



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:36 AM UTC

PDB ID : 1KMM / pdb_00001kmm
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 types of validation reports are described at

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

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

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

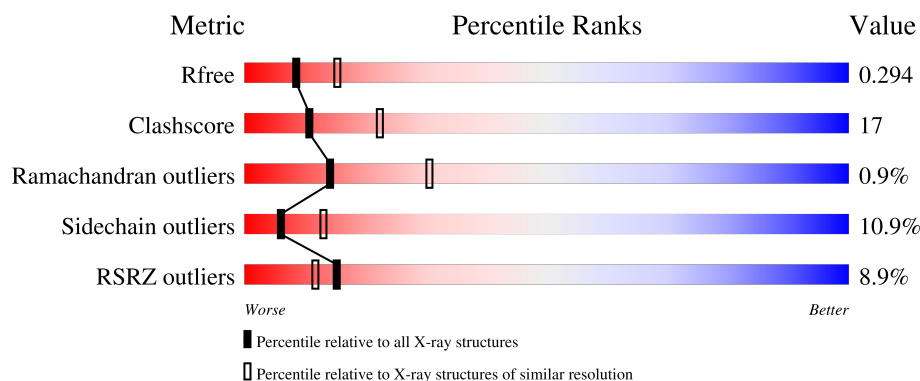
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	424	9% 55% 31% • 9%
1	B	424	7% 50% 29% 6% • 14%
1	C	424	7% 56% 31% • • 9%
1	D	424	8% 55% 26% • 15%

2 Entry composition [i](#)

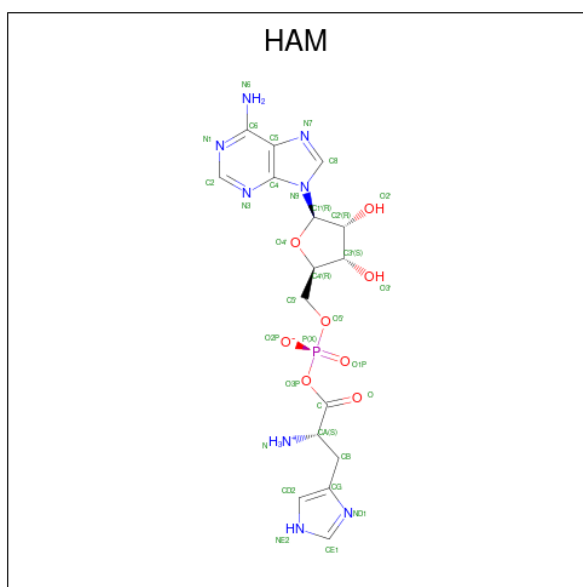
There are 3 unique types of molecules in this entry. The entry contains 14633 atoms, of which 2685 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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	0	0
			40	16	7	8	8	1		
2	D	1	Total	C	H	N	O	P	0	0
			40	16	7	8	8	1		

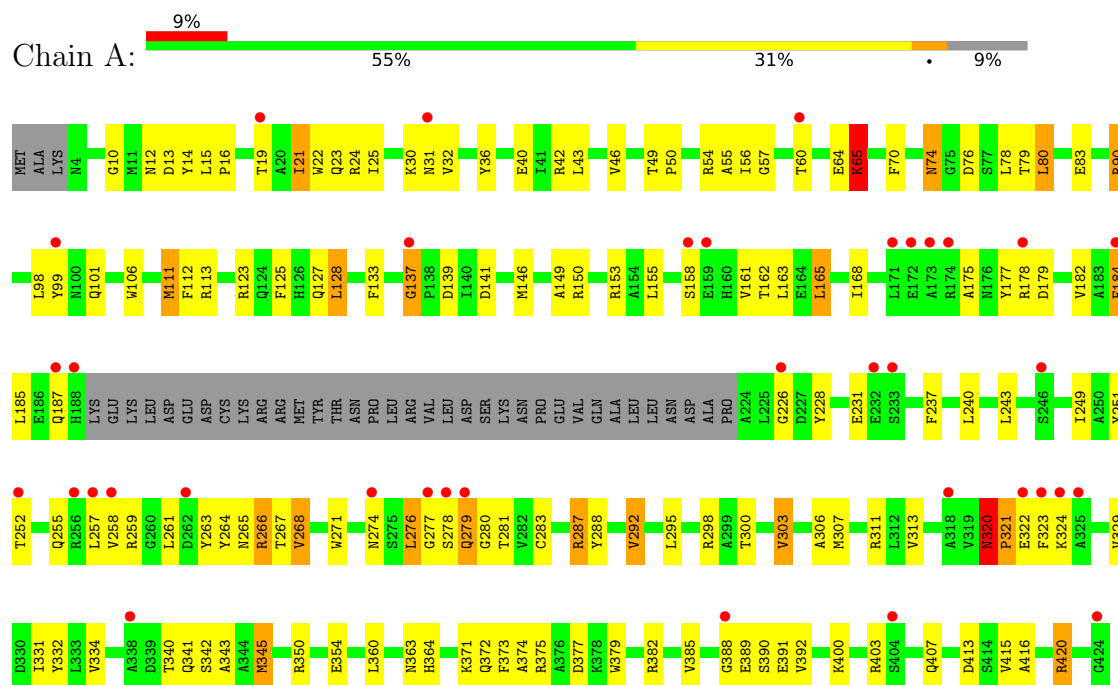
- Molecule 3 is water.

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

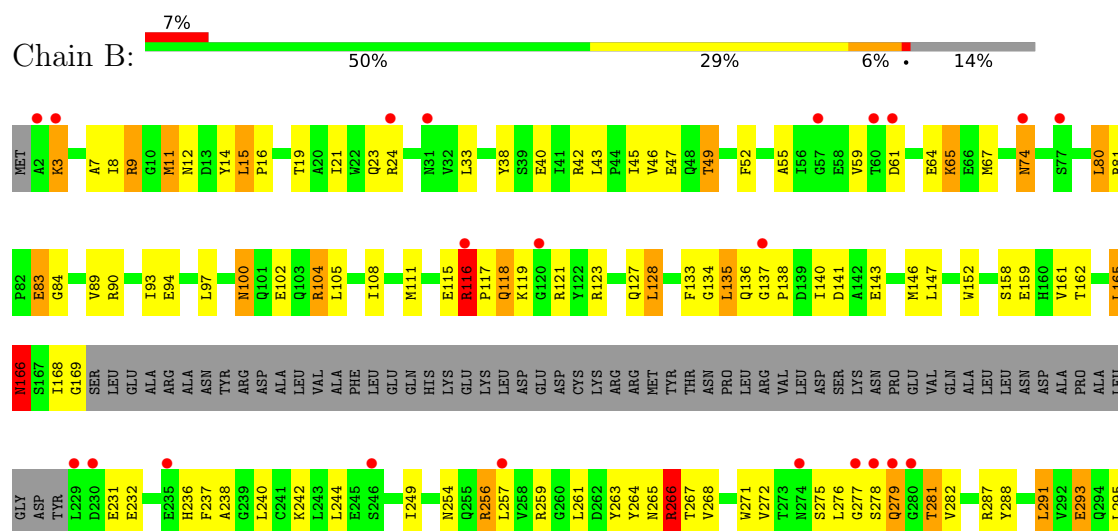
3 Residue-property plots

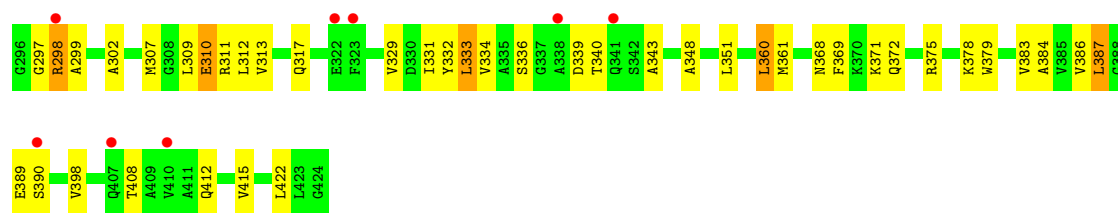
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: HISTIDYL-TRNA SYNTHETASE

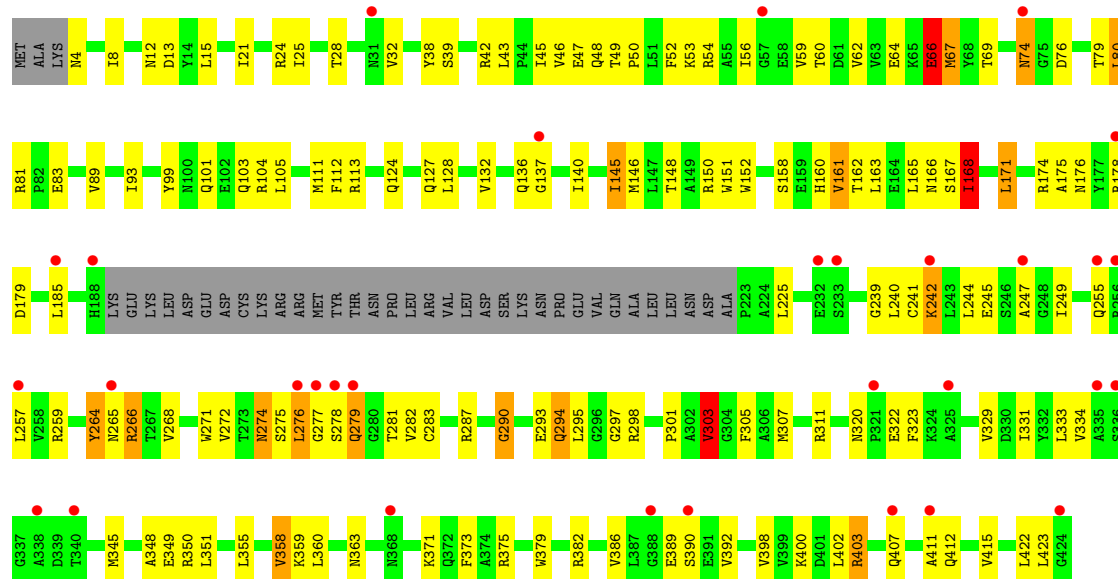


• Molecule 1: HISTIDYL-TRNA SYNTHETASE

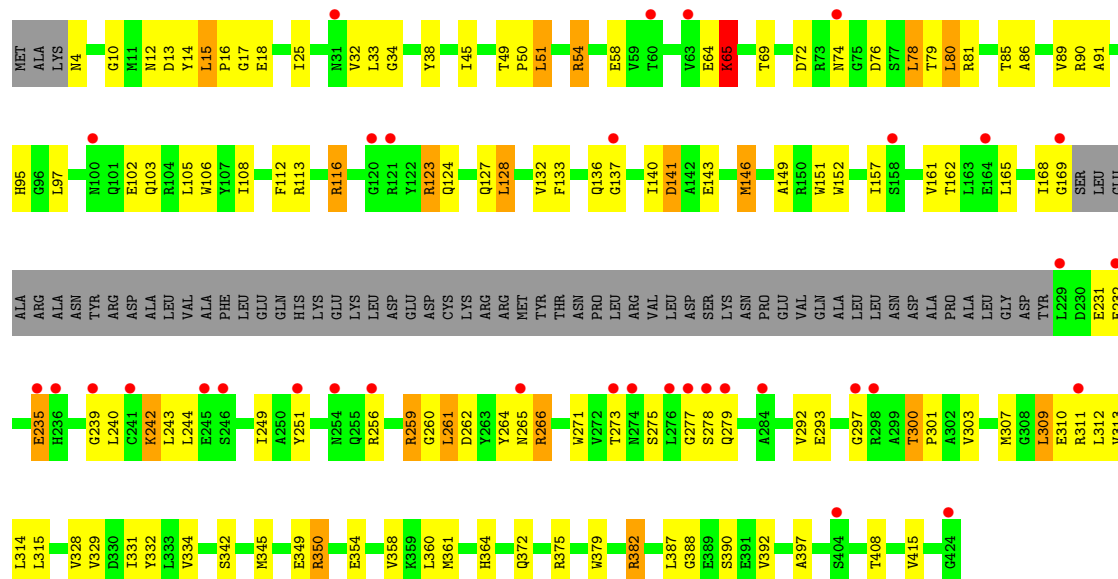




● Molecule 1: HISTIDYL-TRNA SYNTHETASE



● Molecule 1: HISTIDYL-TRNA SYNTHETASE



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 12.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	68.0 (12.00-2.60) 84.1 (12.00-2.60)	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 (Not available) , 0.294	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)	0.31 , 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

5.1 Standard geometry

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	0.71	1/3047 (0.0%)	1.17	21/4123 (0.5%)
1	B	0.73	0/2875	1.13	18/3888 (0.5%)
1	C	0.71	0/3061	1.13	23/4142 (0.6%)
1	D	0.69	0/2861	1.10	12/3870 (0.3%)
All	All	0.71	1/11844 (0.0%)	1.13	74/16023 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	VAL	CA-CB	5.47	1.62	1.54

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	GLN	N-CA-C	-10.22	100.82	113.28
1	A	279	GLN	N-CA-C	-9.72	101.34	113.01
1	C	277	GLY	N-CA-C	-9.67	104.04	114.67
1	B	43	LEU	CA-C-N	8.97	129.00	119.76
1	B	43	LEU	C-N-CA	8.97	129.00	119.76
1	A	320	ASN	CA-C-N	8.81	130.85	119.84
1	A	320	ASN	C-N-CA	8.81	130.85	119.84
1	B	279	GLN	N-CA-C	-8.79	99.48	111.87
1	C	43	LEU	CA-C-N	7.94	127.99	119.89
1	C	43	LEU	C-N-CA	7.94	127.99	119.89
1	A	320	ASN	C-N-CD	-7.90	92.60	125.00
1	A	303	VAL	CB-CA-C	-7.83	100.92	111.80
1	B	128	LEU	N-CA-C	-7.66	96.03	108.52
1	A	277	GLY	N-CA-C	-7.63	106.27	114.67
1	A	137	GLY	CA-C-N	7.50	127.67	119.87
1	A	137	GLY	C-N-CA	7.50	127.67	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	116	ARG	CA-C-N	7.45	127.49	119.90
1	B	116	ARG	C-N-CA	7.45	127.49	119.90
1	B	65	LYS	N-CA-C	7.37	121.74	111.56
1	A	43	LEU	CA-C-N	7.29	127.27	119.76
1	A	43	LEU	C-N-CA	7.29	127.27	119.76
1	C	128	LEU	N-CA-C	-7.25	96.60	108.41
1	C	66	GLU	N-CA-C	7.22	122.76	113.88
1	A	128	LEU	N-CA-C	-7.16	96.75	108.41
1	C	275	SER	N-CA-C	-7.04	104.81	113.19
1	D	65	LYS	N-CA-C	6.99	121.07	111.71
1	C	279	GLN	N-CA-C	-6.88	103.84	111.82
1	C	264	TYR	N-CA-C	6.85	120.42	110.28
1	D	58	GLU	N-CA-C	6.84	118.81	111.36
1	A	323	PHE	N-CA-C	-6.84	94.31	107.57
1	B	277	GLY	N-CA-C	-6.77	107.22	114.67
1	C	56	ILE	N-CA-C	6.74	117.53	110.72
1	D	128	LEU	N-CA-C	-6.64	97.45	108.34
1	A	80	LEU	N-CA-C	-6.62	100.03	109.96
1	C	81	ARG	N-CA-C	6.52	117.58	109.57
1	D	277	GLY	N-CA-C	-6.42	105.52	115.73
1	C	323	PHE	N-CA-C	-6.42	95.12	107.57
1	B	276	LEU	N-CA-C	-6.36	104.10	112.24
1	A	12	ASN	N-CA-C	6.34	119.90	110.52
1	D	12	ASN	N-CA-C	6.25	120.11	110.42
1	D	81	ARG	N-CA-C	6.22	117.22	109.57
1	C	320	ASN	CA-C-N	6.20	127.58	119.84
1	C	320	ASN	C-N-CA	6.20	127.58	119.84
1	D	13	ASP	N-CA-C	-5.92	100.53	109.95
1	C	67	MET	N-CA-C	5.92	118.81	110.23
1	C	290	GLY	N-CA-C	5.84	121.91	114.66
1	A	341	GLN	N-CA-C	5.82	118.37	111.33
1	B	94	GLU	N-CA-C	5.75	117.55	111.28
1	C	358	VAL	CB-CA-C	-5.74	105.28	111.59
1	C	12	ASN	N-CA-C	5.74	119.44	110.32
1	B	387	LEU	N-CA-C	5.73	117.46	107.49
1	D	262	ASP	N-CA-C	5.70	119.85	113.02
1	D	17	GLY	N-CA-C	5.69	119.10	112.50
1	C	168	ILE	CB-CA-C	5.67	119.66	111.88
1	A	55	ALA	N-CA-C	5.62	117.21	111.14
1	B	267	THR	N-CA-C	5.61	118.37	109.96
1	A	65	LYS	N-CA-C	5.58	122.00	113.19
1	A	258	VAL	N-CA-C	-5.47	99.94	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	VAL	N-CA-C	5.42	115.79	107.77
1	C	80	LEU	N-CA-C	-5.40	101.65	109.59
1	D	80	LEU	N-CA-C	-5.37	101.04	109.25
1	C	111	MET	N-CA-C	-5.32	101.09	109.50
1	B	49	THR	CA-C-N	-5.28	114.18	119.56
1	B	49	THR	C-N-CA	-5.28	114.18	119.56
1	B	12	ASN	N-CA-C	5.25	118.30	109.95
1	C	303	VAL	CB-CA-C	-5.19	104.08	111.40
1	A	111	MET	N-CA-C	-5.17	100.27	109.06
1	B	291	LEU	N-CA-C	5.16	117.65	111.71
1	A	263	TYR	N-CA-C	5.15	119.56	113.28
1	C	411	ALA	N-CA-C	-5.08	103.77	110.43
1	B	81	ARG	N-CA-C	5.06	115.79	109.57
1	C	160	HIS	N-CA-C	5.06	118.94	112.26
1	D	141	ASP	N-CA-C	-5.04	105.68	111.07
1	B	74	ASN	N-CA-C	5.02	118.24	112.57

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	97	0
1	B	2824	648	2798	124	0
1	C	3005	684	2962	98	0
1	D	2810	643	2780	94	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	389	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 17.

All (389) 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:HG2	1:D:382:ARG:HH11	1.35	0.90
1:C:67:MET:HE3	1:C:79:THR:HG21	1.52	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
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:H	1:B:116:ARG:HD2	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:HB3	1:B:3:LYS:HZ2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ARG:HA	1:B:378:LYS:HD2	1.76	0.66
1:B:293:GLU:HA	1:B:297:GLY:O	1.96	0.66
1:D:382:ARG:HG2	1:D:382:ARG:NH1	2.07	0.66
1:A:345:MET:HG2	1:B:146:MET:HE1	1.76	0.66
1:C:168:ILE:HG22	1:C:265:ASN:O	1.95	0.65
1:D:256:ARG:HA	1:D:256:ARG:NE	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
1:D:332:TYR:HE1	1:D:361:MET:HE2	1.64	0.62
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:D:345:MET:HE2	1:D:364:HIS:HE1	1.65	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:C:274:ASN:C	1:C:276:LEU:H	2.10	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:HD2	1:B:116:ARG:N	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:HB3	1:B:3:LYS:HZ3	1.70	0.57
1:C:290:GLY:O	1:C:294:GLN:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:361:MET:HE1	1:D:379:TRP:NE1	2.20	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
1:A:184:PHE:CD1	1:A:184:PHE:C	2.84	0.55
1:B:49:THR:HG23	1:B:67:MET:HE1	1.88	0.55
1:B:332:TYR:HE1	1:B:361:MET:HE2	1.71	0.55
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: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:C:74:ASN:HD22	1:C:74:ASN:C	2.16	0.54
1:D:256:ARG:HA	1:D:256:ARG:CZ	2.38	0.54
1:A:112:PHE:HZ	1:B:45:ILE:HG13	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:A:420:ARG:HH11	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:HD12	1:C:21:ILE:N	2.23	0.52
1:C:46:VAL:HG22	1:C:80:LEU:HD12	1.90	0.52
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: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:13:ASP:OD2	1:B:90:ARG:NH2	2.43	0.51
1:A:40:GLU:HB2	1:A:106:TRP:CZ2	2.45	0.51
1:C:278:SER:CB	1:C:311:ARG:HB3	2.41	0.51
1:B:134:GLY:C	1:B:135:LEU:HD13	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:278:SER:C	1:A:280:GLY:N	2.67	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:C:274:ASN:C	1:C:276:LEU:N	2.69	0.50
1:B:291:LEU:HD23	1:B:291:LEU:C	2.37	0.50
1:B:278:SER:C	1:B:311:ARG:HD2	2.37	0.49
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:278:SER:CB	1:B:311:ARG:HB3	2.42	0.49
1:B:298:ARG:HG3	1:B:298:ARG:NH1	2.17	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
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:A:391:GLU:CD	1:A:391:GLU:H	2.20	0.49
1:C:112:PHE:HZ	1:D:45:ILE:HD12	1.78	0.49
1:A:99:TYR:O	1:A:101:GLN:HG3	2.12	0.48
1:A:332:TYR:CZ	1:A:363:ASN:HB2	2.47	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:N	1:B:38:TYR:CD1	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:D:72:ASP:C	1:D:74:ASN:H	2.22	0.47
1:B:361:MET:HE1	1:B:379:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:271:TRP:HB2	1:A:283:CYS:HB3	1.96	0.47
1:B:311:ARG:HG3	1:B:311:ARG:NH1	2.29	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: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:276:LEU:C	1:C:278:SER:N	2.72	0.46
1:D:74:ASN:HB3	1:D:76:ASP:OD2	2.14	0.46
1:D:136:GLN:NE2	1:D:266:ARG:NH1	2.64	0.46
1:B:83:GLU:C	1:B:111:MET:HE3	2.40	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: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: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:D:32:VAL:HB	1:D:151:TRP:HE1	1.82	0.45
1:A:278:SER:C	1:A:280:GLY:H	2.25	0.45
1:B:61:ASP:HA	1:B:64:GLU:HB2	1.99	0.45
1:B:108:ILE:HA	1:B:127:GLN:O	2.15	0.45
1:C:127:GLN:HA	1:C:307:MET:O	2.16	0.45
1:B:38:TYR:N	1:B:38:TYR:HD1	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:C:15:LEU:HD22	1:D:97:LEU:HD11	1.99	0.45
1:C:74:ASN:ND2	1:C:76:ASP:H	2.15	0.45
1:C:375:ARG:O	1:C:379:TRP:HD1	1.98	0.45
1:B:84:GLY:N	1:B:111:MET:HE3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:MET:HG3	1:B:249:ILE:HD11	1.98	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:89:VAL:O	1:C:93:ILE:HG13	2.16	0.45
1:C:333:LEU:HD13	1:C:348:ALA:HB2	1.98	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:C:345:MET:HB3	1:D:146:MET:HE1	1.99	0.45
1:D:361:MET:CE	1:D:379:TRP:NE1	2.80	0.45
1:A:90:ARG:NH2	1:B:7:ALA:HB2	2.31	0.44
1:A:320:ASN:HA	1:A:321:PRO:HD2	1.64	0.44
1:B:261:LEU:HD12	1:B:263:TYR:OH	2.17	0.44
1:B:310:GLU:H	1:B:310:GLU:HG2	1.47	0.44
1:D:361:MET:HE1	1:D:379:TRP:CE2	2.52	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: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
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:62:VAL:HA	1:C:66:GLU:HB2	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: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: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:D:260:GLY:C	1:D:261:LEU:HD23	2.43	0.44
1:B:47:GLU:HB2	1:B:52:PHE:CE2	2.53	0.43
1:C:38:TYR:N	1:C:38:TYR:CD1	2.86	0.43
1:C:178:ARG:O	1:C:179:ASP:C	2.60	0.43
1:C:403:ARG:H	1:C:403:ARG:HG3	1.59	0.43
1:A:64:GLU:CB	1:A:65:LYS:HD3	2.47	0.43
1:A:113:ARG:NH2	2:A:450:HAM:O2P	2.48	0.43
1:D:345:MET:HE2	1:D:364:HIS:CE1	2.49	0.43
1:B:166:ASN:HA	1:B:237:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ILE:O	1:B:169:GLY:C	2.62	0.43
1:B:231:GLU:HG2	1:B:232:GLU:N	2.33	0.43
1:D:38:TYR:N	1:D:38:TYR:CD1	2.86	0.43
1:C:28:THR:O	1:C:32:VAL:HG23	2.19	0.43
1:B:232:GLU:CD	1:B:266:ARG:NH1	2.76	0.43
1:D:146:MET:HG3	1:D:249:ILE:CD1	2.45	0.43
1:D:251:TYR:CD1	1:D:251:TYR:C	2.96	0.43
1:D:388:GLY:O	1:D:392:VAL:HG23	2.18	0.43
1:A:345:MET:HE3	1:B:146:MET:SD	2.58	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:32:VAL:O	1:A:36:TYR:HD1	2.01	0.43
1:A:149:ALA:O	1:A:153:ARG:HG3	2.19	0.43
1:A:274:ASN:C	1:A:276:LEU:H	2.26	0.43
1:B:152:TRP:HE3	1:B:152:TRP:HA	1.84	0.43
1:C:174:ARG:C	1:C:176:ASN:H	2.27	0.43
1:A:16:PRO:HG3	1:B:105:LEU:HD22	2.01	0.42
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: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:B:361:MET:HE1	1:B:379:TRP:NE1	2.35	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
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:A:74:ASN:HD21	1:A:76:ASP:CG	2.27	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:38:TYR:N	1:D:38:TYR:HD1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ALA:HB3	1:D:415:VAL:HG21	2.02	0.42
1:C:146:MET:HE2	1:C:247:ALA:HB2	2.01	0.42
1:C:276:LEU:C	1:C:278:SER:H	2.26	0.42
1:A:15:LEU:O	1:A:16:PRO:C	2.62	0.41
1:B:279:GLN:HA	1:B:279:GLN:NE2	2.35	0.41
1:C:13:ASP:CG	1:D:90:ARG:HH22	2.27	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:A:363:ASN:CG	1:A:372:GLN:HG2	2.45	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:HA	1:B:152:TRP:CE3	2.55	0.41
1:B:307:MET:SD	1:B:312:LEU:HD22	2.60	0.41
1:C:48:GLN:HB3	1:C:50:PRO:HD2	2.02	0.41
1:C:334:VAL:HG21	1:C:373:PHE:HE1	1.85	0.41
1:A:276:LEU:C	1:A:278:SER:N	2.77	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:9:ARG:HE	1:B:123:ARG:NH2	2.19	0.41
1:B:265:ASN:CG	1:B:266:ARG:H	2.29	0.41
1:B:334:VAL:HG13	1:B:372:GLN:OE1	2.21	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:D:112:PHE:CD1	1:D:112:PHE:N	2.89	0.41
1:D:116:ARG:C	1:D:116:ARG:HD2	2.46	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
1:D:165:LEU:HD11	1:D:244:LEU:CD1	2.50	0.41
1:A:70:PHE:HE1	1:A:80:LEU:CD1	2.34	0.41
1:A:113:ARG:O	1:A:123:ARG:HA	2.21	0.41
1:B:42:ARG:HA	3:B:597:HOH:O	2.20	0.41
1:B:118:GLN:HG2	1:B:121:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLN:HE21	1:B:121:ARG:HG3	1.85	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: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: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:HD23	1:B:422:LEU:HA	1.90	0.40
1:C:38:TYR:N	1:C:38:TYR:HD1	2.19	0.40
1:C:161:VAL:HA	1:C:272:VAL:O	2.20	0.40
1:C:305:PHE:CD1	1:C:305:PHE:C	2.99	0.40
1:B:19:THR:O	1:B:23:GLN:HG3	2.21	0.40
1:B:118:GLN:HB2	1:B:119:LYS:H	1.74	0.40
1:B:147:LEU:HD23	1:B:147:LEU:C	2.46	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:A:178:ARG:O	1:A:179:ASP:C	2.63	0.40
1:B:100:ASN:O	1:B:100:ASN:ND2	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
1:D:72:ASP:C	1:D:74:ASN:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	382/424 (90%)	360 (94%)	16 (4%)	6 (2%)	7 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	360/424 (85%)	340 (94%)	17 (5%)	3 (1%)	16	34
1	C	383/424 (90%)	358 (94%)	23 (6%)	2 (0%)	24	46
1	D	358/424 (84%)	342 (96%)	14 (4%)	2 (1%)	21	42
All	All	1483/1696 (87%)	1400 (94%)	70 (5%)	13 (1%)	14	30

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%)	271 (89%)	33 (11%)	6	13
1	B	289/342 (84%)	255 (88%)	34 (12%)	5	10
1	C	306/342 (90%)	273 (89%)	33 (11%)	6	13
1	D	288/342 (84%)	259 (90%)	29 (10%)	7	15
All	All	1187/1368 (87%)	1058 (89%)	129 (11%)	6	13

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	23	GLN
1	A	31	ASN
1	A	54	ARG
1	A	65	LYS
1	A	74	ASN
1	A	78	LEU
1	A	83	GLU
1	A	90	ARG
1	A	128	LEU
1	A	139	ASP
1	A	155	LEU
1	A	158	SER
1	A	165	LEU
1	A	184	PHE
1	A	231	GLU
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	292	VAL
1	A	295	LEU
1	A	303	VAL
1	A	342	SER
1	A	345	MET
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	15	LEU
1	B	16	PRO
1	B	24	ARG
1	B	65	LYS
1	B	74	ASN
1	B	80	LEU
1	B	83	GLU

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Mol	Chain	Res	Type
1	B	100	ASN
1	B	104	ARG
1	B	116	ARG
1	B	118	GLN
1	B	135	LEU
1	B	158	SER
1	B	159	GLU
1	B	165	LEU
1	B	166	ASN
1	B	256	ARG
1	B	257	LEU
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	360	LEU
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	66	GLU
1	C	69	THR
1	C	74	ASN
1	C	83	GLU
1	C	140	ILE
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

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Mol	Chain	Res	Type
1	C	257	LEU
1	C	266	ARG
1	C	274	ASN
1	C	276	LEU
1	C	281	THR
1	C	294	GLN
1	C	295	LEU
1	C	298	ARG
1	C	303	VAL
1	C	322	GLU
1	C	329	VAL
1	C	363	ASN
1	C	371	LYS
1	C	390	SER
1	C	403	ARG
1	D	4	ASN
1	D	15	LEU
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	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	261	LEU
1	D	275	SER
1	D	300	THR
1	D	303	VAL
1	D	309	LEU
1	D	342	SER
1	D	350	ARG
1	D	375	ARG
1	D	382	ARG
1	D	387	LEU

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Mol	Chain	Res	Type
1	D	390	SER
1	D	408	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	23	GLN
1	A	74	ASN
1	A	236	HIS
1	A	255	GLN
1	A	274	ASN
1	A	364	HIS
1	A	372	GLN
1	A	407	GLN
1	A	418	HIS
1	B	23	GLN
1	B	160	HIS
1	B	166	ASN
1	B	274	ASN
1	B	341	GLN
1	B	407	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	C	363	ASN
1	D	31	ASN
1	D	114	HIS
1	D	124	GLN
1	D	136	GLN
1	D	160	HIS
1	D	236	HIS
1	D	364	HIS
1	D	407	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	A	450	-	35,36,36	1.00	2 (5%)	50,53,53	0.90	3 (6%)
2	HAM	C	450	-	35,36,36	1.06	1 (2%)	50,53,53	0.84	3 (6%)
2	HAM	D	450	-	35,36,36	0.88	1 (2%)	50,53,53	0.62	1 (2%)
2	HAM	B	450	-	35,36,36	1.04	2 (5%)	50,53,53	0.79	2 (4%)

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	A	450	-	-	3/21/39/39	0/4/4/4
2	HAM	C	450	-	-	3/21/39/39	0/4/4/4
2	HAM	D	450	-	-	3/21/39/39	0/4/4/4
2	HAM	B	450	-	-	2/21/39/39	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	450	HAM	P-O3P	5.10	1.70	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	HAM	P-O3P	4.86	1.69	1.60
2	A	450	HAM	P-O3P	4.48	1.68	1.60
2	D	450	HAM	P-O3P	3.81	1.67	1.60
2	A	450	HAM	O-C	2.17	1.26	1.21
2	B	450	HAM	CA-C	2.00	1.59	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	450	HAM	O-C-CA	-3.58	108.59	120.62
2	A	450	HAM	O-C-CA	-3.36	109.31	120.62
2	B	450	HAM	O-C-CA	-3.36	109.33	120.62
2	A	450	HAM	O2P-P-O3P	3.08	114.92	104.94
2	D	450	HAM	O-C-CA	-3.02	110.46	120.62
2	B	450	HAM	CB-CA-C	2.13	116.72	110.46
2	C	450	HAM	O3P-P-O5'	2.06	109.19	103.00
2	A	450	HAM	O3P-P-O5'	2.05	109.17	103.00
2	C	450	HAM	O2P-P-O3P	2.03	111.49	104.94

There are no chirality outliers.

All (11) 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	D	450	HAM	CA-CB-CG-ND1
2	A	450	HAM	C5'-O5'-P-O3P
2	B	450	HAM	C5'-O5'-P-O1P
2	C	450	HAM	C5'-O5'-P-O1P
2	C	450	HAM	C-O3P-P-O5'
2	B	450	HAM	C-O3P-P-O5'
2	D	450	HAM	C-O3P-P-O5'
2	C	450	HAM	C-O3P-P-O1P

There are no ring outliers.

4 monomers are involved in 10 short contacts:

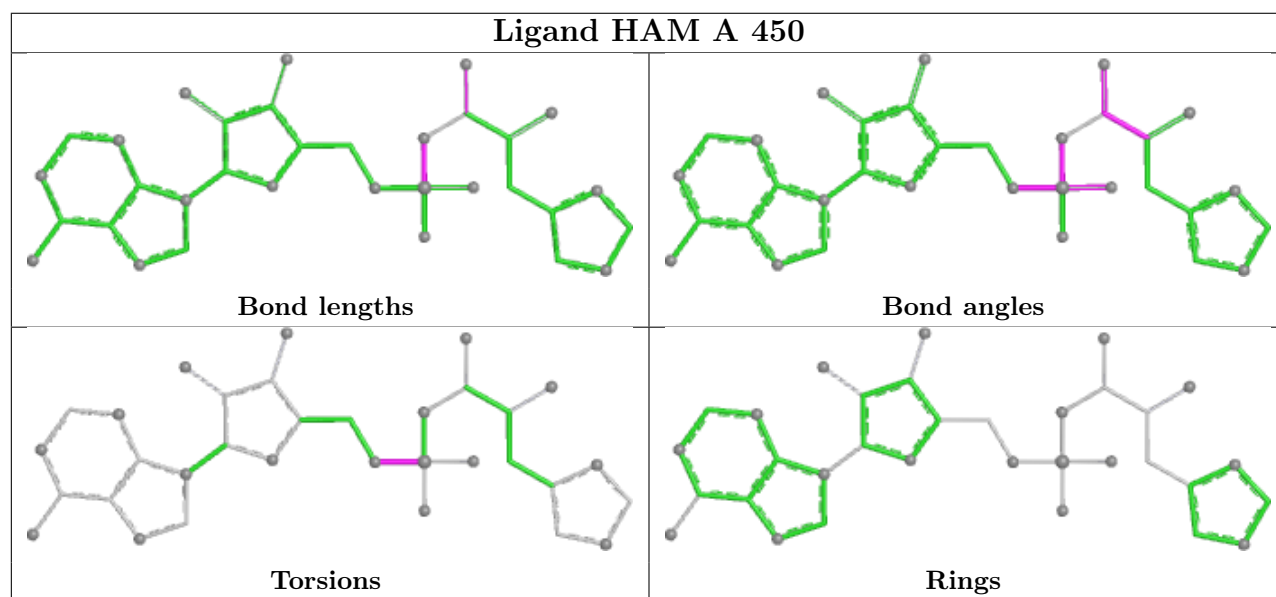
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	450	HAM	2	0
2	C	450	HAM	2	0

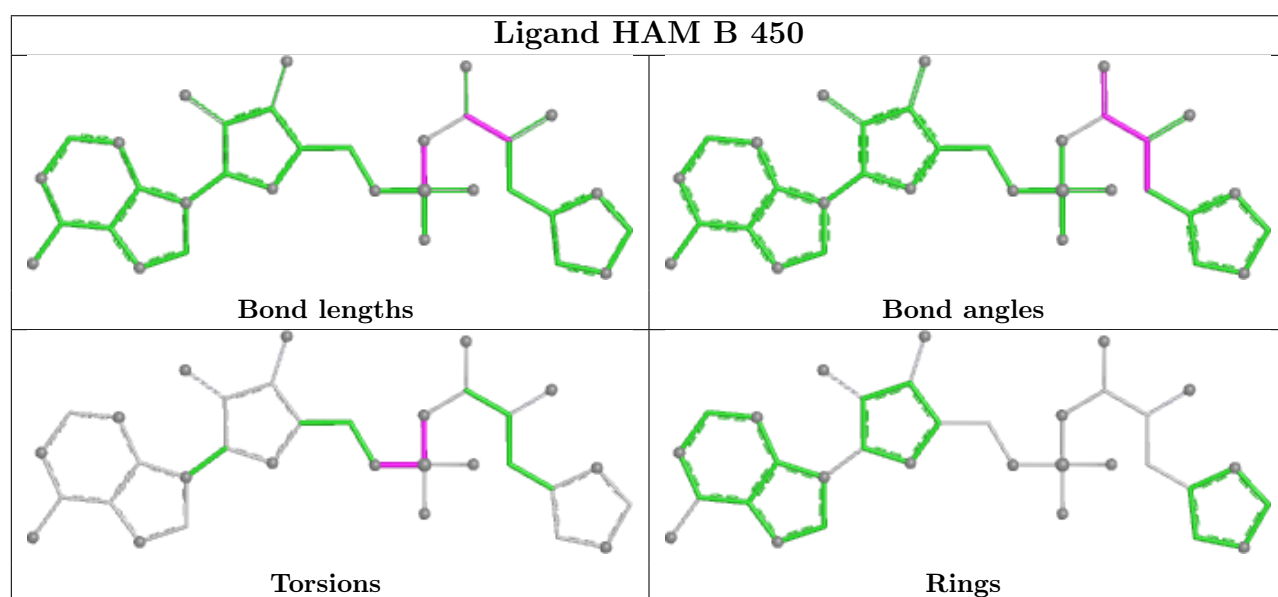
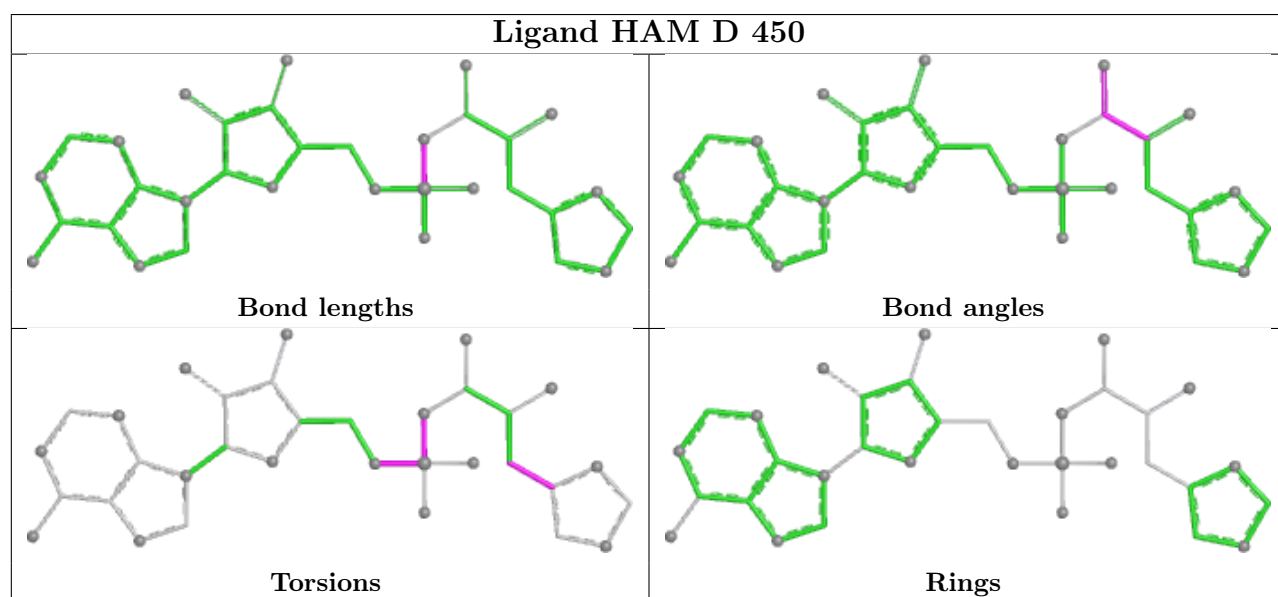
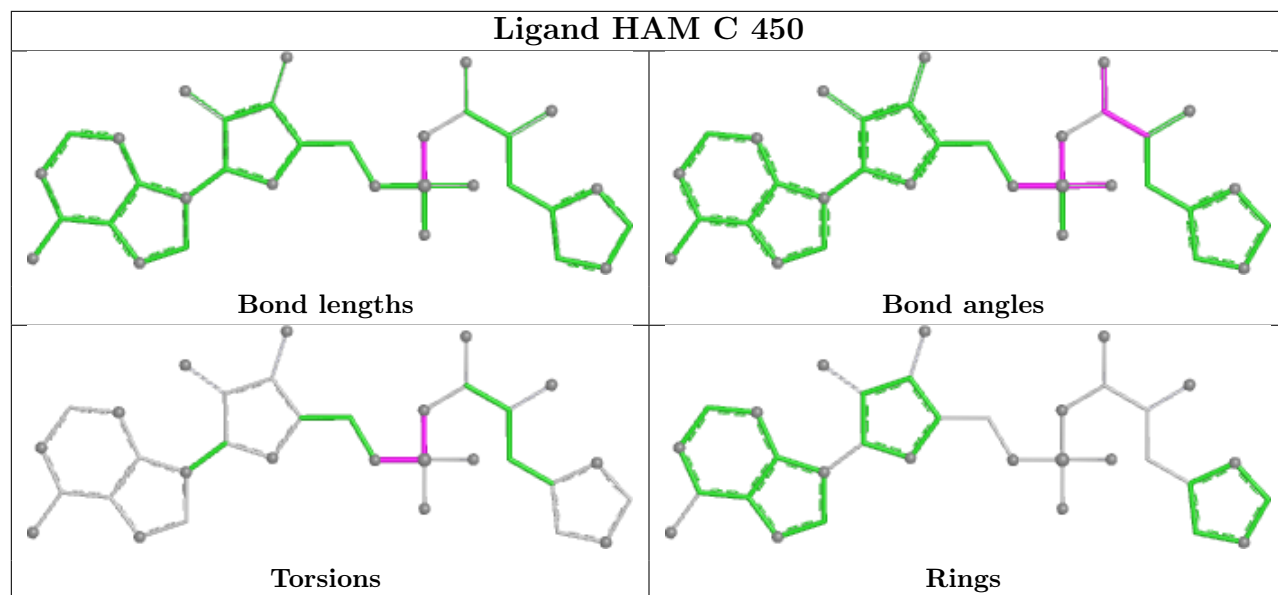
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	450	HAM	5	0
2	B	450	HAM	1	0

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

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	386/424 (91%)	0.57	37 (9%) 13 10	15, 35, 66, 84	0
1	B	364/424 (85%)	0.55	30 (8%) 17 14	16, 36, 65, 90	0
1	C	387/424 (91%)	0.58	31 (8%) 18 14	15, 36, 65, 82	0
1	D	362/424 (85%)	0.63	35 (9%) 13 10	17, 37, 63, 89	0
All	All	1499/1696 (88%)	0.58	133 (8%) 15 12	15, 36, 66, 90	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	SER	6.1
1	A	277	GLY	5.2
1	D	277	GLY	4.9
1	C	278	SER	4.6
1	D	158	SER	4.4
1	C	277	GLY	4.3
1	C	137	GLY	4.0
1	C	338	ALA	3.9
1	A	178	ARG	3.8
1	B	61	ASP	3.8
1	D	120	GLY	3.6
1	D	169	GLY	3.5
1	B	277	GLY	3.4
1	D	265	ASN	3.4
1	D	278	SER	3.4
1	B	74	ASN	3.4
1	A	19	THR	3.3
1	A	60	THR	3.3
1	B	278	SER	3.3
1	B	274	ASN	3.1
1	D	137	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	74	ASN	3.1
1	B	137	GLY	3.1
1	C	325	ALA	3.1
1	B	279	GLN	3.0
1	D	273	THR	3.0
1	C	390	SER	3.0
1	C	424	GLY	3.0
1	D	121	ARG	2.9
1	D	235	GLU	2.9
1	B	116	ARG	2.9
1	A	137	GLY	2.9
1	C	411	ALA	2.9
1	D	229	LEU	2.9
1	A	159	GLU	2.8
1	A	171	LEU	2.8
1	B	120	GLY	2.8
1	D	164	GLU	2.8
1	C	178	ARG	2.8
1	C	256	ARG	2.8
1	A	338	ALA	2.8
1	D	256	ARG	2.8
1	B	390	SER	2.7
1	D	424	GLY	2.7
1	A	256	ARG	2.7
1	B	31	ASN	2.7
1	D	246	SER	2.7
1	B	322	GLU	2.7
1	D	232	GLU	2.7
1	C	255	GLN	2.7
1	D	284	ALA	2.7
1	B	229	LEU	2.6
1	A	172	GLU	2.6
1	B	24	ARG	2.6
1	B	57	GLY	2.6
1	B	338	ALA	2.6
1	B	280	GLY	2.6
1	A	184	PHE	2.6
1	C	368	ASN	2.6
1	C	265	ASN	2.6
1	C	242	LYS	2.5
1	B	2	ALA	2.5
1	B	341	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	31	ASN	2.5
1	D	31	ASN	2.5
1	C	233	SER	2.5
1	D	251	TYR	2.5
1	A	388	GLY	2.5
1	A	279	GLN	2.5
1	A	158	SER	2.5
1	B	298	ARG	2.5
1	C	57	GLY	2.5
1	C	74	ASN	2.4
1	C	257	LEU	2.4
1	B	230	ASP	2.4
1	B	3	LYS	2.4
1	B	60	THR	2.4
1	A	274	ASN	2.4
1	D	241	CYS	2.4
1	B	246	SER	2.4
1	A	322	GLU	2.4
1	C	247	ALA	2.4
1	A	31	ASN	2.4
1	C	336	SER	2.4
1	A	424	GLY	2.4
1	C	279	GLN	2.4
1	A	173	ALA	2.4
1	B	257	LEU	2.3
1	A	99	TYR	2.3
1	A	232	GLU	2.3
1	D	245	GLU	2.3
1	A	262	ASP	2.3
1	D	254	ASN	2.2
1	D	404	SER	2.2
1	D	236	HIS	2.2
1	C	232	GLU	2.2
1	C	340	THR	2.2
1	C	388	GLY	2.2
1	A	188	HIS	2.2
1	A	252	THR	2.2
1	D	274	ASN	2.2
1	A	226	GLY	2.2
1	A	233	SER	2.2
1	A	257	LEU	2.2
1	C	185	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	276	LEU	2.2
1	D	239	GLY	2.2
1	A	323	PHE	2.2
1	B	323	PHE	2.2
1	C	321	PRO	2.1
1	A	324	LYS	2.1
1	D	100	ASN	2.1
1	D	279	GLN	2.1
1	D	297	GLY	2.1
1	B	410	VAL	2.1
1	C	188	HIS	2.1
1	B	235	GLU	2.1
1	A	187	GLN	2.1
1	A	404	SER	2.1
1	D	311	ARG	2.1
1	C	407	GLN	2.1
1	A	246	SER	2.1
1	A	174	ARG	2.1
1	A	318	ALA	2.1
1	D	298	ARG	2.1
1	D	60	THR	2.1
1	C	276	LEU	2.0
1	A	325	ALA	2.0
1	C	335	ALA	2.0
1	B	77	SER	2.0
1	B	407	GLN	2.0
1	A	258	VAL	2.0
1	D	63	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

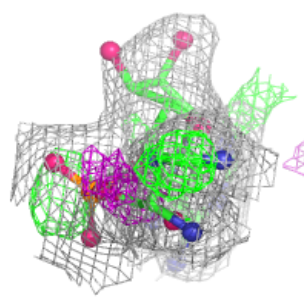
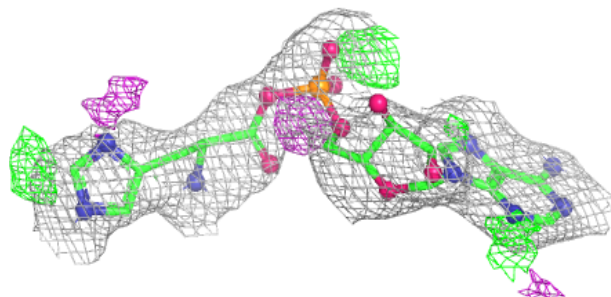
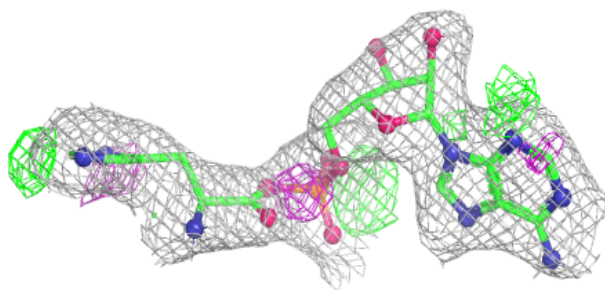
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HAM	B	450	33/33	0.84	0.13	0,42,49,50	0
2	HAM	D	450	33/33	0.84	0.13	0,49,54,54	0
2	HAM	A	450	33/33	0.88	0.11	0,28,35,37	0
2	HAM	C	450	33/33	0.92	0.11	0,31,35,37	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.

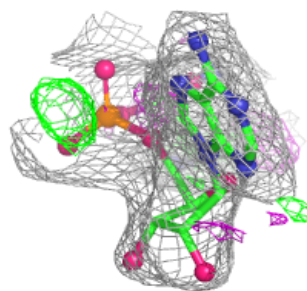
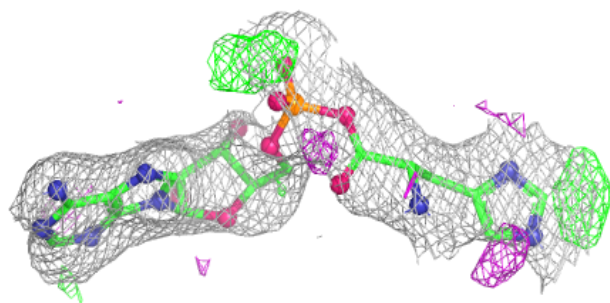
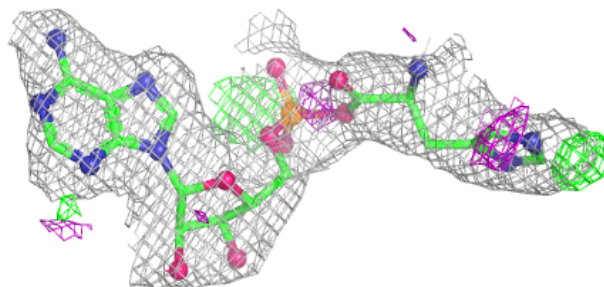
Electron density around HAM B 450:

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

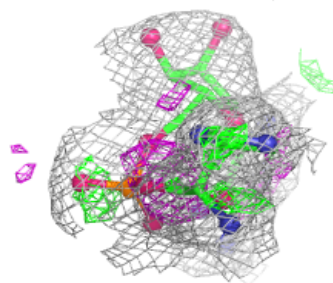
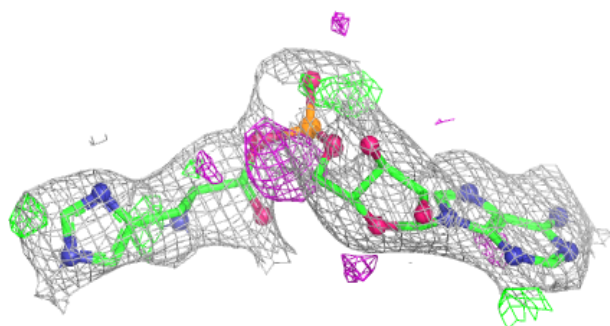
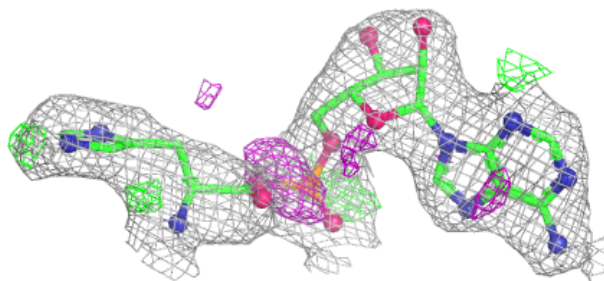


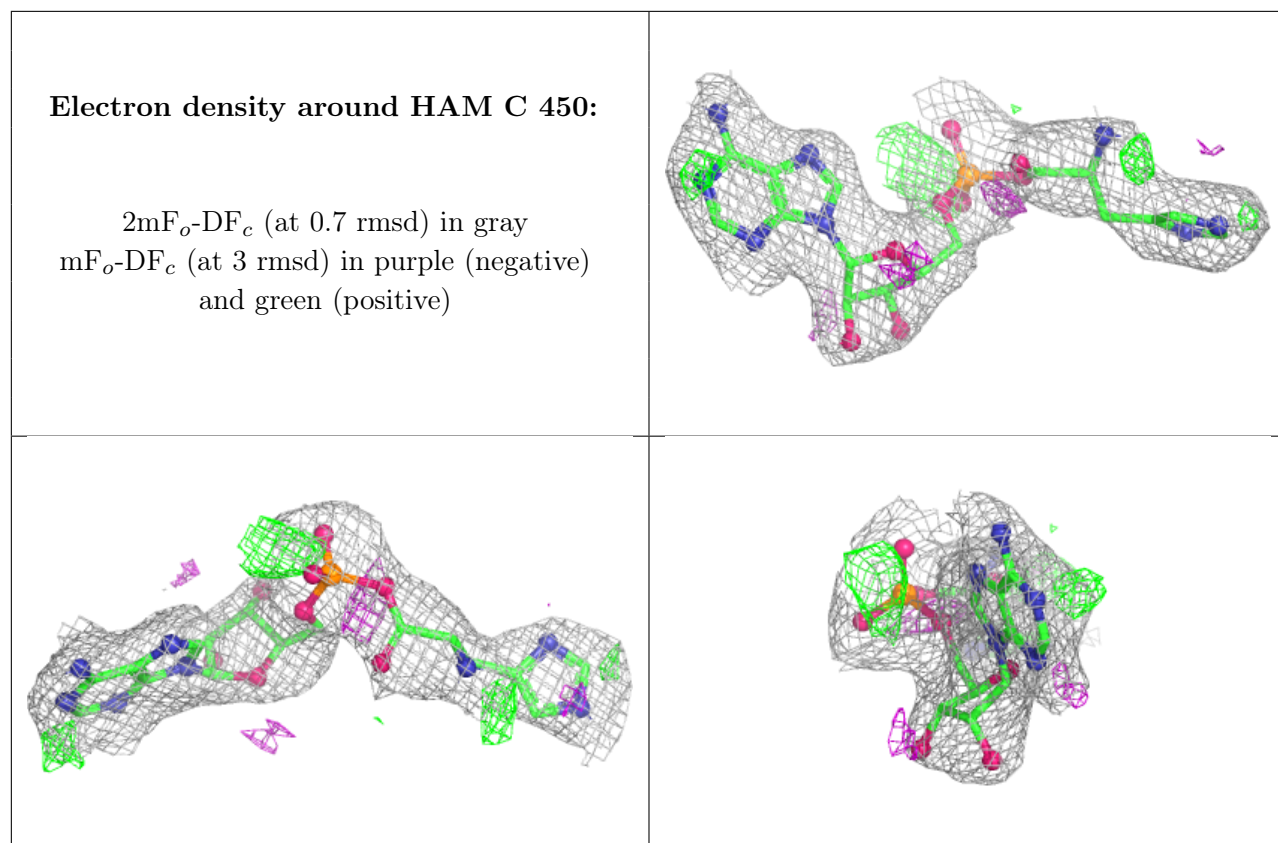
Electron density around HAM D 450:

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

**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)





6.5 Other polymers ⓘ

There are no such residues in this entry.