.70
1:A:246:ARG:HH11	1:A:268:GLN:HE21	1.37	0.70
1:A:4:LYS:HB2	1:A:101:LEU:HD23	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASN:HD22	1:B:306:ASN:H	1.37	0.70
1:D:296:ILE:O	1:D:300:LYS:HG2	1.92	0.70
1:C:516:LYS:HE3	1:C:518:ASP:OD1	1.92	0.69
1:B:246:ARG:HH11	1:B:268:GLN:NE2	1.90	0.69
1:E:289:ARG:HG3	1:E:501:TRP:CE2	2.28	0.69
1:A:202:LEU:HG	1:B:38:LYS:HB3	1.74	0.69
1:D:56:ARG:HD3	4:D:618:NDP:O1X	1.93	0.69
1:A:246:ARG:HH11	1:A:268:GLN:NE2	1.91	0.69
1:A:304:ASN:HD22	1:A:306:ASN:H	1.37	0.69
1:A:315:ILE:HD13	3:A:604:F89:C18	2.21	0.69
1:B:516:LYS:HE3	1:B:518:ASP:OD1	1.92	0.69
1:C:333:ARG:HG3	1:C:337:ASP:HB3	1.75	0.69
1:D:315:ILE:HD12	3:D:616:F89:C8	2.22	0.69
1:B:4:LYS:HE2	1:B:101:LEU:HA	1.75	0.69
1:C:419:ASN:ND2	1:C:457:ALA:HB3	2.08	0.69
1:D:289:ARG:HG3	1:D:501:TRP:CE2	2.28	0.69
1:C:151:PRO:HG2	1:C:154:PHE:HD2	1.57	0.68
1:C:296:ILE:HD12	1:C:297:TRP:H	1.58	0.68
1:B:4:LYS:HB2	1:B:101:LEU:HD23	1.75	0.68
1:D:246:ARG:HH11	1:D:268:GLN:NE2	1.92	0.68
1:A:4:LYS:HE2	1:A:101:LEU:HA	1.75	0.68
1:B:333:ARG:HG3	1:B:337:ASP:HB3	1.76	0.68
1:E:56:ARG:HD3	4:E:622:NDP:O1X	1.94	0.68
1:C:4:LYS:HE2	1:C:101:LEU:HA	1.75	0.68
1:C:206:ILE:HD11	1:D:35:PHE:HA	1.76	0.68
1:D:4:LYS:HB2	1:D:101:LEU:HD23	1.74	0.68
1:A:33:LEU:HB3	3:A:605:F89:HG1	1.76	0.67
1:B:151:PRO:HG2	1:B:154:PHE:HD2	1.59	0.67
1:C:296:ILE:HD12	1:C:297:TRP:N	2.10	0.67
1:A:391:PRO:HD2	1:B:349:TYR:CE2	2.30	0.67
1:E:333:ARG:HG3	1:E:337:ASP:HB3	1.75	0.67
1:C:81:GLN:HE22	1:C:92:ARG:NE	1.93	0.67
1:D:304:ASN:HD22	1:D:306:ASN:H	1.40	0.67
1:E:4:LYS:HE2	1:E:101:LEU:HA	1.76	0.67
1:C:391:PRO:HD2	1:D:349:TYR:CE2	2.29	0.67
1:B:99:GLU:OE2	1:B:99:GLU:C	2.34	0.67
1:C:104:ASP:C	1:C:106:SER:H	1.98	0.67
1:A:333:ARG:HG3	1:A:337:ASP:HB3	1.76	0.67
1:A:34:LYS:HG2	1:B:206:ILE:HG12	1.77	0.67
1:D:104:ASP:C	1:D:106:SER:H	1.99	0.66
1:B:359:ASP:OD2	1:B:361:THR:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ARG:HG3	1:D:337:ASP:HB3	1.77	0.66
1:A:151:PRO:HG2	1:A:154:PHE:HD2	1.60	0.66
1:E:419:ASN:ND2	1:E:457:ALA:HB3	2.10	0.66
1:A:296:ILE:O	1:A:300:LYS:HG2	1.96	0.66
1:B:81:GLN:HE22	1:B:92:ARG:NE	1.93	0.66
1:C:315:ILE:HD13	3:C:612:F89:C18	2.25	0.66
1:B:296:ILE:O	1:B:300:LYS:HG2	1.95	0.66
1:E:217:LYS:N	1:E:250:ASN:HD21	1.93	0.66
1:E:296:ILE:O	1:E:300:LYS:HG2	1.95	0.66
1:B:56:ARG:HD3	4:B:610:NDP:O1X	1.95	0.65
1:C:267:GLY:O	1:D:271:ARG:NH2	2.29	0.65
1:C:359:ASP:OD2	1:C:361:THR:HG22	1.96	0.65
1:A:56:ARG:HD3	4:A:606:NDP:O1X	1.96	0.65
1:C:79:LEU:HD23	1:C:80:PRO:HD2	1.77	0.65
1:D:225:ASN:O	1:D:233:ARG:NH2	2.28	0.65
1:E:79:LEU:HD23	1:E:80:PRO:HD2	1.78	0.65
1:D:217:LYS:N	1:D:250:ASN:HD21	1.94	0.65
1:A:35:PHE:HA	1:B:206:ILE:HD11	1.79	0.65
1:A:81:GLN:HE22	1:A:92:ARG:NE	1.95	0.65
1:B:79:LEU:HD23	1:B:80:PRO:HD2	1.79	0.65
1:B:468:ASN:N	1:B:468:ASN:HD22	1.94	0.65
1:D:4:LYS:HE2	1:D:101:LEU:HA	1.77	0.65
1:E:67:LEU:HG	1:E:72:ILE:HD11	1.77	0.64
1:D:293:GLU:HA	1:D:296:ILE:HD11	1.78	0.64
1:A:349:TYR:CE2	1:B:391:PRO:HD2	2.33	0.64
1:C:296:ILE:O	1:C:300:LYS:HG2	1.97	0.64
1:B:104:ASP:C	1:B:106:SER:H	1.98	0.64
1:C:289:ARG:HG3	1:C:501:TRP:CE2	2.33	0.64
1:D:79:LEU:HD23	1:D:80:PRO:HD2	1.80	0.64
1:A:104:ASP:C	1:A:106:SER:H	1.99	0.64
1:A:267:GLY:O	1:B:271:ARG:NH2	2.31	0.64
1:D:315:ILE:HD13	3:D:616:F89:C18	2.28	0.64
1:B:217:LYS:N	1:B:250:ASN:HD21	1.96	0.63
1:C:67:LEU:HG	1:C:72:ILE:HD11	1.79	0.63
1:E:225:ASN:O	1:E:233:ARG:NH2	2.30	0.63
1:C:99:GLU:C	1:C:99:GLU:OE2	2.37	0.63
1:E:104:ASP:C	1:E:106:SER:H	2.01	0.63
1:A:67:LEU:HG	1:A:72:ILE:HD11	1.81	0.63
1:A:79:LEU:HD23	1:A:80:PRO:HD2	1.81	0.63
1:A:304:ASN:HD21	1:A:306:ASN:HB2	1.62	0.63
1:B:293:GLU:HA	1:B:296:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ASN:HD22	1:B:468:ASN:H	1.44	0.63
1:D:81:GLN:HE22	1:D:92:ARG:NE	1.96	0.63
1:A:225:ASN:O	1:A:233:ARG:NH2	2.31	0.63
3:E:621:F89:C6	4:E:622:NDP:H42N	2.29	0.63
1:C:93:ASN:HD21	1:C:95:GLU:HB3	1.64	0.63
1:C:217:LYS:N	1:C:250:ASN:HD21	1.95	0.63
1:D:260:ILE:HD12	1:D:260:ILE:N	2.13	0.63
1:E:81:GLN:HE22	1:E:92:ARG:NE	1.96	0.63
1:E:151:PRO:HG2	1:E:154:PHE:CD2	2.33	0.63
1:E:304:ASN:HD21	1:E:306:ASN:HB2	1.63	0.63
1:A:296:ILE:HD12	1:A:297:TRP:H	1.64	0.63
1:B:289:ARG:HG3	1:B:501:TRP:CE2	2.33	0.63
1:A:217:LYS:N	1:A:250:ASN:HD21	1.96	0.62
1:E:93:ASN:HD21	1:E:95:GLU:HB3	1.64	0.62
1:D:220:LYS:NZ	5:D:631:HOH:O	2.31	0.62
1:B:67:LEU:HG	1:B:72:ILE:HD11	1.82	0.62
1:C:468:ASN:N	1:C:468:ASN:HD22	1.98	0.62
1:E:52:LEU:HB3	1:E:113:CYS:SG	2.39	0.62
1:B:15:LEU:HB2	1:B:139:GLU:HG2	1.81	0.62
1:B:33:LEU:HB3	3:B:609:F89:HG1	1.80	0.62
1:B:225:ASN:O	1:B:233:ARG:NH2	2.32	0.62
1:D:136:VAL:HG12	1:D:138:LEU:CD2	2.29	0.62
1:A:289:ARG:HG3	1:A:501:TRP:CE2	2.34	0.62
1:E:289:ARG:HB3	1:E:289:ARG:NH1	2.15	0.62
1:D:297:TRP:CD1	1:D:302:ASP:HB3	2.35	0.62
1:A:99:GLU:OE2	1:A:99:GLU:C	2.38	0.61
1:C:304:ASN:HD21	1:C:306:ASN:HB2	1.65	0.61
1:E:296:ILE:HD12	1:E:297:TRP:N	2.15	0.61
1:E:468:ASN:HD22	1:E:468:ASN:N	1.96	0.61
1:D:67:LEU:HG	1:D:72:ILE:HD11	1.82	0.61
1:E:293:GLU:HA	1:E:296:ILE:HD11	1.82	0.61
1:A:293:GLU:HA	1:A:296:ILE:HD11	1.82	0.61
1:D:151:PRO:HG2	1:D:154:PHE:CD2	2.34	0.61
1:E:297:TRP:CG	1:E:308:LEU:HD21	2.35	0.61
1:A:468:ASN:N	1:A:468:ASN:HD22	1.98	0.61
1:C:225:ASN:O	1:C:233:ARG:NH2	2.33	0.61
1:E:260:ILE:N	1:E:260:ILE:HD12	2.15	0.61
1:E:297:TRP:CD1	1:E:302:ASP:HB3	2.35	0.61
1:B:296:ILE:HD12	1:B:297:TRP:H	1.65	0.61
1:E:468:ASN:HD22	1:E:468:ASN:H	1.48	0.61
1:A:296:ILE:HD12	1:A:297:TRP:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG12	1:A:138:LEU:CD2	2.31	0.61
1:B:419:ASN:ND2	1:B:457:ALA:HB3	2.16	0.61
1:E:378:ASN:ND2	1:E:381:ASP:HB2	2.16	0.61
1:B:296:ILE:HD12	1:B:297:TRP:N	2.15	0.61
1:C:151:PRO:HG2	1:C:154:PHE:CD2	2.36	0.61
3:C:613:F89:C6A	4:C:614:NDP:H42N	2.30	0.61
1:E:136:VAL:HG12	1:E:138:LEU:CD2	2.30	0.61
1:B:243:LEU:O	1:B:247:VAL:HG13	2.01	0.60
1:B:297:TRP:CG	1:B:308:LEU:HD21	2.36	0.60
1:D:99:GLU:OE2	1:D:99:GLU:C	2.39	0.60
1:D:490:LYS:HD2	1:D:502:GLU:O	2.02	0.60
1:B:136:VAL:HG12	1:B:138:LEU:CD2	2.30	0.60
1:C:136:VAL:HG12	1:C:138:LEU:CD2	2.30	0.60
1:D:468:ASN:N	1:D:468:ASN:HD22	1.99	0.60
1:D:296:ILE:HD12	1:D:297:TRP:N	2.17	0.60
1:E:99:GLU:C	1:E:99:GLU:OE2	2.39	0.60
1:A:103:ASN:O	1:A:104:ASP:C	2.40	0.60
3:A:605:F89:C6	4:A:606:NDP:H42N	2.30	0.60
1:C:104:ASP:HB3	1:C:107:ILE:HD13	1.84	0.60
1:A:297:TRP:CG	1:A:308:LEU:HD21	2.36	0.60
1:E:389:TRP:HB2	1:E:404:VAL:HG13	1.83	0.60
1:C:468:ASN:HD22	1:C:468:ASN:H	1.50	0.60
1:D:297:TRP:CG	1:D:308:LEU:HD21	2.37	0.60
1:E:104:ASP:HB3	1:E:107:ILE:HD13	1.83	0.60
1:A:419:ASN:ND2	1:A:457:ALA:HB3	2.17	0.60
3:D:617:F89:C6	4:D:618:NDP:H42N	2.32	0.60
1:E:179:GLU:OE2	1:E:179:GLU:HA	2.02	0.60
1:A:315:ILE:HG21	3:A:604:F89:C15	2.31	0.60
1:C:103:ASN:C	1:C:103:ASN:HD22	2.04	0.60
1:D:419:ASN:ND2	1:D:457:ALA:HB3	2.17	0.59
1:A:37:SER:HB2	3:A:605:F89:HB1	1.84	0.59
1:A:297:TRP:CD1	1:A:302:ASP:HB3	2.38	0.59
1:C:15:LEU:HB2	1:C:139:GLU:HG2	1.85	0.59
1:A:490:LYS:HD2	1:A:502:GLU:O	2.01	0.59
1:B:19:ILE:O	4:B:610:NDP:H2N	2.02	0.59
1:D:52:LEU:HB3	1:D:113:CYS:SG	2.42	0.59
1:D:93:ASN:HD21	1:D:95:GLU:HB3	1.67	0.59
1:C:378:ASN:ND2	1:C:381:ASP:HB2	2.17	0.59
1:E:103:ASN:O	1:E:104:ASP:C	2.41	0.59
1:D:15:LEU:HB2	1:D:139:GLU:HG2	1.84	0.59
1:D:33:LEU:CB	3:D:617:F89:HG1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:ILE:HD12	1:E:297:TRP:H	1.66	0.59
1:C:104:ASP:C	1:C:106:SER:N	2.55	0.59
1:D:179:GLU:HA	1:D:179:GLU:OE2	2.02	0.59
1:D:304:ASN:HD21	1:D:306:ASN:HB2	1.65	0.59
1:B:260:ILE:HD12	1:B:260:ILE:N	2.18	0.59
1:D:296:ILE:HD12	1:D:297:TRP:H	1.67	0.59
1:E:315:ILE:HG21	3:E:620:F89:C15	2.32	0.59
1:B:93:ASN:HD21	1:B:95:GLU:HB3	1.67	0.59
1:E:334:GLU:OE2	1:E:357:HIS:HE1	1.85	0.59
1:A:151:PRO:HG2	1:A:154:PHE:CD2	2.38	0.59
1:A:206:ILE:HG12	1:B:34:LYS:HG2	1.84	0.59
1:C:35:PHE:HA	1:D:206:ILE:HD11	1.85	0.59
1:D:289:ARG:HB3	1:D:289:ARG:NH1	2.18	0.59
1:E:490:LYS:HD2	1:E:502:GLU:O	2.03	0.59
1:A:260:ILE:N	1:A:260:ILE:HD12	2.17	0.59
1:C:297:TRP:CG	1:C:308:LEU:HD21	2.38	0.58
1:D:468:ASN:HD22	1:D:468:ASN:H	1.51	0.58
1:B:104:ASP:C	1:B:106:SER:N	2.55	0.58
1:C:389:TRP:HB2	1:C:404:VAL:HG13	1.85	0.58
1:A:15:LEU:HB2	1:A:139:GLU:HG2	1.86	0.58
1:B:304:ASN:HD21	1:B:306:ASN:HB2	1.66	0.58
1:B:378:ASN:ND2	1:B:381:ASP:HB2	2.19	0.58
1:D:103:ASN:O	1:D:104:ASP:C	2.41	0.58
3:E:621:F89:C6A	4:E:622:NDP:H42N	2.33	0.58
1:B:289:ARG:HB3	1:B:289:ARG:NH1	2.18	0.58
1:A:104:ASP:C	1:A:106:SER:N	2.56	0.58
1:B:103:ASN:O	1:B:104:ASP:C	2.41	0.58
1:D:389:TRP:HB2	1:D:404:VAL:HG13	1.86	0.58
3:D:617:F89:C6A	4:D:618:NDP:H42N	2.34	0.58
1:B:103:ASN:C	1:B:103:ASN:HD22	2.05	0.58
1:B:490:LYS:HD2	1:B:502:GLU:O	2.03	0.58
1:C:289:ARG:HB3	1:C:289:ARG:NH1	2.17	0.58
1:E:103:ASN:C	1:E:103:ASN:HD22	2.06	0.58
1:A:289:ARG:HB3	1:A:289:ARG:NH1	2.17	0.58
1:D:126:ASN:HD21	1:D:177:LYS:CE	2.16	0.58
1:A:468:ASN:HD22	1:A:468:ASN:H	1.51	0.58
1:E:19:ILE:O	4:E:622:NDP:H2N	2.03	0.58
1:C:260:ILE:N	1:C:260:ILE:HD12	2.18	0.57
1:C:490:LYS:HD2	1:C:502:GLU:O	2.03	0.57
1:E:126:ASN:HD21	1:E:177:LYS:HE3	1.69	0.57
1:B:52:LEU:HB3	1:B:113:CYS:SG	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:HD3	1:B:514:THR:HG22	1.84	0.57
1:C:439:ALA:O	1:C:443:MET:HG3	2.04	0.57
1:D:114:GLY:HA2	1:D:119:TYR:CZ	2.39	0.57
1:D:126:ASN:HD21	1:D:177:LYS:HE3	1.69	0.57
1:B:179:GLU:HA	1:B:179:GLU:OE2	2.05	0.57
1:D:103:ASN:C	1:D:103:ASN:HD22	2.05	0.57
1:B:334:GLU:OE2	1:B:357:HIS:HE1	1.88	0.57
1:E:15:LEU:HB2	1:E:139:GLU:HG2	1.85	0.57
1:A:179:GLU:OE2	1:A:179:GLU:HA	2.05	0.57
1:A:285:LYS:HD3	1:A:514:THR:HG22	1.87	0.57
1:C:52:LEU:HB3	1:C:113:CYS:SG	2.45	0.57
1:B:151:PRO:HG2	1:B:154:PHE:CD2	2.38	0.57
3:B:609:F89:O1A	3:B:609:F89:C10	2.53	0.57
1:C:285:LYS:HD3	1:C:514:THR:HG22	1.86	0.57
1:C:293:GLU:HA	1:C:296:ILE:HD11	1.85	0.57
1:E:126:ASN:HD21	1:E:177:LYS:CE	2.17	0.57
1:A:126:ASN:HD21	1:A:177:LYS:CE	2.18	0.57
1:A:126:ASN:HD21	1:A:177:LYS:NZ	2.03	0.57
1:B:439:ALA:O	1:B:443:MET:HG3	2.05	0.57
1:C:297:TRP:CD1	1:C:302:ASP:HB3	2.40	0.57
1:D:19:ILE:O	4:D:618:NDP:H2N	2.05	0.57
1:D:104:ASP:C	1:D:106:SER:N	2.56	0.57
1:B:389:TRP:HB2	1:B:404:VAL:HG13	1.87	0.56
1:D:334:GLU:OE2	1:D:357:HIS:HE1	1.87	0.56
1:D:217:LYS:H	1:D:250:ASN:ND2	2.03	0.56
1:E:114:GLY:HA2	1:E:119:TYR:CZ	2.39	0.56
1:A:291:ILE:HD13	1:A:436:ALA:HB3	1.86	0.56
1:A:320:GLY:O	1:A:335:GLU:O	2.23	0.56
1:A:439:ALA:O	1:A:443:MET:HG3	2.05	0.56
1:C:271:ARG:NH2	1:D:267:GLY:O	2.38	0.56
1:C:315:ILE:HG21	3:C:612:F89:C15	2.35	0.56
1:C:334:GLU:OE2	1:C:357:HIS:HE1	1.87	0.56
1:D:439:ALA:O	1:D:443:MET:HG3	2.05	0.56
1:A:93:ASN:HD21	1:A:95:GLU:HB3	1.68	0.56
1:B:468:ASN:H	1:B:468:ASN:ND2	2.04	0.56
1:D:104:ASP:HB3	1:D:107:ILE:HD13	1.87	0.56
1:A:115:GLY:HA3	4:A:606:NDP:PA	2.46	0.56
1:A:126:ASN:ND2	1:A:177:LYS:NZ	2.53	0.56
1:B:291:ILE:HD13	1:B:436:ALA:HB3	1.87	0.56
1:A:206:ILE:HD11	1:B:35:PHE:HA	1.87	0.56
1:A:269:MET:HE1	1:B:269:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ASN:HD21	1:B:177:LYS:CE	2.18	0.56
1:D:291:ILE:HD13	1:D:436:ALA:HB3	1.87	0.56
1:D:495:ASN:OD1	1:D:497:GLU:HG2	2.06	0.56
1:E:217:LYS:H	1:E:250:ASN:ND2	2.04	0.56
1:E:243:LEU:O	1:E:247:VAL:HG13	2.05	0.56
1:B:487:LEU:O	1:B:488:LYS:HD3	2.05	0.56
1:C:103:ASN:O	1:C:104:ASP:C	2.43	0.56
1:E:285:LYS:HD3	1:E:514:THR:HG22	1.87	0.56
1:A:102:MET:HA	1:A:102:MET:CE	2.36	0.56
1:D:285:LYS:HD3	1:D:514:THR:HG22	1.87	0.56
1:E:123:LEU:HD13	1:E:128:VAL:HG11	1.88	0.56
1:B:102:MET:CE	1:B:102:MET:HA	2.36	0.56
1:A:104:ASP:HB3	1:A:107:ILE:HD13	1.87	0.55
1:E:104:ASP:C	1:E:106:SER:N	2.57	0.55
1:E:495:ASN:OD1	1:E:497:GLU:HG2	2.07	0.55
1:A:389:TRP:HB2	1:A:404:VAL:HG13	1.87	0.55
1:C:243:LEU:O	1:C:247:VAL:HG13	2.07	0.55
1:A:52:LEU:HB3	1:A:113:CYS:SG	2.47	0.55
1:A:103:ASN:HD22	1:A:103:ASN:C	2.07	0.55
1:A:334:GLU:OE2	1:A:357:HIS:HE1	1.89	0.55
1:B:126:ASN:HD21	1:B:177:LYS:HE3	1.71	0.55
1:B:297:TRP:CD1	1:B:302:ASP:HB3	2.42	0.55
3:C:612:F89:O1A	3:C:612:F89:C10	2.53	0.55
1:E:291:ILE:HD13	1:E:436:ALA:HB3	1.88	0.55
1:E:304:ASN:ND2	1:E:306:ASN:HB2	2.22	0.55
1:E:320:GLY:O	1:E:335:GLU:O	2.24	0.55
1:A:114:GLY:HA2	1:A:119:TYR:CZ	2.42	0.55
1:A:404:VAL:HG11	1:B:405:LEU:HD11	1.87	0.55
3:B:609:F89:C6	4:B:610:NDP:H42N	2.36	0.55
1:D:378:ASN:ND2	1:D:381:ASP:HB2	2.21	0.55
1:A:115:GLY:HA3	4:A:606:NDP:O1A	2.07	0.55
1:C:284:LYS:HZ1	1:C:432:PRO:HG2	1.72	0.55
1:C:487:LEU:O	1:C:488:LYS:HD3	2.07	0.55
1:C:126:ASN:HD21	1:C:177:LYS:HE3	1.72	0.55
1:A:233:ARG:NH1	1:A:242:ASP:OD1	2.40	0.54
3:C:612:F89:OE1	3:C:612:F89:HA	2.07	0.54
1:A:19:ILE:O	4:A:606:NDP:H2N	2.07	0.54
1:C:509:TYR:HA	5:C:669:HOH:O	2.08	0.54
1:E:284:LYS:HZ1	1:E:432:PRO:HG2	1.72	0.54
1:D:102:MET:HA	1:D:102:MET:CE	2.38	0.54
1:E:102:MET:CE	1:E:102:MET:HA	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA2	1:B:119:TYR:CZ	2.43	0.54
1:C:126:ASN:HD21	1:C:177:LYS:CE	2.20	0.54
1:C:211:LYS:HE3	5:C:682:HOH:O	2.06	0.54
1:D:123:LEU:HD13	1:D:128:VAL:HG11	1.89	0.54
1:B:315:ILE:HD13	3:B:608:F89:C18	2.37	0.54
1:B:320:GLY:O	1:B:335:GLU:O	2.26	0.54
1:C:136:VAL:HG12	1:C:138:LEU:HD23	1.90	0.54
1:D:243:LEU:O	1:D:247:VAL:HG13	2.07	0.54
1:E:439:ALA:O	1:E:443:MET:HG3	2.07	0.54
1:B:130:ARG:HD2	1:B:132:TYR:CE1	2.43	0.54
1:C:291:ILE:HD13	1:C:436:ALA:HB3	1.88	0.54
1:C:519:MET:HG2	1:C:520:ALA:N	2.23	0.54
1:D:315:ILE:HD12	3:D:616:F89:H8	1.90	0.54
1:E:123:LEU:HD13	1:E:128:VAL:CG1	2.38	0.54
1:C:123:LEU:HD13	1:C:128:VAL:HG11	1.89	0.53
1:D:126:ASN:ND2	1:D:177:LYS:NZ	2.56	0.53
1:E:75:ILE:O	4:E:622:NDP:H1B	2.08	0.53
1:A:123:LEU:HD13	1:A:128:VAL:HG11	1.90	0.53
3:B:608:F89:OE1	3:B:608:F89:HA	2.08	0.53
1:C:102:MET:HA	1:C:102:MET:CE	2.37	0.53
1:A:304:ASN:ND2	1:A:306:ASN:HB2	2.22	0.53
1:D:359:ASP:CG	1:D:361:THR:HG22	2.29	0.53
1:B:519:MET:HG2	1:B:520:ALA:N	2.23	0.53
1:D:126:ASN:HD21	1:D:177:LYS:NZ	2.06	0.53
1:D:304:ASN:ND2	1:D:304:ASN:C	2.61	0.53
1:E:126:ASN:ND2	1:E:177:LYS:NZ	2.57	0.53
1:A:215:ARG:NH1	5:A:652:HOH:O	2.41	0.53
1:C:130:ARG:HD2	1:C:132:TYR:CE1	2.43	0.53
1:C:320:GLY:O	1:C:335:GLU:O	2.25	0.53
1:A:243:LEU:O	1:A:247:VAL:HG13	2.09	0.53
1:C:304:ASN:ND2	1:C:304:ASN:C	2.60	0.53
1:D:83:GLU:HA	1:D:83:GLU:OE2	2.07	0.53
1:A:126:ASN:HD21	1:A:177:LYS:HE3	1.73	0.53
1:A:495:ASN:OD1	1:A:497:GLU:HG2	2.09	0.53
1:C:405:LEU:HD11	1:D:404:VAL:HG11	1.90	0.53
1:D:315:ILE:HG21	3:D:616:F89:C15	2.39	0.53
1:C:114:GLY:HA2	1:C:119:TYR:CZ	2.44	0.53
1:E:114:GLY:HA2	1:E:119:TYR:CE2	2.44	0.53
1:E:359:ASP:CG	1:E:361:THR:HG22	2.28	0.53
1:A:51:ALA:C	1:A:52:LEU:HD23	2.29	0.53
1:A:239:GLN:HG3	1:A:271:ARG:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:NH1	1:D:242:ASP:OD1	2.40	0.53
1:A:519:MET:HG2	1:A:520:ALA:N	2.24	0.52
1:B:123:LEU:HD13	1:B:128:VAL:HG11	1.90	0.52
1:B:315:ILE:HG21	3:B:608:F89:C15	2.39	0.52
3:E:620:F89:HA	3:E:620:F89:OE1	2.08	0.52
1:B:115:GLY:HA3	4:B:610:NDP:PA	2.49	0.52
1:B:126:ASN:HD21	1:B:177:LYS:NZ	2.07	0.52
1:B:284:LYS:HZ1	1:B:432:PRO:HG2	1.74	0.52
1:E:136:VAL:HG12	1:E:138:LEU:HD23	1.92	0.52
1:B:126:ASN:ND2	1:B:177:LYS:NZ	2.57	0.52
1:B:495:ASN:OD1	1:B:497:GLU:HG2	2.10	0.52
1:C:495:ASN:OD1	1:C:497:GLU:HG2	2.10	0.52
1:B:217:LYS:H	1:B:250:ASN:ND2	2.05	0.52
1:D:37:SER:O	1:D:41:ASN:HB2	2.10	0.52
1:D:114:GLY:HA2	1:D:119:TYR:CE2	2.44	0.52
1:E:83:GLU:OE2	1:E:83:GLU:HA	2.10	0.52
1:B:41:ASN:HD21	1:B:69:ASN:HB2	1.75	0.52
1:C:103:ASN:C	1:C:103:ASN:ND2	2.62	0.52
1:A:83:GLU:HA	1:A:83:GLU:OE2	2.09	0.52
1:A:217:LYS:H	1:A:250:ASN:ND2	2.06	0.52
1:B:103:ASN:C	1:B:103:ASN:ND2	2.63	0.52
1:C:123:LEU:HD13	1:C:128:VAL:CG1	2.40	0.52
1:D:136:VAL:HG12	1:D:138:LEU:HD23	1.91	0.52
1:E:51:ALA:C	1:E:52:LEU:HD23	2.30	0.52
1:E:340:PRO:HG3	1:E:353:TYR:CB	2.40	0.52
2:A:603:UMP:OP1	1:B:383:ARG:NH1	2.43	0.52
1:B:104:ASP:HB3	1:B:107:ILE:HD13	1.91	0.52
1:B:136:VAL:HG12	1:B:138:LEU:HD23	1.91	0.52
1:E:11:ALA:HB2	3:E:621:F89:H3M2	1.92	0.52
1:E:183:LEU:HD21	5:E:643:HOH:O	2.08	0.52
1:E:423:ARG:NH1	2:E:619:UMP:OP3	2.38	0.52
1:E:468:ASN:H	1:E:468:ASN:ND2	2.07	0.52
1:C:113:CYS:O	3:C:613:F89:H6	2.10	0.52
1:A:359:ASP:CG	1:A:361:THR:HG22	2.30	0.52
3:A:604:F89:OE1	3:A:604:F89:HA	2.10	0.52
1:B:509:TYR:HA	5:B:621:HOH:O	2.10	0.52
1:C:83:GLU:OE2	1:C:83:GLU:HA	2.10	0.51
1:D:51:ALA:C	1:D:52:LEU:HD23	2.31	0.51
1:D:320:GLY:O	1:D:335:GLU:O	2.26	0.51
1:D:519:MET:HG2	1:D:520:ALA:N	2.25	0.51
1:C:126:ASN:ND2	1:C:177:LYS:NZ	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ARG:NH1	1:E:242:ASP:OD1	2.41	0.51
1:C:75:ILE:O	4:C:614:NDP:H1B	2.11	0.51
1:C:468:ASN:H	1:C:468:ASN:ND2	2.08	0.51
1:E:388:ALA:O	1:E:401:PRO:HG2	2.09	0.51
1:A:288:ILE:HD11	1:A:440:ILE:HD11	1.92	0.51
1:E:315:ILE:HD12	3:E:620:F89:C8	2.41	0.51
1:B:304:ASN:ND2	1:B:306:ASN:HB2	2.26	0.51
1:D:304:ASN:ND2	1:D:306:ASN:HB2	2.25	0.51
1:B:115:GLY:HA3	4:B:610:NDP:O1A	2.11	0.51
1:C:4:LYS:HB3	1:C:101:LEU:HD23	1.92	0.51
1:A:136:VAL:HG12	1:A:138:LEU:HD23	1.92	0.51
1:E:288:ILE:HD11	1:E:440:ILE:HD11	1.92	0.51
1:A:340:PRO:HG3	1:A:353:TYR:CB	2.41	0.51
1:B:83:GLU:OE2	1:B:83:GLU:HA	2.10	0.51
1:E:126:ASN:HD21	1:E:177:LYS:NZ	2.07	0.51
1:A:304:ASN:ND2	1:A:304:ASN:C	2.61	0.51
1:C:217:LYS:H	1:C:250:ASN:ND2	2.07	0.51
1:D:33:LEU:HB3	3:D:617:F89:CG	2.34	0.50
1:E:103:ASN:C	1:E:103:ASN:ND2	2.65	0.50
1:E:304:ASN:ND2	1:E:304:ASN:C	2.63	0.50
1:A:41:ASN:HD21	1:A:69:ASN:HB2	1.75	0.50
1:D:287:ALA:HB1	5:D:654:HOH:O	2.10	0.50
1:E:130:ARG:HD2	1:E:132:TYR:CE1	2.47	0.50
1:A:103:ASN:C	1:A:103:ASN:ND2	2.65	0.50
1:B:51:ALA:C	1:B:52:LEU:HD23	2.32	0.50
1:C:239:GLN:HG3	1:C:271:ARG:O	2.11	0.50
1:D:75:ILE:O	4:D:618:NDP:H1B	2.11	0.50
1:D:123:LEU:HD13	1:D:128:VAL:CG1	2.41	0.50
1:C:304:ASN:ND2	1:C:306:ASN:HB2	2.26	0.50
1:D:103:ASN:C	1:D:103:ASN:ND2	2.64	0.50
1:E:4:LYS:HB3	1:E:101:LEU:HD23	1.93	0.50
1:A:123:LEU:HD13	1:A:128:VAL:CG1	2.42	0.50
1:C:233:ARG:NH1	1:C:242:ASP:OD1	2.43	0.50
1:D:340:PRO:HG3	1:D:353:TYR:CB	2.41	0.50
1:E:308:LEU:HD12	1:E:313:VAL:HG11	1.94	0.50
1:C:4:LYS:H	1:C:101:LEU:CD2	2.24	0.50
1:C:115:GLY:HA3	4:C:614:NDP:O1A	2.12	0.50
1:D:41:ASN:HD21	1:D:69:ASN:HB2	1.76	0.50
1:D:193:LEU:N	1:D:193:LEU:HD23	2.27	0.50
1:E:41:ASN:HD21	1:E:69:ASN:HB2	1.75	0.50
1:E:519:MET:HG2	1:E:520:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLY:HA2	1:C:119:TYR:CE2	2.47	0.50
1:C:126:ASN:HD21	1:C:177:LYS:NZ	2.10	0.50
1:D:131:ILE:HB	1:D:175:PHE:HB2	1.94	0.50
1:E:487:LEU:O	1:E:488:LYS:HD3	2.12	0.50
1:A:405:LEU:HD11	1:B:404:VAL:HG11	1.93	0.50
1:D:468:ASN:H	1:D:468:ASN:ND2	2.10	0.50
1:E:239:GLN:HG3	1:E:271:ARG:O	2.12	0.50
1:B:490:LYS:HE2	1:B:505:GLU:HG3	1.94	0.49
1:D:239:GLN:HG3	1:D:271:ARG:O	2.11	0.49
3:D:616:F89:OE1	3:D:616:F89:HA	2.10	0.49
1:A:130:ARG:HD2	1:A:132:TYR:CE1	2.47	0.49
1:C:51:ALA:C	1:C:52:LEU:HD23	2.32	0.49
1:C:179:GLU:OE2	1:C:179:GLU:HA	2.12	0.49
1:D:115:GLY:HA3	4:D:618:NDP:O1A	2.11	0.49
1:E:308:LEU:HD12	1:E:313:VAL:CG1	2.42	0.49
1:B:4:LYS:HB3	1:B:101:LEU:HD23	1.93	0.49
1:C:288:ILE:HD11	1:C:440:ILE:HD11	1.93	0.49
1:C:41:ASN:HD21	1:C:69:ASN:HB2	1.77	0.49
1:C:133:LEU:HD22	1:C:134:THR:N	2.27	0.49
1:D:113:CYS:O	3:D:617:F89:H6	2.11	0.49
1:D:284:LYS:HZ1	1:D:432:PRO:HG2	1.76	0.49
1:A:487:LEU:O	1:A:488:LYS:HD3	2.13	0.49
1:E:402:CYS:SG	2:E:619:UMP:C6	3.05	0.49
1:C:308:LEU:HD12	1:C:313:VAL:HG11	1.95	0.49
1:A:378:ASN:ND2	1:A:381:ASP:HB2	2.27	0.49
1:A:468:ASN:H	1:A:468:ASN:ND2	2.09	0.49
1:B:315:ILE:HD12	3:B:608:F89:C8	2.43	0.49
1:C:19:ILE:O	4:C:614:NDP:H2N	2.12	0.49
1:B:233:ARG:NH1	1:B:242:ASP:OD1	2.43	0.49
1:B:308:LEU:HD12	1:B:313:VAL:HG11	1.93	0.49
2:C:611:UMP:OP1	1:D:383:ARG:NH1	2.46	0.49
1:B:113:CYS:O	3:B:609:F89:H6	2.11	0.49
1:B:359:ASP:CG	1:B:361:THR:HG22	2.33	0.49
1:D:288:ILE:HD11	1:D:440:ILE:HD11	1.94	0.49
1:A:131:ILE:HB	1:A:175:PHE:HB2	1.94	0.48
1:C:388:ALA:O	1:C:401:PRO:HG2	2.13	0.48
1:A:490:LYS:HE2	1:A:505:GLU:HG3	1.96	0.48
1:B:468:ASN:N	1:B:468:ASN:ND2	2.61	0.48
1:C:202:LEU:HG	1:D:38:LYS:HB3	1.94	0.48
1:E:131:ILE:HB	1:E:175:PHE:HB2	1.95	0.48
1:A:37:SER:HB2	3:A:605:F89:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD12	1:B:313:VAL:CG1	2.44	0.48
1:A:280:LEU:HD11	1:A:286:VAL:HB	1.95	0.48
1:A:284:LYS:HZ1	1:A:432:PRO:HG2	1.77	0.48
1:B:37:SER:O	1:B:41:ASN:HB2	2.14	0.48
1:B:193:LEU:N	1:B:193:LEU:HD23	2.28	0.48
1:C:359:ASP:CG	1:C:361:THR:HG22	2.34	0.48
3:C:613:F89:O1A	3:C:613:F89:C10	2.53	0.48
1:C:405:LEU:C	1:C:405:LEU:HD23	2.34	0.48
1:D:4:LYS:H	1:D:101:LEU:CD2	2.26	0.48
1:E:113:CYS:O	3:E:621:F89:H6	2.13	0.48
1:B:239:GLN:HG3	1:B:271:ARG:O	2.13	0.48
1:C:308:LEU:HD12	1:C:313:VAL:CG1	2.43	0.48
1:C:423:ARG:NH1	2:C:611:UMP:OP3	2.42	0.48
1:C:56:ARG:O	1:C:59:TRP:HB3	2.14	0.48
1:E:133:LEU:HD22	1:E:134:THR:N	2.28	0.48
1:E:4:LYS:H	1:E:101:LEU:CD2	2.27	0.48
1:E:315:ILE:CG2	3:E:620:F89:C15	2.92	0.48
1:B:225:ASN:O	1:B:226:THR:C	2.53	0.48
1:E:25:LEU:HD11	3:E:621:F89:H10	1.95	0.48
1:B:62:ILE:N	1:B:62:ILE:HD13	2.28	0.48
1:B:288:ILE:HG23	1:B:501:TRP:HH2	1.79	0.48
1:A:114:GLY:HA2	1:A:119:TYR:CE2	2.49	0.47
1:D:294:GLU:O	1:D:297:TRP:HB3	2.14	0.47
1:D:343:GLY:HA2	1:D:346:TRP:HB2	1.96	0.47
1:E:37:SER:O	1:E:41:ASN:HB2	2.14	0.47
1:A:289:ARG:NH1	5:A:629:HOH:O	2.47	0.47
1:A:304:ASN:HD21	1:A:306:ASN:CB	2.27	0.47
1:B:131:ILE:HB	1:B:175:PHE:HB2	1.95	0.47
1:B:280:LEU:HD11	1:B:286:VAL:HB	1.96	0.47
1:D:115:GLY:HA3	4:D:618:NDP:PA	2.54	0.47
1:D:130:ARG:HD2	1:D:132:TYR:CE1	2.48	0.47
1:D:487:LEU:O	1:D:488:LYS:HD3	2.13	0.47
1:E:304:ASN:HD21	1:E:306:ASN:CB	2.26	0.47
1:A:297:TRP:CD2	1:A:308:LEU:HD21	2.50	0.47
1:B:96:ASP:O	1:B:99:GLU:HG3	2.14	0.47
1:C:404:VAL:HG11	1:D:405:LEU:HD11	1.97	0.47
1:D:388:ALA:O	1:D:401:PRO:HG2	2.15	0.47
1:A:269:MET:HE1	1:B:269:MET:CE	2.44	0.47
1:C:315:ILE:HD12	3:C:612:F89:C8	2.45	0.47
1:A:193:LEU:HD21	1:A:196:ILE:CD1	2.41	0.47
1:D:56:ARG:O	1:D:59:TRP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:LEU:HD11	1:E:286:VAL:HB	1.95	0.47
1:A:37:SER:O	1:A:41:ASN:HB2	2.14	0.47
1:B:123:LEU:HD13	1:B:128:VAL:CG1	2.44	0.47
1:B:297:TRP:CD2	1:B:308:LEU:HD21	2.49	0.47
1:C:62:ILE:HD13	1:C:62:ILE:N	2.30	0.47
1:C:199:THR:OG1	1:D:174:ILE:HD11	2.15	0.47
1:D:4:LYS:HB3	1:D:101:LEU:HD23	1.94	0.47
1:E:472:GLN:HG2	1:E:517:MET:HG2	1.97	0.47
1:A:62:ILE:N	1:A:62:ILE:HD13	2.30	0.47
1:A:75:ILE:O	4:A:606:NDP:H1B	2.14	0.47
1:B:79:LEU:HD23	1:B:80:PRO:CD	2.45	0.47
1:C:206:ILE:HG12	1:D:34:LYS:HG2	1.96	0.47
1:C:340:PRO:HG3	1:C:353:TYR:CB	2.44	0.47
1:E:56:ARG:O	1:E:59:TRP:HB3	2.15	0.47
1:A:101:LEU:O	1:A:103:ASN:N	2.46	0.47
1:B:423:ARG:NH1	2:B:607:UMP:OP3	2.43	0.47
3:D:616:F89:O1A	3:D:616:F89:C10	2.54	0.47
1:E:343:GLY:HA2	1:E:346:TRP:HB2	1.97	0.47
1:E:405:LEU:HD23	1:E:405:LEU:C	2.36	0.47
1:E:490:LYS:HE2	1:E:505:GLU:HG3	1.97	0.47
1:A:308:LEU:HD12	1:A:313:VAL:CG1	2.45	0.47
1:A:383:ARG:NH1	1:B:400:PRO:HD2	2.30	0.47
1:D:171:ASP:OD2	1:D:483:PRO:HD3	2.15	0.47
1:D:339:GLY:HA2	1:D:353:TYR:CE2	2.50	0.47
1:E:248:LEU:HD13	1:E:465:ILE:HD12	1.97	0.47
1:E:315:ILE:HG21	3:E:620:F89:C14	2.45	0.47
1:E:340:PRO:HG3	1:E:353:TYR:CG	2.50	0.47
1:A:4:LYS:HB3	1:A:101:LEU:HD23	1.94	0.46
1:A:459:PHE:CD2	1:B:459:PHE:CD2	3.03	0.46
1:C:53:ILE:HG23	1:C:75:ILE:HD13	1.97	0.46
1:C:193:LEU:HD21	1:C:196:ILE:CD1	2.41	0.46
1:D:233:ARG:NH1	1:D:242:ASP:OD2	2.48	0.46
1:E:62:ILE:HD13	1:E:62:ILE:N	2.29	0.46
1:E:92:ARG:O	4:E:622:NDP:H2A	2.15	0.46
1:E:96:ASP:O	1:E:99:GLU:HG3	2.15	0.46
1:E:288:ILE:HG23	1:E:501:TRP:HH2	1.80	0.46
3:B:609:F89:C6A	4:B:610:NDP:H42N	2.45	0.46
1:C:297:TRP:CD2	1:C:308:LEU:HD21	2.50	0.46
1:D:308:LEU:HD12	1:D:313:VAL:CG1	2.45	0.46
1:C:131:ILE:HB	1:C:175:PHE:HB2	1.95	0.46
1:C:295:LEU:O	1:C:299:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:HD22	1:D:134:THR:N	2.30	0.46
3:E:620:F89:O1A	3:E:620:F89:C10	2.55	0.46
1:A:254:ARG:HB2	1:B:380:LYS:HD2	1.97	0.46
1:A:340:PRO:HG3	1:A:353:TYR:CG	2.50	0.46
1:B:335:GLU:HB3	5:B:682:HOH:O	2.16	0.46
1:E:193:LEU:HD23	1:E:193:LEU:N	2.30	0.46
1:E:224:TYR:O	1:E:227:PRO:HG3	2.16	0.46
1:A:388:ALA:O	1:A:401:PRO:HG2	2.15	0.46
1:A:402:CYS:SG	2:A:603:UMP:C6	3.09	0.46
1:B:53:ILE:HG23	1:B:75:ILE:HD13	1.98	0.46
1:B:99:GLU:OE2	1:B:99:GLU:O	2.34	0.46
1:B:193:LEU:HD21	1:B:196:ILE:CD1	2.44	0.46
1:B:248:LEU:HD13	1:B:465:ILE:HD12	1.97	0.46
1:C:512:TYR:HB3	1:C:513:PRO:HD2	1.97	0.46
1:D:8:ILE:HG12	1:D:112:VAL:HB	1.97	0.46
1:B:56:ARG:O	1:B:59:TRP:HB3	2.16	0.46
1:C:224:TYR:O	1:C:227:PRO:HG3	2.15	0.46
1:A:315:ILE:HG21	3:A:604:F89:C16	2.45	0.46
1:B:4:LYS:H	1:B:101:LEU:CD2	2.28	0.46
1:C:10:VAL:HG22	1:C:11:ALA:N	2.31	0.46
1:C:53:ILE:HG23	1:C:75:ILE:CD1	2.46	0.46
1:C:225:ASN:O	1:C:226:THR:C	2.54	0.46
1:C:293:GLU:HG2	1:C:311:LYS:HB3	1.97	0.46
1:D:224:TYR:O	1:D:227:PRO:HG3	2.15	0.46
1:E:297:TRP:CD2	1:E:308:LEU:HD21	2.50	0.46
1:A:248:LEU:HD13	1:A:465:ILE:HD12	1.98	0.46
1:A:293:GLU:HG2	1:A:311:LYS:HB3	1.98	0.46
1:B:79:LEU:HA	1:B:80:PRO:HD3	1.83	0.46
1:E:14:VAL:HG13	1:E:15:LEU:HG	1.98	0.46
1:C:96:ASP:O	1:C:99:GLU:HG3	2.14	0.46
1:C:472:GLN:HG2	1:C:517:MET:HG2	1.97	0.46
1:D:62:ILE:N	1:D:62:ILE:HD13	2.31	0.46
1:D:288:ILE:HG23	1:D:501:TRP:HH2	1.81	0.46
1:D:470:LEU:HD12	1:D:470:LEU:HA	1.80	0.46
1:A:4:LYS:H	1:A:101:LEU:CD2	2.29	0.46
1:A:288:ILE:HG23	1:A:501:TRP:HH2	1.81	0.46
1:A:315:ILE:HD12	3:A:604:F89:C8	2.46	0.46
1:E:428:GLY:O	1:E:517:MET:HE3	2.16	0.46
1:B:52:LEU:HD23	1:B:52:LEU:N	2.31	0.45
1:D:405:LEU:C	1:D:405:LEU:HD23	2.36	0.45
1:E:380:LYS:HE3	1:E:412:ASN:ND2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA2	1:B:119:TYR:CE2	2.51	0.45
1:B:340:PRO:HG3	1:B:353:TYR:CB	2.46	0.45
3:B:608:F89:O1A	3:B:608:F89:C10	2.54	0.45
1:C:468:ASN:N	1:C:468:ASN:ND2	2.63	0.45
1:D:372:ILE:O	1:D:376:LYS:HG2	2.16	0.45
1:D:423:ARG:NH1	2:D:615:UMP:OP3	2.39	0.45
1:A:383:ARG:NH1	2:B:607:UMP:OP1	2.50	0.45
1:C:280:LEU:HD11	1:C:286:VAL:HB	1.98	0.45
1:D:340:PRO:HG3	1:D:353:TYR:CG	2.51	0.45
1:A:359:ASP:OD2	1:A:361:THR:CG2	2.61	0.45
1:D:193:LEU:HD21	1:D:196:ILE:CD1	2.43	0.45
1:E:8:ILE:HG12	1:E:112:VAL:HB	1.99	0.45
1:A:96:ASP:O	1:A:99:GLU:HG3	2.17	0.45
1:C:163:PHE:HA	1:C:276:GLU:HB3	1.98	0.45
1:C:372:ILE:O	1:C:376:LYS:HG2	2.17	0.45
1:C:519:MET:HA	5:C:624:HOH:O	2.17	0.45
1:D:308:LEU:HD12	1:D:313:VAL:HG11	1.98	0.45
1:B:37:SER:HB2	3:B:609:F89:HB1	1.99	0.45
1:C:490:LYS:HE2	1:C:505:GLU:HG3	1.98	0.45
1:D:10:VAL:HG22	1:D:11:ALA:N	2.31	0.45
1:D:163:PHE:HA	1:D:276:GLU:HB3	1.98	0.45
1:D:311:LYS:NZ	5:D:677:HOH:O	2.49	0.45
1:E:468:ASN:N	1:E:468:ASN:ND2	2.63	0.45
1:A:53:ILE:HG23	1:A:75:ILE:HD13	1.98	0.45
1:A:225:ASN:O	1:A:226:THR:C	2.54	0.45
1:A:284:LYS:HZ3	1:A:517:MET:HE1	1.81	0.45
3:A:605:F89:O1A	3:A:605:F89:C10	2.53	0.45
1:B:10:VAL:HG22	1:B:11:ALA:N	2.32	0.45
1:B:101:LEU:O	1:B:103:ASN:N	2.47	0.45
1:B:163:PHE:HA	1:B:276:GLU:HB3	1.98	0.45
1:B:293:GLU:HG2	1:B:311:LYS:HB3	1.99	0.45
1:C:93:ASN:OD1	1:C:96:ASP:HB2	2.17	0.45
1:E:138:LEU:HD23	1:E:138:LEU:N	2.32	0.45
1:E:359:ASP:OD2	1:E:361:THR:CG2	2.62	0.45
1:A:269:MET:HE2	1:B:269:MET:HE1	1.97	0.45
1:C:8:ILE:HG12	1:C:112:VAL:HB	1.99	0.45
1:C:37:SER:O	1:C:41:ASN:HB2	2.16	0.45
1:D:490:LYS:HE2	1:D:505:GLU:HG3	1.97	0.45
1:E:293:GLU:HG2	1:E:311:LYS:HB3	1.98	0.45
1:A:8:ILE:HG12	1:A:112:VAL:HB	1.99	0.45
1:A:154:PHE:CE1	1:A:177:LYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLU:HG2	1:B:497:GLU:H	1.58	0.45
1:D:280:LEU:HD11	1:D:286:VAL:HB	1.97	0.45
1:A:52:LEU:HD23	1:A:52:LEU:N	2.32	0.45
1:A:383:ARG:CZ	1:B:400:PRO:HG2	2.47	0.45
1:B:264:SER:CB	1:B:464:HIS:HB3	2.47	0.45
1:D:79:LEU:HD23	1:D:80:PRO:CD	2.47	0.45
1:D:304:ASN:HD21	1:D:306:ASN:CB	2.29	0.45
1:E:93:ASN:OD1	1:E:96:ASP:HB2	2.17	0.45
1:A:294:GLU:O	1:A:297:TRP:HB3	2.17	0.44
1:B:304:ASN:ND2	1:B:304:ASN:C	2.63	0.44
1:C:38:LYS:HB3	1:D:202:LEU:HG	1.98	0.44
1:C:304:ASN:HD21	1:C:306:ASN:CB	2.29	0.44
1:C:308:LEU:HD12	1:C:313:VAL:HB	1.99	0.44
1:C:402:CYS:SG	2:C:611:UMP:C6	3.11	0.44
1:D:472:GLN:HG2	1:D:517:MET:HG2	1.98	0.44
1:E:193:LEU:HD21	1:E:196:ILE:CD1	2.44	0.44
1:E:295:LEU:O	1:E:299:ILE:HG13	2.16	0.44
1:A:380:LYS:HE3	1:A:412:ASN:ND2	2.32	0.44
1:C:101:LEU:O	1:C:103:ASN:N	2.50	0.44
1:D:81:GLN:NE2	1:D:92:ARG:NE	2.64	0.44
1:D:308:LEU:HD12	1:D:313:VAL:HB	1.99	0.44
1:A:133:LEU:HD22	1:A:134:THR:N	2.32	0.44
1:B:288:ILE:HD11	1:B:440:ILE:HD11	1.98	0.44
1:C:99:GLU:C	1:C:101:LEU:N	2.69	0.44
1:C:193:LEU:HD23	1:C:193:LEU:N	2.31	0.44
1:D:99:GLU:C	1:D:101:LEU:N	2.69	0.44
1:E:10:VAL:HG22	1:E:11:ALA:N	2.32	0.44
1:E:226:THR:N	1:E:227:PRO:HD3	2.33	0.44
1:A:308:LEU:HD12	1:A:313:VAL:HG11	1.98	0.44
1:C:288:ILE:HG23	1:C:501:TRP:HH2	1.80	0.44
1:D:56:ARG:HG3	1:D:79:LEU:HD12	1.99	0.44
1:E:96:ASP:O	1:E:99:GLU:CG	2.66	0.44
1:E:100:ASN:HB2	1:E:110:ILE:HD11	1.99	0.44
1:A:53:ILE:HG23	1:A:75:ILE:CD1	2.47	0.44
1:A:371:LEU:O	1:A:374:THR:HG22	2.18	0.44
1:A:405:LEU:C	1:A:405:LEU:HD23	2.37	0.44
1:B:388:ALA:O	1:B:401:PRO:HG2	2.17	0.44
1:C:37:SER:HB2	3:C:613:F89:HB1	1.98	0.44
1:A:114:GLY:HA3	4:A:606:NDP:H5N	2.00	0.44
1:A:472:GLN:HG2	1:A:517:MET:HG2	2.00	0.44
3:A:604:F89:O1A	3:A:604:F89:C10	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LEU:HD22	1:C:133:LEU:C	2.38	0.44
1:C:181:LYS:O	1:C:182:THR:HB	2.17	0.44
1:C:380:LYS:HE3	1:C:412:ASN:ND2	2.33	0.44
1:C:470:LEU:HD12	1:C:470:LEU:HA	1.79	0.44
1:E:339:GLY:HA2	1:E:353:TYR:CE2	2.53	0.44
1:A:79:LEU:HD23	1:A:80:PRO:CD	2.46	0.44
1:A:193:LEU:N	1:A:193:LEU:HD23	2.32	0.44
1:A:233:ARG:NH1	1:A:242:ASP:OD2	2.50	0.44
1:D:126:ASN:ND2	1:D:177:LYS:HZ2	2.16	0.44
1:D:154:PHE:CE1	1:D:177:LYS:HB2	2.53	0.44
1:D:248:LEU:HD13	1:D:465:ILE:HD12	2.00	0.44
1:D:297:TRP:CD2	1:D:308:LEU:HD21	2.51	0.44
1:D:512:TYR:HB3	1:D:513:PRO:HD2	1.99	0.44
1:E:163:PHE:HA	1:E:276:GLU:HB3	2.00	0.44
1:A:56:ARG:O	1:A:59:TRP:HB3	2.17	0.44
1:B:183:LEU:O	1:B:184:GLN:HB3	2.18	0.44
1:B:470:LEU:HD12	1:B:470:LEU:HA	1.79	0.44
1:C:34:LYS:HE3	1:C:34:LYS:HB2	1.77	0.44
1:E:308:LEU:HD12	1:E:313:VAL:HB	1.99	0.44
1:E:372:ILE:O	1:E:376:LYS:HG2	2.18	0.44
3:A:605:F89:C6A	4:A:606:NDP:H42N	2.47	0.44
1:C:114:GLY:HA3	4:C:614:NDP:H5N	2.00	0.44
1:C:154:PHE:CE1	1:C:177:LYS:HB2	2.52	0.44
1:E:52:LEU:HD23	1:E:52:LEU:N	2.32	0.44
1:E:512:TYR:HB3	1:E:513:PRO:HD2	1.99	0.44
1:B:372:ILE:O	1:B:376:LYS:HG2	2.18	0.43
1:C:183:LEU:O	1:C:184:GLN:HB3	2.18	0.43
1:D:428:GLY:O	1:D:517:MET:HE3	2.17	0.43
1:E:115:GLY:HA3	4:E:622:NDP:O1A	2.17	0.43
1:E:181:LYS:O	1:E:182:THR:HB	2.18	0.43
1:B:53:ILE:HG23	1:B:75:ILE:CD1	2.49	0.43
1:C:56:ARG:HG3	1:C:79:LEU:HD12	1.99	0.43
3:D:617:F89:O1A	3:D:617:F89:C10	2.53	0.43
1:E:53:ILE:HG23	1:E:75:ILE:HD13	2.00	0.43
1:E:154:PHE:CE1	1:E:177:LYS:HB2	2.53	0.43
1:B:56:ARG:HG3	1:B:79:LEU:HD12	2.00	0.43
1:B:512:TYR:HB3	1:B:513:PRO:HD2	1.99	0.43
1:C:96:ASP:O	1:C:99:GLU:CG	2.66	0.43
1:C:174:ILE:HD11	1:D:199:THR:OG1	2.18	0.43
1:D:293:GLU:HG2	1:D:311:LYS:HB3	1.99	0.43
1:E:99:GLU:C	1:E:101:LEU:N	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:CYS:O	3:A:605:F89:H6	2.18	0.43
1:A:183:LEU:O	1:A:184:GLN:HB3	2.19	0.43
1:A:383:ARG:HH12	1:B:400:PRO:HD2	1.82	0.43
1:B:78:SER:O	1:B:79:LEU:C	2.57	0.43
1:B:304:ASN:HD21	1:B:306:ASN:CB	2.30	0.43
1:C:104:ASP:CB	1:C:107:ILE:HD13	2.48	0.43
1:D:468:ASN:N	1:D:468:ASN:ND2	2.65	0.43
1:A:224:TYR:O	1:A:227:PRO:HG3	2.18	0.43
1:A:308:LEU:HD12	1:A:313:VAL:HB	2.01	0.43
1:C:79:LEU:HA	1:C:80:PRO:HD3	1.81	0.43
1:D:96:ASP:O	1:D:99:GLU:HG3	2.17	0.43
1:E:133:LEU:HD13	1:E:135:ARG:HG2	2.00	0.43
1:A:115:GLY:CA	4:A:606:NDP:PA	3.07	0.43
1:A:163:PHE:HA	1:A:276:GLU:HB3	2.00	0.43
1:B:93:ASN:OD1	1:B:96:ASP:HB2	2.18	0.43
1:B:102:MET:O	1:B:103:ASN:HB3	2.18	0.43
1:B:181:LYS:O	1:B:182:THR:HB	2.18	0.43
1:D:359:ASP:OD2	1:D:361:THR:CG2	2.62	0.43
1:E:81:GLN:NE2	1:E:92:ARG:NE	2.65	0.43
1:E:101:LEU:O	1:E:103:ASN:N	2.50	0.43
1:A:31:GLU:HG2	1:B:207:PHE:CE1	2.54	0.43
1:D:101:LEU:O	1:D:103:ASN:N	2.49	0.43
1:D:429:LEU:CD2	1:D:519:MET:HB2	2.49	0.43
1:E:75:ILE:HG22	4:E:622:NDP:C4A	2.49	0.43
1:E:225:ASN:O	1:E:226:THR:C	2.56	0.43
1:A:400:PRO:HG2	1:B:383:ARG:CZ	2.49	0.43
1:A:429:LEU:CD2	1:A:519:MET:HB2	2.49	0.43
1:B:154:PHE:CE1	1:B:177:LYS:HB2	2.53	0.43
1:C:248:LEU:HD13	1:C:465:ILE:HD12	1.99	0.43
1:D:203:LEU:HD12	1:D:203:LEU:HA	1.90	0.43
1:C:78:SER:O	1:C:79:LEU:C	2.57	0.43
1:C:115:GLY:O	1:C:116:GLU:C	2.57	0.43
1:C:343:GLY:HA2	1:C:346:TRP:HB2	2.01	0.43
1:D:34:LYS:HE3	1:D:34:LYS:HB2	1.82	0.43
1:D:52:LEU:HD23	1:D:52:LEU:N	2.33	0.43
1:D:78:SER:O	1:D:79:LEU:C	2.57	0.43
1:A:126:ASN:ND2	1:A:177:LYS:HZ2	2.17	0.43
1:A:181:LYS:O	1:A:182:THR:HB	2.19	0.43
1:A:372:ILE:O	1:A:376:LYS:HG2	2.19	0.43
1:B:43:LYS:NZ	1:B:48:LYS:O	2.42	0.43
1:B:101:LEU:C	1:B:103:ASN:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:GLY:HA2	1:B:346:TRP:HB2	2.00	0.43
1:C:247:VAL:HG21	1:C:465:ILE:HG13	2.01	0.43
1:D:53:ILE:HG23	1:D:75:ILE:HD13	2.01	0.43
1:C:383:ARG:NH1	2:D:615:UMP:OP1	2.52	0.42
1:C:428:GLY:O	1:C:517:MET:HE3	2.18	0.42
1:E:126:ASN:ND2	1:E:177:LYS:HZ2	2.17	0.42
1:A:512:TYR:HB3	1:A:513:PRO:HD2	2.01	0.42
1:B:472:GLN:HG2	1:B:517:MET:HG2	1.99	0.42
1:C:429:LEU:CD2	1:C:519:MET:HB2	2.49	0.42
1:D:225:ASN:O	1:D:226:THR:C	2.57	0.42
1:A:81:GLN:NE2	1:A:92:ARG:NE	2.65	0.42
1:A:226:THR:N	1:A:227:PRO:HD3	2.34	0.42
1:A:380:LYS:HD2	1:B:254:ARG:HB2	2.01	0.42
1:B:81:GLN:NE2	1:B:92:ARG:NE	2.63	0.42
1:B:323:GLU:OE2	1:B:323:GLU:N	2.44	0.42
1:C:14:VAL:HG13	1:C:15:LEU:HG	2.00	0.42
1:C:339:GLY:HA2	1:C:353:TYR:CE2	2.54	0.42
1:C:340:PRO:HG3	1:C:353:TYR:CG	2.53	0.42
1:D:93:ASN:OD1	1:D:96:ASP:HB2	2.19	0.42
1:D:247:VAL:HG21	1:D:465:ILE:HG13	2.02	0.42
1:D:315:ILE:HD13	3:D:616:F89:C13	2.48	0.42
1:E:104:ASP:CB	1:E:107:ILE:HD13	2.48	0.42
1:E:209:ILE:CD1	1:E:209:ILE:N	2.70	0.42
3:E:621:F89:O1A	3:E:621:F89:C10	2.53	0.42
1:A:10:VAL:HG22	1:A:11:ALA:N	2.34	0.42
1:A:115:GLY:HA2	4:A:606:NDP:O5D	2.19	0.42
1:A:264:SER:CB	1:A:464:HIS:HB3	2.49	0.42
1:A:497:GLU:HG2	1:A:497:GLU:H	1.60	0.42
1:B:8:ILE:HG12	1:B:112:VAL:HB	2.02	0.42
1:B:114:GLY:HA3	4:B:610:NDP:H5N	2.01	0.42
1:B:247:VAL:HG21	1:B:465:ILE:HG13	2.00	0.42
1:B:295:LEU:O	1:B:299:ILE:HG13	2.19	0.42
1:E:133:LEU:CD1	1:E:135:ARG:HG2	2.49	0.42
1:E:247:VAL:HG21	1:E:465:ILE:HG13	2.01	0.42
1:E:264:SER:CB	1:E:464:HIS:HB3	2.50	0.42
1:E:294:GLU:O	1:E:297:TRP:HB3	2.19	0.42
1:A:284:LYS:NZ	1:A:517:MET:HE1	2.34	0.42
1:B:34:LYS:HB2	1:B:34:LYS:HE3	1.82	0.42
1:C:115:GLY:HA3	4:C:614:NDP:PA	2.59	0.42
1:E:183:LEU:O	1:E:184:GLN:HB3	2.19	0.42
1:A:203:LEU:HD11	1:B:172:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:LEU:CD2	1:B:519:MET:HB2	2.50	0.42
1:C:233:ARG:NH1	1:C:242:ASP:OD2	2.53	0.42
1:C:371:LEU:O	1:C:374:THR:HG22	2.20	0.42
1:D:181:LYS:O	1:D:182:THR:HB	2.20	0.42
1:D:264:SER:CB	1:D:464:HIS:HB3	2.50	0.42
1:E:34:LYS:HB2	1:E:34:LYS:HE3	1.80	0.42
1:E:248:LEU:HD12	1:E:248:LEU:HA	1.91	0.42
1:E:371:LEU:O	1:E:374:THR:HG22	2.20	0.42
1:A:33:LEU:HD22	3:A:605:F89:H14	2.02	0.42
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.90	0.42
1:C:100:ASN:HB2	1:C:110:ILE:HD11	2.01	0.42
1:C:248:LEU:HD13	1:C:465:ILE:CD1	2.50	0.42
1:D:497:GLU:HG2	1:D:497:GLU:H	1.59	0.42
1:E:53:ILE:HG23	1:E:75:ILE:CD1	2.49	0.42
1:E:56:ARG:HG3	1:E:79:LEU:HD12	2.00	0.42
1:E:133:LEU:HD22	1:E:133:LEU:C	2.40	0.42
1:E:207:PHE:HB3	1:E:210:ARG:HB2	2.02	0.42
1:A:96:ASP:O	1:A:99:GLU:CG	2.68	0.42
1:A:223:ILE:HD11	1:A:249:GLU:OE1	2.20	0.42
1:A:284:LYS:NZ	1:A:517:MET:CE	2.83	0.42
1:A:295:LEU:O	1:A:299:ILE:HG13	2.20	0.42
1:B:220:LYS:NZ	5:B:705:HOH:O	2.52	0.42
1:C:248:LEU:HD12	1:C:248:LEU:HA	1.91	0.42
1:A:101:LEU:C	1:A:103:ASN:H	2.22	0.42
1:B:96:ASP:O	1:B:99:GLU:CG	2.68	0.42
1:E:79:LEU:HD23	1:E:80:PRO:CD	2.46	0.42
1:E:361:THR:HG23	1:E:361:THR:O	2.20	0.42
1:A:47:ASN:HD22	1:A:47:ASN:HA	1.66	0.42
1:A:310:GLU:C	1:A:312:LYS:H	2.24	0.42
1:A:461:GLY:HA3	1:B:407:GLN:OE1	2.20	0.42
1:B:226:THR:N	1:B:227:PRO:HD3	2.35	0.42
1:B:371:LEU:O	1:B:374:THR:HG22	2.20	0.42
1:C:39:ILE:CG2	1:C:40:THR:N	2.83	0.42
1:C:126:ASN:ND2	1:C:177:LYS:HZ2	2.17	0.42
1:C:220:LYS:NZ	5:C:690:HOH:O	2.51	0.42
1:C:238:PHE:O	1:C:242:ASP:HB2	2.20	0.42
1:C:284:LYS:NZ	1:C:517:MET:HE1	2.35	0.42
1:D:183:LEU:O	1:D:184:GLN:HB3	2.19	0.42
1:E:429:LEU:CD2	1:E:519:MET:HB2	2.50	0.42
1:A:238:PHE:O	1:A:242:ASP:HB2	2.20	0.41
1:B:133:LEU:HD13	1:B:135:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:CG2	1:D:40:THR:N	2.82	0.41
1:D:209:ILE:CD1	1:D:209:ILE:N	2.70	0.41
1:A:126:ASN:CG	1:A:177:LYS:HZ1	2.24	0.41
1:C:101:LEU:C	1:C:103:ASN:H	2.23	0.41
1:C:138:LEU:HD23	1:C:138:LEU:N	2.35	0.41
1:D:371:LEU:O	1:D:374:THR:HG22	2.20	0.41
1:A:207:PHE:CE1	1:B:31:GLU:HG2	2.55	0.41
1:B:133:LEU:HD22	1:B:134:THR:N	2.34	0.41
1:B:224:TYR:O	1:B:227:PRO:HG3	2.20	0.41
1:C:271:ARG:HD3	1:D:212:MET:CE	2.50	0.41
1:D:138:LEU:HD23	1:D:138:LEU:N	2.35	0.41
1:E:133:LEU:HD13	1:E:135:ARG:CG	2.50	0.41
1:E:470:LEU:HD12	1:E:470:LEU:HA	1.81	0.41
1:A:102:MET:O	1:A:103:ASN:HB3	2.20	0.41
1:B:133:LEU:HD13	1:B:135:ARG:CG	2.49	0.41
1:C:81:GLN:NE2	1:C:92:ARG:NE	2.64	0.41
1:D:96:ASP:O	1:D:99:GLU:CG	2.69	0.41
1:D:133:LEU:HD22	1:D:133:LEU:C	2.41	0.41
1:D:380:LYS:HE3	1:D:412:ASN:ND2	2.36	0.41
1:D:479:ARG:HD3	1:D:512:TYR:CG	2.55	0.41
1:E:39:ILE:CG2	1:E:40:THR:N	2.83	0.41
1:E:233:ARG:NH1	1:E:242:ASP:OD2	2.52	0.41
1:A:343:GLY:HA2	1:A:346:TRP:HB2	2.02	0.41
1:B:99:GLU:C	1:B:101:LEU:N	2.72	0.41
1:C:226:THR:N	1:C:227:PRO:HD3	2.36	0.41
1:C:497:GLU:HG2	1:C:497:GLU:H	1.58	0.41
1:D:37:SER:HB2	3:D:617:F89:HB1	2.03	0.41
1:D:101:LEU:C	1:D:103:ASN:H	2.24	0.41
1:E:62:ILE:HG22	1:E:62:ILE:O	2.20	0.41
1:E:208:GLY:C	1:E:210:ARG:N	2.74	0.41
1:A:93:ASN:OD1	1:A:96:ASP:HB2	2.20	0.41
1:B:115:GLY:CA	4:B:610:NDP:PA	3.09	0.41
1:C:25:LEU:HD11	3:C:613:F89:H10	2.03	0.41
1:E:102:MET:O	1:E:103:ASN:HB3	2.21	0.41
1:C:19:ILE:HD11	1:C:145:THR:HG22	2.03	0.41
1:C:102:MET:O	1:C:103:ASN:HB3	2.21	0.41
3:C:612:F89:HB2	3:C:612:F89:O	2.20	0.41
1:D:104:ASP:CB	1:D:107:ILE:HD13	2.50	0.41
1:E:248:LEU:HD13	1:E:465:ILE:CD1	2.50	0.41
1:A:269:MET:CE	1:B:269:MET:CE	2.98	0.41
1:B:248:LEU:HD13	1:B:465:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:NE2	1:C:92:ARG:CZ	2.84	0.41
1:D:102:MET:O	1:D:103:ASN:HB3	2.21	0.41
1:D:220:LYS:NZ	1:D:220:LYS:HB2	2.36	0.41
1:E:62:ILE:HD12	3:E:621:F89:C18	2.51	0.41
1:E:310:GLU:C	1:E:312:LYS:H	2.23	0.41
1:A:78:SER:O	1:A:79:LEU:C	2.59	0.41
1:A:248:LEU:HD13	1:A:465:ILE:CD1	2.51	0.41
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.85	0.41
1:B:181:LYS:HB2	1:B:182:THR:H	1.47	0.41
1:B:308:LEU:HD12	1:B:313:VAL:HB	2.03	0.41
1:B:340:PRO:HG3	1:B:353:TYR:CG	2.56	0.41
1:B:402:CYS:SG	2:B:607:UMP:C6	3.14	0.41
1:B:405:LEU:C	1:B:405:LEU:HD23	2.41	0.41
1:C:354:LYS:HD2	1:C:358:ASP:OD2	2.21	0.41
1:D:53:ILE:HG23	1:D:75:ILE:CD1	2.51	0.41
1:E:78:SER:O	1:E:79:LEU:C	2.58	0.41
1:E:203:LEU:HD12	1:E:203:LEU:HA	1.93	0.41
1:E:340:PRO:HG3	1:E:353:TYR:HB2	2.03	0.41
1:A:99:GLU:C	1:A:101:LEU:N	2.71	0.41
1:A:133:LEU:HD13	1:A:135:ARG:HG2	2.03	0.41
1:B:138:LEU:HD23	1:B:138:LEU:N	2.36	0.41
1:B:294:GLU:O	1:B:297:TRP:HB3	2.21	0.41
1:B:310:GLU:C	1:B:312:LYS:H	2.25	0.41
1:D:223:ILE:HD11	1:D:249:GLU:OE1	2.21	0.41
1:A:14:VAL:HG13	1:A:15:LEU:HG	2.03	0.40
1:A:339:GLY:HA2	1:A:353:TYR:CE2	2.56	0.40
1:C:79:LEU:HD23	1:C:80:PRO:CD	2.45	0.40
1:C:480:THR:HA	1:C:481:PRO:HD3	1.96	0.40
1:D:238:PHE:O	1:D:242:ASP:HB2	2.21	0.40
1:D:310:GLU:C	1:D:312:LYS:H	2.23	0.40
1:E:62:ILE:HD11	3:E:621:F89:H8	2.02	0.40
1:E:101:LEU:C	1:E:103:ASN:H	2.24	0.40
1:A:158:TYR:O	1:A:173:MET:CB	2.70	0.40
1:B:133:LEU:CD1	1:B:135:ARG:HG2	2.51	0.40
1:C:52:LEU:HD23	1:C:52:LEU:N	2.35	0.40
1:C:182:THR:O	1:C:183:LEU:C	2.60	0.40
1:D:14:VAL:HG13	1:D:15:LEU:HG	2.02	0.40
1:E:238:PHE:O	1:E:242:ASP:HB2	2.20	0.40
1:A:264:SER:HB3	1:A:464:HIS:HB3	2.03	0.40
1:B:380:LYS:HE3	1:B:412:ASN:ND2	2.36	0.40
1:C:405:LEU:CD1	1:D:404:VAL:HG11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:THR:HG23	1:D:361:THR:O	2.21	0.40
1:E:182:THR:O	1:E:183:LEU:C	2.60	0.40
1:A:58:THR:O	1:A:61:SER:HB2	2.22	0.40
1:A:138:LEU:HD23	1:A:138:LEU:N	2.36	0.40
1:A:400:PRO:HD2	1:B:383:ARG:NH1	2.37	0.40
1:B:3:GLU:OE2	1:B:3:GLU:HA	2.22	0.40
1:C:247:VAL:O	1:C:251:GLY:N	2.51	0.40
1:E:220:LYS:NZ	1:E:220:LYS:HB2	2.36	0.40
1:A:207:PHE:HB3	1:A:210:ARG:HB2	2.04	0.40
1:B:354:LYS:HD2	1:B:358:ASP:OD2	2.22	0.40
1:D:92:ARG:O	4:D:618:NDP:H2A	2.22	0.40
1:E:260:ILE:N	1:E:260:ILE:CD1	2.83	0.40
1:E:308:LEU:HD12	1:E:313:VAL:CB	2.52	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	517/521 (99%)	472 (91%)	36 (7%)	9 (2%)	9	28
1	B	517/521 (99%)	472 (91%)	36 (7%)	9 (2%)	9	28
1	C	517/521 (99%)	470 (91%)	38 (7%)	9 (2%)	9	28
1	D	517/521 (99%)	473 (92%)	35 (7%)	9 (2%)	9	28
1	E	517/521 (99%)	469 (91%)	39 (8%)	9 (2%)	9	28
All	All	2585/2605 (99%)	2356 (91%)	184 (7%)	45 (2%)	9	28

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA

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Mol	Chain	Res	Type
1	A	102	MET
1	A	179	GLU
1	A	182	THR
1	B	84	ALA
1	B	102	MET
1	B	179	GLU
1	B	182	THR
1	C	84	ALA
1	C	102	MET
1	C	179	GLU
1	C	182	THR
1	D	84	ALA
1	D	102	MET
1	D	179	GLU
1	D	182	THR
1	E	84	ALA
1	E	102	MET
1	E	179	GLU
1	E	182	THR
1	A	103	ASN
1	A	335	GLU
1	B	103	ASN
1	B	335	GLU
1	C	103	ASN
1	C	335	GLU
1	D	103	ASN
1	D	335	GLU
1	E	103	ASN
1	E	335	GLU
1	A	183	LEU
1	B	183	LEU
1	C	183	LEU
1	D	183	LEU
1	E	183	LEU
1	A	184	GLN
1	B	184	GLN
1	C	184	GLN
1	D	184	GLN
1	E	184	GLN
1	C	341	ILE
1	D	341	ILE
1	E	341	ILE

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Mol	Chain	Res	Type
1	A	341	ILE
1	B	341	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/470 (100%)	432 (92%)	36 (8%)	13	34
1	B	468/470 (100%)	431 (92%)	37 (8%)	12	32
1	C	468/470 (100%)	432 (92%)	36 (8%)	13	34
1	D	468/470 (100%)	433 (92%)	35 (8%)	13	35
1	E	468/470 (100%)	434 (93%)	34 (7%)	14	36
All	All	2340/2350 (100%)	2162 (92%)	178 (8%)	13	35

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	41	ASN
1	A	79	LEU
1	A	81	GLN
1	A	99	GLU
1	A	102	MET
1	A	103	ASN
1	A	104	ASP
1	A	126	ASN
1	A	128	VAL
1	A	133	LEU
1	A	138	LEU
1	A	142	GLU
1	A	176	GLU
1	A	179	GLU
1	A	181	LYS
1	A	202	LEU

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Mol	Chain	Res	Type
1	A	203	LEU
1	A	209	ILE
1	A	220	LYS
1	A	247	VAL
1	A	248	LEU
1	A	289	ARG
1	A	295	LEU
1	A	296	ILE
1	A	304	ASN
1	A	371	LEU
1	A	383	ARG
1	A	427	LEU
1	A	468	ASN
1	A	470	LEU
1	A	471	THR
1	A	474	LYS
1	A	506	LEU
1	A	514	THR
1	A	516	LYS
1	B	4	LYS
1	B	41	ASN
1	B	79	LEU
1	B	81	GLN
1	B	99	GLU
1	B	102	MET
1	B	103	ASN
1	B	104	ASP
1	B	126	ASN
1	B	128	VAL
1	B	133	LEU
1	B	138	LEU
1	B	142	GLU
1	B	176	GLU
1	B	179	GLU
1	B	181	LYS
1	B	202	LEU
1	B	203	LEU
1	B	209	ILE
1	B	220	LYS
1	B	247	VAL
1	B	248	LEU
1	B	289	ARG

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Mol	Chain	Res	Type
1	B	295	LEU
1	B	296	ILE
1	B	304	ASN
1	B	311	LYS
1	B	371	LEU
1	B	383	ARG
1	B	427	LEU
1	B	468	ASN
1	B	470	LEU
1	B	471	THR
1	B	474	LYS
1	B	506	LEU
1	B	514	THR
1	B	516	LYS
1	C	4	LYS
1	C	41	ASN
1	C	79	LEU
1	C	81	GLN
1	C	99	GLU
1	C	102	MET
1	C	103	ASN
1	C	104	ASP
1	C	126	ASN
1	C	128	VAL
1	C	133	LEU
1	C	138	LEU
1	C	142	GLU
1	C	176	GLU
1	C	179	GLU
1	C	181	LYS
1	C	203	LEU
1	C	209	ILE
1	C	220	LYS
1	C	247	VAL
1	C	248	LEU
1	C	289	ARG
1	C	295	LEU
1	C	296	ILE
1	C	304	ASN
1	C	311	LYS
1	C	371	LEU
1	C	383	ARG

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Mol	Chain	Res	Type
1	C	427	LEU
1	C	468	ASN
1	C	470	LEU
1	C	471	THR
1	C	474	LYS
1	C	506	LEU
1	C	514	THR
1	C	516	LYS
1	D	4	LYS
1	D	41	ASN
1	D	79	LEU
1	D	81	GLN
1	D	99	GLU
1	D	102	MET
1	D	103	ASN
1	D	104	ASP
1	D	126	ASN
1	D	128	VAL
1	D	133	LEU
1	D	138	LEU
1	D	142	GLU
1	D	176	GLU
1	D	179	GLU
1	D	181	LYS
1	D	203	LEU
1	D	209	ILE
1	D	220	LYS
1	D	247	VAL
1	D	248	LEU
1	D	295	LEU
1	D	296	ILE
1	D	304	ASN
1	D	311	LYS
1	D	371	LEU
1	D	383	ARG
1	D	427	LEU
1	D	468	ASN
1	D	470	LEU
1	D	471	THR
1	D	474	LYS
1	D	506	LEU
1	D	514	THR

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Mol	Chain	Res	Type
1	D	516	LYS
1	E	4	LYS
1	E	41	ASN
1	E	79	LEU
1	E	81	GLN
1	E	99	GLU
1	E	102	MET
1	E	103	ASN
1	E	104	ASP
1	E	126	ASN
1	E	128	VAL
1	E	133	LEU
1	E	138	LEU
1	E	142	GLU
1	E	176	GLU
1	E	179	GLU
1	E	181	LYS
1	E	203	LEU
1	E	209	ILE
1	E	220	LYS
1	E	247	VAL
1	E	248	LEU
1	E	289	ARG
1	E	295	LEU
1	E	304	ASN
1	E	371	LEU
1	E	383	ARG
1	E	427	LEU
1	E	468	ASN
1	E	470	LEU
1	E	471	THR
1	E	474	LYS
1	E	506	LEU
1	E	514	THR
1	E	516	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	41	ASN
1	A	47	ASN

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Mol	Chain	Res	Type
1	A	69	ASN
1	A	81	GLN
1	A	103	ASN
1	A	126	ASN
1	A	167	ASN
1	A	250	ASN
1	A	256	ASN
1	A	268	GLN
1	A	304	ASN
1	A	306	ASN
1	A	336	ASN
1	A	357	HIS
1	A	412	ASN
1	A	419	ASN
1	A	422	GLN
1	A	468	ASN
1	A	476	GLN
1	B	24	GLN
1	B	41	ASN
1	B	47	ASN
1	B	81	GLN
1	B	103	ASN
1	B	126	ASN
1	B	167	ASN
1	B	250	ASN
1	B	256	ASN
1	B	268	GLN
1	B	304	ASN
1	B	306	ASN
1	B	336	ASN
1	B	357	HIS
1	B	378	ASN
1	B	412	ASN
1	B	419	ASN
1	B	422	GLN
1	B	468	ASN
1	B	476	GLN
1	C	24	GLN
1	C	41	ASN
1	C	47	ASN
1	C	69	ASN
1	C	81	GLN

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Mol	Chain	Res	Type
1	C	103	ASN
1	C	126	ASN
1	C	167	ASN
1	C	192	GLN
1	C	250	ASN
1	C	256	ASN
1	C	268	GLN
1	C	304	ASN
1	C	306	ASN
1	C	336	ASN
1	C	357	HIS
1	C	378	ASN
1	C	412	ASN
1	C	419	ASN
1	C	422	GLN
1	C	468	ASN
1	C	476	GLN
1	D	24	GLN
1	D	41	ASN
1	D	47	ASN
1	D	81	GLN
1	D	103	ASN
1	D	126	ASN
1	D	167	ASN
1	D	192	GLN
1	D	250	ASN
1	D	256	ASN
1	D	268	GLN
1	D	304	ASN
1	D	306	ASN
1	D	336	ASN
1	D	357	HIS
1	D	378	ASN
1	D	412	ASN
1	D	419	ASN
1	D	422	GLN
1	D	468	ASN
1	D	476	GLN
1	E	24	GLN
1	E	41	ASN
1	E	47	ASN
1	E	69	ASN

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Mol	Chain	Res	Type
1	E	81	GLN
1	E	103	ASN
1	E	126	ASN
1	E	167	ASN
1	E	250	ASN
1	E	256	ASN
1	E	268	GLN
1	E	304	ASN
1	E	306	ASN
1	E	336	ASN
1	E	357	HIS
1	E	378	ASN
1	E	412	ASN
1	E	419	ASN
1	E	422	GLN
1	E	468	ASN
1	E	476	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NDP	C	614	-	45,52,52	1.79	10 (22%)	53,80,80	1.54	11 (20%)
3	F89	D	616	-	40,41,41	3.91	9 (22%)	53,60,60	3.92	17 (32%)
2	UMP	D	615	-	21,21,21	2.87	8 (38%)	31,31,31	2.19	9 (29%)
3	F89	B	608	-	40,41,41	3.91	9 (22%)	53,60,60	3.90	18 (33%)
3	F89	E	621	-	40,41,41	3.90	9 (22%)	53,60,60	3.92	17 (32%)
2	UMP	A	603	-	21,21,21	2.84	8 (38%)	31,31,31	2.19	9 (29%)
4	NDP	D	618	-	45,52,52	1.78	8 (17%)	53,80,80	1.54	11 (20%)
3	F89	D	617	-	40,41,41	3.90	9 (22%)	53,60,60	3.92	17 (32%)
2	UMP	C	611	-	21,21,21	2.81	7 (33%)	31,31,31	2.19	9 (29%)
3	F89	C	613	-	40,41,41	3.90	9 (22%)	53,60,60	3.92	16 (30%)
4	NDP	E	622	-	45,52,52	1.79	10 (22%)	53,80,80	1.54	11 (20%)
4	NDP	B	610	-	45,52,52	1.76	9 (20%)	53,80,80	1.55	11 (20%)
2	UMP	B	607	-	21,21,21	2.83	7 (33%)	31,31,31	2.19	9 (29%)
3	F89	B	609	-	40,41,41	3.90	9 (22%)	53,60,60	3.94	17 (32%)
2	UMP	E	619	-	21,21,21	2.84	7 (33%)	31,31,31	2.18	9 (29%)
3	F89	A	604	-	40,41,41	3.90	9 (22%)	53,60,60	3.88	17 (32%)
4	NDP	A	606	-	45,52,52	1.79	9 (20%)	53,80,80	1.54	12 (22%)
3	F89	C	612	-	40,41,41	3.91	9 (22%)	53,60,60	3.90	17 (32%)
3	F89	A	605	-	40,41,41	3.91	9 (22%)	53,60,60	3.93	17 (32%)
3	F89	E	620	-	40,41,41	3.90	9 (22%)	53,60,60	3.85	16 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDP	C	614	-	-	5/30/77/77	0/5/5/5
3	F89	D	616	-	-	4/18/30/30	0/5/5/5
2	UMP	D	615	-	-	1/10/22/22	0/2/2/2
3	F89	B	608	-	-	4/18/30/30	0/5/5/5
3	F89	E	621	-	-	4/18/30/30	0/5/5/5
2	UMP	A	603	-	-	1/10/22/22	0/2/2/2
4	NDP	D	618	-	-	5/30/77/77	0/5/5/5
3	F89	D	617	-	-	4/18/30/30	0/5/5/5
2	UMP	C	611	-	-	1/10/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F89	C	613	-	-	4/18/30/30	0/5/5/5
4	NDP	E	622	-	-	5/30/77/77	0/5/5/5
4	NDP	B	610	-	-	5/30/77/77	0/5/5/5
2	UMP	B	607	-	-	1/10/22/22	0/2/2/2
3	F89	B	609	-	-	4/18/30/30	0/5/5/5
2	UMP	E	619	-	-	1/10/22/22	0/2/2/2
3	F89	A	604	-	-	4/18/30/30	0/5/5/5
4	NDP	A	606	-	-	5/30/77/77	0/5/5/5
3	F89	C	612	-	-	4/18/30/30	0/5/5/5
3	F89	A	605	-	-	4/18/30/30	0/5/5/5
3	F89	E	620	-	-	4/18/30/30	0/5/5/5

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	612	F89	C19-N	-17.63	1.33	1.46
3	B	608	F89	C19-N	-17.59	1.33	1.46
3	E	620	F89	C19-N	-17.54	1.33	1.46
3	D	616	F89	C19-N	-17.54	1.33	1.46
3	A	604	F89	C19-N	-17.54	1.33	1.46
3	A	605	F89	C19-N	-17.54	1.33	1.46
3	E	621	F89	C19-N	-17.54	1.33	1.46
3	D	617	F89	C19-N	-17.50	1.33	1.46
3	C	613	F89	C19-N	-17.46	1.33	1.46
3	B	609	F89	C19-N	-17.44	1.33	1.46
3	B	609	F89	C19-C15	-12.48	1.33	1.50
3	E	621	F89	C19-C15	-12.45	1.33	1.50
3	A	605	F89	C19-C15	-12.44	1.33	1.50
3	C	613	F89	C19-C15	-12.44	1.33	1.50
3	D	616	F89	C19-C15	-12.43	1.33	1.50
3	B	608	F89	C19-C15	-12.42	1.33	1.50
3	C	612	F89	C19-C15	-12.41	1.33	1.50
3	D	617	F89	C19-C15	-12.38	1.33	1.50
3	E	620	F89	C19-C15	-12.35	1.33	1.50
3	A	604	F89	C19-C15	-12.35	1.33	1.50
2	A	603	UMP	C6-C5	7.86	1.53	1.35
2	D	615	UMP	C6-C5	7.85	1.53	1.35
2	E	619	UMP	C6-C5	7.85	1.53	1.35
2	B	607	UMP	C6-C5	7.82	1.53	1.35
2	C	611	UMP	C6-C5	7.77	1.53	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	620	F89	C6-C5	6.36	1.52	1.35
3	B	609	F89	C6-C5	6.29	1.52	1.35
3	D	616	F89	C6-C5	6.29	1.52	1.35
3	C	612	F89	C6-C5	6.28	1.52	1.35
3	C	613	F89	C6-C5	6.28	1.52	1.35
3	A	604	F89	C6-C5	6.28	1.52	1.35
3	A	605	F89	C6-C5	6.26	1.52	1.35
3	B	608	F89	C6-C5	6.26	1.52	1.35
3	E	621	F89	C6-C5	6.25	1.52	1.35
3	D	617	F89	C6-C5	6.19	1.52	1.35
3	D	616	F89	C16-C	-5.92	1.39	1.48
3	B	609	F89	C16-C	-5.88	1.39	1.48
3	D	617	F89	C16-C	-5.87	1.39	1.48
3	A	605	F89	C16-C	-5.87	1.39	1.48
3	A	604	F89	C16-C	-5.82	1.39	1.48
3	B	608	F89	C16-C	-5.81	1.39	1.48
3	C	612	F89	C16-C	-5.81	1.39	1.48
3	E	620	F89	C16-C	-5.81	1.39	1.48
3	C	613	F89	C16-C	-5.80	1.39	1.48
3	E	621	F89	C16-C	-5.79	1.39	1.48
4	E	622	NDP	O4B-C1B	5.56	1.48	1.41
4	D	618	NDP	O4B-C1B	5.54	1.48	1.41
4	C	614	NDP	O4B-C1B	5.46	1.48	1.41
4	A	606	NDP	O4B-C1B	5.44	1.48	1.41
2	B	607	UMP	C6-N1	5.27	1.50	1.38
2	C	611	UMP	C6-N1	5.23	1.50	1.38
2	D	615	UMP	C6-N1	5.22	1.50	1.38
2	E	619	UMP	C6-N1	5.21	1.50	1.38
2	A	603	UMP	C6-N1	5.20	1.50	1.38
4	B	610	NDP	O4B-C1B	5.18	1.48	1.41
2	D	615	UMP	C5-C4	4.86	1.54	1.43
2	E	619	UMP	C5-C4	4.78	1.54	1.43
4	A	606	NDP	C4N-C3N	-4.71	1.40	1.49
2	C	611	UMP	C5-C4	4.70	1.54	1.43
2	B	607	UMP	C5-C4	4.70	1.54	1.43
2	A	603	UMP	C5-C4	4.64	1.53	1.43
4	B	610	NDP	C4N-C3N	-4.63	1.40	1.49
2	D	615	UMP	C2'-C1'	-4.63	1.39	1.52
2	A	603	UMP	C2'-C1'	-4.63	1.39	1.52
2	B	607	UMP	C2'-C1'	-4.61	1.39	1.52
2	C	611	UMP	C2'-C1'	-4.61	1.39	1.52
2	E	619	UMP	C2'-C1'	-4.61	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	618	NDP	C4N-C3N	-4.48	1.41	1.49
4	C	614	NDP	C4N-C3N	-4.43	1.41	1.49
3	E	620	F89	C1-N2	4.35	1.40	1.33
3	D	616	F89	C1-N2	4.34	1.40	1.33
3	A	604	F89	C1-N2	4.34	1.40	1.33
4	E	622	NDP	C4N-C3N	-4.32	1.41	1.49
3	D	617	F89	C1-N2	4.31	1.40	1.33
3	C	613	F89	C1-N2	4.29	1.40	1.33
3	C	612	F89	C1-N2	4.28	1.40	1.33
3	B	608	F89	C1-N2	4.28	1.40	1.33
3	E	621	F89	C1-N2	4.27	1.40	1.33
3	A	605	F89	C1-N2	4.26	1.40	1.33
3	B	609	F89	C1-N2	4.25	1.40	1.33
4	C	614	NDP	C6N-C5N	4.18	1.40	1.33
4	E	622	NDP	C6N-C5N	4.18	1.40	1.33
4	D	618	NDP	C6N-C5N	4.06	1.40	1.33
4	A	606	NDP	C6N-C5N	3.95	1.40	1.33
4	C	614	NDP	P2B-O1X	3.93	1.63	1.50
4	B	610	NDP	C6N-C5N	3.92	1.40	1.33
4	A	606	NDP	P2B-O1X	3.91	1.63	1.50
4	E	622	NDP	P2B-O1X	3.91	1.63	1.50
4	B	610	NDP	P2B-O1X	3.74	1.62	1.50
4	D	618	NDP	P2B-O1X	3.72	1.62	1.50
3	A	604	F89	C3-N2	3.63	1.40	1.34
3	D	616	F89	C3-N2	3.62	1.40	1.34
3	E	620	F89	C3-N2	3.61	1.40	1.34
3	B	608	F89	C3-N2	3.60	1.40	1.34
3	C	613	F89	C3-N2	3.60	1.40	1.34
3	C	612	F89	C3-N2	3.58	1.40	1.34
3	E	621	F89	C3-N2	3.58	1.40	1.34
3	B	609	F89	C3-N2	3.57	1.40	1.34
3	D	617	F89	C3-N2	3.57	1.40	1.34
3	A	605	F89	C3-N2	3.54	1.40	1.34
4	B	610	NDP	C4N-C5N	-3.18	1.40	1.48
4	A	606	NDP	C4N-C5N	-3.16	1.40	1.48
2	E	619	UMP	P-OP1	3.15	1.60	1.50
4	C	614	NDP	C4N-C5N	-3.10	1.40	1.48
4	D	618	NDP	C4N-C5N	-3.03	1.41	1.48
4	E	622	NDP	C4N-C5N	-3.02	1.41	1.48
2	D	615	UMP	P-OP1	3.01	1.60	1.50
3	C	613	F89	C-N	-2.89	1.33	1.36
3	A	605	F89	C-N	-2.88	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	607	UMP	P-OP1	2.82	1.59	1.50
2	C	611	UMP	P-OP1	2.80	1.59	1.50
3	B	609	F89	C-N	-2.77	1.33	1.36
2	A	603	UMP	P-OP1	2.77	1.59	1.50
3	D	617	F89	C-N	-2.74	1.33	1.36
2	A	603	UMP	C2-N1	2.72	1.42	1.38
3	D	616	F89	C-N	-2.72	1.33	1.36
3	E	621	F89	C-N	-2.72	1.33	1.36
3	B	608	F89	C-N	-2.71	1.33	1.36
3	E	620	F89	C-N	-2.68	1.33	1.36
2	D	615	UMP	C2-N1	2.68	1.42	1.38
2	E	619	UMP	C2-N1	2.63	1.42	1.38
3	C	612	F89	C-N	-2.60	1.33	1.36
3	A	604	F89	C-N	-2.60	1.33	1.36
4	D	618	NDP	P2B-O2X	-2.53	1.45	1.54
2	B	607	UMP	C2-N1	2.52	1.42	1.38
4	A	606	NDP	P2B-O2X	-2.50	1.45	1.54
4	C	614	NDP	P2B-O2X	-2.49	1.45	1.54
2	C	611	UMP	C2-N1	2.46	1.42	1.38
4	E	622	NDP	P2B-O2X	-2.46	1.45	1.54
4	B	610	NDP	P2B-O2X	-2.45	1.45	1.54
4	D	618	NDP	C6N-N1N	2.35	1.43	1.37
4	E	622	NDP	C6N-N1N	2.34	1.43	1.37
4	B	610	NDP	O4D-C1D	2.33	1.47	1.42
4	C	614	NDP	C6N-N1N	2.32	1.43	1.37
4	E	622	NDP	C7N-C3N	2.31	1.53	1.48
4	C	614	NDP	O4D-C1D	2.25	1.47	1.42
4	C	614	NDP	C7N-C3N	2.24	1.53	1.48
4	E	622	NDP	O4D-C1D	2.23	1.47	1.42
2	D	615	UMP	O4'-C1'	2.22	1.47	1.42
3	D	617	F89	O2-CT	-2.19	1.23	1.30
2	A	603	UMP	O4'-C1'	2.19	1.47	1.42
3	A	605	F89	O2-CT	-2.18	1.23	1.30
3	B	609	F89	O2-CT	-2.18	1.23	1.30
3	A	605	F89	OE2-CD	-2.17	1.23	1.30
3	C	613	F89	O2-CT	-2.17	1.23	1.30
4	D	618	NDP	C7N-C3N	2.17	1.53	1.48
3	E	621	F89	O2-CT	-2.17	1.23	1.30
3	E	621	F89	OE2-CD	-2.17	1.23	1.30
4	A	606	NDP	C6N-N1N	2.16	1.42	1.37
3	D	617	F89	OE2-CD	-2.16	1.23	1.30
3	A	604	F89	OE2-CD	-2.16	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	620	F89	O2-CT	-2.16	1.23	1.30
3	D	616	F89	OE2-CD	-2.15	1.23	1.30
3	C	612	F89	OE2-CD	-2.15	1.23	1.30
3	B	608	F89	OE2-CD	-2.15	1.23	1.30
3	A	604	F89	O2-CT	-2.15	1.23	1.30
3	B	609	F89	OE2-CD	-2.15	1.23	1.30
3	C	612	F89	O2-CT	-2.15	1.23	1.30
3	E	620	F89	OE2-CD	-2.14	1.23	1.30
3	D	616	F89	O2-CT	-2.14	1.23	1.30
3	C	613	F89	OE2-CD	-2.14	1.23	1.30
3	B	608	F89	O2-CT	-2.14	1.23	1.30
2	D	615	UMP	C4-N3	-2.13	1.34	1.38
4	A	606	NDP	C7N-C3N	2.12	1.53	1.48
2	E	619	UMP	O4'-C1'	2.10	1.47	1.42
2	C	611	UMP	C4-N3	-2.10	1.34	1.38
4	B	610	NDP	C7N-C3N	2.08	1.53	1.48
2	B	607	UMP	C4-N3	-2.08	1.34	1.38
4	B	610	NDP	C6N-N1N	2.07	1.42	1.37
4	C	614	NDP	C2N-C3N	2.04	1.40	1.34
2	A	603	UMP	C4-N3	-2.03	1.34	1.38
4	E	622	NDP	C2N-C3N	2.03	1.40	1.34
4	A	606	NDP	O4D-C1D	2.02	1.46	1.42

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	621	F89	C15-C19-N	21.81	109.45	102.18
3	B	609	F89	C15-C19-N	21.73	109.42	102.18
3	D	617	F89	C15-C19-N	21.70	109.41	102.18
3	C	613	F89	C15-C19-N	21.65	109.39	102.18
3	A	605	F89	C15-C19-N	21.64	109.39	102.18
3	D	616	F89	C15-C19-N	21.49	109.34	102.18
3	B	608	F89	C15-C19-N	21.42	109.32	102.18
3	C	612	F89	C15-C19-N	21.41	109.31	102.18
3	A	604	F89	C15-C19-N	21.23	109.25	102.18
3	E	620	F89	C15-C19-N	20.93	109.16	102.18
3	B	609	F89	C19-N-C	-9.64	109.15	113.12
3	A	605	F89	C19-N-C	-9.60	109.17	113.12
3	D	616	F89	C19-N-C	-9.56	109.19	113.12
3	C	613	F89	C19-N-C	-9.51	109.21	113.12
3	D	617	F89	C19-N-C	-9.49	109.22	113.12
3	B	608	F89	C19-N-C	-9.46	109.23	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	612	F89	C19-N-C	-9.44	109.24	113.12
3	E	621	F89	C19-N-C	-9.38	109.26	113.12
3	A	604	F89	C19-N-C	-9.35	109.27	113.12
3	E	620	F89	C19-N-C	-9.24	109.32	113.12
3	E	620	F89	C3-N4-C4A	8.37	122.21	116.54
3	A	605	F89	C3-N4-C4A	8.35	122.20	116.54
3	D	616	F89	C3-N4-C4A	8.35	122.20	116.54
3	B	609	F89	C3-N4-C4A	8.34	122.19	116.54
3	C	612	F89	C3-N4-C4A	8.32	122.18	116.54
3	A	604	F89	C3-N4-C4A	8.31	122.17	116.54
3	B	608	F89	C3-N4-C4A	8.30	122.17	116.54
3	E	621	F89	C3-N4-C4A	8.24	122.13	116.54
3	D	617	F89	C3-N4-C4A	8.21	122.11	116.54
3	C	613	F89	C3-N4-C4A	8.09	122.03	116.54
3	E	620	F89	C15-C16-C	-6.91	105.24	108.94
3	B	608	F89	C15-C16-C	-6.74	105.33	108.94
3	C	612	F89	C15-C16-C	-6.72	105.34	108.94
3	D	616	F89	C15-C16-C	-6.66	105.37	108.94
3	A	604	F89	C15-C16-C	-6.62	105.40	108.94
3	C	613	F89	C15-C16-C	-6.54	105.43	108.94
3	A	605	F89	C15-C16-C	-6.53	105.44	108.94
3	B	609	F89	C15-C16-C	-6.52	105.45	108.94
3	D	617	F89	C15-C16-C	-6.40	105.51	108.94
3	E	621	F89	C15-C16-C	-6.29	105.57	108.94
2	D	615	UMP	C5-C6-N1	-5.91	111.91	121.81
2	C	611	UMP	C5-C6-N1	-5.90	111.93	121.81
2	A	603	UMP	C5-C6-N1	-5.88	111.96	121.81
2	B	607	UMP	C5-C6-N1	-5.87	111.97	121.81
2	B	607	UMP	C6-C5-C4	-5.87	111.49	119.52
2	C	611	UMP	C6-C5-C4	-5.86	111.51	119.52
2	E	619	UMP	C5-C6-N1	-5.86	112.00	121.81
2	A	603	UMP	C6-C5-C4	-5.82	111.56	119.52
2	D	615	UMP	C6-C5-C4	-5.80	111.59	119.52
2	E	619	UMP	C6-C5-C4	-5.80	111.59	119.52
4	C	614	NDP	N3A-C2A-N1A	-5.23	120.50	128.68
4	D	618	NDP	N3A-C2A-N1A	-5.20	120.55	128.68
4	E	622	NDP	N3A-C2A-N1A	-5.18	120.58	128.68
4	A	606	NDP	N3A-C2A-N1A	-5.17	120.59	128.68
4	B	610	NDP	N3A-C2A-N1A	-5.17	120.60	128.68
3	C	613	F89	C1A-C1-N2	-4.54	120.06	124.09
3	E	621	F89	C1A-C1-N2	-4.46	120.13	124.09
3	D	617	F89	C1A-C1-N2	-4.43	120.16	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	609	F89	C1A-C1-N2	-4.40	120.19	124.09
3	C	612	F89	C1A-C1-N2	-4.35	120.23	124.09
3	A	605	F89	C1A-C1-N2	-4.30	120.27	124.09
3	E	620	F89	C1A-C1-N2	-4.28	120.29	124.09
3	A	604	F89	C1A-C1-N2	-4.26	120.31	124.09
2	D	615	UMP	N3-C2-N1	4.24	120.51	114.89
3	B	608	F89	C1A-C1-N2	-4.22	120.34	124.09
3	D	616	F89	C1A-C1-N2	-4.21	120.35	124.09
2	A	603	UMP	N3-C2-N1	4.19	120.45	114.89
2	B	607	UMP	N3-C2-N1	4.18	120.44	114.89
2	E	619	UMP	N3-C2-N1	4.14	120.39	114.89
2	C	611	UMP	N3-C2-N1	4.14	120.38	114.89
2	B	607	UMP	C5-C4-N3	4.08	120.95	114.84
2	C	611	UMP	C5-C4-N3	4.08	120.94	114.84
2	D	615	UMP	C5-C4-N3	4.03	120.86	114.84
2	E	619	UMP	C5-C4-N3	3.97	120.78	114.84
2	A	603	UMP	C5-C4-N3	3.96	120.76	114.84
3	D	616	F89	C1B-C1A-C4A	3.72	121.25	117.78
3	B	608	F89	C1B-C1A-C4A	3.69	121.22	117.78
3	C	612	F89	C1B-C1A-C4A	3.69	121.22	117.78
3	C	612	F89	N4-C3-N2	-3.65	119.00	125.72
3	B	608	F89	N4-C3-N2	-3.65	119.00	125.72
3	D	616	F89	N4-C3-N2	-3.64	119.02	125.72
3	A	604	F89	N4-C3-N2	-3.63	119.04	125.72
3	A	605	F89	N4-C3-N2	-3.63	119.05	125.72
3	B	609	F89	N4-C3-N2	-3.62	119.05	125.72
3	D	617	F89	C1B-C1A-C4A	3.62	121.16	117.78
3	E	620	F89	N4-C3-N2	-3.62	119.07	125.72
4	E	622	NDP	PN-O3-PA	-3.61	120.44	132.83
3	A	604	F89	C1B-C1A-C4A	3.60	121.14	117.78
3	C	613	F89	N4-C3-N2	-3.60	119.10	125.72
3	E	621	F89	N4-C3-N2	-3.59	119.12	125.72
3	C	613	F89	C1B-C1A-C4A	3.58	121.12	117.78
3	E	621	F89	C1B-C1A-C4A	3.57	121.11	117.78
4	D	618	NDP	PN-O3-PA	-3.57	120.58	132.83
3	D	617	F89	N4-C3-N2	-3.55	119.19	125.72
3	A	605	F89	C1B-C1A-C4A	3.54	121.08	117.78
3	B	609	F89	C1B-C1A-C4A	3.53	121.07	117.78
3	E	620	F89	C1B-C1A-C4A	3.50	121.05	117.78
4	C	614	NDP	PN-O3-PA	-3.47	120.93	132.83
3	A	604	F89	CA-N-C	3.42	127.26	121.81
4	B	610	NDP	PN-O3-PA	-3.39	121.20	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	606	NDP	PN-O3-PA	-3.35	121.31	132.83
3	E	620	F89	CA-N-C	3.35	127.14	121.81
3	D	616	F89	CA-N-C	3.33	127.11	121.81
3	C	612	F89	CA-N-C	3.30	127.06	121.81
2	E	619	UMP	O4-C4-C5	-3.27	119.41	125.16
2	C	611	UMP	O4-C4-C5	-3.24	119.46	125.16
2	A	603	UMP	O4-C4-C5	-3.22	119.49	125.16
3	E	621	F89	C19-C15-C16	-3.22	107.74	109.75
2	B	607	UMP	O4-C4-C5	-3.22	119.50	125.16
3	D	617	F89	C19-C15-C16	-3.22	107.74	109.75
3	B	608	F89	CA-N-C	3.21	126.93	121.81
3	B	609	F89	C1A-C1B-C6A	3.19	121.27	118.85
2	D	615	UMP	O4-C4-C5	-3.17	119.58	125.16
3	A	605	F89	C1A-C1B-C6A	3.17	121.25	118.85
3	B	609	F89	C19-C15-C16	-3.12	107.80	109.75
3	C	613	F89	C19-C15-C16	-3.10	107.82	109.75
3	A	605	F89	C19-C15-C16	-3.09	107.82	109.75
3	E	621	F89	C1A-C1B-C6A	3.07	121.18	118.85
3	C	613	F89	C1A-C1B-C6A	3.07	121.18	118.85
4	B	610	NDP	O5B-PA-O1A	-3.06	97.13	109.07
4	C	614	NDP	O5B-PA-O1A	-3.04	97.17	109.07
3	D	617	F89	C1A-C1B-C6A	3.03	121.15	118.85
4	E	622	NDP	O5B-PA-O1A	-3.02	97.25	109.07
3	D	616	F89	C16-C-N	2.99	108.21	106.44
3	D	616	F89	C19-C15-C16	-2.99	107.88	109.75
4	A	606	NDP	O5B-PA-O1A	-2.97	97.46	109.07
3	E	620	F89	C16-C-N	2.96	108.19	106.44
3	E	620	F89	C1A-C1B-C6A	2.95	121.09	118.85
4	D	618	NDP	O5B-PA-O1A	-2.95	97.55	109.07
3	B	608	F89	C17-C16-C	2.94	134.42	129.63
3	D	616	F89	C17-C16-C	2.93	134.41	129.63
3	A	605	F89	C16-C-N	2.93	108.17	106.44
3	C	613	F89	C17-C16-C	2.93	134.40	129.63
3	B	608	F89	C16-C-N	2.91	108.16	106.44
3	B	609	F89	C16-C-N	2.91	108.16	106.44
2	C	611	UMP	OP3-P-OP2	2.90	118.72	107.64
3	B	609	F89	C17-C16-C	2.89	134.35	129.63
3	A	604	F89	C1A-C1B-C6A	2.88	121.03	118.85
3	C	612	F89	C17-C16-C	2.88	134.33	129.63
3	C	613	F89	C16-C-N	2.88	108.14	106.44
2	A	603	UMP	OP3-P-OP2	2.87	118.61	107.64
2	B	607	UMP	OP3-P-OP2	2.87	118.61	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	608	F89	C19-C15-C16	-2.87	107.96	109.75
3	D	617	F89	C17-C16-C	2.86	134.30	129.63
3	C	612	F89	C16-C-N	2.85	108.13	106.44
3	A	604	F89	C19-C15-C16	-2.85	107.97	109.75
3	A	604	F89	C17-C16-C	2.84	134.27	129.63
2	E	619	UMP	OP3-P-OP2	2.84	118.48	107.64
3	C	612	F89	C19-C15-C16	-2.84	107.98	109.75
2	D	615	UMP	OP3-P-OP2	2.83	118.46	107.64
3	A	605	F89	C17-C16-C	2.83	134.24	129.63
3	D	617	F89	C16-C-N	2.82	108.11	106.44
3	E	621	F89	C17-C16-C	2.82	134.23	129.63
3	A	604	F89	C16-C-N	2.81	108.10	106.44
3	E	620	F89	C17-C16-C	2.79	134.18	129.63
3	D	616	F89	C1A-C1B-C6A	2.77	120.95	118.85
3	C	612	F89	C1A-C1B-C6A	2.75	120.93	118.85
4	B	610	NDP	O2X-P2B-O2B	2.74	118.25	105.99
4	D	618	NDP	O2X-P2B-O2B	2.72	118.19	105.99
4	A	606	NDP	O2X-P2B-O2B	2.72	118.18	105.99
4	B	610	NDP	O4D-C1D-N1N	2.70	113.34	108.06
3	B	608	F89	C1A-C1B-C6A	2.70	120.89	118.85
4	C	614	NDP	O2X-P2B-O2B	2.67	117.94	105.99
4	E	622	NDP	O2X-P2B-O2B	2.66	117.91	105.99
3	E	620	F89	C19-C15-C16	-2.65	108.09	109.75
3	E	621	F89	C16-C-N	2.59	107.97	106.44
4	B	610	NDP	O2A-PA-O1A	2.57	124.93	112.24
4	C	614	NDP	O2A-PA-O1A	2.55	124.85	112.24
4	D	618	NDP	O2N-PN-O1N	2.55	124.84	112.24
4	C	614	NDP	O2N-PN-O1N	2.53	124.75	112.24
4	A	606	NDP	O2A-PA-O1A	2.52	124.72	112.24
4	D	618	NDP	O2A-PA-O1A	2.52	124.69	112.24
4	E	622	NDP	O2N-PN-O1N	2.52	124.68	112.24
4	A	606	NDP	O3X-P2B-O1X	-2.51	100.86	110.68
4	E	622	NDP	O2A-PA-O1A	2.51	124.65	112.24
4	A	606	NDP	O2N-PN-O1N	2.49	124.56	112.24
4	B	610	NDP	O2N-PN-O1N	2.49	124.54	112.24
4	C	614	NDP	O3X-P2B-O1X	-2.48	100.97	110.68
4	C	614	NDP	O4D-C1D-N1N	2.47	112.89	108.06
4	E	622	NDP	O3X-P2B-O1X	-2.46	101.05	110.68
4	B	610	NDP	O3X-P2B-O1X	-2.46	101.05	110.68
4	D	618	NDP	O3X-P2B-O1X	-2.45	101.09	110.68
4	E	622	NDP	C3N-C2N-N1N	-2.44	119.61	123.10
4	D	618	NDP	C3N-C2N-N1N	-2.43	119.63	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	610	NDP	O2A-PA-O5B	-2.42	96.49	107.75
4	A	606	NDP	O4D-C1D-N1N	2.42	112.78	108.06
4	A	606	NDP	O2A-PA-O5B	-2.41	96.57	107.75
4	A	606	NDP	C3N-C2N-N1N	-2.40	119.67	123.10
4	B	610	NDP	C3N-C2N-N1N	-2.38	119.70	123.10
4	C	614	NDP	C3N-C2N-N1N	-2.37	119.71	123.10
4	E	622	NDP	O4D-C1D-N1N	2.36	112.67	108.06
4	C	614	NDP	O2A-PA-O5B	-2.34	96.89	107.75
4	D	618	NDP	O2A-PA-O5B	-2.33	96.93	107.75
2	E	619	UMP	O2-C2-N1	-2.31	119.71	122.79
3	C	613	F89	C3M-C3-N2	2.31	120.76	117.15
2	C	611	UMP	C4-N3-C2	-2.29	123.56	126.58
2	C	611	UMP	O2-C2-N1	-2.28	119.75	122.79
4	E	622	NDP	O2A-PA-O5B	-2.28	97.15	107.75
3	B	608	F89	C3M-C3-N2	2.28	120.71	117.15
3	D	616	F89	C3M-C3-N2	2.26	120.69	117.15
2	D	615	UMP	O2-C2-N1	-2.26	119.78	122.79
3	B	608	F89	O2-CT-O1	-2.26	118.97	124.09
2	B	607	UMP	O2-C2-N1	-2.25	119.79	122.79
2	B	607	UMP	C4-N3-C2	-2.24	123.63	126.58
3	A	605	F89	C3M-C3-N4	2.24	120.64	117.16
2	E	619	UMP	C4-N3-C2	-2.22	123.65	126.58
3	D	616	F89	O2-CT-O1	-2.22	119.04	124.09
3	E	620	F89	C3M-C3-N4	2.22	120.62	117.16
2	A	603	UMP	O2-C2-N1	-2.22	119.83	122.79
2	D	615	UMP	C4-N3-C2	-2.22	123.66	126.58
3	E	621	F89	O2-CT-O1	-2.20	119.10	124.09
3	D	617	F89	O2-CT-O1	-2.19	119.13	124.09
4	D	618	NDP	O4D-C1D-N1N	2.18	112.33	108.06
2	A	603	UMP	C4-N3-C2	-2.18	123.70	126.58
3	C	612	F89	C3M-C3-N2	2.18	120.56	117.15
2	A	603	UMP	O4'-C1'-N1	2.17	111.74	107.86
3	A	604	F89	C3M-C3-N2	2.17	120.54	117.15
4	E	622	NDP	O2N-PN-O5D	2.17	117.82	107.75
3	A	604	F89	O2-CT-O1	-2.17	119.17	124.09
3	C	613	F89	C5-C6-C6A	-2.15	118.03	121.36
3	C	612	F89	O2-CT-O1	-2.15	119.22	124.09
2	D	615	UMP	O4'-C1'-N1	2.14	111.68	107.86
4	A	606	NDP	O2N-PN-O5D	2.14	117.66	107.75
3	E	621	F89	C3M-C3-N2	2.13	120.48	117.15
3	A	605	F89	C5-C6-C6A	-2.13	118.06	121.36
4	B	610	NDP	O2N-PN-O5D	2.13	117.65	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	609	F89	C3M-C3-N2	2.13	120.48	117.15
3	B	609	F89	C3M-C3-N4	2.13	120.47	117.16
3	B	609	F89	C5-C6-C6A	-2.11	118.09	121.36
4	D	618	NDP	O2N-PN-O5D	2.11	117.54	107.75
3	C	612	F89	C3M-C3-N4	2.11	120.44	117.16
3	A	604	F89	C5-C6-C6A	-2.11	118.10	121.36
4	C	614	NDP	O2N-PN-O5D	2.10	117.48	107.75
3	E	621	F89	C5-C6-C6A	-2.10	118.12	121.36
3	A	604	F89	C3M-C3-N4	2.09	120.41	117.16
3	D	617	F89	C3M-C3-N4	2.09	120.41	117.16
3	D	616	F89	C5-C6-C6A	-2.09	118.13	121.36
3	E	621	F89	C3M-C3-N4	2.08	120.39	117.16
3	B	608	F89	C5-C6-C6A	-2.08	118.15	121.36
3	C	612	F89	C5-C6-C6A	-2.08	118.15	121.36
3	D	617	F89	C5-C6-C6A	-2.08	118.15	121.36
3	D	617	F89	C3M-C3-N2	2.08	120.39	117.15
3	A	605	F89	O2-CT-O1	-2.08	119.38	124.09
2	E	619	UMP	O4'-C1'-N1	2.07	111.56	107.86
3	E	620	F89	C7-C6A-C6	-2.07	118.35	123.19
3	B	608	F89	C7-C6A-C6	-2.06	118.37	123.19
3	C	613	F89	O2-CT-O1	-2.06	119.41	124.09
3	E	620	F89	C5-C6-C6A	-2.06	118.18	121.36
3	B	609	F89	O2-CT-O1	-2.05	119.42	124.09
3	A	604	F89	C7-C6A-C6	-2.05	118.39	123.19
3	C	613	F89	CA-N-C	2.05	125.07	121.81
3	A	605	F89	C19-N-CA	2.05	125.65	123.69
3	D	617	F89	CA-N-C	2.05	125.07	121.81
3	B	609	F89	CA-N-C	2.04	125.07	121.81
3	D	616	F89	C7-C6A-C6	-2.04	118.41	123.19
3	A	605	F89	CA-N-C	2.04	125.06	121.81
2	C	611	UMP	O4'-C1'-N1	2.03	111.49	107.86
4	A	606	NDP	O2X-P2B-O1X	2.03	118.61	110.68
3	E	620	F89	C3M-C3-N2	2.03	120.31	117.15
3	A	605	F89	C3M-C3-N2	2.03	120.31	117.15
2	B	607	UMP	O4'-C1'-N1	2.02	111.47	107.86
3	B	609	F89	C19-N-CA	2.02	125.62	123.69
3	B	608	F89	O2-CT-CA	2.02	120.38	113.38
3	D	616	F89	C3M-C3-N4	2.02	120.30	117.16
3	E	621	F89	CA-N-C	2.01	125.01	121.81
3	B	608	F89	C3M-C3-N4	2.01	120.28	117.16
3	E	621	F89	C19-N-CA	2.01	125.61	123.69
3	D	617	F89	C19-N-CA	2.01	125.61	123.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	613	F89	C7-C6A-C6	-2.01	118.50	123.19
3	C	612	F89	C7-C6A-C6	-2.00	118.50	123.19

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	F89	CB-CA-N-C
3	A	605	F89	CB-CA-N-C19
3	B	608	F89	CB-CA-N-C
3	B	609	F89	CB-CA-N-C19
3	C	612	F89	CB-CA-N-C
3	C	613	F89	CB-CA-N-C19
3	D	616	F89	CB-CA-N-C
3	D	617	F89	CB-CA-N-C19
3	E	620	F89	CB-CA-N-C
3	E	621	F89	CB-CA-N-C19
4	A	606	NDP	C2B-O2B-P2B-O3X
4	A	606	NDP	C5D-O5D-PN-O2N
4	B	610	NDP	C2B-O2B-P2B-O3X
4	B	610	NDP	C5D-O5D-PN-O2N
4	C	614	NDP	C2B-O2B-P2B-O3X
4	C	614	NDP	C5D-O5D-PN-O2N
4	D	618	NDP	C2B-O2B-P2B-O3X
4	D	618	NDP	C5D-O5D-PN-O2N
4	E	622	NDP	C2B-O2B-P2B-O3X
4	E	622	NDP	C5D-O5D-PN-O2N
3	A	604	F89	N-CA-CT-O2
3	B	608	F89	N-CA-CT-O2
3	C	612	F89	N-CA-CT-O2
3	D	616	F89	N-CA-CT-O2
3	E	620	F89	N-CA-CT-O2
3	A	604	F89	CB-CA-N-C19
3	B	608	F89	CB-CA-N-C19
3	C	612	F89	CB-CA-N-C19
3	D	616	F89	CB-CA-N-C19
3	E	620	F89	CB-CA-N-C19
4	C	614	NDP	C4D-C5D-O5D-PN
4	D	618	NDP	C4D-C5D-O5D-PN
4	E	622	NDP	C4D-C5D-O5D-PN
4	A	606	NDP	C4D-C5D-O5D-PN
4	B	610	NDP	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
4	C	614	NDP	PA-O3-PN-O5D
3	A	604	F89	N-CA-CT-O1
3	B	608	F89	N-CA-CT-O1
3	C	612	F89	N-CA-CT-O1
3	D	616	F89	N-CA-CT-O1
3	E	620	F89	N-CA-CT-O1
4	A	606	NDP	O4D-C1D-N1N-C2N
4	B	610	NDP	O4D-C1D-N1N-C2N
4	C	614	NDP	O4D-C1D-N1N-C2N
4	D	618	NDP	O4D-C1D-N1N-C2N
4	E	622	NDP	O4D-C1D-N1N-C2N
2	C	611	UMP	O4'-C4'-C5'-O5'
2	A	603	UMP	O4'-C4'-C5'-O5'
2	B	607	UMP	O4'-C4'-C5'-O5'
2	D	615	UMP	O4'-C4'-C5'-O5'
3	C	613	F89	OE2-CD-CG-CB
4	A	606	NDP	PA-O3-PN-O5D
4	B	610	NDP	PA-O3-PN-O5D
4	D	618	NDP	PA-O3-PN-O5D
4	E	622	NDP	PA-O3-PN-O5D
3	E	621	F89	OE2-CD-CG-CB
3	B	609	F89	OE2-CD-CG-CB
3	A	605	F89	OE2-CD-CG-CB
2	E	619	UMP	O4'-C4'-C5'-O5'
3	D	617	F89	OE2-CD-CG-CB
3	D	617	F89	OE1-CD-CG-CB
3	B	609	F89	OE1-CD-CG-CB
3	A	605	F89	OE1-CD-CG-CB
3	C	613	F89	OE1-CD-CG-CB
3	E	621	F89	OE1-CD-CG-CB
3	A	605	F89	CA-CB-CG-CD
3	B	609	F89	CA-CB-CG-CD
3	C	613	F89	CA-CB-CG-CD
3	D	617	F89	CA-CB-CG-CD
3	E	621	F89	CA-CB-CG-CD

There are no ring outliers.

20 monomers are involved in 122 short contacts:

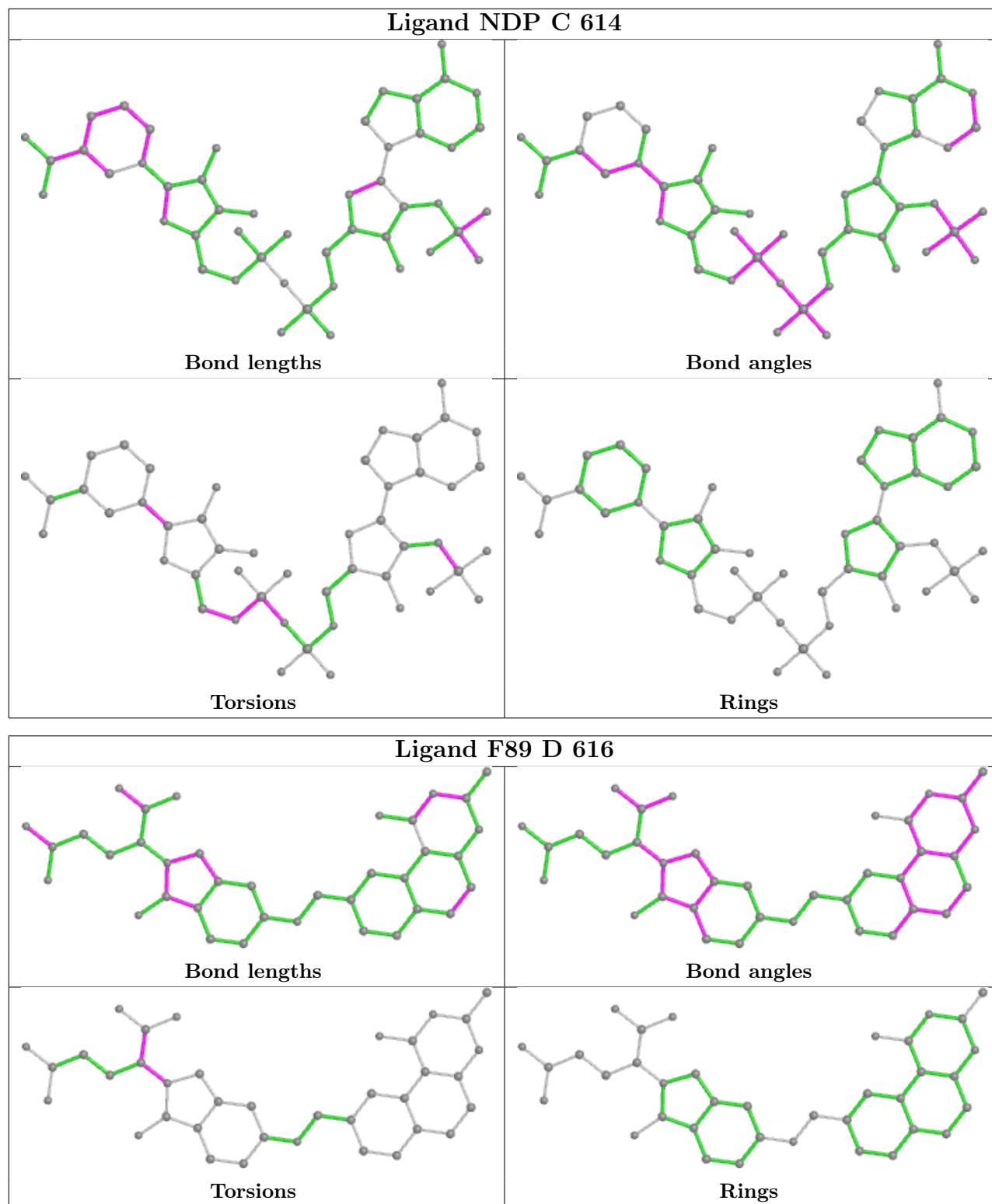
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	614	NDP	8	0
3	D	616	F89	8	0

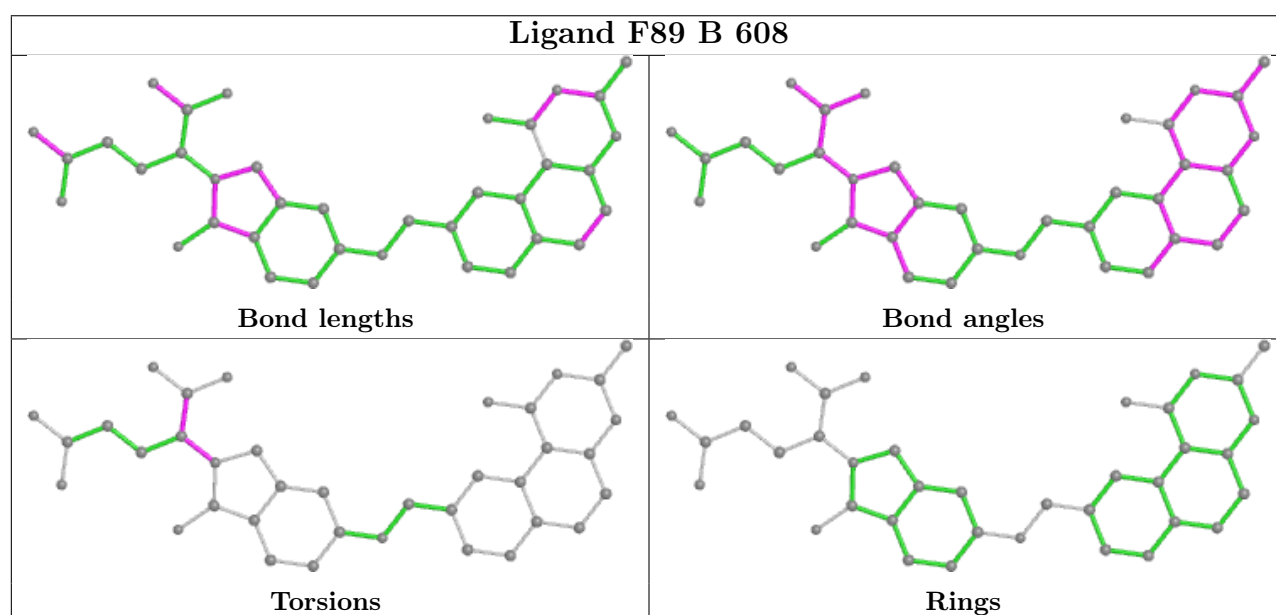
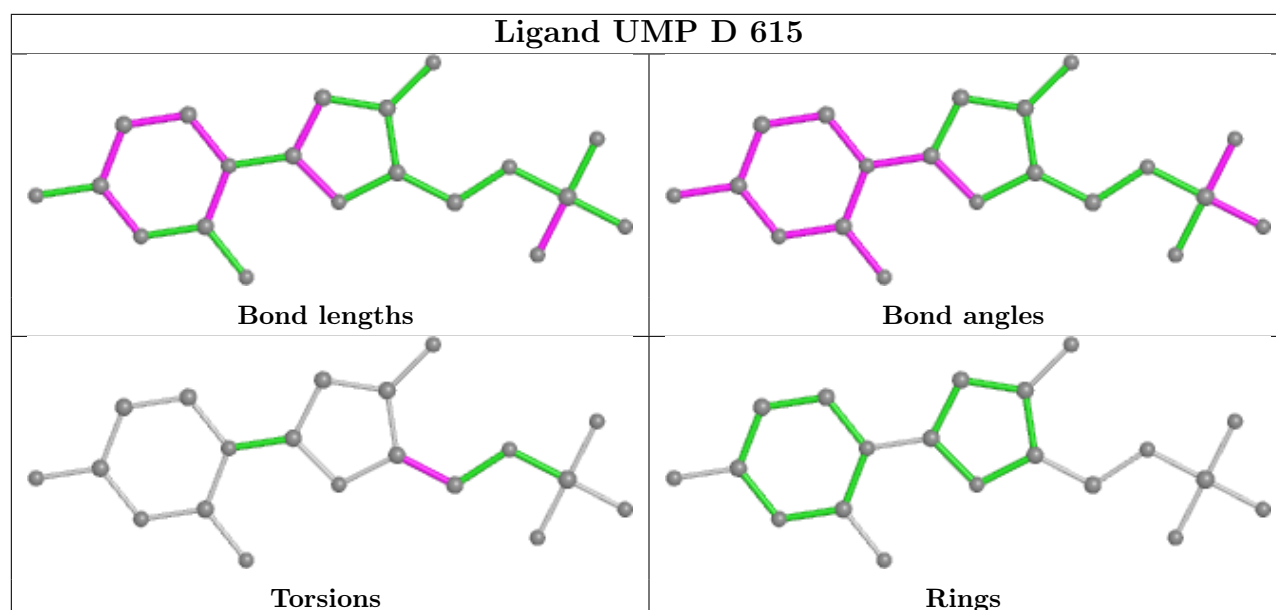
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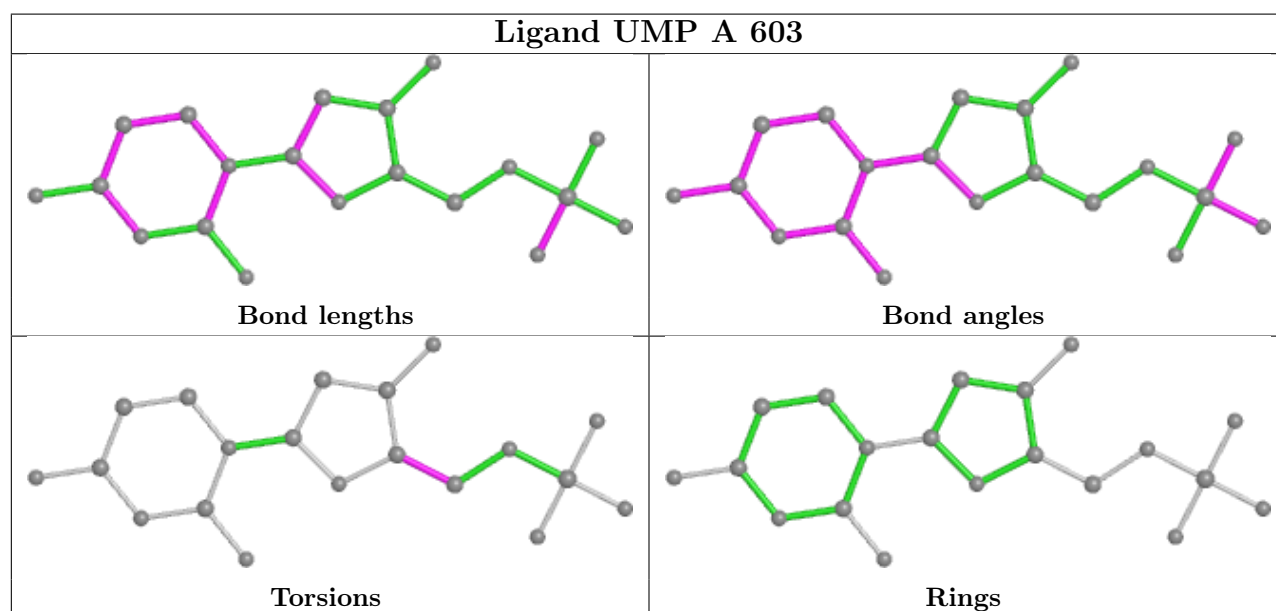
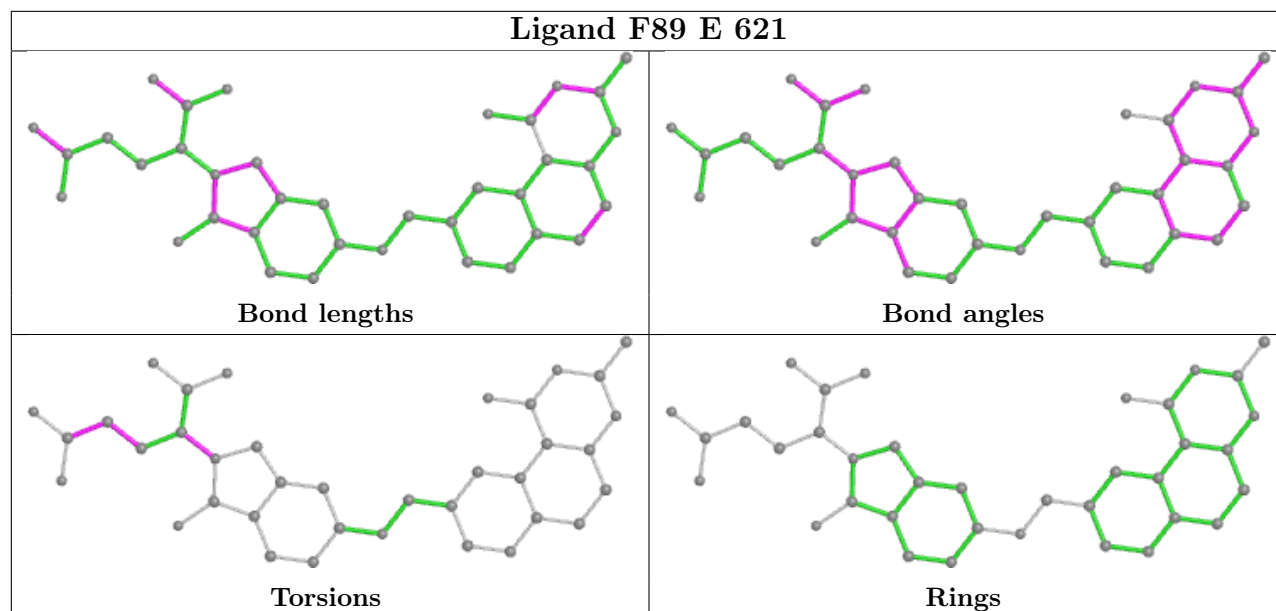
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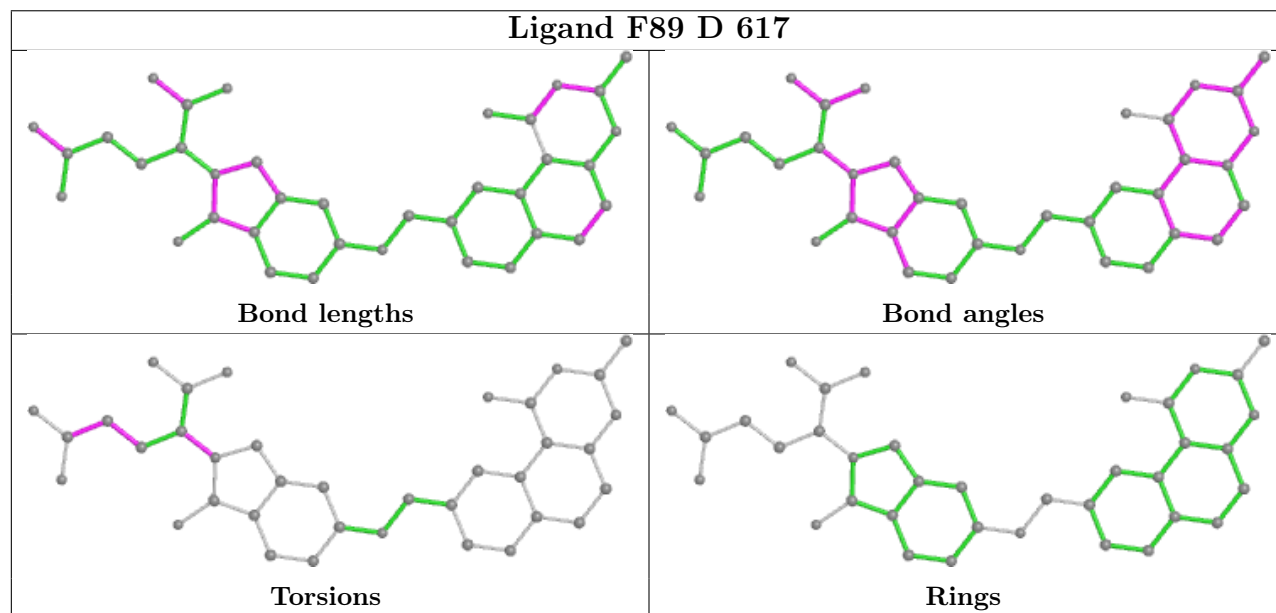
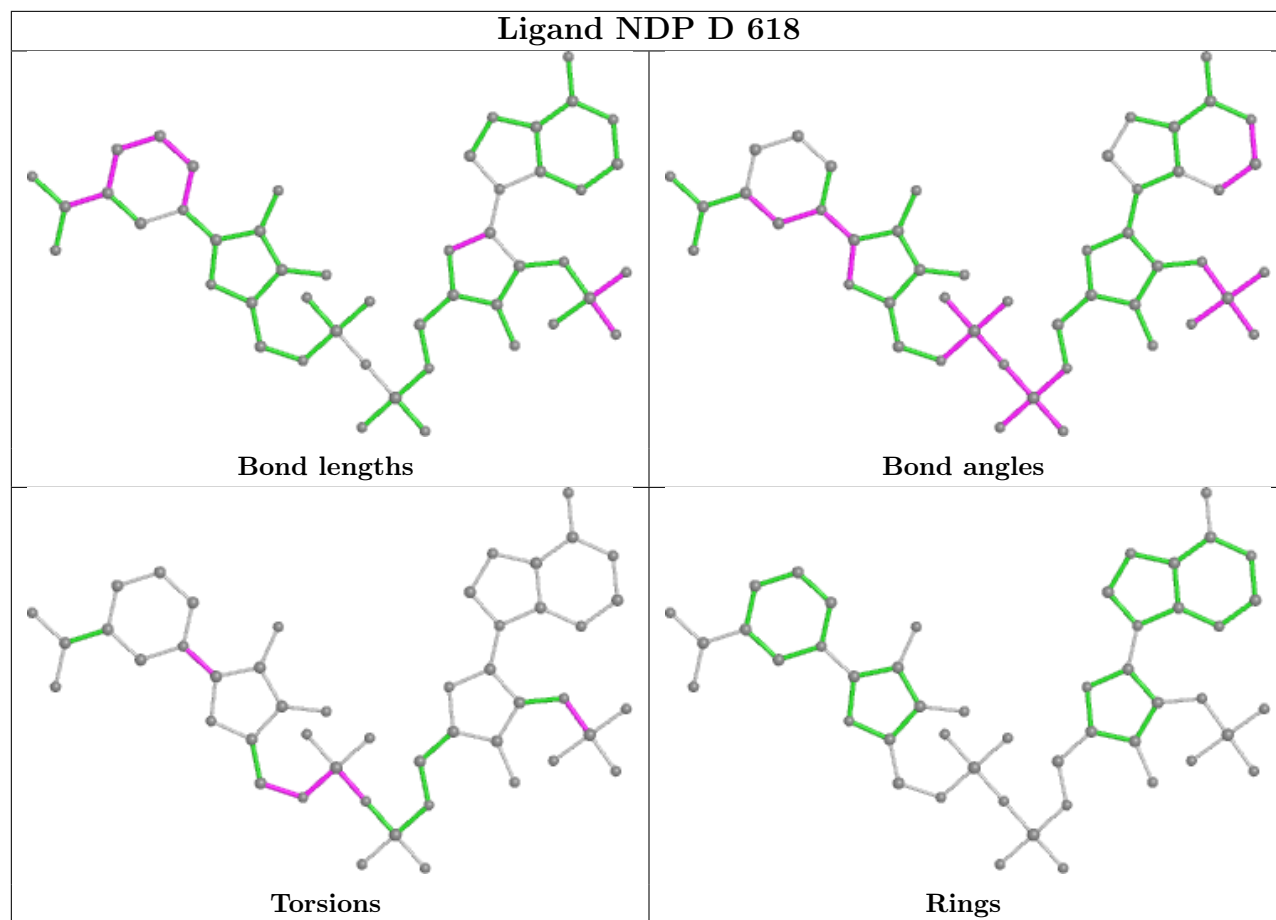
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	615	UMP	2	0
3	B	608	F89	6	0
3	E	621	F89	10	0
2	A	603	UMP	2	0
4	D	618	NDP	8	0
3	D	617	F89	9	0
2	C	611	UMP	3	0
3	C	613	F89	8	0
4	E	622	NDP	8	0
4	B	610	NDP	8	0
2	B	607	UMP	3	0
3	B	609	F89	7	0
2	E	619	UMP	2	0
3	A	604	F89	7	0
4	A	606	NDP	10	0
3	C	612	F89	7	0
3	A	605	F89	9	0
3	E	620	F89	7	0

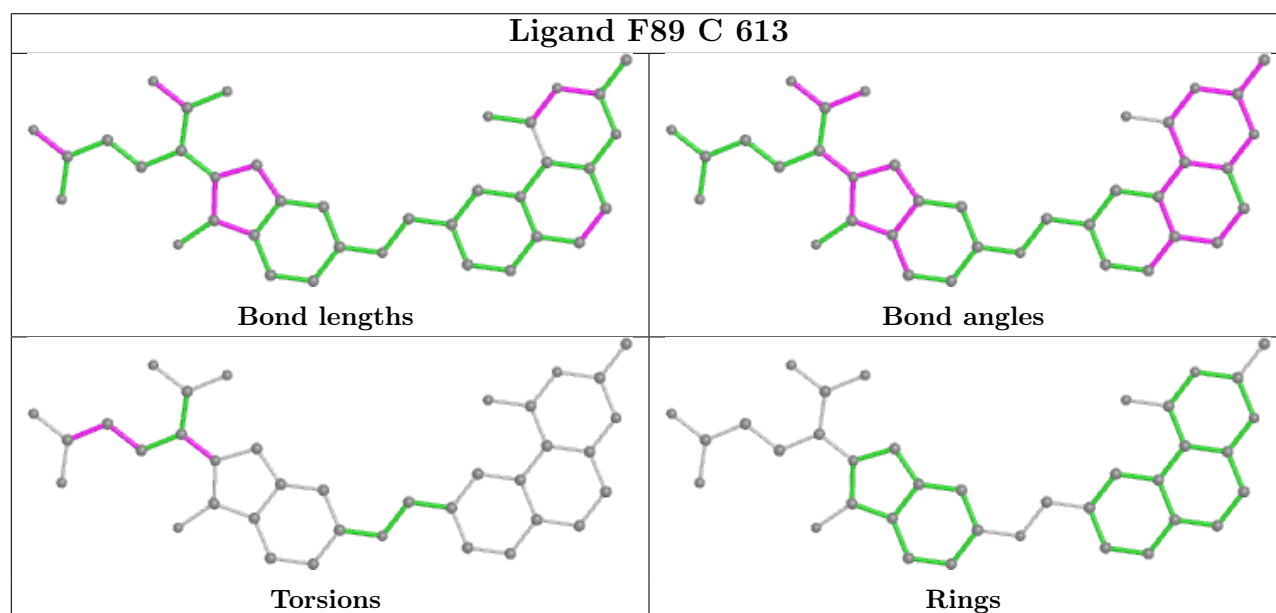
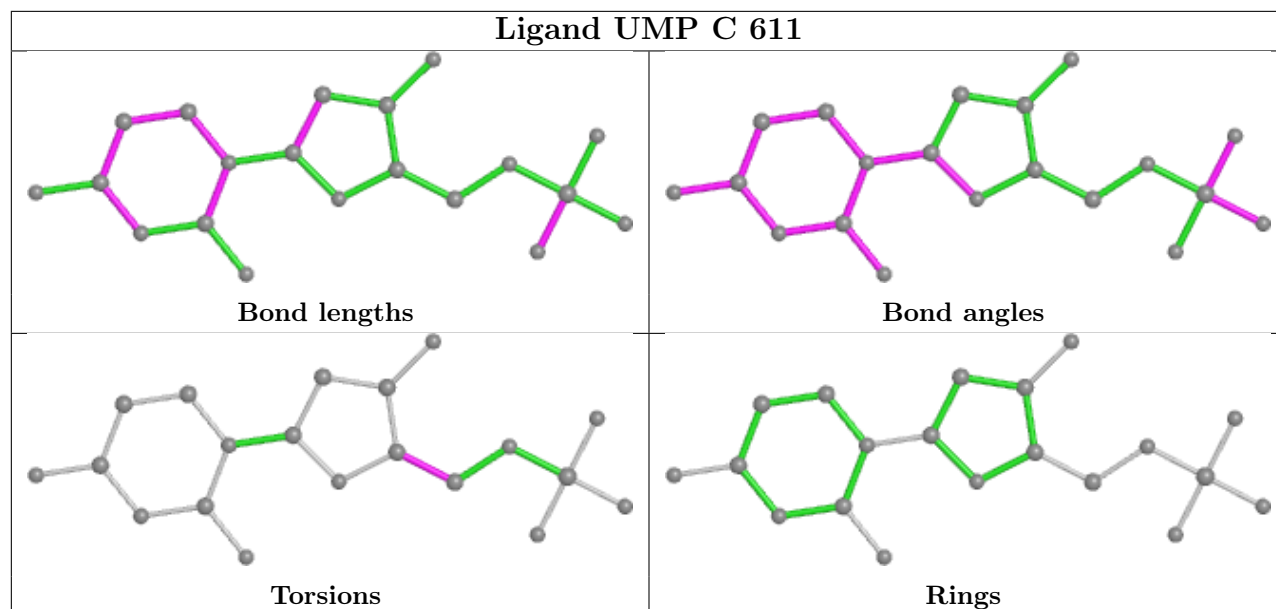
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

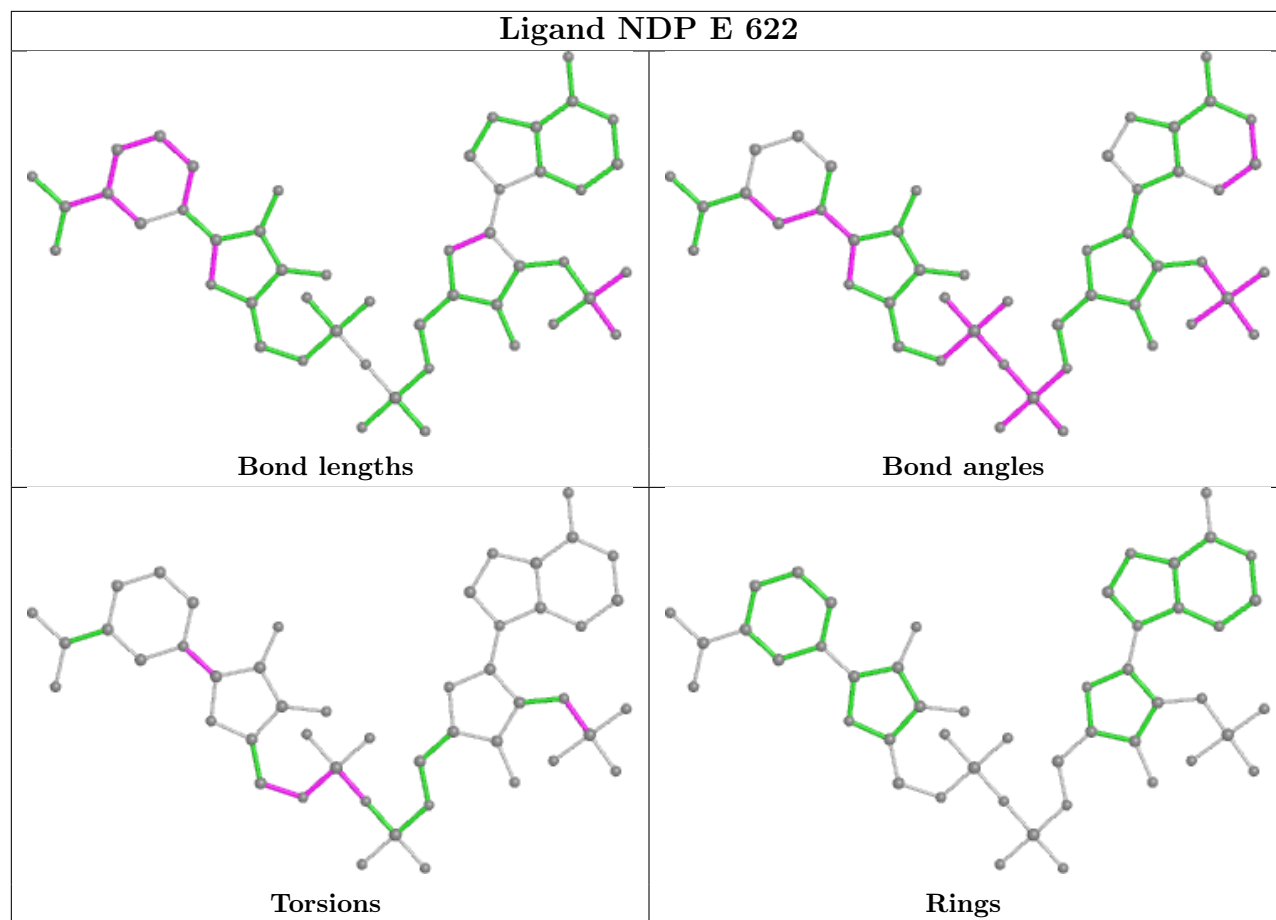


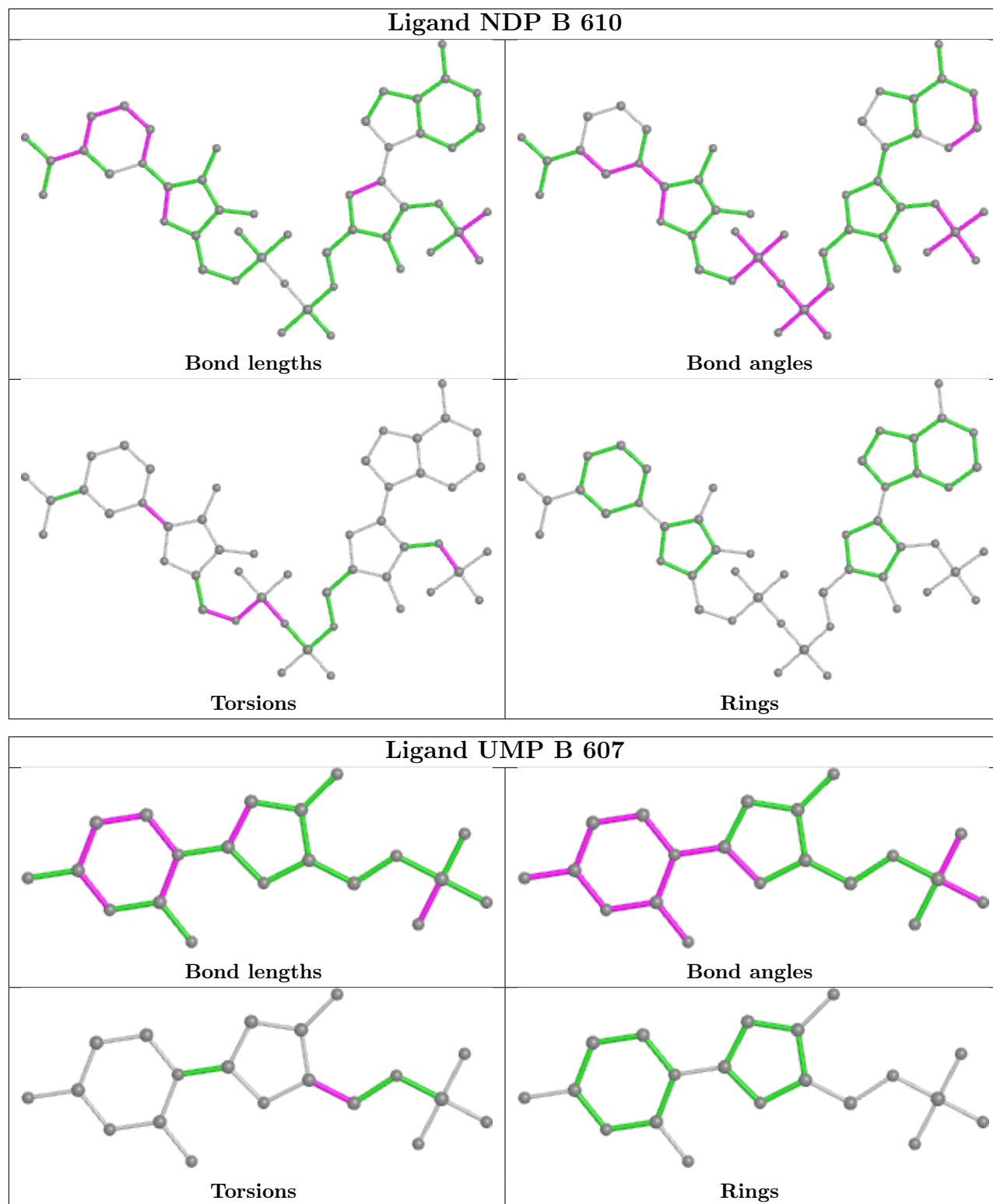


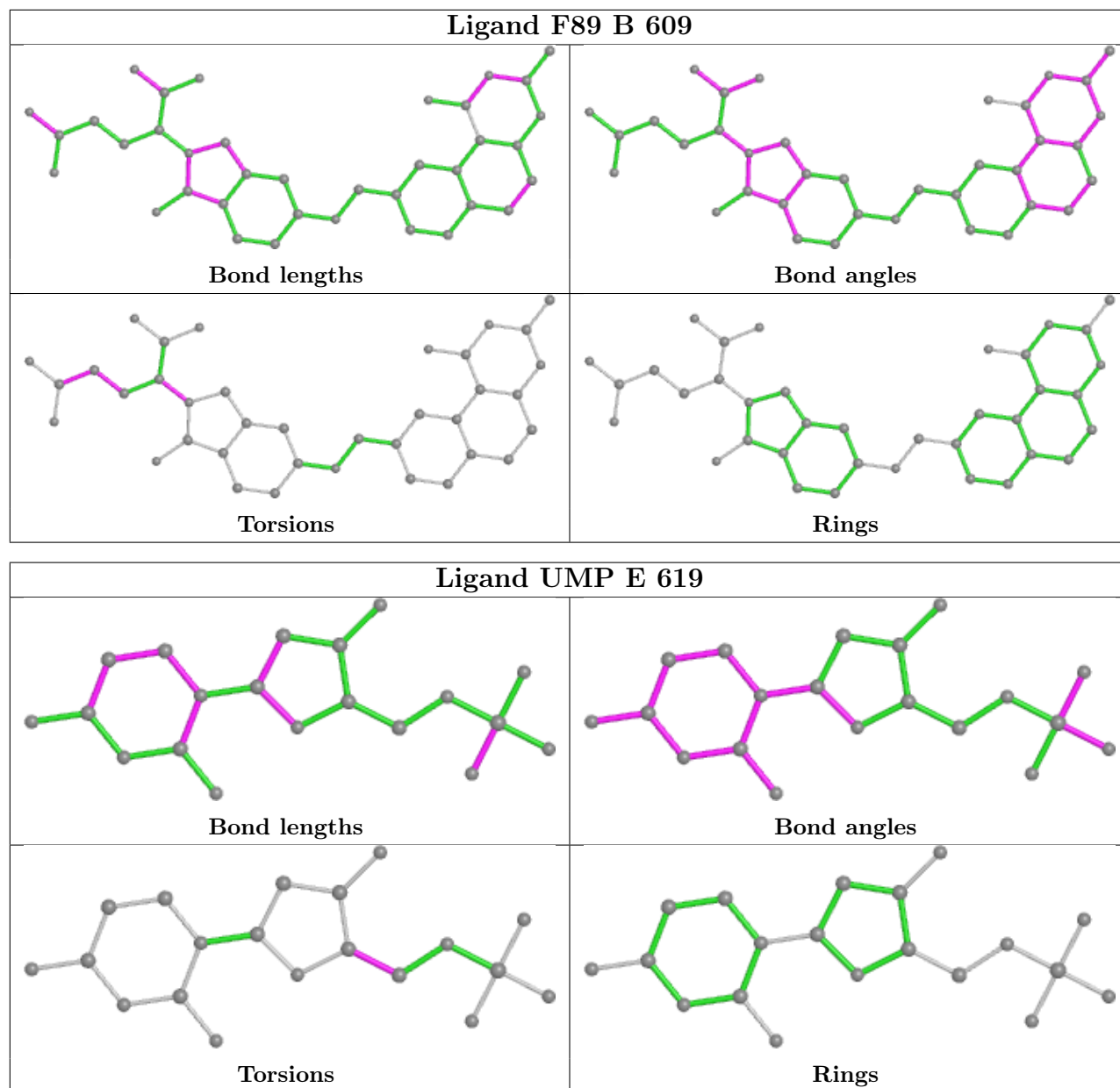


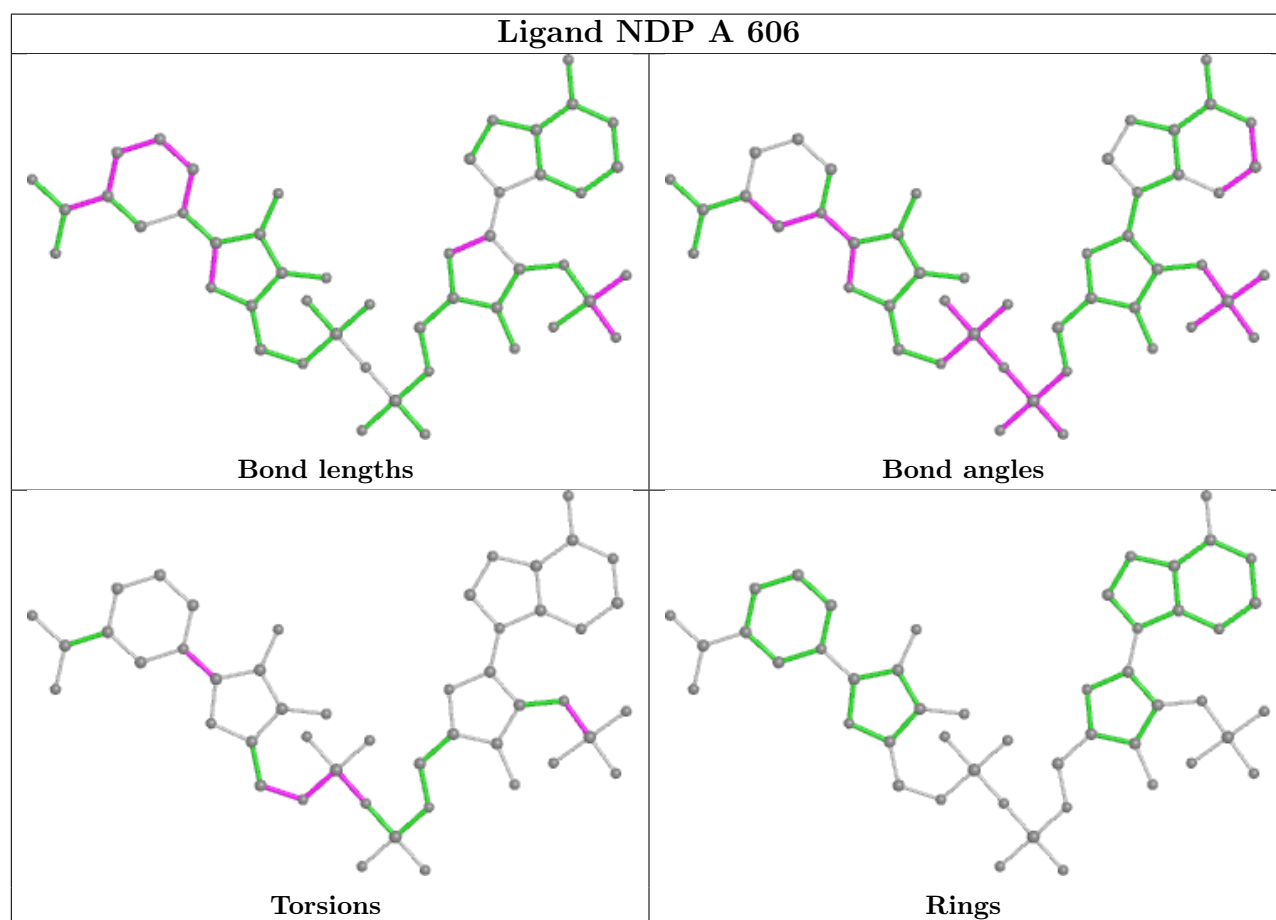
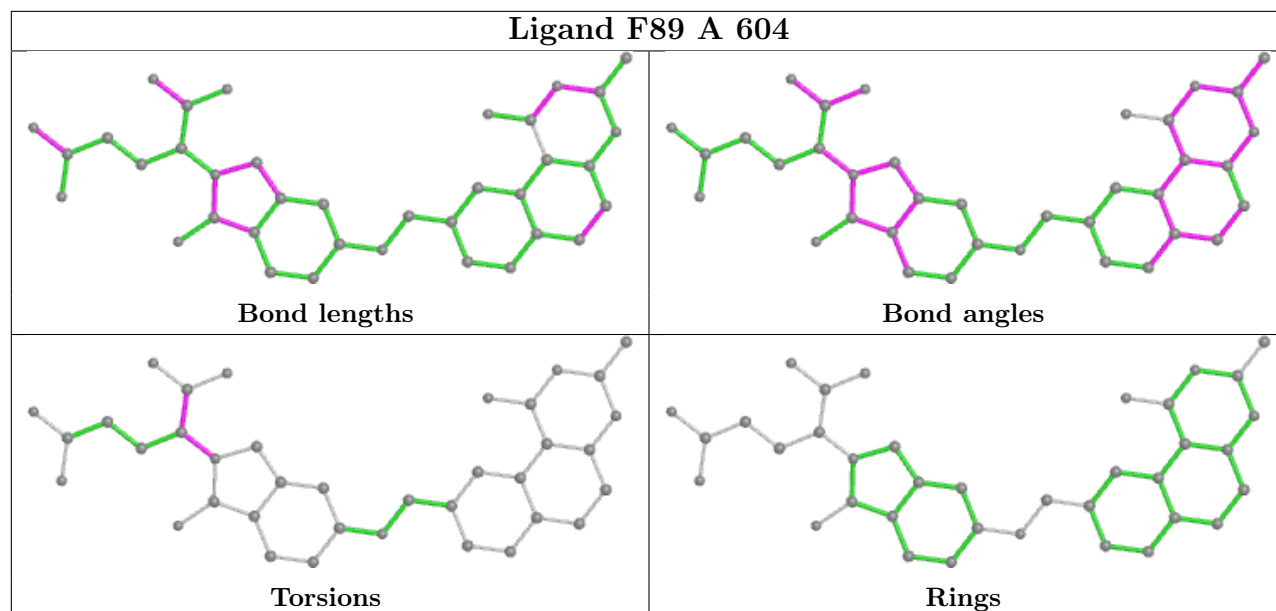


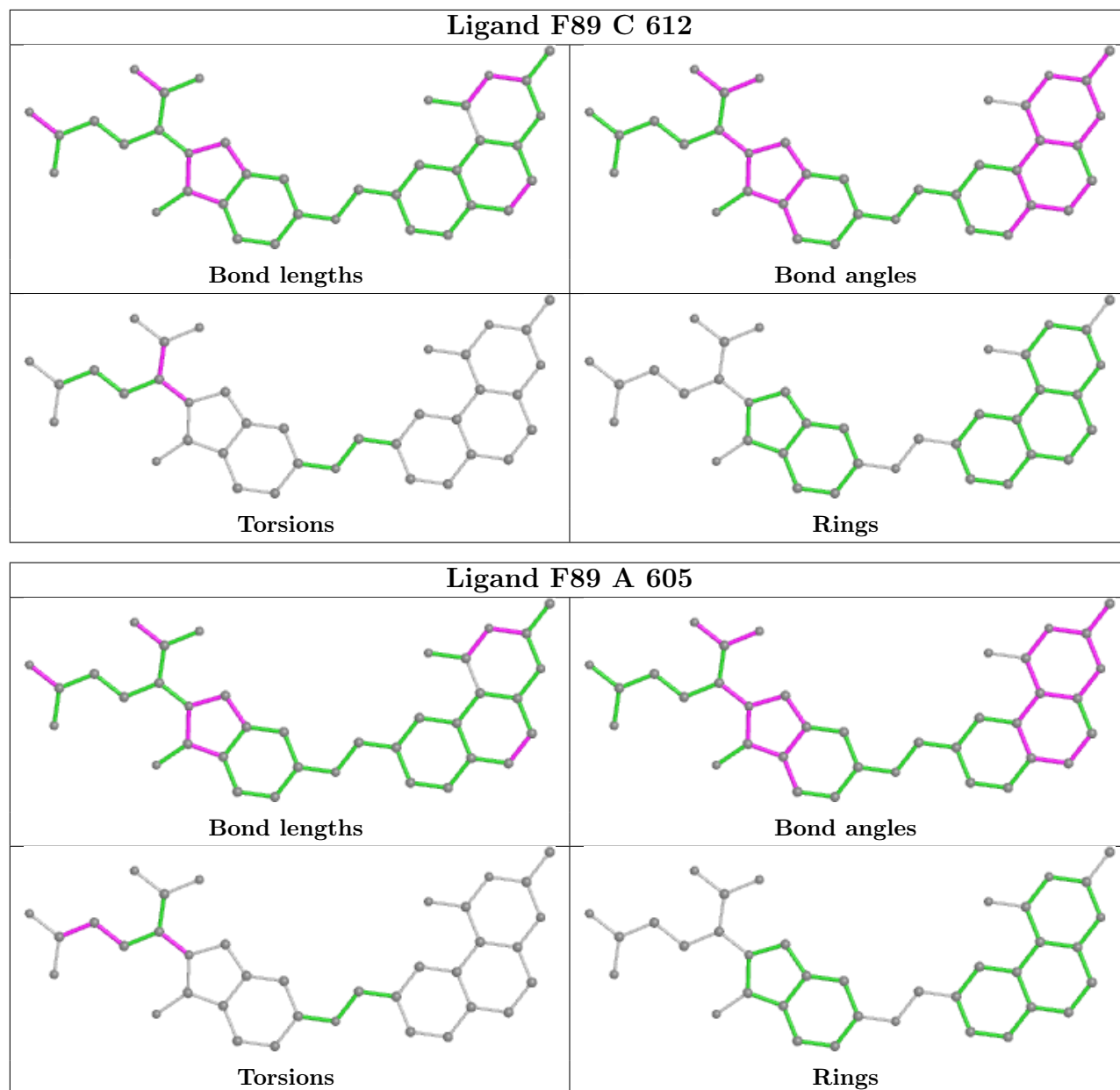


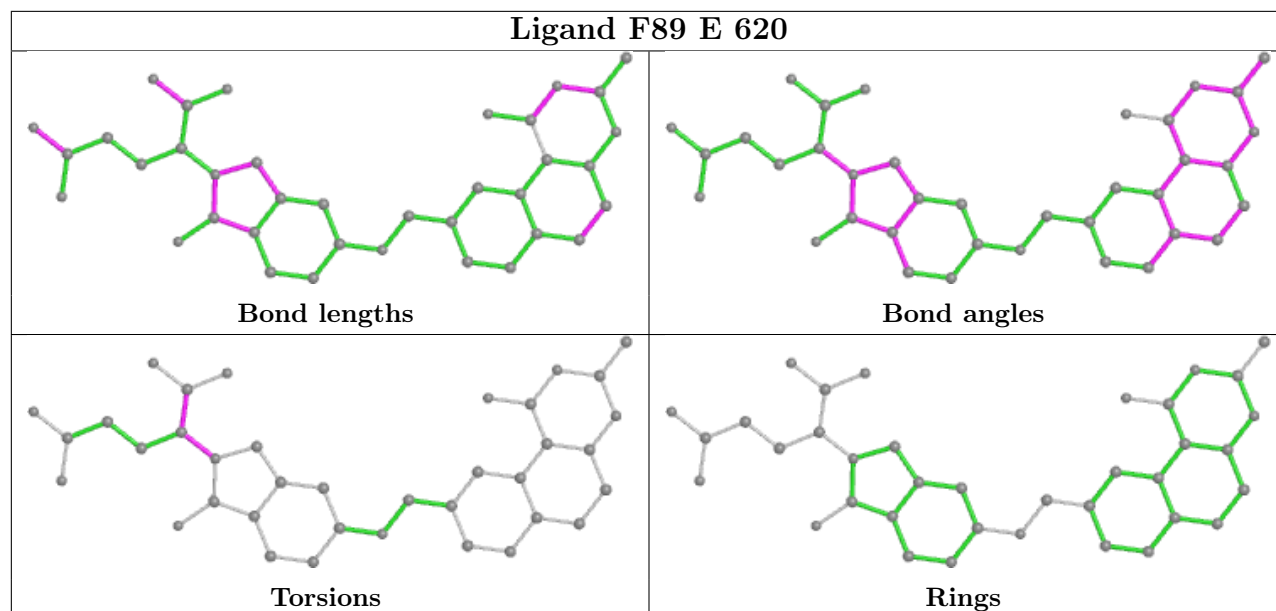












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/521 (99%)	-0.28	10 (1%) 66 65	16, 30, 54, 76	0
1	B	519/521 (99%)	-0.25	9 (1%) 70 70	16, 29, 51, 76	0
1	C	519/521 (99%)	-0.31	9 (1%) 70 70	17, 30, 52, 76	0
1	D	519/521 (99%)	-0.29	13 (2%) 57 55	18, 31, 55, 76	0
1	E	519/521 (99%)	-0.19	15 (2%) 51 48	19, 32, 55, 76	0
All	All	2595/2605 (99%)	-0.26	56 (2%) 62 60	16, 31, 54, 76	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	521	VAL	6.1
1	D	521	VAL	6.0
1	B	180	LYS	5.1
1	D	182	THR	5.0
1	B	521	VAL	5.0
1	C	182	THR	5.0
1	B	182	THR	4.9
1	A	182	THR	4.8
1	E	180	LYS	4.8
1	C	180	LYS	4.6
1	E	182	THR	4.2
1	A	180	LYS	4.2
1	E	521	VAL	3.9
1	D	180	LYS	3.8
1	C	183	LEU	3.7
1	D	183	LEU	3.7
1	E	183	LEU	3.7
1	D	102	MET	3.4
1	A	183	LEU	3.4
1	A	179	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	179	GLU	3.3
1	C	521	VAL	3.3
1	B	102	MET	3.3
1	E	102	MET	3.2
1	E	520	ALA	3.1
1	C	179	GLU	3.1
1	C	82	ASP	3.1
1	B	183	LEU	3.0
1	D	520	ALA	3.0
1	D	179	GLU	2.9
1	C	102	MET	2.9
1	D	181	LYS	2.8
1	E	184	GLN	2.7
1	A	102	MET	2.7
1	E	181	LYS	2.6
1	B	179	GLU	2.6
1	A	181	LYS	2.5
1	B	103	ASN	2.5
1	C	3	GLU	2.4
1	C	181	LYS	2.4
1	D	84	ALA	2.4
1	E	84	ALA	2.4
1	D	82	ASP	2.3
1	E	82	ASP	2.3
1	A	520	ALA	2.2
1	D	3	GLU	2.2
1	B	3	GLU	2.2
1	B	520	ALA	2.1
1	D	184	GLN	2.1
1	E	328	ILE	2.1
1	E	519	MET	2.1
1	A	331	GLY	2.1
1	D	47	ASN	2.1
1	E	324	TYR	2.0
1	A	184	GLN	2.0
1	E	178	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

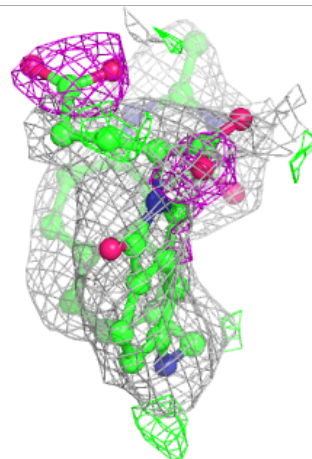
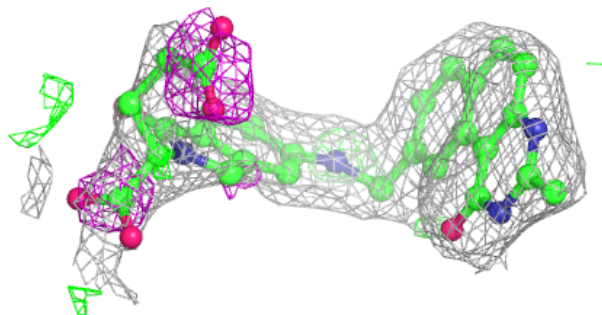
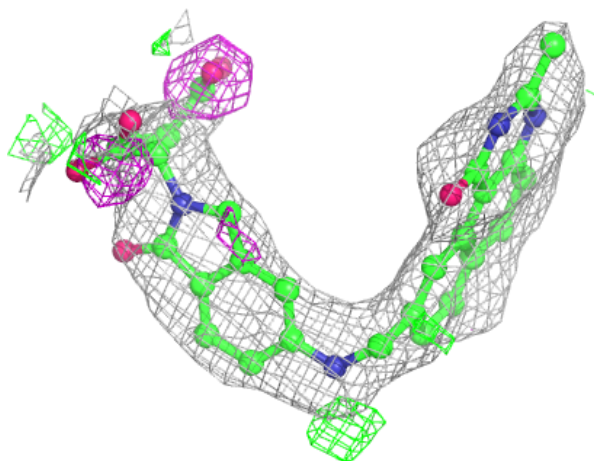
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	F89	D	616	37/37	0.83	0.28	42,50,56,56	0
3	F89	A	604	37/37	0.84	0.27	42,50,56,56	0
3	F89	E	620	37/37	0.84	0.36	42,50,56,56	0
3	F89	C	612	37/37	0.85	0.27	42,50,56,56	0
3	F89	B	608	37/37	0.86	0.28	42,50,56,56	0
3	F89	D	617	37/37	0.91	0.23	42,50,56,56	0
3	F89	C	613	37/37	0.91	0.23	42,50,56,56	0
3	F89	E	621	37/37	0.91	0.21	42,50,56,56	0
3	F89	B	609	37/37	0.92	0.24	42,50,56,56	0
3	F89	A	605	37/37	0.93	0.24	42,50,56,56	0
2	UMP	D	615	20/20	0.94	0.20	52,64,69,69	0
2	UMP	B	607	20/20	0.95	0.22	47,61,67,67	0
2	UMP	E	619	20/20	0.95	0.17	54,64,69,69	0
2	UMP	C	611	20/20	0.95	0.21	49,61,68,68	0
4	NDP	C	614	48/48	0.95	0.17	31,43,53,54	0
2	UMP	A	603	20/20	0.96	0.24	50,63,68,69	0
4	NDP	D	618	48/48	0.96	0.17	33,42,52,52	0
4	NDP	E	622	48/48	0.96	0.14	33,43,52,53	0
4	NDP	B	610	48/48	0.98	0.17	29,38,49,50	0
4	NDP	A	606	48/48	0.98	0.17	29,38,48,50	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.

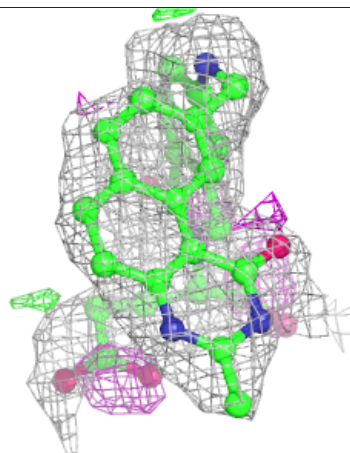
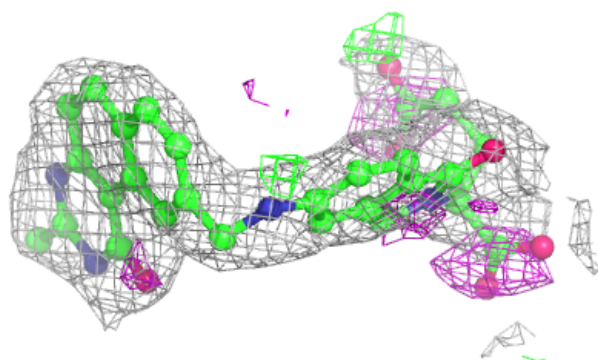
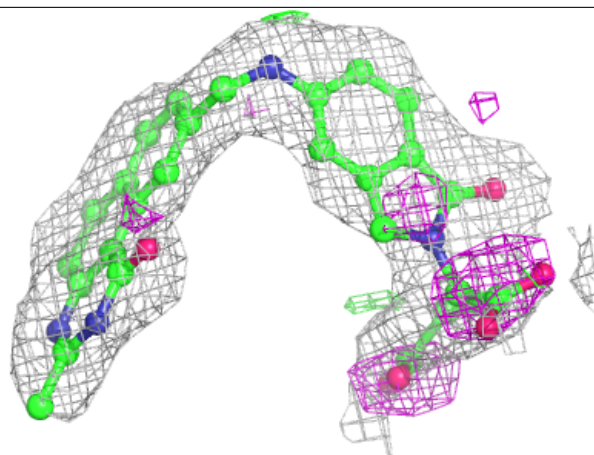
Electron density around F89 D 616:

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



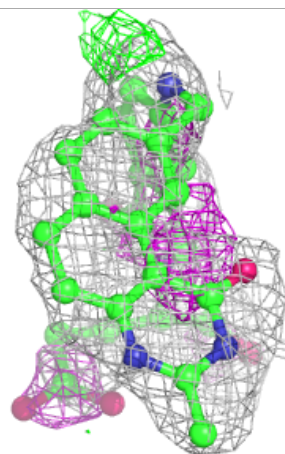
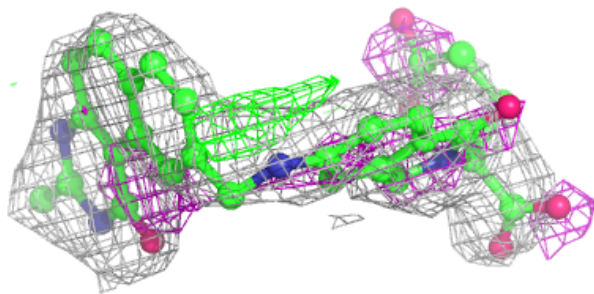
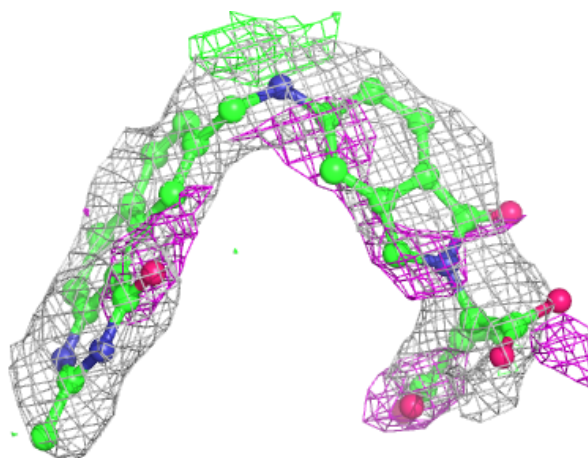
Electron density around F89 A 604:

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



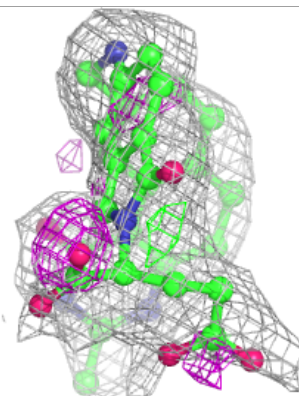
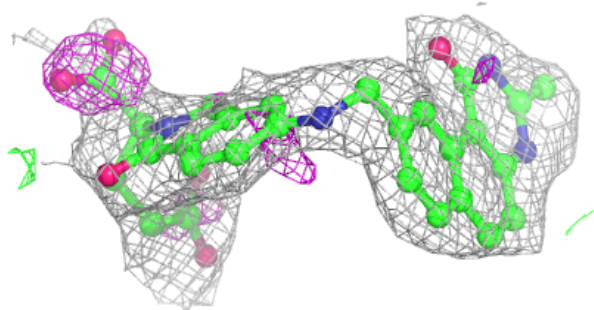
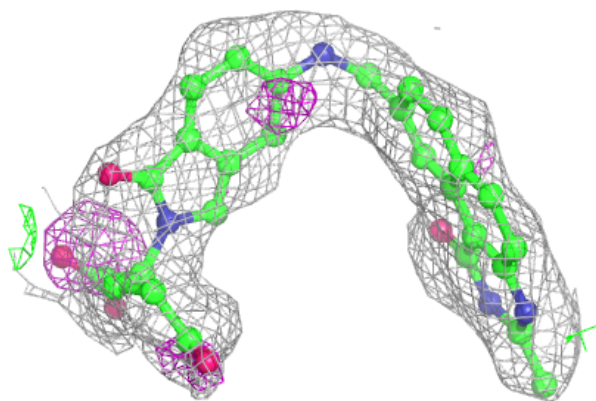
Electron density around F89 E 620:

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

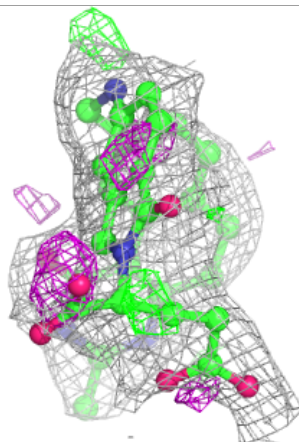
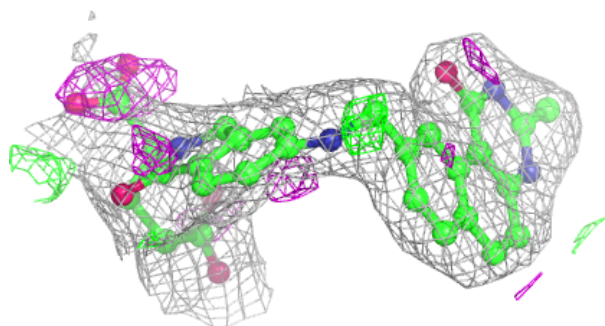
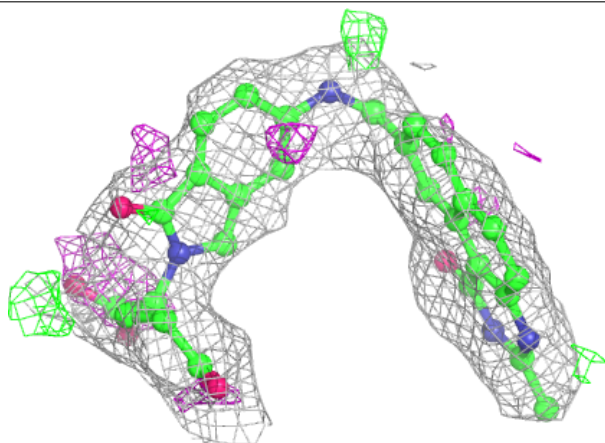


Electron density around F89 C 612:

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

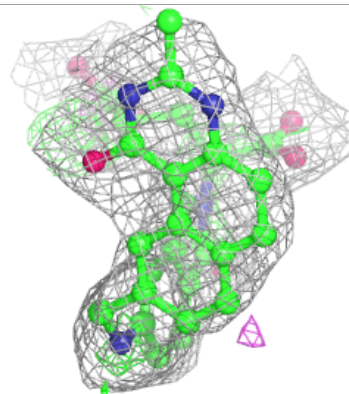
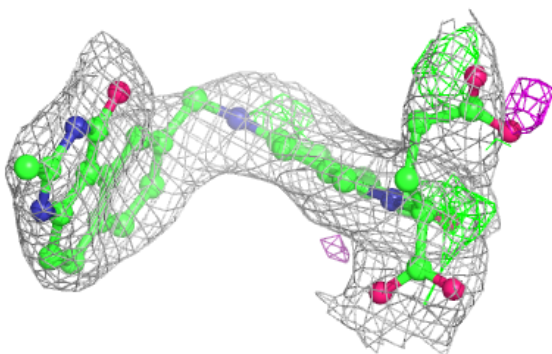
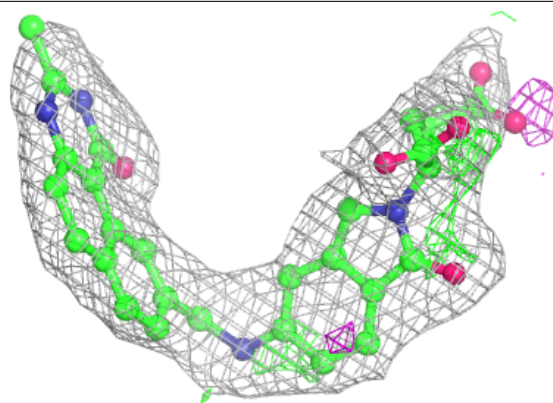
**Electron density around F89 B 608:**

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



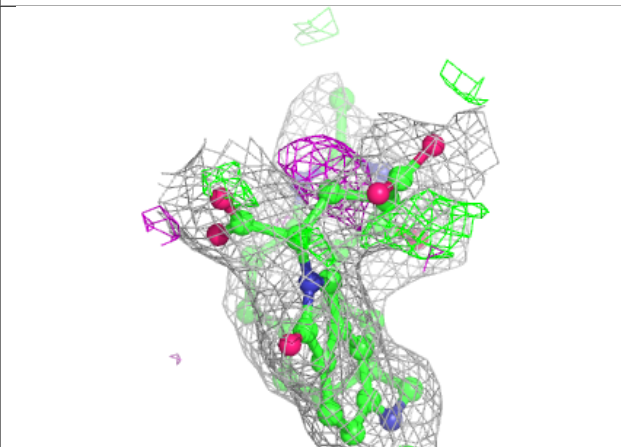
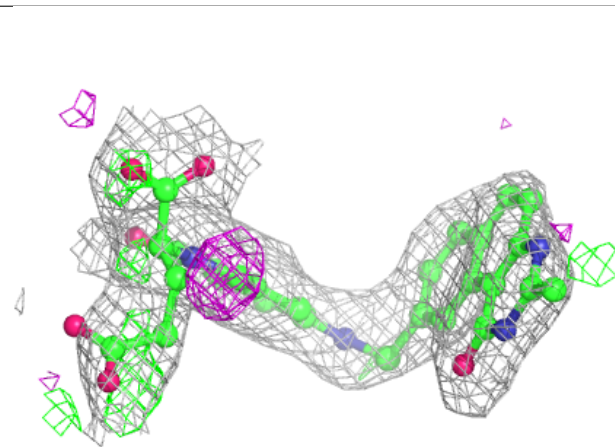
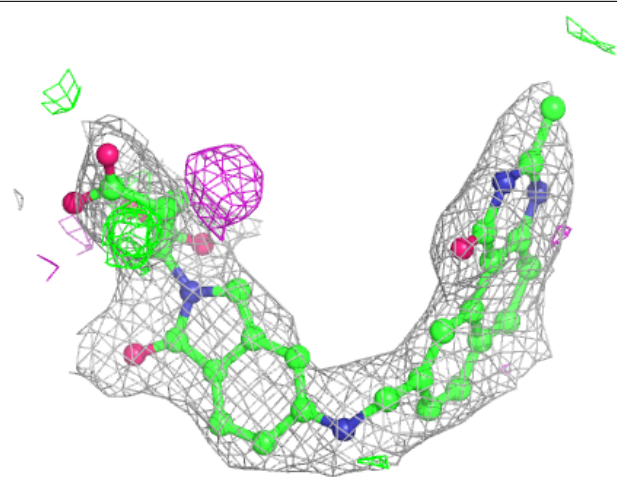
Electron density around F89 D 617:

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



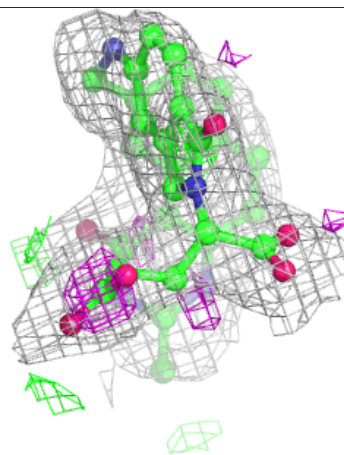
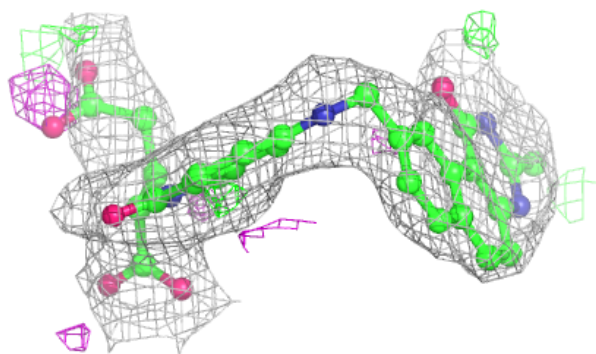
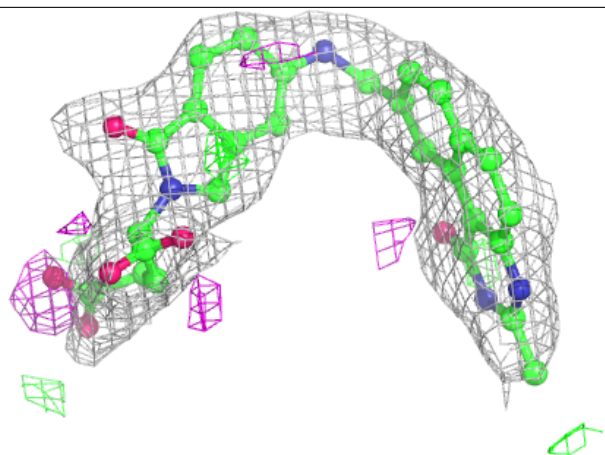
Electron density around F89 C 613:

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



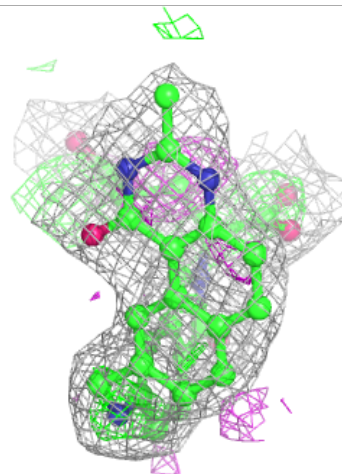
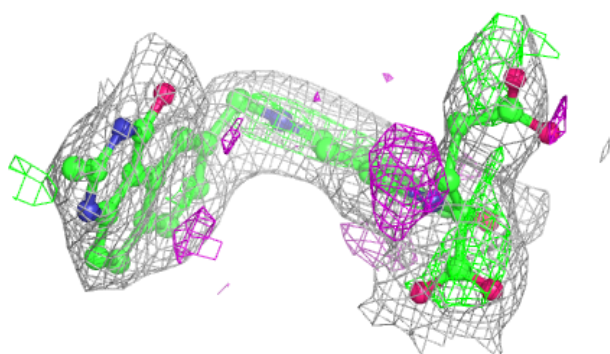
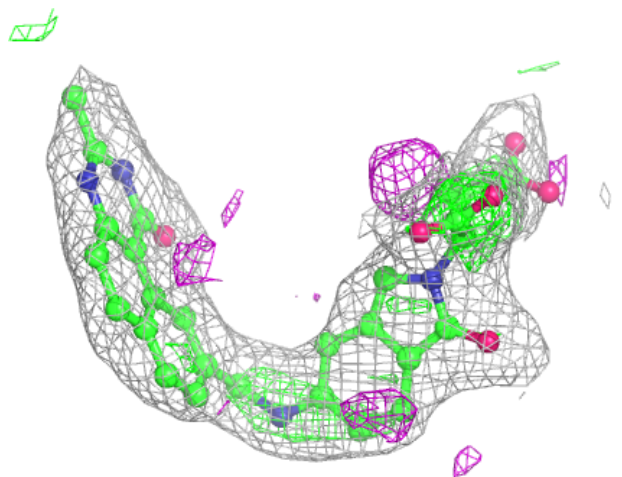
Electron density around F89 E 621:

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



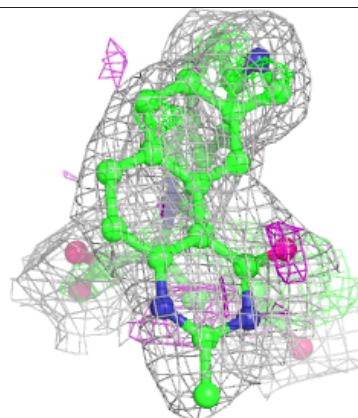
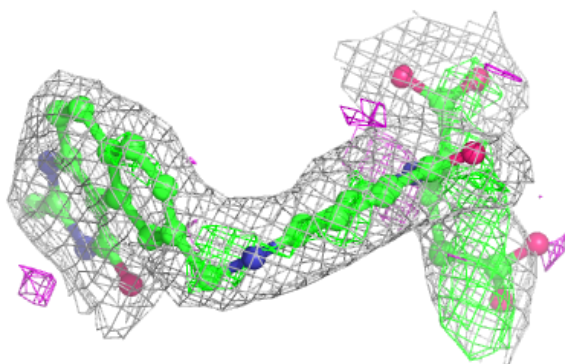
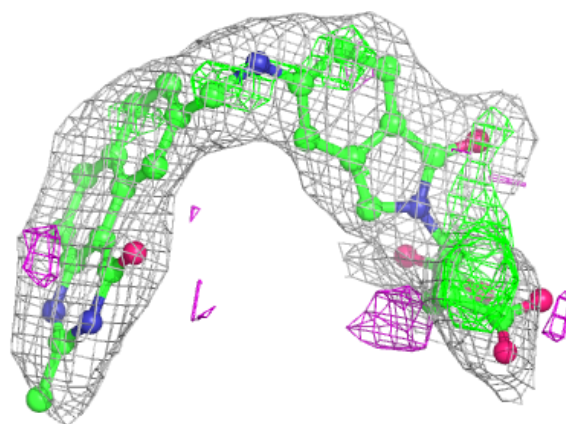
Electron density around F89 B 609:

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

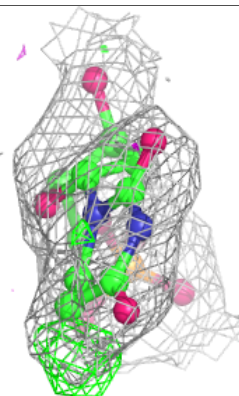
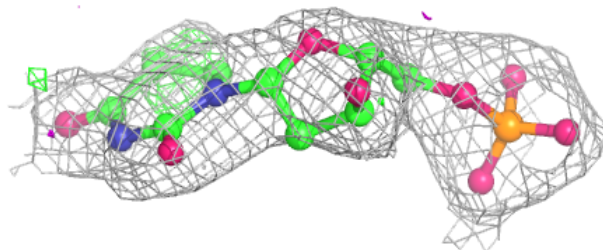
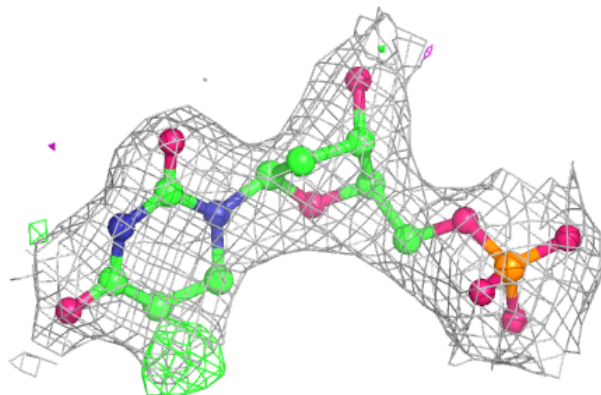


Electron density around F89 A 605:

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

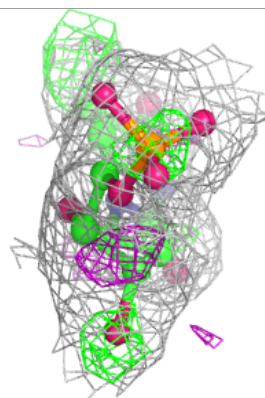
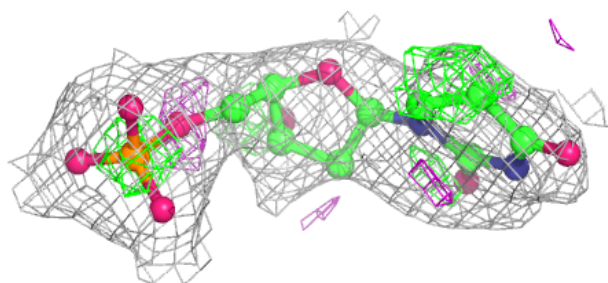
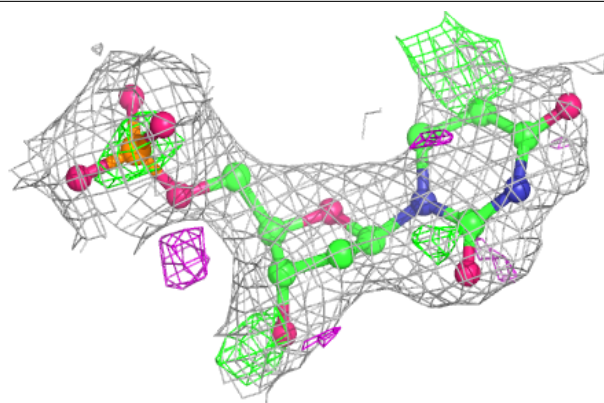
**Electron density around UMP D 615:**

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

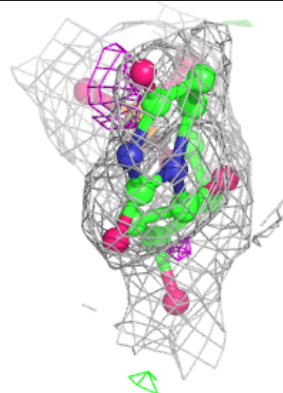
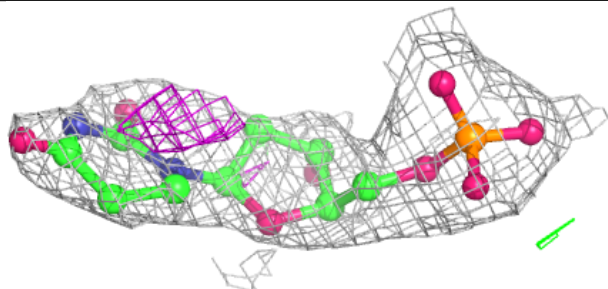
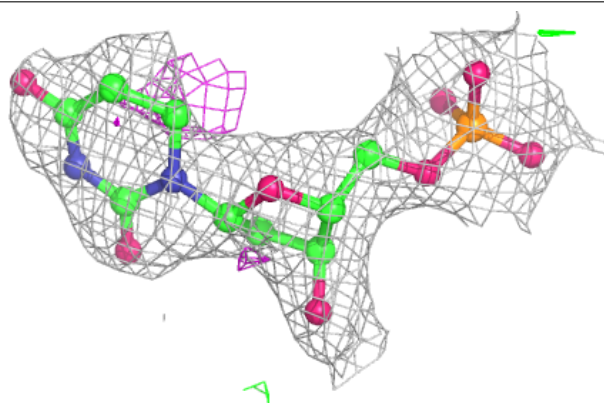


Electron density around UMP B 607:

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

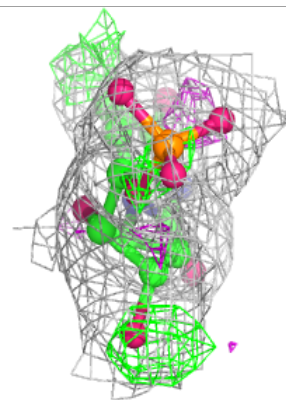
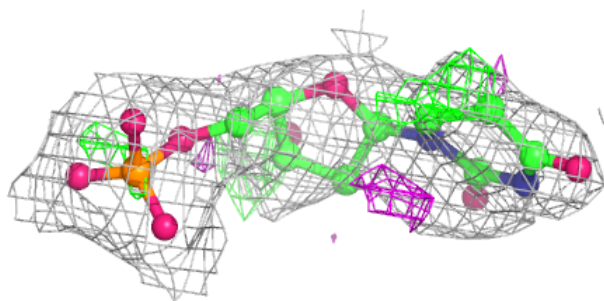
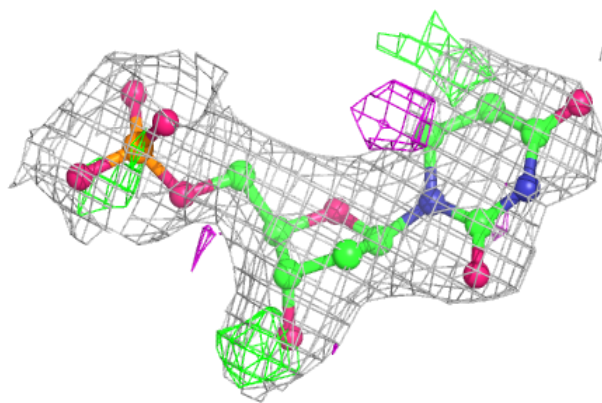
**Electron density around UMP E 619:**

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

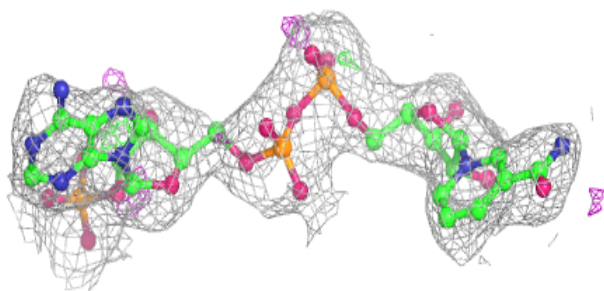
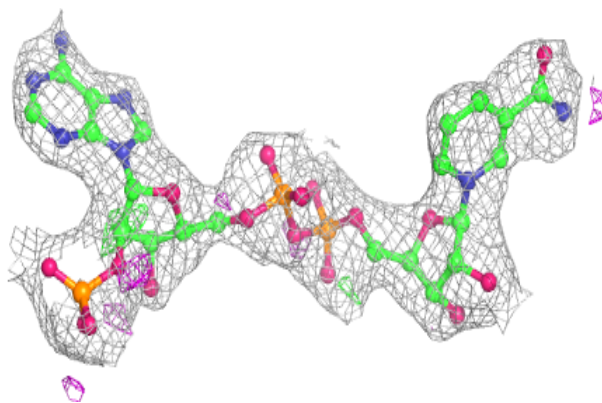


Electron density around UMP C 611:

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

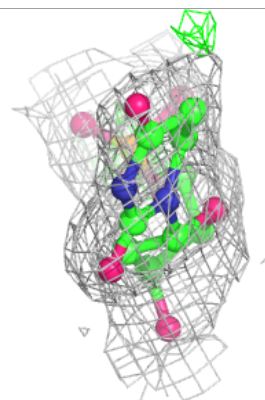
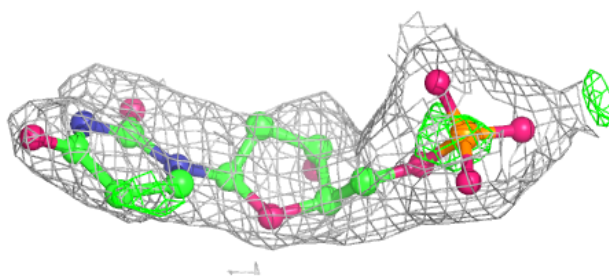
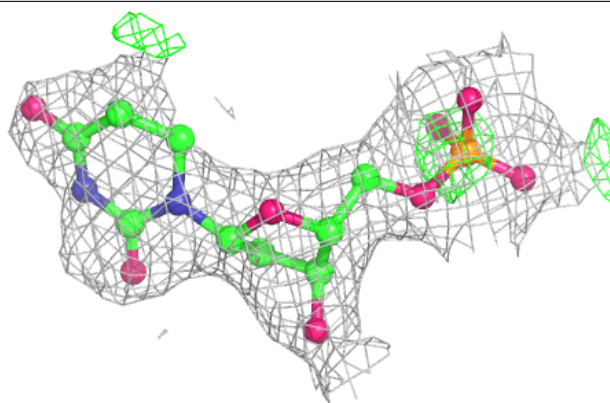
**Electron density around NDP C 614:**

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

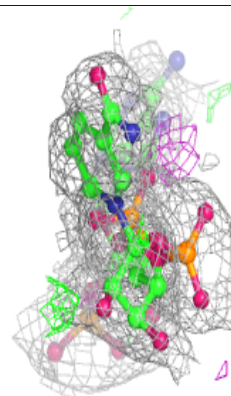
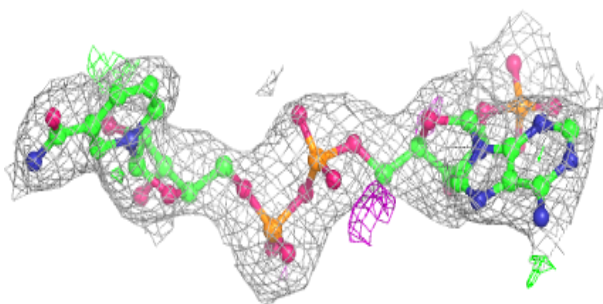
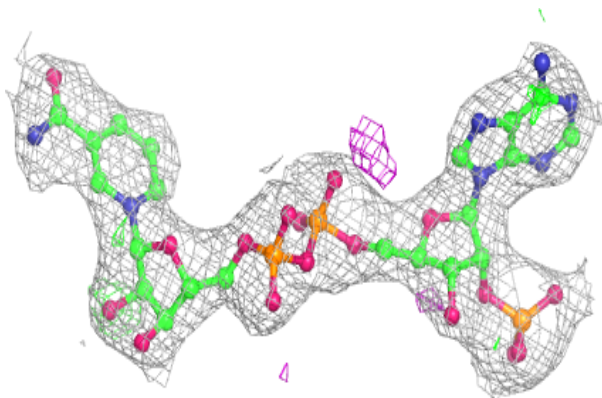


Electron density around UMP A 603:

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

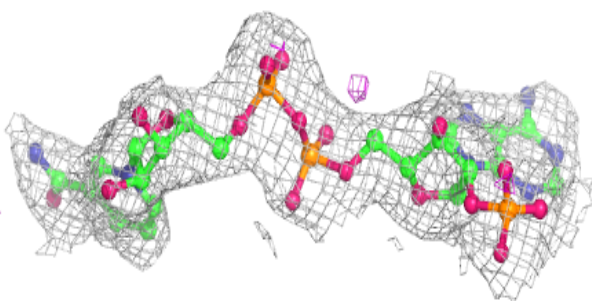
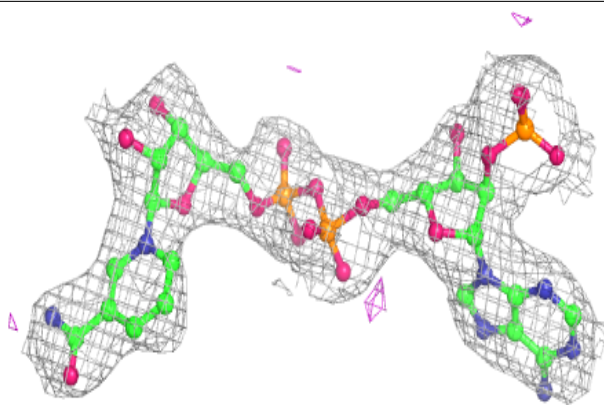
**Electron density around NDP D 618:**

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

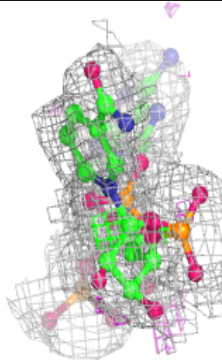
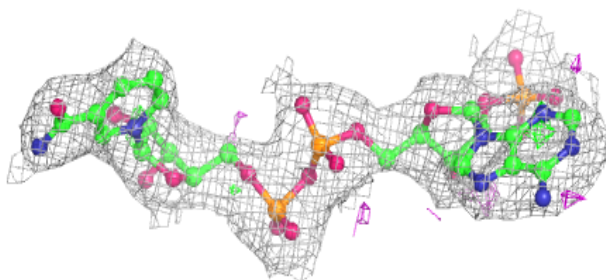
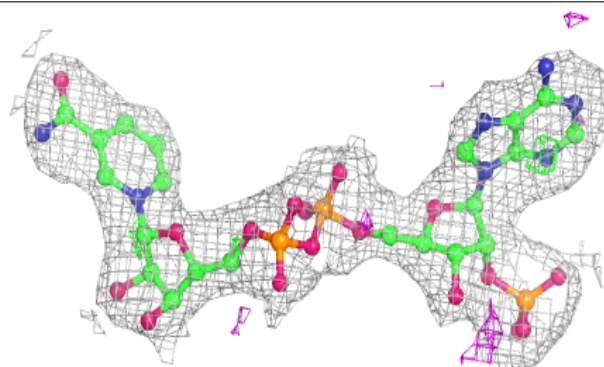


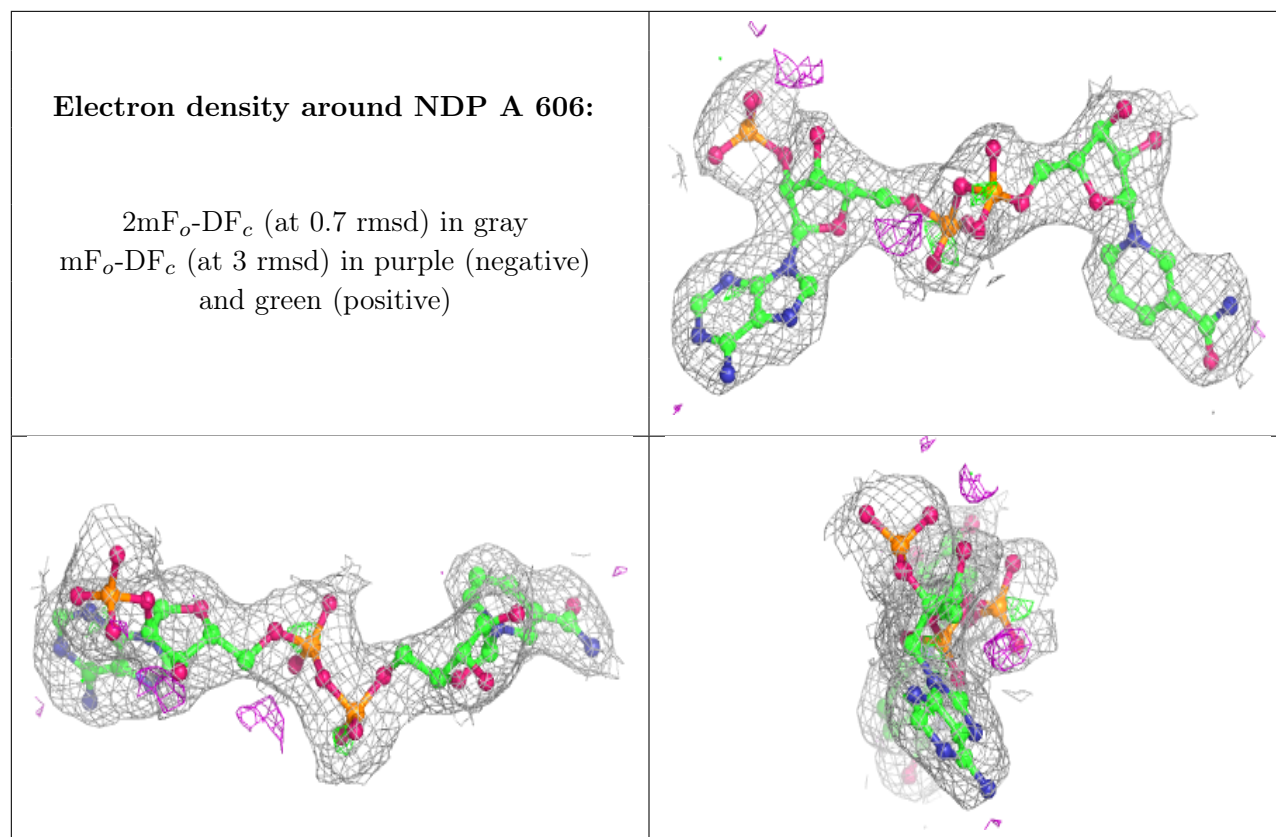
Electron density around NDP E 622:

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

**Electron density around NDP B 610:**

$2mF_o-DF_c$ (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.