



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:44 PM UTC

PDB ID : 1KZJ / pdb_00001kzj
Title : Crystal Structure of EcTS W80G/dUMP/CB3717 Complex
Authors : Fritz, T.A.; Liu, L.; Finer-Moore, J.S.; Stroud, R.M.
Deposited on : 2002-02-06
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

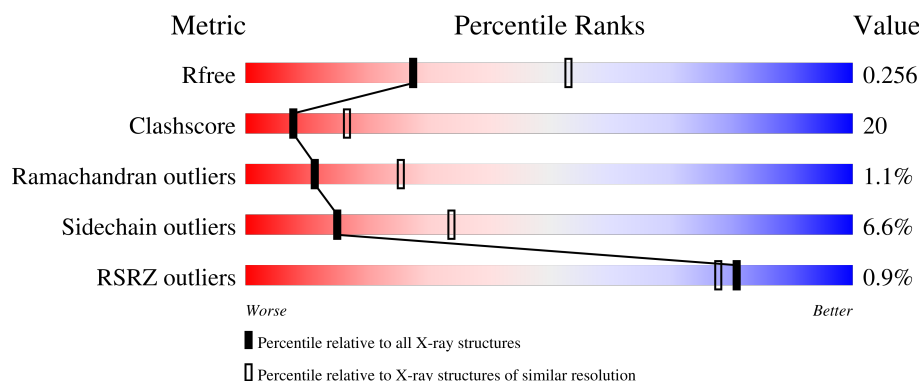
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	264	
1	B	264	
1	C	264	
1	D	264	
1	E	264	

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Mol	Chain	Length	Quality of chain
1	F	264	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 61%, a yellow segment representing 34%, and a small orange segment representing 5%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13459 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.

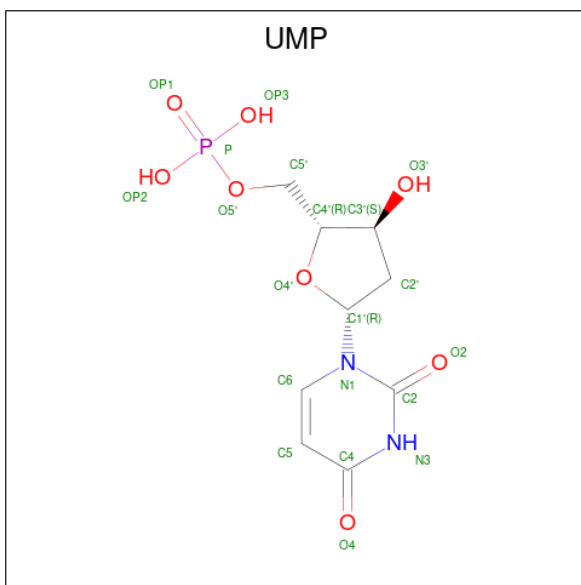
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2143	1366	370	395	12			
1	B	264	Total	C	N	O	S	0	0	0
			2143	1366	370	395	12			
1	C	264	Total	C	N	O	S	0	0	0
			2143	1366	370	395	12			
1	D	264	Total	C	N	O	S	0	0	0
			2143	1366	370	395	12			
1	E	261	Total	C	N	O	S	0	0	0
			2122	1352	367	391	12			
1	F	264	Total	C	N	O	S	0	0	0
			2143	1366	370	395	12			

There are 12 discrepancies between the modelled and reference sequences:

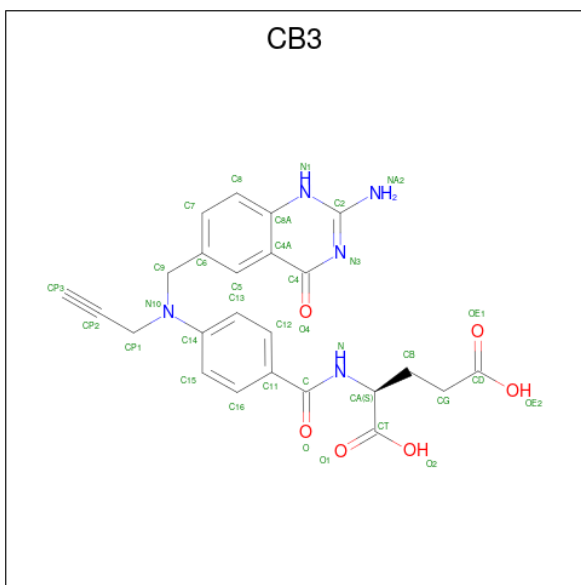
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	modified residue	UNP P0A884
A	80	GLY	TRP	engineered mutation	UNP P0A884
B	1	CXM	MET	modified residue	UNP P0A884
B	80	GLY	TRP	engineered mutation	UNP P0A884
C	1	CXM	MET	modified residue	UNP P0A884
C	80	GLY	TRP	engineered mutation	UNP P0A884
D	1	CXM	MET	modified residue	UNP P0A884
D	80	GLY	TRP	engineered mutation	UNP P0A884
E	1	CXM	MET	modified residue	UNP P0A884
E	80	GLY	TRP	engineered mutation	UNP P0A884
F	1	CXM	MET	modified residue	UNP P0A884
F	80	GLY	TRP	engineered mutation	UNP P0A884

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



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

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (CCD ID: CB3) (formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		
3	C	1	Total	C	N	O	0	0
			35	24	5	6		
3	D	1	Total	C	N	O	0	0
			35	24	5	6		
3	E	1	Total	C	N	O	0	0
			35	24	5	6		
3	F	1	Total	C	N	O	0	0
			35	24	5	6		

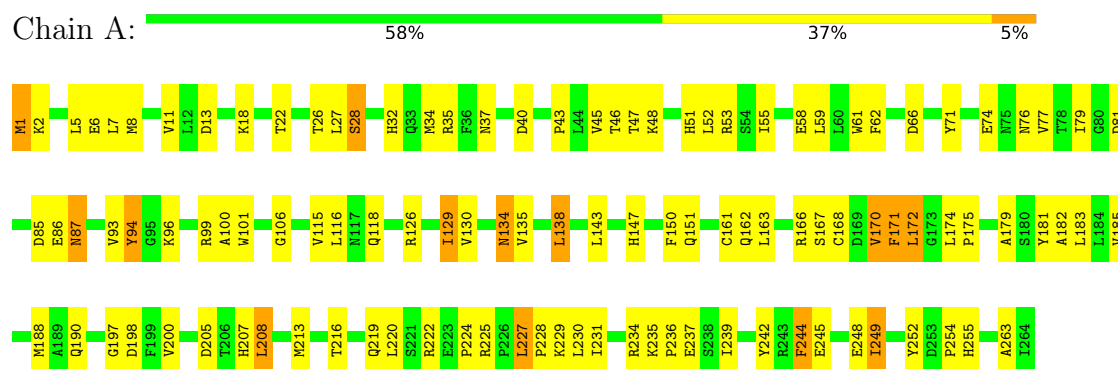
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	54	Total	O	0	0
			54	54		
4	C	62	Total	O	0	0
			62	62		
4	D	34	Total	O	0	0
			34	34		
4	E	36	Total	O	0	0
			36	36		
4	F	52	Total	O	0	0
			52	52		

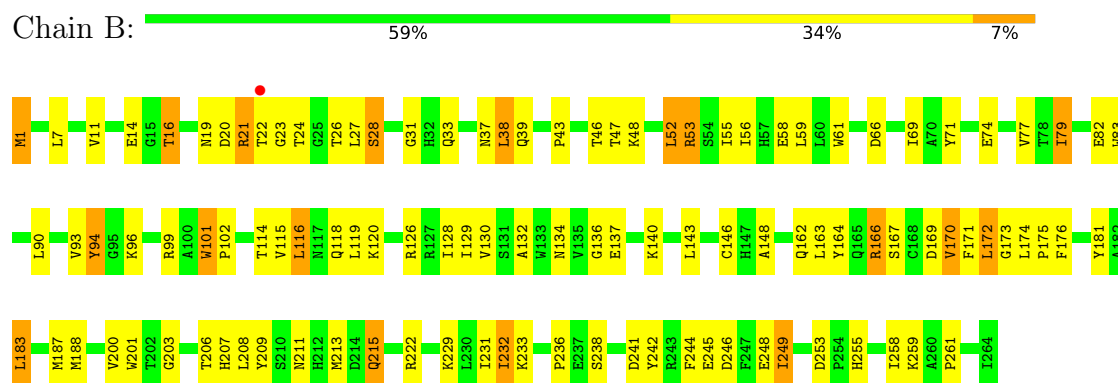
3 Residue-property plots

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

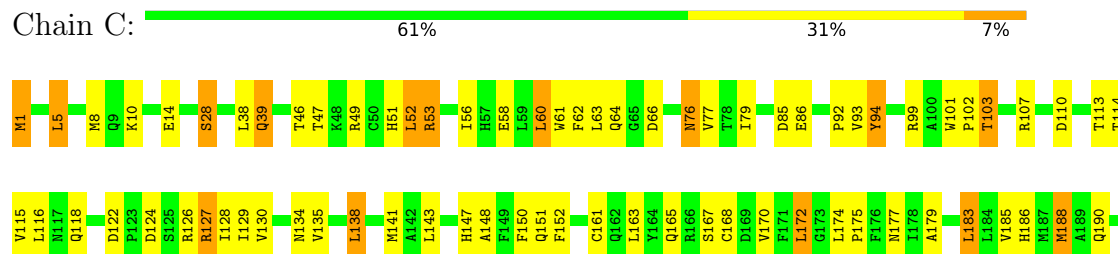
• Molecule 1: Thymidylate synthase

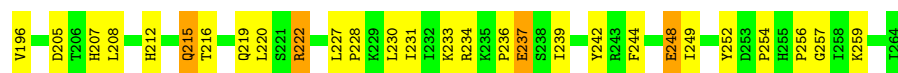


• Molecule 1: Thymidylate synthase

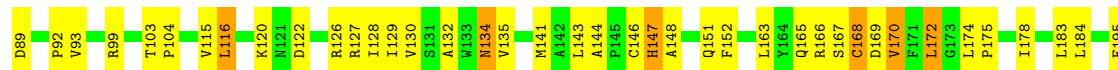


• Molecule 1: Thymidylate synthase

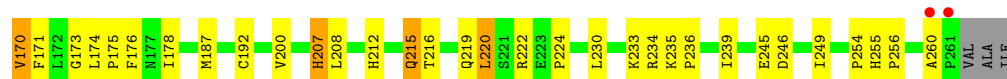
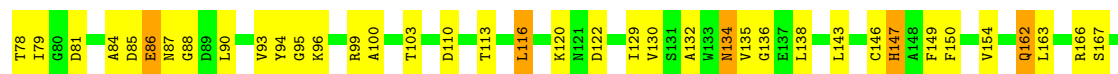




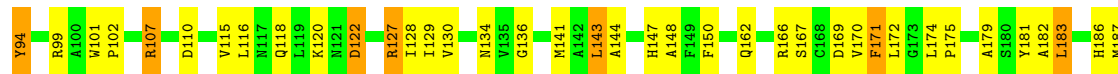
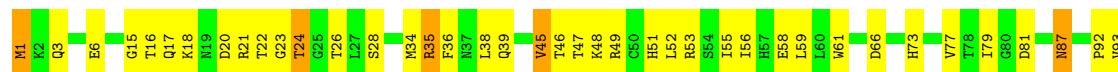
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.55Å 84.57Å 111.52Å 90.00° 111.37° 90.00°	Depositor
Resolution (Å)	25.35 – 2.60 25.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.35-2.60) 98.2 (25.35-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.258 0.213 , 0.256	Depositor DCC
R_{free} test set	3545 reflections (7.06%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13459	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4247e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, CXM, CB3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/2190	0.95	10/2972 (0.3%)
1	B	0.45	0/2190	0.95	12/2972 (0.4%)
1	C	0.44	0/2190	0.91	5/2972 (0.2%)
1	D	0.44	0/2190	0.91	11/2972 (0.4%)
1	E	0.46	0/2169	0.95	8/2944 (0.3%)
1	F	0.46	0/2190	0.95	7/2972 (0.2%)
All	All	0.45	0/13119	0.94	53/17804 (0.3%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	170	VAL	N-CA-C	7.05	117.77	110.36
1	F	24	THR	N-CA-C	6.98	118.54	111.07
1	D	168	CYS	N-CA-C	6.84	119.51	107.61
1	A	27	LEU	N-CA-C	-6.76	97.26	108.34
1	B	170	VAL	N-CA-C	6.63	118.18	110.62
1	C	28	SER	N-CA-C	6.37	119.91	109.85
1	B	146	CYS	N-CA-C	-6.37	103.03	111.24
1	A	28	SER	N-CA-C	6.33	118.80	109.24
1	F	122	ASP	CA-C-N	6.32	126.24	119.28
1	F	122	ASP	C-N-CA	6.32	126.24	119.28
1	A	81	ASP	N-CA-C	6.29	118.93	111.33
1	B	148	ALA	N-CA-C	6.20	120.92	113.23
1	E	147	HIS	N-CA-C	-6.12	96.47	107.98
1	F	171	PHE	N-CA-C	6.04	117.67	111.14
1	B	232	ILE	N-CA-C	-6.03	99.19	107.99
1	A	182	ALA	N-CA-C	-5.99	104.75	111.28
1	D	132	ALA	N-CA-C	-5.93	106.00	113.72
1	E	207	HIS	N-CA-C	5.88	118.81	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	LEU	N-CA-C	5.86	118.55	111.40
1	D	148	ALA	N-CA-C	5.70	120.94	113.30
1	A	171	PHE	N-CA-C	5.67	117.26	111.14
1	B	253	ASP	CA-C-N	5.62	125.60	120.21
1	B	253	ASP	C-N-CA	5.62	125.60	120.21
1	D	207	HIS	N-CA-C	5.61	118.21	109.52
1	C	148	ALA	N-CA-C	5.56	120.76	113.30
1	C	129	ILE	N-CA-C	5.54	117.78	108.81
1	A	170	VAL	N-CA-C	5.51	116.14	110.36
1	E	132	ALA	N-CA-C	-5.46	106.66	113.38
1	F	129	ILE	N-CA-C	5.46	116.59	108.46
1	A	129	ILE	N-CA-C	5.39	117.64	108.86
1	B	28	SER	N-CA-C	5.38	117.59	109.41
1	B	132	ALA	N-CA-C	-5.36	106.12	113.30
1	C	172	LEU	N-CA-C	5.35	117.93	111.40
1	A	13	ASP	N-CA-C	5.32	116.89	111.14
1	E	255	HIS	N-CA-C	-5.30	102.34	110.07
1	C	168	CYS	N-CA-C	5.28	117.22	108.13
1	F	148	ALA	N-CA-C	5.26	119.86	113.38
1	F	207	HIS	N-CA-C	5.25	117.39	109.41
1	B	173	GLY	N-CA-C	5.23	119.46	112.77
1	D	255	HIS	N-CA-C	-5.23	102.44	110.07
1	D	26	THR	N-CA-C	5.22	116.23	108.60
1	D	170	VAL	N-CA-C	5.19	116.54	110.62
1	D	122	ASP	CA-C-N	5.18	124.84	119.56
1	D	122	ASP	C-N-CA	5.18	124.84	119.56
1	B	140	LYS	N-CA-C	-5.17	107.00	113.72
1	E	122	ASP	CA-C-N	5.14	124.85	119.82
1	E	122	ASP	C-N-CA	5.14	124.85	119.82
1	B	90	LEU	N-CA-C	-5.13	107.05	113.72
1	B	102	PRO	N-CA-C	5.12	118.60	110.21
1	A	168	CYS	N-CA-C	5.10	116.91	108.13
1	A	106	GLY	N-CA-C	5.05	120.73	114.37
1	D	147	HIS	N-CA-C	-5.02	98.54	107.98
1	E	233	LYS	N-CA-C	5.02	118.50	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2143	0	2072	95	0
1	B	2143	0	2072	77	0
1	C	2143	0	2072	83	0
1	D	2143	0	2073	88	0
1	E	2122	0	2048	93	0
1	F	2143	0	2072	82	0
2	A	20	0	10	0	0
2	B	20	0	10	1	0
2	C	20	0	10	1	0
2	D	20	0	11	1	0
2	E	20	0	11	1	0
2	F	20	0	10	2	0
3	A	35	0	21	2	0
3	B	35	0	21	2	0
3	C	35	0	21	3	0
3	D	35	0	21	6	0
3	E	35	0	21	5	0
3	F	35	0	21	1	0
4	A	54	0	0	2	0
4	B	54	0	0	4	0
4	C	62	0	0	6	0
4	D	34	0	0	1	0
4	E	36	0	0	1	0
4	F	52	0	0	3	0
All	All	13459	0	12597	509	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 20.

All (509) 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:F:183:LEU:HD22	1:F:187:MET:HE2	1.36	1.07
1:C:127:ARG:HH21	1:C:127:ARG:HG3	1.27	0.99
1:D:83:TRP:HH2	3:D:307:CB3:H8	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LYS:HD2	1:B:248:GLU:HG2	1.44	0.97
1:A:59:LEU:HD23	1:A:183:LEU:HD23	1.45	0.96
1:E:1:CXM:HE1	1:E:43:PRO:HA	1.47	0.96
1:C:127:ARG:HH21	1:C:127:ARG:CG	1.83	0.91
1:D:129:ILE:HG12	1:D:151:GLN:HB2	1.53	0.90
1:E:173:GLY:HA2	3:E:309:CB3:HP3	1.54	0.88
1:A:231:ILE:HB	1:A:248:GLU:HB3	1.55	0.85
1:C:116:LEU:HG	1:C:188:MET:HE1	1.57	0.84
1:B:115:VAL:HA	1:B:118:GLN:HE21	1.43	0.83
1:A:229:LYS:HE2	1:A:231:ILE:HD11	1.61	0.82
1:C:102:PRO:HG2	4:C:441:HOH:O	1.77	0.82
1:E:215:GLN:H	1:E:215:GLN:HE21	1.27	0.82
1:E:174:LEU:HG	1:E:178:ILE:HD11	1.62	0.82
1:D:83:TRP:CH2	3:D:307:CB3:H8	2.15	0.81
1:C:8:MET:HE2	1:C:216:THR:HG23	1.62	0.81
1:C:177:ASN:HD21	2:C:304:UMP:HN3	1.26	0.81
1:F:107:ARG:HH11	1:F:107:ARG:HG3	1.45	0.81
1:D:116:LEU:HD12	1:D:120:LYS:HE3	1.61	0.81
1:B:21:ARG:HG2	1:B:21:ARG:HH21	1.47	0.79
1:C:51:HIS:CD2	1:C:53:ARG:HB3	2.18	0.78
1:E:134:ASN:C	1:E:134:ASN:HD22	1.90	0.78
1:D:134:ASN:C	1:D:134:ASN:HD22	1.88	0.78
1:C:127:ARG:HG3	1:C:127:ARG:NH2	1.96	0.78
1:F:116:LEU:HD22	1:F:188:MET:CE	2.14	0.78
1:E:51:HIS:HD2	1:E:53:ARG:H	1.32	0.77
1:A:222:ARG:NH2	1:A:255:HIS:HB3	1.98	0.77
1:A:59:LEU:CD2	1:A:183:LEU:HD23	2.13	0.77
1:F:59:LEU:HD23	1:F:187:MET:HE1	1.65	0.77
1:A:86:GLU:CD	1:A:86:GLU:H	1.93	0.77
1:C:103:THR:HG23	1:C:107:ARG:O	1.85	0.76
1:E:51:HIS:CD2	1:E:53:ARG:H	2.03	0.76
1:F:127:ARG:HG3	1:F:127:ARG:HH11	1.50	0.76
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.51	0.75
1:C:116:LEU:HG	1:C:188:MET:CE	2.16	0.74
1:C:28:SER:HB3	1:C:207:HIS:HB3	1.71	0.73
1:A:8:MET:HE2	1:A:216:THR:HG23	1.69	0.73
1:C:53:ARG:HD3	1:C:244:PHE:CE1	2.24	0.73
1:C:212:HIS:O	1:C:215:GLN:HG2	1.88	0.72
1:B:233:LYS:HD2	1:B:248:GLU:CG	2.20	0.72
1:A:51:HIS:CD2	1:A:53:ARG:HB3	2.23	0.72
1:F:116:LEU:HD22	1:F:188:MET:HE1	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:CXM:HE1	1:E:43:PRO:CA	2.20	0.72
1:E:215:GLN:HE21	1:E:215:GLN:N	1.88	0.71
1:F:234:ARG:HG2	1:F:235:LYS:N	2.06	0.70
1:E:1:CXM:ON1	1:E:47:THR:OG1	2.08	0.70
1:F:59:LEU:CD2	1:F:187:MET:HE1	2.22	0.70
1:F:51:HIS:CD2	1:F:53:ARG:HB2	2.26	0.70
1:F:51:HIS:HD2	1:F:53:ARG:HB2	1.56	0.70
1:D:52:LEU:HD12	1:D:55:ILE:HD12	1.74	0.70
1:B:11:VAL:HG11	1:B:208:LEU:HB2	1.74	0.69
1:B:208:LEU:HG	1:B:213:MET:HE1	1.73	0.69
1:D:262:VAL:HG12	1:D:263:ALA:H	1.56	0.69
1:E:170:VAL:HB	1:E:208:LEU:HD13	1.74	0.69
1:B:21:ARG:HG2	1:B:21:ARG:NH2	2.04	0.69
1:C:127:ARG:HG3	1:C:127:ARG:O	1.91	0.69
1:C:143:LEU:HD13	4:C:663:HOH:O	1.93	0.69
1:E:234:ARG:HD3	1:E:246:ASP:OD1	1.93	0.69
1:E:53:ARG:NH2	1:E:75:ASN:O	2.27	0.68
1:A:222:ARG:HH21	1:A:255:HIS:HB3	1.55	0.68
1:D:1:CXM:HE1	1:D:43:PRO:CB	2.23	0.68
1:F:170:VAL:HB	1:F:208:LEU:HD13	1.74	0.68
1:F:26:THR:HG22	1:F:209:TYR:HA	1.75	0.68
1:B:53:ARG:HA	1:B:244:PHE:HE1	1.58	0.67
1:C:5:LEU:HD21	1:C:47:THR:HG21	1.75	0.67
1:A:2:LYS:O	1:A:6:GLU:HG3	1.94	0.67
1:B:22:THR:O	1:B:24:THR:N	2.26	0.67
1:C:135:VAL:HA	1:C:138:LEU:HD22	1.75	0.67
1:E:69:ILE:HG22	1:E:72:LEU:HD12	1.76	0.67
1:E:234:ARG:O	1:E:236:PRO:HD3	1.95	0.66
1:F:107:ARG:HG3	1:F:107:ARG:NH1	2.09	0.66
1:A:22:THR:HG21	1:A:263:ALA:HB1	1.78	0.66
1:A:222:ARG:HH21	1:A:255:HIS:CB	2.08	0.66
1:B:116:LEU:HD12	1:B:120:LYS:HE3	1.76	0.66
1:B:174:LEU:HB3	1:B:175:PRO:HD3	1.77	0.66
1:B:238:SER:HB3	1:B:241:ASP:OD2	1.96	0.66
1:C:230:LEU:HA	1:C:249:ILE:HD13	1.77	0.66
1:D:170:VAL:HB	1:D:208:LEU:HD13	1.78	0.66
1:D:262:VAL:HG12	1:D:263:ALA:N	2.11	0.65
1:F:92:PRO:O	1:F:141:MET:HE2	1.96	0.65
1:A:222:ARG:HD3	1:A:255:HIS:ND1	2.11	0.65
1:E:215:GLN:H	1:E:215:GLN:NE2	1.94	0.65
1:F:116:LEU:CD2	1:F:188:MET:CE	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:GLY:CA	3:E:309:CB3:HP3	2.26	0.64
1:D:228:PRO:O	1:D:229:LYS:HD2	1.98	0.64
1:E:47:THR:HB	1:E:219:GLN:HG3	1.78	0.64
1:A:87:ASN:N	1:A:87:ASN:HD22	1.93	0.64
1:A:96:LYS:HE2	1:A:100:ALA:O	1.97	0.64
1:C:135:VAL:HA	1:C:138:LEU:CD2	2.28	0.64
1:A:51:HIS:NE2	1:A:53:ARG:HB3	2.13	0.64
1:A:55:ILE:HD13	1:A:179:ALA:HB3	1.80	0.64
1:B:115:VAL:HG13	1:B:128:ILE:CG2	2.28	0.64
1:B:119:LEU:HD23	1:B:128:ILE:HD13	1.80	0.64
1:B:172:LEU:HD21	3:B:303:CB3:C	2.28	0.63
3:C:305:CB3:HA	4:C:513:HOH:O	1.97	0.63
1:A:5:LEU:HD11	1:A:47:THR:HG21	1.80	0.63
1:B:136:GLY:HA3	4:B:573:HOH:O	1.97	0.63
1:D:116:LEU:CD1	1:D:120:LYS:HE3	2.29	0.63
1:A:126:ARG:HD3	1:B:167:SER:OG	1.99	0.62
1:E:8:MET:HE2	1:E:216:THR:HG23	1.81	0.62
1:B:28:SER:HB3	1:B:207:HIS:HB3	1.80	0.62
1:E:21:ARG:HB3	1:E:21:ARG:NH1	2.14	0.62
1:C:8:MET:CE	1:C:216:THR:HG23	2.29	0.62
1:D:212:HIS:O	1:D:215:GLN:HG2	2.00	0.62
4:C:441:HOH:O	1:D:104:PRO:HG3	2.00	0.62
1:C:219:GLN:HA	1:C:222:ARG:HG3	1.82	0.61
1:E:116:LEU:O	1:E:120:LYS:HG3	2.00	0.61
1:A:7:LEU:HD22	1:A:34:MET:HE1	1.83	0.61
1:A:170:VAL:HB	1:A:208:LEU:HD13	1.82	0.61
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.36	0.60
1:A:134:ASN:C	1:A:134:ASN:HD22	2.07	0.60
1:A:222:ARG:HB3	1:A:255:HIS:CE1	2.35	0.60
1:E:110:ASP:CG	1:E:113:THR:HG22	2.26	0.60
1:F:116:LEU:CD2	1:F:188:MET:HE2	2.32	0.60
1:B:20:ASP:OD2	1:B:22:THR:HB	2.02	0.60
1:B:134:ASN:C	1:B:134:ASN:HD22	2.10	0.60
1:E:96:LYS:HE2	1:E:100:ALA:HB3	1.84	0.60
1:E:99:ARG:HG3	1:E:99:ARG:HH11	1.66	0.60
1:E:47:THR:HG22	1:E:222:ARG:HB2	1.83	0.60
1:A:135:VAL:HA	1:A:138:LEU:HD22	1.83	0.59
3:A:301:CB3:HB1	1:F:259:LYS:HE3	1.84	0.59
1:C:130:VAL:HB	1:C:150:PHE:CZ	2.37	0.59
1:A:5:LEU:CD1	1:A:224:PRO:HG3	2.32	0.59
1:F:116:LEU:HD22	1:F:188:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ARG:HH11	1:D:255:HIS:HB3	1.67	0.59
3:E:309:CB3:H5	3:E:309:CB3:CP3	2.33	0.59
1:F:127:ARG:HG3	1:F:127:ARG:NH1	2.18	0.59
1:A:170:VAL:HG23	1:A:207:HIS:O	2.01	0.59
1:A:225:ARG:CZ	1:A:255:HIS:CD2	2.86	0.58
1:C:61:TRP:CD1	1:C:66:ASP:HB3	2.38	0.58
1:C:205:ASP:OD2	1:D:126:ARG:HG2	2.03	0.58
1:F:232:ILE:HG22	1:F:234:ARG:O	2.04	0.58
1:D:28:SER:HB3	1:D:207:HIS:HB3	1.85	0.58
1:C:233:LYS:NZ	1:C:248:GLU:HG3	2.18	0.58
1:C:228:PRO:HB2	1:C:249:ILE:HG23	1.83	0.58
3:E:309:CB3:H13	3:E:309:CB3:C6	2.34	0.58
1:B:47:THR:HA	1:B:255:HIS:HD2	1.68	0.57
1:C:51:HIS:NE2	1:C:53:ARG:HB3	2.19	0.57
1:C:234:ARG:O	1:C:236:PRO:HD3	2.04	0.57
1:E:134:ASN:HD22	1:E:136:GLY:H	1.51	0.57
1:E:21:ARG:NH1	2:E:308:UMP:OP1	2.36	0.57
1:E:245:GLU:CD	1:E:245:GLU:H	2.12	0.57
1:A:1:CXM:HE1	1:A:43:PRO:HA	1.85	0.57
1:B:245:GLU:CD	1:B:245:GLU:H	2.11	0.57
1:E:216:THR:HG22	1:E:220:LEU:HD23	1.87	0.57
1:F:174:LEU:HB3	1:F:175:PRO:HD3	1.87	0.57
1:B:22:THR:C	1:B:24:THR:H	2.12	0.56
3:E:309:CB3:H5	3:E:309:CB3:CP2	2.34	0.56
1:F:15:GLY:HA2	1:F:28:SER:O	2.05	0.56
1:F:144:ALA:HB3	1:F:166:ARG:NH2	2.21	0.56
1:A:222:ARG:HB3	1:A:255:HIS:ND1	2.20	0.56
1:C:47:THR:HB	1:C:219:GLN:HG3	1.87	0.56
1:E:10:LYS:NZ	1:E:32:HIS:HD2	2.03	0.56
1:F:3:GLN:HB3	1:F:34:MET:CG	2.35	0.56
1:C:28:SER:CB	1:C:207:HIS:HB3	2.35	0.56
1:A:35:ARG:HD3	1:A:198:ASP:OD2	2.06	0.56
1:D:216:THR:HG22	1:D:220:LEU:HD12	1.87	0.55
1:A:32:HIS:NE2	1:A:34:MET:HE2	2.21	0.55
1:C:134:ASN:C	1:C:134:ASN:HD22	2.15	0.55
1:E:187:MET:HB3	1:E:239:ILE:CD1	2.37	0.55
1:C:56:ILE:HG12	1:C:183:LEU:HD11	1.87	0.55
1:E:44:LEU:HD13	1:E:52:LEU:HD21	1.88	0.55
1:B:222:ARG:HD3	1:B:255:HIS:CG	2.40	0.55
1:A:87:ASN:N	1:A:87:ASN:ND2	2.54	0.55
1:E:134:ASN:ND2	1:E:136:GLY:H	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:ASN:C	1:E:134:ASN:ND2	2.61	0.55
1:A:22:THR:HG21	1:A:263:ALA:CB	2.36	0.55
1:E:162:GLN:HB2	1:E:200:VAL:HB	1.89	0.55
1:C:127:ARG:CG	1:C:127:ARG:NH2	2.53	0.54
1:D:222:ARG:NH1	1:D:255:HIS:HB3	2.22	0.54
1:C:170:VAL:HB	1:C:208:LEU:CD1	2.37	0.54
1:D:85:ASP:OD2	1:D:89:ASP:HB2	2.07	0.54
1:B:215:GLN:HB2	1:B:258:ILE:HG21	1.88	0.54
1:F:45:VAL:HG23	4:F:475:HOH:O	2.07	0.54
1:F:162:GLN:HA	1:F:200:VAL:O	2.08	0.54
1:D:17:GLN:HA	1:D:26:THR:O	2.08	0.54
1:E:68:ASN:HA	1:E:88:GLY:O	2.08	0.54
1:D:7:LEU:O	1:D:11:VAL:HG23	2.08	0.54
1:D:48:LYS:HE2	4:D:497:HOH:O	2.08	0.54
1:A:197:GLY:HA2	4:A:544:HOH:O	2.08	0.54
1:A:37:ASN:HB3	1:A:40:ASP:OD2	2.08	0.53
1:D:263:ALA:HB3	3:D:307:CB3:HN21	1.73	0.53
1:F:234:ARG:CG	1:F:235:LYS:N	2.71	0.53
1:D:99:ARG:HG3	1:D:99:ARG:HH11	1.73	0.53
1:D:134:ASN:C	1:D:134:ASN:ND2	2.61	0.53
1:A:8:MET:CE	1:A:216:THR:HG23	2.37	0.53
1:A:32:HIS:HE2	1:A:34:MET:HE2	1.72	0.53
1:B:58:GLU:O	1:B:61:TRP:HB3	2.09	0.53
1:D:5:LEU:HD11	1:D:47:THR:HG21	1.90	0.53
1:E:49:ARG:HG3	1:E:254:PRO:HG2	1.89	0.53
1:E:171:PHE:HE2	1:E:260:ALA:CB	2.22	0.53
1:A:162:GLN:HA	1:A:200:VAL:O	2.08	0.53
1:D:45:VAL:HG21	1:D:175:PRO:HB3	1.91	0.53
1:F:45:VAL:HG21	1:F:175:PRO:HB3	1.91	0.53
1:B:208:LEU:HD12	4:B:617:HOH:O	2.09	0.53
1:E:21:ARG:CB	1:E:21:ARG:HH11	2.21	0.53
1:E:129:ILE:HD13	1:E:149:PHE:HZ	1.72	0.53
1:A:190:GLN:NE2	1:A:235:LYS:HA	2.24	0.53
1:C:124:ASP:OD1	1:D:18:LYS:HD2	2.09	0.53
1:E:84:ALA:HA	1:E:90:LEU:HD23	1.91	0.53
1:F:34:MET:HE3	1:F:36:PHE:CZ	2.44	0.53
1:A:32:HIS:CD2	1:A:34:MET:HE2	2.43	0.52
1:A:234:ARG:O	1:A:236:PRO:HD3	2.09	0.52
1:D:222:ARG:HD3	1:D:255:HIS:CG	2.44	0.52
1:A:7:LEU:O	1:A:11:VAL:HG23	2.09	0.52
1:A:147:HIS:HD2	1:A:181:TYR:OH	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:TRP:CH2	1:A:134:ASN:HA	2.45	0.52
1:E:37:ASN:HB3	1:E:40:ASP:OD2	2.08	0.52
1:E:116:LEU:HD23	1:E:192:CYS:SG	2.49	0.52
1:C:114:THR:O	1:C:118:GLN:HG3	2.09	0.52
1:D:53:ARG:HG3	1:D:244:PHE:CZ	2.45	0.52
1:E:1:CXM:HA	1:E:224:PRO:HB3	1.90	0.52
1:E:86:GLU:CD	1:E:86:GLU:H	2.16	0.52
1:B:129:ILE:HG22	1:B:130:VAL:N	2.24	0.52
1:C:110:ASP:CG	1:C:113:THR:HG23	2.34	0.52
1:E:174:LEU:HG	1:E:178:ILE:CD1	2.38	0.52
1:B:1:CXM:CN	1:B:46:THR:H	2.23	0.52
1:B:59:LEU:HD23	1:B:183:LEU:HD12	1.91	0.52
1:B:129:ILE:CG2	1:B:130:VAL:N	2.73	0.52
1:D:228:PRO:C	1:D:229:LYS:HD2	2.35	0.52
1:E:129:ILE:HD13	1:E:149:PHE:CZ	2.45	0.52
1:E:187:MET:HB3	1:E:239:ILE:HD11	1.90	0.52
1:E:147:HIS:H	1:E:147:HIS:CD2	2.27	0.52
1:A:47:THR:HB	1:A:219:GLN:HG2	1.92	0.51
1:A:61:TRP:CD1	1:A:66:ASP:HB3	2.45	0.51
1:C:143:LEU:HD12	1:C:143:LEU:O	2.10	0.51
1:F:186:HIS:CG	1:F:230:LEU:HD23	2.45	0.51
1:D:17:GLN:HE21	1:D:27:LEU:CD2	2.23	0.51
1:D:83:TRP:HH2	3:D:307:CB3:C8	2.11	0.51
1:E:7:LEU:O	1:E:11:VAL:HG23	2.10	0.51
1:E:55:ILE:HG13	1:E:176:PHE:CE1	2.45	0.51
1:F:169:ASP:OD2	3:F:311:CB3:N3	2.44	0.51
1:C:165:GLN:HG2	1:C:167:SER:O	2.10	0.50
1:C:222:ARG:NH2	1:C:256:PRO:O	2.44	0.50
1:C:230:LEU:HD13	1:C:231:ILE:N	2.25	0.50
1:D:1:CXM:HE1	1:D:43:PRO:HB3	1.93	0.50
1:A:96:LYS:HE2	1:A:100:ALA:HB3	1.92	0.50
1:F:77:VAL:HG12	1:F:79:ILE:HG12	1.92	0.50
1:C:170:VAL:HB	1:C:208:LEU:HD12	1.92	0.50
1:C:64:GLN:HG2	4:C:444:HOH:O	2.12	0.50
1:B:82:GLU:HB2	1:B:83:TRP:CZ3	2.47	0.50
1:A:1:CXM:CN	1:A:46:THR:H	2.25	0.50
1:A:116:LEU:HD11	1:A:239:ILE:CG2	2.42	0.50
1:D:38:LEU:HD21	1:D:199:PHE:HB2	1.94	0.50
1:D:82:GLU:CD	1:D:82:GLU:H	2.19	0.50
1:F:102:PRO:HA	1:F:107:ARG:O	2.12	0.50
1:B:47:THR:HA	1:B:255:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HB3	1:A:213:MET:HE1	1.93	0.49
3:B:303:CB3:HG1	3:B:303:CB3:O2	2.12	0.49
1:B:170:VAL:HB	1:B:208:LEU:HD13	1.95	0.49
1:E:170:VAL:HG23	1:E:207:HIS:O	2.12	0.49
1:A:5:LEU:HD12	1:A:224:PRO:HG3	1.93	0.49
1:B:207:HIS:NE2	2:B:302:UMP:O3'	2.37	0.49
1:D:59:LEU:HD23	1:D:183:LEU:HD23	1.93	0.49
1:B:116:LEU:HD22	1:B:188:MET:SD	2.52	0.49
1:D:211:ASN:ND2	1:D:261:PRO:HG2	2.27	0.49
1:F:172:LEU:HD13	1:F:262:VAL:HG22	1.93	0.49
1:A:229:LYS:HE2	1:A:231:ILE:CD1	2.36	0.49
1:F:1:CXM:HA	4:F:422:HOH:O	2.10	0.49
1:C:188:MET:HE3	1:C:239:ILE:CD1	2.42	0.49
1:D:12:LEU:CD1	1:D:208:LEU:HD23	2.43	0.49
1:E:171:PHE:HE2	1:E:260:ALA:HB3	1.76	0.49
1:D:9:GLN:O	1:D:12:LEU:HB2	2.12	0.49
1:E:146:CYS:SG	1:E:167:SER:O	2.70	0.49
1:A:58:GLU:HG2	1:A:62:PHE:CZ	2.48	0.49
1:F:115:VAL:HG21	1:F:130:VAL:HG23	1.94	0.49
1:B:232:ILE:HA	1:B:246:ASP:O	2.13	0.48
1:C:126:ARG:HD3	1:D:167:SER:OG	2.13	0.48
1:D:168:CYS:SG	1:D:174:LEU:HB2	2.53	0.48
1:F:52:LEU:O	1:F:56:ILE:HG13	2.14	0.48
1:E:5:LEU:HD22	1:E:220:LEU:HD13	1.94	0.48
1:F:239:ILE:HG13	1:F:239:ILE:O	2.12	0.48
1:E:1:CXM:CN	1:E:46:THR:H	2.27	0.48
1:E:77:VAL:HG12	1:E:79:ILE:HG12	1.95	0.48
1:A:7:LEU:HD22	1:A:34:MET:CE	2.43	0.48
1:D:52:LEU:O	1:D:56:ILE:HG13	2.13	0.48
1:E:222:ARG:NH2	1:E:256:PRO:O	2.43	0.48
1:A:174:LEU:HB3	1:A:175:PRO:HD3	1.95	0.48
1:C:58:GLU:O	1:C:61:TRP:HB3	2.13	0.48
1:D:59:LEU:HD11	1:D:184:LEU:HD13	1.95	0.48
1:A:86:GLU:C	1:A:87:ASN:HD22	2.21	0.48
1:E:212:HIS:O	1:E:215:GLN:HG2	2.14	0.48
1:F:53:ARG:HA	1:F:244:PHE:HE1	1.78	0.48
1:B:169:ASP:OD2	1:B:172:LEU:CB	2.62	0.48
1:B:231:ILE:HB	1:B:248:GLU:HB2	1.94	0.48
1:D:44:LEU:HD11	1:D:50:CYS:HB2	1.94	0.48
1:A:28:SER:HB3	1:A:207:HIS:HB3	1.96	0.48
1:A:22:THR:CB	1:A:263:ALA:HB1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:CD2	1:B:188:MET:SD	3.02	0.47
1:E:154:VAL:O	1:F:18:LYS:NZ	2.30	0.47
1:D:61:TRP:CD1	1:D:66:ASP:HB3	2.49	0.47
1:F:182:ALA:O	1:F:186:HIS:HD2	1.97	0.47
1:F:55:ILE:HD13	1:F:179:ALA:HB3	1.96	0.47
1:B:33:GLN:HA	1:B:201:TRP:O	2.15	0.47
1:F:61:TRP:CD1	1:F:66:ASP:HB3	2.50	0.47
1:F:120:LYS:HE2	1:F:191:GLN:O	2.13	0.47
1:F:134:ASN:C	1:F:134:ASN:HD22	2.23	0.47
1:F:143:LEU:N	1:F:143:LEU:CD2	2.77	0.47
1:A:76:ASN:HA	1:F:53:ARG:HH11	1.79	0.47
1:A:171:PHE:CD2	1:A:172:LEU:HD13	2.50	0.47
1:E:10:LYS:HZ3	1:E:32:HIS:HD2	1.61	0.47
1:E:30:PHE:O	1:F:35:ARG:NH2	2.39	0.47
1:E:130:VAL:HB	1:E:150:PHE:CZ	2.50	0.47
1:F:147:HIS:CD2	1:F:147:HIS:H	2.31	0.47
1:A:237:GLU:OE2	1:A:237:GLU:HA	2.15	0.47
1:C:174:LEU:HB3	1:C:175:PRO:HD3	1.96	0.47
1:D:144:ALA:HB3	1:D:166:ARG:NH2	2.30	0.47
1:E:58:GLU:O	1:E:61:TRP:HB3	2.15	0.47
1:B:114:THR:O	1:B:118:GLN:HG3	2.15	0.47
1:C:128:ILE:CG2	1:C:152:PHE:HB2	2.45	0.47
1:F:166:ARG:HD2	1:F:167:SER:N	2.30	0.47
1:A:22:THR:CG2	1:A:263:ALA:HB1	2.44	0.46
1:E:15:GLY:HA2	1:E:29:ILE:HG22	1.97	0.46
1:B:46:THR:C	1:B:48:LYS:H	2.23	0.46
1:A:181:TYR:O	1:A:185:VAL:HG23	2.16	0.46
1:D:92:PRO:O	1:D:141:MET:HE2	2.15	0.46
1:F:118:GLN:NE2	1:F:128:ILE:HA	2.30	0.46
1:A:129:ILE:HD11	1:B:166:ARG:HD3	1.98	0.46
1:C:85:ASP:OD1	1:C:85:ASP:C	2.59	0.46
1:C:230:LEU:HD23	1:C:249:ILE:HD11	1.98	0.46
1:D:147:HIS:H	1:D:147:HIS:CD2	2.33	0.46
1:D:174:LEU:O	1:D:178:ILE:HG13	2.16	0.46
1:E:21:ARG:NH1	1:E:21:ARG:CB	2.77	0.46
1:B:16:THR:C	1:B:27:LEU:HD23	2.41	0.46
1:C:127:ARG:CG	1:C:127:ARG:O	2.61	0.46
1:E:166:ARG:NH1	1:E:167:SER:HB2	2.30	0.46
1:C:126:ARG:NH2	1:D:20:ASP:HB3	2.30	0.46
1:F:115:VAL:HA	1:F:118:GLN:HE21	1.80	0.46
1:A:222:ARG:NH2	1:A:255:HIS:CB	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:THR:HA	1:E:81:ASP:OD1	2.15	0.46
1:A:93:VAL:O	1:A:94:TYR:C	2.58	0.46
1:B:52:LEU:O	1:B:56:ILE:HG13	2.16	0.46
1:B:169:ASP:OD2	1:B:172:LEU:HB2	2.16	0.46
1:B:229:LYS:HA	4:B:545:HOH:O	2.15	0.46
1:C:126:ARG:NH2	1:D:20:ASP:CB	2.79	0.46
1:D:165:GLN:HG2	1:D:167:SER:O	2.16	0.46
1:E:86:GLU:CD	1:E:86:GLU:N	2.74	0.46
1:A:85:ASP:OD1	1:A:85:ASP:C	2.59	0.46
1:A:134:ASN:C	1:A:134:ASN:ND2	2.73	0.46
1:C:8:MET:HE2	1:C:216:THR:CG2	2.41	0.46
1:A:1:CXM:HE2	1:A:227:LEU:HD21	1.97	0.45
1:C:52:LEU:HD11	1:C:249:ILE:CG1	2.46	0.45
1:F:171:PHE:CD1	1:F:171:PHE:C	2.93	0.45
1:A:228:PRO:HB2	1:A:249:ILE:HD12	1.97	0.45
1:E:17:GLN:HA	1:E:26:THR:O	2.15	0.45
1:A:77:VAL:HG12	1:A:79:ILE:HG12	1.98	0.45
1:F:170:VAL:HB	1:F:208:LEU:CD1	2.42	0.45
1:B:99:ARG:HG3	1:B:99:ARG:HH11	1.81	0.45
1:D:129:ILE:CG2	1:D:130:VAL:N	2.78	0.45
1:D:147:HIS:HB2	1:D:163:LEU:HD11	1.99	0.45
1:C:1:CXM:CN	1:C:46:THR:H	2.30	0.45
1:E:58:GLU:HB2	1:E:79:ILE:HD11	1.99	0.45
1:A:46:THR:C	1:A:48:LYS:H	2.25	0.45
1:A:163:LEU:HD22	1:A:181:TYR:CE1	2.52	0.45
1:B:7:LEU:HD11	1:B:206:THR:HG21	1.97	0.45
1:A:147:HIS:HB2	1:A:163:LEU:HD11	1.99	0.45
1:B:53:ARG:HA	1:B:244:PHE:CE1	2.46	0.45
1:C:115:VAL:HA	1:C:118:GLN:HE21	1.82	0.45
1:E:110:ASP:OD1	1:E:113:THR:HG22	2.17	0.45
1:A:163:LEU:HD22	1:A:181:TYR:CD1	2.52	0.45
1:C:116:LEU:HD11	1:C:239:ILE:CG2	2.47	0.45
1:E:235:LYS:HE2	4:E:589:HOH:O	2.16	0.45
1:A:55:ILE:HD13	1:A:179:ALA:CB	2.47	0.45
1:A:71:TYR:O	1:A:74:GLU:HB2	2.17	0.45
1:B:71:TYR:O	1:B:74:GLU:HB3	2.17	0.45
1:D:36:PHE:O	1:D:38:LEU:HD22	2.16	0.45
1:D:115:VAL:HG13	1:D:128:ILE:CG2	2.47	0.45
1:D:263:ALA:HB3	3:D:307:CB3:NA2	2.31	0.45
1:E:149:PHE:CD1	1:E:149:PHE:C	2.94	0.45
1:F:53:ARG:NH2	4:F:678:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASN:ND2	1:B:261:PRO:HG2	2.31	0.44
1:C:151:GLN:O	1:C:161:CYS:HA	2.17	0.44
1:C:94:TYR:CE1	1:C:147:HIS:CE1	3.05	0.44
1:B:77:VAL:HG12	1:B:79:ILE:HG12	1.99	0.44
1:D:170:VAL:HB	1:D:208:LEU:CD1	2.46	0.44
1:E:129:ILE:HG21	1:E:149:PHE:CZ	2.53	0.44
1:F:150:PHE:HA	1:F:162:GLN:O	2.17	0.44
1:B:171:PHE:CD1	1:B:171:PHE:C	2.95	0.44
1:C:76:ASN:HD22	1:C:76:ASN:HA	1.63	0.44
1:D:212:HIS:HA	1:D:215:GLN:OE1	2.17	0.44
1:A:1:CXM:ON2	1:A:45:VAL:HG13	2.18	0.44
1:C:101:TRP:CD2	1:D:135:VAL:HB	2.53	0.44
1:E:162:GLN:HA	1:E:200:VAL:O	2.17	0.44
1:F:236:PRO:HG2	1:F:242:TYR:CG	2.53	0.44
1:C:5:LEU:HD12	1:C:5:LEU:HA	1.81	0.44
1:F:93:VAL:O	1:F:94:TYR:C	2.61	0.44
1:D:53:ARG:HG3	1:D:244:PHE:HZ	1.81	0.44
1:C:38:LEU:HD12	1:C:185:VAL:HG11	1.99	0.43
1:C:237:GLU:CD	1:C:237:GLU:O	2.61	0.43
1:D:57:HIS:CE1	1:D:75:ASN:ND2	2.86	0.43
1:D:201:TRP:CH2	1:D:203:GLY:HA3	2.53	0.43
1:E:167:SER:OG	1:E:207:HIS:HE1	2.01	0.43
1:A:166:ARG:NH1	1:A:167:SER:HB2	2.32	0.43
1:C:215:GLN:H	1:C:215:GLN:NE2	2.16	0.43
1:C:252:TYR:CE2	1:C:254:PRO:HG3	2.53	0.43
1:D:183:LEU:HD12	1:D:230:LEU:HD21	2.00	0.43
1:D:247:PHE:O	1:D:248:GLU:HG2	2.19	0.43
1:E:69:ILE:HD12	1:E:73:HIS:CE1	2.52	0.43
1:F:233:LYS:HD2	1:F:248:GLU:HG2	2.00	0.43
1:B:31:GLY:HA2	1:B:203:GLY:O	2.18	0.43
1:E:4:TYR:OH	1:E:171:PHE:HA	2.18	0.43
1:E:135:VAL:HB	1:F:101:TRP:CD2	2.54	0.43
1:A:171:PHE:HD2	1:A:172:LEU:HD13	1.83	0.43
1:C:56:ILE:HG22	1:C:60:LEU:HD22	2.00	0.43
1:E:65:GLY:HA2	1:E:95:GLY:O	2.18	0.43
1:B:101:TRP:CD1	1:B:101:TRP:C	2.97	0.43
1:B:162:GLN:HA	1:B:200:VAL:O	2.19	0.43
1:D:215:GLN:HE21	1:D:215:GLN:HB3	1.63	0.43
1:D:228:PRO:HB3	1:D:252:TYR:HB2	2.00	0.43
1:E:10:LYS:NZ	1:E:32:HIS:CD2	2.85	0.43
1:F:47:THR:HA	1:F:255:HIS:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:TRP:CD1	1:F:101:TRP:C	2.96	0.43
1:F:210:SER:O	1:F:213:MET:HG2	2.18	0.43
1:B:208:LEU:CG	1:B:213:MET:HE1	2.47	0.43
1:B:249:ILE:HD13	1:B:249:ILE:HA	1.72	0.43
1:C:39:GLN:HE21	1:C:39:GLN:HB3	1.49	0.43
1:C:77:VAL:HG12	1:C:79:ILE:HG12	2.00	0.43
1:D:1:CXM:CN	1:D:1:CXM:HG2	2.48	0.43
1:E:8:MET:O	1:E:12:LEU:HG	2.19	0.43
1:E:75:ASN:O	1:E:77:VAL:HG23	2.17	0.43
1:F:3:GLN:HB3	1:F:34:MET:HG2	2.01	0.43
1:B:22:THR:C	1:B:24:THR:N	2.76	0.43
1:B:37:ASN:OD1	1:B:39:GLN:HB2	2.19	0.43
1:D:46:THR:HG21	1:D:225:ARG:O	2.18	0.43
1:D:222:ARG:HD3	1:D:255:HIS:ND1	2.33	0.43
1:F:34:MET:HE3	1:F:36:PHE:HZ	1.83	0.43
1:A:147:HIS:CD2	1:A:181:TYR:OH	2.70	0.43
1:A:252:TYR:CE2	1:A:254:PRO:HG3	2.54	0.43
3:A:301:CB3:HA	4:A:472:HOH:O	2.19	0.43
1:F:58:GLU:O	1:F:61:TRP:HB3	2.18	0.43
1:D:115:VAL:HG21	1:D:130:VAL:HG23	2.00	0.43
1:E:143:LEU:HD12	1:E:143:LEU:C	2.44	0.43
1:F:208:LEU:HD12	1:F:208:LEU:HA	1.82	0.42
1:E:174:LEU:O	1:E:178:ILE:HG13	2.19	0.42
1:A:151:GLN:NE2	1:B:164:TYR:OH	2.52	0.42
1:A:245:GLU:CD	1:A:245:GLU:H	2.27	0.42
1:D:146:CYS:SG	2:D:306:UMP:C6	3.12	0.42
1:A:53:ARG:NH2	1:A:244:PHE:CZ	2.87	0.42
1:B:259:LYS:HE3	3:C:305:CB3:HB1	2.02	0.42
1:C:179:ALA:O	1:C:183:LEU:HB2	2.20	0.42
4:C:465:HOH:O	1:D:126:ARG:HD3	2.19	0.42
1:F:21:ARG:NH2	2:F:310:UMP:O5'	2.52	0.42
1:C:58:GLU:OE2	3:C:305:CB3:HP11	2.19	0.42
1:F:46:THR:C	1:F:48:LYS:H	2.28	0.42
1:A:26:THR:HB	1:A:207:HIS:HB2	2.01	0.42
1:A:96:LYS:HE2	1:A:100:ALA:CB	2.50	0.42
1:B:163:LEU:HD22	1:B:181:TYR:CD1	2.54	0.42
1:C:10:LYS:O	1:C:14:GLU:HG2	2.19	0.42
1:D:22:THR:HG22	1:D:23:GLY:N	2.35	0.42
1:D:48:LYS:HB3	1:D:219:GLN:NE2	2.35	0.42
1:D:115:VAL:HG11	1:D:152:PHE:CD2	2.55	0.42
1:F:73:HIS:HE2	1:F:81:ASP:CG	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LEU:HB3	1:D:175:PRO:HD3	2.02	0.42
1:E:52:LEU:O	1:E:53:ARG:C	2.63	0.42
1:B:236:PRO:HG2	1:B:242:TYR:CD2	2.55	0.42
1:C:49:ARG:H	1:C:257:GLY:HA2	1.85	0.42
1:C:186:HIS:CE1	1:C:196:VAL:HG11	2.55	0.42
1:C:190:GLN:NE2	1:C:242:TYR:OH	2.51	0.42
1:C:228:PRO:HB2	1:C:249:ILE:CG2	2.48	0.42
1:B:38:LEU:HD12	1:B:43:PRO:HD3	2.01	0.42
1:D:115:VAL:HG21	1:D:130:VAL:CG2	2.50	0.42
1:D:232:ILE:HG22	1:D:234:ARG:O	2.19	0.42
1:A:190:GLN:NE2	1:A:242:TYR:OH	2.53	0.41
1:D:169:ASP:OD2	3:D:307:CB3:N3	2.53	0.41
1:F:49:ARG:HG3	1:F:49:ARG:HH11	1.85	0.41
1:F:87:ASN:ND2	1:F:87:ASN:N	2.67	0.41
1:F:181:TYR:HB3	1:F:199:PHE:CE1	2.55	0.41
1:A:205:ASP:OD2	1:B:126:ARG:HG2	2.19	0.41
1:C:172:LEU:HD12	1:C:172:LEU:HA	1.91	0.41
1:D:210:SER:O	1:D:213:MET:HG2	2.21	0.41
1:E:103:THR:HG22	1:F:136:GLY:HA2	2.02	0.41
1:B:118:GLN:NE2	4:B:612:HOH:O	2.44	0.41
1:C:92:PRO:O	1:C:141:MET:HE2	2.20	0.41
1:A:151:GLN:O	1:A:161:CYS:HA	2.19	0.41
1:C:63:LEU:O	1:C:99:ARG:NH1	2.50	0.41
1:D:116:LEU:HD12	1:D:120:LYS:CE	2.39	0.41
1:E:174:LEU:HB3	1:E:175:PRO:HD3	2.02	0.41
1:F:21:ARG:HH21	2:F:310:UMP:P	2.43	0.41
1:D:262:VAL:CG1	1:D:263:ALA:N	2.80	0.41
1:F:22:THR:C	1:F:24:THR:H	2.28	0.41
1:B:187:MET:HE3	1:B:242:TYR:CD1	2.56	0.41
1:B:187:MET:HE3	1:B:242:TYR:CG	2.56	0.41
1:E:147:HIS:HB2	1:E:163:LEU:HD11	2.01	0.41
1:F:183:LEU:HD22	1:F:187:MET:CE	2.26	0.41
1:E:85:ASP:C	1:E:87:ASN:H	2.29	0.41
1:E:220:LEU:HD13	1:E:220:LEU:HA	1.79	0.41
1:A:130:VAL:HB	1:A:150:PHE:CZ	2.55	0.41
1:F:99:ARG:HE	1:F:110:ASP:CG	2.29	0.41
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.85	0.41
1:B:82:GLU:HB2	1:B:83:TRP:CE3	2.56	0.41
1:B:222:ARG:HD3	1:B:255:HIS:CB	2.51	0.41
1:C:52:LEU:HD11	1:C:249:ILE:HG12	2.03	0.41
1:D:103:THR:HB	1:D:104:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:GLN:O	1:F:122:ASP:C	2.64	0.41
1:A:129:ILE:CG2	1:A:130:VAL:N	2.84	0.41
1:C:147:HIS:HB2	1:C:163:LEU:HD11	2.03	0.41
1:B:55:ILE:HG13	1:B:176:PHE:CE2	2.56	0.40
1:D:225:ARG:O	1:D:226:PRO:C	2.64	0.40
1:F:52:LEU:HB3	1:F:56:ILE:HG13	2.03	0.40
1:A:244:PHE:CD2	1:A:244:PHE:C	2.99	0.40
1:C:58:GLU:HG2	1:C:62:PHE:CE2	2.57	0.40
1:E:166:ARG:HG3	1:E:167:SER:N	2.36	0.40
1:F:20:ASP:CG	1:F:22:THR:O	2.65	0.40
1:F:215:GLN:HE21	1:F:260:ALA:HA	1.85	0.40
1:B:26:THR:HG22	1:B:209:TYR:CD1	2.56	0.40
1:B:93:VAL:O	1:B:94:TYR:C	2.64	0.40
1:D:34:MET:HE3	1:D:34:MET:HB2	1.88	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	262/264 (99%)	246 (94%)	15 (6%)	1 (0%)	30	51
1	B	262/264 (99%)	240 (92%)	18 (7%)	4 (2%)	8	18
1	C	262/264 (99%)	244 (93%)	15 (6%)	3 (1%)	11	25
1	D	262/264 (99%)	240 (92%)	20 (8%)	2 (1%)	16	34
1	E	259/264 (98%)	235 (91%)	20 (8%)	4 (2%)	8	18
1	F	262/264 (99%)	244 (93%)	15 (6%)	3 (1%)	11	25
All	All	1569/1584 (99%)	1449 (92%)	103 (7%)	17 (1%)	11	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	TYR
1	A	94	TYR
1	B	23	GLY
1	B	79	ILE
1	E	94	TYR
1	F	23	GLY
1	E	86	GLU
1	F	94	TYR
1	C	94	TYR
1	D	24	THR
1	E	48	LYS
1	C	93	VAL
1	E	93	VAL
1	B	69	ILE
1	F	45	VAL
1	C	122	ASP
1	D	93	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/231 (100%)	217 (94%)	14 (6%)	17	37
1	B	231/231 (100%)	214 (93%)	17 (7%)	13	29
1	C	231/231 (100%)	212 (92%)	19 (8%)	10	24
1	D	231/231 (100%)	216 (94%)	15 (6%)	15	35
1	E	229/231 (99%)	216 (94%)	13 (6%)	18	40
1	F	231/231 (100%)	218 (94%)	13 (6%)	19	40
All	All	1384/1386 (100%)	1293 (93%)	91 (7%)	15	34

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	87	ASN
1	A	134	ASN
1	A	138	LEU
1	A	143	LEU
1	A	172	LEU
1	A	188	MET
1	A	208	LEU
1	A	220	LEU
1	A	227	LEU
1	A	230	LEU
1	A	244	PHE
1	A	249	ILE
1	B	14	GLU
1	B	16	THR
1	B	19	ASN
1	B	21	ARG
1	B	38	LEU
1	B	52	LEU
1	B	53	ARG
1	B	96	LYS
1	B	101	TRP
1	B	116	LEU
1	B	137	GLU
1	B	143	LEU
1	B	166	ARG
1	B	172	LEU
1	B	183	LEU
1	B	215	GLN
1	B	249	ILE
1	C	5	LEU
1	C	39	GLN
1	C	52	LEU
1	C	53	ARG
1	C	60	LEU
1	C	76	ASN
1	C	86	GLU
1	C	103	THR
1	C	127	ARG
1	C	138	LEU
1	C	183	LEU
1	C	188	MET
1	C	215	GLN

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Mol	Chain	Res	Type
1	C	220	LEU
1	C	222	ARG
1	C	227	LEU
1	C	237	GLU
1	C	248	GLU
1	C	259	LYS
1	D	12	LEU
1	D	39	GLN
1	D	82	GLU
1	D	116	LEU
1	D	127	ARG
1	D	134	ASN
1	D	143	LEU
1	D	172	LEU
1	D	195	GLU
1	D	215	GLN
1	D	223	GLU
1	D	231	ILE
1	D	238	SER
1	D	243	ARG
1	D	249	ILE
1	E	17	GLN
1	E	47	THR
1	E	49	ARG
1	E	50	CYS
1	E	60	LEU
1	E	116	LEU
1	E	134	ASN
1	E	138	LEU
1	E	162	GLN
1	E	215	GLN
1	E	220	LEU
1	E	230	LEU
1	E	249	ILE
1	F	6	GLU
1	F	16	THR
1	F	17	GLN
1	F	35	ARG
1	F	38	LEU
1	F	39	GLN
1	F	87	ASN
1	F	107	ARG

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Mol	Chain	Res	Type
1	F	127	ARG
1	F	143	LEU
1	F	183	LEU
1	F	188	MET
1	F	238	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	39	GLN
1	A	64	GLN
1	A	75	ASN
1	A	87	ASN
1	A	97	GLN
1	A	117	ASN
1	A	118	GLN
1	A	121	ASN
1	A	134	ASN
1	A	147	HIS
1	A	151	GLN
1	A	190	GLN
1	A	217	HIS
1	B	17	GLN
1	B	19	ASN
1	B	32	HIS
1	B	57	HIS
1	B	75	ASN
1	B	76	ASN
1	B	108	HIS
1	B	117	ASN
1	B	118	GLN
1	B	121	ASN
1	B	134	ASN
1	C	3	GLN
1	C	9	GLN
1	C	33	GLN
1	C	39	GLN
1	C	64	GLN
1	C	76	ASN
1	C	87	ASN
1	C	117	ASN

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Mol	Chain	Res	Type
1	C	118	GLN
1	C	134	ASN
1	C	151	GLN
1	C	162	GLN
1	C	177	ASN
1	C	190	GLN
1	C	191	GLN
1	C	215	GLN
1	C	219	GLN
1	D	9	GLN
1	D	17	GLN
1	D	33	GLN
1	D	64	GLN
1	D	75	ASN
1	D	117	ASN
1	D	134	ASN
1	D	191	GLN
1	D	219	GLN
1	E	19	ASN
1	E	32	HIS
1	E	51	HIS
1	E	75	ASN
1	E	76	ASN
1	E	97	GLN
1	E	117	ASN
1	E	134	ASN
1	E	215	GLN
1	F	32	HIS
1	F	39	GLN
1	F	51	HIS
1	F	87	ASN
1	F	108	HIS
1	F	117	ASN
1	F	118	GLN
1	F	134	ASN
1	F	186	HIS
1	F	217	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	CXM	B	1	1	9,10,11	1.34	2 (22%)	9,11,13	1.24	1 (11%)
1	CXM	D	1	1	9,10,11	1.30	1 (11%)	9,11,13	1.45	1 (11%)
1	CXM	E	1	1	9,10,11	1.07	0	9,11,13	1.29	1 (11%)
1	CXM	F	1	1	9,10,11	1.61	2 (22%)	9,11,13	1.14	1 (11%)
1	CXM	A	1	1	9,10,11	1.06	0	9,11,13	1.36	1 (11%)
1	CXM	C	1	1	9,10,11	1.07	1 (11%)	9,11,13	1.51	2 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	B	1	1	-	0/9/10/12	-
1	CXM	D	1	1	-	4/9/10/12	-
1	CXM	E	1	1	-	2/9/10/12	-
1	CXM	F	1	1	-	4/9/10/12	-
1	CXM	A	1	1	-	1/9/10/12	-
1	CXM	C	1	1	-	2/9/10/12	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	1	CXM	CA-N	3.05	1.51	1.46
1	B	1	CXM	CA-N	2.80	1.50	1.46
1	F	1	CXM	CN-N	2.77	1.40	1.35
1	D	1	CXM	CA-N	2.32	1.49	1.46
1	B	1	CXM	ON1-CN	2.12	1.25	1.21
1	C	1	CXM	CA-N	2.05	1.49	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1	CXM	ON1-CN-N	-4.05	118.22	124.86
1	C	1	CXM	ON1-CN-N	-3.83	118.58	124.86
1	A	1	CXM	ON1-CN-N	-3.72	118.75	124.86
1	E	1	CXM	ON1-CN-N	-3.56	119.03	124.86
1	B	1	CXM	ON1-CN-N	-2.92	120.06	124.86
1	F	1	CXM	ON1-CN-N	-2.39	120.93	124.86
1	C	1	CXM	C-CA-N	2.02	113.39	109.50

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	1	CXM	ON1-CN-N-CA
1	D	1	CXM	ON2-CN-N-CA
1	D	1	CXM	O-C-CA-CB
1	F	1	CXM	N-CA-CB-CG
1	F	1	CXM	C-CA-CB-CG
1	F	1	CXM	O-C-CA-CB
1	C	1	CXM	ON1-CN-N-CA
1	E	1	CXM	CA-CB-CG-SD
1	A	1	CXM	CA-CB-CG-SD
1	F	1	CXM	CB-CG-SD-CE
1	D	1	CXM	C-CA-N-CN
1	C	1	CXM	CA-CB-CG-SD
1	E	1	CXM	ON1-CN-N-CA

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	CXM	1	0
1	D	1	CXM	3	0
1	E	1	CXM	5	0
1	F	1	CXM	1	0
1	A	1	CXM	4	0
1	C	1	CXM	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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
2	UMP	F	310	1	21,21,21	3.59	5 (23%)	30,31,31	2.86	12 (40%)
3	CB3	E	309	-	37,37,37	1.51	4 (10%)	50,51,51	2.31	7 (14%)
2	UMP	D	306	-	21,21,21	2.84	4 (19%)	30,31,31	3.03	8 (26%)
3	CB3	A	301	-	37,37,37	1.41	5 (13%)	50,51,51	2.40	10 (20%)
3	CB3	F	311	-	37,37,37	1.88	7 (18%)	50,51,51	2.91	13 (26%)
3	CB3	C	305	-	37,37,37	1.44	6 (16%)	50,51,51	2.77	15 (30%)
2	UMP	A	300	1	21,21,21	3.27	4 (19%)	30,31,31	3.13	9 (30%)
3	CB3	B	303	-	37,37,37	1.47	5 (13%)	50,51,51	1.77	6 (12%)
3	CB3	D	307	-	37,37,37	1.70	9 (24%)	50,51,51	1.78	10 (20%)
2	UMP	E	308	-	21,21,21	3.29	5 (23%)	30,31,31	2.78	9 (30%)
2	UMP	B	302	1	21,21,21	3.41	6 (28%)	30,31,31	3.32	12 (40%)
2	UMP	C	304	1	21,21,21	3.29	5 (23%)	30,31,31	2.95	11 (36%)

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
2	UMP	F	310	1	-	1/10/22/22	0/2/2/2
3	CB3	E	309	-	-	6/27/28/28	0/3/3/3
2	UMP	D	306	-	-	0/10/22/22	0/2/2/2
3	CB3	A	301	-	-	3/27/28/28	0/3/3/3
3	CB3	F	311	-	-	5/27/28/28	0/3/3/3
3	CB3	C	305	-	-	8/27/28/28	0/3/3/3
2	UMP	A	300	1	-	0/10/22/22	0/2/2/2
3	CB3	B	303	-	-	5/27/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CB3	D	307	-	-	2/27/28/28	0/3/3/3
2	UMP	E	308	-	-	0/10/22/22	0/2/2/2
2	UMP	B	302	1	-	3/10/22/22	0/2/2/2
2	UMP	C	304	1	-	0/10/22/22	0/2/2/2

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	UMP	O4-C4	10.21	1.44	1.24
2	C	304	UMP	C6-C5	9.79	1.57	1.35
2	E	308	UMP	O4-C4	9.46	1.43	1.24
2	B	302	UMP	C6-C5	9.10	1.56	1.35
2	F	310	UMP	O4-C4	9.06	1.42	1.24
2	B	302	UMP	O4-C4	9.06	1.42	1.24
2	D	306	UMP	O4-C4	8.85	1.41	1.24
2	F	310	UMP	C6-C5	8.78	1.55	1.35
2	F	310	UMP	C6-N1	8.13	1.57	1.38
2	E	308	UMP	C6-C5	8.03	1.53	1.35
2	A	300	UMP	C6-C5	7.81	1.53	1.35
2	C	304	UMP	O4-C4	7.69	1.39	1.24
2	D	306	UMP	C6-C5	7.06	1.51	1.35
2	E	308	UMP	C5-C4	6.05	1.56	1.43
2	B	302	UMP	C6-N1	5.89	1.52	1.38
2	C	304	UMP	C6-N1	5.64	1.51	1.38
2	F	310	UMP	C5-C4	5.51	1.55	1.43
3	F	311	CB3	CP1-N10	5.35	1.51	1.46
2	A	300	UMP	C6-N1	5.21	1.50	1.38
3	E	309	CB3	CP1-N10	5.07	1.51	1.46
2	B	302	UMP	C5-C4	4.88	1.54	1.43
2	E	308	UMP	C6-N1	4.83	1.49	1.38
2	C	304	UMP	C5-C4	4.70	1.53	1.43
3	D	307	CB3	CP1-N10	4.20	1.50	1.46
2	D	306	UMP	C6-N1	3.94	1.47	1.38
2	D	306	UMP	C5-C4	3.88	1.52	1.43
2	A	300	UMP	C5-C4	3.84	1.52	1.43
3	F	311	CB3	CP1-CP2	-3.54	1.41	1.46
3	F	311	CB3	C9-N10	3.45	1.51	1.46
3	F	311	CB3	C2-N3	3.27	1.41	1.33
3	A	301	CB3	C2-N3	3.23	1.41	1.33
3	B	303	CB3	CA-N	3.19	1.52	1.45
3	E	309	CB3	C2-N3	3.13	1.40	1.33
3	C	305	CB3	CP1-N10	3.11	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	307	CB3	C2-N3	3.06	1.40	1.33
3	D	307	CB3	C4A-C4	-3.03	1.43	1.48
3	B	303	CB3	C2-N3	2.94	1.40	1.33
3	C	305	CB3	CP1-CP2	2.76	1.50	1.46
3	F	311	CB3	CG-CD	2.72	1.56	1.50
3	A	301	CB3	C9-N10	2.64	1.50	1.46
3	D	307	CB3	C-N	2.59	1.40	1.34
3	C	305	CB3	C2-N3	2.49	1.39	1.33
2	C	304	UMP	C2-N3	2.42	1.42	1.38
3	E	309	CB3	CA-N	2.42	1.50	1.45
3	D	307	CB3	CB-CA	2.39	1.59	1.53
3	D	307	CB3	C7-C6	2.33	1.43	1.38
3	F	311	CB3	C14-N10	2.30	1.45	1.38
3	E	309	CB3	O2-CT	-2.25	1.23	1.30
3	A	301	CB3	CP1-N10	2.24	1.48	1.46
3	B	303	CB3	C-N	2.24	1.39	1.34
3	F	311	CB3	C16-C11	2.23	1.42	1.39
3	A	301	CB3	C2-NA2	2.20	1.39	1.34
3	C	305	CB3	O2-CT	-2.20	1.23	1.30
3	B	303	CB3	C16-C11	2.18	1.42	1.39
3	A	301	CB3	O2-CT	-2.16	1.23	1.30
2	B	302	UMP	C3'-C4'	2.14	1.58	1.53
3	C	305	CB3	CA-N	2.14	1.50	1.45
3	C	305	CB3	C4-N3	2.13	1.43	1.38
3	D	307	CB3	CP1-CP2	2.13	1.50	1.46
2	E	308	UMP	P-OP2	-2.13	1.46	1.54
3	D	307	CB3	C9-N10	2.11	1.49	1.46
2	B	302	UMP	C2-N3	2.09	1.41	1.38
3	D	307	CB3	C12-C11	2.04	1.42	1.39
3	B	303	CB3	CP1-N10	2.01	1.48	1.46
2	F	310	UMP	P-OP2	-2.01	1.47	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	311	CB3	CP1-N10-C9	-14.96	102.12	117.19
3	C	305	CB3	CP1-N10-C9	-12.17	104.93	117.19
3	E	309	CB3	CP2-CP1-N10	-11.30	103.02	113.45
3	A	301	CB3	CP2-CP1-N10	-10.74	103.54	113.45
2	A	300	UMP	C6-C5-C4	-9.46	107.45	119.53
2	B	302	UMP	C5-C6-N1	-9.33	106.67	121.84
3	B	303	CB3	CP1-N10-C9	-9.04	108.08	117.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	310	UMP	C5-C6-N1	-8.78	107.56	121.84
2	D	306	UMP	O4-C4-C5	-8.78	110.03	125.16
2	B	302	UMP	C6-C5-C4	-8.01	109.30	119.53
3	A	301	CB3	CP1-N10-C9	-7.89	109.25	117.19
3	C	305	CB3	CP2-CP1-N10	-7.87	106.19	113.45
2	C	304	UMP	C5-C6-N1	-7.45	109.72	121.84
2	D	306	UMP	C5-C4-N3	7.17	124.85	114.80
3	F	311	CB3	C9-N10-C14	7.02	132.88	120.72
2	C	304	UMP	C6-C5-C4	-6.82	110.81	119.53
2	A	300	UMP	C5-C6-N1	-6.74	110.88	121.84
2	E	308	UMP	C5-C4-N3	6.68	124.16	114.80
2	A	300	UMP	O4-C4-C5	-6.66	113.68	125.16
3	E	309	CB3	CP1-N10-C9	-6.63	110.51	117.19
2	E	308	UMP	O4-C4-C5	-6.54	113.89	125.16
2	F	310	UMP	C6-C5-C4	-6.39	111.37	119.53
2	C	304	UMP	O4-C4-C5	-6.04	114.74	125.16
2	B	302	UMP	C6-N1-C2	5.98	128.27	121.00
2	D	306	UMP	C6-N1-C2	5.79	128.04	121.00
2	B	302	UMP	O4-C4-C5	-5.68	115.36	125.16
3	D	307	CB3	CP1-N10-C9	-5.68	111.46	117.19
3	A	301	CB3	C9-N10-C14	5.58	130.40	120.72
2	B	302	UMP	C1'-N1-C6	-5.36	110.99	121.53
2	E	308	UMP	C6-N1-C2	5.19	127.31	121.00
3	C	305	CB3	C9-C6-C7	-5.04	111.45	120.75
2	C	304	UMP	C4-N3-C2	-5.00	120.41	126.61
2	E	308	UMP	C5-C6-N1	-4.92	113.85	121.84
2	F	310	UMP	C5-C4-N3	4.88	121.63	114.80
3	D	307	CB3	CP2-CP1-N10	-4.87	108.95	113.45
2	D	306	UMP	C1'-N1-C6	-4.82	112.05	121.53
2	C	304	UMP	C5-C4-N3	4.73	121.43	114.80
3	F	311	CB3	CP2-CP1-N10	-4.72	109.09	113.45
2	F	310	UMP	O4-C4-C5	-4.68	117.08	125.16
2	D	306	UMP	C4-N3-C2	-4.65	120.83	126.61
2	E	308	UMP	C1'-N1-C6	-4.60	112.48	121.53
2	A	300	UMP	C5-C4-N3	4.52	121.13	114.80
2	E	308	UMP	C4-N3-C2	-4.50	121.03	126.61
3	C	305	CB3	C9-N10-C14	4.45	128.43	120.72
2	A	300	UMP	C6-N1-C2	4.37	126.31	121.00
2	D	306	UMP	C5-C6-N1	-4.31	114.84	121.84
2	D	306	UMP	C6-C5-C4	-4.30	114.05	119.53
2	E	308	UMP	C6-C5-C4	-4.24	114.12	119.53
2	C	304	UMP	C6-N1-C2	4.21	126.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	UMP	C4-N3-C2	-4.17	121.44	126.61
3	C	305	CB3	O4-C4-C4A	4.15	128.01	121.33
3	D	307	CB3	CP1-N10-C14	4.10	126.73	119.03
3	F	311	CB3	C9-C6-C7	-4.09	113.21	120.75
3	E	309	CB3	C9-N10-C14	4.06	127.75	120.72
3	C	305	CB3	C8-C8A-C4A	4.05	124.66	119.37
2	A	300	UMP	O4-C4-N3	4.01	125.09	119.27
2	B	302	UMP	O4-C4-N3	3.94	124.98	119.27
2	F	310	UMP	C4-N3-C2	-3.73	121.98	126.61
3	F	311	CB3	O-C-C11	3.71	128.25	120.90
2	A	300	UMP	C4-N3-C2	-3.71	122.01	126.61
2	F	310	UMP	C6-N1-C2	3.63	125.42	121.00
2	A	300	UMP	C1'-N1-C6	-3.63	114.40	121.53
2	E	308	UMP	N3-C2-N1	3.51	119.46	114.89
2	F	310	UMP	C2'-C1'-N1	-3.49	105.09	113.81
2	B	302	UMP	C5-C4-N3	3.45	119.63	114.80
2	D	306	UMP	O4-C4-N3	3.44	124.26	119.27
3	D	307	CB3	C5-C4A-C8A	3.43	122.17	119.09
3	B	303	CB3	C9-N10-C14	3.34	126.50	120.72
2	C	304	UMP	C1'-N1-C6	-3.32	115.01	121.53
3	F	311	CB3	C9-C6-C5	3.19	126.29	120.27
3	D	307	CB3	C4A-C5-C6	-3.16	116.48	121.38
2	C	304	UMP	O4-C4-N3	3.14	123.83	119.27
3	E	309	CB3	O4-C4-C4A	3.12	126.36	121.33
2	A	300	UMP	O2-C2-N3	-3.11	115.76	121.49
2	F	310	UMP	N3-C2-N1	3.08	118.91	114.89
3	C	305	CB3	C9-C6-C5	3.08	126.09	120.27
3	C	305	CB3	C8-C8A-N1	-3.07	114.75	119.91
3	D	307	CB3	C15-C14-N10	-2.91	117.35	121.39
3	A	301	CB3	NA2-C2-N1	2.84	122.74	116.77
3	C	305	CB3	C7-C6-C5	2.83	122.46	118.55
2	F	310	UMP	C1'-N1-C6	-2.82	115.98	121.53
3	D	307	CB3	C4A-C8A-N1	2.81	121.66	119.46
2	C	304	UMP	C1'-N1-C2	-2.81	112.17	117.66
2	C	304	UMP	O2-C2-N3	-2.79	116.35	121.49
3	A	301	CB3	N1-C2-N3	-2.78	118.24	123.32
2	B	302	UMP	C2'-C1'-N1	-2.77	106.88	113.81
3	F	311	CB3	N1-C2-N3	-2.76	118.27	123.32
2	E	308	UMP	O2-C2-N3	-2.75	116.42	121.49
3	B	303	CB3	O4-C4-C4A	2.69	125.66	121.33
3	B	303	CB3	C9-C6-C7	-2.68	115.82	120.75
3	C	305	CB3	CP1-N10-C14	2.67	124.04	119.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	CB3	C9-C6-C7	-2.54	116.07	120.75
3	C	305	CB3	O-C-N	-2.52	117.67	122.47
3	F	311	CB3	CP1-CP2-CP3	-2.51	173.56	177.63
3	A	301	CB3	O4-C4-C4A	2.48	125.32	121.33
2	B	302	UMP	N3-C2-N1	-2.44	111.71	114.89
3	E	309	CB3	C9-C6-C7	-2.39	116.34	120.75
2	C	304	UMP	C2'-C1'-N1	-2.37	107.88	113.81
3	C	305	CB3	OE1-CD-CG	-2.36	115.60	123.09
3	A	301	CB3	OE1-CD-CG	-2.36	115.61	123.09
3	D	307	CB3	O-C-N	-2.33	118.04	122.47
3	F	311	CB3	NA2-C2-N1	2.32	121.65	116.77
3	A	301	CB3	CG-CB-CA	-2.29	108.94	113.16
3	C	305	CB3	CB-CA-CT	2.27	115.74	110.35
2	B	302	UMP	O2-C2-N3	-2.26	117.31	121.49
3	E	309	CB3	C8-C8A-C4A	2.26	122.33	119.37
3	F	311	CB3	C11-C-N	-2.23	112.90	117.04
3	C	305	CB3	C4A-C4-N3	-2.21	114.22	118.33
3	B	303	CB3	CG-CB-CA	-2.20	109.11	113.16
2	F	310	UMP	O2-C2-N1	-2.16	119.98	122.80
2	F	310	UMP	O2-C2-N3	-2.16	117.50	121.49
2	F	310	UMP	OP3-P-OP2	2.16	115.90	107.80
3	F	311	CB3	C15-C14-N10	-2.15	118.40	121.39
3	A	301	CB3	CA-N-C	-2.14	116.43	121.56
3	D	307	CB3	N1-C2-N3	-2.14	119.41	123.32
3	F	311	CB3	O-C-N	-2.13	118.42	122.47
3	F	311	CB3	C8-C8A-C4A	2.10	122.11	119.37
3	D	307	CB3	C7-C6-C5	2.09	121.44	118.55
3	B	303	CB3	C9-C6-C5	2.07	124.18	120.27
2	B	302	UMP	C1'-N1-C2	-2.01	113.72	117.66
3	E	309	CB3	C9-C6-C5	2.01	124.07	120.27
3	C	305	CB3	C4A-C5-C6	-2.01	118.26	121.38

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	302	UMP	C5'-O5'-P-OP2
2	B	302	UMP	C5'-O5'-P-OP3
3	F	311	CB3	C6-C9-N10-C14
3	E	309	CB3	N-CA-CB-CG
3	B	303	CB3	C6-C9-N10-C14
3	C	305	CB3	C6-C9-N10-C14

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Mol	Chain	Res	Type	Atoms
3	E	309	CB3	CT-CA-CB-CG
3	F	311	CB3	C13-C14-N10-C9
3	F	311	CB3	C15-C14-N10-C9
3	A	301	CB3	C6-C9-N10-C14
3	B	303	CB3	C15-C14-N10-C9
2	B	302	UMP	C5'-O5'-P-OP1
3	B	303	CB3	C13-C14-N10-C9
3	E	309	CB3	C15-C14-N10-CP1
3	E	309	CB3	CA-CB-CG-CD
3	C	305	CB3	CB-CA-CT-O2
3	F	311	CB3	C6-C9-N10-CP1
3	C	305	CB3	CB-CA-CT-O1
3	C	305	CB3	CT-CA-CB-CG
3	D	307	CB3	OE2-CD-CG-CB
3	F	311	CB3	CA-CB-CG-CD
3	B	303	CB3	OE1-CD-CG-CB
3	B	303	CB3	OE2-CD-CG-CB
3	C	305	CB3	CA-CB-CG-CD
3	C	305	CB3	OE2-CD-CG-CB
3	D	307	CB3	OE1-CD-CG-CB
3	A	301	CB3	OE1-CD-CG-CB
3	C	305	CB3	OE1-CD-CG-CB
3	A	301	CB3	OE2-CD-CG-CB
3	E	309	CB3	OE1-CD-CG-CB
3	E	309	CB3	OE2-CD-CG-CB
3	C	305	CB3	C6-C9-N10-CP1
2	F	310	UMP	O4'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 25 short contacts:

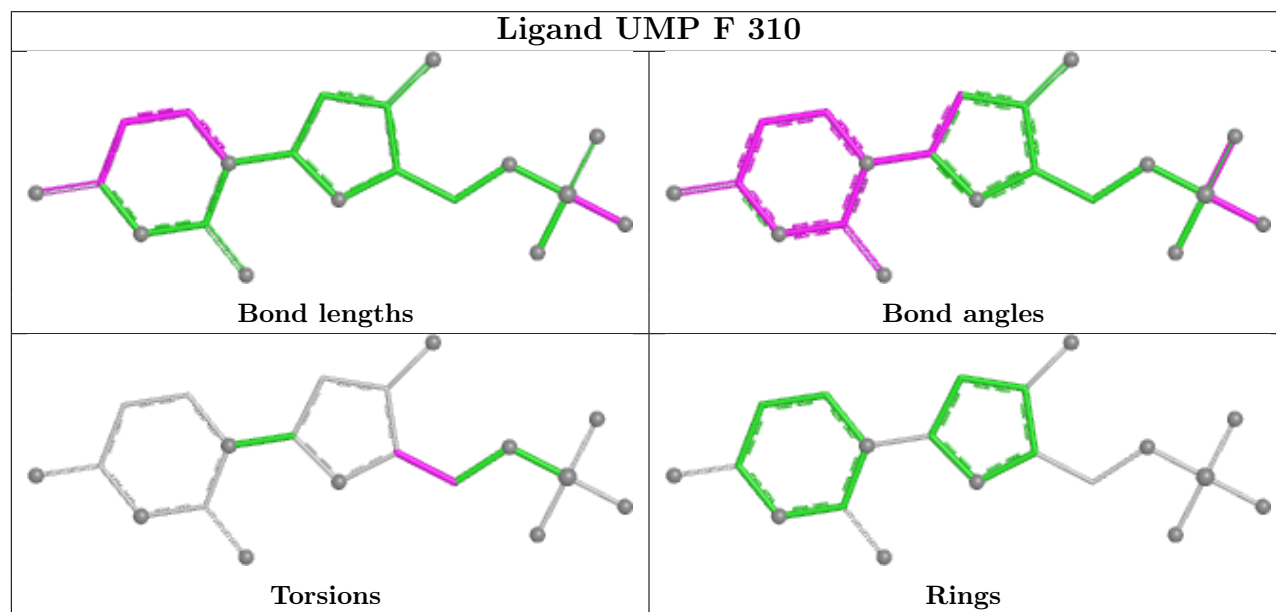
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	310	UMP	2	0
3	E	309	CB3	5	0
2	D	306	UMP	1	0
3	A	301	CB3	2	0
3	F	311	CB3	1	0
3	C	305	CB3	3	0
3	B	303	CB3	2	0
3	D	307	CB3	6	0
2	E	308	UMP	1	0
2	B	302	UMP	1	0

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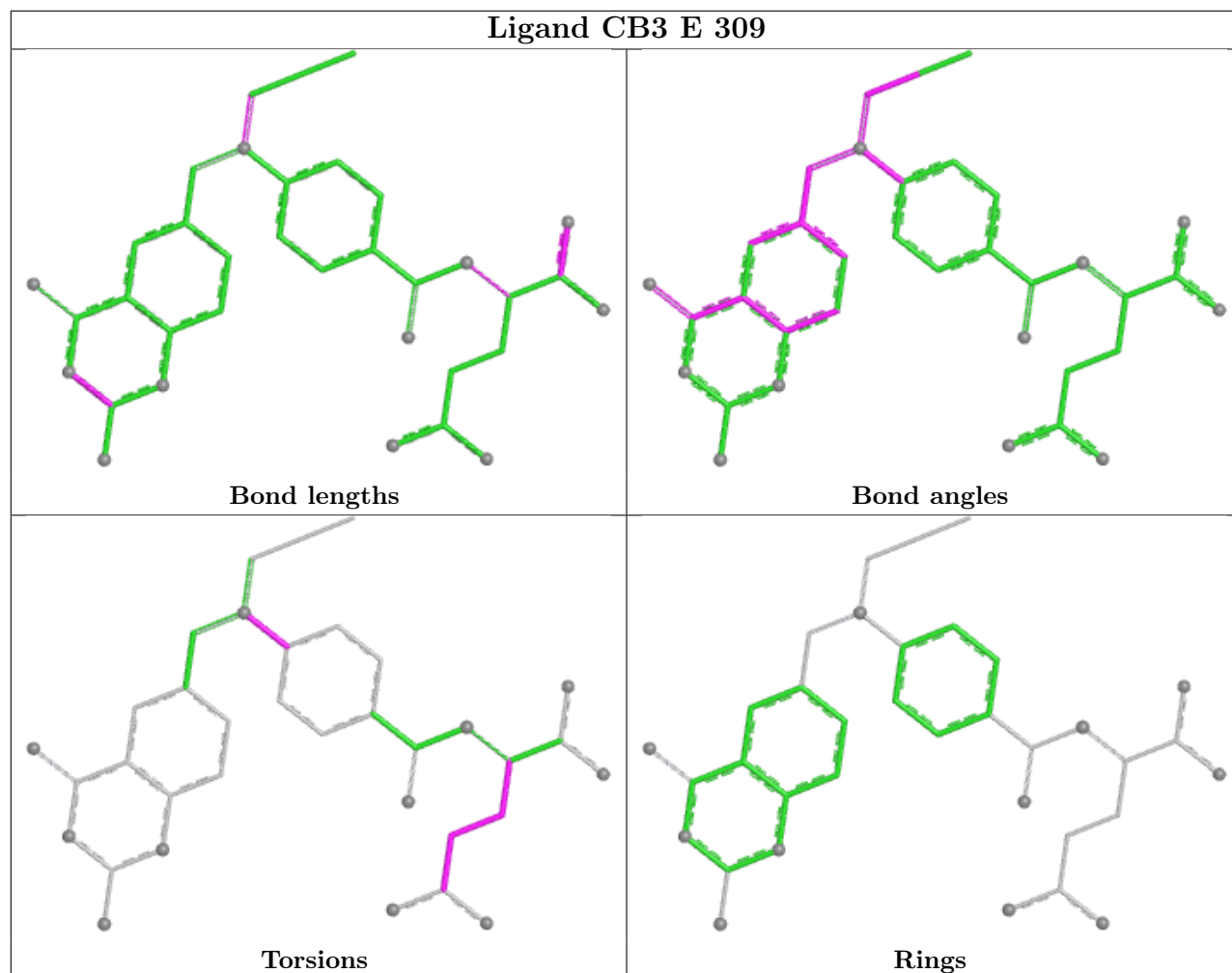
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	304	UMP	1	0

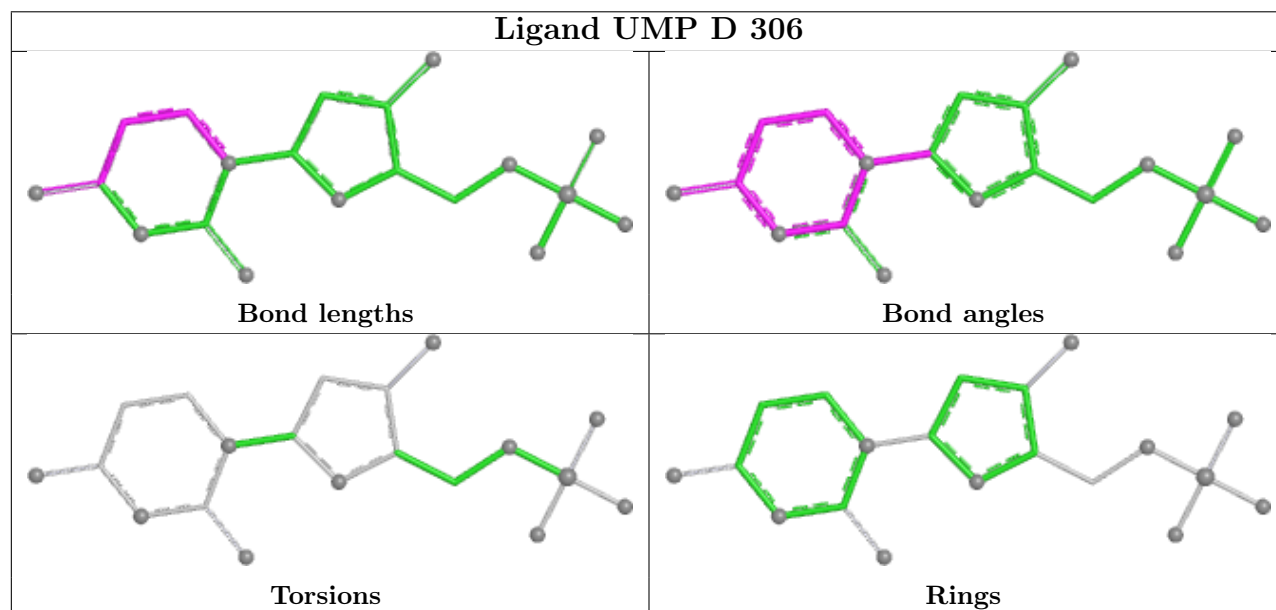
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

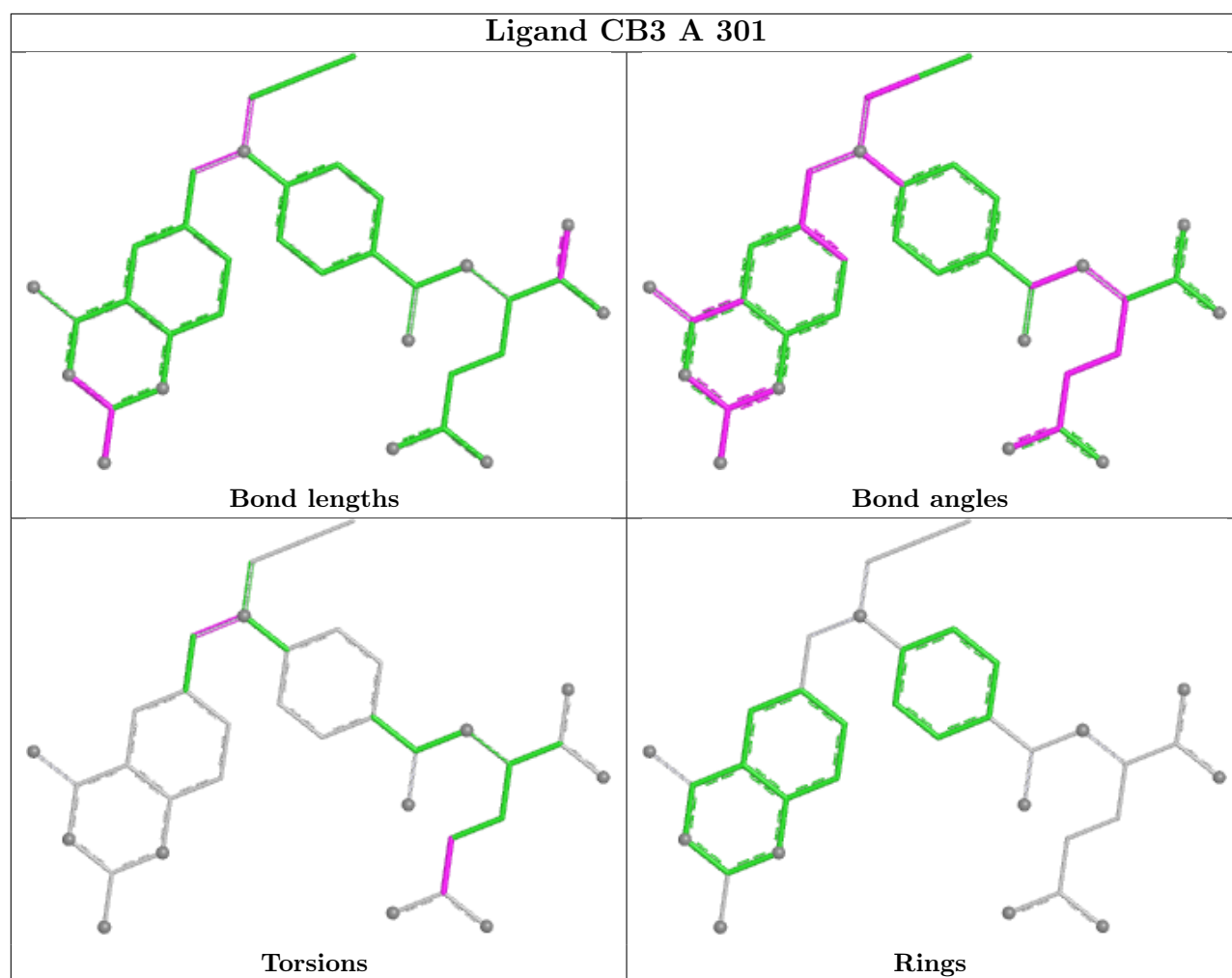


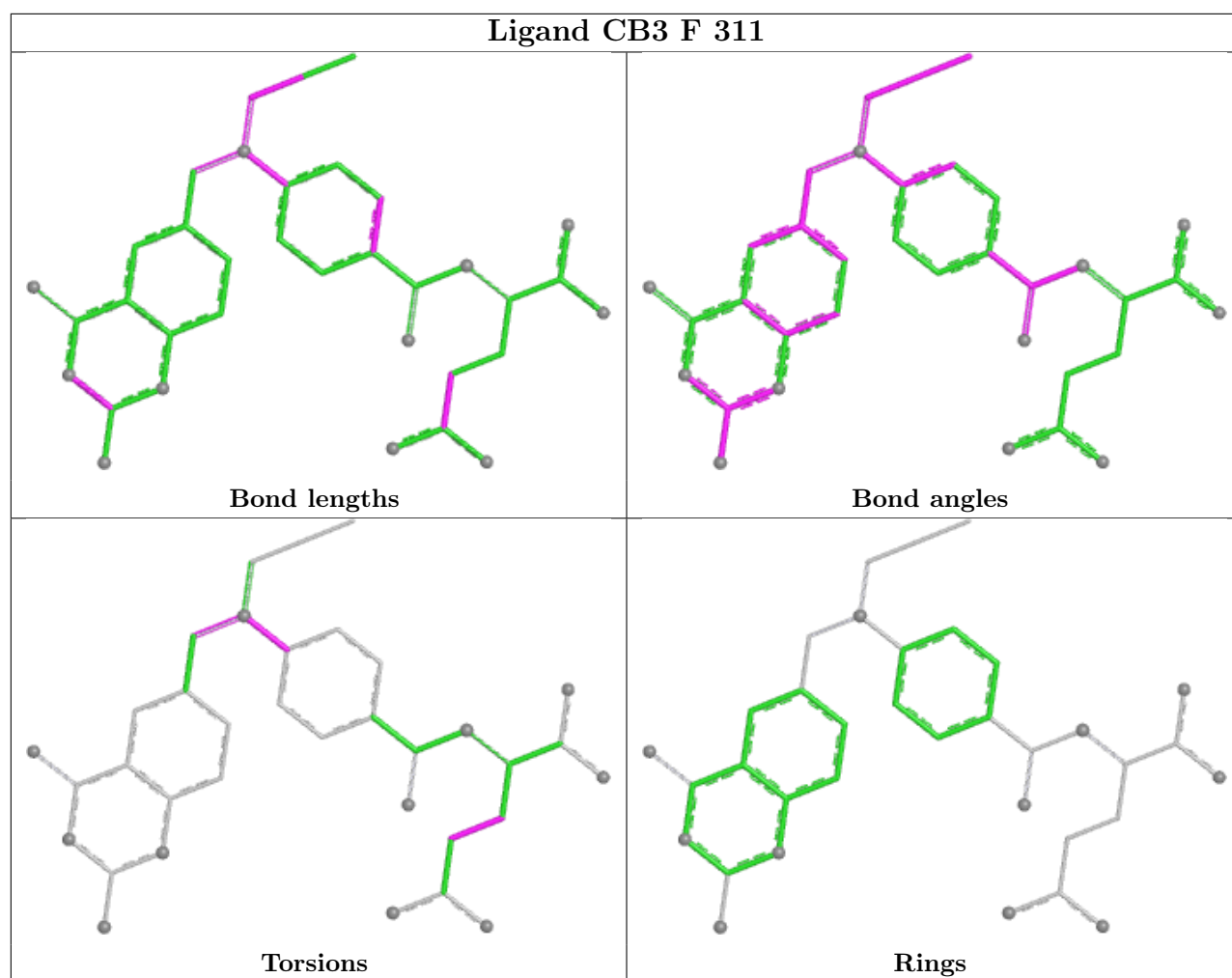
Ligand CB3 E 309



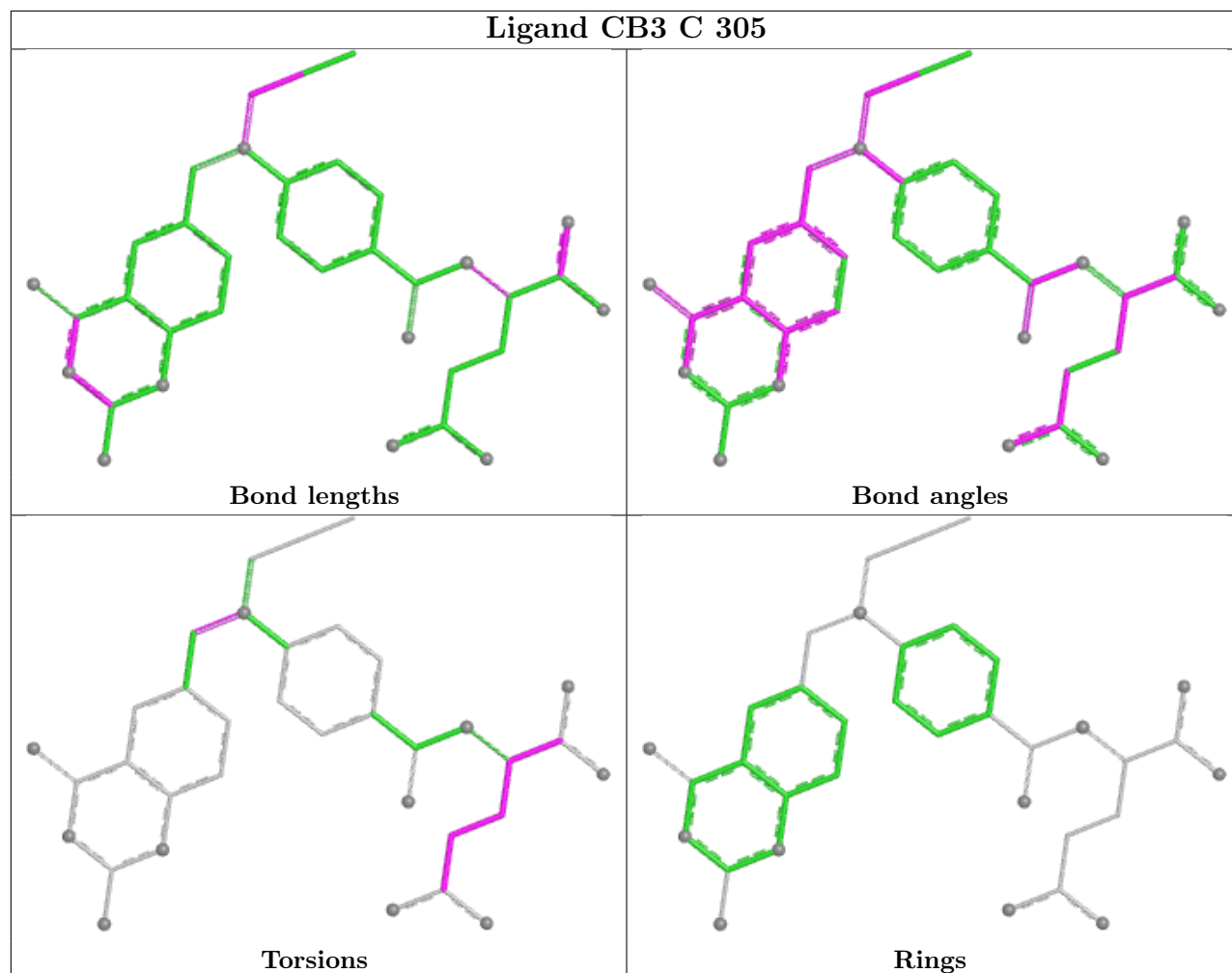
Ligand UMP D 306



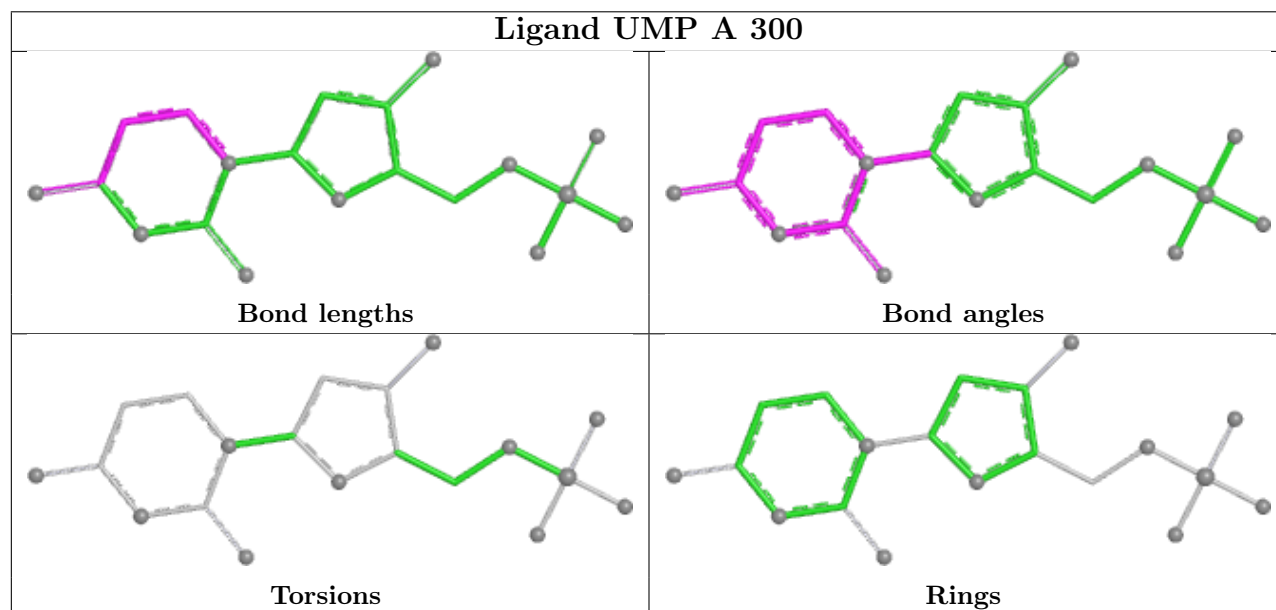


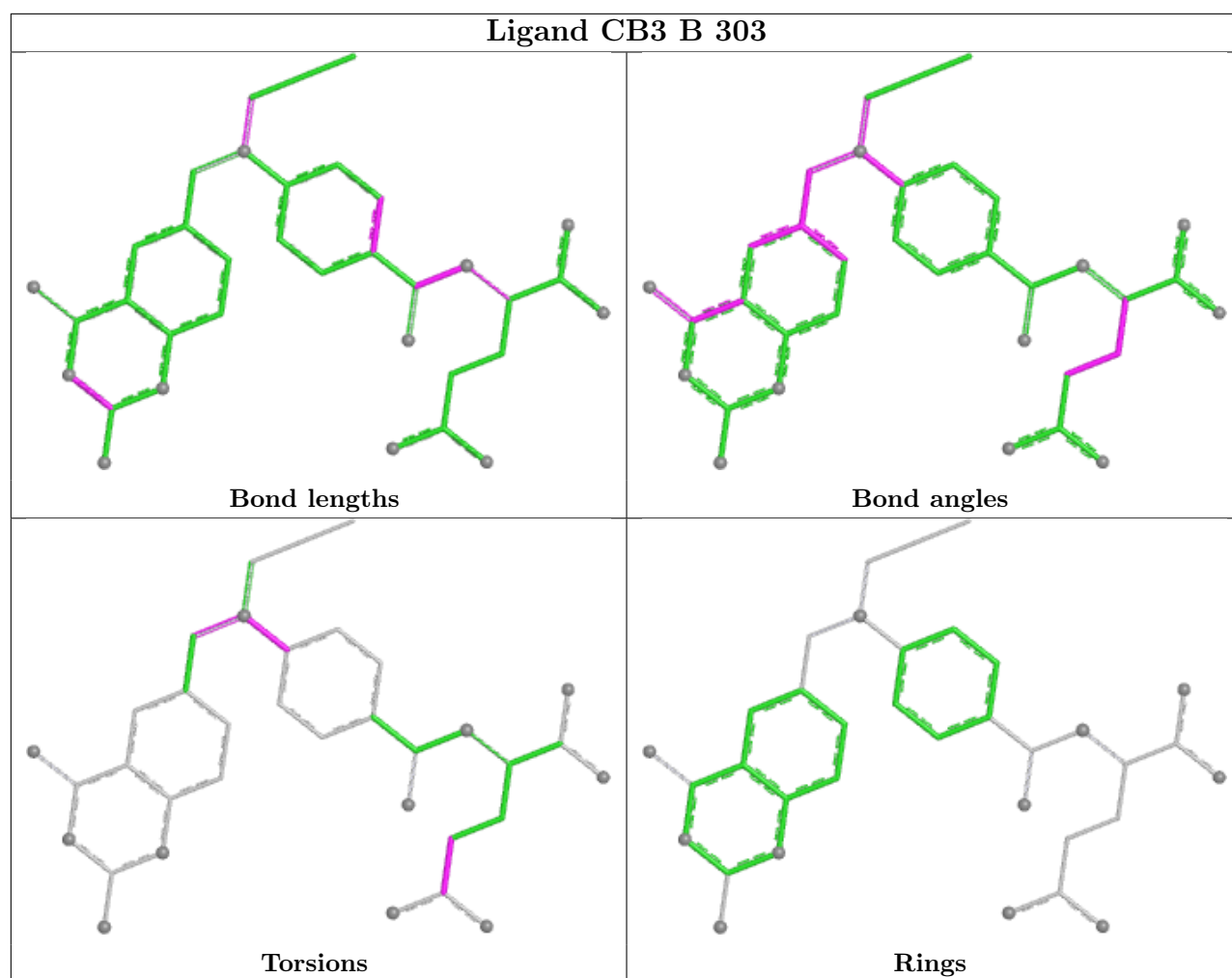


Ligand CB3 C 305

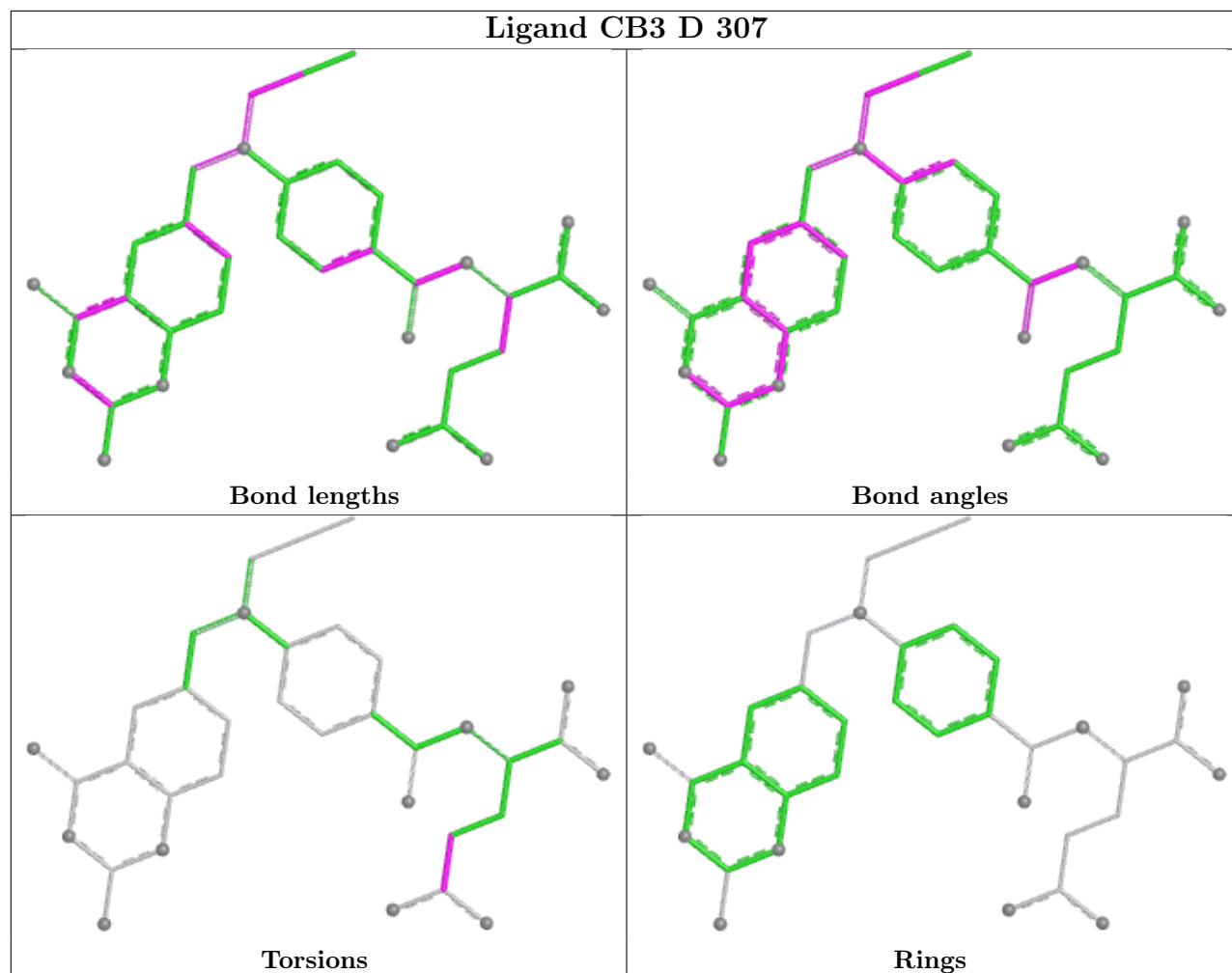


Ligand UMP A 300

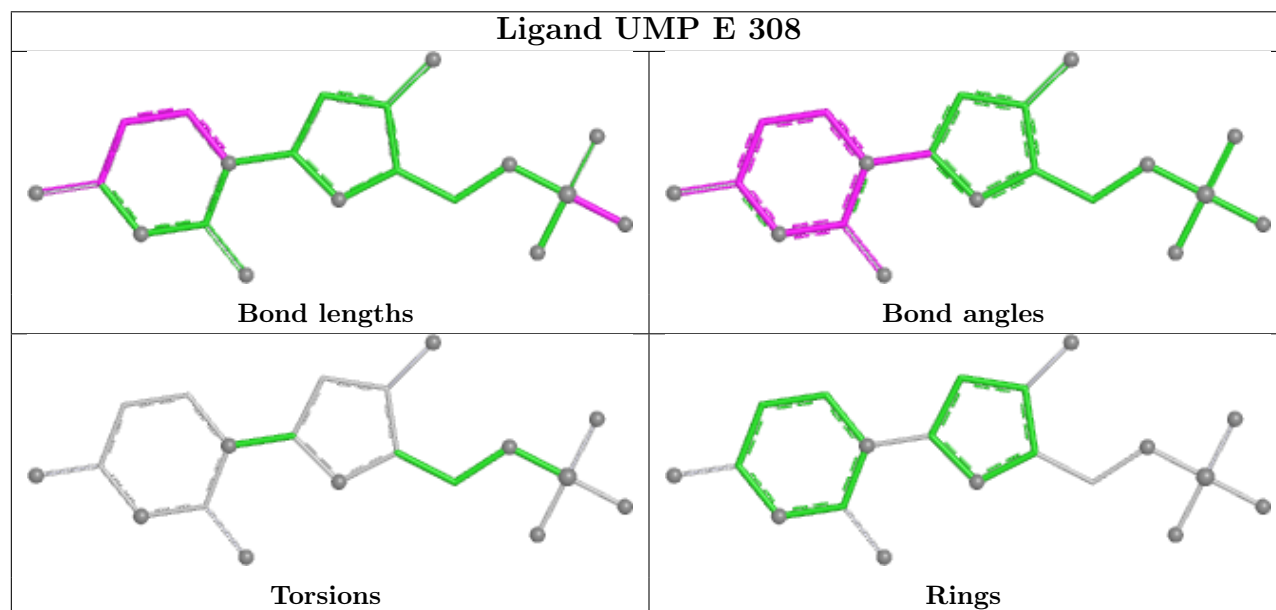


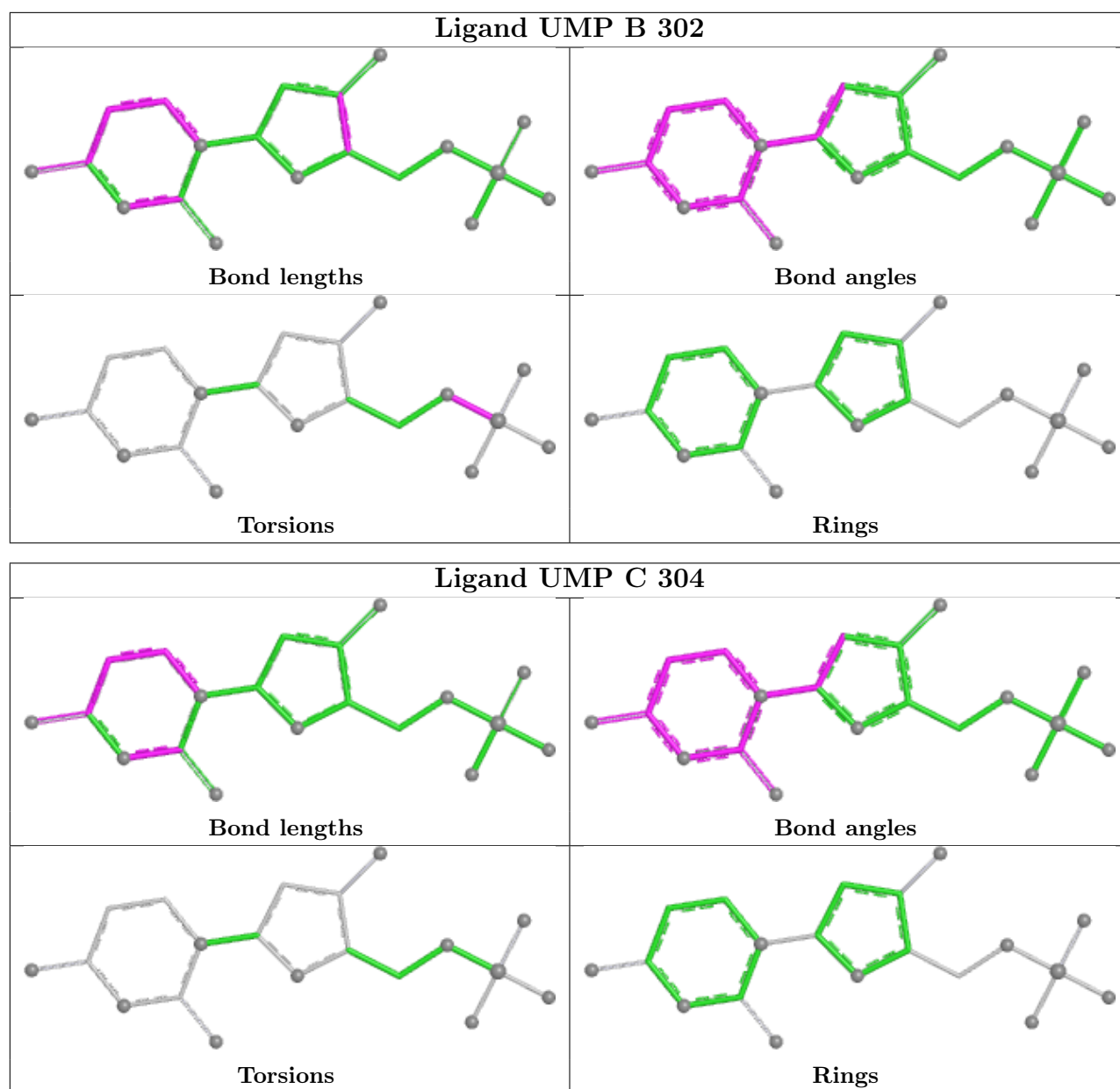


Ligand CB3 D 307



Ligand UMP E 308





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	263/264 (99%)	-0.36	0 100 100	3, 16, 29, 39	0
1	B	263/264 (99%)	-0.25	1 (0%) 88 86	4, 17, 36, 45	0
1	C	263/264 (99%)	-0.25	0 100 100	3, 19, 33, 50	0
1	D	263/264 (99%)	-0.06	9 (3%) 48 42	5, 22, 42, 62	0
1	E	260/264 (98%)	-0.04	4 (1%) 72 68	6, 22, 43, 60	0
1	F	263/264 (99%)	-0.22	0 100 100	7, 20, 31, 44	0
All	All	1575/1584 (99%)	-0.20	14 (0%) 81 78	3, 19, 37, 62	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	22	THR	3.8
1	E	261	PRO	3.5
1	D	262	VAL	3.5
1	E	22	THR	3.2
1	D	263	ALA	3.1
1	D	23	GLY	3.0
1	D	21	ARG	2.9
1	E	260	ALA	2.7
1	D	260	ALA	2.6
1	D	83	TRP	2.3
1	E	17	GLN	2.3
1	B	22	THR	2.3
1	D	237	GLU	2.2
1	D	264	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CXM	E	1	11/12	0.92	0.11	27,30,34,34	0
1	CXM	D	1	11/12	0.93	0.10	21,22,24,25	0
1	CXM	F	1	11/12	0.93	0.10	21,24,26,27	0
1	CXM	C	1	11/12	0.94	0.08	22,26,28,28	0
1	CXM	A	1	11/12	0.95	0.10	13,17,24,27	0
1	CXM	B	1	11/12	0.96	0.07	12,15,24,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

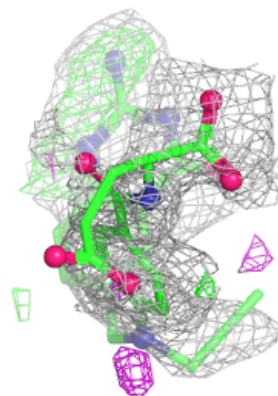
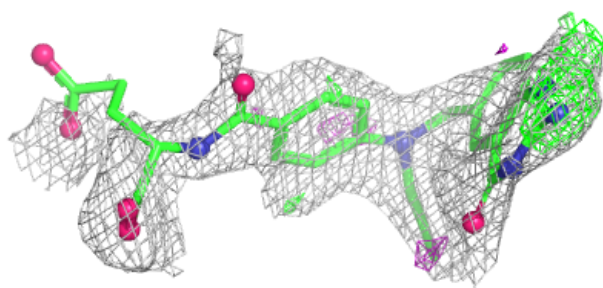
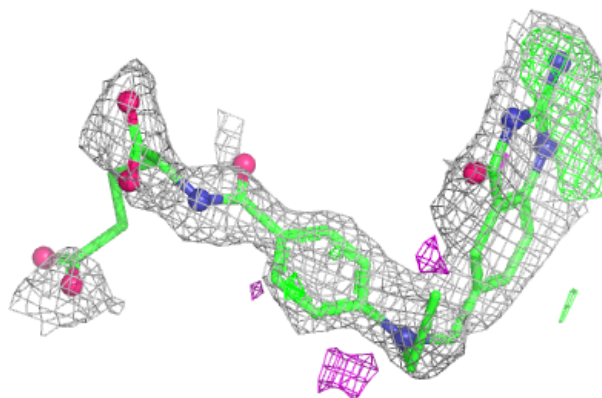
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CB3	E	309	35/35	0.69	0.27	67,78,92,92	0
3	CB3	D	307	35/35	0.76	0.16	43,49,63,64	0
3	CB3	B	303	35/35	0.82	0.14	24,31,50,52	0
3	CB3	F	311	35/35	0.85	0.13	18,26,47,48	0
3	CB3	C	305	35/35	0.88	0.12	10,24,51,53	0
3	CB3	A	301	35/35	0.88	0.12	9,24,36,37	0
2	UMP	E	308	20/20	0.94	0.09	12,15,21,23	0
2	UMP	D	306	20/20	0.95	0.09	18,21,23,24	0
2	UMP	B	302	20/20	0.95	0.09	16,17,21,21	0
2	UMP	F	310	20/20	0.96	0.07	12,15,20,20	0
2	UMP	C	304	20/20	0.97	0.07	12,14,17,18	0
2	UMP	A	300	20/20	0.98	0.06	4,7,11,12	0

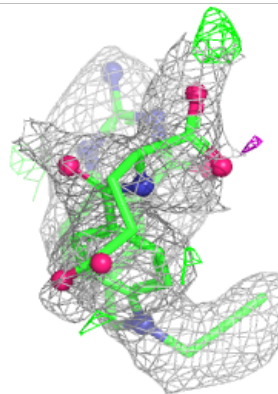
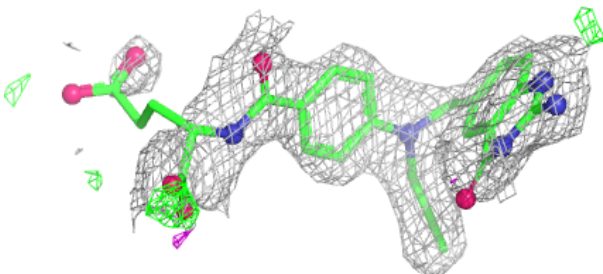
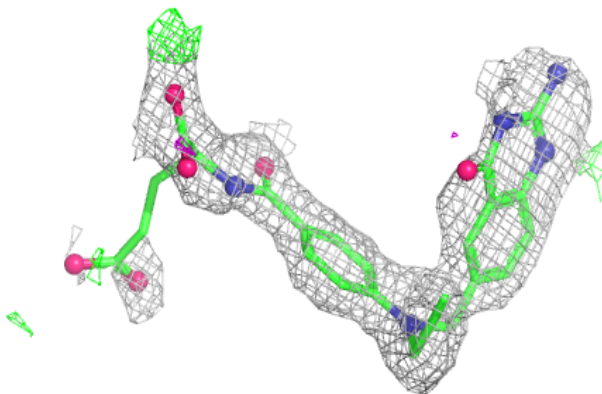
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CB3 E 309:

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

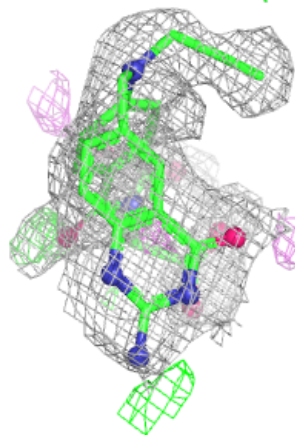
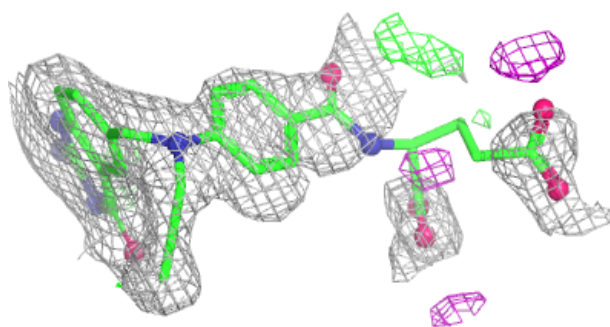
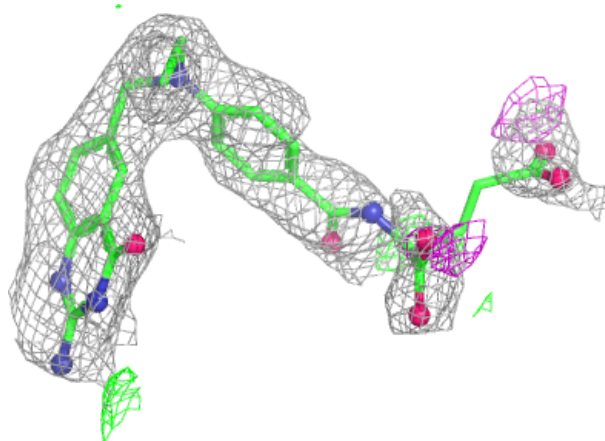
**Electron density around CB3 D 307:**

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



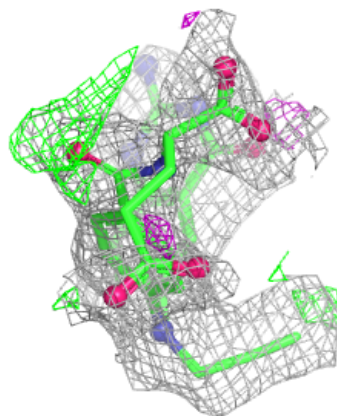
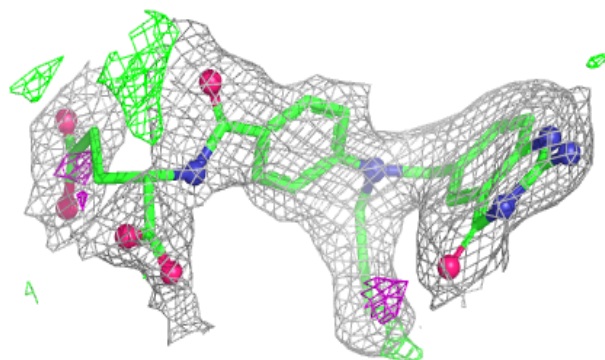
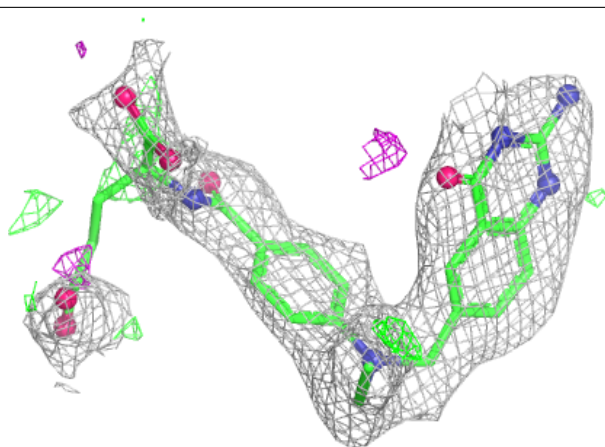
Electron density around CB3 B 303:

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



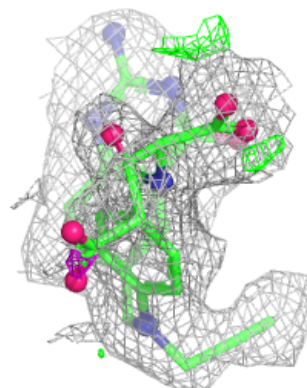
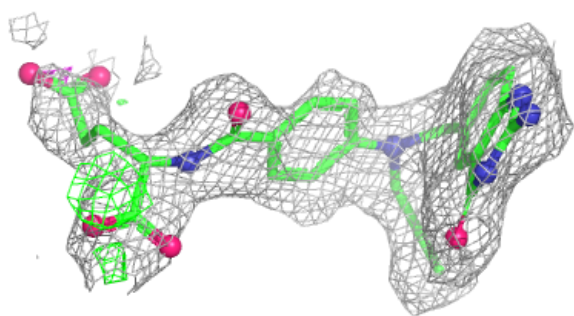
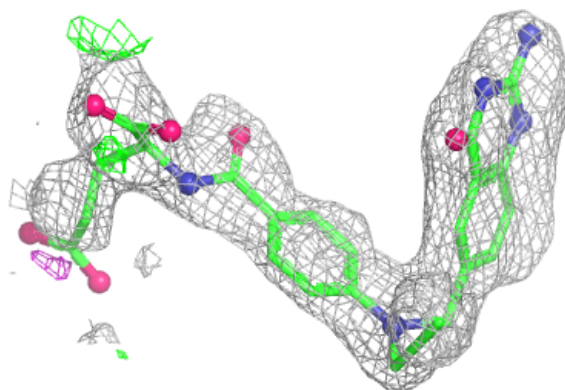
Electron density around CB3 F 311:

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

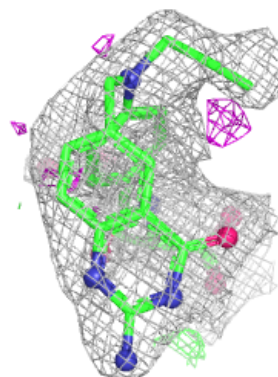
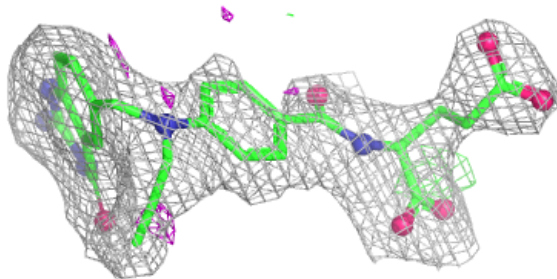
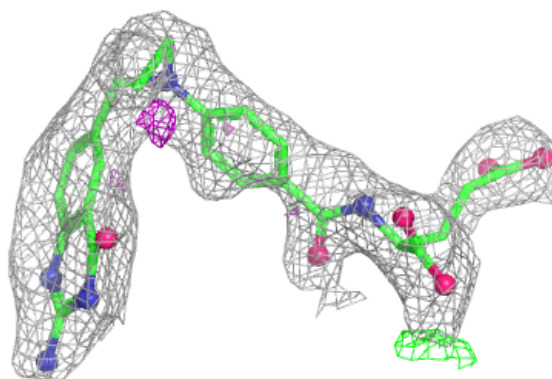


Electron density around CB3 C 305:

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

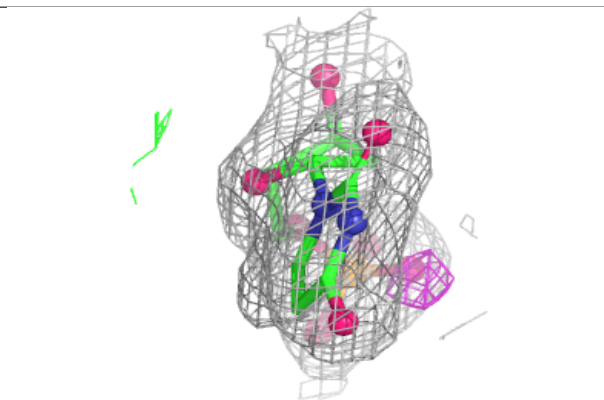
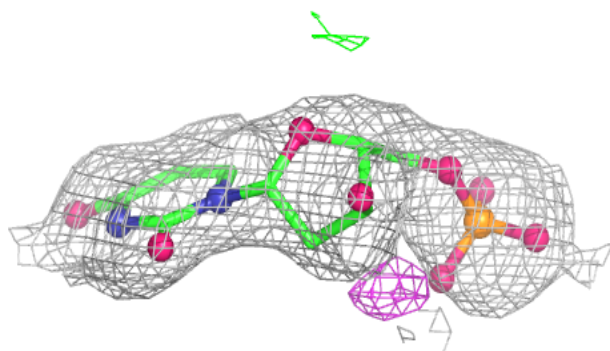
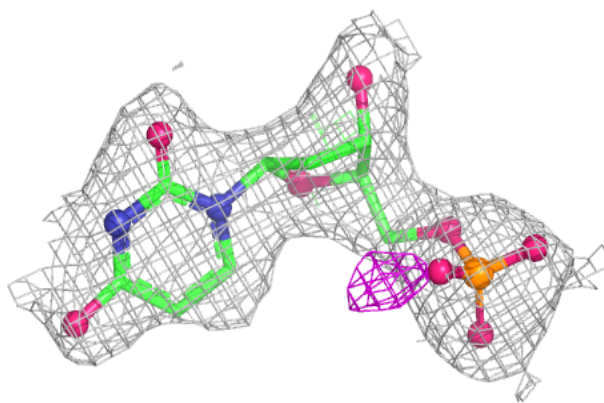
**Electron density around CB3 A 301:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

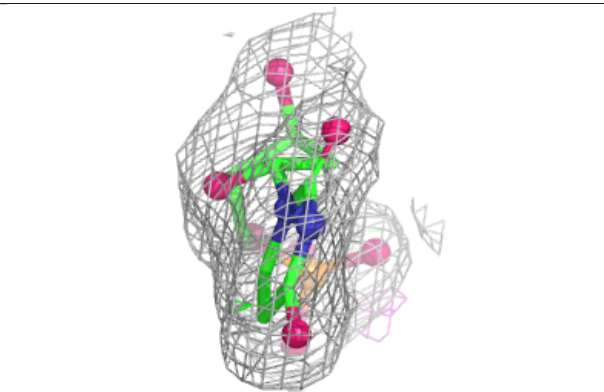
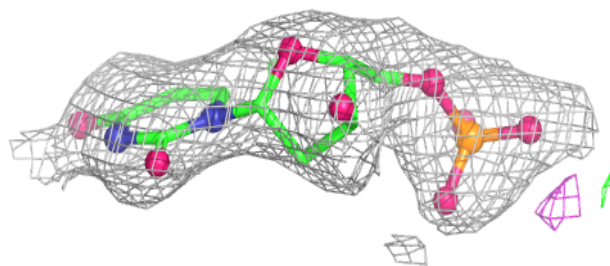
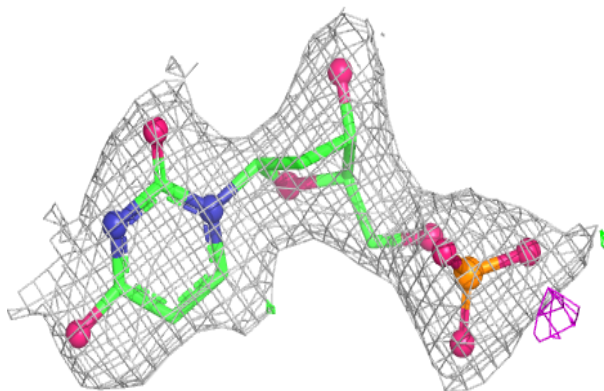


Electron density around UMP E 308:

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

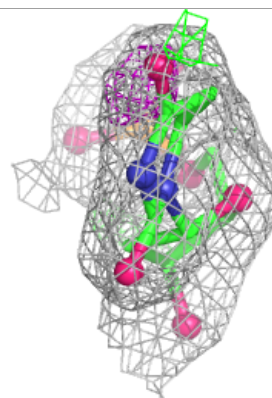
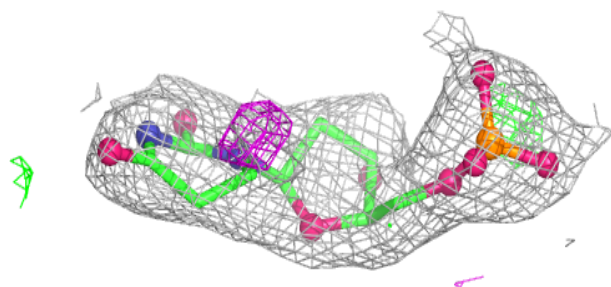
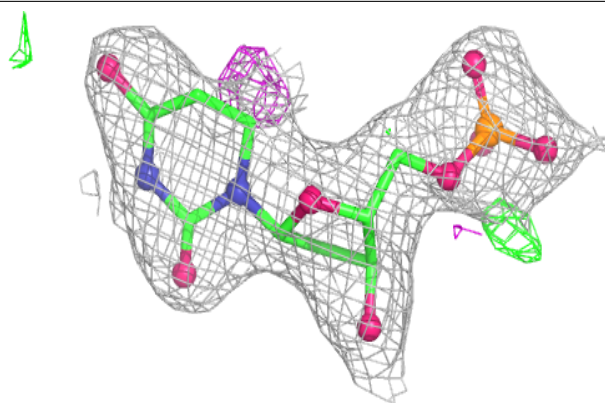
**Electron density around UMP D 306:**

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

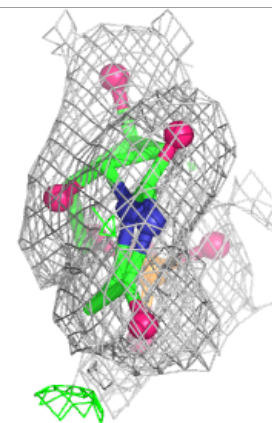
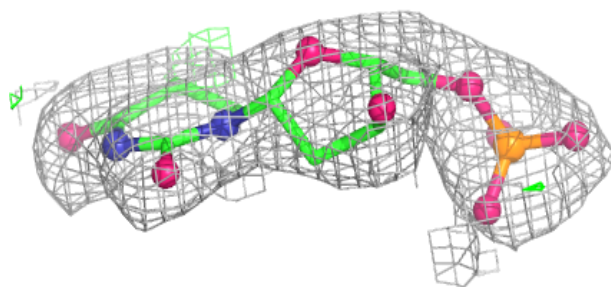
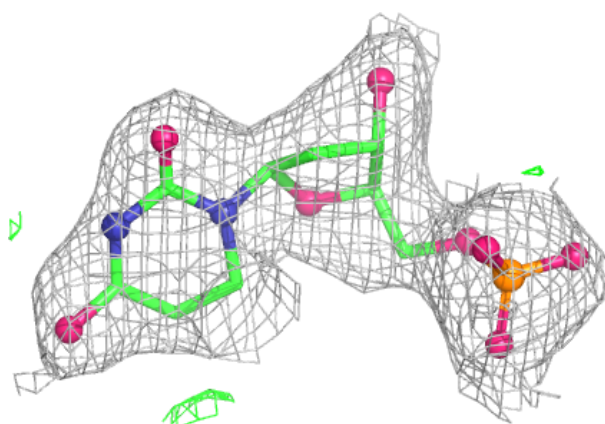


Electron density around UMP B 302:

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

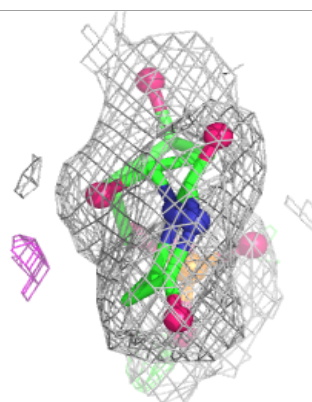
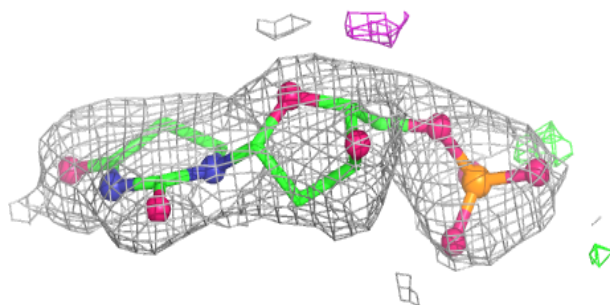
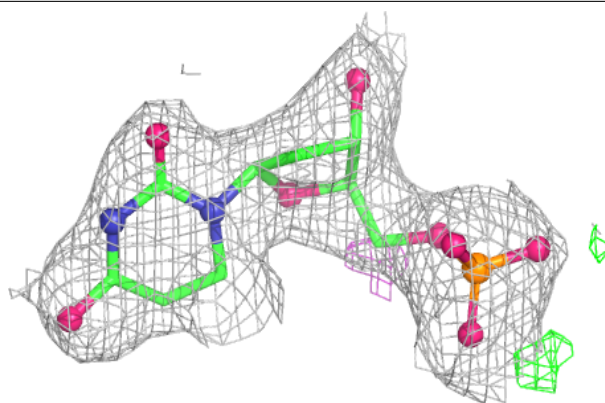
**Electron density around UMP F 310:**

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

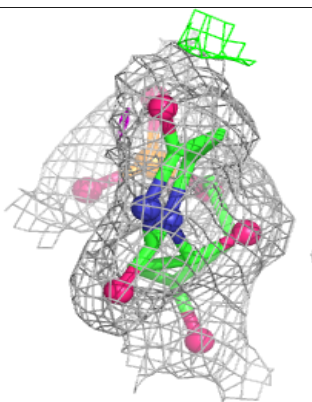
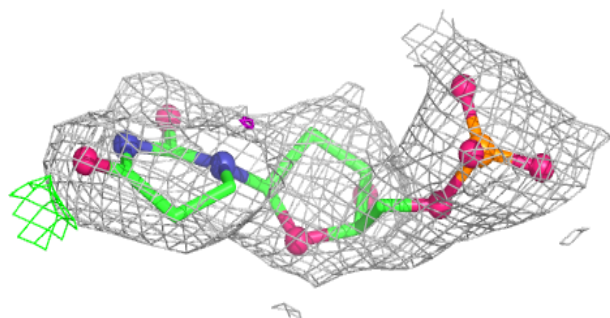
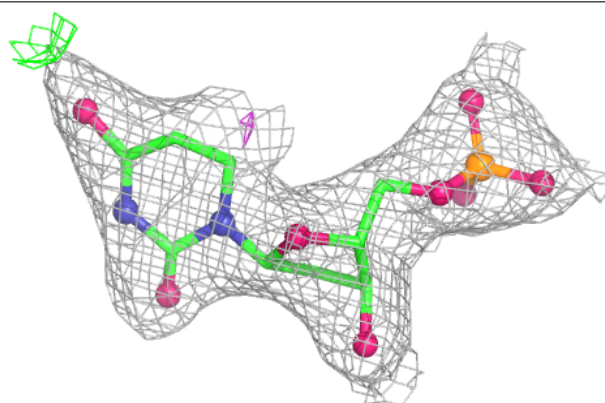


Electron density around UMP C 304:

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

**Electron density around UMP A 300:**

$2mF_o-DF_c$ (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.