Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 01:21 PM JST

PDB ID	:	5HS3
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 (i) 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 (i)) were used in the production of this report:

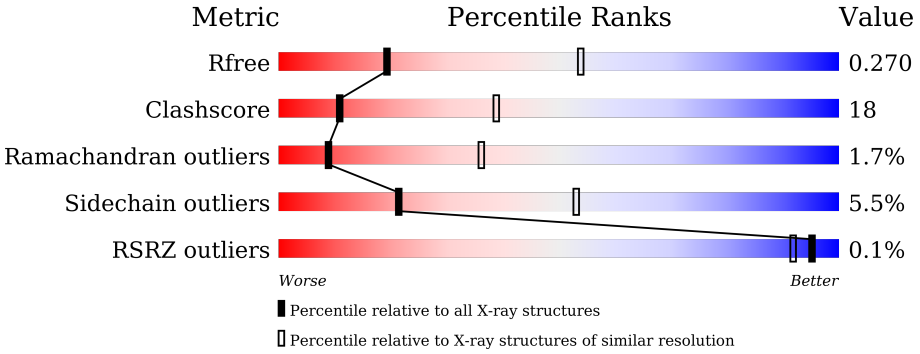
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	65% 31% •
1	B	289	65% 32% •
1	C	289	69% 25% • •
1	D	289	63% 31% • •
1	E	289	64% 30% • •

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Mol	Chain	Length	Quality of chain
1	F	289	51% 40% 6% •

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 (i)

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.

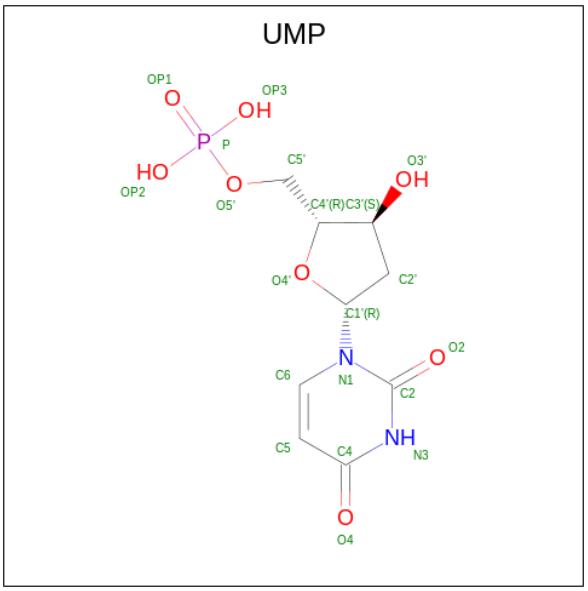
- Molecule 1 is a protein called Thymidylate synthase.

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

There are 6 discrepancies between the modelled and reference sequences:

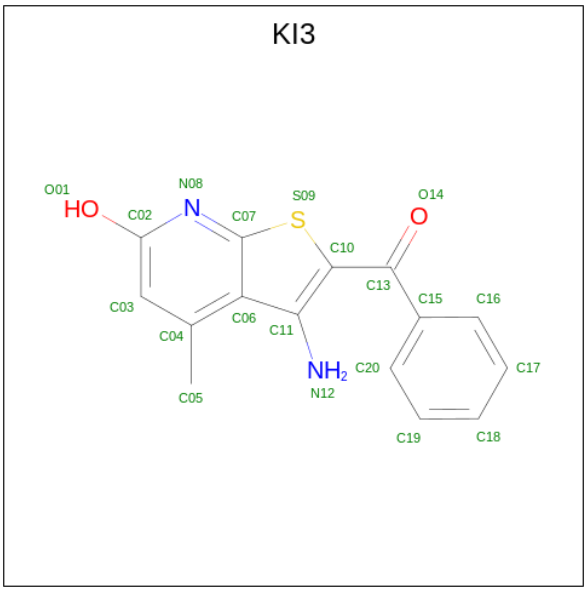
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	expression tag	UNP P04818
B	25	MET	-	expression tag	UNP P04818
C	25	MET	-	expression tag	UNP P04818
D	25	MET	-	expression tag	UNP P04818
E	25	MET	-	expression tag	UNP P04818
F	25	MET	-	expression tag	UNP P04818

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



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 (three-letter code: KI3) (formula: $C_{15}H_{12}N_2O_2S$).



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

- Molecule 4 is water.

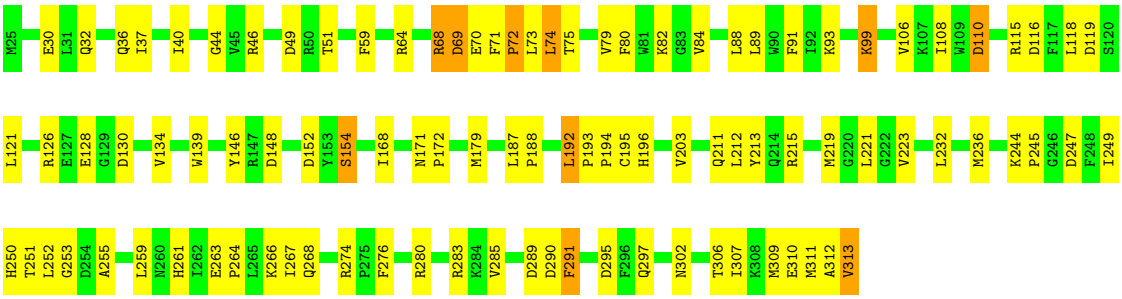
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	6	6	6	0	0
			Total	O		
4	B	3	3	3	0	0
			Total	O		
4	C	1	1	1	0	0
			Total	O		
4	D	1	1	1	0	0

3 Residue-property plots (i)

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.

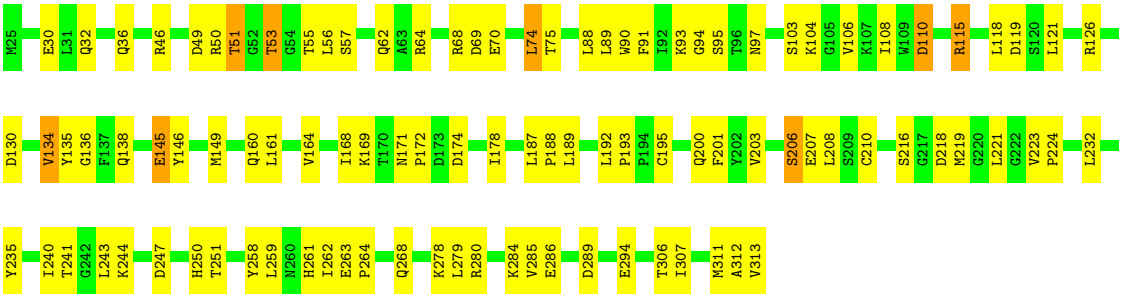
- Molecule 1: Thymidylate synthase

Chain A:



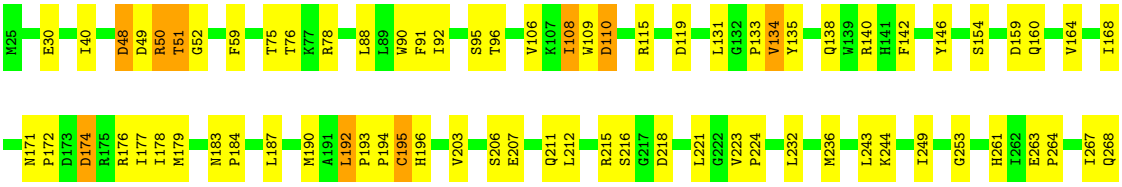
- Molecule 1: Thymidylate synthase

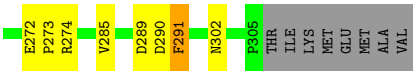
Chain B:



- Molecule 1: Thymidylate synthase

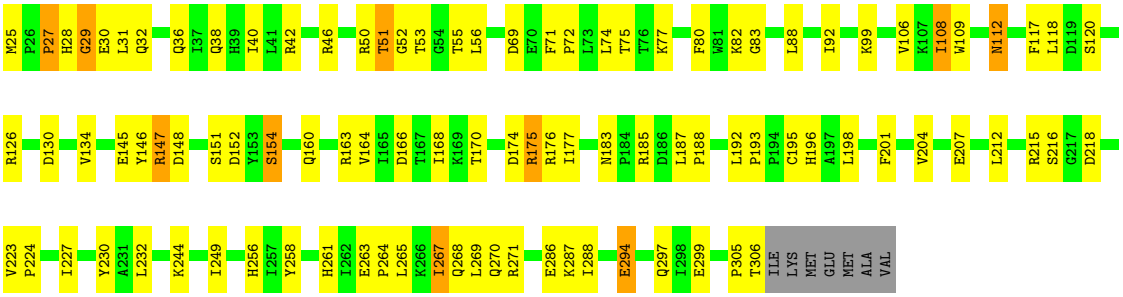
Chain C:





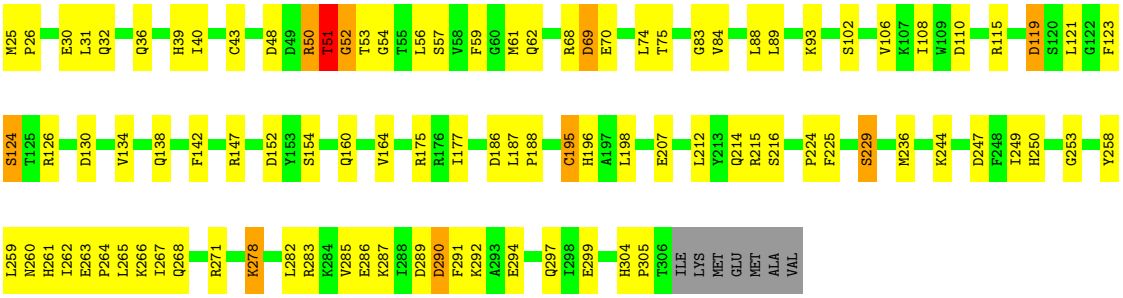
- Molecule 1: Thymidylate synthase

Chain D:



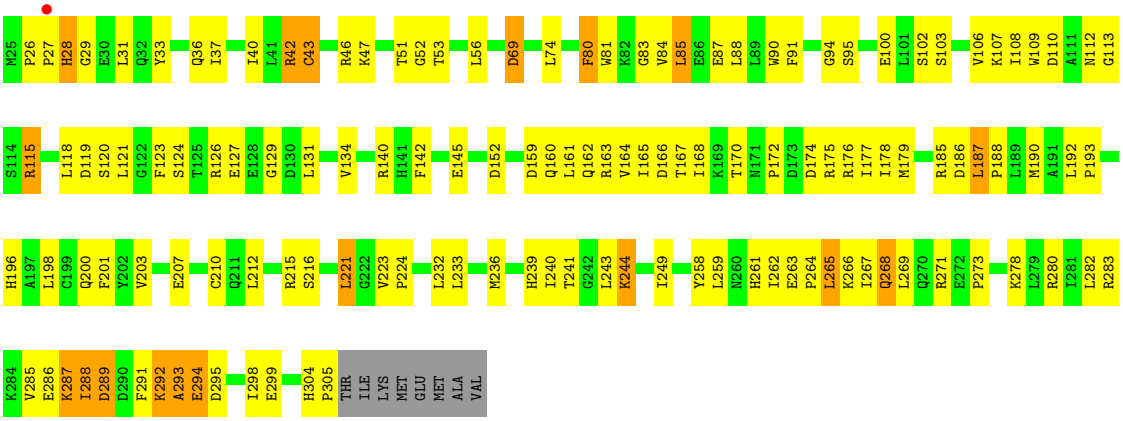
- Molecule 1: Thymidylate synthase

Chain E:



- Molecule 1: Thymidylate synthase

Chain F:



4 Data and refinement statistics (i)

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) 99.8 (28.11-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.180 , 0.268 0.185 , 0.270	Depositor DCC
R_{free} test set	1674 reflections (4.83%)	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 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.73	0/2369	0.57	0/3210
1	B	0.62	0/2357	0.57	0/3195
1	C	0.61	0/2283	0.56	0/3100
1	D	0.73	1/2320 (0.0%)	0.59	0/3143
1	E	0.64	1/2325 (0.0%)	0.56	0/3149
1	F	0.59	0/2300	0.56	0/3117
All	All	0.66	2/13954 (0.0%)	0.57	0/18914

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	195	CYS	CB-SG	-5.73	1.72	1.81
1	E	195	CYS	CB-SG	-5.03	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2309	0	2254	81	0
1	B	2297	0	2242	76	0
1	C	2223	0	2142	64	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2260	0	2215	76	3
1	E	2265	0	2221	68	2
1	F	2240	0	2189	138	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	494	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 18.

All (494) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:F:28:HIS:ND1	1:F:31:LEU:HG	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:270:GLN:HA	1:D:270:GLN:OE1	1.99	0.62
1:D:294:GLU:CD	1:D:294:GLU:H	2.01	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: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:E:88:LEU:HG	1:E:236:MET:HE1	1.84	0.60
1:F:177:ILE:HG21	1:F:201:PHE:HB2	1.82	0.60
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: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:A:232:LEU:HG	1:A:236:MET:HE3	1.84	0.58
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:F:140:ARG:HG2	1:F:140:ARG:NH1	2.18	0.58
1:A:69:ASP:N	1:A:69:ASP:OD1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:N	1:A:172:PRO:HD3	2.19	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:F:198:LEU:C	1:F:198:LEU:HD12	2.25	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: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:F:292:LYS:NZ	1:F:295:ASP:OD1	2.34	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
1:D:152:ASP:OD1	1:D:154:SER:OG	2.23	0.55
1:F:120:SER:OG	1:F:120:SER:O	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: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:236:MET:HB3	1:C:291:PHE:HE2	1.70	0.55
1:A:99:LYS:HZ1	1:D:99:LYS:HD2	1.72	0.55
1:C:48:ASP:CG	1:F:46:ARG:HH12	2.10	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ARG:HH12	1:F:126:ARG:C	2.10	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:A:139:TRP:CD1	1:A:179:MET:HE2	2.43	0.54
1:F:91:PHE:O	1:F:94:GLY:N	2.40	0.54
1:C:59:PHE:HA	1:C:253:GLY:O	2.09	0.53
1:D:198:LEU:HD12	1:D:198:LEU:C	2.29	0.53
1:F:83:GLY:HA2	1:F:106:VAL:HG21	1.89	0.53
1:B:145:GLU:HG2	1:D:145:GLU:CD	2.28	0.53
1:E:152:ASP:OD1	1:E:154:SER:OG	2.22	0.53
1:D:130:ASP:OD1	1:D:146:TYR:OH	2.25	0.53
1:A:219:MET:HE1	1:A:252:LEU:CD1	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:E:294:GLU:CD	1:E:294:GLU:H	2.14	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:272:GLU:CD	1:C:273:PRO:HD2	2.31	0.50
1:C:168:ILE:HG12	1:C:177:ILE:HD13	1.93	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:B:55:THR:C	1:B:56:LEU:HD23	2.32	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:A:219:MET:HE1	1:A:252:LEU:HD13	1.96	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
1:F:162:GLN:HE22	1:F:287:LYS:HE2	1.79	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:C:232:LEU:HD11	1:C:236:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:232:LEU:HD12	1:B:232:LEU:C	2.36	0.46
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: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:A:99:LYS:HZ1	1:D:99:LYS:HB3	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:ARG:HH22	1:E:247:ASP:CG	2.19	0.46
1:F:90:TRP:NE1	1:F:95:SER:OG	2.48	0.46
1:A:232:LEU:CG	1:A:236:MET:HE3	2.46	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: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: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: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
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:172:PRO:HB3	1:F:203:VAL:HG11	1.99	0.45
1:E:102:SER:HB2	1:E:110:ASP:CG	2.38	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:F:85:LEU:HD12	1:F:85:LEU:C	2.37	0.44
1:E:62:GLN:HA	1:E:250:HIS:O	2.18	0.44
1:A:261:HIS:C	1:A:264:PRO:HD2	2.38	0.44
1:B:160:GLN:O	1:B:164:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:28:HIS:C	1:D:31:LEU:HD13	2.38	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:219:MET:HE2	1:A:255:ALA:HB1	2.00	0.43
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
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:HG22	1:C:40:ILE:O	2.19	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:VAL:HG12	1:E:287:LYS:O	2.18	0.43
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:F:51:THR:C	1:F:53:THR:H	2.22	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: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:A:179:MET:HE2	1:A:179:MET:HB3	1.89	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
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
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:B:216:SER:OG	2:B:400:UMP:H2'	2.20	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: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:D:30:GLU:CD	1:D:75:THR:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLN:HB2	1:A:249:ILE:HB	2.02	0.41
1:B:69:ASP:O	1:B:70:GLU:HB3	2.20	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: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: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:A:219:MET:HE1	1:A:252:LEU:HD11	2.01	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:B:187:LEU:C	1:B:189:LEU:H	2.24	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: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: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:267:ILE:HG22	1:A:268:GLN:N	2.35	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	1:D:216:SER:N	2.36	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: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:259:LEU:HA	1:F:262:ILE:CG1	2.51	0.40
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:E:261:HIS:C	1:E:264:PRO:HD2	2.41	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:A:108:ILE:HG12	1:A:108:ILE:H	1.72	0.40
1:A:219:MET:CE	1:A:255:ALA:HB1	2.52	0.40
1:F:142:PHE:CD1	1:F:142:PHE:C	2.95	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%)	22	57
1	B	287/289 (99%)	258 (90%)	26 (9%)	3 (1%)	15	49
1	C	279/289 (96%)	258 (92%)	19 (7%)	2 (1%)	22	57
1	D	280/289 (97%)	251 (90%)	22 (8%)	7 (2%)	5	27
1	E	280/289 (97%)	252 (90%)	23 (8%)	5 (2%)	8	34
1	F	279/289 (96%)	246 (88%)	24 (9%)	9 (3%)	4	22
All	All	1692/1734 (98%)	1531 (90%)	133 (8%)	28 (2%)	9	36

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/252 (98%)	233 (94%)	14 (6%)	20	52
1	B	244/252 (97%)	233 (96%)	11 (4%)	27	60
1	C	234/252 (93%)	225 (96%)	9 (4%)	33	66
1	D	241/252 (96%)	227 (94%)	14 (6%)	20	51
1	E	243/252 (96%)	230 (95%)	13 (5%)	22	54
1	F	237/252 (94%)	218 (92%)	19 (8%)	12	40
All	All	1446/1512 (96%)	1366 (94%)	80 (6%)	21	53

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	69	ASP
1	A	70	GLU
1	A	74	LEU
1	A	99	LYS
1	A	110	ASP
1	A	148	ASP
1	A	154	SER
1	A	192	LEU
1	A	266	LYS

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Mol	Chain	Res	Type
1	A	289	ASP
1	A	291	PHE
1	A	310	GLU
1	A	313	VAL
1	B	51	THR
1	B	53	THR
1	B	57	SER
1	B	74	LEU
1	B	110	ASP
1	B	115	ARG
1	B	145	GLU
1	B	174	ASP
1	B	206	SER
1	B	221	LEU
1	B	289	ASP
1	C	48	ASP
1	C	50	ARG
1	C	108	ILE
1	C	110	ASP
1	C	154	SER
1	C	174	ASP
1	C	192	LEU
1	C	195	CYS
1	C	291	PHE
1	D	38	GLN
1	D	51	THR
1	D	56	LEU
1	D	69	ASP
1	D	108	ILE
1	D	112	ASN
1	D	147	ARG
1	D	154	SER
1	D	163	ARG
1	D	175	ARG
1	D	204	VAL
1	D	267	ILE
1	D	269	LEU
1	D	294	GLU
1	E	51	THR
1	E	57	SER
1	E	61	MET
1	E	69	ASP

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Mol	Chain	Res	Type
1	E	119	ASP
1	E	186	ASP
1	E	195	CYS
1	E	198	LEU
1	E	229	SER
1	E	278	LYS
1	E	286	GLU
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	102	SER
1	F	115	ARG
1	F	119	ASP
1	F	175	ARG
1	F	185	ARG
1	F	187	LEU
1	F	221	LEU
1	F	244	LYS
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	B	211	GLN
1	C	256	HIS
1	F	62	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	UMP	A	400	-	21,21,21	2.78	15 (71%)	31,31,31	2.47	11 (35%)
2	UMP	D	400	-	21,21,21	2.78	15 (71%)	31,31,31	2.46	11 (35%)
2	UMP	E	400	-	21,21,21	2.78	15 (71%)	31,31,31	2.48	11 (35%)
3	KI3	B	401	-	20,22,22	1.06	2 (10%)	19,32,32	1.57	3 (15%)
3	KI3	A	401	-	20,22,22	1.01	1 (5%)	19,32,32	1.47	3 (15%)
2	UMP	B	400	-	21,21,21	2.77	15 (71%)	31,31,31	2.47	11 (35%)
2	UMP	F	400	-	21,21,21	2.78	15 (71%)	31,31,31	2.47	11 (35%)
2	UMP	C	400	-	21,21,21	2.78	15 (71%)	31,31,31	2.47	11 (35%)
3	KI3	E	401	-	20,22,22	0.91	2 (10%)	19,32,32	1.63	3 (15%)

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	A	400	-	-	7/10/22/22	0/2/2/2
2	UMP	D	400	-	-	7/10/22/22	0/2/2/2
2	UMP	E	400	-	-	7/10/22/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KI3	B	401	-	-	0/4/8/8	0/3/3/3
3	KI3	A	401	-	-	0/4/8/8	0/3/3/3
2	UMP	B	400	-	-	7/10/22/22	0/2/2/2
2	UMP	F	400	-	-	7/10/22/22	0/2/2/2
2	UMP	C	400	-	-	7/10/22/22	0/2/2/2
3	KI3	E	401	-	-	1/4/8/8	0/3/3/3

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	UMP	C2'-C3'	-4.81	1.40	1.52
2	E	400	UMP	C2'-C3'	-4.79	1.40	1.52
2	F	400	UMP	C2'-C3'	-4.78	1.40	1.52
2	B	400	UMP	C2'-C3'	-4.77	1.40	1.52
2	D	400	UMP	C2'-C3'	-4.76	1.40	1.52
2	A	400	UMP	C2'-C3'	-4.74	1.40	1.52
2	C	400	UMP	C6-C5	4.54	1.45	1.35
2	B	400	UMP	C6-C5	4.52	1.45	1.35
2	F	400	UMP	C6-C5	4.52	1.45	1.35
2	E	400	UMP	C6-C5	4.50	1.45	1.35
2	A	400	UMP	C6-C5	4.50	1.45	1.35
2	D	400	UMP	C6-C5	4.48	1.45	1.35
2	D	400	UMP	C3'-C4'	-3.86	1.42	1.53
2	C	400	UMP	C3'-C4'	-3.85	1.42	1.53
2	E	400	UMP	C3'-C4'	-3.84	1.42	1.53
2	A	400	UMP	C3'-C4'	-3.84	1.42	1.53
2	F	400	UMP	C3'-C4'	-3.83	1.42	1.53
2	B	400	UMP	C3'-C4'	-3.83	1.42	1.53
2	D	400	UMP	O2-C2	-3.40	1.16	1.23
2	E	400	UMP	O2-C2	-3.38	1.16	1.23
2	A	400	UMP	O2-C2	-3.35	1.16	1.23
2	F	400	UMP	O2-C2	-3.35	1.16	1.23
2	C	400	UMP	O2-C2	-3.35	1.16	1.23
2	B	400	UMP	O2-C2	-3.33	1.17	1.23
2	E	400	UMP	P-O5'	-3.19	1.49	1.60
2	B	400	UMP	P-O5'	-3.19	1.49	1.60
2	D	400	UMP	P-O5'	-3.19	1.50	1.60
2	F	400	UMP	P-O5'	-3.19	1.50	1.60
2	C	400	UMP	P-O5'	-3.18	1.50	1.60
2	A	400	UMP	P-O5'	-3.16	1.50	1.60
2	B	400	UMP	C2'-C1'	-3.02	1.43	1.52
2	E	400	UMP	O4-C4	-3.02	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	UMP	O4-C4	-3.01	1.18	1.24
2	D	400	UMP	C2'-C1'	-3.00	1.44	1.52
2	C	400	UMP	O4-C4	-3.00	1.18	1.24
2	B	400	UMP	O4-C4	-2.99	1.18	1.24
2	C	400	UMP	C2'-C1'	-2.99	1.44	1.52
2	A	400	UMP	C2'-C1'	-2.99	1.44	1.52
2	E	400	UMP	C2'-C1'	-2.98	1.44	1.52
2	F	400	UMP	C2'-C1'	-2.97	1.44	1.52
2	D	400	UMP	O4-C4	-2.97	1.18	1.24
2	F	400	UMP	O4-C4	-2.96	1.18	1.24
2	B	400	UMP	O3'-C3'	-2.91	1.37	1.43
2	F	400	UMP	O3'-C3'	-2.91	1.37	1.43
2	A	400	UMP	O3'-C3'	-2.87	1.37	1.43
2	D	400	UMP	O3'-C3'	-2.87	1.37	1.43
2	E	400	UMP	O3'-C3'	-2.87	1.37	1.43
2	C	400	UMP	O3'-C3'	-2.86	1.37	1.43
3	A	401	KI3	C07-C06	-2.82	1.37	1.42
2	A	400	UMP	O5'-C5'	-2.82	1.33	1.44
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	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'	-2.79	1.34	1.44
2	F	400	UMP	C2-N3	2.77	1.42	1.38
2	A	400	UMP	O4'-C4'	-2.77	1.38	1.45
2	D	400	UMP	P-OP3	-2.77	1.44	1.54
2	C	400	UMP	C2-N3	2.75	1.42	1.38
2	C	400	UMP	P-OP3	-2.75	1.44	1.54
2	F	400	UMP	P-OP3	-2.75	1.44	1.54
2	A	400	UMP	C2-N3	2.75	1.42	1.38
2	B	400	UMP	C2-N3	2.75	1.42	1.38
2	E	400	UMP	P-OP3	-2.75	1.44	1.54
2	C	400	UMP	O4'-C4'	-2.75	1.38	1.45
2	A	400	UMP	P-OP3	-2.74	1.44	1.54
2	D	400	UMP	C2-N3	2.73	1.42	1.38
2	E	400	UMP	C2-N3	2.73	1.42	1.38
2	D	400	UMP	O4'-C4'	-2.73	1.38	1.45
2	B	400	UMP	P-OP3	-2.73	1.44	1.54
2	E	400	UMP	O4'-C4'	-2.72	1.38	1.45
2	F	400	UMP	O4'-C4'	-2.71	1.38	1.45
2	B	400	UMP	O4'-C4'	-2.71	1.38	1.45
3	B	401	KI3	C07-C06	-2.71	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	UMP	P-OP2	-2.47	1.45	1.54
2	A	400	UMP	P-OP2	-2.46	1.45	1.54
2	C	400	UMP	P-OP2	-2.45	1.45	1.54
2	D	400	UMP	C2-N1	2.34	1.42	1.38
2	C	400	UMP	C2-N1	2.31	1.42	1.38
2	A	400	UMP	C2-N1	2.30	1.42	1.38
2	D	400	UMP	P-OP2	-2.30	1.46	1.54
2	F	400	UMP	P-OP2	-2.30	1.46	1.54
2	E	400	UMP	P-OP2	-2.29	1.46	1.54
2	B	400	UMP	C2-N1	2.28	1.42	1.38
2	E	400	UMP	C2-N1	2.28	1.42	1.38
2	F	400	UMP	C2-N1	2.27	1.42	1.38
3	E	401	KI3	C07-C06	-2.25	1.38	1.42
2	A	400	UMP	O4'-C1'	-2.12	1.37	1.42
2	B	400	UMP	O4'-C1'	-2.12	1.37	1.42
2	C	400	UMP	O4'-C1'	-2.11	1.37	1.42
2	E	400	UMP	O4'-C1'	-2.10	1.37	1.42
2	D	400	UMP	O4'-C1'	-2.10	1.37	1.42
2	F	400	UMP	O4'-C1'	-2.10	1.37	1.42
3	E	401	KI3	C11-N12	2.09	1.42	1.36
3	B	401	KI3	C11-N12	2.05	1.42	1.36

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	400	UMP	C2'-C1'-N1	9.33	135.26	113.77
2	C	400	UMP	C2'-C1'-N1	9.32	135.24	113.77
2	B	400	UMP	C2'-C1'-N1	9.32	135.23	113.77
2	E	400	UMP	C2'-C1'-N1	9.31	135.22	113.77
2	A	400	UMP	C2'-C1'-N1	9.31	135.20	113.77
2	D	400	UMP	C2'-C1'-N1	9.31	135.20	113.77
3	B	401	KI3	C11-C06-C07	4.40	114.51	107.94
3	A	401	KI3	C11-C06-C07	4.25	114.28	107.94
3	E	401	KI3	C11-C06-C07	4.19	114.19	107.94
2	A	400	UMP	O4'-C1'-N1	3.47	114.07	107.86
2	E	400	UMP	O4'-C1'-N1	3.45	114.03	107.86
2	C	400	UMP	O4'-C1'-N1	3.44	114.02	107.86
2	F	400	UMP	O4'-C1'-N1	3.43	114.00	107.86
2	D	400	UMP	O4'-C1'-N1	3.43	113.99	107.86
2	B	400	UMP	O4'-C1'-N1	3.42	113.97	107.86
3	E	401	KI3	C05-C04-C03	-3.34	115.86	120.74
3	B	401	KI3	C02-N08-C07	3.32	121.29	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	401	KI3	C02-N08-C07	3.29	121.25	116.73
3	B	401	KI3	C05-C04-C03	-3.16	116.12	120.74
3	A	401	KI3	C02-N08-C07	3.06	120.94	116.73
2	D	400	UMP	OP2-P-O5'	3.00	114.72	106.73
2	E	400	UMP	OP2-P-O5'	3.00	114.72	106.73
2	F	400	UMP	OP2-P-O5'	2.98	114.66	106.73
3	A	401	KI3	C05-C04-C03	-2.94	116.45	120.74
2	C	400	UMP	O5'-P-OP1	2.93	114.70	106.47
2	C	400	UMP	N3-C2-N1	2.93	118.78	114.89
2	B	400	UMP	O5'-P-OP1	2.93	114.68	106.47
2	B	400	UMP	N3-C2-N1	2.92	118.77	114.89
2	F	400	UMP	O5'-C5'-C4'	2.91	119.02	108.99
2	A	400	UMP	O5'-C5'-C4'	2.91	119.02	108.99
2	E	400	UMP	N3-C2-N1	2.91	118.75	114.89
2	F	400	UMP	N3-C2-N1	2.91	118.75	114.89
2	A	400	UMP	O5'-P-OP1	2.91	114.62	106.47
2	A	400	UMP	N3-C2-N1	2.91	118.75	114.89
2	E	400	UMP	O5'-C5'-C4'	2.90	118.99	108.99
2	C	400	UMP	O5'-C5'-C4'	2.90	118.98	108.99
2	B	400	UMP	O5'-C5'-C4'	2.90	118.96	108.99
2	D	400	UMP	O5'-C5'-C4'	2.89	118.95	108.99
2	D	400	UMP	N3-C2-N1	2.85	118.67	114.89
2	B	400	UMP	OP2-P-O5'	2.84	114.29	106.73
2	A	400	UMP	OP2-P-O5'	2.83	114.27	106.73
2	C	400	UMP	C1'-N1-C2	2.83	123.22	117.64
2	C	400	UMP	OP2-P-O5'	2.83	114.26	106.73
2	A	400	UMP	C1'-N1-C2	2.83	123.21	117.64
2	E	400	UMP	C1'-N1-C2	2.82	123.19	117.64
2	F	400	UMP	C1'-N1-C2	2.82	123.19	117.64
2	B	400	UMP	C1'-N1-C2	2.81	123.18	117.64
2	D	400	UMP	C1'-N1-C2	2.80	123.15	117.64
2	E	400	UMP	O5'-P-OP1	2.78	114.27	106.47
2	F	400	UMP	O5'-P-OP1	2.77	114.26	106.47
2	D	400	UMP	O5'-P-OP1	2.76	114.22	106.47
2	C	400	UMP	O2-C2-N1	-2.58	119.36	122.79
2	A	400	UMP	O2-C2-N1	-2.57	119.36	122.79
2	E	400	UMP	O2-C2-N1	-2.57	119.36	122.79
2	B	400	UMP	O2-C2-N1	-2.57	119.38	122.79
2	D	400	UMP	O2-C2-N1	-2.55	119.39	122.79
2	F	400	UMP	O2-C2-N1	-2.53	119.42	122.79
2	E	400	UMP	C3'-C2'-C1'	2.51	108.83	102.54
2	B	400	UMP	C3'-C2'-C1'	2.51	108.82	102.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	UMP	C3'-C2'-C1'	2.51	108.82	102.54
2	F	400	UMP	C3'-C2'-C1'	2.51	108.82	102.54
2	A	400	UMP	C3'-C2'-C1'	2.50	108.80	102.54
2	D	400	UMP	C3'-C2'-C1'	2.50	108.80	102.54
2	F	400	UMP	O4-C4-C5	-2.39	120.97	125.16
2	A	400	UMP	O4-C4-C5	-2.38	120.98	125.16
2	D	400	UMP	O4-C4-C5	-2.37	120.98	125.16
2	C	400	UMP	O4-C4-C5	-2.37	120.99	125.16
2	E	400	UMP	O4-C4-C5	-2.36	121.00	125.16
2	B	400	UMP	O4-C4-C5	-2.35	121.02	125.16
2	B	400	UMP	OP3-P-O5'	-2.05	101.29	106.73
2	A	400	UMP	OP3-P-O5'	-2.04	101.29	106.73
2	E	400	UMP	OP3-P-O5'	-2.04	101.30	106.73
2	F	400	UMP	OP3-P-O5'	-2.04	101.30	106.73
2	C	400	UMP	OP3-P-O5'	-2.04	101.31	106.73
2	D	400	UMP	OP3-P-O5'	-2.03	101.33	106.73

There are no chirality outliers.

All (43) 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	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'

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Mol	Chain	Res	Type	Atoms
2	D	400	UMP	O4'-C4'-C5'-O5'
2	F	400	UMP	O4'-C4'-C5'-O5'
2	A	400	UMP	C2'-C1'-N1-C2
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	D	400	UMP	C5'-O5'-P-OP1
2	E	400	UMP	C5'-O5'-P-OP1
2	F	400	UMP	C5'-O5'-P-OP1
2	E	400	UMP	O4'-C4'-C5'-O5'
3	E	401	KI3	O14-C13-C15-C20
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.

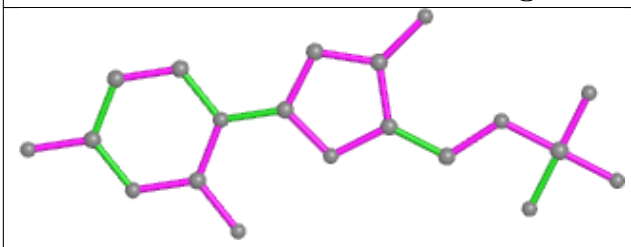
8 monomers are involved in 24 short contacts:

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

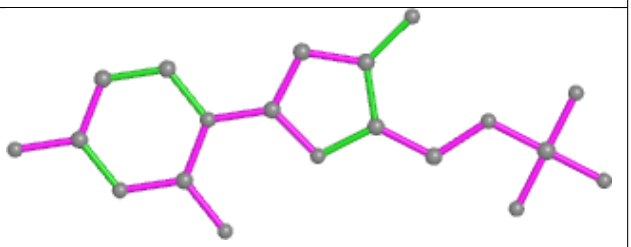
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

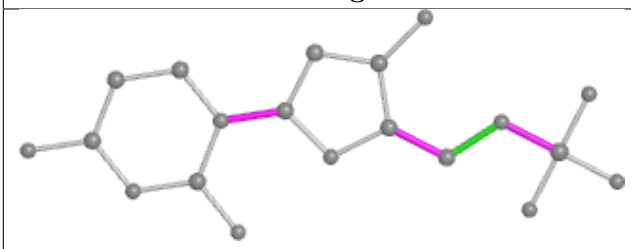
Ligand UMP A 400



Bond lengths



Bond angles



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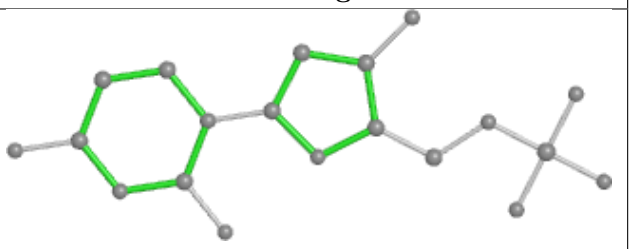
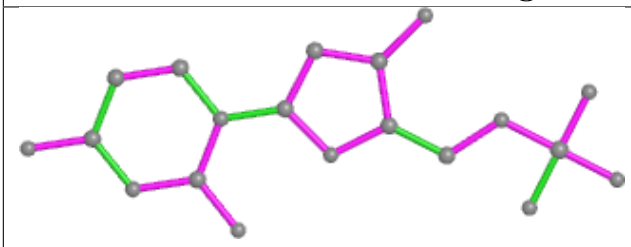
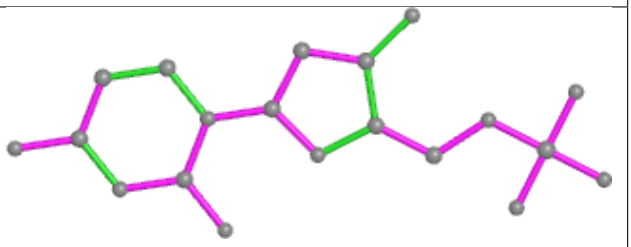


Rings

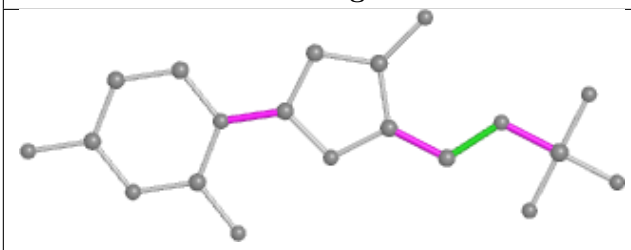
Ligand UMP D 400



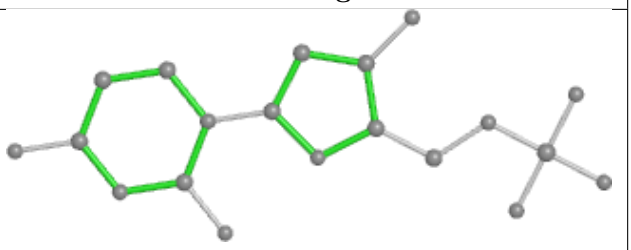
Bond lengths



Bond angles

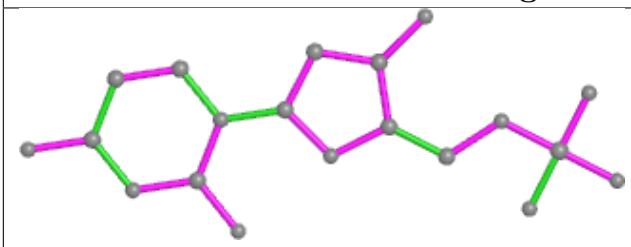


Torsions

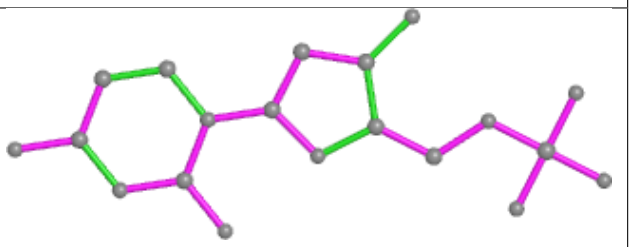


Rings

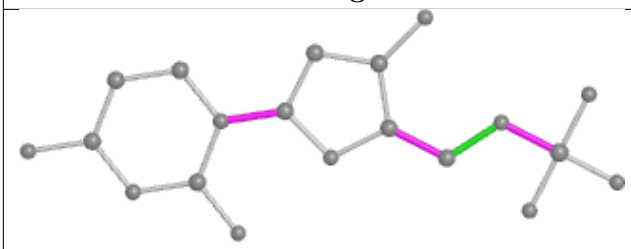
Ligand UMP E 400



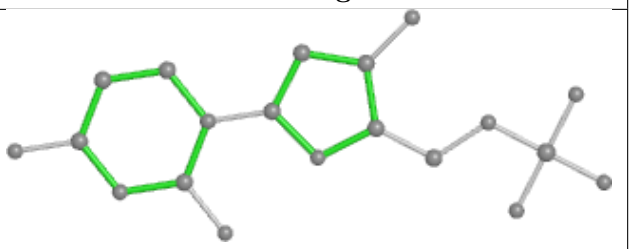
Bond lengths



Bond angles

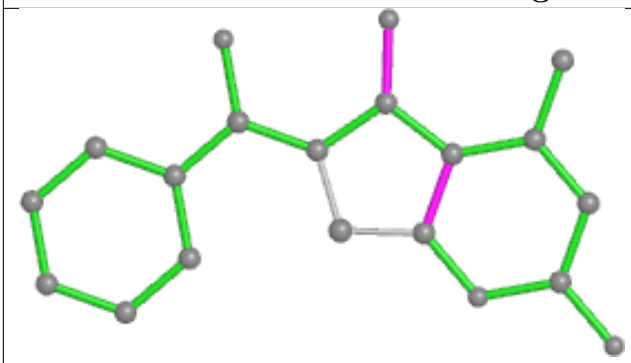


Torsions

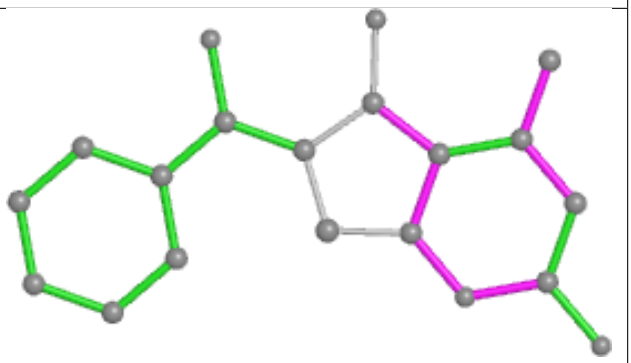


Rings

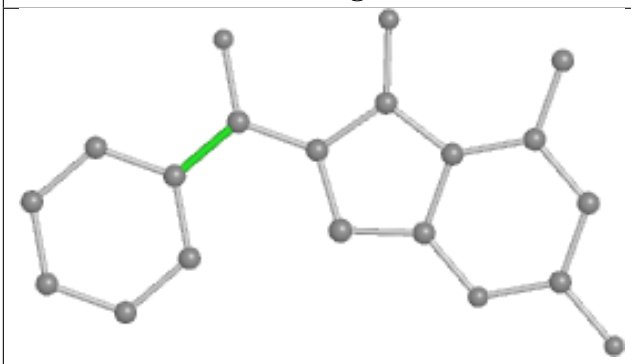
Ligand KI3 B 401



Bond lengths



Bond angles



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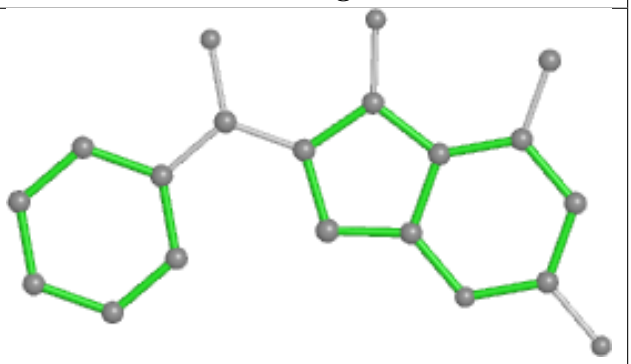
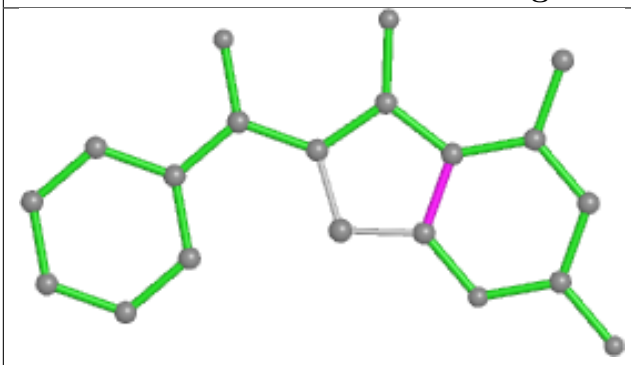
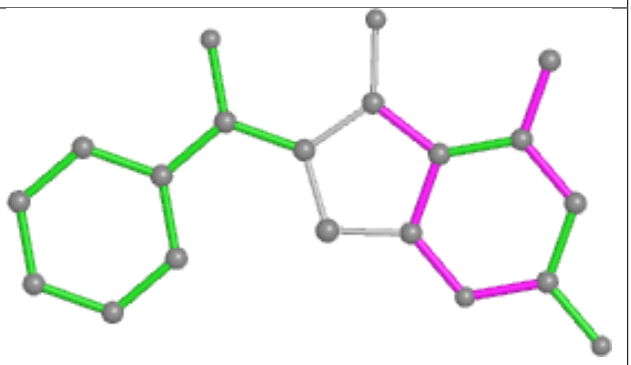


Rings

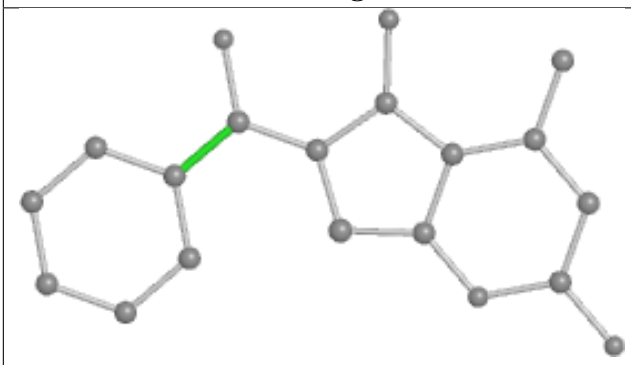
Ligand KI3 A 401



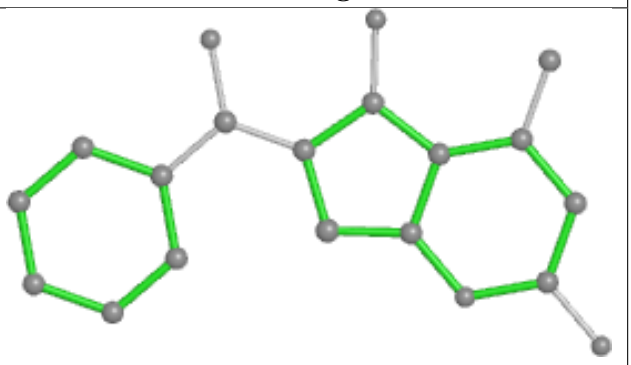
Bond lengths



Bond angles

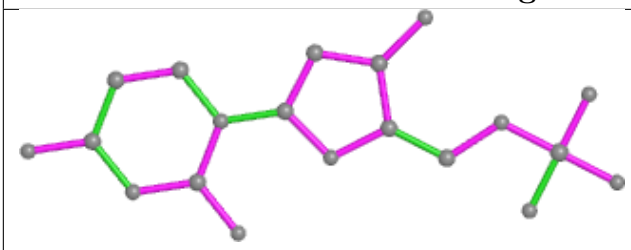


Torsions

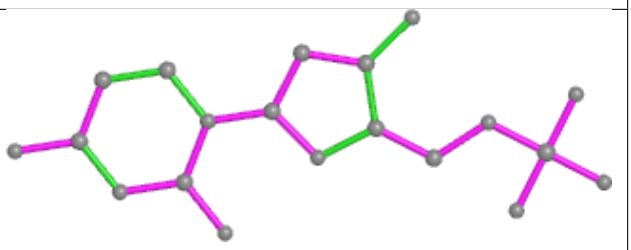


Rings

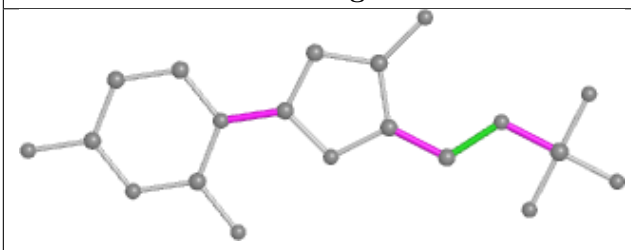
Ligand UMP B 400



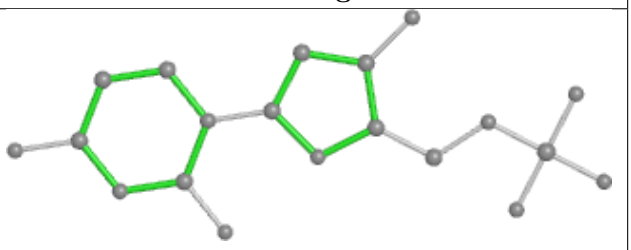
Bond lengths



Bond angles

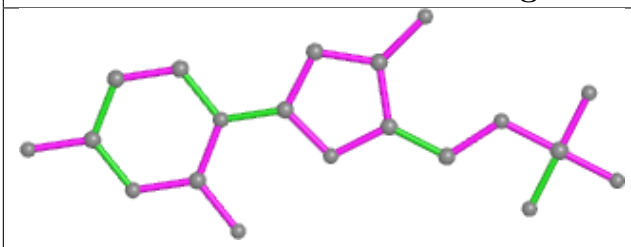


Torsions



Rings

Ligand UMP F 400



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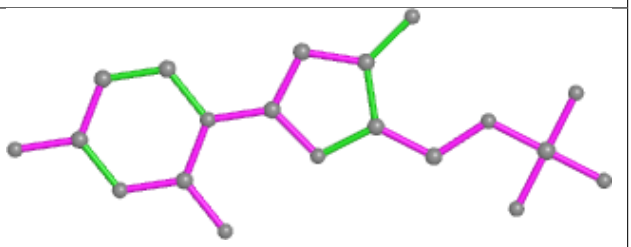
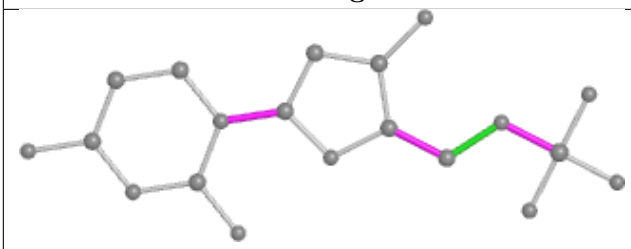


Bond angles



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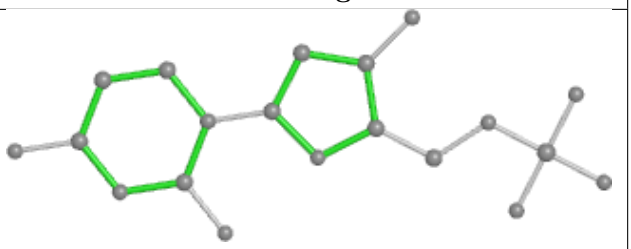
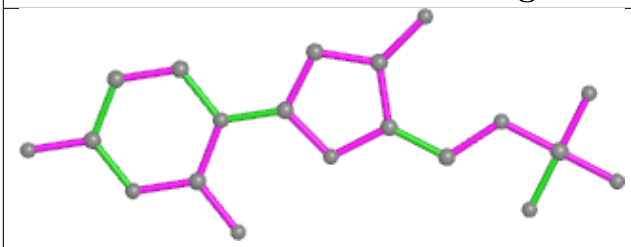
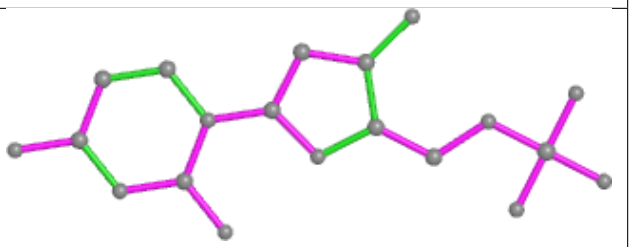


Rings

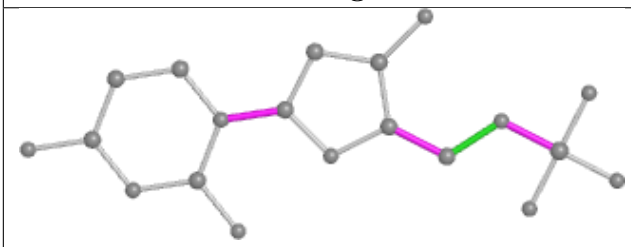
Ligand UMP C 400



Bond lengths



Bond angles



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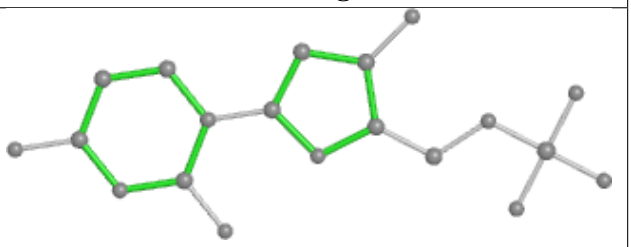
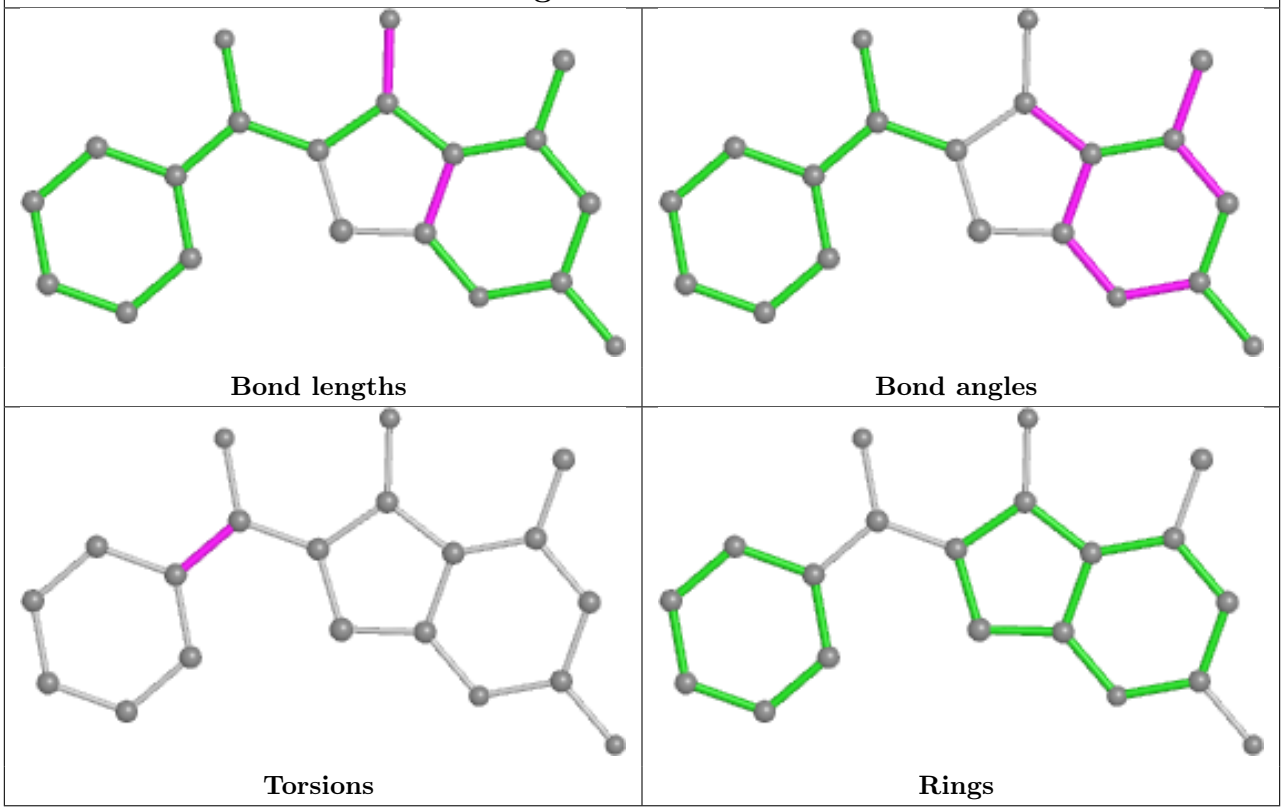


Rings

Ligand KI3 E 401



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%)	-0.65	0	100	100	26, 39, 56, 67	0
1	B	289/289 (100%)	-0.60	0	100	100	28, 44, 59, 73	0
1	C	281/289 (97%)	-0.53	0	100	100	31, 45, 62, 80	0
1	D	282/289 (97%)	-0.53	0	100	100	25, 42, 63, 82	0
1	E	282/289 (97%)	-0.52	0	100	100	28, 44, 68, 81	0
1	F	281/289 (97%)	-0.40	1 (0%)	92	84	33, 49, 71, 86	0
All	All	1704/1734 (98%)	-0.54	1 (0%)	95	92	25, 44, 65, 86	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	27	PRO	2.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

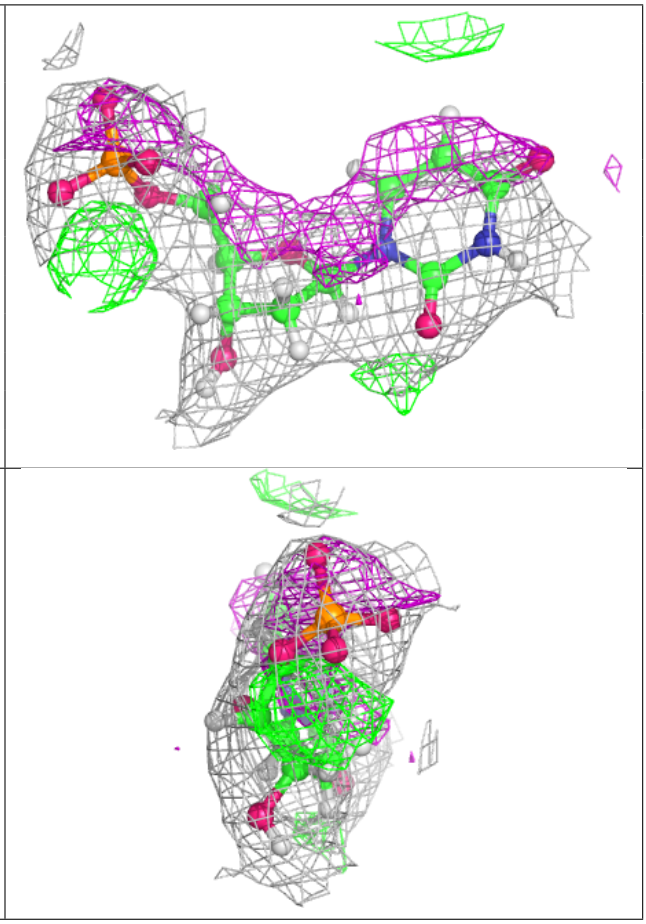
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UMP	E	400	20/20	0.86	0.26	34,40,48,49	0
2	UMP	F	400	20/20	0.87	0.24	34,40,48,49	0
2	UMP	D	400	20/20	0.88	0.23	34,40,48,49	0
2	UMP	C	400	20/20	0.89	0.21	34,40,48,49	0
3	KI3	E	401	20/20	0.93	0.28	51,61,80,85	0
3	KI3	B	401	20/20	0.95	0.14	43,52,59,64	0
2	UMP	B	400	20/20	0.95	0.15	34,40,48,49	0
3	KI3	A	401	20/20	0.96	0.18	36,47,58,69	0
2	UMP	A	400	20/20	0.97	0.13	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.

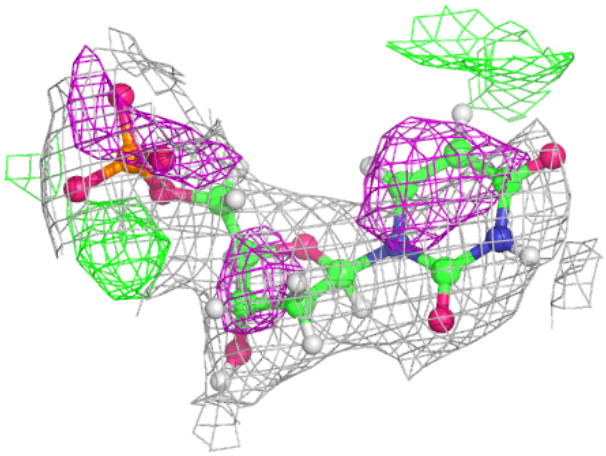
Electron density around UMP E 400:

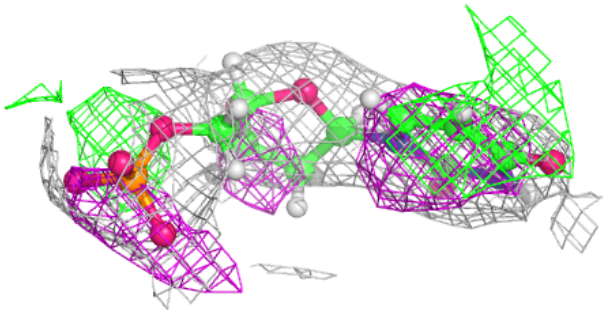
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

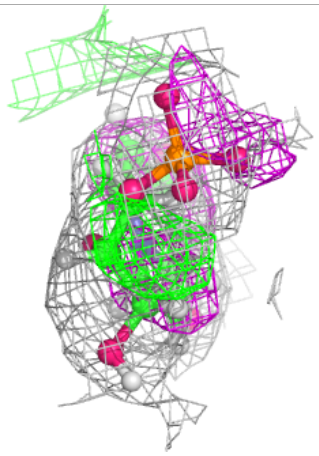


Electron density around UMP F 400:

$2mF_o$-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 D 400:

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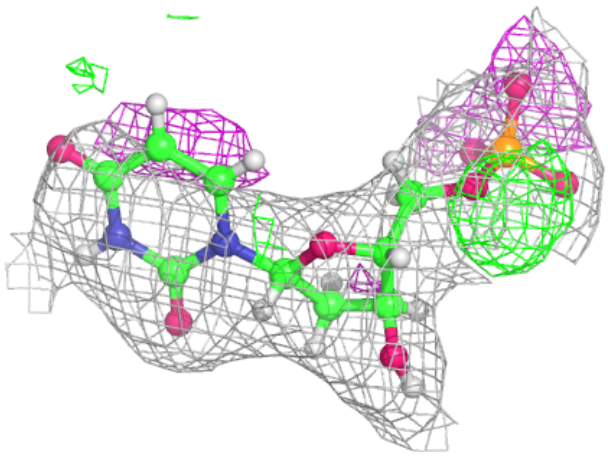
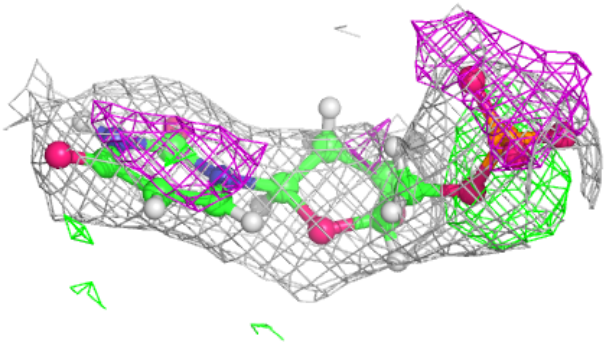
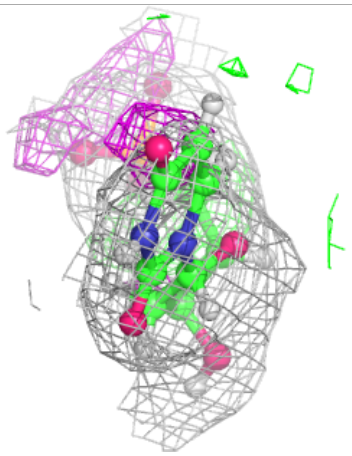
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

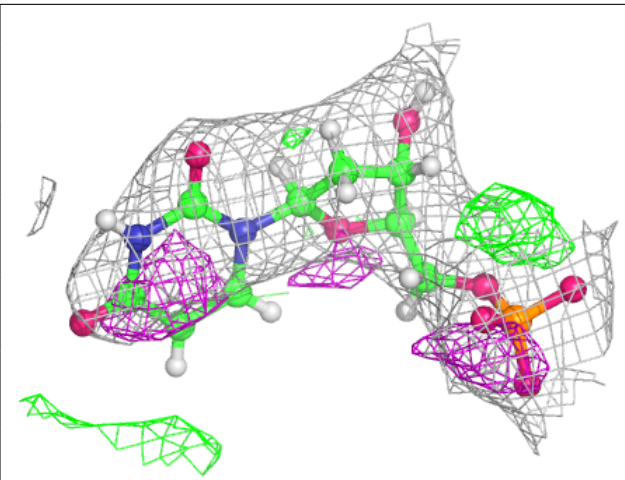


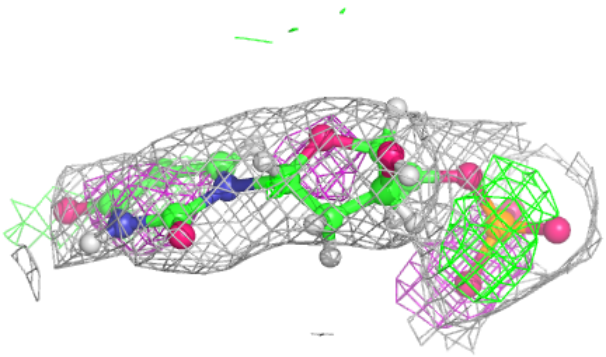


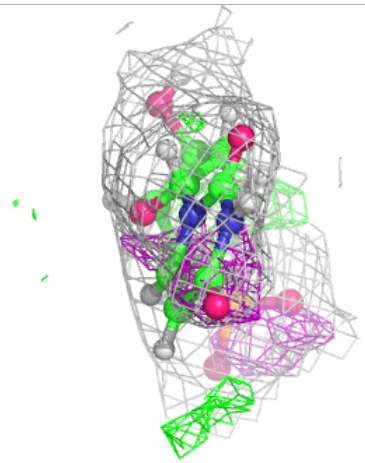


Electron density around UMP C 400:

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

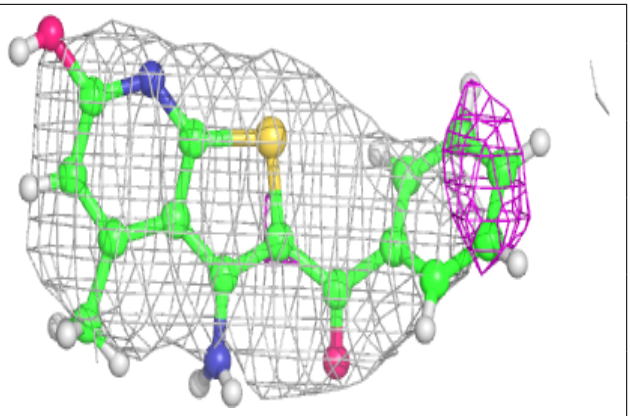


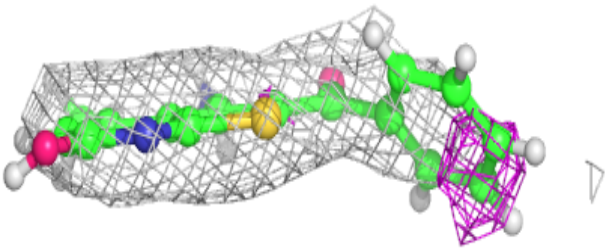


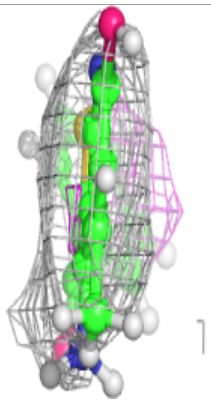


Electron density around KI3 E 401:

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

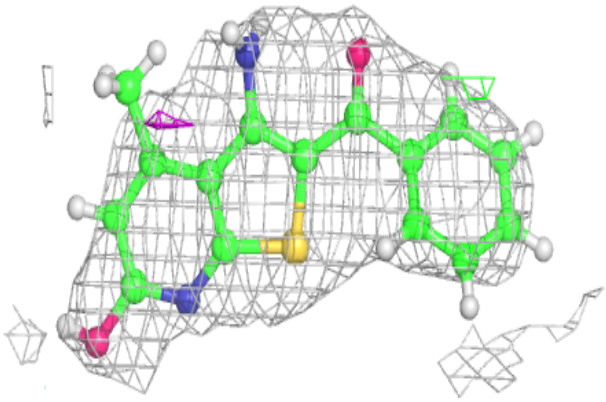


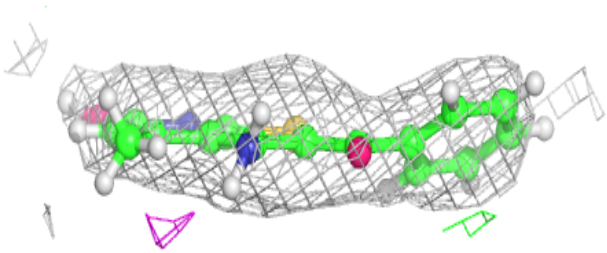


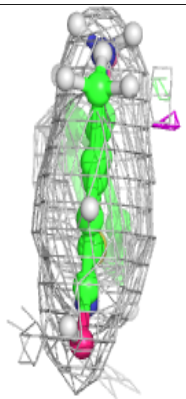


Electron density around KI3 B 401:

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

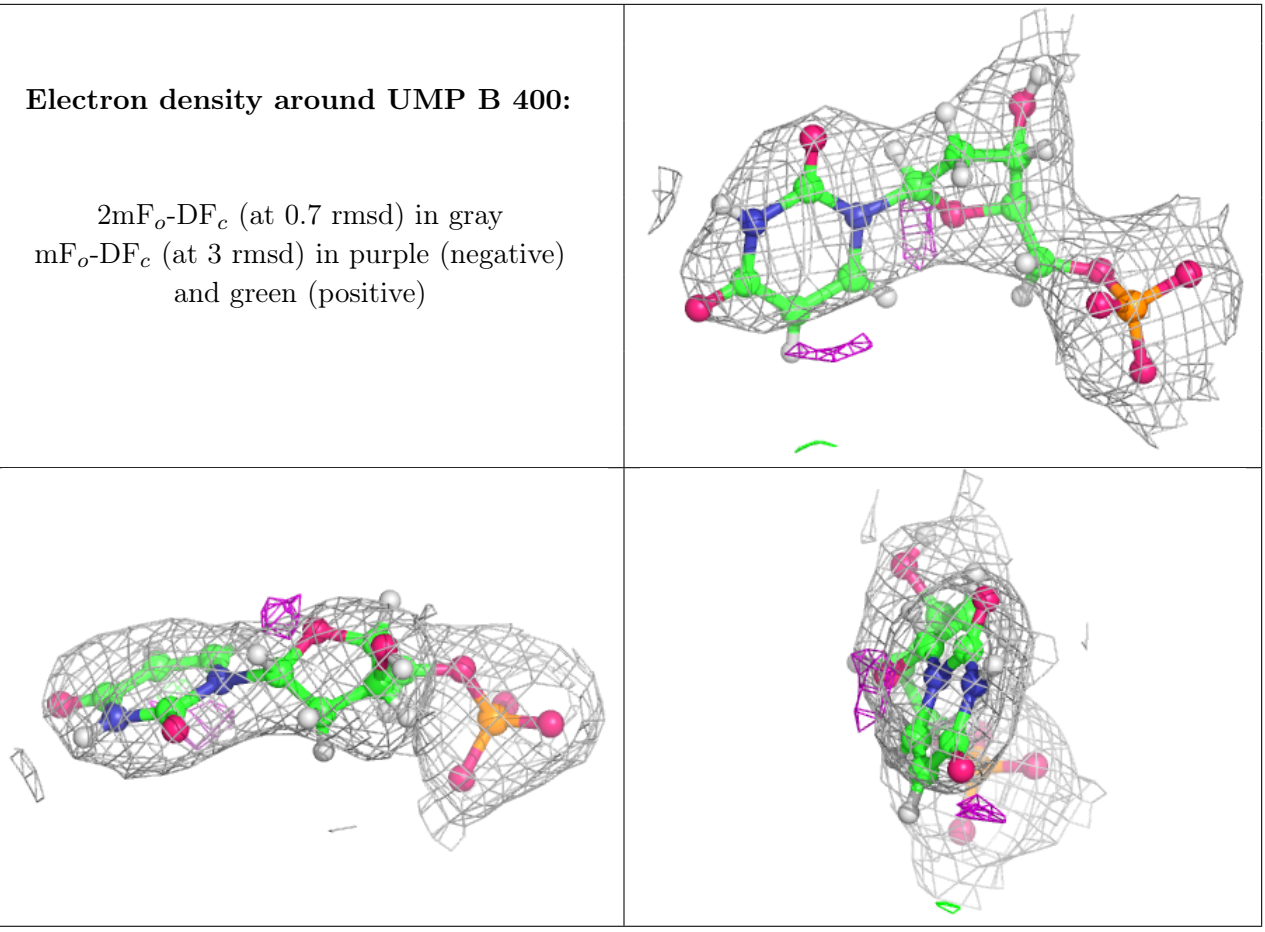






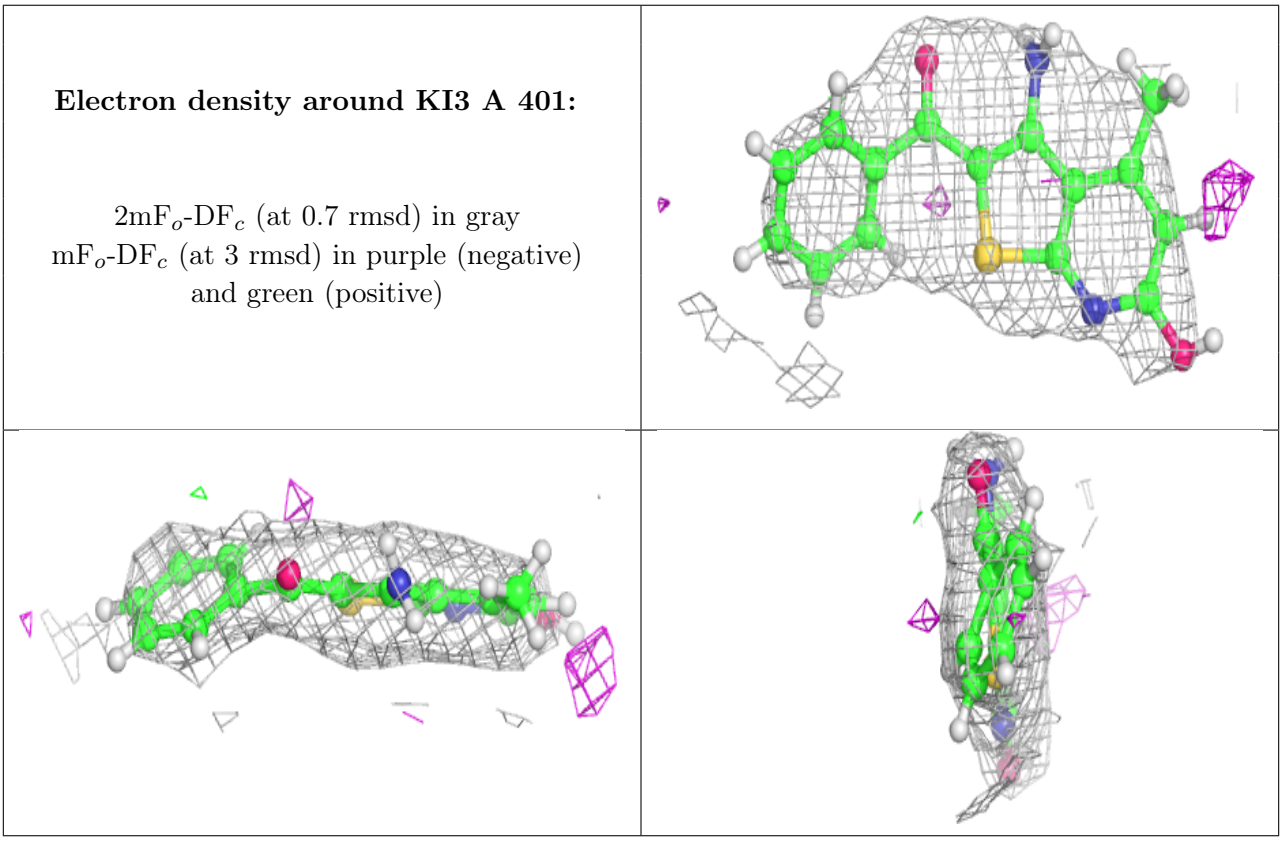
Electron density around UMP B 400:

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



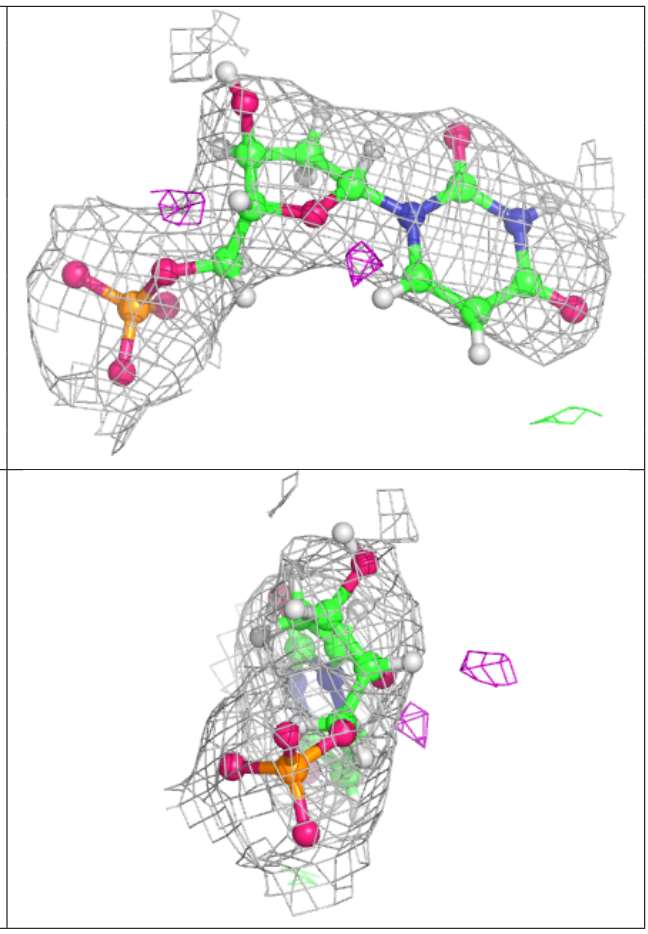
Electron density around KI3 A 401:

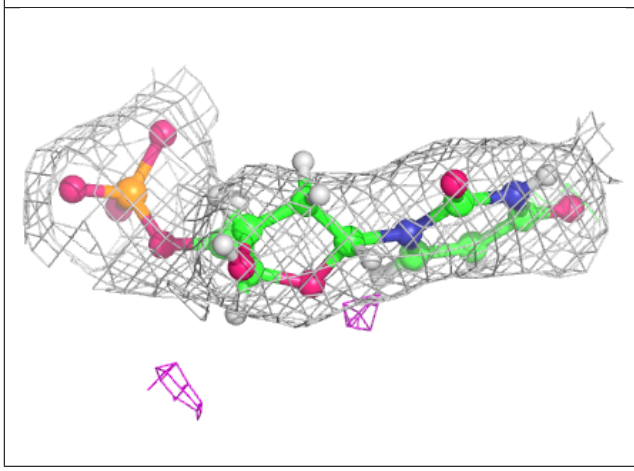
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.