



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:55 PM UTC

PDB ID : 5HS3 / pdb_00005hs3
Title : Human thymidylate synthase complexed with dUMP and 3-amino-2-benzoyl-4-methylthieno[2,3-b]pyridin-6-ol
Authors : Chen, D.; Almqvist, H.; Axelsson, H.; Jafari, R.; Mateus, A.; Haraldsson, M.; Larsson, A.; Artursson, P.; Molina, D.M.; Lundback, T.; Nordlund, P.
Deposited on : 2016-01-25
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

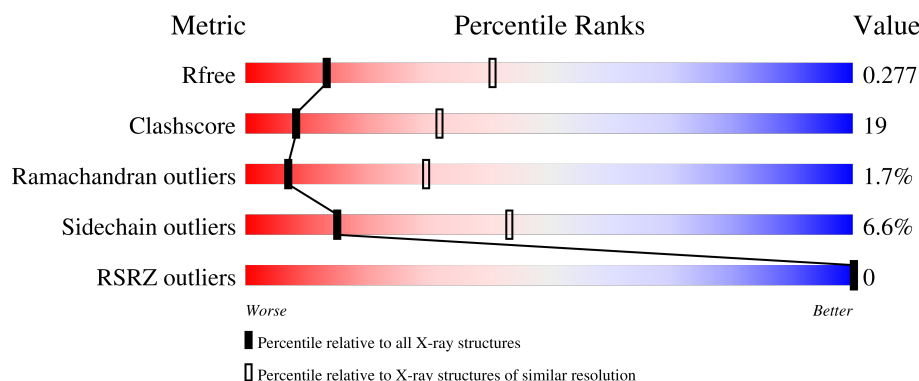
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

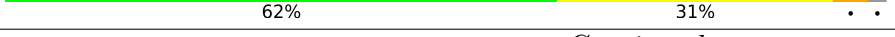
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	289	 62% 33% 5%
1	B	289	 62% 34% 5%
1	C	289	 67% 25% 5% 5%
1	D	289	 62% 31% 5% 5%

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Mol	Chain	Length	Quality of chain
1	E	289	
1	F	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	400	-	X	-	-
2	UMP	B	400	-	X	-	-
2	UMP	C	400	-	X	-	-
2	UMP	D	400	-	X	-	-
2	UMP	E	400	-	X	-	-
2	UMP	F	400	-	X	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13887 atoms, of which 102 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.

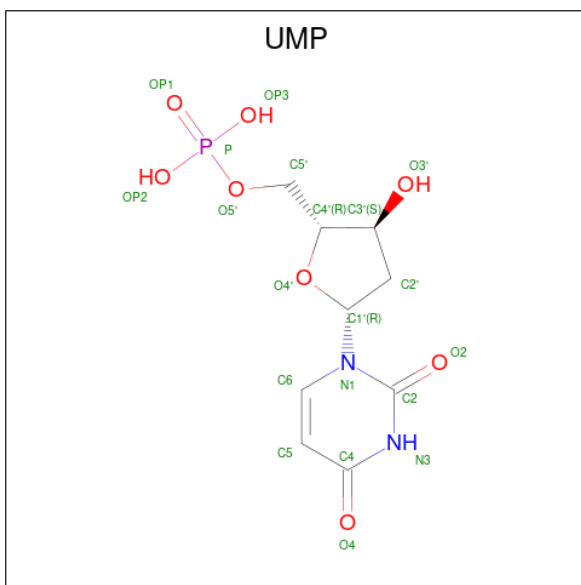
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2309	1477	398	421	13			
1	B	289	Total	C	N	O	S	0	0	0
			2297	1471	398	415	13			
1	C	281	Total	C	N	O	S	0	0	0
			2223	1424	384	404	11			
1	D	282	Total	C	N	O	S	0	0	0
			2260	1446	397	406	11			
1	E	282	Total	C	N	O	S	0	0	0
			2265	1449	395	410	11			
1	F	281	Total	C	N	O	S	0	0	0
			2240	1436	392	401	11			

There are 6 discrepancies between the modelled and reference sequences:

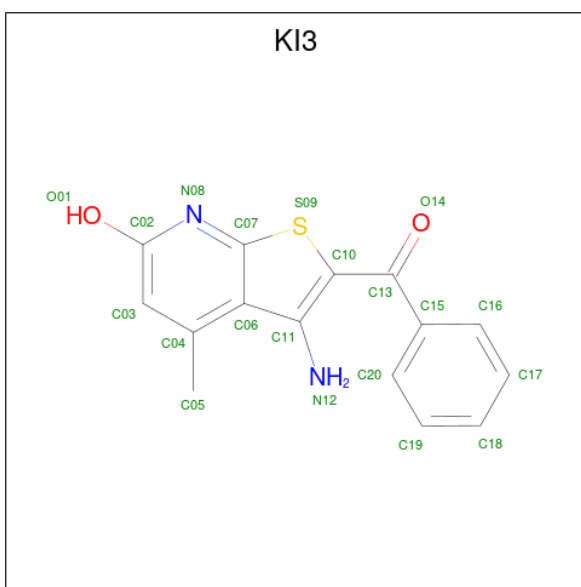
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP P04818
B	25	MET	-	expression tag	UNP P04818
C	25	MET	-	expression tag	UNP P04818
D	25	MET	-	expression tag	UNP P04818
E	25	MET	-	expression tag	UNP P04818
F	25	MET	-	expression tag	UNP P04818

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			31	9	11	2	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			31	9	11	2	8	1		
2	C	1	Total	C	H	N	O	P	0	0
			31	9	11	2	8	1		
2	D	1	Total	C	H	N	O	P	0	0
			31	9	11	2	8	1		
2	E	1	Total	C	H	N	O	P	0	0
			31	9	11	2	8	1		
2	F	1	Total	C	H	N	O	P	0	0
			31	9	11	2	8	1		

- Molecule 3 is 3-amino-2-benzoyl-4-methylthieno[2,3-b]pyridin-6-ol (CCD ID: KI3) (formula: C₁₅H₁₂N₂O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			32	15	12	2	2	1		
3	B	1	Total	C	H	N	O	S	0	0
			32	15	12	2	2	1		
3	E	1	Total	C	H	N	O	S	0	0
			32	15	12	2	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	3	Total	O	0	0
			3	3		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

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.

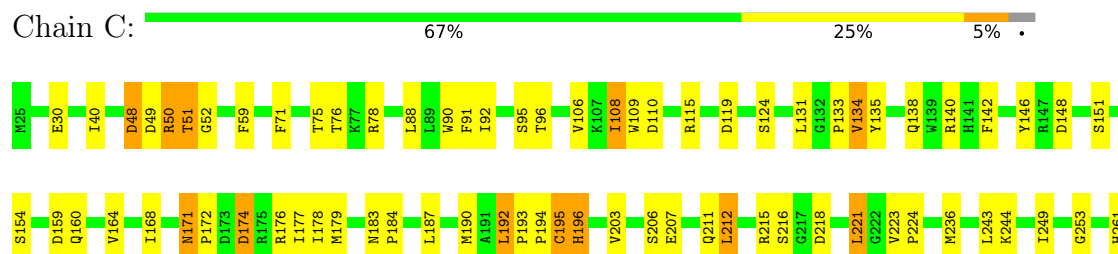
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase



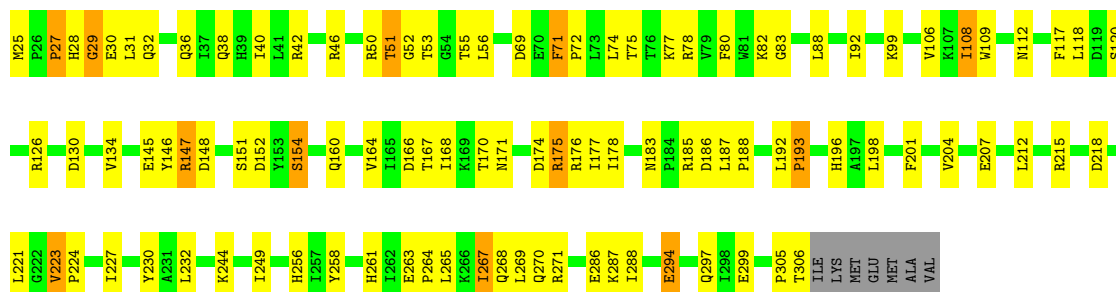
• Molecule 1: Thymidylate synthase





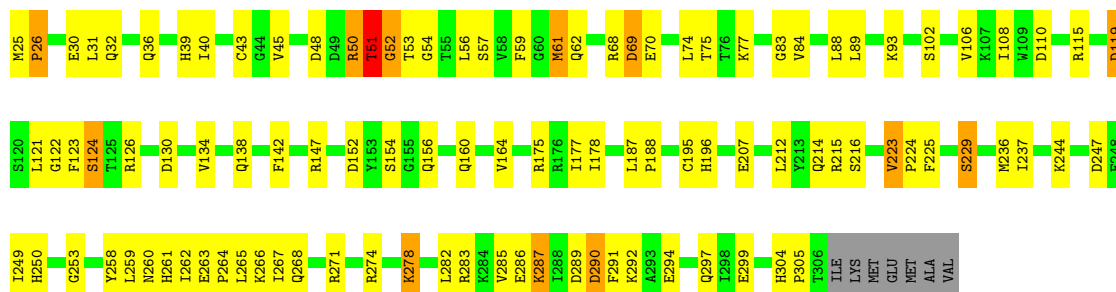
• Molecule 1: Thymidylate synthase

Chain D: 62% 31%



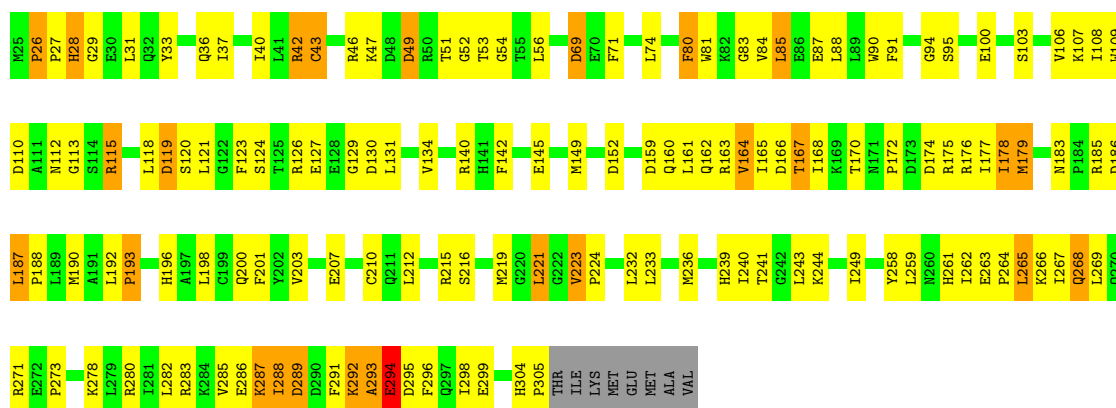
• Molecule 1: Thymidylate synthase

Chain E: 62% 31%



• Molecule 1: Thymidylate synthase

Chain F: 48% 40% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.20Å 108.20Å 313.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.11 – 3.10 28.11 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.11-3.10) 99.6 (28.11-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.268 0.188 , 0.277	Depositor DCC
R_{free} test set	1675 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13887	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 58.10 % 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 2.1489e-05. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KI3, UMP

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	0.98	0/2369	0.92	6/3210 (0.2%)
1	B	0.83	0/2357	0.89	7/3195 (0.2%)
1	C	0.81	0/2283	0.87	6/3100 (0.2%)
1	D	0.95	0/2320	0.94	7/3143 (0.2%)
1	E	0.82	0/2325	0.86	5/3149 (0.2%)
1	F	0.78	1/2300 (0.0%)	0.94	10/3117 (0.3%)
All	All	0.86	1/13954 (0.0%)	0.90	41/18914 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	223	VAL	CA-CB	-6.12	1.51	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	LYS	CA-C-N	7.65	127.94	119.90
1	A	244	LYS	C-N-CA	7.65	127.94	119.90
1	F	26	PRO	CA-C-N	7.18	126.94	119.76
1	F	26	PRO	C-N-CA	7.18	126.94	119.76
1	B	223	VAL	CB-CA-C	-7.17	106.75	114.35
1	D	71	PHE	CA-C-N	6.81	128.35	119.84
1	D	71	PHE	C-N-CA	6.81	128.35	119.84
1	C	71	PHE	CA-C-N	6.55	128.03	119.84
1	C	71	PHE	C-N-CA	6.55	128.03	119.84
1	D	171	ASN	CA-C-N	6.48	126.17	119.82
1	D	171	ASN	C-N-CA	6.48	126.17	119.82
1	A	71	PHE	CA-C-N	6.29	127.71	119.84
1	A	71	PHE	C-N-CA	6.29	127.71	119.84
1	B	171	ASN	CA-C-N	6.29	127.71	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASN	C-N-CA	6.29	127.71	119.84
1	C	171	ASN	CA-C-N	6.18	127.56	119.84
1	C	171	ASN	C-N-CA	6.18	127.56	119.84
1	F	183	ASN	CA-C-N	6.04	126.21	119.32
1	F	183	ASN	C-N-CA	6.04	126.21	119.32
1	D	223	VAL	CB-CA-C	-6.00	107.98	114.35
1	E	26	PRO	CA-C-N	5.99	127.33	119.84
1	E	26	PRO	C-N-CA	5.99	127.33	119.84
1	F	193	PRO	CA-C-N	5.87	125.89	119.90
1	F	193	PRO	C-N-CA	5.87	125.89	119.90
1	F	71	PHE	CA-C-N	5.77	127.06	119.84
1	F	71	PHE	C-N-CA	5.77	127.06	119.84
1	F	49	ASP	N-CA-C	5.71	115.38	107.73
1	B	183	ASN	CA-C-N	5.67	125.78	119.32
1	B	183	ASN	C-N-CA	5.67	125.78	119.32
1	A	171	ASN	CA-C-N	5.51	126.73	119.84
1	A	171	ASN	C-N-CA	5.51	126.73	119.84
1	B	193	PRO	CA-C-N	5.36	125.36	119.90
1	B	193	PRO	C-N-CA	5.36	125.36	119.90
1	F	294	GLU	N-CA-C	-5.25	106.38	112.89
1	D	193	PRO	CA-C-N	5.24	125.24	119.90
1	D	193	PRO	C-N-CA	5.24	125.24	119.90
1	E	274	ARG	CA-C-N	5.19	124.95	119.76
1	E	274	ARG	C-N-CA	5.19	124.95	119.76
1	E	223	VAL	CB-CA-C	-5.14	108.90	114.35
1	C	272	GLU	CA-C-N	5.01	126.10	119.84
1	C	272	GLU	C-N-CA	5.01	126.10	119.84

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	2309	0	2254	84	0
1	B	2297	0	2242	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2223	0	2142	67	3
1	D	2260	0	2215	77	3
1	E	2265	0	2221	72	2
1	F	2240	0	2189	146	2
2	A	20	11	10	2	2
2	B	20	11	10	2	1
2	C	20	11	10	2	1
2	D	20	11	10	3	0
2	E	20	11	10	1	0
2	F	20	11	10	5	3
3	A	20	12	0	1	0
3	B	20	12	0	1	0
3	E	20	12	0	0	0
4	A	6	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	13785	102	13323	519	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (519) 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:27:PRO:HA	1:F:28:HIS:HB3	1.21	1.16
1:F:42:ARG:HG2	1:F:42:ARG:HH11	1.20	1.04
1:C:215:ARG:NH1	2:C:400:UMP:OP1	1.92	1.01
1:B:97:ASN:ND2	1:B:149:MET:SD	2.43	0.91
1:F:263:GLU:HB3	1:F:264:PRO:HD3	1.54	0.90
1:F:192:LEU:HD12	1:F:193:PRO:HD2	1.52	0.90
1:D:192:LEU:HD12	1:D:193:PRO:HD2	1.54	0.88
1:F:27:PRO:HA	1:F:28:HIS:CB	2.02	0.86
1:F:42:ARG:NH1	1:F:43:CYS:SG	2.51	0.84
1:E:30:GLU:OE2	1:E:75:THR:N	2.11	0.83
1:F:259:LEU:HD23	1:F:262:ILE:HD11	1.60	0.82
1:F:37:ILE:HG21	1:F:269:LEU:HD11	1.61	0.82
1:A:219:MET:HE3	1:A:255:ALA:HB1	1.60	0.82
1:B:104:LYS:NZ	1:F:100:GLU:OE2	2.11	0.82
1:D:77:LYS:HG3	1:D:306:THR:HG22	1.61	0.82
1:F:196:HIS:HB3	1:F:212:LEU:HD11	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:NH1	1:B:259:LEU:HD11	1.95	0.81
1:B:88:LEU:HD23	1:B:232:LEU:HG	1.60	0.81
1:D:27:PRO:HA	1:D:28:HIS:HB3	1.63	0.80
1:A:146:TYR:O	1:E:147:ARG:NH1	2.16	0.78
1:C:192:LEU:HD12	1:C:193:PRO:HD2	1.65	0.78
1:D:263:GLU:HB2	1:D:264:PRO:HD3	1.66	0.77
1:C:196:HIS:HB3	1:C:212:LEU:HD11	1.66	0.76
1:E:268:GLN:HA	1:E:271:ARG:HD2	1.69	0.74
1:A:64:ARG:HD3	1:A:247:ASP:OD2	1.87	0.74
1:A:219:MET:HE1	1:A:252:LEU:HD13	1.69	0.74
1:F:27:PRO:CA	1:F:28:HIS:HB3	2.12	0.74
1:F:215:ARG:NH1	2:F:400:UMP:OP2	2.21	0.74
1:C:274:ARG:NH1	1:C:302:ASN:O	2.20	0.73
1:D:28:HIS:O	1:D:31:LEU:HD13	1.89	0.73
1:A:116:ASP:OD1	1:C:78:ARG:NH1	2.22	0.72
1:B:49:ASP:OD2	1:B:51:THR:HG23	1.91	0.71
1:B:115:ARG:NH1	1:B:119:ASP:OD1	2.24	0.71
1:A:219:MET:HE1	1:A:252:LEU:CD1	2.21	0.70
1:F:74:LEU:HD12	1:F:224:PRO:HB3	1.71	0.70
1:F:42:ARG:HG2	1:F:42:ARG:NH1	1.94	0.70
1:E:263:GLU:HB2	1:E:264:PRO:HD3	1.73	0.70
1:C:140:ARG:NH2	1:C:289:ASP:OD1	2.24	0.70
1:B:187:LEU:HB2	1:B:188:PRO:HD3	1.74	0.69
1:D:51:THR:O	1:D:53:THR:N	2.22	0.68
1:F:240:ILE:HD11	1:F:291:PHE:CE2	2.28	0.68
1:B:311:MET:HE3	1:B:313:VAL:CG1	2.23	0.68
1:E:215:ARG:NH1	2:E:400:UMP:OP2	2.27	0.68
1:B:126:ARG:HD3	1:B:130:ASP:HB3	1.76	0.68
1:E:50:ARG:O	1:E:52:GLY:N	2.26	0.68
1:E:271:ARG:NH2	1:E:305:PRO:O	2.27	0.67
1:B:278:LYS:HE3	1:B:280:ARG:NH1	2.09	0.67
1:A:97:ASN:ND2	1:A:149:MET:HE3	2.08	0.67
1:F:28:HIS:ND1	1:F:31:LEU:HG	2.09	0.67
1:D:294:GLU:CD	1:D:294:GLU:H	2.01	0.67
1:E:115:ARG:O	1:E:119:ASP:HB2	1.95	0.67
1:A:221:LEU:HD13	1:A:309:MET:HB2	1.76	0.66
1:D:196:HIS:HB3	1:D:212:LEU:HD11	1.76	0.66
1:D:126:ARG:HD3	1:D:130:ASP:HB3	1.77	0.66
1:F:177:ILE:CG2	1:F:201:PHE:HB2	2.24	0.66
1:B:294:GLU:N	1:B:294:GLU:OE1	2.28	0.66
1:F:292:LYS:HE3	1:F:294:GLU:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HD23	1:A:236:MET:HE3	1.79	0.65
1:E:51:THR:O	1:E:53:THR:N	2.29	0.65
1:A:115:ARG:NH2	1:A:126:ARG:O	2.29	0.65
1:F:241:THR:OG1	1:F:243:LEU:HD12	1.97	0.64
1:F:215:ARG:NH2	2:F:400:UMP:OP2	2.30	0.64
1:A:115:ARG:H	1:A:128:GLU:HG3	1.61	0.64
1:A:126:ARG:HD3	1:A:130:ASP:HB3	1.80	0.64
1:E:258:TYR:O	1:E:261:HIS:N	2.25	0.64
1:C:49:ASP:OD2	1:C:51:THR:OG1	2.12	0.63
1:D:207:GLU:HA	1:D:244:LYS:O	1.98	0.63
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.79	0.63
1:F:107:LYS:HG3	1:F:110:ASP:OD2	1.99	0.63
1:B:30:GLU:HG2	1:B:74:LEU:HD22	1.81	0.63
1:B:207:GLU:HA	1:B:244:LYS:O	1.99	0.63
1:D:215:ARG:NH1	2:D:400:UMP:OP2	2.30	0.63
1:A:263:GLU:HB2	1:A:264:PRO:HD3	1.81	0.62
1:F:36:GLN:O	1:F:40:ILE:HG13	2.00	0.62
1:F:287:LYS:HE3	1:F:288:ILE:N	2.14	0.62
1:D:268:GLN:HA	1:D:271:ARG:HD2	1.80	0.62
1:F:236:MET:HE2	1:F:296:PHE:CZ	2.33	0.62
1:F:293:ALA:HB3	1:F:294:GLU:OE2	2.00	0.62
1:E:31:LEU:H	1:E:31:LEU:HD12	1.63	0.62
1:F:207:GLU:HA	1:F:244:LYS:O	2.00	0.62
1:A:99:LYS:HZ1	1:D:99:LYS:HD2	1.64	0.62
1:D:270:GLN:HA	1:D:270:GLN:OE1	1.99	0.62
1:F:198:LEU:C	1:F:198:LEU:HD12	2.25	0.62
1:B:68:ARG:NH1	1:B:247:ASP:OD1	2.28	0.61
1:C:164:VAL:O	1:C:168:ILE:HG13	2.00	0.61
1:A:32:GLN:O	1:A:36:GLN:HG3	2.01	0.61
1:D:31:LEU:N	1:D:31:LEU:HD12	2.15	0.61
1:B:64:ARG:HD3	1:B:247:ASP:OD2	2.01	0.61
1:E:88:LEU:HG	1:E:236:MET:HE1	1.84	0.60
1:D:106:VAL:CG1	1:D:108:ILE:HD13	2.31	0.60
1:F:140:ARG:HG2	1:F:140:ARG:HH11	1.66	0.60
1:B:30:GLU:OE2	1:B:75:THR:N	2.24	0.60
1:F:174:ASP:OD1	1:F:176:ARG:N	2.35	0.60
1:F:177:ILE:HG21	1:F:201:PHE:HB2	1.82	0.60
1:C:48:ASP:CG	1:F:46:ARG:HH12	2.10	0.59
1:C:142:PHE:CE1	1:C:183:ASN:HB2	2.36	0.59
1:A:88:LEU:HD23	1:A:232:LEU:HG	1.85	0.59
1:F:115:ARG:HH12	1:F:126:ARG:C	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:THR:HG22	1:C:134:VAL:CG2	2.33	0.59
1:F:33:TYR:O	1:F:37:ILE:HG12	2.01	0.59
1:C:263:GLU:HB2	1:C:264:PRO:HD3	1.85	0.59
1:F:259:LEU:HD23	1:F:262:ILE:CD1	2.31	0.59
1:F:26:PRO:HB2	1:F:27:PRO:HD2	1.85	0.59
1:F:115:ARG:NH2	1:F:124:SER:O	2.35	0.58
1:D:166:ASP:O	1:D:170:THR:HG23	2.03	0.58
1:F:127:GLU:OE1	1:F:127:GLU:N	2.36	0.58
1:F:263:GLU:HB3	1:F:264:PRO:CD	2.31	0.58
1:D:198:LEU:HD12	1:D:198:LEU:C	2.29	0.58
1:F:140:ARG:HG2	1:F:140:ARG:NH1	2.18	0.58
1:B:145:GLU:HG2	1:D:145:GLU:CD	2.28	0.58
1:A:69:ASP:N	1:A:69:ASP:OD1	2.35	0.58
1:A:171:ASN:N	1:A:172:PRO:HD3	2.19	0.58
1:F:292:LYS:NZ	1:F:295:ASP:OD1	2.34	0.58
1:F:259:LEU:HA	1:F:262:ILE:CD1	2.34	0.58
1:C:138:GLN:O	1:C:160:GLN:NE2	2.37	0.57
1:F:108:ILE:HG13	1:F:109:TRP:CD1	2.40	0.57
1:A:219:MET:CE	1:A:252:LEU:HD13	2.33	0.57
1:B:51:THR:OG1	1:B:53:THR:OG1	2.16	0.57
1:A:46:ARG:HH11	1:A:259:LEU:HD11	1.68	0.57
1:B:232:LEU:HD12	1:B:232:LEU:O	2.03	0.57
1:B:115:ARG:NH2	1:B:126:ARG:O	2.38	0.57
1:A:196:HIS:HB3	1:A:212:LEU:HD11	1.87	0.57
1:E:285:VAL:HG13	1:E:290:ASP:HB3	1.87	0.57
1:E:297:GLN:NE2	1:E:299:GLU:OE2	2.38	0.56
1:F:236:MET:O	1:F:239:HIS:HB3	2.04	0.56
1:A:51:THR:HG21	1:A:312:ALA:HB1	1.87	0.56
1:B:241:THR:OG1	1:B:243:LEU:HD12	2.06	0.56
1:B:46:ARG:HH12	1:B:259:LEU:HD11	1.70	0.56
1:C:218:ASP:OD2	1:C:221:LEU:HB2	2.05	0.56
1:D:152:ASP:OD1	1:D:154:SER:OG	2.23	0.56
1:E:214:GLN:NE2	1:E:216:SER:O	2.30	0.56
1:F:287:LYS:HE3	1:F:288:ILE:H	1.70	0.56
1:A:115:ARG:N	1:A:128:GLU:HG3	2.21	0.56
1:B:89:LEU:O	1:B:93:LYS:HG2	2.06	0.56
1:B:93:LYS:HD3	1:B:93:LYS:N	2.20	0.56
1:B:90:TRP:NE1	1:B:95:SER:OG	2.39	0.55
1:A:232:LEU:HG	1:A:236:MET:HE3	1.89	0.55
1:A:302:ASN:OD1	1:B:50:ARG:HB3	2.06	0.55
1:C:106:VAL:HG12	1:C:108:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ASP:OD1	1:E:154:SER:OG	2.22	0.55
1:F:120:SER:O	1:F:120:SER:OG	2.23	0.55
1:F:163:ARG:NH2	1:F:166:ASP:HB2	2.21	0.55
1:D:80:PHE:CE1	1:D:82:LYS:HB3	2.42	0.55
1:D:187:LEU:N	1:D:188:PRO:CD	2.70	0.55
1:F:87:GLU:O	1:F:90:TRP:HB3	2.06	0.55
1:D:88:LEU:HD23	1:D:232:LEU:HG	1.88	0.55
1:E:106:VAL:HG12	1:E:108:ILE:HG12	1.89	0.55
1:E:294:GLU:CD	1:E:294:GLU:H	2.14	0.55
1:A:285:VAL:HG21	1:A:291:PHE:CD1	2.42	0.55
1:B:110:ASP:OD1	1:B:110:ASP:N	2.38	0.55
1:B:219:MET:SD	1:B:223:VAL:HG21	2.47	0.55
1:C:272:GLU:CD	1:C:273:PRO:HD2	2.31	0.55
1:C:236:MET:HB3	1:C:291:PHE:HE2	1.70	0.55
1:B:55:THR:C	1:B:56:LEU:HD23	2.32	0.55
1:D:261:HIS:O	1:D:265:LEU:HB2	2.06	0.55
1:A:30:GLU:HG3	1:A:74:LEU:HD13	1.89	0.54
1:A:187:LEU:HB3	1:A:188:PRO:HD3	1.90	0.54
1:A:30:GLU:OE2	1:A:75:THR:OG1	2.17	0.54
1:C:174:ASP:OD2	1:C:176:ARG:HB2	2.06	0.54
1:C:171:ASN:N	1:C:172:PRO:HD3	2.21	0.54
1:D:148:ASP:OD1	1:D:151:SER:OG	2.23	0.54
1:B:30:GLU:OE2	1:B:75:THR:OG1	2.18	0.54
1:C:164:VAL:HG13	1:C:177:ILE:CG2	2.38	0.54
1:F:91:PHE:O	1:F:94:GLY:N	2.40	0.54
1:B:133:PRO:O	1:B:190:MET:HE2	2.08	0.53
1:C:59:PHE:HA	1:C:253:GLY:O	2.09	0.53
1:F:83:GLY:HA2	1:F:106:VAL:HG21	1.89	0.53
1:D:130:ASP:OD1	1:D:146:TYR:OH	2.25	0.53
1:E:102:SER:HB2	1:E:110:ASP:OD2	2.09	0.53
1:F:186:ASP:O	1:F:190:MET:HG3	2.09	0.53
1:F:268:GLN:HA	1:F:271:ARG:HD2	1.91	0.53
1:F:85:LEU:HD12	1:F:85:LEU:O	2.09	0.53
1:F:215:ARG:HH22	2:F:400:UMP:P	2.31	0.53
1:B:311:MET:HG3	1:B:313:VAL:HG13	1.91	0.53
1:D:30:GLU:HG3	1:D:74:LEU:HD22	1.89	0.53
1:F:51:THR:O	1:F:53:THR:N	2.41	0.53
1:E:263:GLU:O	1:E:267:ILE:HG12	2.09	0.52
1:C:192:LEU:HD12	1:C:193:PRO:CD	2.35	0.52
1:D:286:GLU:HG3	1:D:287:LYS:N	2.25	0.52
1:C:168:ILE:HG23	1:C:203:VAL:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:O	1:D:92:ILE:HG13	2.09	0.52
1:F:292:LYS:HE3	1:F:294:GLU:CG	2.39	0.52
1:A:110:ASP:N	1:A:110:ASP:OD1	2.43	0.52
1:C:190:MET:SD	1:C:194:PRO:HD3	2.50	0.52
1:F:90:TRP:HH2	1:F:131:LEU:HD12	1.75	0.52
1:F:113:GLY:O	1:F:129:GLY:N	2.40	0.52
1:D:174:ASP:OD1	1:D:176:ARG:N	2.37	0.52
1:B:201:PHE:CE1	1:B:210:CYS:HB2	2.46	0.51
1:D:183:ASN:OD1	1:D:185:ARG:N	2.42	0.51
1:F:282:LEU:HD12	1:F:294:GLU:O	2.10	0.51
1:F:304:HIS:HB3	1:F:305:PRO:CD	2.40	0.51
1:C:268:GLN:HG2	1:C:268:GLN:O	2.09	0.51
1:C:90:TRP:NE1	1:C:95:SER:HB3	2.24	0.51
1:F:88:LEU:HD23	1:F:232:LEU:CD2	2.41	0.51
1:F:166:ASP:O	1:F:170:THR:HG23	2.11	0.51
1:E:126:ARG:HD3	1:E:130:ASP:O	2.11	0.51
1:F:187:LEU:HD23	1:F:187:LEU:O	2.10	0.51
1:B:178:ILE:HD13	1:B:200:GLN:HG3	1.93	0.51
1:B:232:LEU:HD12	1:B:232:LEU:C	2.36	0.51
1:A:280:ARG:HB3	1:A:297:GLN:HB3	1.92	0.51
1:E:304:HIS:HB3	1:E:305:PRO:HD2	1.91	0.51
1:F:215:ARG:CZ	2:F:400:UMP:OP2	2.59	0.51
1:C:76:THR:OG1	1:C:268:GLN:NE2	2.34	0.51
1:E:68:ARG:HH22	1:E:247:ASP:CG	2.19	0.51
1:A:187:LEU:CB	1:A:188:PRO:HD3	2.40	0.50
1:E:196:HIS:HB3	1:E:212:LEU:HD11	1.93	0.50
1:C:96:THR:HG22	1:C:134:VAL:HG23	1.93	0.50
1:E:39:HIS:O	1:E:43:CYS:N	2.43	0.50
1:E:123:PHE:O	1:E:126:ARG:HB3	2.11	0.50
1:F:28:HIS:CE1	1:F:31:LEU:HG	2.46	0.50
1:F:259:LEU:HA	1:F:262:ILE:HD11	1.92	0.50
1:C:168:ILE:HG12	1:C:177:ILE:HD13	1.93	0.50
1:C:236:MET:HE2	1:C:296:PHE:CZ	2.47	0.50
1:D:215:ARG:NH2	2:D:400:UMP:OP2	2.42	0.50
1:F:28:HIS:ND1	1:F:28:HIS:O	2.45	0.50
1:A:264:PRO:O	1:A:267:ILE:HB	2.12	0.50
1:D:177:ILE:HG21	1:D:201:PHE:HB2	1.93	0.50
1:D:185:ARG:HG2	1:D:185:ARG:O	2.10	0.50
1:F:163:ARG:O	1:F:167:THR:OG1	2.29	0.50
1:B:56:LEU:HD23	1:B:56:LEU:N	2.26	0.50
1:F:240:ILE:HD11	1:F:291:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ARG:HG3	1:E:50:ARG:HH21	1.75	0.50
1:E:138:GLN:O	1:E:142:PHE:HB2	2.12	0.50
1:E:249:ILE:H	1:E:249:ILE:HD12	1.77	0.50
1:A:285:VAL:HG13	1:A:290:ASP:OD1	2.12	0.49
1:B:32:GLN:O	1:B:36:GLN:HG3	2.12	0.49
1:C:211:GLN:HG3	1:C:249:ILE:HB	1.94	0.49
1:F:140:ARG:NH1	1:F:159:ASP:OD2	2.45	0.49
1:B:90:TRP:CD1	1:B:95:SER:HG	2.30	0.49
1:B:146:TYR:O	1:D:147:ARG:NH2	2.45	0.49
1:C:110:ASP:OD1	1:C:110:ASP:N	2.45	0.49
1:E:249:ILE:HD12	1:E:249:ILE:N	2.27	0.49
1:F:37:ILE:CG2	1:F:269:LEU:HD11	2.37	0.49
1:F:258:TYR:O	1:F:261:HIS:N	2.33	0.49
1:A:285:VAL:HG21	1:A:291:PHE:CE1	2.47	0.49
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.94	0.49
1:C:206:SER:HA	1:C:243:LEU:CD2	2.42	0.49
1:F:85:LEU:HD12	1:F:85:LEU:C	2.37	0.49
1:B:178:ILE:CD1	1:B:200:GLN:HG3	2.43	0.49
1:C:48:ASP:OD2	1:F:46:ARG:NH1	2.39	0.49
1:E:102:SER:HB2	1:E:110:ASP:CG	2.38	0.49
1:F:26:PRO:CB	1:F:27:PRO:HD2	2.43	0.49
1:F:259:LEU:HA	1:F:262:ILE:HG13	1.95	0.49
1:F:90:TRP:CD1	1:F:95:SER:HB3	2.48	0.49
1:F:287:LYS:HE2	1:F:288:ILE:HG22	1.94	0.49
1:A:261:HIS:C	1:A:264:PRO:HD2	2.38	0.49
1:E:187:LEU:N	1:E:188:PRO:CD	2.75	0.49
1:E:48:ASP:HA	1:E:54:GLY:HA2	1.95	0.49
1:E:291:PHE:O	1:E:292:LYS:HE3	2.13	0.49
1:F:81:TRP:CZ2	1:F:298:ILE:HD11	2.48	0.49
1:D:28:HIS:C	1:D:31:LEU:HD13	2.38	0.48
1:B:106:VAL:HG12	1:B:108:ILE:HG12	1.96	0.48
1:C:236:MET:HB3	1:C:291:PHE:CE2	2.48	0.48
1:D:55:THR:HG22	1:D:258:TYR:CD1	2.49	0.48
1:F:107:LYS:HG2	1:F:107:LYS:O	2.13	0.48
1:B:284:LYS:HD2	1:B:285:VAL:N	2.28	0.48
1:F:187:LEU:N	1:F:188:PRO:CD	2.76	0.48
1:F:241:THR:CB	1:F:243:LEU:HD12	2.43	0.48
1:B:161:LEU:O	1:B:161:LEU:HD12	2.13	0.48
1:E:259:LEU:HD23	1:E:262:ILE:HD11	1.94	0.48
1:F:115:ARG:NH1	1:F:126:ARG:O	2.45	0.48
1:F:145:GLU:OE1	1:F:145:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:GLN:HE22	1:F:287:LYS:HE2	1.79	0.48
1:A:205:ASN:O	1:A:206:SER:OG	2.29	0.48
1:B:258:TYR:O	1:B:261:HIS:HB2	2.13	0.48
1:A:99:LYS:HD2	1:A:99:LYS:O	2.13	0.48
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.73	0.48
1:D:223:VAL:HB	1:D:224:PRO:HD3	1.96	0.48
1:E:84:VAL:HG23	1:E:225:PHE:CE1	2.49	0.48
1:F:261:HIS:O	1:F:265:LEU:HB2	2.13	0.48
1:F:292:LYS:CE	1:F:294:GLU:HG2	2.43	0.48
1:D:36:GLN:O	1:D:40:ILE:HG13	2.14	0.47
1:D:218:ASP:HB3	1:D:256:HIS:NE2	2.29	0.47
1:F:163:ARG:HD2	1:F:163:ARG:HA	1.72	0.47
1:F:283:ARG:HE	1:F:292:LYS:HD3	1.79	0.47
1:A:80:PHE:O	1:A:84:VAL:HG23	2.14	0.47
1:F:80:PHE:O	1:F:84:VAL:HG23	2.14	0.47
1:F:292:LYS:O	1:F:293:ALA:HB2	2.14	0.47
1:A:72:PRO:HA	1:A:276:PHE:CE2	2.49	0.47
1:D:212:LEU:HD13	1:D:230:TYR:CE2	2.49	0.47
1:F:177:ILE:HG22	1:F:201:PHE:HB2	1.94	0.47
1:D:223:VAL:O	1:D:227:ILE:HG13	2.14	0.47
1:E:36:GLN:O	1:E:40:ILE:HG13	2.14	0.47
1:F:51:THR:C	1:F:53:THR:H	2.22	0.47
1:F:115:ARG:NH2	1:F:124:SER:HA	2.30	0.47
1:D:117:PHE:O	1:D:120:SER:HB3	2.15	0.47
1:D:263:GLU:O	1:D:267:ILE:HG12	2.14	0.47
1:B:263:GLU:HB2	1:B:264:PRO:HD3	1.95	0.47
1:B:294:GLU:HG2	1:F:152:ASP:OD1	2.14	0.47
1:A:194:PRO:O	1:A:215:ARG:NE	2.45	0.47
1:B:56:LEU:CD2	1:B:259:LEU:HD21	2.44	0.47
1:B:88:LEU:O	1:B:91:PHE:HB2	2.15	0.47
1:E:160:GLN:O	1:E:164:VAL:HG23	2.15	0.47
1:F:100:GLU:O	1:F:103:SER:OG	2.31	0.47
1:E:258:TYR:O	1:E:260:ASN:N	2.48	0.47
1:A:306:THR:HG22	1:A:307:ILE:N	2.29	0.47
1:C:50:ARG:O	1:C:52:GLY:N	2.47	0.47
1:F:27:PRO:HB3	1:F:31:LEU:CB	2.45	0.47
1:F:178:ILE:HG12	1:F:200:GLN:HG3	1.96	0.47
1:A:118:LEU:O	1:A:121:LEU:HB2	2.15	0.47
1:B:286:GLU:HA	1:B:286:GLU:OE1	2.14	0.47
1:C:96:THR:HG22	1:C:134:VAL:HG22	1.96	0.47
1:B:46:ARG:HH11	1:B:46:ARG:HG2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:MET:HG3	1:B:311:MET:O	2.14	0.46
1:E:265:LEU:HD23	1:E:265:LEU:HA	1.73	0.46
1:F:262:ILE:O	1:F:266:LYS:HG3	2.15	0.46
1:A:80:PHE:CE1	1:A:82:LYS:HB3	2.49	0.46
1:D:30:GLU:CD	1:D:75:THR:H	2.21	0.46
1:F:160:GLN:HB3	1:F:179:MET:HG2	1.97	0.46
1:A:49:ASP:OD2	1:A:51:THR:HG23	2.16	0.46
1:C:142:PHE:HE1	1:C:183:ASN:HB2	1.78	0.46
1:F:164:VAL:O	1:F:168:ILE:HG13	2.15	0.46
1:A:152:ASP:OD1	1:A:154:SER:OG	2.33	0.46
1:A:36:GLN:O	1:A:40:ILE:HG13	2.16	0.46
1:B:169:LYS:HE3	1:B:241:THR:HG22	1.96	0.46
1:C:90:TRP:CZ3	1:C:91:PHE:HE1	2.33	0.46
1:D:112:ASN:OD1	1:D:112:ASN:N	2.49	0.46
1:F:90:TRP:NE1	1:F:95:SER:OG	2.48	0.46
1:B:187:LEU:C	1:B:189:LEU:H	2.24	0.46
1:D:160:GLN:O	1:D:164:VAL:HG23	2.16	0.46
1:E:31:LEU:HD12	1:E:31:LEU:N	2.29	0.46
1:F:263:GLU:CB	1:F:264:PRO:HD3	2.35	0.46
1:A:75:THR:HG21	1:A:274:ARG:O	2.16	0.46
1:F:88:LEU:HD11	1:F:233:LEU:HD13	1.98	0.46
1:B:268:GLN:HB2	1:B:307:ILE:CD1	2.45	0.45
1:D:297:GLN:NE2	1:D:299:GLU:OE2	2.47	0.45
1:F:126:ARG:CG	1:F:127:GLU:H	2.29	0.45
1:B:311:MET:O	1:B:313:VAL:N	2.42	0.45
1:D:187:LEU:N	1:D:188:PRO:HD2	2.32	0.45
1:E:164:VAL:HG13	1:E:177:ILE:HG23	1.98	0.45
1:B:195:CYS:SG	2:B:400:UMP:C6	3.09	0.45
1:F:121:LEU:HB2	1:F:123:PHE:CD2	2.51	0.45
1:F:271:ARG:O	1:F:273:PRO:HD3	2.16	0.45
1:A:59:PHE:HA	1:A:253:GLY:O	2.15	0.45
1:A:219:MET:HE3	1:A:255:ALA:CB	2.38	0.45
1:C:215:ARG:HG3	1:C:216:SER:N	2.31	0.45
1:D:71:PHE:HA	1:D:72:PRO:HD2	1.79	0.45
1:E:261:HIS:C	1:E:264:PRO:HD2	2.41	0.45
1:B:235:TYR:CD2	1:B:279:LEU:HD23	2.52	0.45
1:D:198:LEU:HD12	1:D:198:LEU:O	2.15	0.45
1:E:59:PHE:HA	1:E:253:GLY:O	2.17	0.45
1:E:61:MET:HE2	1:E:61:MET:HB3	1.80	0.45
1:F:210:CYS:O	1:F:249:ILE:HD12	2.16	0.45
1:A:221:LEU:CD1	1:A:309:MET:HB2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD12	1:B:208:LEU:HA	1.71	0.45
1:C:221:LEU:HD22	1:C:261:HIS:NE2	2.31	0.45
1:F:287:LYS:HG3	1:F:288:ILE:H	1.82	0.45
1:F:142:PHE:CD1	1:F:142:PHE:C	2.95	0.45
1:F:172:PRO:HB3	1:F:203:VAL:HG11	1.99	0.45
1:B:103:SER:OG	1:B:104:LYS:N	2.50	0.44
1:B:306:THR:HG22	1:B:307:ILE:N	2.32	0.44
1:F:223:VAL:HB	1:F:224:PRO:HD3	2.00	0.44
1:C:171:ASN:N	1:C:172:PRO:CD	2.79	0.44
1:E:207:GLU:HA	1:E:244:LYS:O	2.17	0.44
1:B:62:GLN:HA	1:B:250:HIS:O	2.18	0.44
1:D:46:ARG:HA	1:D:55:THR:O	2.17	0.44
1:E:62:GLN:HA	1:E:250:HIS:O	2.18	0.44
1:B:160:GLN:O	1:B:164:VAL:HG23	2.17	0.44
1:A:115:ARG:NH1	1:A:119:ASP:OD1	2.51	0.44
1:C:108:ILE:HG13	1:C:109:TRP:CD1	2.52	0.44
1:E:69:ASP:O	1:E:70:GLU:HB3	2.17	0.44
1:E:74:LEU:HD12	1:E:224:PRO:HB3	1.98	0.44
1:E:187:LEU:HB2	1:E:188:PRO:HD3	1.99	0.44
1:F:49:ASP:C	1:F:51:THR:H	2.24	0.44
1:A:74:LEU:O	1:A:301:TYR:OH	2.32	0.44
1:C:135:TYR:OH	1:C:195:CYS:N	2.37	0.44
1:C:207:GLU:HA	1:C:244:LYS:O	2.17	0.44
1:D:29:GLY:N	1:D:31:LEU:HD13	2.33	0.44
1:B:206:SER:HA	1:B:243:LEU:CD2	2.48	0.44
1:E:119:ASP:OD1	1:E:124:SER:HB3	2.17	0.44
1:A:268:GLN:O	1:A:268:GLN:HG2	2.18	0.43
1:B:94:GLY:HA2	1:B:136:GLY:O	2.18	0.43
1:C:215:ARG:CZ	2:C:400:UMP:OP1	2.63	0.43
1:F:263:GLU:HA	1:F:263:GLU:OE2	2.17	0.43
1:C:263:GLU:N	1:C:264:PRO:CD	2.81	0.43
1:A:89:LEU:O	1:A:93:LYS:HG3	2.17	0.43
1:C:223:VAL:HB	1:C:224:PRO:HD3	2.00	0.43
1:F:140:ARG:HH11	1:F:140:ARG:CG	2.28	0.43
1:F:223:VAL:N	1:F:224:PRO:CD	2.81	0.43
1:A:223:VAL:HG13	1:A:250:HIS:HE1	1.83	0.43
1:A:283:ARG:NH2	1:A:295:ASP:OD2	2.52	0.43
1:D:223:VAL:N	1:D:224:PRO:CD	2.81	0.43
1:F:292:LYS:HB2	1:F:292:LYS:HE2	1.61	0.43
1:A:68:ARG:HA	1:A:69:ASP:HA	1.68	0.43
1:B:313:VAL:HG23	1:B:313:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:ASP:OD1	1:D:218:ASP:N	2.48	0.43
1:E:25:MET:N	1:E:26:PRO:CD	2.81	0.43
1:A:215:ARG:NH2	2:A:400:UMP:OP1	2.47	0.43
1:C:40:ILE:O	1:C:40:ILE:HG22	2.19	0.43
1:D:51:THR:C	1:D:53:THR:H	2.18	0.43
1:F:28:HIS:HD1	1:F:31:LEU:HG	1.79	0.43
1:F:161:LEU:O	1:F:165:ILE:HG13	2.18	0.43
1:A:71:PHE:O	1:A:73:LEU:N	2.43	0.43
1:F:168:ILE:O	1:F:172:PRO:HG3	2.19	0.43
1:F:219:MET:HE3	1:F:219:MET:HB3	1.74	0.43
1:D:32:GLN:O	1:D:36:GLN:HG3	2.19	0.43
1:E:75:THR:O	1:E:304:HIS:HD2	2.02	0.43
1:F:118:LEU:O	1:F:123:PHE:HB2	2.18	0.43
1:E:102:SER:HB2	1:E:110:ASP:OD1	2.18	0.43
1:B:139:TRP:C	1:B:140:ARG:HG2	2.44	0.43
1:C:88:LEU:O	1:C:92:ILE:HG13	2.19	0.43
1:C:108:ILE:HG12	1:C:108:ILE:H	1.58	0.43
1:E:285:VAL:HG12	1:E:287:LYS:O	2.18	0.43
1:F:232:LEU:HG	1:F:236:MET:HE3	2.01	0.43
1:C:148:ASP:OD1	1:C:151:SER:OG	2.35	0.42
1:D:27:PRO:HB2	1:D:31:LEU:HB2	2.01	0.42
1:E:262:ILE:CG2	1:E:266:LYS:HE3	2.48	0.42
1:C:184:PRO:O	1:C:187:LEU:HB2	2.19	0.42
1:D:108:ILE:HG13	1:D:109:TRP:CD1	2.53	0.42
1:D:218:ASP:HB3	1:D:256:HIS:CD2	2.55	0.42
1:F:31:LEU:HD23	1:F:31:LEU:HA	1.73	0.42
1:A:311:MET:HG2	1:A:313:VAL:HG22	2.02	0.42
1:C:133:PRO:HB3	1:C:146:TYR:CD2	2.55	0.42
1:D:30:GLU:HG2	1:D:30:GLU:O	2.20	0.42
1:D:30:GLU:OE2	1:D:75:THR:N	2.43	0.42
1:F:285:VAL:HG12	1:F:286:GLU:N	2.34	0.42
1:B:168:ILE:HG23	1:B:203:VAL:HG21	2.00	0.42
1:B:259:LEU:HD22	1:B:262:ILE:HD11	2.01	0.42
1:C:285:VAL:CG1	1:C:290:ASP:HB2	2.50	0.42
1:D:177:ILE:O	1:D:177:ILE:HG22	2.20	0.42
1:A:79:VAL:HG12	1:A:80:PHE:N	2.34	0.42
1:B:33:TYR:OH	1:B:219:MET:O	2.33	0.42
1:F:69:ASP:O	1:F:278:LYS:HE3	2.20	0.42
1:A:88:LEU:O	1:A:91:PHE:HB2	2.19	0.42
1:C:267:ILE:HD13	1:C:267:ILE:HA	1.94	0.42
1:D:288:ILE:O	1:D:288:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:SER:C	1:E:156:GLN:H	2.26	0.42
1:F:81:TRP:CH2	1:F:298:ILE:HD11	2.55	0.42
1:A:168:ILE:HG23	1:A:203:VAL:HG21	2.01	0.42
1:A:198:LEU:C	1:A:198:LEU:HD12	2.45	0.42
3:B:401:KI3:C20	3:B:401:KI3:S09	3.08	0.42
1:C:140:ARG:HD2	1:C:159:ASP:OD1	2.19	0.42
1:C:215:ARG:NH1	1:C:216:SER:HB3	2.35	0.42
1:E:89:LEU:O	1:E:93:LYS:HG3	2.20	0.42
1:E:164:VAL:HG13	1:E:177:ILE:CG2	2.48	0.42
1:A:33:TYR:OH	1:A:219:MET:O	2.35	0.42
1:B:216:SER:OG	2:B:400:UMP:H2'	2.20	0.42
1:C:115:ARG:HH22	1:C:124:SER:C	2.28	0.42
1:F:221:LEU:HD12	1:F:221:LEU:HA	1.69	0.42
1:C:263:GLU:CB	1:C:264:PRO:HD3	2.49	0.42
1:D:118:LEU:HD23	1:D:118:LEU:HA	1.95	0.42
1:D:186:ASP:C	1:D:188:PRO:HD2	2.44	0.42
1:A:106:VAL:HG12	1:A:108:ILE:HG12	2.02	0.42
1:A:195:CYS:SG	2:A:400:UMP:C6	3.13	0.42
1:B:118:LEU:O	1:B:121:LEU:N	2.39	0.42
1:E:278:LYS:HE3	1:E:278:LYS:HB3	1.87	0.42
1:C:115:ARG:NH1	1:C:119:ASP:OD1	2.53	0.41
1:A:192:LEU:HD22	1:A:193:PRO:O	2.19	0.41
1:A:211:GLN:HB2	1:A:249:ILE:HB	2.02	0.41
1:C:178:ILE:CG2	1:C:179:MET:N	2.82	0.41
1:F:216:SER:OG	2:F:400:UMP:H2'	2.20	0.41
1:A:139:TRP:CD1	1:A:179:MET:HE2	2.55	0.41
1:D:117:PHE:CD1	1:D:117:PHE:C	2.98	0.41
1:F:33:TYR:O	1:F:36:GLN:HB2	2.20	0.41
1:F:42:ARG:HH11	1:F:42:ARG:CG	2.07	0.41
1:F:112:ASN:OD1	1:F:112:ASN:N	2.53	0.41
1:C:50:ARG:C	1:C:52:GLY:N	2.78	0.41
1:D:27:PRO:CB	1:D:31:LEU:HB2	2.51	0.41
1:D:29:GLY:H	1:D:31:LEU:HD13	1.86	0.41
1:D:249:ILE:N	1:D:249:ILE:HD12	2.35	0.41
1:E:32:GLN:O	1:E:36:GLN:HG3	2.21	0.41
1:F:249:ILE:HD12	1:F:249:ILE:N	2.35	0.41
1:C:168:ILE:HG22	1:C:168:ILE:O	2.20	0.41
1:E:50:ARG:HH21	1:E:50:ARG:CG	2.33	0.41
1:E:56:LEU:HD23	1:E:56:LEU:HA	1.76	0.41
1:F:126:ARG:CG	1:F:127:GLU:N	2.84	0.41
1:A:206:SER:C	1:A:243:LEU:HD22	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASN:N	1:B:172:PRO:HD3	2.34	0.41
1:B:192:LEU:HA	1:B:193:PRO:HD2	1.85	0.41
1:C:193:PRO:HA	1:C:194:PRO:HD3	1.94	0.41
1:D:126:ARG:CD	1:D:130:ASP:HB3	2.48	0.41
1:F:27:PRO:HB3	1:F:31:LEU:HB3	2.02	0.41
1:F:115:ARG:HH21	1:F:124:SER:HA	1.84	0.41
1:F:119:ASP:C	1:F:121:LEU:H	2.29	0.41
1:A:171:ASN:N	1:A:172:PRO:CD	2.84	0.41
1:E:84:VAL:HG13	1:E:229:SER:HA	2.03	0.41
1:F:88:LEU:HD23	1:F:232:LEU:HG	2.02	0.41
1:F:289:ASP:OD1	1:F:289:ASP:N	2.53	0.41
1:A:40:ILE:O	1:A:44:GLY:HA3	2.20	0.41
1:A:263:GLU:CB	1:A:264:PRO:HD3	2.51	0.41
1:A:294:GLU:CD	1:A:294:GLU:H	2.28	0.41
1:B:223:VAL:HG13	1:B:250:HIS:HE1	1.85	0.41
1:D:175:ARG:HH11	1:D:175:ARG:HD2	1.70	0.41
1:D:187:LEU:HB2	1:D:188:PRO:HD3	2.03	0.41
1:E:121:LEU:HB2	1:E:123:PHE:CD2	2.55	0.41
1:E:122:GLY:C	1:E:124:SER:H	2.29	0.41
1:E:263:GLU:N	1:E:264:PRO:CD	2.83	0.41
1:E:282:LEU:O	1:E:283:ARG:HB3	2.20	0.41
1:A:88:LEU:CD2	1:A:232:LEU:HG	2.50	0.41
3:A:401:KI3:C16	3:A:401:KI3:S09	3.09	0.41
1:B:69:ASP:O	1:B:70:GLU:HB3	2.20	0.41
1:B:134:VAL:HG23	1:B:135:TYR:N	2.36	0.41
1:B:138:GLN:OE1	1:B:138:GLN:HA	2.19	0.41
1:B:218:ASP:O	1:B:223:VAL:HG23	2.21	0.41
1:C:90:TRP:HH2	1:C:131:LEU:HD12	1.86	0.41
1:D:286:GLU:HG3	1:D:287:LYS:H	1.86	0.41
1:A:126:ARG:CD	1:A:130:ASP:HB3	2.50	0.40
1:A:232:LEU:HD12	1:A:232:LEU:O	2.21	0.40
1:D:215:ARG:HH22	2:D:400:UMP:P	2.44	0.40
1:E:83:GLY:HA2	1:E:106:VAL:HG21	2.03	0.40
1:F:294:GLU:CD	1:F:294:GLU:N	2.79	0.40
1:A:37:ILE:CD1	1:A:219:MET:HB3	2.52	0.40
1:A:192:LEU:HD23	1:A:193:PRO:HD2	2.03	0.40
1:A:213:TYR:HD2	1:A:251:THR:HG21	1.86	0.40
1:E:108:ILE:HG12	1:E:108:ILE:H	1.65	0.40
1:F:54:GLY:C	1:F:259:LEU:HD12	2.46	0.40
1:F:130:ASP:CG	1:F:149:MET:HG2	2.46	0.40
1:F:259:LEU:HA	1:F:262:ILE:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:ARG:HD2	1:F:299:GLU:OE2	2.21	0.40
1:B:56:LEU:HD23	1:B:259:LEU:HD21	2.03	0.40
1:B:62:GLN:HE21	1:B:251:THR:HG1	1.68	0.40
1:C:30:GLU:OE2	1:C:75:THR:OG1	2.32	0.40
1:D:177:ILE:CG2	1:D:201:PHE:HB2	2.51	0.40
1:E:74:LEU:HD23	1:E:74:LEU:HA	1.78	0.40
1:F:88:LEU:HD23	1:F:232:LEU:HD23	2.04	0.40
1:F:287:LYS:CE	1:F:288:ILE:HG22	2.51	0.40
1:E:142:PHE:CD1	1:E:142:PHE:C	2.99	0.40
1:A:108:ILE:HG12	1:A:108:ILE:H	1.72	0.40
1:F:244:LYS:N	1:F:244:LYS:HD2	2.36	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ARG:NH1	2:F:400:UMP:OP1[6_465]	1.63	0.57
1:E:175:ARG:NH1	2:B:400:UMP:OP3[6_455]	1.77	0.43
1:C:176:ARG:NE	2:F:400:UMP:OP1[6_465]	1.92	0.28
1:C:176:ARG:CZ	2:F:400:UMP:OP1[6_465]	2.00	0.20
1:D:25:MET:O	1:D:42:ARG:NH2[8_665]	2.12	0.08
1:E:25:MET:O	1:F:42:ARG:NH2[8_665]	2.13	0.07
1:F:176:ARG:NH1	2:C:400:UMP:OP2[6_565]	2.15	0.05
1:D:176:ARG:NH1	2:A:400:UMP:OP2[6_555]	2.18	0.02
1:D:175:ARG:NH1	2:A:400:UMP:OP3[6_555]	2.18	0.02

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	287/289 (99%)	266 (93%)	19 (7%)	2 (1%)	18 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	287/289 (99%)	258 (90%)	26 (9%)	3 (1%)	12	41
1	C	279/289 (96%)	258 (92%)	19 (7%)	2 (1%)	18	49
1	D	280/289 (97%)	251 (90%)	22 (8%)	7 (2%)	4	21
1	E	280/289 (97%)	252 (90%)	23 (8%)	5 (2%)	6	28
1	F	279/289 (96%)	246 (88%)	24 (9%)	9 (3%)	3	18
All	All	1692/1734 (98%)	1531 (90%)	133 (8%)	28 (2%)	7	30

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	51	THR
1	E	52	GLY
1	F	293	ALA
1	C	51	THR
1	D	52	GLY
1	D	134	VAL
1	D	305	PRO
1	F	29	GLY
1	F	52	GLY
1	B	134	VAL
1	D	29	GLY
1	D	50	ARG
1	E	50	ARG
1	E	134	VAL
1	F	134	VAL
1	D	168	ILE
1	E	124	SER
1	F	28	HIS
1	F	80	PHE
1	A	72	PRO
1	A	134	VAL
1	B	240	ILE
1	B	312	ALA
1	F	47	LYS
1	F	268	GLN
1	C	134	VAL
1	F	267	ILE
1	D	27	PRO

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	247/252 (98%)	231 (94%)	16 (6%)	15	44
1	B	244/252 (97%)	230 (94%)	14 (6%)	18	49
1	C	234/252 (93%)	223 (95%)	11 (5%)	23	55
1	D	241/252 (96%)	225 (93%)	16 (7%)	15	43
1	E	243/252 (96%)	226 (93%)	17 (7%)	14	41
1	F	237/252 (94%)	216 (91%)	21 (9%)	9	33
All	All	1446/1512 (96%)	1351 (93%)	95 (7%)	15	43

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	69	ASP
1	A	74	LEU
1	A	78	ARG
1	A	99	LYS
1	A	148	ASP
1	A	154	SER
1	A	178	ILE
1	A	187	LEU
1	A	192	LEU
1	A	262	ILE
1	A	266	LYS
1	A	267	ILE
1	A	291	PHE
1	A	310	GLU
1	A	313	VAL
1	B	51	THR
1	B	53	THR
1	B	56	LEU
1	B	57	SER
1	B	74	LEU
1	B	108	ILE

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Mol	Chain	Res	Type
1	B	115	ARG
1	B	145	GLU
1	B	158	VAL
1	B	174	ASP
1	B	206	SER
1	B	221	LEU
1	B	289	ASP
1	B	309	MET
1	C	48	ASP
1	C	50	ARG
1	C	108	ILE
1	C	154	SER
1	C	174	ASP
1	C	192	LEU
1	C	195	CYS
1	C	196	HIS
1	C	212	LEU
1	C	221	LEU
1	C	291	PHE
1	D	38	GLN
1	D	51	THR
1	D	56	LEU
1	D	69	ASP
1	D	78	ARG
1	D	108	ILE
1	D	147	ARG
1	D	154	SER
1	D	167	THR
1	D	175	ARG
1	D	178	ILE
1	D	204	VAL
1	D	221	LEU
1	D	267	ILE
1	D	269	LEU
1	D	294	GLU
1	E	45	VAL
1	E	51	THR
1	E	57	SER
1	E	61	MET
1	E	69	ASP
1	E	77	LYS
1	E	119	ASP

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Mol	Chain	Res	Type
1	E	178	ILE
1	E	195	CYS
1	E	223	VAL
1	E	229	SER
1	E	237	ILE
1	E	278	LYS
1	E	286	GLU
1	E	287	LYS
1	E	289	ASP
1	E	290	ASP
1	F	42	ARG
1	F	43	CYS
1	F	56	LEU
1	F	69	ASP
1	F	85	LEU
1	F	115	ARG
1	F	119	ASP
1	F	164	VAL
1	F	167	THR
1	F	175	ARG
1	F	178	ILE
1	F	179	MET
1	F	185	ARG
1	F	187	LEU
1	F	221	LEU
1	F	265	LEU
1	F	287	LYS
1	F	288	ILE
1	F	289	ASP
1	F	292	LYS
1	F	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	62	GLN
1	C	62	GLN
1	C	141	HIS
1	C	256	HIS
1	D	39	HIS
1	D	62	GLN

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Mol	Chain	Res	Type
1	E	302	ASN
1	F	62	GLN
1	F	138	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
3	KI3	B	401	-	22,22,22	1.38	4 (18%)	31,32,32	3.37	11 (35%)
2	UMP	A	400	-	21,21,21	2.84	15 (71%)	30,31,31	2.45	12 (40%)
2	UMP	D	400	-	21,21,21	2.84	15 (71%)	30,31,31	2.44	11 (36%)
3	KI3	E	401	-	22,22,22	1.41	4 (18%)	31,32,32	3.25	14 (45%)
2	UMP	F	400	-	21,21,21	2.84	15 (71%)	30,31,31	2.45	12 (40%)
3	KI3	A	401	-	22,22,22	1.39	4 (18%)	31,32,32	3.28	11 (35%)
2	UMP	C	400	-	21,21,21	2.84	15 (71%)	30,31,31	2.45	12 (40%)
2	UMP	B	400	-	21,21,21	2.84	15 (71%)	30,31,31	2.44	12 (40%)
2	UMP	E	400	-	21,21,21	2.84	15 (71%)	30,31,31	2.45	12 (40%)

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
3	KI3	B	401	-	-	0/8/8/8	0/3/3/3
2	UMP	A	400	-	-	7/10/22/22	0/2/2/2
2	UMP	D	400	-	-	7/10/22/22	0/2/2/2
3	KI3	E	401	-	-	0/8/8/8	0/3/3/3
2	UMP	F	400	-	-	7/10/22/22	0/2/2/2
3	KI3	A	401	-	-	0/8/8/8	0/3/3/3
2	UMP	C	400	-	-	7/10/22/22	0/2/2/2
2	UMP	B	400	-	-	7/10/22/22	0/2/2/2
2	UMP	E	400	-	-	7/10/22/22	0/2/2/2

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	UMP	C2'-C3'	-5.01	1.40	1.52
2	E	400	UMP	C2'-C3'	-4.98	1.40	1.52
2	F	400	UMP	C2'-C3'	-4.97	1.40	1.52
2	B	400	UMP	C2'-C3'	-4.96	1.40	1.52
2	D	400	UMP	C2'-C3'	-4.96	1.40	1.52
2	A	400	UMP	C2'-C3'	-4.94	1.40	1.52
2	C	400	UMP	C6-C5	4.53	1.45	1.35
2	B	400	UMP	C6-C5	4.52	1.45	1.35
2	F	400	UMP	C6-C5	4.51	1.45	1.35
2	E	400	UMP	C6-C5	4.50	1.45	1.35
2	A	400	UMP	C6-C5	4.49	1.45	1.35
2	D	400	UMP	C6-C5	4.48	1.45	1.35
2	D	400	UMP	C3'-C4'	-4.04	1.42	1.53
2	C	400	UMP	C3'-C4'	-4.02	1.42	1.53
2	E	400	UMP	C3'-C4'	-4.01	1.42	1.53
2	A	400	UMP	C3'-C4'	-4.01	1.42	1.53
2	F	400	UMP	C3'-C4'	-4.00	1.42	1.53
2	B	400	UMP	C3'-C4'	-4.00	1.42	1.53
2	D	400	UMP	O2-C2	-3.52	1.16	1.23
2	E	400	UMP	O2-C2	-3.50	1.16	1.23
2	A	400	UMP	O2-C2	-3.47	1.16	1.23
2	F	400	UMP	O2-C2	-3.47	1.16	1.23
2	C	400	UMP	O2-C2	-3.46	1.16	1.23
2	B	400	UMP	O2-C2	-3.45	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	KI3	C11-N12	3.43	1.42	1.35
3	B	401	KI3	C11-N12	3.37	1.42	1.35
2	E	400	UMP	P-O5'	-3.29	1.49	1.60
2	B	400	UMP	P-O5'	-3.28	1.49	1.60
2	D	400	UMP	P-O5'	-3.28	1.50	1.60
2	F	400	UMP	P-O5'	-3.28	1.50	1.60
2	C	400	UMP	P-O5'	-3.28	1.50	1.60
2	A	400	UMP	P-O5'	-3.25	1.50	1.60
3	A	401	KI3	C11-N12	3.18	1.41	1.35
2	B	400	UMP	C2'-C1'	-3.11	1.43	1.52
2	D	400	UMP	C2'-C1'	-3.09	1.44	1.52
2	C	400	UMP	C2'-C1'	-3.08	1.44	1.52
2	A	400	UMP	C2'-C1'	-3.07	1.44	1.52
2	E	400	UMP	C2'-C1'	-3.07	1.44	1.52
2	F	400	UMP	C2'-C1'	-3.06	1.44	1.52
2	E	400	UMP	O4-C4	-3.01	1.18	1.24
2	A	400	UMP	O4-C4	-3.00	1.18	1.24
2	C	400	UMP	O4-C4	-2.99	1.18	1.24
2	B	400	UMP	O4-C4	-2.98	1.18	1.24
2	D	400	UMP	O4-C4	-2.96	1.18	1.24
2	F	400	UMP	O4-C4	-2.95	1.18	1.24
2	B	400	UMP	O3'-C3'	-2.93	1.37	1.43
2	F	400	UMP	O3'-C3'	-2.93	1.37	1.43
2	A	400	UMP	O3'-C3'	-2.90	1.37	1.43
2	D	400	UMP	O3'-C3'	-2.90	1.37	1.43
2	E	400	UMP	O3'-C3'	-2.89	1.37	1.43
2	C	400	UMP	O3'-C3'	-2.89	1.37	1.43
2	D	400	UMP	P-OP3	-2.86	1.44	1.54
2	C	400	UMP	P-OP3	-2.84	1.44	1.54
2	F	400	UMP	P-OP3	-2.84	1.44	1.54
2	E	400	UMP	P-OP3	-2.84	1.44	1.54
2	F	400	UMP	C2-N3	2.84	1.42	1.38
2	A	400	UMP	P-OP3	-2.84	1.44	1.54
2	C	400	UMP	C2-N3	2.82	1.42	1.38
2	A	400	UMP	O5'-C5'	-2.82	1.33	1.44
2	B	400	UMP	P-OP3	-2.82	1.44	1.54
2	A	400	UMP	C2-N3	2.81	1.42	1.38
2	B	400	UMP	C2-N3	2.81	1.42	1.38
2	C	400	UMP	O5'-C5'	-2.81	1.33	1.44
2	F	400	UMP	O5'-C5'	-2.81	1.34	1.44
2	D	400	UMP	C2-N3	2.80	1.42	1.38
2	E	400	UMP	C2-N3	2.80	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	KI3	C06-C11	-2.79	1.42	1.45
2	E	400	UMP	O5'-C5'	-2.79	1.34	1.44
2	B	400	UMP	O5'-C5'	-2.79	1.34	1.44
2	D	400	UMP	O5'-C5'	-2.78	1.34	1.44
2	A	400	UMP	O4'-C4'	-2.78	1.38	1.45
2	C	400	UMP	O4'-C4'	-2.76	1.38	1.45
2	D	400	UMP	O4'-C4'	-2.74	1.38	1.45
2	E	400	UMP	O4'-C4'	-2.73	1.38	1.45
2	F	400	UMP	O4'-C4'	-2.73	1.38	1.45
2	B	400	UMP	O4'-C4'	-2.72	1.38	1.45
2	B	400	UMP	P-OP2	-2.55	1.45	1.54
2	A	400	UMP	P-OP2	-2.54	1.45	1.54
2	C	400	UMP	P-OP2	-2.53	1.45	1.54
3	E	401	KI3	C06-C04	2.47	1.44	1.40
3	E	401	KI3	C07-N08	2.44	1.36	1.33
2	D	400	UMP	C2-N1	2.39	1.42	1.38
2	D	400	UMP	P-OP2	-2.37	1.46	1.54
2	F	400	UMP	P-OP2	-2.37	1.46	1.54
2	E	400	UMP	P-OP2	-2.37	1.46	1.54
2	C	400	UMP	C2-N1	2.36	1.42	1.38
2	A	400	UMP	C2-N1	2.35	1.42	1.38
2	B	400	UMP	C2-N1	2.33	1.42	1.38
2	E	400	UMP	C2-N1	2.32	1.42	1.38
2	F	400	UMP	C2-N1	2.32	1.42	1.38
3	B	401	KI3	C06-C04	2.32	1.43	1.40
3	A	401	KI3	C06-C04	2.30	1.43	1.40
3	A	401	KI3	C06-C07	-2.30	1.37	1.40
3	A	401	KI3	C06-C11	-2.24	1.43	1.45
2	A	400	UMP	O4'-C1'	-2.15	1.37	1.42
2	B	400	UMP	O4'-C1'	-2.14	1.37	1.42
3	B	401	KI3	C06-C07	-2.14	1.38	1.40
2	C	400	UMP	O4'-C1'	-2.14	1.37	1.42
2	E	400	UMP	O4'-C1'	-2.13	1.37	1.42
2	D	400	UMP	O4'-C1'	-2.13	1.37	1.42
2	F	400	UMP	O4'-C1'	-2.12	1.37	1.42
3	B	401	KI3	C07-N08	2.02	1.36	1.33

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	KI3	C07-S09-C10	8.64	97.65	90.54
2	F	400	UMP	C2'-C1'-N1	8.58	135.26	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	UMP	C2'-C1'-N1	8.57	135.24	113.81
2	B	400	UMP	C2'-C1'-N1	8.57	135.23	113.81
2	E	400	UMP	C2'-C1'-N1	8.56	135.22	113.81
2	A	400	UMP	C2'-C1'-N1	8.55	135.20	113.81
2	D	400	UMP	C2'-C1'-N1	8.55	135.20	113.81
3	A	401	KI3	C07-S09-C10	8.43	97.47	90.54
3	E	401	KI3	C06-C07-N08	-7.61	120.01	126.44
3	E	401	KI3	S09-C07-N08	7.47	132.94	121.69
3	B	401	KI3	S09-C07-N08	7.14	132.44	121.69
3	B	401	KI3	C11-C10-S09	-7.05	106.12	112.74
3	A	401	KI3	C11-C10-S09	-6.94	106.23	112.74
3	A	401	KI3	S09-C07-N08	6.91	132.10	121.69
3	E	401	KI3	C07-S09-C10	6.58	95.96	90.54
3	B	401	KI3	C06-C07-N08	-6.04	121.33	126.44
3	A	401	KI3	C06-C07-N08	-5.85	121.49	126.44
3	E	401	KI3	C11-C10-S09	-5.85	107.25	112.74
3	B	401	KI3	C07-C06-C11	5.15	114.51	111.29
3	B	401	KI3	C06-C07-S09	-5.01	106.23	112.40
3	A	401	KI3	C06-C11-C10	4.93	115.61	112.09
3	A	401	KI3	C06-C07-S09	-4.87	106.41	112.40
3	E	401	KI3	C06-C11-C10	4.84	115.55	112.09
3	A	401	KI3	C07-C06-C11	4.79	114.28	111.29
3	B	401	KI3	C06-C11-C10	4.76	115.49	112.09
3	E	401	KI3	C07-C06-C11	4.64	114.19	111.29
3	B	401	KI3	C02-N08-C07	4.61	121.29	117.15
3	E	401	KI3	C02-N08-C07	4.56	121.25	117.15
3	E	401	KI3	C06-C07-S09	-4.35	107.05	112.40
3	A	401	KI3	C02-N08-C07	4.22	120.94	117.15
3	E	401	KI3	C10-C11-N12	-4.00	118.74	124.01
3	B	401	KI3	C10-C11-N12	-3.58	119.29	124.01
3	A	401	KI3	C10-C11-N12	-3.52	119.38	124.01
2	A	400	UMP	O4'-C1'-N1	3.50	114.07	107.86
2	E	400	UMP	O4'-C1'-N1	3.47	114.03	107.86
2	C	400	UMP	O4'-C1'-N1	3.47	114.02	107.86
2	F	400	UMP	O4'-C1'-N1	3.46	114.00	107.86
2	D	400	UMP	O4'-C1'-N1	3.45	113.99	107.86
2	B	400	UMP	O4'-C1'-N1	3.44	113.97	107.86
3	A	401	KI3	C11-C10-C13	3.19	127.30	124.43
2	D	400	UMP	OP2-P-O5'	3.09	114.72	106.67
2	E	400	UMP	OP2-P-O5'	3.09	114.72	106.67
2	F	400	UMP	OP2-P-O5'	3.06	114.66	106.67
2	C	400	UMP	O5'-P-OP1	3.06	114.70	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	UMP	O5'-P-OP1	3.05	114.68	106.44
2	A	400	UMP	O5'-P-OP1	3.03	114.62	106.44
2	C	400	UMP	N3-C2-N1	2.99	118.78	114.89
2	B	400	UMP	N3-C2-N1	2.98	118.77	114.89
2	E	400	UMP	N3-C2-N1	2.97	118.75	114.89
2	F	400	UMP	N3-C2-N1	2.96	118.75	114.89
2	A	400	UMP	N3-C2-N1	2.96	118.75	114.89
2	F	400	UMP	O5'-C5'-C4'	2.95	119.02	108.99
2	A	400	UMP	O5'-C5'-C4'	2.95	119.02	108.99
2	E	400	UMP	O5'-C5'-C4'	2.93	118.99	108.99
2	C	400	UMP	O5'-C5'-C4'	2.93	118.98	108.99
2	B	400	UMP	O5'-C5'-C4'	2.93	118.96	108.99
2	D	400	UMP	O5'-C5'-C4'	2.93	118.95	108.99
2	B	400	UMP	OP2-P-O5'	2.92	114.29	106.67
2	A	400	UMP	OP2-P-O5'	2.91	114.27	106.67
2	C	400	UMP	OP2-P-O5'	2.91	114.26	106.67
2	D	400	UMP	N3-C2-N1	2.91	118.67	114.89
2	E	400	UMP	O5'-P-OP1	2.90	114.27	106.44
2	F	400	UMP	O5'-P-OP1	2.89	114.26	106.44
2	D	400	UMP	O5'-P-OP1	2.88	114.22	106.44
2	C	400	UMP	C1'-N1-C2	2.84	123.22	117.66
2	A	400	UMP	C1'-N1-C2	2.84	123.21	117.66
2	E	400	UMP	C1'-N1-C2	2.83	123.19	117.66
2	F	400	UMP	C1'-N1-C2	2.83	123.19	117.66
2	B	400	UMP	C1'-N1-C2	2.82	123.18	117.66
2	D	400	UMP	C1'-N1-C2	2.81	123.15	117.66
3	E	401	KI3	C05-C04-C06	2.80	125.35	121.67
3	B	401	KI3	C11-C10-C13	2.72	126.88	124.43
2	C	400	UMP	O2-C2-N1	-2.64	119.36	122.80
2	A	400	UMP	O2-C2-N1	-2.64	119.36	122.80
2	E	400	UMP	O2-C2-N1	-2.64	119.36	122.80
2	B	400	UMP	O2-C2-N1	-2.63	119.38	122.80
2	D	400	UMP	O2-C2-N1	-2.61	119.39	122.80
2	F	400	UMP	O2-C2-N1	-2.60	119.42	122.80
3	A	401	KI3	C05-C04-C06	2.59	125.08	121.67
3	B	401	KI3	C05-C04-C06	2.55	125.03	121.67
2	E	400	UMP	C3'-C2'-C1'	2.55	108.83	102.60
2	B	400	UMP	C3'-C2'-C1'	2.54	108.82	102.60
2	C	400	UMP	C3'-C2'-C1'	2.54	108.82	102.60
2	F	400	UMP	C3'-C2'-C1'	2.54	108.82	102.60
2	A	400	UMP	C3'-C2'-C1'	2.54	108.80	102.60
2	D	400	UMP	C3'-C2'-C1'	2.53	108.80	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	400	UMP	O4-C4-C5	-2.43	120.97	125.16
2	A	400	UMP	O4-C4-C5	-2.43	120.98	125.16
2	D	400	UMP	O4-C4-C5	-2.42	120.98	125.16
2	C	400	UMP	O4-C4-C5	-2.42	120.99	125.16
2	E	400	UMP	O4-C4-C5	-2.41	121.00	125.16
2	B	400	UMP	O4-C4-C5	-2.40	121.02	125.16
3	E	401	KI3	C04-C06-C07	2.36	119.34	117.75
3	E	401	KI3	C05-C04-C03	-2.11	115.86	119.57
2	B	400	UMP	OP3-P-O5'	-2.06	101.29	106.67
2	A	400	UMP	OP3-P-O5'	-2.06	101.29	106.67
2	E	400	UMP	OP3-P-O5'	-2.06	101.30	106.67
2	F	400	UMP	OP3-P-O5'	-2.06	101.30	106.67
2	F	400	UMP	C5-C4-N3	2.05	117.68	114.80
2	C	400	UMP	C5-C4-N3	2.05	117.67	114.80
2	C	400	UMP	OP3-P-O5'	-2.05	101.31	106.67
2	D	400	UMP	OP3-P-O5'	-2.05	101.33	106.67
2	A	400	UMP	C5-C4-N3	2.03	117.64	114.80
3	E	401	KI3	C13-C10-S09	2.03	128.11	119.41
2	B	400	UMP	C5-C4-N3	2.02	117.62	114.80
2	E	400	UMP	C5-C4-N3	2.01	117.61	114.80
3	E	401	KI3	C20-C15-C16	2.01	121.12	118.57

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	UMP	C5'-O5'-P-OP2
2	A	400	UMP	C5'-O5'-P-OP3
2	B	400	UMP	C5'-O5'-P-OP2
2	B	400	UMP	C5'-O5'-P-OP3
2	C	400	UMP	C5'-O5'-P-OP2
2	C	400	UMP	C5'-O5'-P-OP3
2	D	400	UMP	C5'-O5'-P-OP2
2	D	400	UMP	C5'-O5'-P-OP3
2	E	400	UMP	C5'-O5'-P-OP2
2	E	400	UMP	C5'-O5'-P-OP3
2	F	400	UMP	C5'-O5'-P-OP2
2	F	400	UMP	C5'-O5'-P-OP3
2	D	400	UMP	C5'-O5'-P-OP1
2	E	400	UMP	C5'-O5'-P-OP1
2	F	400	UMP	C5'-O5'-P-OP1
2	A	400	UMP	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
2	B	400	UMP	C2'-C1'-N1-C2
2	C	400	UMP	C2'-C1'-N1-C2
2	D	400	UMP	C2'-C1'-N1-C2
2	E	400	UMP	C2'-C1'-N1-C2
2	F	400	UMP	C2'-C1'-N1-C2
2	A	400	UMP	C3'-C4'-C5'-O5'
2	B	400	UMP	C3'-C4'-C5'-O5'
2	C	400	UMP	C3'-C4'-C5'-O5'
2	D	400	UMP	C3'-C4'-C5'-O5'
2	E	400	UMP	C3'-C4'-C5'-O5'
2	F	400	UMP	C3'-C4'-C5'-O5'
2	A	400	UMP	O4'-C4'-C5'-O5'
2	B	400	UMP	O4'-C4'-C5'-O5'
2	C	400	UMP	O4'-C4'-C5'-O5'
2	D	400	UMP	O4'-C4'-C5'-O5'
2	F	400	UMP	O4'-C4'-C5'-O5'
2	E	400	UMP	O4'-C4'-C5'-O5'
2	A	400	UMP	C5'-O5'-P-OP1
2	B	400	UMP	C5'-O5'-P-OP1
2	C	400	UMP	C5'-O5'-P-OP1
2	A	400	UMP	C2'-C1'-N1-C6
2	B	400	UMP	C2'-C1'-N1-C6
2	C	400	UMP	C2'-C1'-N1-C6
2	E	400	UMP	C2'-C1'-N1-C6
2	F	400	UMP	C2'-C1'-N1-C6
2	D	400	UMP	C2'-C1'-N1-C6

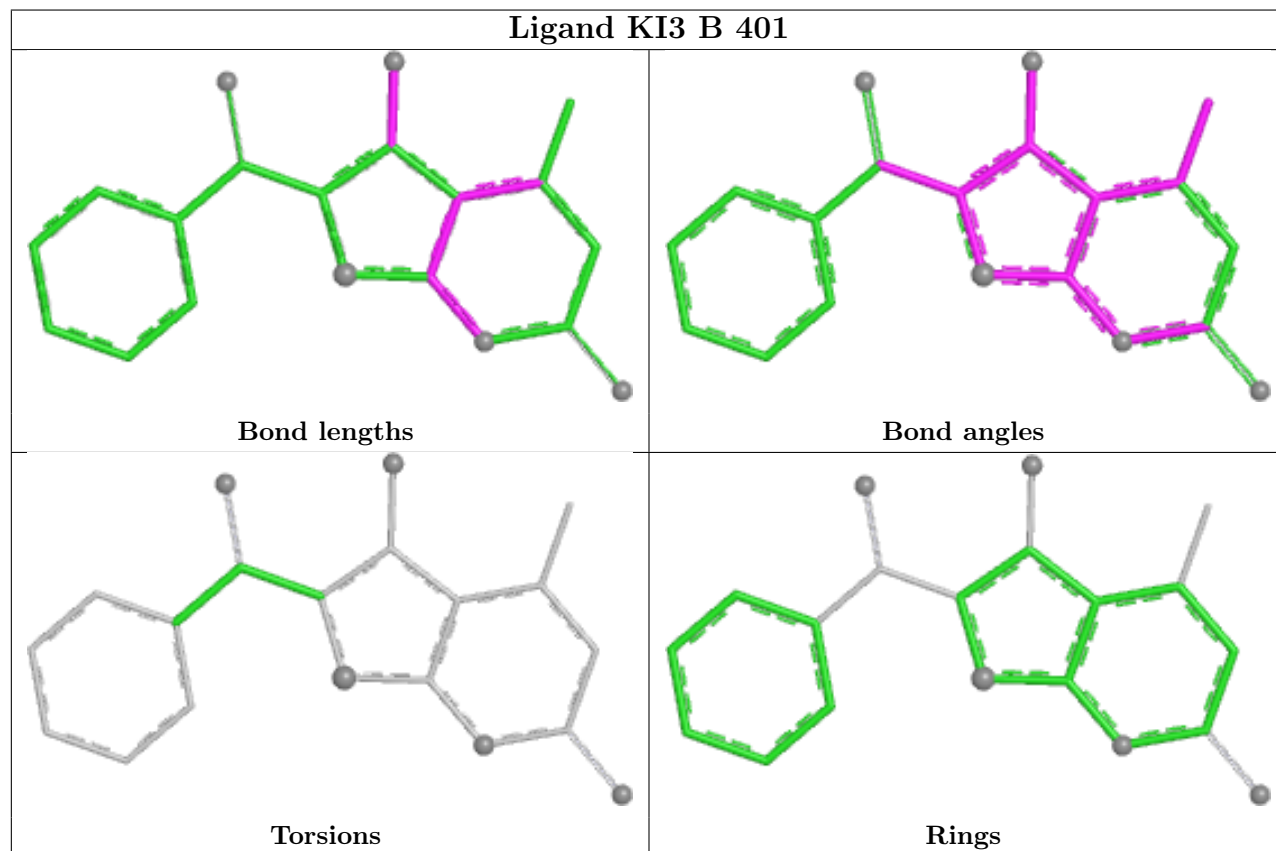
There are no ring outliers.

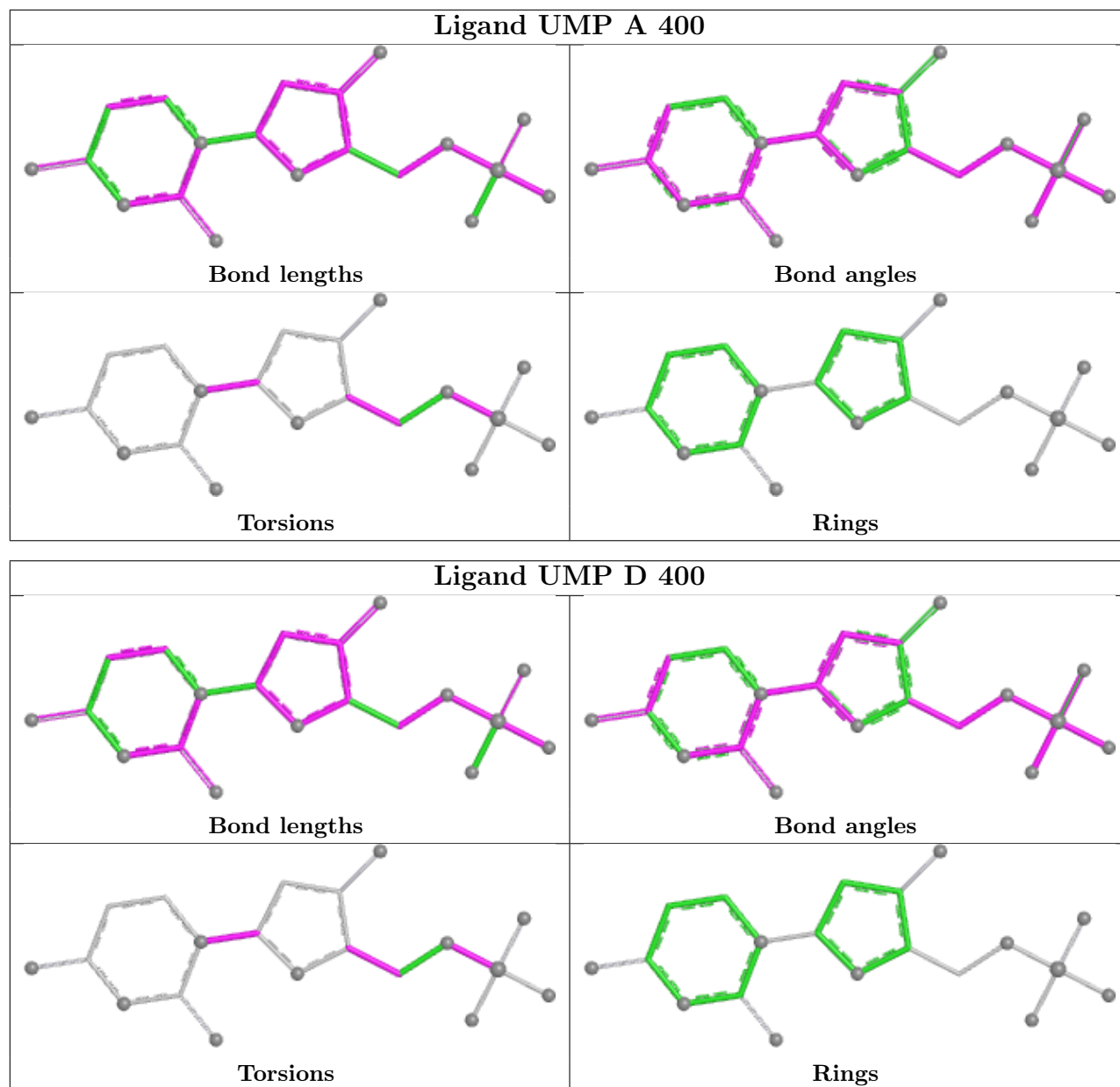
8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	KI3	1	0
2	A	400	UMP	2	2
2	D	400	UMP	3	0
2	F	400	UMP	5	3
3	A	401	KI3	1	0
2	C	400	UMP	2	1
2	B	400	UMP	2	1
2	E	400	UMP	1	0

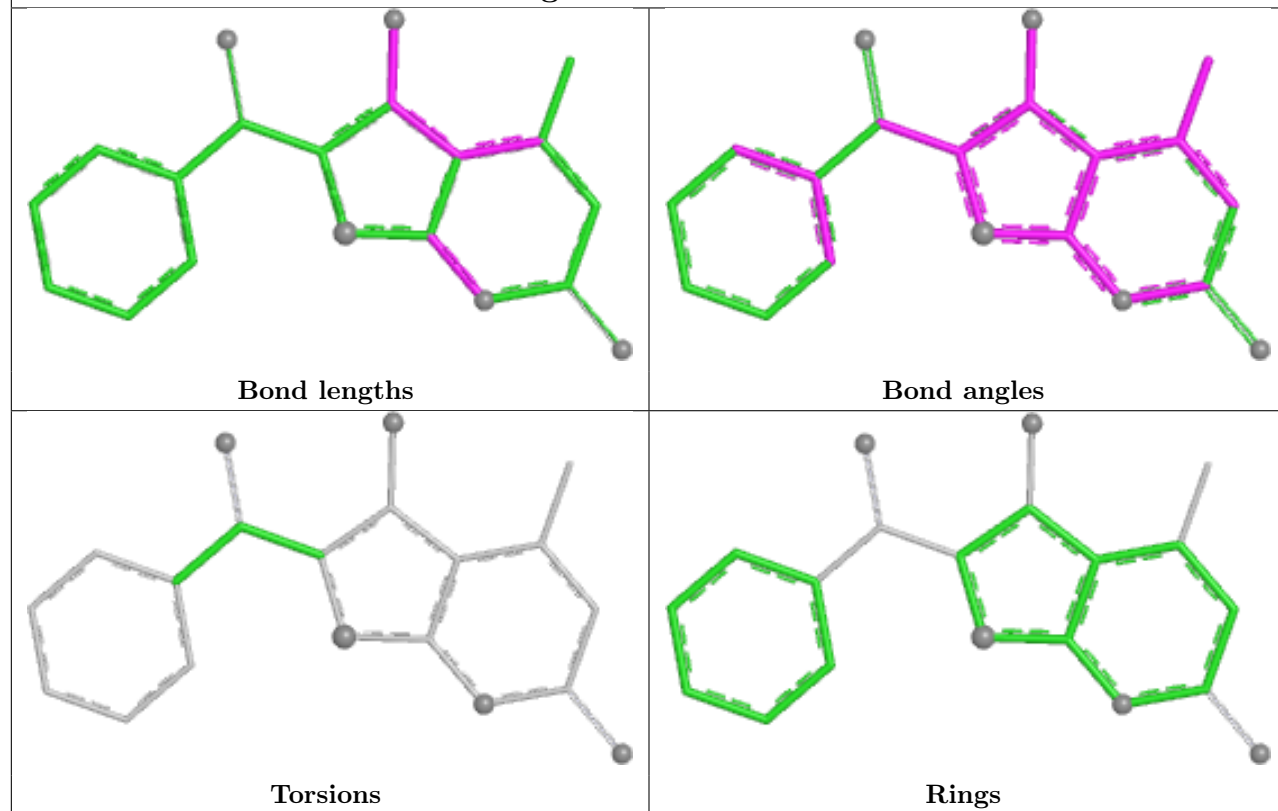
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

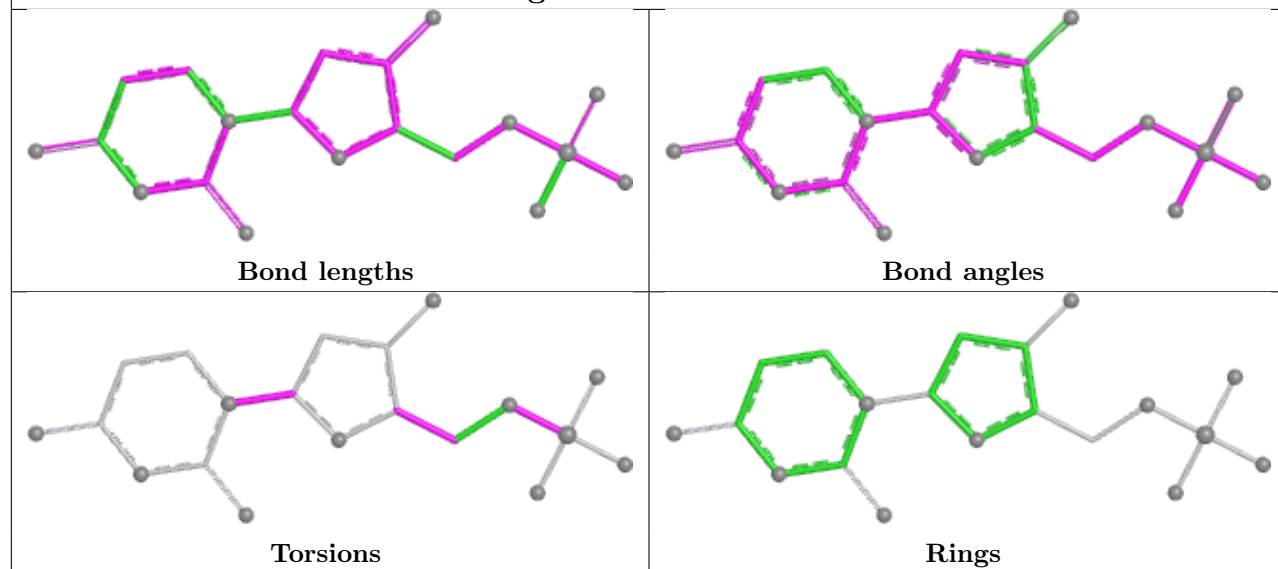




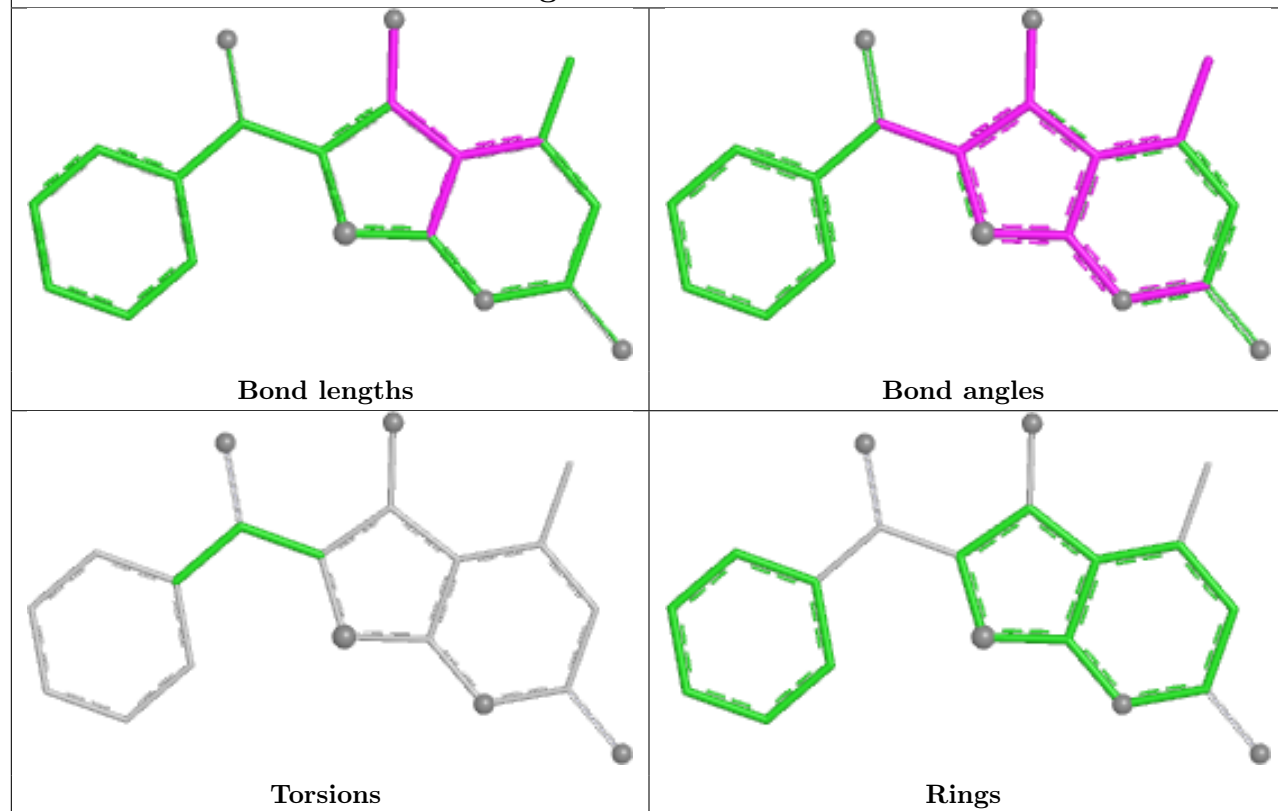
Ligand KI3 E 401



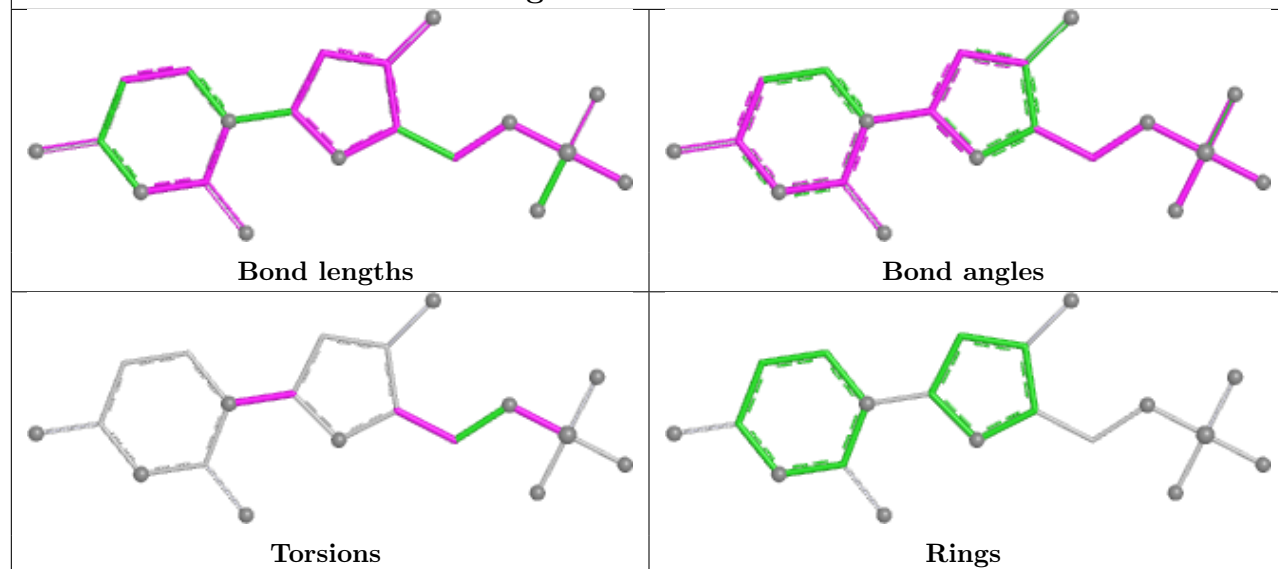
Ligand UMP F 400

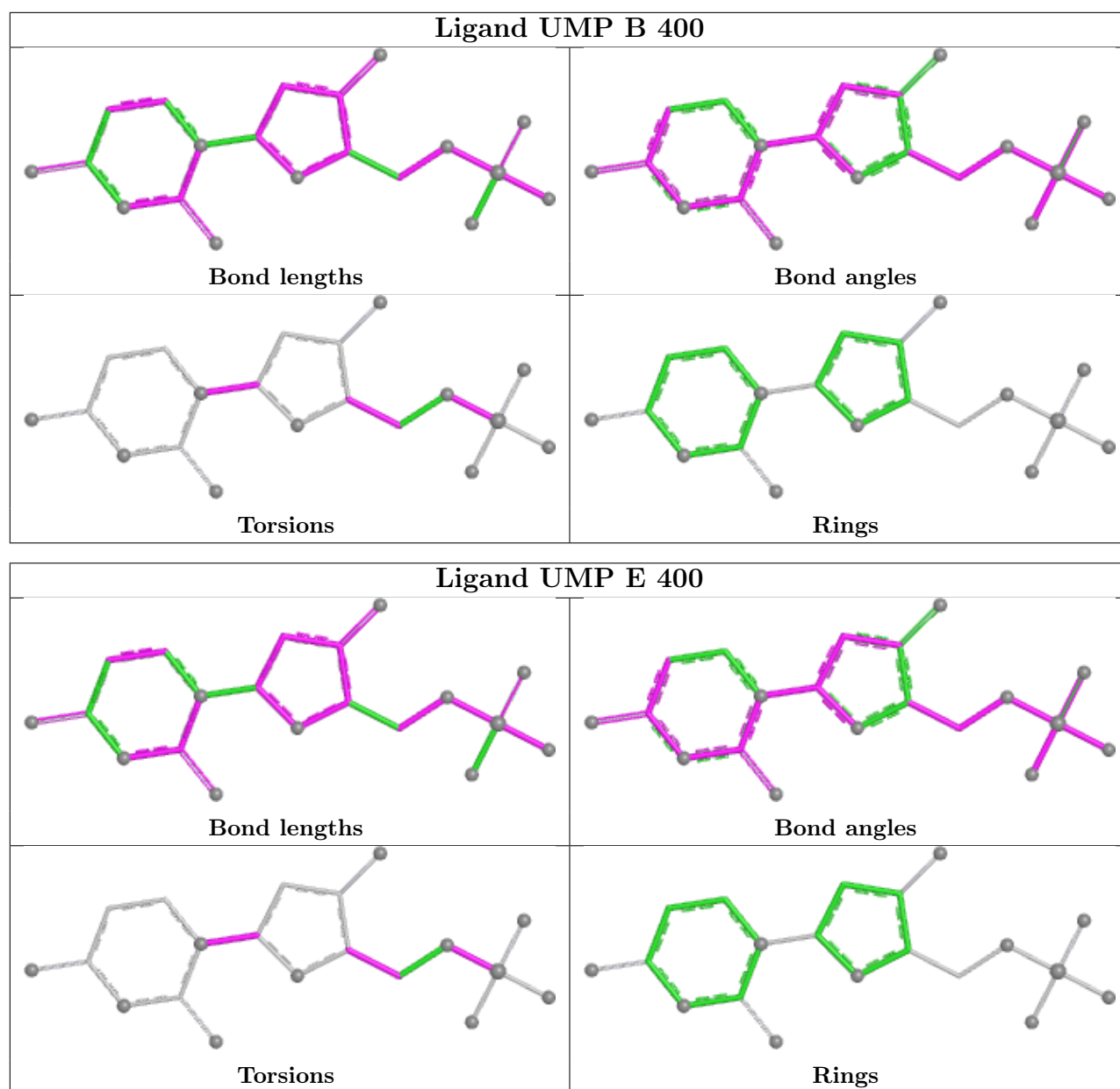


Ligand KI3 A 401



Ligand UMP C 400





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	289/289 (100%)	-0.69	0 100 100	26, 39, 56, 67	0
1	B	289/289 (100%)	-0.72	0 100 100	28, 44, 59, 73	0
1	C	281/289 (97%)	-0.66	0 100 100	31, 45, 62, 80	0
1	D	282/289 (97%)	-0.62	0 100 100	25, 42, 63, 82	0
1	E	282/289 (97%)	-0.65	0 100 100	28, 44, 68, 81	0
1	F	281/289 (97%)	-0.50	0 100 100	33, 49, 71, 86	0
All	All	1704/1734 (98%)	-0.64	0 100 100	25, 44, 65, 86	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

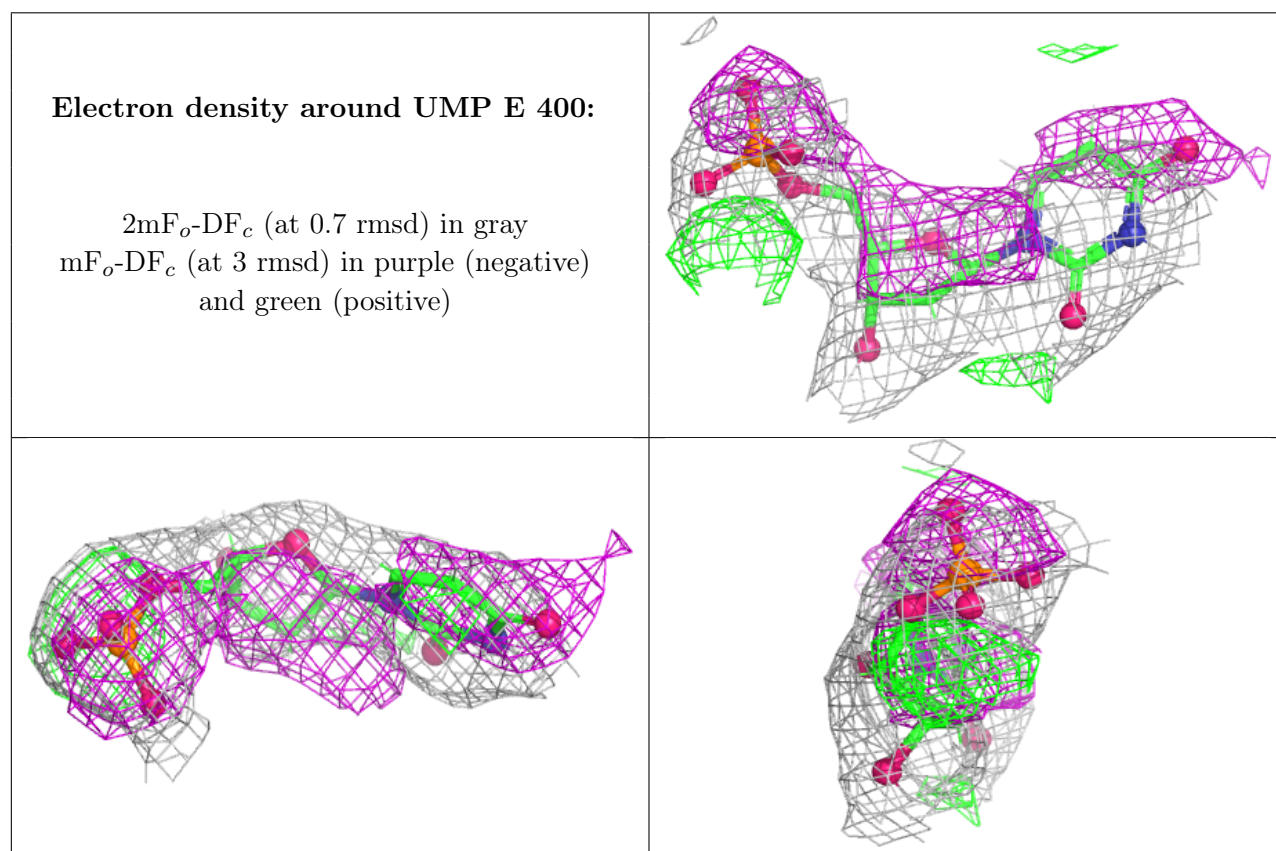
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	UMP	E	400	20/20	0.73	0.13	34,40,48,49	0

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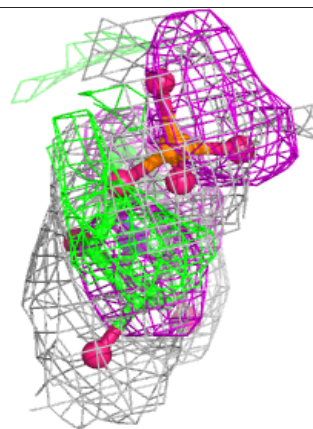
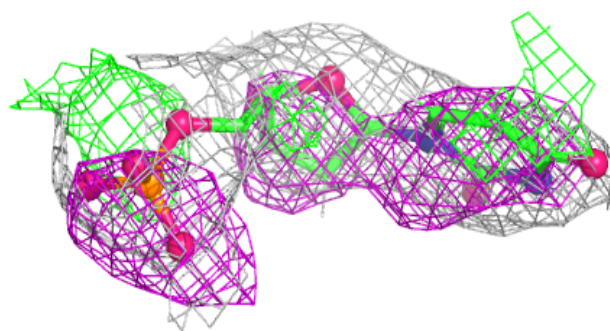
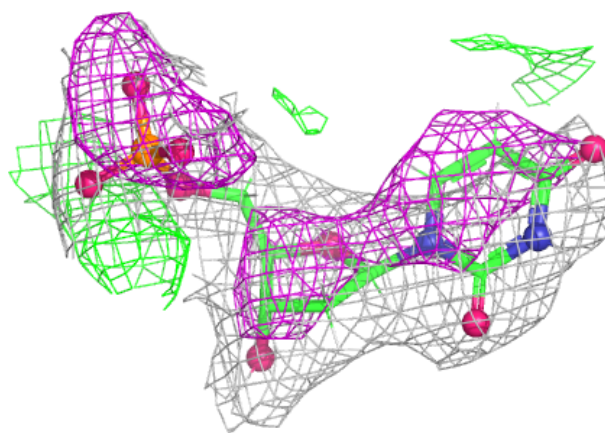
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UMP	F	400	20/20	0.78	0.12	34,40,48,49	0
2	UMP	C	400	20/20	0.79	0.12	34,40,48,49	0
2	UMP	D	400	20/20	0.81	0.13	34,40,48,49	0
3	KI3	E	401	20/20	0.81	0.11	51,61,80,85	0
3	KI3	B	401	20/20	0.92	0.07	43,52,59,64	0
2	UMP	B	400	20/20	0.92	0.08	34,40,48,49	0
3	KI3	A	401	20/20	0.94	0.07	36,47,58,69	0
2	UMP	A	400	20/20	0.97	0.06	34,40,48,49	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.



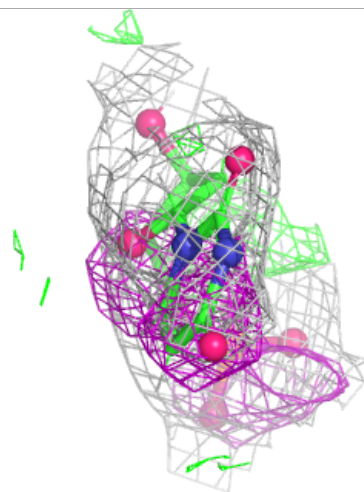
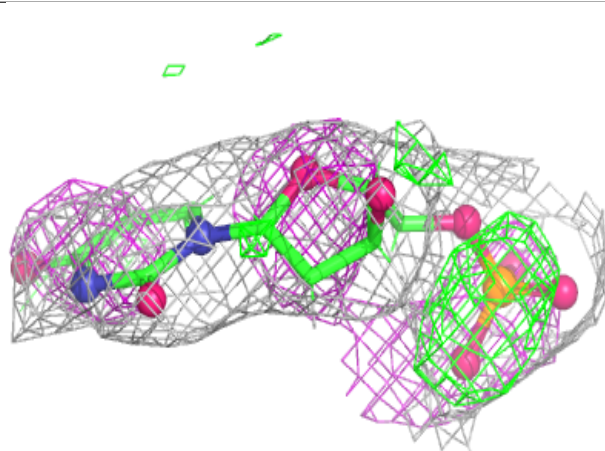
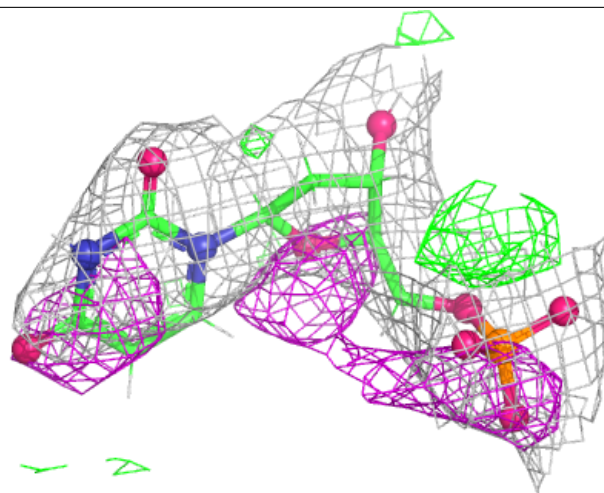
Electron density around UMP F 400:

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



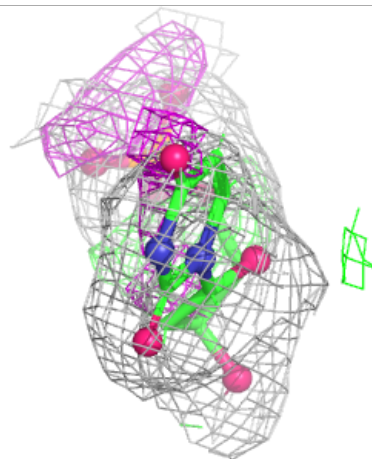
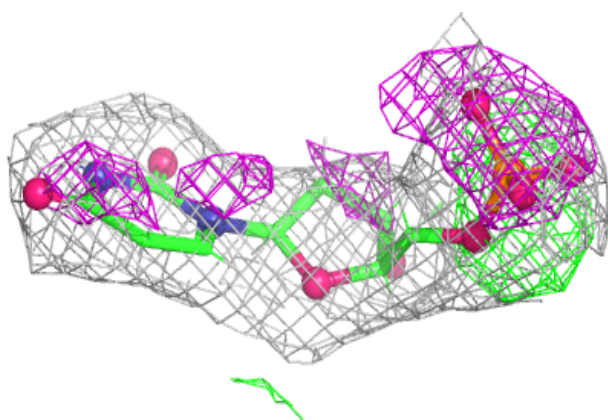
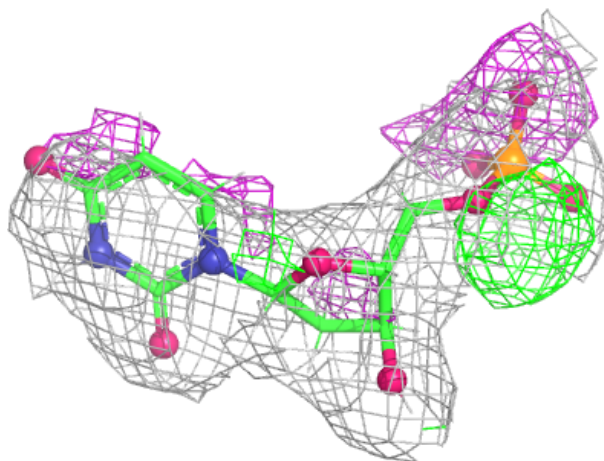
Electron density around UMP C 400:

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



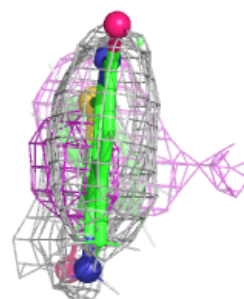
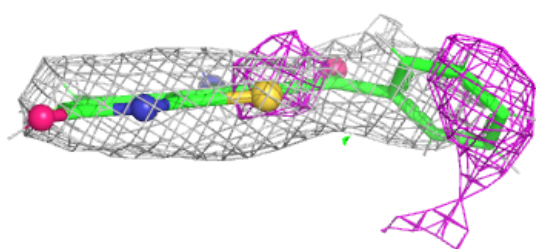
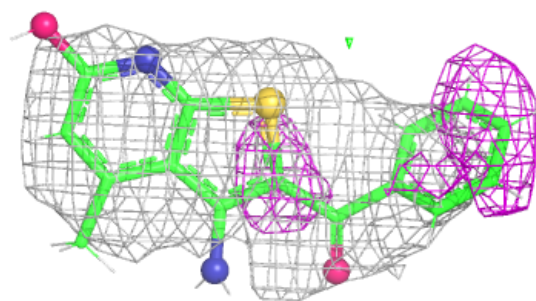
Electron density around UMP D 400:

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

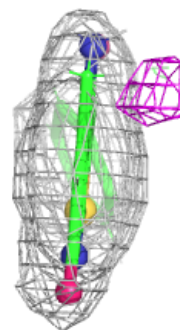
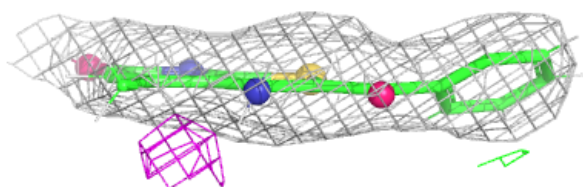
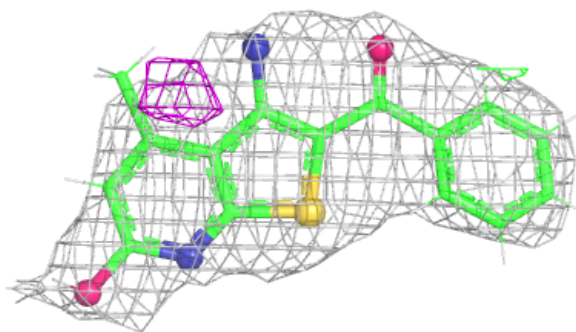


Electron density around KI3 E 401:

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

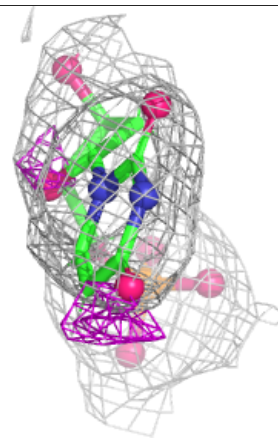
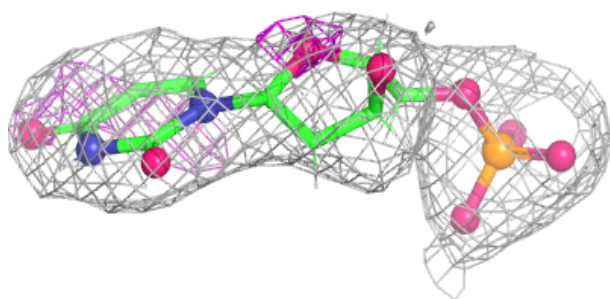
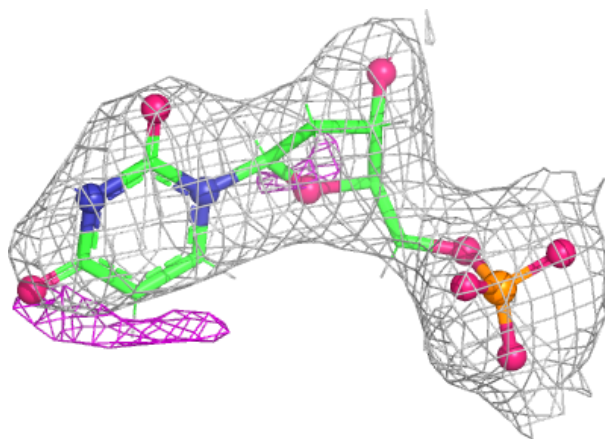
**Electron density around KI3 B 401:**

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



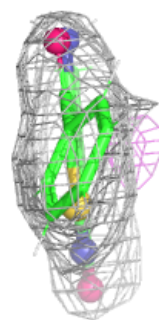
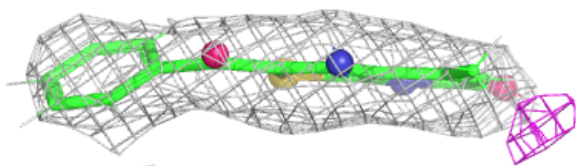
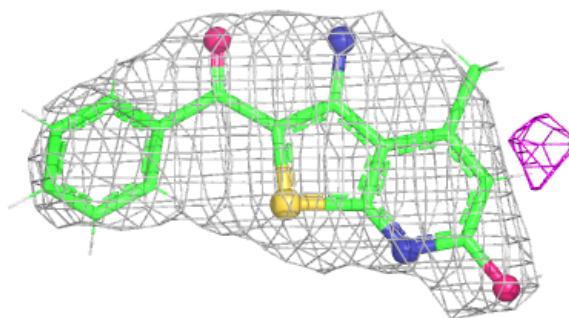
Electron density around UMP B 400:

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

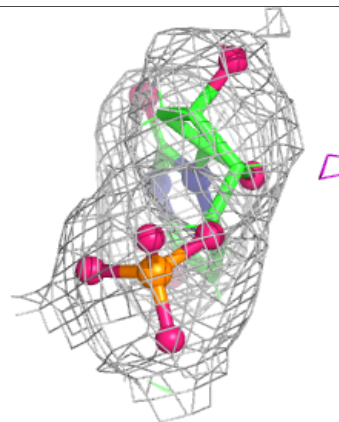
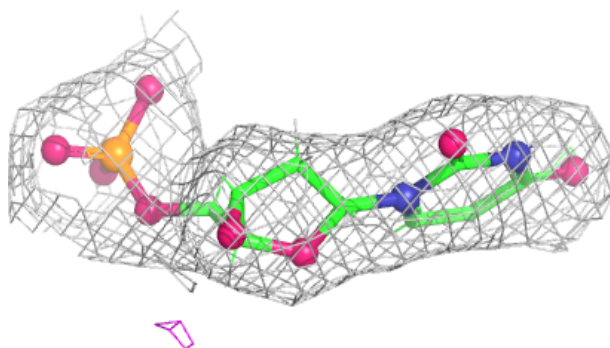
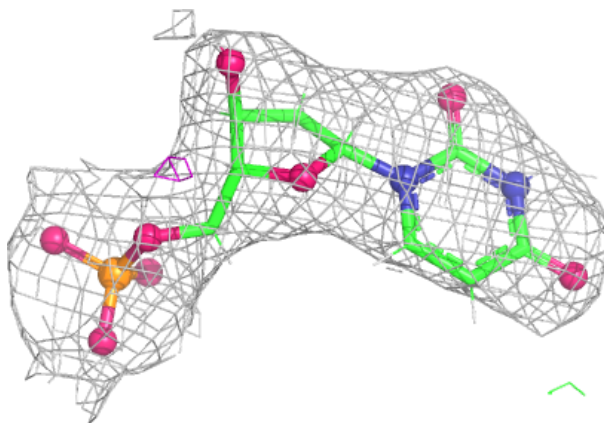


Electron density around KI3 A 401:

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

**Electron density around UMP A 400:**

$2mF_o-DF_c$ (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.