



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:33 am BST

PDB ID : 1KMM
Title : HISTIDYL-TRNA SYNTHETASE COMPLEXED WITH HISTIDYL-ADENYLATE
Authors : Arnez, J.G.; Francklyn, C.S.; Moras, D.
Deposited on : 1997-05-09
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

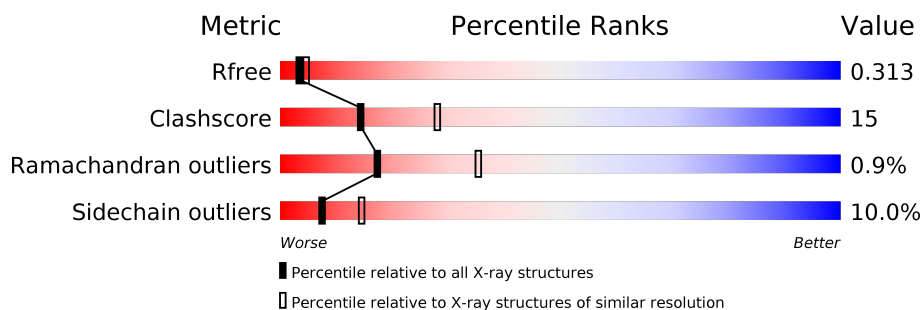
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	424	
1	B	424	
1	C	424	
1	D	424	

2 Entry composition [i](#)

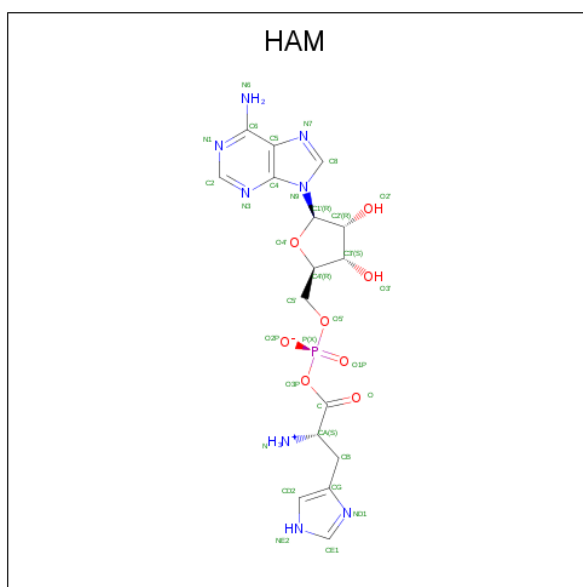
There are 3 unique types of molecules in this entry. The entry contains 14633 atoms, of which 2685 are hydrogens and 0 are deuteriums.

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 HISTIDYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	H	N	O	S	0	0	0
			3675	1884	682	535	563	11			
1	B	364	Total	C	H	N	O	S	0	0	0
			3472	1777	648	507	529	11			
1	C	387	Total	C	H	N	O	S	0	0	0
			3689	1892	684	538	564	11			
1	D	362	Total	C	H	N	O	S	0	0	0
			3453	1768	643	504	527	11			

- Molecule 2 is HISTIDYL-ADENOSINE MONOPHOSPHATE (three-letter code: HAM) (formula: $C_{16}H_{21}N_8O_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			40	16	7	8	8	1		
2	B	1	Total	C	H	N	O	P	0	0
			40	16	7	8	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	P	
			40	16	7	8	8	1	
2	D	1	Total	C	H	N	O	P	
			40	16	7	8	8	1	

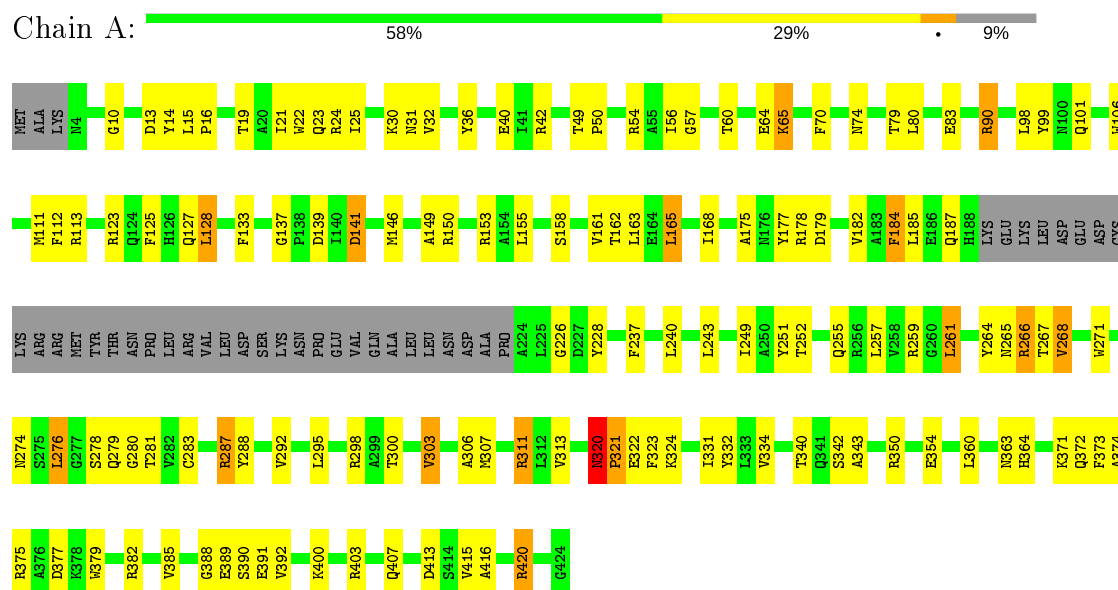
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O		
			45	45	0	0
3	B	50	Total	O		
			50	50	0	0
3	C	55	Total	O		
			55	55	0	0
3	D	34	Total	O		
			34	34	0	0

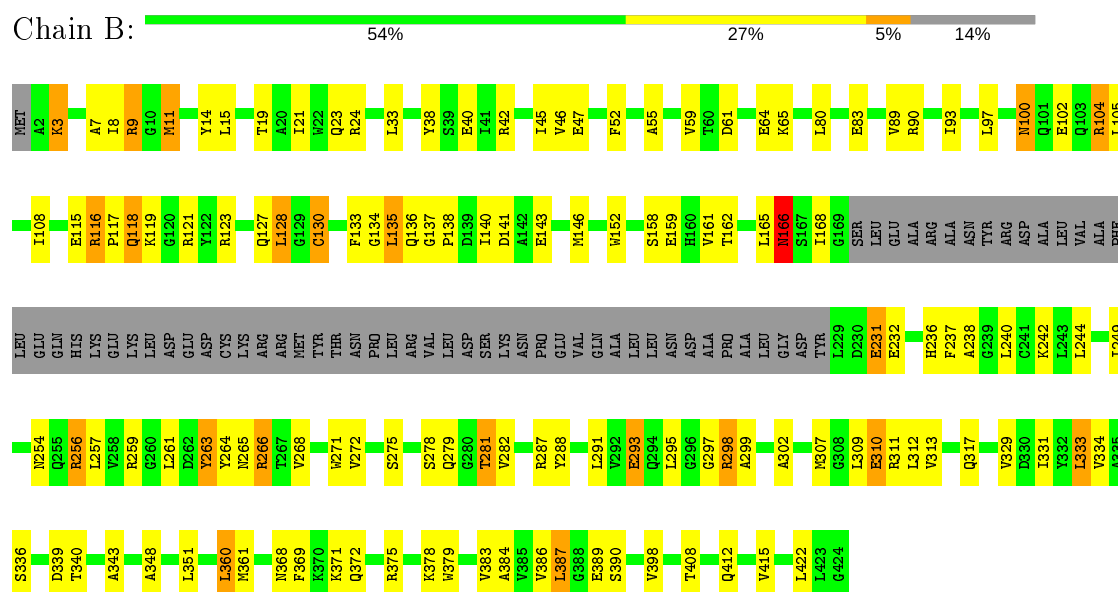
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: HISTIDYL-TRNA SYNTHETASE

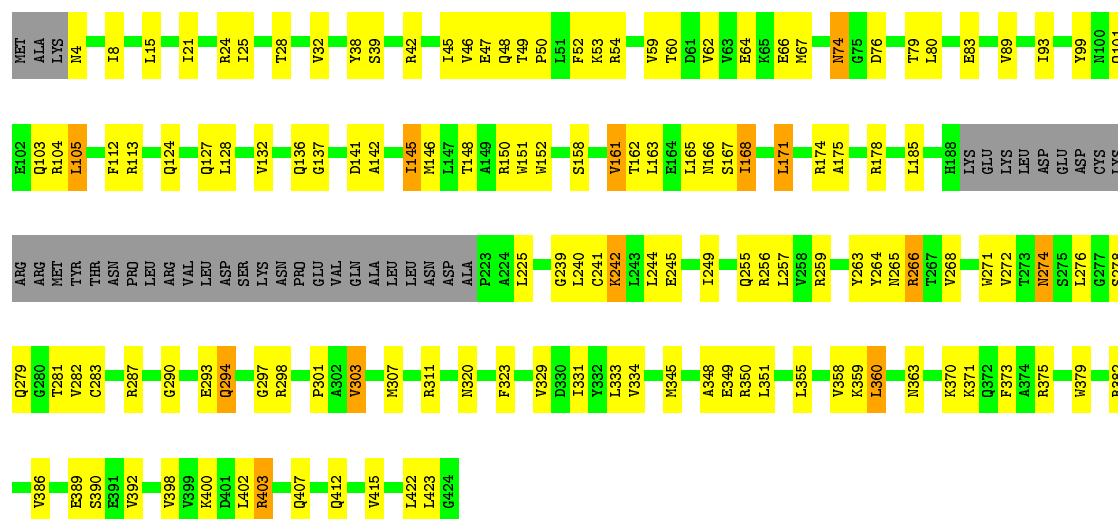


• Molecule 1: HISTIDYL-TRNA SYNTHETASE



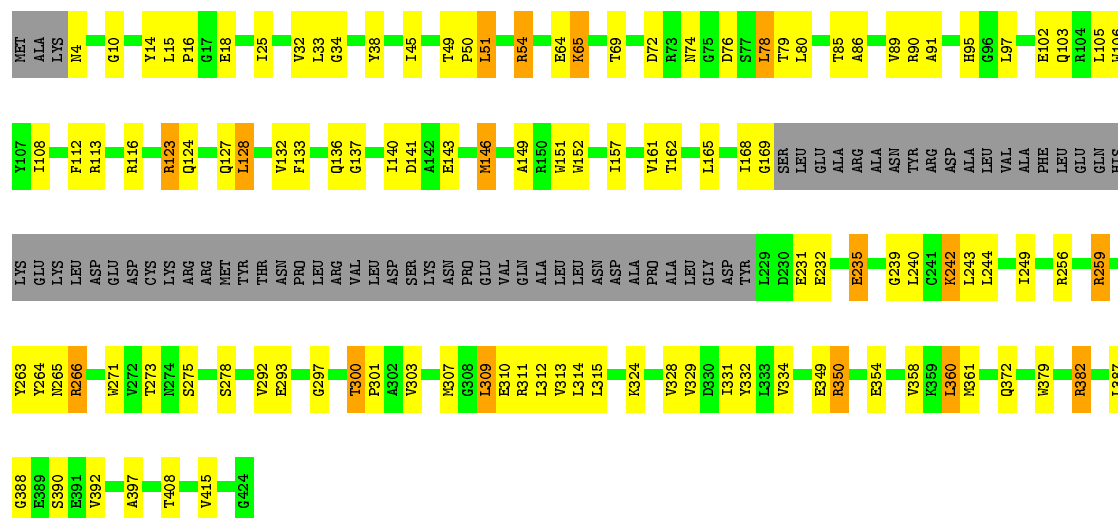
• Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain C: 



• Molecule 1: HISTIDYL-TRNA SYNTHETASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.40Å 110.70Å 108.70Å 115.00° 97.40° 90.00°	Depositor
Resolution (Å)	12.00 – 2.60 12.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	68.0 (12.00-2.60) 84.9 (12.04-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.66 (at 2.59Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.221 , 0.297 0.255 , 0.313	Depositor DCC
R_{free} test set	1684 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 89.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14633	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.59	0/3047	0.85	6/4123 (0.1%)
1	B	0.60	1/2875 (0.0%)	0.80	5/3888 (0.1%)
1	C	0.58	0/3061	0.80	4/4142 (0.1%)
1	D	0.57	0/2861	0.77	2/3870 (0.1%)
All	All	0.59	1/11844 (0.0%)	0.81	17/16023 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	CYS	CB-SG	-6.51	1.71	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASN	C-N-CD	-12.73	92.60	120.60
1	B	387	LEU	CA-CB-CG	7.16	131.76	115.30
1	A	323	PHE	N-CA-C	-6.18	94.31	111.00
1	C	323	PHE	N-CA-C	-5.88	95.12	111.00
1	D	360	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	128	LEU	N-CA-C	-5.54	96.03	111.00
1	A	303	VAL	CB-CA-C	-5.51	100.92	111.40
1	B	360	LEU	CA-CB-CG	5.47	127.87	115.30
1	B	257	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	128	LEU	CA-CB-CG	-5.36	102.98	115.30
1	C	128	LEU	N-CA-C	-5.33	96.60	111.00
1	C	360	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	128	LEU	N-CA-C	-5.28	96.75	111.00
1	A	261	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	105	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	311	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	LEU	N-CA-C	-5.02	97.45	111.00

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	2993	682	2949	88	0
1	B	2824	648	2798	113	0
1	C	3005	684	2962	95	0
1	D	2810	643	2780	85	0
2	A	33	7	21	2	0
2	B	33	7	21	1	0
2	C	33	7	21	2	0
2	D	33	7	21	5	0
3	A	45	0	0	1	0
3	B	50	0	0	1	0
3	C	55	0	0	1	0
3	D	34	0	0	0	0
All	All	11948	2685	11573	361	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (361) 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:D:382:ARG:HH11	1:D:382:ARG:HG2	1.35	0.90
1:B:3:LYS:NZ	1:B:3:LYS:HB3	1.87	0.89
1:B:89:VAL:HG21	1:B:291:LEU:HD22	1.55	0.89
1:D:311:ARG:NH1	2:D:450:HAM:H2'	1.88	0.89
1:A:161:VAL:HG12	1:A:271:TRP:HE3	1.38	0.88
1:B:8:ILE:HB	1:B:11:MET:HG3	1.55	0.85
1:D:311:ARG:HH12	2:D:450:HAM:H2'	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PRO:O	1:A:19:THR:HG22	1.75	0.85
1:B:298:ARG:HG3	1:B:298:ARG:HH11	1.42	0.85
1:B:116:ARG:HD2	1:B:116:ARG:H	1.45	0.82
1:B:278:SER:HA	1:B:311:ARG:HD2	1.62	0.81
1:A:278:SER:CB	1:A:311:ARG:HD3	2.11	0.80
1:B:278:SER:CA	1:B:311:ARG:HD2	2.14	0.78
1:B:9:ARG:H	1:B:9:ARG:HD3	1.52	0.74
1:C:239:GLY:O	1:C:242:LYS:HG3	1.88	0.73
1:A:161:VAL:HG12	1:A:271:TRP:CE3	2.24	0.73
1:A:292:VAL:HG21	1:A:300:THR:HG22	1.69	0.72
1:C:168:ILE:HG23	1:C:174:ARG:HE	1.55	0.72
1:B:115:GLU:HA	1:B:116:ARG:NH1	2.05	0.71
1:B:333:LEU:HD23	1:B:348:ALA:HB2	1.72	0.71
1:A:334:VAL:HG21	1:A:373:PHE:CE1	2.26	0.71
1:B:240:LEU:O	1:B:244:LEU:HD23	1.89	0.70
1:C:355:LEU:O	1:C:358:VAL:HG22	1.91	0.69
1:C:278:SER:CB	1:C:311:ARG:HD3	2.23	0.69
1:B:3:LYS:HZ2	1:B:3:LYS:HB3	1.57	0.69
1:D:328:VAL:HG23	1:D:329:VAL:HG23	1.75	0.69
1:A:165:LEU:HD22	1:A:237:PHE:HE1	1.57	0.69
1:A:146:MET:HG2	1:A:249:ILE:HD11	1.75	0.68
1:D:146:MET:HG3	1:D:249:ILE:HD11	1.74	0.68
1:A:19:THR:HG21	1:B:40:GLU:O	1.94	0.67
1:C:171:LEU:HA	1:C:174:ARG:NH1	2.09	0.67
1:C:175:ALA:HA	1:C:178:ARG:HE	1.57	0.67
1:D:273:THR:HG21	1:D:315:LEU:HD22	1.76	0.67
1:A:364:HIS:HD2	1:B:104:ARG:HH22	1.42	0.67
1:A:364:HIS:HD2	1:B:104:ARG:NH2	1.92	0.67
1:D:157:ILE:HD12	1:D:315:LEU:HD23	1.76	0.67
1:B:375:ARG:HA	1:B:378:LYS:HD2	1.76	0.66
1:C:67:MET:HE2	1:C:79:THR:HG21	1.77	0.66
1:B:293:GLU:HA	1:B:297:GLY:O	1.96	0.66
1:D:382:ARG:NH1	1:D:382:ARG:HG2	2.07	0.66
1:C:168:ILE:HG22	1:C:265:ASN:O	1.95	0.65
1:D:256:ARG:NE	1:D:256:ARG:HA	2.12	0.65
1:A:165:LEU:HD22	1:A:237:PHE:CE1	2.32	0.65
1:A:382:ARG:HD2	1:A:403:ARG:HH21	1.61	0.65
1:A:14:TYR:HB2	1:B:42:ARG:HB2	1.80	0.64
1:D:310:GLU:O	1:D:314:LEU:HG	1.98	0.63
1:C:311:ARG:NH1	2:C:450:HAM:H2'	2.14	0.63
1:A:57:GLY:O	1:A:60:THR:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:HG	1:C:174:ARG:HH12	1.64	0.62
1:A:15:LEU:HD22	1:B:97:LEU:HD11	1.80	0.62
1:C:45:ILE:H	1:D:124:GLN:HE22	1.47	0.62
1:C:279:GLN:HB2	1:C:311:ARG:NH2	2.14	0.62
1:B:102:GLU:HA	1:B:133:PHE:O	2.00	0.61
1:D:311:ARG:NH1	2:D:450:HAM:C2'	2.62	0.61
1:A:388:GLY:O	1:A:392:VAL:HG23	2.01	0.60
1:B:412:GLN:O	1:B:415:VAL:HG22	2.01	0.60
1:A:49:THR:N	1:A:50:PRO:HD2	2.17	0.60
1:B:115:GLU:HA	1:B:116:ARG:HH11	1.67	0.60
1:D:331:ILE:HD12	1:D:358:VAL:HG11	1.83	0.60
1:B:152:TRP:CD1	1:B:161:VAL:HG21	2.37	0.60
1:D:239:GLY:O	1:D:242:LYS:HG3	2.02	0.59
1:B:168:ILE:HG13	1:B:265:ASN:O	2.02	0.59
1:C:136:GLN:HG3	1:C:301:PRO:HG2	1.83	0.59
1:B:116:ARG:N	1:B:116:ARG:HD2	2.17	0.59
1:D:259:ARG:HB2	1:D:264:TYR:CD2	2.38	0.58
1:D:51:LEU:HD22	1:D:86:ALA:HB1	1.85	0.58
1:D:89:VAL:HG13	1:D:292:VAL:HG22	1.86	0.58
1:B:15:LEU:HD22	1:B:15:LEU:H	1.67	0.58
1:A:24:ARG:NH1	1:A:324:LYS:O	2.36	0.57
1:D:334:VAL:HG13	1:D:372:GLN:OE1	2.04	0.57
1:A:175:ALA:O	1:A:178:ARG:HG2	2.04	0.57
1:A:22:TRP:CE2	1:A:313:VAL:HG21	2.38	0.57
1:B:3:LYS:HZ3	1:B:3:LYS:HB3	1.70	0.57
1:C:290:GLY:O	1:C:294:GLN:HB2	2.04	0.57
1:B:336:SER:HB3	1:B:369:PHE:CZ	2.39	0.57
1:A:30:LYS:HE2	1:A:106:TRP:HH2	1.70	0.57
1:D:168:ILE:HB	1:D:265:ASN:O	2.05	0.56
1:D:293:GLU:HA	1:D:297:GLY:O	2.06	0.56
1:C:412:GLN:HA	1:C:415:VAL:HG23	1.86	0.56
1:D:49:THR:N	1:D:50:PRO:HD2	2.20	0.56
1:A:30:LYS:HE2	1:A:106:TRP:CH2	2.41	0.56
1:B:89:VAL:O	1:B:93:ILE:HG13	2.05	0.56
1:D:85:THR:O	1:D:89:VAL:HG23	2.05	0.56
1:A:10:GLY:HA3	1:A:123:ARG:HG3	1.87	0.56
1:B:259:ARG:HG3	1:B:259:ARG:HH11	1.71	0.56
1:D:242:LYS:HE2	1:D:243:LEU:HG	1.88	0.56
1:B:166:ASN:ND2	1:B:268:VAL:HG23	2.21	0.55
1:A:320:ASN:O	1:A:322:GLU:N	2.39	0.55
1:B:89:VAL:HG21	1:B:291:LEU:CD2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:O	1:B:166:ASN:HB3	2.06	0.55
1:C:259:ARG:NH1	1:C:264:TYR:OH	2.39	0.55
1:D:72:ASP:HB2	1:D:78:LEU:HD22	1.89	0.55
1:D:64:GLU:HB3	1:D:65:LYS:HD3	1.89	0.55
1:C:112:PHE:CE2	1:C:124:GLN:HG3	2.42	0.55
1:C:274:ASN:C	1:C:276:LEU:H	2.10	0.55
1:C:42:ARG:HB2	1:D:14:TYR:HB2	1.88	0.55
1:A:226:GLY:H	1:A:255:GLN:HE21	1.53	0.55
1:A:276:LEU:HD13	1:A:278:SER:O	2.07	0.54
1:C:350:ARG:HD2	1:C:351:LEU:HD12	1.87	0.54
1:D:128:LEU:HB2	1:D:309:LEU:HD11	1.89	0.54
1:A:36:TYR:HE1	1:A:150:ARG:HD2	1.71	0.54
1:A:49:THR:HG23	1:A:79:THR:OG1	2.07	0.54
1:C:375:ARG:O	1:C:379:TRP:CD1	2.61	0.54
1:A:364:HIS:CD2	1:B:104:ARG:NH2	2.75	0.54
1:C:163:LEU:HG	1:C:165:LEU:HD12	1.90	0.54
1:A:266:ARG:HB3	3:A:576:HOH:O	2.06	0.54
1:A:279:GLN:HG2	1:A:311:ARG:NH2	2.23	0.54
1:A:400:LYS:HE2	1:A:407:GLN:HE21	1.72	0.54
1:B:254:ASN:OD1	1:B:256:ARG:HG3	2.08	0.54
1:D:256:ARG:CZ	1:D:256:ARG:HA	2.38	0.54
1:A:112:PHE:HZ	1:B:45:ILE:HG13	1.73	0.54
1:C:8:ILE:HD11	1:D:78:LEU:HG	1.90	0.54
1:D:102:GLU:HA	1:D:133:PHE:O	2.07	0.54
1:A:182:VAL:HA	1:A:185:LEU:HD12	1.90	0.53
1:C:148:THR:O	1:C:151:TRP:HB2	2.08	0.53
1:A:21:ILE:O	1:A:25:ILE:HG13	2.07	0.53
1:A:42:ARG:HB2	1:B:14:TYR:HB2	1.91	0.53
1:C:271:TRP:HB2	1:C:283:CYS:HB3	1.90	0.53
1:D:259:ARG:NH1	1:D:264:TYR:OH	2.41	0.53
1:D:329:VAL:CG2	1:D:379:TRP:HB3	2.38	0.53
1:B:115:GLU:OE1	1:B:121:ARG:HD2	2.08	0.53
1:A:178:ARG:HG3	1:A:179:ASP:H	1.74	0.53
1:A:420:ARG:HH11	1:A:420:ARG:HG2	1.72	0.53
1:C:175:ALA:HA	1:C:178:ARG:NE	2.23	0.53
1:A:400:LYS:HG3	1:A:407:GLN:HB3	1.91	0.52
1:C:4:ASN:N	1:D:54:ARG:HH22	2.07	0.52
1:B:33:LEU:HD11	1:B:128:LEU:HD21	1.91	0.52
1:D:162:THR:O	1:D:271:TRP:HA	2.10	0.52
1:C:21:ILE:N	1:C:21:ILE:HD12	2.23	0.52
1:C:46:VAL:HG22	1:C:80:LEU:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD23	1:A:251:TYR:HB3	1.92	0.52
1:C:287:ARG:NH2	1:C:303:VAL:CG2	2.73	0.52
1:C:287:ARG:NH2	1:C:303:VAL:HG21	2.25	0.52
1:D:265:ASN:OD1	1:D:266:ARG:HG3	2.09	0.52
1:A:161:VAL:CG1	1:A:271:TRP:HE3	2.17	0.52
1:C:241:CYS:O	1:C:245:GLU:HG3	2.09	0.52
1:D:361:MET:HE2	1:D:379:TRP:NE1	2.24	0.52
1:A:264:TYR:HA	1:A:287:ARG:O	2.10	0.52
1:C:99:TYR:O	1:C:101:GLN:HG3	2.10	0.52
1:A:40:GLU:HB2	1:A:106:TRP:CZ2	2.45	0.51
1:A:13:ASP:OD2	1:B:90:ARG:NH2	2.43	0.51
1:C:278:SER:CB	1:C:311:ARG:HB3	2.41	0.51
1:C:47:GLU:HB2	1:C:52:PHE:CE2	2.45	0.51
1:A:350:ARG:NH2	1:A:413:ASP:HA	2.26	0.51
1:B:291:LEU:O	1:B:291:LEU:HD23	2.11	0.51
1:D:33:LEU:HD13	1:D:106:TRP:CG	2.45	0.51
1:A:178:ARG:HG3	1:A:179:ASP:N	2.26	0.51
1:A:184:PHE:CD1	1:A:184:PHE:C	2.84	0.51
1:B:102:GLU:OE2	1:B:135:LEU:HD11	2.10	0.51
1:C:171:LEU:HA	1:C:174:ARG:HH12	1.76	0.51
1:C:389:GLU:O	1:C:392:VAL:HG22	2.11	0.51
1:D:350:ARG:HD3	1:D:354:GLU:OE1	2.11	0.51
1:A:267:THR:H	1:A:287:ARG:HG3	1.76	0.50
1:B:162:THR:O	1:B:271:TRP:HA	2.10	0.50
1:D:278:SER:CB	1:D:311:ARG:HG3	2.40	0.50
1:C:333:LEU:CD1	1:C:348:ALA:HB2	2.42	0.50
1:C:171:LEU:HD23	1:C:178:ARG:HH22	1.75	0.50
1:B:311:ARG:HH11	1:B:311:ARG:HG3	1.76	0.50
1:D:49:THR:HG23	1:D:79:THR:OG1	2.12	0.50
1:B:281:THR:O	1:B:311:ARG:NH1	2.45	0.49
1:D:169:GLY:H	1:D:266:ARG:HA	1.77	0.49
1:A:332:TYR:CE2	1:A:363:ASN:HB2	2.47	0.49
1:C:171:LEU:CD2	1:C:178:ARG:HH22	2.25	0.49
1:D:232:GLU:HG3	1:D:266:ARG:NH2	2.27	0.49
1:A:177:TYR:HD1	1:A:228:TYR:CD1	2.30	0.49
1:B:298:ARG:HG3	1:B:298:ARG:NH1	2.17	0.49
1:B:278:SER:CB	1:B:311:ARG:HB3	2.42	0.49
1:C:74:ASN:HD22	1:C:74:ASN:C	2.16	0.49
1:D:265:ASN:OD1	1:D:266:ARG:N	2.46	0.49
1:C:175:ALA:HB2	1:C:178:ARG:HH21	1.77	0.49
1:D:15:LEU:HD22	1:D:15:LEU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:NH2	1:C:422:LEU:O	2.46	0.49
1:B:59:VAL:HG22	1:B:59:VAL:O	2.13	0.49
1:D:307:MET:SD	1:D:312:LEU:HD22	2.52	0.49
1:C:112:PHE:HZ	1:D:45:ILE:HD12	1.78	0.49
1:A:332:TYR:CZ	1:A:363:ASN:HB2	2.47	0.48
1:A:99:TYR:O	1:A:101:GLN:HG3	2.12	0.48
1:B:264:TYR:HA	1:B:287:ARG:O	2.13	0.48
1:C:331:ILE:O	1:C:360:LEU:HA	2.13	0.48
1:A:259:ARG:HG2	1:A:268:VAL:HG22	1.95	0.48
1:B:136:GLN:HA	1:B:287:ARG:NH1	2.28	0.48
1:A:259:ARG:HG2	1:A:268:VAL:CG2	2.44	0.48
1:A:259:ARG:NH1	1:A:264:TYR:OH	2.46	0.48
1:C:49:THR:HG22	1:C:53:LYS:HE2	1.96	0.48
1:B:38:TYR:CD1	1:B:38:TYR:N	2.82	0.48
1:C:168:ILE:CG2	1:C:174:ARG:HE	2.26	0.48
1:D:141:ASP:HB2	1:D:240:LEU:HD13	1.96	0.48
1:C:334:VAL:HG21	1:C:373:PHE:CE1	2.49	0.47
1:C:8:ILE:CD1	1:D:78:LEU:HG	2.45	0.47
1:B:238:ALA:O	1:B:242:LYS:HG2	2.15	0.47
1:C:21:ILE:O	1:C:25:ILE:HG13	2.15	0.47
1:D:141:ASP:CB	1:D:240:LEU:HD13	2.45	0.47
1:B:311:ARG:NH1	1:B:311:ARG:HG3	2.29	0.47
1:A:271:TRP:HB2	1:A:283:CYS:HB3	1.96	0.47
1:D:103:GLN:O	1:D:132:VAL:HA	2.15	0.47
1:D:140:ILE:HD12	1:D:143:GLU:HB3	1.97	0.47
1:B:134:GLY:C	1:B:135:LEU:HD13	2.34	0.47
1:B:21:ILE:N	1:B:21:ILE:HD12	2.29	0.47
1:B:313:VAL:O	1:B:317:GLN:HG3	2.15	0.47
1:B:102:GLU:OE2	1:B:135:LEU:HD21	2.15	0.46
1:C:142:ALA:HB1	1:C:146:MET:HE3	1.97	0.46
1:D:136:GLN:NE2	1:D:266:ARG:NH1	2.64	0.46
1:D:74:ASN:HB3	1:D:76:ASP:OD2	2.14	0.46
1:C:166:ASN:HB3	1:C:268:VAL:HG23	1.96	0.46
1:A:354:GLU:OE1	1:A:416:ALA:HB2	2.15	0.46
1:B:161:VAL:HA	1:B:272:VAL:O	2.16	0.46
1:C:163:LEU:HG	1:C:165:LEU:CD1	2.45	0.46
1:C:168:ILE:HG23	1:C:174:ARG:NE	2.26	0.46
1:D:108:ILE:HA	1:D:127:GLN:O	2.16	0.46
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.70	0.46
1:C:400:LYS:HD3	1:C:407:GLN:NE2	2.31	0.46
1:C:67:MET:CE	1:C:79:THR:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ALA:O	1:D:95:HIS:HD2	1.99	0.46
1:C:359:LYS:HG2	1:D:34:GLY:O	2.16	0.46
1:A:278:SER:C	1:A:280:GLY:N	2.67	0.46
1:B:329:VAL:CG2	1:B:379:TRP:HB3	2.45	0.46
1:C:104:ARG:HG2	1:C:132:VAL:HG13	1.98	0.46
1:C:163:LEU:HD21	1:C:165:LEU:HD11	1.98	0.46
1:D:334:VAL:HG22	1:D:372:GLN:HB3	1.98	0.46
1:B:361:MET:HE2	1:B:379:TRP:NE1	2.32	0.45
1:D:32:VAL:HB	1:D:151:TRP:HE1	1.82	0.45
1:B:108:ILE:HA	1:B:127:GLN:O	2.15	0.45
1:B:61:ASP:HA	1:B:64:GLU:HB2	1.99	0.45
1:C:127:GLN:HA	1:C:307:MET:O	2.16	0.45
1:B:38:TYR:HD1	1:B:38:TYR:N	2.15	0.45
1:A:298:ARG:HG3	1:A:298:ARG:HH11	1.82	0.45
1:B:115:GLU:O	1:B:117:PRO:HD3	2.16	0.45
1:B:291:LEU:C	1:B:291:LEU:HD23	2.37	0.45
1:C:15:LEU:HD22	1:D:97:LEU:HD11	1.99	0.45
1:C:375:ARG:O	1:C:379:TRP:HD1	1.98	0.45
1:C:74:ASN:ND2	1:C:76:ASP:H	2.15	0.45
1:B:146:MET:HG3	1:B:249:ILE:HD11	1.98	0.45
1:B:278:SER:C	1:B:311:ARG:HD2	2.37	0.45
1:B:278:SER:HA	1:B:311:ARG:HB3	1.98	0.45
1:C:386:VAL:HB	1:C:398:VAL:HB	1.97	0.45
1:D:232:GLU:O	1:D:235:GLU:HG2	2.16	0.45
1:A:127:GLN:HA	1:A:307:MET:O	2.15	0.45
1:D:146:MET:O	1:D:149:ALA:HB3	2.16	0.45
1:D:278:SER:CB	1:D:311:ARG:CG	2.95	0.45
1:C:333:LEU:HD13	1:C:348:ALA:HB2	1.98	0.45
1:C:89:VAL:O	1:C:93:ILE:HG13	2.16	0.45
1:B:138:PRO:HD3	1:B:236:HIS:CD2	2.52	0.45
1:B:278:SER:CB	1:B:282:VAL:HG22	2.47	0.45
1:D:361:MET:CE	1:D:379:TRP:NE1	2.80	0.45
1:A:320:ASN:HA	1:A:321:PRO:HD2	1.64	0.44
1:A:90:ARG:NH2	1:B:7:ALA:HB2	2.31	0.44
1:B:261:LEU:HD12	1:B:263:TYR:OH	2.17	0.44
1:B:310:GLU:HG2	1:B:310:GLU:H	1.47	0.44
1:B:288:TYR:CD2	1:B:288:TYR:O	2.70	0.44
1:C:113:ARG:NH2	2:C:450:HAM:O2P	2.47	0.44
1:C:67:MET:HE2	1:C:67:MET:HB3	1.74	0.44
1:D:152:TRP:CD1	1:D:161:VAL:HG21	2.52	0.44
1:A:340:THR:O	1:A:343:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLU:H	1:A:391:GLU:CD	2.20	0.44
1:B:55:ALA:HB2	1:B:295:LEU:HD11	1.99	0.44
1:B:386:VAL:HB	1:B:398:VAL:HB	2.00	0.44
1:C:145:ILE:HG22	1:C:249:ILE:HD13	1.98	0.44
1:C:282:VAL:O	1:C:307:MET:HG3	2.17	0.44
1:C:62:VAL:HA	1:C:66:GLU:HB2	2.00	0.44
1:D:331:ILE:O	1:D:360:LEU:HA	2.18	0.44
1:A:363:ASN:OD1	1:A:372:GLN:HG2	2.18	0.44
1:B:133:PHE:CD1	1:B:302:ALA:HB2	2.53	0.44
1:C:274:ASN:C	1:C:276:LEU:N	2.69	0.44
1:B:128:LEU:HB2	1:B:309:LEU:HD21	1.98	0.44
1:C:266:ARG:HB3	3:C:505:HOH:O	2.18	0.44
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.53	0.43
1:C:38:TYR:CD1	1:C:38:TYR:N	2.86	0.43
1:C:403:ARG:HG3	1:C:403:ARG:H	1.59	0.43
1:A:113:ARG:NH2	2:A:450:HAM:O2P	2.48	0.43
1:A:64:GLU:CB	1:A:65:LYS:HD3	2.47	0.43
1:B:166:ASN:HA	1:B:237:PHE:CZ	2.53	0.43
1:B:231:GLU:HG2	1:B:232:GLU:N	2.33	0.43
1:D:38:TYR:CD1	1:D:38:TYR:N	2.86	0.43
1:C:28:THR:O	1:C:32:VAL:HG23	2.19	0.43
1:D:146:MET:HG3	1:D:249:ILE:CD1	2.45	0.43
1:D:388:GLY:O	1:D:392:VAL:HG23	2.18	0.43
1:A:385:VAL:HG23	1:A:385:VAL:O	2.18	0.43
1:B:259:ARG:HB2	1:B:264:TYR:CD2	2.53	0.43
1:C:103:GLN:HB3	1:C:105:LEU:HD21	2.01	0.43
1:A:111:MET:HB2	1:A:125:PHE:CZ	2.54	0.43
1:A:149:ALA:O	1:A:153:ARG:HG3	2.19	0.43
1:A:32:VAL:O	1:A:36:TYR:HD1	2.01	0.43
1:B:152:TRP:HE3	1:B:152:TRP:HA	1.84	0.43
1:A:371:LYS:O	1:A:374:ALA:HB3	2.20	0.42
1:A:375:ARG:O	1:A:379:TRP:CD1	2.72	0.42
1:A:16:PRO:HG3	1:B:105:LEU:HD22	2.01	0.42
1:B:121:ARG:NH1	2:B:450:HAM:N7	2.66	0.42
1:A:98:LEU:HD22	1:A:133:PHE:CG	2.54	0.42
1:D:259:ARG:HB2	1:D:264:TYR:HD2	1.82	0.42
1:D:331:ILE:CD1	1:D:358:VAL:HG11	2.47	0.42
1:A:374:ALA:HA	1:A:377:ASP:OD2	2.19	0.42
1:B:46:VAL:HG22	1:B:80:LEU:HD13	2.02	0.42
1:C:293:GLU:HA	1:C:297:GLY:O	2.18	0.42
1:D:69:THR:HG23	1:D:79:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:HG21	1:A:373:PHE:HE1	1.81	0.42
1:B:259:ARG:NH1	1:B:264:TYR:OH	2.50	0.42
1:B:331:ILE:O	1:B:360:LEU:HA	2.19	0.42
1:C:150:ARG:NH2	1:D:349:GLU:OE1	2.49	0.42
1:C:167:SER:HA	1:C:266:ARG:O	2.19	0.42
1:C:345:MET:O	1:C:349:GLU:HG2	2.20	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.70	0.42
1:B:141:ASP:HB2	1:B:240:LEU:HD13	2.02	0.42
1:D:300:THR:HA	1:D:301:PRO:HD3	1.90	0.42
1:D:72:ASP:C	1:D:74:ASN:H	2.22	0.42
1:C:276:LEU:C	1:C:278:SER:N	2.72	0.42
1:D:38:TYR:HD1	1:D:38:TYR:N	2.18	0.42
1:D:397:ALA:HB3	1:D:415:VAL:HG21	2.02	0.42
1:B:279:GLN:HA	1:B:279:GLN:NE2	2.35	0.41
1:C:60:THR:O	1:C:64:GLU:HG3	2.20	0.41
1:D:329:VAL:HG21	1:D:379:TRP:HB3	2.02	0.41
1:A:306:ALA:HB3	2:A:450:HAM:HB2	2.01	0.41
1:C:32:VAL:HG13	1:C:150:ARG:HD2	2.01	0.41
1:C:259:ARG:CZ	1:C:259:ARG:HB3	2.50	0.41
1:A:161:VAL:CG1	1:A:271:TRP:CE3	2.97	0.41
1:B:298:ARG:HH11	1:B:298:ARG:CG	2.23	0.41
1:C:74:ASN:HD22	1:C:76:ASP:H	1.68	0.41
1:D:33:LEU:HG	1:D:151:TRP:HZ2	1.85	0.41
1:D:113:ARG:NH1	2:D:450:HAM:O2P	2.52	0.41
1:A:56:ILE:HG22	1:A:60:THR:HG21	2.03	0.41
1:B:152:TRP:CE3	1:B:152:TRP:HA	2.55	0.41
1:B:307:MET:SD	1:B:312:LEU:HD22	2.60	0.41
1:C:334:VAL:HG21	1:C:373:PHE:HE1	1.85	0.41
1:C:48:GLN:HB3	1:C:50:PRO:HD2	2.02	0.41
1:B:152:TRP:CE3	1:B:152:TRP:CA	3.03	0.41
1:B:368:ASN:H	1:B:371:LYS:HZ2	1.68	0.41
1:D:25:ILE:HD12	1:D:313:VAL:HG22	2.03	0.41
1:B:334:VAL:HG13	1:B:372:GLN:OE1	2.21	0.41
1:B:9:ARG:HE	1:B:123:ARG:NH2	2.19	0.41
1:A:331:ILE:O	1:A:360:LEU:HA	2.21	0.41
1:B:298:ARG:HD2	1:B:299:ALA:N	2.36	0.41
1:C:382:ARG:O	1:C:402:LEU:HB2	2.20	0.41
1:C:67:MET:HE2	1:C:79:THR:CG2	2.50	0.41
1:D:112:PHE:N	1:D:112:PHE:CD1	2.89	0.41
1:D:259:ARG:NH2	2:D:450:HAM:O1P	2.54	0.41
1:B:140:ILE:HD12	1:B:143:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LEU:HD11	1:D:244:LEU:CD1	2.50	0.41
1:B:118:GLN:HE21	1:B:121:ARG:HG3	1.85	0.41
1:B:118:GLN:HG2	1:B:121:ARG:HB2	2.03	0.41
1:B:278:SER:HA	1:B:311:ARG:CD	2.42	0.41
1:B:298:ARG:NH1	1:B:299:ALA:O	2.54	0.41
1:B:42:ARG:HA	3:B:597:HOH:O	2.20	0.41
1:A:113:ARG:O	1:A:123:ARG:HA	2.21	0.41
1:A:70:PHE:HE1	1:A:80:LEU:CD1	2.34	0.41
1:C:331:ILE:HD11	1:C:423:LEU:HD11	2.03	0.41
1:B:133:PHE:HD1	1:B:302:ALA:HB2	1.85	0.41
1:B:383:VAL:HG12	1:B:384:ALA:N	2.36	0.41
1:D:10:GLY:HA3	1:D:123:ARG:HG3	2.02	0.41
1:D:332:TYR:HE1	1:D:361:MET:HE2	1.85	0.41
1:A:141:ASP:HB2	1:A:240:LEU:HD13	2.03	0.40
1:A:168:ILE:HG12	1:A:265:ASN:O	2.21	0.40
1:B:295:LEU:HD23	1:B:295:LEU:HA	1.85	0.40
1:B:422:LEU:HA	1:B:422:LEU:HD23	1.90	0.40
1:C:161:VAL:HA	1:C:272:VAL:O	2.20	0.40
1:C:38:TYR:HD1	1:C:38:TYR:N	2.19	0.40
1:B:118:GLN:HB2	1:B:119:LYS:H	1.74	0.40
1:B:19:THR:O	1:B:23:GLN:HG3	2.21	0.40
1:B:340:THR:O	1:B:343:ALA:HB3	2.21	0.40
1:A:162:THR:HG22	1:A:163:LEU:N	2.36	0.40
1:B:100:ASN:ND2	1:B:100:ASN:O	2.54	0.40
1:B:351:LEU:HD21	1:B:415:VAL:HG23	2.03	0.40
1:C:152:TRP:HB3	1:C:158:SER:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	382/424 (90%)	360 (94%)	16 (4%)	6 (2%)	9	19
1	B	360/424 (85%)	340 (94%)	17 (5%)	3 (1%)	19	39
1	C	383/424 (90%)	358 (94%)	23 (6%)	2 (0%)	29	52
1	D	358/424 (84%)	342 (96%)	14 (4%)	2 (1%)	25	47
All	All	1483/1696 (87%)	1400 (94%)	70 (5%)	13 (1%)	17	35

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	PRO
1	A	137	GLY
1	B	137	GLY
1	C	137	GLY
1	A	266	ARG
1	D	137	GLY
1	A	187	GLN
1	A	288	TYR
1	B	166	ASN
1	B	266	ARG
1	D	266	ARG
1	A	320	ASN
1	C	59	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/342 (89%)	275 (90%)	29 (10%)	8	16
1	B	289/342 (84%)	259 (90%)	30 (10%)	7	13
1	C	306/342 (90%)	274 (90%)	32 (10%)	7	13
1	D	288/342 (84%)	260 (90%)	28 (10%)	8	15
All	All	1187/1368 (87%)	1068 (90%)	119 (10%)	7	14

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	31	ASN
1	A	54	ARG
1	A	65	LYS
1	A	74	ASN
1	A	83	GLU
1	A	90	ARG
1	A	128	LEU
1	A	139	ASP
1	A	141	ASP
1	A	155	LEU
1	A	158	SER
1	A	165	LEU
1	A	184	PHE
1	A	243	LEU
1	A	252	THR
1	A	257	LEU
1	A	261	LEU
1	A	268	VAL
1	A	276	LEU
1	A	281	THR
1	A	287	ARG
1	A	295	LEU
1	A	303	VAL
1	A	342	SER
1	A	389	GLU
1	A	390	SER
1	A	415	VAL
1	A	420	ARG
1	B	3	LYS
1	B	9	ARG
1	B	11	MET
1	B	24	ARG
1	B	65	LYS
1	B	83	GLU
1	B	100	ASN
1	B	104	ARG
1	B	116	ARG
1	B	118	GLN
1	B	130	CYS
1	B	135	LEU
1	B	158	SER
1	B	159	GLU

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Mol	Chain	Res	Type
1	B	166	ASN
1	B	231	GLU
1	B	256	ARG
1	B	263	TYR
1	B	266	ARG
1	B	275	SER
1	B	281	THR
1	B	293	GLU
1	B	298	ARG
1	B	310	GLU
1	B	333	LEU
1	B	339	ASP
1	B	387	LEU
1	B	389	GLU
1	B	390	SER
1	B	408	THR
1	C	24	ARG
1	C	39	SER
1	C	54	ARG
1	C	74	ASN
1	C	83	GLU
1	C	141	ASP
1	C	145	ILE
1	C	161	VAL
1	C	162	THR
1	C	168	ILE
1	C	171	LEU
1	C	225	LEU
1	C	240	LEU
1	C	242	LYS
1	C	244	LEU
1	C	255	GLN
1	C	256	ARG
1	C	257	LEU
1	C	263	TYR
1	C	266	ARG
1	C	274	ASN
1	C	281	THR
1	C	294	GLN
1	C	298	ARG
1	C	303	VAL
1	C	320	ASN

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Mol	Chain	Res	Type
1	C	329	VAL
1	C	363	ASN
1	C	370	LYS
1	C	371	LYS
1	C	390	SER
1	C	403	ARG
1	D	4	ASN
1	D	16	PRO
1	D	18	GLU
1	D	51	LEU
1	D	54	ARG
1	D	65	LYS
1	D	78	LEU
1	D	80	LEU
1	D	90	ARG
1	D	105	LEU
1	D	116	ARG
1	D	123	ARG
1	D	146	MET
1	D	231	GLU
1	D	235	GLU
1	D	242	LYS
1	D	259	ARG
1	D	263	TYR
1	D	275	SER
1	D	300	THR
1	D	303	VAL
1	D	309	LEU
1	D	324	LYS
1	D	350	ARG
1	D	382	ARG
1	D	387	LEU
1	D	390	SER
1	D	408	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	12	ASN
1	A	23	GLN
1	A	74	ASN

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Mol	Chain	Res	Type
1	A	160	HIS
1	A	236	HIS
1	A	255	GLN
1	A	274	ASN
1	A	364	HIS
1	A	407	GLN
1	B	23	GLN
1	B	166	ASN
1	B	341	GLN
1	B	418	HIS
1	C	48	GLN
1	C	74	ASN
1	C	100	ASN
1	C	160	HIS
1	C	274	ASN
1	D	114	HIS
1	D	124	GLN
1	D	136	GLN
1	D	236	HIS
1	D	364	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	HAM	C	450	-	28,36,36	1.21	2 (7%)	30,53,53	1.20	4 (13%)
2	HAM	A	450	-	28,36,36	1.20	3 (10%)	30,53,53	1.30	4 (13%)
2	HAM	D	450	-	28,36,36	1.04	1 (3%)	30,53,53	0.99	2 (6%)
2	HAM	B	450	-	28,36,36	1.17	1 (3%)	30,53,53	1.15	2 (6%)

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	HAM	C	450	-	-	5/17/39/39	0/4/4/4
2	HAM	A	450	-	-	3/17/39/39	0/4/4/4
2	HAM	D	450	-	-	4/17/39/39	0/4/4/4
2	HAM	B	450	-	-	3/17/39/39	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	450	HAM	P-O3P	4.63	1.70	1.60
2	B	450	HAM	P-O3P	4.40	1.69	1.60
2	A	450	HAM	P-O3P	4.04	1.68	1.60
2	D	450	HAM	P-O3P	3.41	1.67	1.60
2	A	450	HAM	O-C	2.19	1.26	1.21
2	C	450	HAM	C8-N7	-2.01	1.31	1.34
2	A	450	HAM	C2-N3	2.00	1.35	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	450	HAM	O-C-CA	-3.75	108.59	120.95
2	A	450	HAM	O-C-CA	-3.54	109.31	120.95
2	B	450	HAM	O-C-CA	-3.53	109.33	120.95
2	A	450	HAM	O2P-P-O3P	3.30	114.92	104.14
2	D	450	HAM	O-C-CA	-3.19	110.46	120.95
2	B	450	HAM	C5-C6-N6	2.72	124.48	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	450	HAM	C5-C6-N6	2.35	123.92	120.35
2	D	450	HAM	C5-C6-N6	2.32	123.88	120.35
2	C	450	HAM	O2P-P-O3P	2.25	111.49	104.14
2	C	450	HAM	C5-C6-N6	2.24	123.75	120.35
2	C	450	HAM	O3P-P-O5'	2.15	109.19	102.92
2	A	450	HAM	O3P-P-O5'	2.14	109.17	102.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	450	HAM	C5'-O5'-P-O1P
2	A	450	HAM	C5'-O5'-P-O2P
2	D	450	HAM	C5'-O5'-P-O1P
2	B	450	HAM	CA-CB-CG-ND1
2	A	450	HAM	C5'-O5'-P-O3P
2	C	450	HAM	C-O3P-P-O5'
2	C	450	HAM	C5'-O5'-P-O3P
2	D	450	HAM	C5'-O5'-P-O3P
2	D	450	HAM	C-O3P-P-O5'
2	B	450	HAM	C-O3P-P-O5'
2	C	450	HAM	C-O3P-P-O1P
2	C	450	HAM	C5'-O5'-P-O1P
2	B	450	HAM	C5'-O5'-P-O1P
2	D	450	HAM	CA-CB-CG-CD2
2	C	450	HAM	O3P-C-CA-N

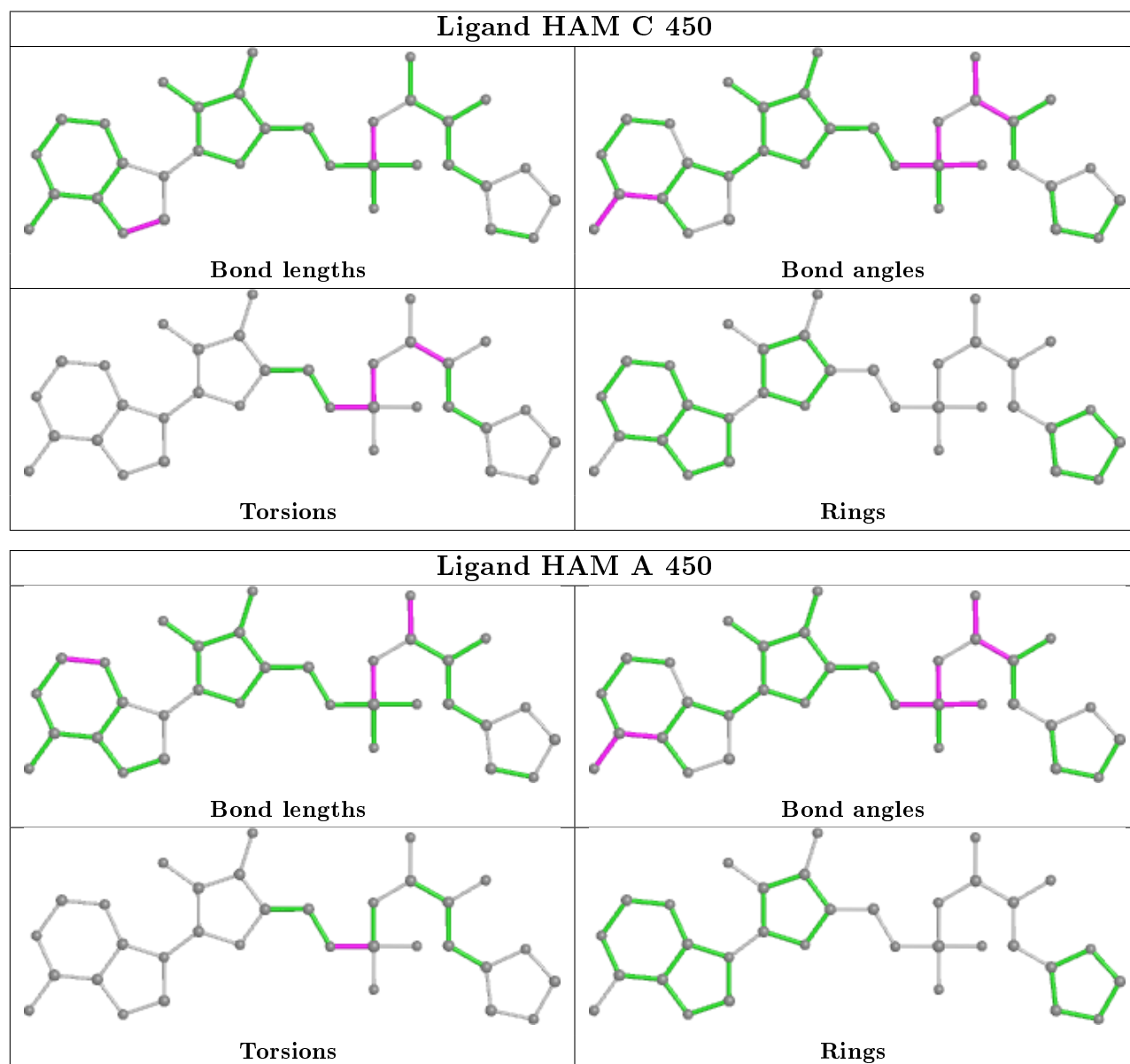
There are no ring outliers.

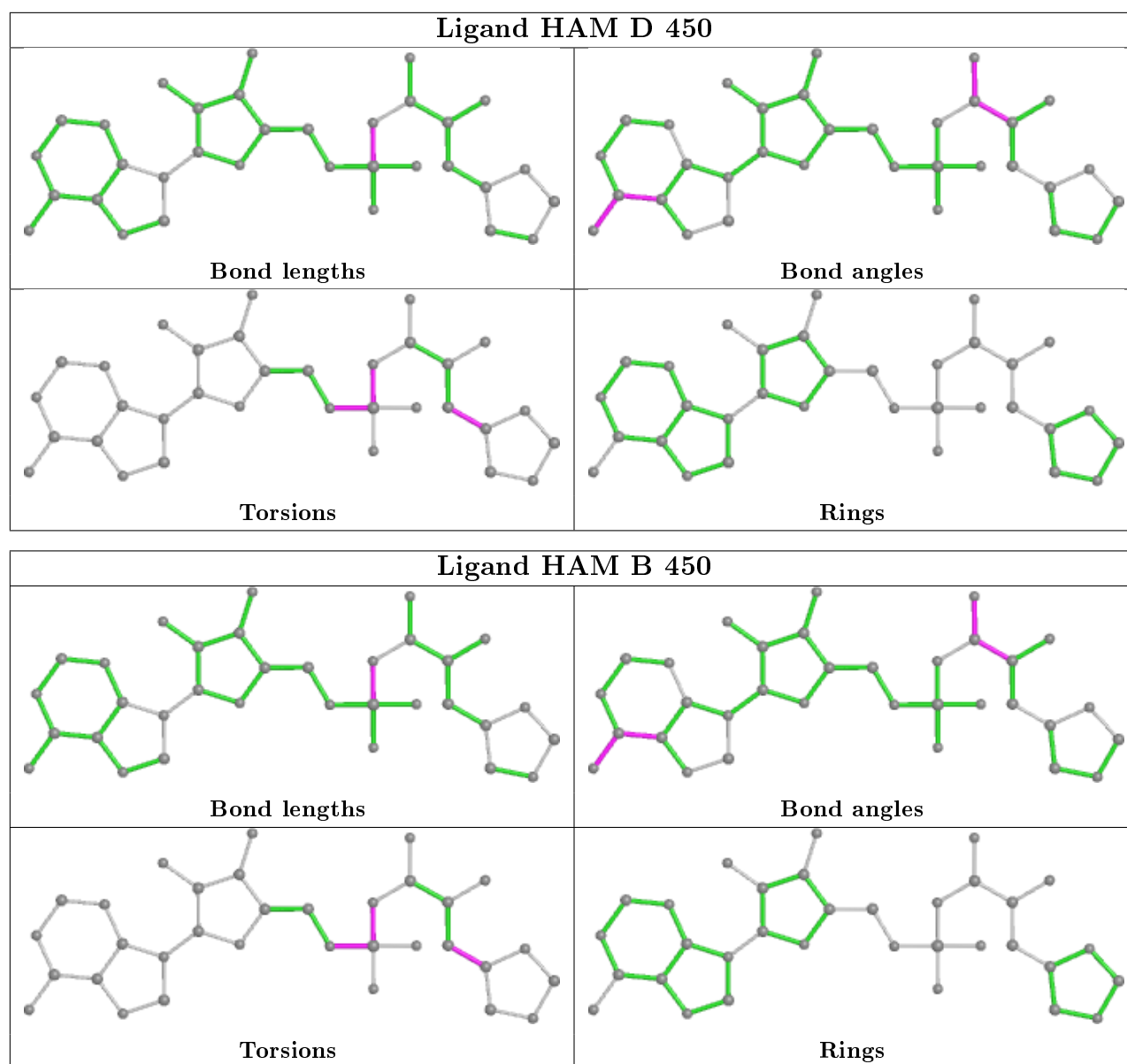
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	450	HAM	2	0
2	A	450	HAM	2	0
2	D	450	HAM	5	0
2	B	450	HAM	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

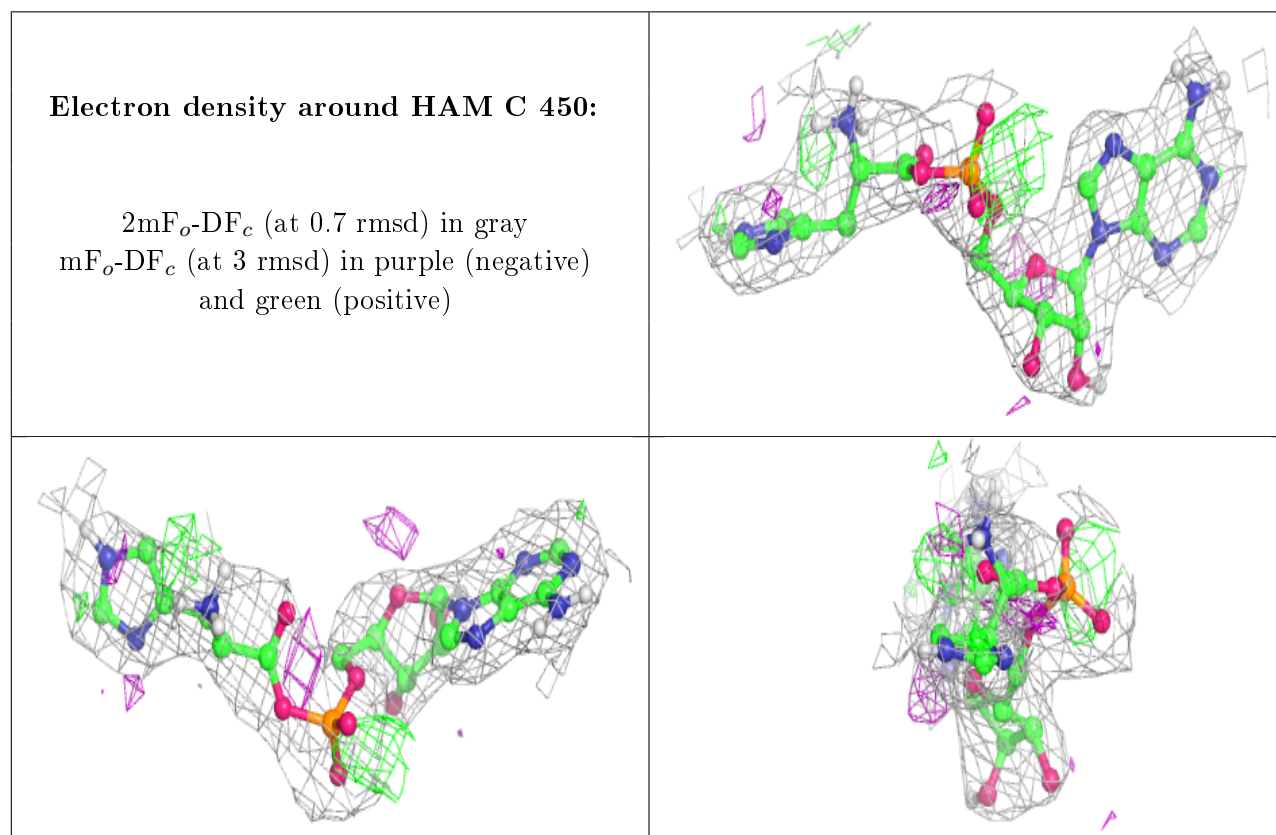
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

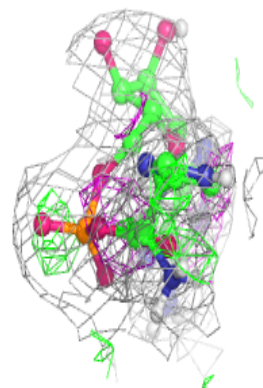
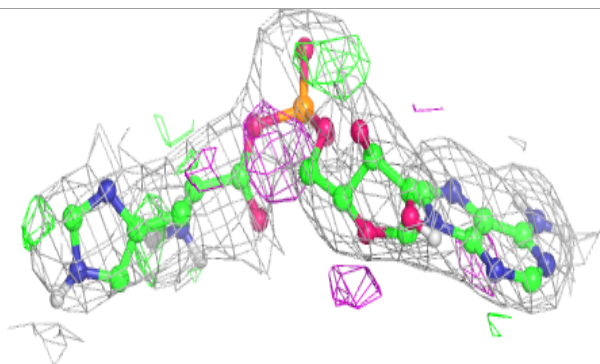
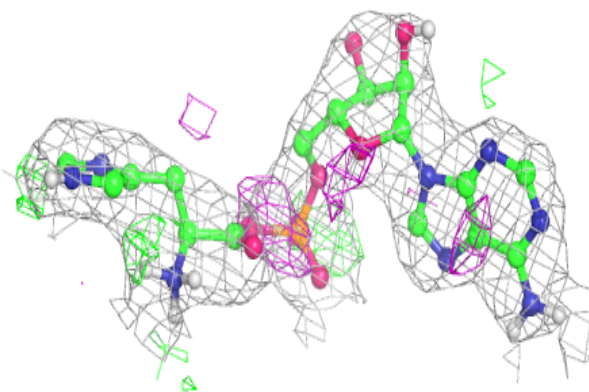
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

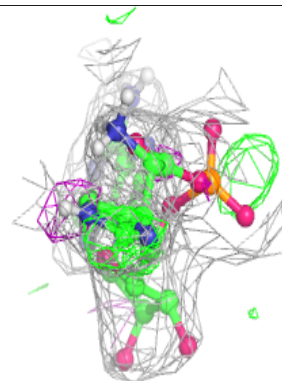
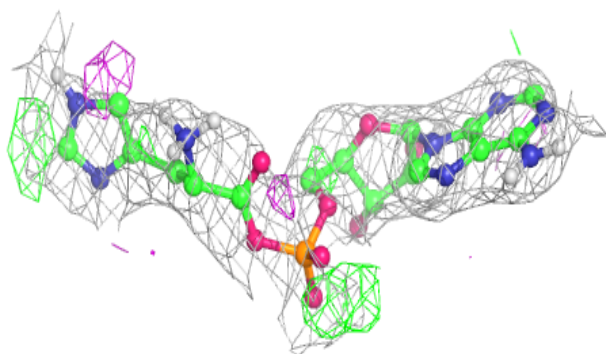
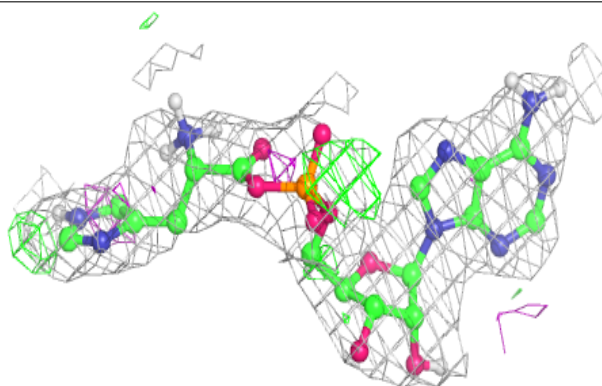


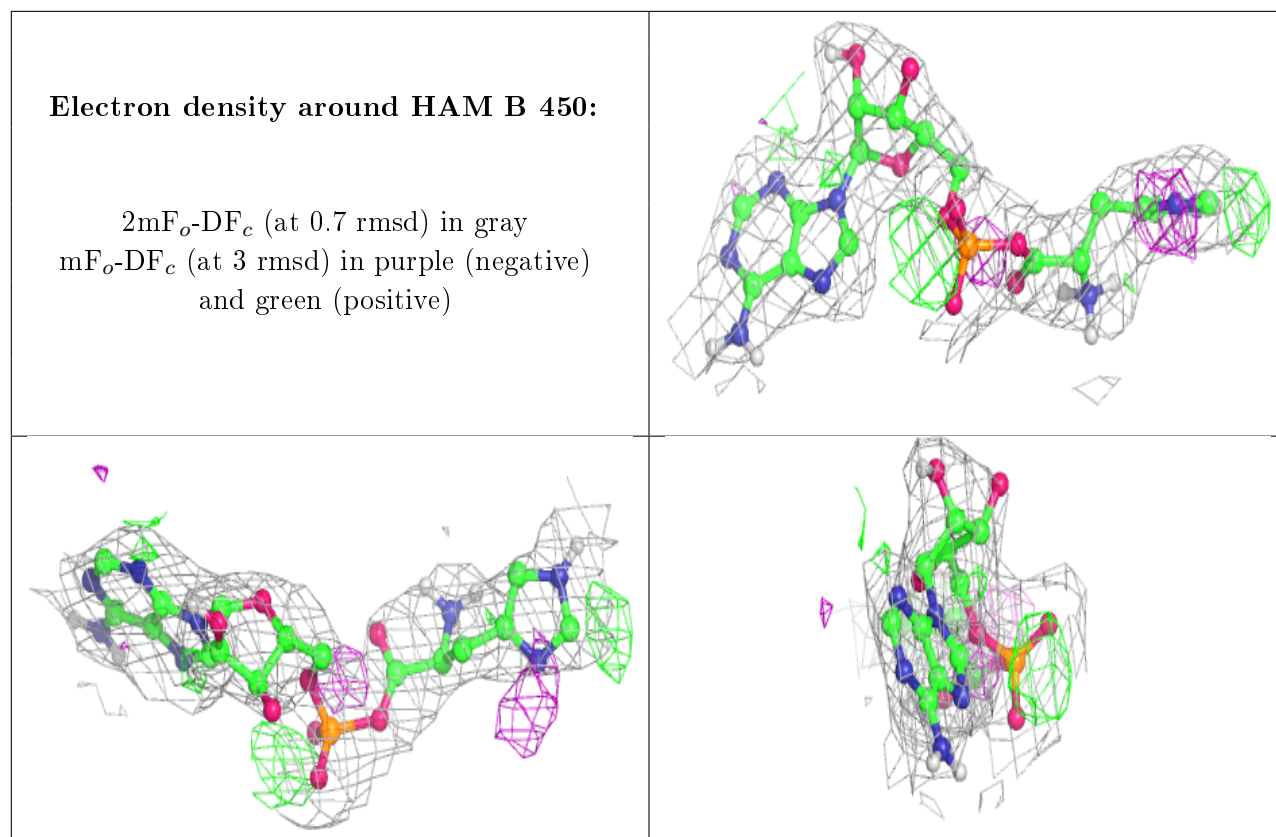
Electron density around HAM A 450:

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

**Electron density around HAM D 450:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.