



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:48 AM UTC

PDB ID : 3TMK / pdb_00003tmk
Title : CRYSTAL STRUCTURE OF YEAST THYMIDYLATE KINASE COM-
PLEXED WITH THE BISUBSTRATE INHIBITOR TP5A AT 2.0 Å RESO-
LUTION: IMPLICATIONS FOR CATALYSIS AND AZT ACTIVATION
Authors : Lavie, A.; Schlichting, I.; Konrad, M.; Goody, R.S.; Brundiers, R.; Reinstein,
J.
Deposited on : 1998-01-26
Resolution : 2.00 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](#) ①) 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

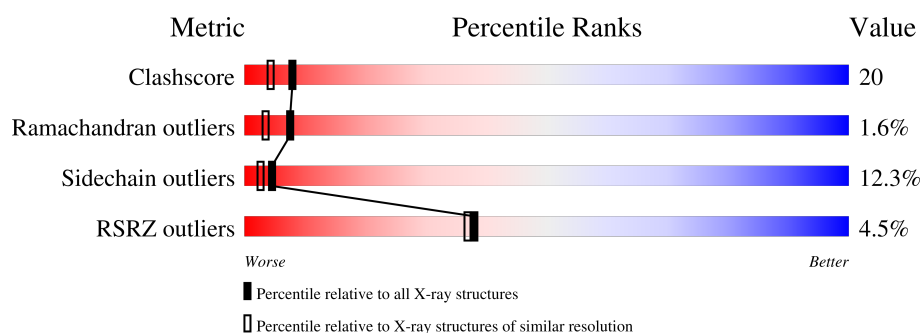
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	216	6% 54% 36% 10% •
1	B	216	4% 66% 31% •
1	C	216	5% 49% 31% 13% 5% •
1	D	216	3% 64% 30% 5% •
1	E	216	6% 60% 31% 8%
1	F	216	2% 67% 29% •
1	G	216	5% 60% 29% 11%

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Mol	Chain	Length	Quality of chain
1	H	216	5% 66% 29%

2 Entry composition

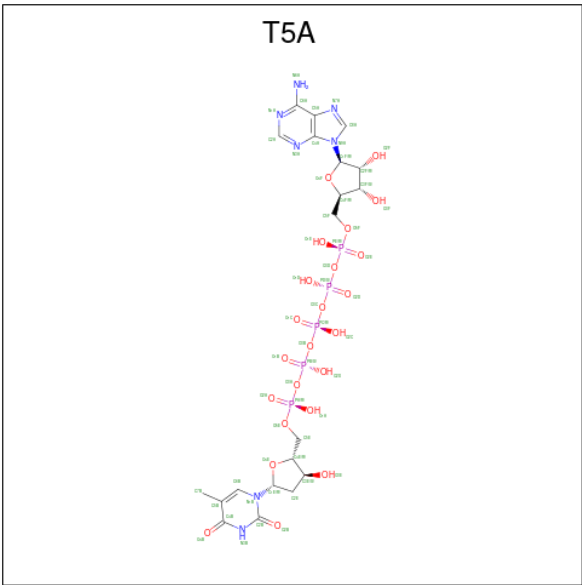
There are 3 unique types of molecules in this entry. The entry contains 15240 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called THYMIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1107	289	332	8			
1	B	216	Total	C	N	O	S	0	0	0
			1733	1106	289	330	8			
1	C	205	Total	C	N	O	S	0	0	0
			1657	1060	275	314	8			
1	D	214	Total	C	N	O	S	0	0	0
			1707	1092	286	323	6			
1	E	215	Total	C	N	O	S	0	0	0
			1722	1096	288	331	7			
1	F	216	Total	C	N	O	S	0	0	0
			1729	1104	288	329	8			
1	G	215	Total	C	N	O	S	0	0	0
			1722	1096	288	331	7			
1	H	214	Total	C	N	O	S	0	0	0
			1706	1090	285	325	6			

- Molecule 2 is P1-(5'-ADENOSYL)P5-(5'-THYMIDYL)PENTAPHOSPHATE (CCD ID: T5A) (formula: C₂₀H₃₀N₇O₂₃P₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	B	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	C	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	D	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	E	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	F	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	G	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	H	1	Total	C	N	O	P	0	0
			55	20	7	23	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	161	Total	O	0	0
			161	161		
3	C	134	Total	O	0	0
			134	134		
3	D	144	Total	O	0	0
			144	144		

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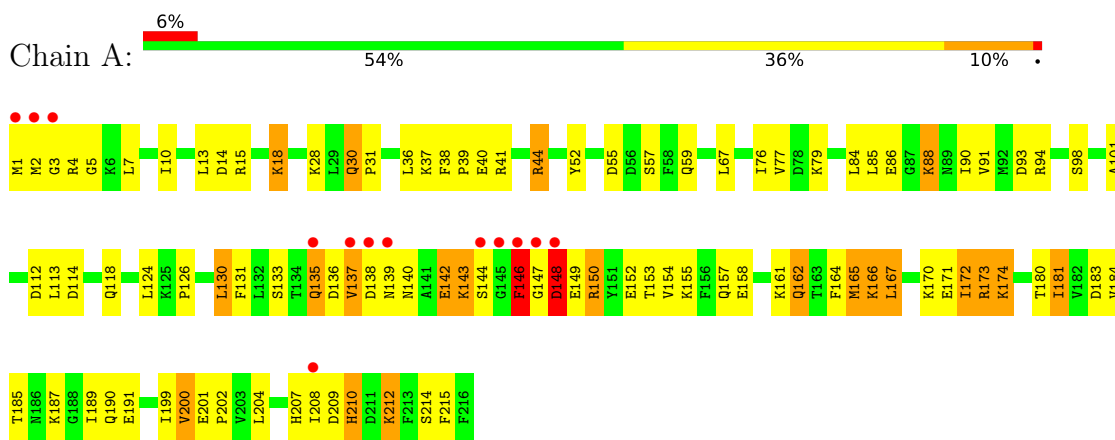
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	126	Total 126	O 126	0	0
3	F	147	Total 147	O 147	0	0
3	G	136	Total 136	O 136	0	0
3	H	111	Total 111	O 111	0	0

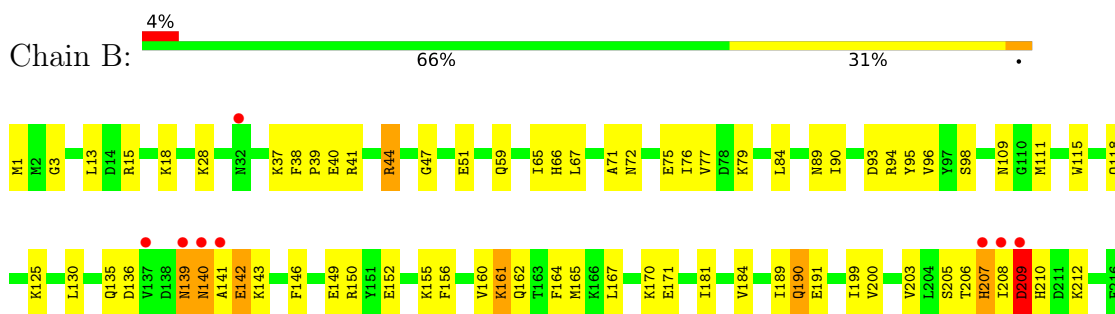
3 Residue-property plots [i](#)

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.

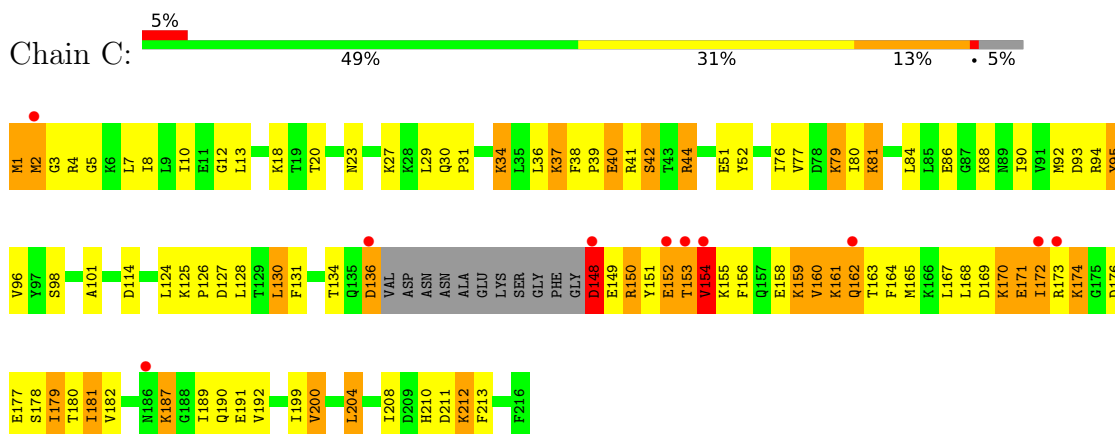
• Molecule 1: THYMIDYLATE KINASE



• Molecule 1: THYMIDYLATE KINASE

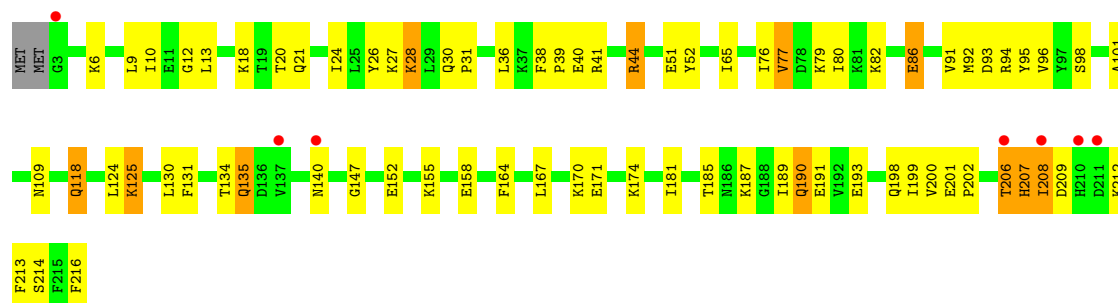


• Molecule 1: THYMIDYLATE KINASE



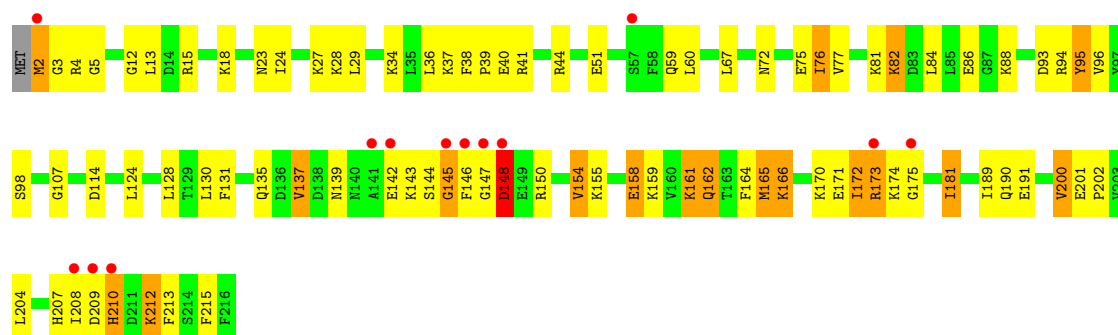
● Molecule 1: THYMIDYLATE KINASE

Chain D: 



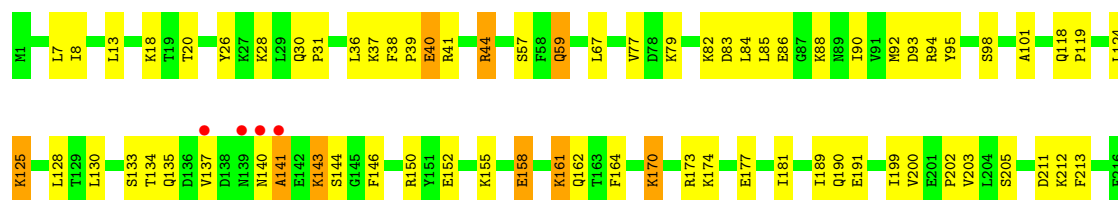
● Molecule 1: THYMIDYLATE KINASE

Chain E: 



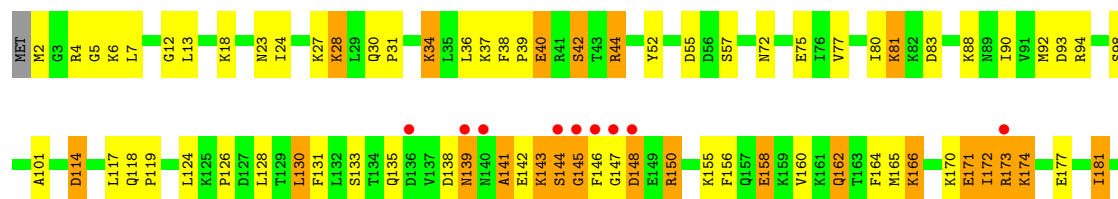
● Molecule 1: THYMIDYLATE KINASE

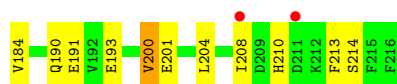
Chain F: 



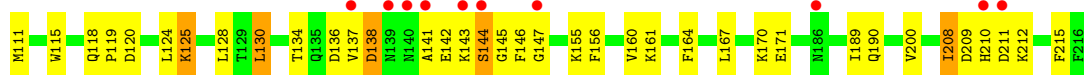
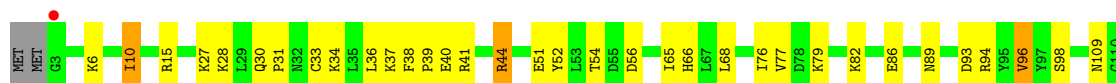
● Molecule 1: THYMIDYLATE KINASE

Chain G: 





- Molecule 1: THYMIDYLATE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.57Å 87.32Å 155.02Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	43.80 – 2.00 43.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.80-2.00) 82.0 (43.80-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.279 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	1.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15240	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.18 % 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 1.1888e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: T5A

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	0.58	0/1765	0.98	11/2375 (0.5%)
1	B	0.60	0/1762	0.96	7/2371 (0.3%)
1	C	0.67	1/1684 (0.1%)	1.02	9/2265 (0.4%)
1	D	0.58	0/1736	0.96	10/2338 (0.4%)
1	E	0.54	0/1750	0.95	7/2356 (0.3%)
1	F	0.60	0/1758	0.98	6/2366 (0.3%)
1	G	0.56	0/1750	0.96	6/2356 (0.3%)
1	H	0.60	0/1735	0.98	8/2338 (0.3%)
All	All	0.59	1/13940 (0.0%)	0.97	64/18765 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	ASP	C-N	13.29	1.55	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	ARG	N-CA-C	8.54	120.51	111.03
1	C	148	ASP	CA-C-N	-8.52	107.32	122.15
1	C	148	ASP	C-N-CA	-8.52	107.32	122.15
1	D	200	VAL	N-CA-C	7.16	117.26	110.53
1	H	145	GLY	N-CA-C	-7.03	106.72	115.08
1	H	41	ARG	N-CA-C	6.75	121.12	113.01
1	F	41	ARG	N-CA-C	6.72	120.93	112.87
1	G	144	SER	N-CA-C	-6.53	105.19	113.02
1	B	200	VAL	N-CA-C	6.47	116.61	110.53
1	E	150	ARG	N-CA-C	6.33	118.99	111.33
1	C	77	VAL	N-CA-C	6.11	119.60	111.17
1	F	200	VAL	N-CA-C	6.09	116.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	41	ARG	N-CA-C	6.07	120.42	113.19
1	F	150	ARG	N-CA-C	6.07	117.56	111.07
1	G	200	VAL	N-CA-C	6.05	116.22	110.53
1	G	150	ARG	N-CA-C	6.04	118.64	111.33
1	C	154	VAL	N-CA-C	-6.04	104.63	110.42
1	A	146	PHE	N-CA-C	6.02	118.47	110.53
1	E	77	VAL	N-CA-C	6.02	119.48	111.17
1	B	96	VAL	N-CA-C	6.01	116.75	110.62
1	E	200	VAL	N-CA-C	5.98	116.15	110.53
1	G	101	ALA	N-CA-C	5.96	117.44	111.07
1	C	101	ALA	N-CA-C	5.89	117.38	111.07
1	C	200	VAL	N-CA-C	5.89	116.67	110.72
1	A	189	ILE	N-CA-C	5.88	116.62	110.62
1	A	41	ARG	N-CA-C	5.83	120.13	113.19
1	A	77	VAL	N-CA-C	5.76	119.12	111.17
1	A	149	GLU	N-CA-C	5.66	117.62	110.33
1	C	179	ILE	N-CA-C	5.58	116.14	107.99
1	E	135	GLN	N-CA-C	-5.56	106.67	113.50
1	B	77	VAL	N-CA-C	5.54	118.82	111.17
1	H	138	ASP	N-CA-C	-5.50	105.70	112.90
1	D	152	GLU	N-CA-C	5.42	118.02	109.39
1	E	137	VAL	N-CA-C	5.39	116.04	109.30
1	D	91	VAL	N-CA-C	-5.35	100.68	108.17
1	F	101	ALA	N-CA-C	5.35	116.79	111.07
1	H	54	THR	N-CA-C	5.34	120.06	113.50
1	A	18	LYS	N-CA-C	5.33	117.09	111.28
1	B	118	GLN	N-CA-C	5.33	120.17	113.25
1	H	200	VAL	N-CA-C	5.31	115.52	110.53
1	D	101	ALA	N-CA-C	5.30	117.06	111.28
1	G	117	LEU	N-CA-C	5.29	117.12	111.36
1	B	150	ARG	N-CA-C	5.27	116.71	111.07
1	D	147	GLY	N-CA-C	-5.26	107.53	114.95
1	G	214	SER	N-CA-C	-5.25	101.55	109.85
1	D	96	VAL	N-CA-C	5.24	115.97	110.62
1	A	150	ARG	N-CA-C	5.22	119.98	111.37
1	A	101	ALA	N-CA-C	5.20	116.64	111.07
1	H	77	VAL	N-CA-C	5.20	118.35	111.17
1	D	118	GLN	N-CA-C	5.19	120.00	113.25
1	H	147	GLY	N-CA-C	-5.17	107.86	114.37
1	D	77	VAL	N-CA-C	5.16	118.30	111.17
1	H	96	VAL	N-CA-C	5.15	115.87	110.62
1	D	86	GLU	N-CA-C	-5.13	106.99	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ARG	N-CA-C	5.13	119.30	113.19
1	A	118	GLN	N-CA-C	5.13	119.92	113.25
1	F	152	GLU	N-CA-C	5.13	117.48	108.56
1	A	91	VAL	N-CA-C	-5.11	101.02	108.17
1	B	89	ASN	N-CA-C	-5.09	103.81	110.53
1	C	41	ARG	N-CA-C	5.08	119.24	113.19
1	E	189	ILE	N-CA-C	5.08	115.29	110.42
1	A	200	VAL	N-CA-C	5.04	115.81	110.72
1	F	77	VAL	N-CA-C	5.03	118.11	111.17
1	D	41	ARG	N-CA-C	5.02	119.16	113.19

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	1736	0	1757	103	1
1	B	1733	0	1755	46	0
1	C	1657	0	1687	115	0
1	D	1707	0	1724	57	0
1	E	1722	0	1738	81	0
1	F	1729	0	1749	44	1
1	G	1722	0	1738	79	0
1	H	1706	0	1715	47	0
2	A	55	0	25	1	0
2	B	55	0	25	1	0
2	C	55	0	25	2	0
2	D	55	0	25	0	0
2	E	55	0	25	1	0
2	F	55	0	25	0	0
2	G	55	0	25	0	0
2	H	55	0	25	0	0
3	A	129	0	0	12	0
3	B	161	0	0	14	0
3	C	134	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	144	0	0	13	0
3	E	126	0	0	14	0
3	F	147	0	0	15	0
3	G	136	0	0	17	0
3	H	111	0	0	8	0
All	All	15240	0	14063	556	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (556) 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:C:162:GLN:H	1:C:162:GLN:NE2	1.33	1.24
1:C:162:GLN:N	1:C:162:GLN:HE21	1.44	1.12
1:A:2:MET:HG3	1:A:3:GLY:H	1.08	1.11
1:D:44:ARG:HG2	3:D:4143:HOH:O	1.51	1.10
1:H:44:ARG:HG3	1:H:44:ARG:HH11	1.15	1.09
1:E:139:ASN:HA	3:E:4681:HOH:O	1.56	1.05
1:G:200:VAL:HG12	1:G:204:LEU:HD11	1.41	0.99
1:E:13:LEU:HD11	1:E:161:LYS:HG3	1.44	0.98
1:H:134:THR:HG22	3:H:4688:HOH:O	1.63	0.98
1:A:162:GLN:HE21	1:A:162:GLN:N	1.61	0.97
1:C:174:LYS:HB2	1:C:174:LYS:NZ	1.80	0.97
1:B:37:LYS:HE3	3:B:4579:HOH:O	1.64	0.97
1:G:147:GLY:O	1:G:148:ASP:HB2	1.63	0.96
1:D:6:LYS:HD2	1:D:208:ILE:HD11	1.47	0.95
1:G:200:VAL:CG1	1:G:204:LEU:HD11	1.97	0.94
1:F:44:ARG:HG2	3:F:4965:HOH:O	1.65	0.94
1:C:190:GLN:HG2	3:C:5001:HOH:O	1.67	0.93
1:G:28:LYS:HE3	3:G:5321:HOH:O	1.69	0.92
1:C:174:LYS:HB2	1:C:174:LYS:HZ3	1.31	0.92
1:A:2:MET:HG3	1:A:3:GLY:N	1.83	0.91
1:E:162:GLN:H	1:E:162:GLN:HE21	0.97	0.91
1:E:15:ARG:HG2	1:E:143:LYS:HA	1.51	0.91
1:H:10:ILE:HD11	1:H:130:LEU:HD12	1.50	0.91
1:A:162:GLN:HE21	1:A:162:GLN:H	0.99	0.90
1:A:200:VAL:CG1	1:A:204:LEU:HD11	2.00	0.90
1:B:161:LYS:HD2	3:B:4437:HOH:O	1.72	0.89
1:C:200:VAL:HG12	1:C:204:LEU:CD2	2.03	0.88
1:A:146:PHE:H	1:A:146:PHE:HD1	1.21	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HG12	1:A:204:LEU:CD1	2.02	0.88
1:E:158:GLU:O	1:E:162:GLN:NE2	2.06	0.88
1:E:147:GLY:O	1:E:148:ASP:HB2	1.72	0.88
1:H:10:ILE:CD1	1:H:130:LEU:HD12	2.04	0.87
1:C:153:THR:HB	1:C:156:PHE:HB3	1.53	0.87
1:C:13:LEU:HD11	1:C:161:LYS:HD2	1.55	0.87
1:A:200:VAL:HG12	1:A:204:LEU:HD11	1.54	0.86
1:G:166:LYS:HD3	1:G:170:LYS:HE3	1.57	0.86
1:G:200:VAL:HG12	1:G:204:LEU:CD1	2.05	0.86
1:A:146:PHE:CD1	1:A:146:PHE:N	2.41	0.85
1:C:155:LYS:O	1:C:159:LYS:HD3	1.78	0.84
1:C:159:LYS:H	1:C:159:LYS:HD2	1.41	0.83
1:H:44:ARG:HG3	1:H:44:ARG:NH1	1.86	0.83
1:G:200:VAL:O	1:G:204:LEU:HD12	1.79	0.82
1:D:28:LYS:HE3	3:D:4223:HOH:O	1.77	0.82
1:E:162:GLN:HE21	1:E:162:GLN:N	1.77	0.82
1:A:166:LYS:O	1:A:170:LYS:HG3	1.80	0.81
1:A:146:PHE:HD1	1:A:146:PHE:N	1.76	0.81
1:A:131:PHE:HB3	1:A:181:ILE:HD12	1.61	0.81
1:E:200:VAL:CG1	1:E:204:LEU:HD11	2.11	0.81
1:G:171:GLU:HG2	3:G:4576:HOH:O	1.78	0.81
1:A:2:MET:CG	1:A:3:GLY:H	1.92	0.80
1:E:23:ASN:O	1:E:27:LYS:HD2	1.82	0.80
1:H:6:LYS:HE3	1:H:208:ILE:HG13	1.62	0.80
1:E:143:LYS:C	1:E:145:GLY:H	1.90	0.80
1:A:5:GLY:HA3	1:A:88:LYS:O	1.83	0.79
1:C:212:LYS:HD3	1:C:212:LYS:C	2.07	0.79
1:C:156:PHE:O	1:C:159:LYS:HG2	1.83	0.78
1:C:159:LYS:HD2	1:C:159:LYS:N	1.99	0.78
1:C:13:LEU:CD2	1:C:160:VAL:HG22	2.15	0.77
1:G:173:ARG:HG3	1:G:173:ARG:O	1.84	0.76
1:F:37:LYS:HG3	3:F:4841:HOH:O	1.85	0.76
1:G:171:GLU:HG3	3:G:5194:HOH:O	1.85	0.76
1:B:203:VAL:HG23	3:B:4786:HOH:O	1.85	0.75
1:D:6:LYS:CD	1:D:208:ILE:HD11	2.16	0.75
1:C:187:LYS:HG3	1:C:191:GLU:CD	2.12	0.75
1:H:167:LEU:O	1:H:171:GLU:HG2	1.87	0.75
1:C:37:LYS:HG3	3:C:4946:HOH:O	1.86	0.74
1:A:137:VAL:HG23	3:A:4743:HOH:O	1.88	0.74
1:B:208:ILE:HG22	1:B:209:ASP:CG	2.12	0.74
1:E:212:LYS:HD2	1:E:213:PHE:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:O	1:D:86:GLU:HG3	1.87	0.74
1:G:36:LEU:CD2	1:G:80:ILE:HD11	2.18	0.74
1:E:172:ILE:HG12	3:E:4898:HOH:O	1.87	0.74
1:H:6:LYS:CD	1:H:208:ILE:HD11	2.18	0.74
1:A:165:MET:HG2	3:A:4689:HOH:O	1.86	0.74
1:A:172:ILE:HG22	1:A:173:ARG:N	2.03	0.74
1:C:200:VAL:CG1	1:C:204:LEU:CD2	2.67	0.73
1:D:124:LEU:HD21	1:D:213:PHE:CD1	2.22	0.73
1:G:36:LEU:HD21	1:G:80:ILE:HD11	1.70	0.72
1:E:200:VAL:HG12	1:E:204:LEU:HD11	1.71	0.72
1:A:170:LYS:O	1:A:174:LYS:HB2	1.90	0.72
1:C:154:VAL:O	1:C:158:GLU:HG3	1.89	0.72
1:H:27:LYS:HE2	3:H:4805:HOH:O	1.89	0.72
1:B:136:ASP:OD2	1:B:139:ASN:HB3	1.89	0.71
1:C:31:PRO:HD2	3:C:4458:HOH:O	1.89	0.71
1:A:44:ARG:HH22	1:B:51:GLU:CD	1.99	0.71
1:B:44:ARG:HG2	3:B:4605:HOH:O	1.89	0.71
1:C:162:GLN:NE2	1:C:162:GLN:N	2.18	0.71
1:E:200:VAL:HG12	1:E:204:LEU:CD1	2.21	0.70
1:H:141:ALA:HA	1:H:146:PHE:CD2	2.27	0.70
1:C:156:PHE:HA	1:C:159:LYS:HD3	1.74	0.70
1:D:209:ASP:HB2	1:D:212:LYS:CB	2.22	0.69
1:B:162:GLN:HG3	3:B:5155:HOH:O	1.92	0.69
1:A:173:ARG:O	1:A:173:ARG:HG3	1.91	0.69
1:A:162:GLN:H	1:A:162:GLN:NE2	1.83	0.69
1:C:13:LEU:HD21	1:C:160:VAL:HG22	1.72	0.69
1:F:125:LYS:HE3	3:F:4275:HOH:O	1.92	0.69
1:A:13:LEU:HD11	1:A:161:LYS:HG3	1.74	0.69
1:G:166:LYS:O	1:G:170:LYS:HG3	1.93	0.68
1:C:13:LEU:CD1	1:C:161:LYS:HD2	2.23	0.68
1:A:167:LEU:HD12	1:A:167:LEU:O	1.94	0.68
1:E:166:LYS:O	1:E:170:LYS:HG3	1.93	0.68
1:C:153:THR:HB	1:C:156:PHE:CB	2.22	0.68
1:C:210:HIS:HE1	3:C:4490:HOH:O	1.76	0.67
1:D:9:LEU:C	1:D:10:ILE:HD12	2.20	0.67
1:G:210:HIS:HE1	3:G:4867:HOH:O	1.77	0.67
1:G:131:PHE:HB3	1:G:181:ILE:HD12	1.76	0.66
1:D:174:LYS:O	3:D:5295:HOH:O	2.13	0.66
1:F:83:ASP:OD2	3:F:4280:HOH:O	2.13	0.66
1:H:93:ASP:O	1:H:94:ARG:HB2	1.94	0.66
1:A:2:MET:HG3	1:A:210:HIS:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:GLN:HG2	3:G:5294:HOH:O	1.96	0.66
1:H:6:LYS:HD2	1:H:208:ILE:HD11	1.78	0.66
1:F:86:GLU:OE1	1:F:88:LYS:HE3	1.96	0.66
1:E:172:ILE:HG22	1:E:173:ARG:N	2.11	0.65
1:G:143:LYS:HG3	1:G:145:GLY:H	1.61	0.65
1:D:51:GLU:OE1	3:D:4213:HOH:O	2.15	0.65
1:C:159:LYS:N	1:C:159:LYS:CD	2.60	0.65
1:G:200:VAL:O	1:G:204:LEU:CD1	2.45	0.65
1:H:6:LYS:HE3	1:H:208:ILE:CG1	2.26	0.65
1:G:12:GLY:HA2	1:G:131:PHE:CE1	2.32	0.65
1:E:207:HIS:O	3:E:4951:HOH:O	2.14	0.64
1:H:34:LYS:NZ	3:H:5030:HOH:O	2.29	0.64
1:C:212:LYS:HD3	1:C:213:PHE:N	2.13	0.64
1:C:162:GLN:H	1:C:162:GLN:HE21	0.70	0.64
1:B:191:GLU:OE2	1:E:191:GLU:CG	2.45	0.64
1:A:165:MET:HA	1:A:165:MET:HE3	1.80	0.63
1:D:209:ASP:HB2	1:D:212:LYS:HB3	1.81	0.63
1:D:6:LYS:CD	1:D:208:ILE:CD1	2.77	0.63
1:E:82:LYS:O	1:E:86:GLU:HG3	1.97	0.63
1:E:173:ARG:HG3	1:E:173:ARG:O	1.97	0.63
1:A:158:GLU:O	1:A:162:GLN:NE2	2.31	0.63
1:E:200:VAL:O	1:E:204:LEU:CD1	2.46	0.63
1:G:23:ASN:O	1:G:27:LYS:HD2	1.98	0.63
1:G:171:GLU:CG	3:G:5194:HOH:O	2.43	0.62
1:A:59:GLN:NE2	3:A:4830:HOH:O	2.32	0.62
1:C:167:LEU:HD12	1:C:170:LYS:HD3	1.81	0.62
1:A:15:ARG:HB3	1:A:142:GLU:HB3	1.80	0.62
1:A:30:GLN:HG2	1:A:31:PRO:HA	1.82	0.62
1:E:147:GLY:O	1:E:148:ASP:CB	2.46	0.61
1:A:140:ASN:OD1	1:A:143:LYS:HE3	2.01	0.61
1:C:124:LEU:HD22	1:C:213:PHE:CD1	2.36	0.61
1:D:216:PHE:HD1	3:D:4879:HOH:O	1.81	0.61
1:C:12:GLY:HA2	1:C:131:PHE:CE1	2.35	0.61
1:G:172:ILE:HG22	1:G:173:ARG:N	2.15	0.61
1:B:72:ASN:O	1:B:76:ILE:HD12	2.01	0.61
1:A:146:PHE:O	1:A:148:ASP:N	2.29	0.61
1:C:131:PHE:HB3	1:C:181:ILE:HD12	1.83	0.61
1:D:191:GLU:OE2	1:G:191:GLU:OE2	2.17	0.61
1:C:155:LYS:HA	1:C:158:GLU:CD	2.25	0.61
1:D:134:THR:HG21	1:D:140:ASN:HD21	1.66	0.61
1:B:139:ASN:O	1:B:142:GLU:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:LYS:HA	3:C:5086:HOH:O	2.01	0.60
1:A:130:LEU:HD11	1:A:199:ILE:HG21	1.82	0.60
1:E:143:LYS:C	1:E:145:GLY:N	2.59	0.60
1:C:125:LYS:NZ	1:C:171:GLU:OE2	2.27	0.60
1:G:2:MET:N	3:G:5235:HOH:O	2.35	0.60
1:G:34:LYS:HD2	1:G:88:LYS:HD2	1.83	0.60
1:E:131:PHE:HB3	1:E:181:ILE:HD12	1.84	0.60
1:B:93:ASP:O	1:B:94:ARG:HB2	2.03	0.59
1:C:169:ASP:HB3	1:C:173:ARG:NH2	2.17	0.59
1:F:143:LYS:HG2	3:F:5096:HOH:O	2.02	0.59
1:G:13:LEU:O	1:G:18:LYS:NZ	2.34	0.59
1:A:200:VAL:O	1:A:204:LEU:CD1	2.50	0.59
1:B:3:GLY:HA3	1:B:207:HIS:CE1	2.37	0.59
1:B:191:GLU:OE2	1:E:191:GLU:OE2	2.19	0.59
1:B:208:ILE:HG22	1:B:209:ASP:OD2	2.02	0.59
1:C:30:GLN:HG2	1:C:31:PRO:HA	1.83	0.59
1:A:28:LYS:HD2	3:A:4971:HOH:O	2.01	0.59
1:C:158:GLU:O	1:C:162:GLN:NE2	2.33	0.59
1:C:200:VAL:HG12	1:C:204:LEU:HD22	1.84	0.59
1:E:166:LYS:CE	1:E:170:LYS:HE3	2.32	0.59
1:B:167:LEU:O	1:B:171:GLU:HG2	2.03	0.59
1:A:93:ASP:O	1:A:94:ARG:HB2	2.02	0.58
1:C:37:LYS:CG	3:C:4946:HOH:O	2.45	0.58
1:E:165:MET:HE3	1:E:165:MET:HA	1.84	0.58
1:D:10:ILE:HD12	1:D:10:ILE:N	2.19	0.58
1:E:175:GLY:C	3:E:4949:HOH:O	2.45	0.58
1:H:10:ILE:HD12	1:H:130:LEU:HD12	1.86	0.58
1:A:15:ARG:HD3	1:A:139:ASN:O	2.04	0.58
1:E:142:GLU:O	2:E:217:T5A:HA51	2.03	0.58
1:C:181:ILE:HD13	1:C:181:ILE:N	2.19	0.58
1:E:72:ASN:O	1:E:76:ILE:HD12	2.03	0.58
1:B:37:LYS:HG3	1:B:93:ASP:HB3	1.86	0.58
1:B:141:ALA:HA	1:B:146:PHE:CD2	2.39	0.57
1:E:13:LEU:CD1	1:E:161:LYS:HG3	2.27	0.57
1:A:36:LEU:HD12	1:A:37:LYS:H	1.69	0.57
1:C:29:LEU:HB3	3:C:4202:HOH:O	2.05	0.57
1:A:200:VAL:HG12	1:A:204:LEU:HD13	1.85	0.57
1:C:13:LEU:O	1:C:18:LYS:NZ	2.36	0.57
1:C:161:LYS:HB3	1:C:162:GLN:HE21	1.70	0.57
1:C:36:LEU:CD2	1:C:80:ILE:HD11	2.33	0.57
1:F:130:LEU:HD21	1:F:199:ILE:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LYS:HE2	3:C:4181:HOH:O	2.05	0.57
1:C:161:LYS:HB3	1:C:162:GLN:NE2	2.20	0.57
1:D:21:GLN:OE1	3:D:4168:HOH:O	2.17	0.57
1:A:200:VAL:CG1	1:A:204:LEU:CD1	2.71	0.57
1:G:55:ASP:OD1	1:G:57:SER:HB2	2.04	0.57
1:C:23:ASN:O	1:C:27:LYS:HD2	2.05	0.57
1:E:67:LEU:HD22	1:F:67:LEU:HD22	1.87	0.57
1:C:155:LYS:HA	1:C:158:GLU:OE2	2.04	0.57
1:C:158:GLU:OE1	1:C:159:LYS:NZ	2.38	0.56
1:E:143:LYS:HG2	1:E:143:LYS:O	2.06	0.56
1:A:180:THR:HG21	1:A:199:ILE:HD13	1.87	0.56
1:C:174:LYS:HB2	1:C:174:LYS:HZ2	1.69	0.56
1:B:206:THR:HG22	1:B:207:HIS:N	2.20	0.56
1:E:181:ILE:HD13	1:E:181:ILE:N	2.21	0.56
1:C:151:TYR:O	1:C:153:THR:N	2.37	0.56
1:E:166:LYS:HE2	1:E:170:LYS:HE3	1.88	0.56
1:C:149:GLU:H	1:C:152:GLU:HG3	1.70	0.56
1:G:141:ALA:O	1:G:143:LYS:N	2.39	0.55
1:C:200:VAL:CG1	1:C:204:LEU:HD22	2.37	0.55
1:C:173:ARG:HD3	1:C:173:ARG:N	2.21	0.55
1:H:109:ASN:ND2	3:H:4704:HOH:O	2.38	0.55
1:A:183:ASP:O	1:A:187:LYS:HE2	2.06	0.55
1:A:155:LYS:HD2	3:A:4691:HOH:O	2.06	0.55
1:B:206:THR:HG22	1:B:207:HIS:H	1.71	0.55
1:C:155:LYS:O	1:C:159:LYS:CD	2.52	0.55
1:H:209:ASP:HB2	1:H:212:LYS:HB3	1.89	0.55
1:E:124:LEU:HD21	1:E:213:PHE:CD1	2.42	0.55
1:F:155:LYS:HD3	3:F:5173:HOH:O	2.06	0.55
1:G:38:PHE:HA	1:G:39:PRO:C	2.32	0.55
1:G:171:GLU:CG	3:G:4576:HOH:O	2.48	0.55
1:F:128:LEU:HD22	1:F:203:VAL:HG21	1.89	0.55
1:G:162:GLN:HE21	1:G:162:GLN:N	2.04	0.55
1:E:212:LYS:HD2	1:E:212:LYS:C	2.31	0.54
1:E:137:VAL:HG11	1:E:158:GLU:OE1	2.08	0.54
1:D:6:LYS:HD2	1:D:208:ILE:CD1	2.27	0.54
1:D:93:ASP:O	1:D:94:ARG:HB2	2.08	0.54
1:D:209:ASP:HB2	1:D:212:LYS:HB2	1.88	0.54
1:F:93:ASP:O	1:F:94:ARG:HB2	2.07	0.54
1:G:52:TYR:O	1:G:150:ARG:NH1	2.37	0.54
1:C:40:GLU:OE1	1:C:42:SER:HB3	2.07	0.54
1:D:6:LYS:HE3	1:D:208:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASP:N	1:C:136:ASP:OD1	2.38	0.54
1:E:38:PHE:HA	1:E:39:PRO:C	2.33	0.54
1:G:7:LEU:HD23	1:G:126:PRO:HA	1.90	0.54
1:A:148:ASP:OD1	1:A:152:GLU:HB2	2.08	0.54
1:D:207:HIS:HA	3:D:4677:HOH:O	2.08	0.54
1:E:200:VAL:HG13	1:E:204:LEU:HD11	1.88	0.54
1:A:140:ASN:O	1:A:143:LYS:HD2	2.09	0.53
1:B:13:LEU:O	1:B:18:LYS:NZ	2.41	0.53
1:D:198:GLN:HG3	3:D:4417:HOH:O	2.08	0.53
1:A:146:PHE:C	1:A:148:ASP:H	2.16	0.53
1:C:165:MET:HE3	1:C:165:MET:HA	1.88	0.53
1:G:83:ASP:HB2	1:G:90:ILE:HD11	1.90	0.53
1:G:138:ASP:O	1:G:139:ASN:C	2.51	0.53
1:A:52:TYR:CE2	1:A:150:ARG:HD3	2.44	0.53
1:C:171:GLU:O	1:C:176:ASP:HB3	2.08	0.53
1:B:111:MET:HG2	1:B:115:TRP:CZ3	2.43	0.53
1:C:156:PHE:O	1:C:159:LYS:CG	2.57	0.52
1:H:44:ARG:HH11	1:H:44:ARG:CG	1.99	0.52
1:C:200:VAL:CG1	1:C:204:LEU:HD21	2.39	0.52
1:A:131:PHE:HB3	1:A:181:ILE:CD1	2.35	0.52
1:C:81:LYS:CG	1:C:124:LEU:HD11	2.39	0.52
1:A:162:GLN:N	1:A:162:GLN:NE2	2.43	0.52
1:G:114:ASP:HB2	3:G:4522:HOH:O	2.10	0.52
1:A:199:ILE:O	1:A:202:PRO:HD2	2.10	0.52
1:D:125:LYS:HD3	3:D:4889:HOH:O	2.09	0.52
1:E:170:LYS:O	1:E:174:LYS:HB2	2.09	0.52
1:A:113:LEU:HD11	1:A:166:LYS:HD2	1.91	0.52
1:B:37:LYS:HG2	3:B:4579:HOH:O	2.08	0.52
1:C:5:GLY:HA3	1:C:88:LYS:O	2.09	0.52
1:C:187:LYS:HB3	1:C:192:VAL:HG23	1.92	0.52
1:E:3:GLY:HA2	1:E:208:ILE:O	2.09	0.52
1:G:93:ASP:O	1:G:94:ARG:HB2	2.10	0.52
1:C:7:LEU:HD23	1:C:126:PRO:HA	1.92	0.52
1:C:20:THR:OG1	2:C:217:T5A:HA8	2.09	0.52
1:F:189:ILE:HD12	3:F:5031:HOH:O	2.10	0.52
1:A:172:ILE:C	1:A:174:LYS:H	2.18	0.51
1:C:168:LEU:HD22	1:C:179:ILE:HG21	1.92	0.51
1:C:52:TYR:O	1:C:150:ARG:HD2	2.10	0.51
1:G:6:LYS:HE2	3:G:5264:HOH:O	2.11	0.51
1:H:125:LYS:HD3	3:H:4364:HOH:O	2.09	0.51
1:F:40:GLU:C	1:F:40:GLU:OE1	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:NH2	1:B:51:GLU:CD	2.68	0.51
1:F:57:SER:O	1:F:59:GLN:HG2	2.10	0.51
1:G:37:LYS:HG3	3:G:4928:HOH:O	2.10	0.51
1:G:143:LYS:HD3	3:G:5247:HOH:O	2.11	0.51
1:C:171:GLU:OE1	1:C:171:GLU:HA	2.10	0.50
1:E:5:GLY:HA3	1:E:88:LYS:O	2.11	0.50
1:D:24:ILE:HG21	1:D:193:GLU:HG3	1.93	0.50
1:D:118:GLN:HB2	3:D:4718:HOH:O	2.11	0.50
1:F:8:ILE:N	1:F:8:ILE:HD12	2.26	0.50
1:G:143:LYS:HG3	1:G:145:GLY:N	2.26	0.50
1:C:38:PHE:HA	1:C:39:PRO:C	2.36	0.50
1:C:169:ASP:HB3	1:C:173:ARG:CZ	2.41	0.50
1:H:38:PHE:HA	1:H:39:PRO:C	2.35	0.50
1:A:67:LEU:HD22	1:B:67:LEU:HD22	1.94	0.50
1:E:12:GLY:HA2	1:E:131:PHE:CE1	2.47	0.50
1:B:44:ARG:NE	3:B:4566:HOH:O	2.42	0.50
1:C:156:PHE:HA	1:C:159:LYS:CD	2.40	0.50
1:A:7:LEU:HD23	1:A:126:PRO:HA	1.93	0.50
1:E:166:LYS:HE3	1:E:170:LYS:HE3	1.94	0.50
3:E:4777:HOH:O	1:F:118:GLN:HB2	2.11	0.49
1:A:4:ARG:HG2	1:A:210:HIS:HA	1.93	0.49
1:B:37:LYS:CG	3:B:4579:HOH:O	2.60	0.49
1:B:84:LEU:HG	1:B:90:ILE:HD12	1.93	0.49
1:C:174:LYS:NZ	1:C:174:LYS:CB	2.56	0.49
1:E:200:VAL:O	1:E:204:LEU:HD13	2.11	0.49
1:B:161:LYS:HZ3	1:B:165:MET:HE2	1.76	0.49
1:D:77:VAL:HA	1:D:80:ILE:HD12	1.94	0.49
1:H:109:ASN:HB2	3:H:4356:HOH:O	2.12	0.49
1:B:191:GLU:OE2	1:E:191:GLU:HG2	2.12	0.49
1:A:36:LEU:HD12	1:A:37:LYS:N	2.26	0.49
1:C:167:LEU:CD1	1:C:170:LYS:HD3	2.43	0.49
1:A:135:GLN:HG3	1:A:185:THR:HG21	1.94	0.48
1:E:143:LYS:O	1:E:145:GLY:N	2.45	0.48
1:F:203:VAL:HG23	3:F:4314:HOH:O	2.13	0.48
1:B:143:LYS:HE2	3:B:4784:HOH:O	2.13	0.48
1:E:107:GLY:HA3	1:G:2:MET:HB2	1.95	0.48
1:G:166:LYS:HD3	1:G:170:LYS:CE	2.38	0.48
1:H:6:LYS:CD	1:H:208:ILE:CD1	2.91	0.48
1:A:137:VAL:CG2	3:A:4743:HOH:O	2.55	0.48
1:F:141:ALA:HA	1:F:146:PHE:CD1	2.47	0.48
1:G:18:LYS:HB2	1:G:18:LYS:HE2	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:VAL:O	1:E:204:LEU:HD12	2.12	0.48
1:G:181:ILE:HD13	1:G:181:ILE:N	2.28	0.48
1:A:200:VAL:O	1:A:204:LEU:HD12	2.13	0.48
1:E:37:LYS:HG3	3:E:4307:HOH:O	2.12	0.48
1:F:37:LYS:CG	3:F:4841:HOH:O	2.51	0.48
1:G:5:GLY:HA3	1:G:88:LYS:O	2.14	0.48
1:G:37:LYS:CG	3:G:4928:HOH:O	2.62	0.48
1:G:143:LYS:HE3	1:G:143:LYS:HB3	1.43	0.48
1:G:143:LYS:C	1:G:145:GLY:H	2.21	0.48
1:C:13:LEU:HD23	1:C:160:VAL:HG22	1.93	0.48
1:C:153:THR:CB	1:C:156:PHE:HB3	2.36	0.48
1:H:30:GLN:HB3	1:H:31:PRO:HA	1.95	0.48
1:A:144:SER:OG	1:A:144:SER:O	2.31	0.47
1:H:156:PHE:O	1:H:160:VAL:HG23	2.14	0.47
1:A:38:PHE:HA	1:A:39:PRO:C	2.38	0.47
1:C:154:VAL:O	1:C:158:GLU:CG	2.61	0.47
1:B:156:PHE:O	1:B:160:VAL:HG23	2.14	0.47
1:A:13:LEU:O	1:A:18:LYS:NZ	2.45	0.47
1:A:172:ILE:C	1:A:174:LYS:N	2.72	0.47
1:B:15:ARG:O	1:B:140:ASN:ND2	2.47	0.47
1:C:79:LYS:HG2	3:C:5151:HOH:O	2.14	0.47
1:B:130:LEU:CD2	1:B:199:ILE:HG21	2.44	0.47
1:D:6:LYS:HE2	1:D:206:THR:O	2.14	0.47
1:E:143:LYS:HG3	1:E:145:GLY:CA	2.45	0.47
1:E:28:LYS:NZ	3:E:4300:HOH:O	2.48	0.47
1:E:159:LYS:HD2	3:E:5377:HOH:O	2.15	0.47
1:G:172:ILE:C	1:G:174:LYS:H	2.21	0.47
1:C:148:ASP:OD1	1:C:152:GLU:CB	2.62	0.47
1:C:159:LYS:H	1:C:159:LYS:CD	2.09	0.47
1:D:135:GLN:HB2	1:D:185:THR:HG21	1.96	0.47
1:D:167:LEU:O	1:D:171:GLU:HG2	2.15	0.47
1:F:170:LYS:CD	3:F:4575:HOH:O	2.62	0.47
1:G:158:GLU:O	1:G:162:GLN:NE2	2.47	0.47
1:E:37:LYS:CG	3:E:4307:HOH:O	2.63	0.47
1:A:2:MET:CG	1:A:210:HIS:HB2	2.45	0.47
1:A:200:VAL:O	1:A:204:LEU:HD13	2.13	0.47
1:C:4:ARG:CZ	1:C:208:ILE:HG21	2.45	0.47
1:C:36:LEU:O	1:C:92:MET:HA	2.15	0.47
1:C:134:THR:O	1:C:161:LYS:NZ	2.37	0.47
1:D:44:ARG:HH11	1:D:44:ARG:HB3	1.80	0.47
1:A:18:LYS:HE2	1:A:18:LYS:HB2	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:O	1:A:184:VAL:HG22	2.16	0.46
1:A:136:ASP:O	1:A:137:VAL:O	2.33	0.46
1:A:37:LYS:HG3	3:A:4084:HOH:O	2.15	0.46
1:D:30:GLN:HB3	1:D:31:PRO:HA	1.97	0.46
1:E:201:GLU:N	1:E:202:PRO:HD2	2.31	0.46
1:A:15:ARG:HD2	1:A:138:ASP:O	2.15	0.46
1:C:125:LYS:HZ3	1:C:171:GLU:HG3	1.80	0.46
1:B:149:GLU:HB2	1:B:152:GLU:CD	2.40	0.46
1:C:44:ARG:HH22	1:D:51:GLU:CD	2.24	0.46
1:D:187:LYS:HD3	1:D:191:GLU:CD	2.41	0.46
1:D:191:GLU:OE2	1:G:191:GLU:CG	2.64	0.46
1:G:144:SER:O	1:G:145:GLY:O	2.33	0.46
1:G:162:GLN:HE21	1:G:162:GLN:H	1.62	0.46
1:B:190:GLN:HG2	3:E:4599:HOH:O	2.16	0.46
1:F:13:LEU:HD11	1:F:161:LYS:HB2	1.97	0.46
3:B:4336:HOH:O	1:E:28:LYS:HD3	2.15	0.46
1:F:20:THR:HG21	1:F:189:ILE:HG12	1.97	0.46
1:A:44:ARG:CG	3:A:4603:HOH:O	2.64	0.46
1:A:55:ASP:OD1	1:A:57:SER:HB2	2.16	0.46
1:F:38:PHE:HA	1:F:39:PRO:C	2.40	0.46
1:E:29:LEU:HB3	3:E:4316:HOH:O	2.15	0.46
1:E:36:LEU:HD12	1:E:37:LYS:N	2.30	0.46
1:F:30:GLN:HB3	1:F:31:PRO:HA	1.98	0.46
1:G:44:ARG:NH1	3:G:5129:HOH:O	2.48	0.46
1:G:72:ASN:O	1:G:75:GLU:HG2	2.15	0.46
1:A:2:MET:O	1:A:207:HIS:HE1	1.99	0.46
1:C:148:ASP:OD1	1:C:152:GLU:HB3	2.15	0.46
1:D:201:GLU:OE2	1:G:201:GLU:OE2	2.33	0.46
1:H:52:TYR:CD2	1:H:65:ILE:HG12	2.51	0.46
1:C:189:ILE:HG12	2:C:217:T5A:N7A	2.31	0.45
1:F:13:LEU:O	1:F:18:LYS:NZ	2.48	0.45
1:G:44:ARG:HH22	1:H:51:GLU:CD	2.23	0.45
1:H:36:LEU:HD12	1:H:37:LYS:H	1.81	0.45
1:H:52:TYR:CE2	1:H:65:ILE:HG12	2.51	0.45
1:D:10:ILE:N	1:D:10:ILE:CD1	2.79	0.45
1:E:93:ASP:O	1:E:94:ARG:HB2	2.15	0.45
1:F:143:LYS:HG3	1:F:144:SER:H	1.81	0.45
1:F:170:LYS:HE2	3:F:4575:HOH:O	2.15	0.45
1:H:65:ILE:HG23	1:H:66:HIS:N	2.31	0.45
1:A:180:THR:HG21	1:A:199:ILE:CD1	2.46	0.45
1:D:20:THR:HG21	1:D:189:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ILE:HD12	3:D:4597:HOH:O	2.16	0.45
1:E:4:ARG:HB2	1:E:84:LEU:O	2.16	0.45
1:G:124:LEU:CD2	1:G:213:PHE:HB3	2.47	0.45
1:H:56:ASP:OD1	1:H:56:ASP:C	2.60	0.45
1:C:36:LEU:HD21	1:C:80:ILE:HD11	1.97	0.45
1:A:146:PHE:HD2	3:A:4692:HOH:O	1.99	0.45
1:C:84:LEU:HG	1:C:90:ILE:HD12	1.99	0.45
1:G:156:PHE:O	1:G:160:VAL:HG23	2.16	0.45
1:A:4:ARG:CZ	1:A:208:ILE:HG21	2.47	0.45
1:G:118:GLN:HB2	1:G:119:PRO:HD3	1.99	0.45
1:A:2:MET:HG2	1:A:210:HIS:HB3	1.99	0.45
1:A:167:LEU:HD12	1:A:167:LEU:C	2.41	0.45
1:C:8:ILE:HD12	1:C:128:LEU:HD23	1.98	0.45
1:G:18:LYS:HE2	3:G:4413:HOH:O	2.17	0.45
1:D:201:GLU:HB3	1:D:202:PRO:HD3	1.97	0.45
1:E:44:ARG:H	1:E:44:ARG:HG2	1.62	0.45
1:A:14:ASP:OD2	1:A:157:GLN:NE2	2.45	0.45
1:E:209:ASP:HB3	1:E:212:LYS:HB2	1.98	0.45
1:H:137:VAL:HG12	1:H:137:VAL:O	2.17	0.45
1:A:85:LEU:HD22	1:A:210:HIS:CE1	2.52	0.44
1:H:44:ARG:NH1	1:H:44:ARG:CG	2.62	0.44
1:H:15:ARG:NE	3:H:4430:HOH:O	2.44	0.44
1:H:134:THR:CG2	3:H:4688:HOH:O	2.41	0.44
1:E:95:TYR:CG	1:E:96:VAL:N	2.86	0.44
1:E:200:VAL:CG1	1:E:204:LEU:CD1	2.83	0.44
1:G:128:LEU:HD21	1:G:130:LEU:HD21	2.00	0.44
1:A:201:GLU:N	1:A:202:PRO:CD	2.81	0.44
1:E:51:GLU:OE2	1:F:44:ARG:NH2	2.50	0.44
1:G:24:ILE:HG21	1:G:193:GLU:HG3	1.99	0.44
1:C:86:GLU:OE1	1:C:88:LYS:HE3	2.18	0.44
1:D:44:ARG:HG2	1:D:44:ARG:H	1.56	0.44
1:E:24:ILE:HG23	3:E:4318:HOH:O	2.18	0.44
1:B:184:VAL:HB	3:B:4646:HOH:O	2.18	0.43
1:C:173:ARG:HD3	1:C:173:ARG:H	1.82	0.43
1:G:77:VAL:O	1:G:77:VAL:HG22	2.18	0.43
1:A:200:VAL:HG13	1:A:204:LEU:HD11	1.90	0.43
1:C:149:GLU:N	1:C:152:GLU:HG3	2.32	0.43
1:F:26:TYR:O	1:F:30:GLN:HG3	2.18	0.43
1:F:118:GLN:HB2	1:F:119:PRO:HD3	1.99	0.43
1:H:118:GLN:HB2	1:H:119:PRO:HD3	1.99	0.43
1:H:128:LEU:HD21	1:H:130:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:GLY:O	1:B:51:GLU:HG3	2.19	0.43
1:B:143:LYS:HE3	2:B:217:T5A:O4F	2.18	0.43
1:G:40:GLU:OE1	1:G:42:SER:HB3	2.18	0.43
1:C:172:ILE:HG22	1:C:173:ARG:N	2.32	0.43
1:A:142:GLU:O	2:A:217:T5A:HA51	2.19	0.43
1:E:72:ASN:O	1:E:75:GLU:HG2	2.18	0.43
1:E:172:ILE:C	1:E:174:LYS:H	2.26	0.43
1:F:134:THR:HG21	1:F:140:ASN:HD21	1.83	0.43
1:G:30:GLN:HG2	1:G:31:PRO:HA	2.01	0.43
1:A:86:GLU:HG3	3:A:4452:HOH:O	2.19	0.43
1:A:209:ASP:O	1:A:212:LYS:N	2.45	0.43
1:C:44:ARG:NH2	1:D:51:GLU:OE2	2.46	0.43
1:F:199:ILE:O	1:F:202:PRO:HD2	2.19	0.43
1:G:201:GLU:HA	1:G:204:LEU:HD13	2.01	0.43
1:H:6:LYS:HD3	1:H:208:ILE:CD1	2.49	0.43
1:H:82:LYS:O	1:H:86:GLU:HG3	2.19	0.43
1:A:138:ASP:HB2	1:A:154:VAL:CG2	2.49	0.43
1:D:207:HIS:ND1	1:D:207:HIS:C	2.75	0.43
1:E:2:MET:HE2	1:E:210:HIS:NE2	2.33	0.43
1:H:208:ILE:O	1:H:209:ASP:C	2.61	0.43
1:A:44:ARG:HG2	3:A:4603:HOH:O	2.19	0.43
1:C:1:MET:HB2	1:C:2:MET:H	1.71	0.43
1:G:200:VAL:HG13	1:G:204:LEU:HD11	1.94	0.43
3:B:4313:HOH:O	1:E:190:GLN:CG	2.67	0.42
1:C:34:LYS:HD2	1:C:88:LYS:HD2	2.01	0.42
1:C:174:LYS:HZ3	1:C:174:LYS:CB	2.15	0.42
1:D:36:LEU:O	1:D:92:MET:HA	2.19	0.42
1:A:15:ARG:CB	1:A:142:GLU:HB3	2.48	0.42
1:A:131:PHE:CB	1:A:181:ILE:HD12	2.41	0.42
1:A:154:VAL:O	1:A:158:GLU:HB2	2.18	0.42
1:C:95:TYR:CG	1:C:96:VAL:N	2.86	0.42
1:F:36:LEU:HD21	1:F:38:PHE:CE2	2.54	0.42
1:G:81:LYS:HG3	1:G:124:LEU:HD11	2.00	0.42
1:C:127:ASP:O	1:C:178:SER:HB2	2.19	0.42
1:A:135:GLN:HG3	1:A:185:THR:CG2	2.48	0.42
1:A:148:ASP:OD1	1:A:148:ASP:C	2.62	0.42
1:C:79:LYS:CG	3:C:5151:HOH:O	2.66	0.42
1:C:211:ASP:OD1	1:C:211:ASP:C	2.62	0.42
1:F:174:LYS:O	3:F:4959:HOH:O	2.22	0.42
1:C:93:ASP:O	1:C:94:ARG:HB2	2.19	0.42
1:C:172:ILE:HG21	1:C:173:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4:ARG:CZ	1:G:208:ILE:HG21	2.49	0.42
1:G:143:LYS:CD	3:G:5247:HOH:O	2.67	0.42
1:D:44:ARG:HB3	1:D:44:ARG:NH1	2.35	0.42
1:D:124:LEU:CD2	1:D:213:PHE:CD1	3.01	0.42
1:E:143:LYS:CG	1:E:145:GLY:H	2.33	0.42
1:G:139:ASN:O	1:G:141:ALA:O	2.38	0.42
1:A:124:LEU:HD23	1:A:215:PHE:CE1	2.54	0.42
1:F:85:LEU:HD23	1:F:85:LEU:HA	1.85	0.42
1:A:1:MET:SD	1:A:1:MET:C	3.03	0.42
1:A:1:MET:SD	1:A:2:MET:HB2	2.60	0.42
1:A:166:LYS:HD3	1:A:170:LYS:HE3	2.01	0.42
1:E:128:LEU:CD1	3:E:4460:HOH:O	2.66	0.42
1:G:52:TYR:CE1	1:G:150:ARG:HD3	2.55	0.42
1:H:68:LEU:HD23	1:H:68:LEU:HA	1.85	0.42
1:C:130:LEU:HD11	1:C:199:ILE:HD13	2.02	0.42
1:C:171:GLU:OE1	1:C:171:GLU:CA	2.67	0.42
1:E:18:LYS:HB2	1:E:18:LYS:HE2	1.77	0.42
1:F:141:ALA:HA	1:F:146:PHE:CE1	2.55	0.42
1:B:142:GLU:O	1:B:143:LYS:C	2.63	0.41
1:C:51:GLU:OE2	1:D:44:ARG:NH2	2.53	0.41
1:F:84:LEU:HG	1:F:90:ILE:HD12	2.02	0.41
1:F:158:GLU:OE2	1:F:162:GLN:NE2	2.53	0.41
1:A:84:LEU:CD2	1:A:90:ILE:HD12	2.50	0.41
1:A:136:ASP:O	1:A:137:VAL:C	2.63	0.41
1:B:140:ASN:HD22	1:B:140:ASN:HA	1.59	0.41
1:D:52:TYR:CD1	1:D:65:ILE:HG12	2.54	0.41
1:B:1:MET:N	3:B:4787:HOH:O	2.39	0.41
1:D:38:PHE:HA	1:D:39:PRO:C	2.44	0.41
1:F:36:LEU:O	1:F:92:MET:HA	2.20	0.41
1:E:86:GLU:OE1	1:E:88:LYS:HE3	2.20	0.41
1:D:155:LYS:HD3	3:D:4441:HOH:O	2.20	0.41
1:G:4:ARG:NH2	1:G:208:ILE:HG21	2.35	0.41
1:C:130:LEU:HD12	1:C:182:VAL:HG23	2.02	0.41
1:E:44:ARG:HG2	3:E:4910:HOH:O	2.21	0.41
1:E:200:VAL:HG12	1:E:204:LEU:HD13	2.00	0.41
1:G:141:ALA:C	1:G:143:LYS:N	2.79	0.41
1:B:38:PHE:HA	1:B:39:PRO:C	2.46	0.41
1:D:130:LEU:HD21	1:D:199:ILE:HG21	2.01	0.41
1:F:177:GLU:HG2	3:F:5075:HOH:O	2.20	0.41
1:G:155:LYS:HG2	3:G:5210:HOH:O	2.19	0.41
1:H:209:ASP:C	1:H:211:ASP:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MET:CG	1:A:210:HIS:CB	2.98	0.41
1:E:139:ASN:HB3	1:E:142:GLU:HB2	2.02	0.41
1:F:124:LEU:CD2	1:F:213:PHE:CD1	3.04	0.41
1:A:112:ASP:O	1:A:113:LEU:C	2.64	0.41
1:A:135:GLN:CG	1:A:185:THR:HG21	2.51	0.41
1:B:161:LYS:HZ3	1:B:165:MET:CE	2.33	0.41
1:C:180:THR:HG21	1:C:199:ILE:HD13	2.02	0.41
1:G:36:LEU:O	1:G:92:MET:HA	2.21	0.41
1:G:133:SER:O	1:G:184:VAL:HG22	2.21	0.41
1:H:124:LEU:HD23	1:H:215:PHE:CE1	2.56	0.41
1:A:79:LYS:HD3	3:A:4814:HOH:O	2.21	0.41
1:B:65:ILE:HG23	1:B:66:HIS:N	2.36	0.41
1:D:13:LEU:O	1:D:18:LYS:NZ	2.53	0.41
1:A:2:MET:O	1:A:207:HIS:CE1	2.74	0.40
1:C:3:GLY:O	1:C:210:HIS:CE1	2.75	0.40
1:E:154:VAL:O	1:E:158:GLU:HB2	2.21	0.40
1:G:143:LYS:HG3	1:G:145:GLY:CA	2.51	0.40
1:C:1:MET:HB2	1:C:1:MET:HE2	1.85	0.40
1:C:18:LYS:HE2	1:C:18:LYS:HB2	1.88	0.40
1:C:169:ASP:O	1:C:172:ILE:HB	2.21	0.40
1:D:12:GLY:HA2	1:D:131:PHE:CE1	2.56	0.40
1:D:134:THR:HG22	3:D:4962:HOH:O	2.20	0.40
1:F:133:SER:C	3:F:5073:HOH:O	2.64	0.40
1:F:173:ARG:NE	3:F:4660:HOH:O	2.31	0.40
1:H:33:CYS:HA	1:H:89:ASN:O	2.21	0.40
1:H:209:ASP:O	1:H:210:HIS:C	2.65	0.40
1:B:71:ALA:O	1:B:75:GLU:HG2	2.22	0.40
3:B:4313:HOH:O	1:E:190:GLN:HB3	2.21	0.40
1:D:26:TYR:O	1:D:30:GLN:HG3	2.20	0.40
1:D:82:LYS:HE2	1:D:86:GLU:OE2	2.22	0.40
1:F:7:LEU:C	1:F:8:ILE:HD12	2.46	0.40
1:H:136:ASP:C	1:H:138:ASP:H	2.28	0.40
1:C:81:LYS:HG2	1:C:124:LEU:HD11	2.02	0.40
1:E:215:PHE:CD1	1:E:215:PHE:N	2.89	0.40
1:H:96:VAL:HG22	1:H:120:ASP:CG	2.46	0.40
1:H:111:MET:HG2	1:H:115:TRP:CZ3	2.56	0.40

All (1) 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:A:191:GLU:OE2	1:F:191:GLU:OE2[1_556]	2.11	0.09

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	214/216 (99%)	194 (91%)	16 (8%)	4 (2%)	6	3
1	B	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	9	4
1	C	201/216 (93%)	191 (95%)	8 (4%)	2 (1%)	12	8
1	D	212/216 (98%)	205 (97%)	6 (3%)	1 (0%)	24	21
1	E	213/216 (99%)	196 (92%)	11 (5%)	6 (3%)	4	1
1	F	214/216 (99%)	204 (95%)	8 (4%)	2 (1%)	14	9
1	G	213/216 (99%)	193 (91%)	14 (7%)	6 (3%)	4	1
1	H	212/216 (98%)	198 (93%)	11 (5%)	3 (1%)	9	4
All	All	1693/1728 (98%)	1582 (93%)	84 (5%)	27 (2%)	7	3

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	VAL
1	G	142	GLU
1	G	145	GLY
1	G	146	PHE
1	G	148	ASP
1	H	142	GLU
1	A	147	GLY
1	B	209	ASP
1	B	210	HIS
1	C	152	GLU
1	E	145	GLY
1	E	146	PHE

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Mol	Chain	Res	Type
1	E	148	ASP
1	H	144	SER
1	A	210	HIS
1	E	210	HIS
1	H	143	LYS
1	B	95	TYR
1	C	95	TYR
1	D	95	TYR
1	F	95	TYR
1	F	141	ALA
1	G	139	ASN
1	G	141	ALA
1	A	148	ASP
1	E	95	TYR
1	E	144	SER

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	194/194 (100%)	166 (86%)	28 (14%)	3	2
1	B	193/194 (100%)	170 (88%)	23 (12%)	5	3
1	C	186/194 (96%)	153 (82%)	33 (18%)	2	1
1	D	188/194 (97%)	169 (90%)	19 (10%)	7	4
1	E	192/194 (99%)	167 (87%)	25 (13%)	4	2
1	F	192/194 (99%)	172 (90%)	20 (10%)	7	4
1	G	192/194 (99%)	169 (88%)	23 (12%)	5	3
1	H	188/194 (97%)	171 (91%)	17 (9%)	9	6
All	All	1525/1552 (98%)	1337 (88%)	188 (12%)	4	3

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	30	GLN
1	A	40	GLU
1	A	44	ARG
1	A	76	ILE
1	A	88	LYS
1	A	98	SER
1	A	114	ASP
1	A	130	LEU
1	A	135	GLN
1	A	142	GLU
1	A	143	LYS
1	A	146	PHE
1	A	148	ASP
1	A	153	THR
1	A	162	GLN
1	A	164	PHE
1	A	165	MET
1	A	166	LYS
1	A	167	LEU
1	A	171	GLU
1	A	172	ILE
1	A	173	ARG
1	A	174	LYS
1	A	181	ILE
1	A	190	GLN
1	A	212	LYS
1	A	214	SER
1	B	28	LYS
1	B	40	GLU
1	B	44	ARG
1	B	59	GLN
1	B	79	LYS
1	B	98	SER
1	B	109	ASN
1	B	125	LYS
1	B	135	GLN
1	B	139	ASN
1	B	140	ASN
1	B	142	GLU
1	B	155	LYS
1	B	161	LYS
1	B	164	PHE

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Mol	Chain	Res	Type
1	B	170	LYS
1	B	181	ILE
1	B	189	ILE
1	B	190	GLN
1	B	205	SER
1	B	207	HIS
1	B	209	ASP
1	B	212	LYS
1	C	1	MET
1	C	2	MET
1	C	10	ILE
1	C	34	LYS
1	C	37	LYS
1	C	40	GLU
1	C	42	SER
1	C	44	ARG
1	C	76	ILE
1	C	79	LYS
1	C	81	LYS
1	C	98	SER
1	C	114	ASP
1	C	130	LEU
1	C	136	ASP
1	C	148	ASP
1	C	153	THR
1	C	154	VAL
1	C	159	LYS
1	C	160	VAL
1	C	161	LYS
1	C	162	GLN
1	C	163	THR
1	C	164	PHE
1	C	170	LYS
1	C	171	GLU
1	C	172	ILE
1	C	174	LYS
1	C	177	GLU
1	C	181	ILE
1	C	187	LYS
1	C	204	LEU
1	C	212	LYS
1	D	27	LYS

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Mol	Chain	Res	Type
1	D	28	LYS
1	D	40	GLU
1	D	44	ARG
1	D	76	ILE
1	D	79	LYS
1	D	98	SER
1	D	109	ASN
1	D	125	LYS
1	D	135	GLN
1	D	158	GLU
1	D	164	PHE
1	D	170	LYS
1	D	181	ILE
1	D	190	GLN
1	D	206	THR
1	D	207	HIS
1	D	208	ILE
1	D	214	SER
1	E	2	MET
1	E	34	LYS
1	E	40	GLU
1	E	59	GLN
1	E	60	LEU
1	E	76	ILE
1	E	81	LYS
1	E	82	LYS
1	E	98	SER
1	E	114	ASP
1	E	130	LEU
1	E	148	ASP
1	E	154	VAL
1	E	155	LYS
1	E	158	GLU
1	E	161	LYS
1	E	162	GLN
1	E	164	PHE
1	E	165	MET
1	E	166	LYS
1	E	171	GLU
1	E	172	ILE
1	E	173	ARG
1	E	181	ILE

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Mol	Chain	Res	Type
1	E	212	LYS
1	F	28	LYS
1	F	40	GLU
1	F	44	ARG
1	F	59	GLN
1	F	79	LYS
1	F	82	LYS
1	F	98	SER
1	F	125	LYS
1	F	135	GLN
1	F	137	VAL
1	F	143	LYS
1	F	158	GLU
1	F	161	LYS
1	F	164	PHE
1	F	170	LYS
1	F	181	ILE
1	F	190	GLN
1	F	205	SER
1	F	211	ASP
1	F	212	LYS
1	G	28	LYS
1	G	34	LYS
1	G	40	GLU
1	G	42	SER
1	G	44	ARG
1	G	81	LYS
1	G	98	SER
1	G	114	ASP
1	G	130	LEU
1	G	135	GLN
1	G	143	LYS
1	G	158	GLU
1	G	162	GLN
1	G	164	PHE
1	G	165	MET
1	G	166	LYS
1	G	171	GLU
1	G	172	ILE
1	G	173	ARG
1	G	174	LYS
1	G	177	GLU

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Mol	Chain	Res	Type
1	G	181	ILE
1	G	190	GLN
1	H	10	ILE
1	H	28	LYS
1	H	40	GLU
1	H	44	ARG
1	H	76	ILE
1	H	79	LYS
1	H	98	SER
1	H	125	LYS
1	H	130	LEU
1	H	144	SER
1	H	155	LYS
1	H	161	LYS
1	H	164	PHE
1	H	170	LYS
1	H	189	ILE
1	H	190	GLN
1	H	208	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	118	GLN
1	A	162	GLN
1	A	186	ASN
1	A	207	HIS
1	B	23	ASN
1	B	32	ASN
1	B	135	GLN
1	B	140	ASN
1	B	207	HIS
1	C	118	GLN
1	C	135	GLN
1	C	162	GLN
1	C	207	HIS
1	C	210	HIS
1	D	23	ASN
1	D	32	ASN
1	D	140	ASN
1	D	190	GLN

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Mol	Chain	Res	Type
1	E	140	ASN
1	E	162	GLN
1	E	186	ASN
1	F	23	ASN
1	F	32	ASN
1	F	109	ASN
1	G	139	ASN
1	G	162	GLN
1	G	186	ASN
1	G	210	HIS
1	H	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	T5A	A	217	-	59,59,59	2.03	7 (11%)	84,93,93	1.30	11 (13%)
2	T5A	H	217	-	59,59,59	1.91	13 (22%)	84,93,93	1.63	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	T5A	C	217	-	59,59,59	1.76	10 (16%)	84,93,93	1.52	15 (17%)
2	T5A	F	217	-	59,59,59	2.03	13 (22%)	84,93,93	1.38	14 (16%)
2	T5A	E	217	-	59,59,59	1.75	12 (20%)	84,93,93	1.50	17 (20%)
2	T5A	B	217	-	59,59,59	2.19	9 (15%)	84,93,93	1.45	14 (16%)
2	T5A	D	217	-	59,59,59	2.60	9 (15%)	84,93,93	1.44	16 (19%)
2	T5A	G	217	-	59,59,59	1.77	11 (18%)	84,93,93	1.47	15 (17%)

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	T5A	A	217	-	-	9/44/72/72	0/5/5/5
2	T5A	H	217	-	-	5/44/72/72	0/5/5/5
2	T5A	C	217	-	-	6/44/72/72	0/5/5/5
2	T5A	F	217	-	-	6/44/72/72	0/5/5/5
2	T5A	E	217	-	-	8/44/72/72	0/5/5/5
2	T5A	B	217	-	-	7/44/72/72	0/5/5/5
2	T5A	D	217	-	-	5/44/72/72	0/5/5/5
2	T5A	G	217	-	-	8/44/72/72	0/5/5/5

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	217	T5A	PC-O3C	10.14	1.70	1.59
2	D	217	T5A	PA-O3A	-8.93	1.49	1.59
2	D	217	T5A	PB-O3A	8.39	1.68	1.59
2	A	217	T5A	PD-O3D	8.28	1.68	1.59
2	A	217	T5A	PC-O3C	7.71	1.67	1.59
2	B	217	T5A	PA-O3A	-7.31	1.51	1.59
2	F	217	T5A	PC-O3C	7.26	1.67	1.59
2	B	217	T5A	PB-O3A	6.72	1.66	1.59
2	B	217	T5A	PC-O3C	6.59	1.66	1.59
2	B	217	T5A	PD-O3D	6.48	1.66	1.59
2	F	217	T5A	PB-O3A	6.21	1.66	1.59
2	G	217	T5A	PB-O3A	6.15	1.66	1.59
2	E	217	T5A	PA-O3A	-6.07	1.52	1.59
2	C	217	T5A	PD-O3D	5.72	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	217	T5A	PA-O3A	-5.69	1.53	1.59
2	A	217	T5A	PB-O3A	5.36	1.65	1.59
2	E	217	T5A	PB-O3A	5.30	1.65	1.59
2	D	217	T5A	PC-O3B	-5.19	1.53	1.59
2	F	217	T5A	PD-O3C	-5.07	1.54	1.59
2	D	217	T5A	PD-O3C	-5.05	1.54	1.59
2	F	217	T5A	PA-O3A	-4.91	1.54	1.59
2	C	217	T5A	PC-O3C	4.88	1.64	1.59
2	H	217	T5A	PB-O3B	4.55	1.64	1.59
2	C	217	T5A	PB-O3A	4.42	1.64	1.59
2	G	217	T5A	PC-O3C	4.41	1.64	1.59
2	D	217	T5A	PD-O3D	4.35	1.64	1.59
2	G	217	T5A	PC-O3B	-4.31	1.54	1.59
2	H	217	T5A	PD-O3C	-4.23	1.54	1.59
2	E	217	T5A	PC-O3C	4.13	1.64	1.59
2	H	217	T5A	PB-O3A	3.86	1.63	1.59
2	B	217	T5A	PE-O3D	3.84	1.63	1.59
2	G	217	T5A	PD-O3D	3.83	1.63	1.59
2	F	217	T5A	PC-O3B	-3.82	1.55	1.59
2	H	217	T5A	C4B-C5B	3.78	1.51	1.44
2	F	217	T5A	C4B-N3B	-3.70	1.31	1.38
2	B	217	T5A	PC-O3B	-3.62	1.55	1.59
2	G	217	T5A	PB-O3B	-3.56	1.55	1.59
2	H	217	T5A	PC-O3C	3.48	1.63	1.59
2	C	217	T5A	PB-O3B	-3.46	1.55	1.59
2	A	217	T5A	C4B-C5B	3.43	1.50	1.44
2	A	217	T5A	PB-O3B	-3.40	1.55	1.59
2	H	217	T5A	PC-O3B	-3.35	1.55	1.59
2	A	217	T5A	C1F-N9A	3.11	1.54	1.46
2	H	217	T5A	C2E-C1E	3.08	1.60	1.52
2	A	217	T5A	PC-O3B	-3.04	1.56	1.59
2	C	217	T5A	C4B-C5B	2.99	1.49	1.44
2	C	217	T5A	PE-O3D	2.92	1.62	1.59
2	E	217	T5A	C4B-N3B	-2.91	1.33	1.38
2	C	217	T5A	C2B-N3B	2.89	1.43	1.38
2	C	217	T5A	C1F-N9A	2.85	1.54	1.46
2	B	217	T5A	C4B-C5B	2.84	1.49	1.44
2	H	217	T5A	O4F-C1F	2.72	1.48	1.42
2	E	217	T5A	O3F-C3F	2.64	1.49	1.43
2	F	217	T5A	C1F-N9A	2.64	1.53	1.46
2	H	217	T5A	PD-O3D	2.64	1.62	1.59
2	G	217	T5A	C4A-N3A	2.62	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	217	T5A	PC-O3B	-2.62	1.56	1.59
2	H	217	T5A	C2B-N1B	2.60	1.42	1.38
2	E	217	T5A	PE-O3D	2.59	1.62	1.59
2	F	217	T5A	PE-O3D	-2.59	1.56	1.59
2	D	217	T5A	C2B-N1B	2.52	1.42	1.38
2	E	217	T5A	PD-O3D	2.52	1.62	1.59
2	G	217	T5A	PD-O1D	-2.51	1.43	1.55
2	G	217	T5A	PA-O3A	-2.46	1.56	1.59
2	D	217	T5A	C4A-N3A	2.40	1.38	1.34
2	C	217	T5A	C4A-N9A	2.38	1.42	1.37
2	E	217	T5A	C6B-N1B	-2.36	1.34	1.38
2	B	217	T5A	C5F-C4F	2.31	1.58	1.51
2	C	217	T5A	PB-O2X	-2.31	1.44	1.55
2	D	217	T5A	PB-O3B	2.27	1.62	1.59
2	G	217	T5A	C2A-N3A	2.26	1.37	1.33
2	B	217	T5A	C2B-N1B	2.20	1.41	1.38
2	F	217	T5A	C2B-N3B	-2.19	1.34	1.38
2	G	217	T5A	C4B-C5B	2.18	1.48	1.44
2	E	217	T5A	PD-O3C	-2.15	1.57	1.59
2	E	217	T5A	O4F-C1F	2.14	1.46	1.42
2	F	217	T5A	C4A-N3A	2.12	1.38	1.34
2	F	217	T5A	O4B-C4B	-2.11	1.19	1.23
2	F	217	T5A	O3F-C3F	2.09	1.48	1.43
2	H	217	T5A	C6B-N1B	-2.06	1.34	1.38
2	H	217	T5A	C5A-N7A	2.03	1.42	1.39
2	G	217	T5A	O4E-C1E	2.02	1.46	1.42
2	F	217	T5A	C2B-N1B	2.02	1.41	1.38
2	E	217	T5A	C4A-N3A	2.00	1.38	1.34

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	217	T5A	O4E-C1E-C2E	-4.26	98.28	106.25
2	B	217	T5A	C4E-O4E-C1E	-4.09	99.80	109.51
2	C	217	T5A	C5B-C4B-N3B	-4.06	111.80	115.32
2	E	217	T5A	O4E-C1E-C2E	-4.02	98.74	106.25
2	F	217	T5A	C4E-O4E-C1E	-3.97	100.08	109.51
2	H	217	T5A	C4E-O4E-C1E	-3.90	100.25	109.51
2	H	217	T5A	C7B-C5B-C6B	-3.89	117.59	122.85
2	E	217	T5A	C6B-C5B-C4B	3.79	121.14	118.02
2	C	217	T5A	O3C-PD-O2D	-3.78	99.33	110.70
2	G	217	T5A	C5B-C4B-N3B	-3.78	112.04	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	217	T5A	C4E-O4E-C1E	-3.67	100.78	109.51
2	A	217	T5A	O2C-PC-O3B	3.63	117.08	107.27
2	A	217	T5A	C4E-O4E-C1E	-3.61	100.93	109.51
2	G	217	T5A	O3B-PB-O1B	-3.58	99.92	110.70
2	B	217	T5A	C6B-C5B-C4B	3.53	120.93	118.02
2	G	217	T5A	C7B-C5B-C6B	-3.42	118.22	122.85
2	D	217	T5A	O4F-C1F-N9A	3.33	114.48	108.09
2	D	217	T5A	O2X-PB-O1B	3.32	127.89	112.44
2	E	217	T5A	C5B-C4B-N3B	-3.31	112.45	115.32
2	G	217	T5A	O2F-C2F-C1F	3.30	121.46	110.10
2	C	217	T5A	O1D-PD-O2D	3.27	127.64	112.44
2	C	217	T5A	O2X-PB-O3B	3.25	116.06	107.27
2	B	217	T5A	O2X-PB-O1B	3.24	127.50	112.44
2	H	217	T5A	C6B-C5B-C4B	3.17	120.63	118.02
2	E	217	T5A	O3C-PD-O2D	-3.14	101.27	110.70
2	D	217	T5A	O2C-PC-O1C	3.11	126.93	112.44
2	B	217	T5A	C7B-C5B-C6B	-3.11	118.64	122.85
2	H	217	T5A	C2F-C3F-C4F	-3.11	96.61	102.61
2	D	217	T5A	O4B-C4B-C5B	-3.10	121.37	124.92
2	F	217	T5A	O2C-PC-O1C	3.08	126.78	112.44
2	C	217	T5A	C4E-O4E-C1E	-3.08	102.20	109.51
2	F	217	T5A	O2C-PC-O3C	-3.06	99.00	107.27
2	H	217	T5A	O4E-C1E-C2E	-3.02	100.60	106.25
2	A	217	T5A	O4E-C1E-C2E	-3.02	100.61	106.25
2	C	217	T5A	C7B-C5B-C6B	-3.00	118.80	122.85
2	G	217	T5A	C4E-O4E-C1E	-2.99	102.41	109.51
2	E	217	T5A	C2F-C3F-C4F	-2.93	96.94	102.61
2	H	217	T5A	O4E-C4E-C3E	2.92	112.30	105.65
2	F	217	T5A	O1E-PE-O5F	2.88	120.61	107.57
2	H	217	T5A	O2X-PB-O1B	2.85	125.72	112.44
2	C	217	T5A	C6B-C5B-C4B	2.84	120.36	118.02
2	H	217	T5A	O2C-PC-O1C	2.83	125.62	112.44
2	H	217	T5A	O4F-C1F-N9A	2.81	113.48	108.09
2	B	217	T5A	O4E-C1E-C2E	-2.81	101.00	106.25
2	E	217	T5A	O4E-C1E-N1B	2.80	112.84	107.86
2	H	217	T5A	C7B-C5B-C4B	2.80	121.77	118.78
2	F	217	T5A	O2X-PB-O1B	2.80	125.46	112.44
2	H	217	T5A	O4E-C1E-N1B	2.77	112.78	107.86
2	E	217	T5A	O1D-PD-O3C	2.72	114.63	107.27
2	D	217	T5A	O2B-C2B-N1B	-2.68	119.30	122.80
2	G	217	T5A	C7B-C5B-C4B	2.68	121.64	118.78
2	G	217	T5A	O2X-PB-O1B	2.67	124.88	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	217	T5A	O2C-PC-O3B	2.67	114.48	107.27
2	C	217	T5A	O4F-C1F-N9A	2.66	113.20	108.09
2	H	217	T5A	O3C-PD-O2D	-2.66	102.70	110.70
2	A	217	T5A	O3F-C3F-C4F	-2.66	103.44	111.08
2	F	217	T5A	O1D-PD-O3C	2.64	114.42	107.27
2	B	217	T5A	O3A-PB-O1B	-2.63	102.80	110.70
2	G	217	T5A	O2C-PC-O3B	2.62	114.37	107.27
2	F	217	T5A	C2F-C3F-C4F	-2.61	97.56	102.61
2	D	217	T5A	O3F-C3F-C4F	-2.59	103.64	111.08
2	A	217	T5A	C5B-C4B-N3B	-2.58	113.08	115.32
2	E	217	T5A	O4F-C1F-N9A	2.58	113.04	108.09
2	H	217	T5A	O2F-C2F-C3F	2.58	120.08	111.82
2	H	217	T5A	O1D-PD-O3C	2.56	114.19	107.27
2	E	217	T5A	O3E-C3E-C2E	-2.56	101.99	110.88
2	D	217	T5A	C1F-N9A-C8A	2.55	132.76	127.09
2	C	217	T5A	O1A-PA-O5E	2.55	119.14	107.57
2	G	217	T5A	C6B-C5B-C4B	2.54	120.12	118.02
2	B	217	T5A	O1D-PD-O3C	2.53	114.11	107.27
2	G	217	T5A	O3E-C3E-C2E	-2.50	102.19	110.88
2	E	217	T5A	O1D-PD-O2D	2.48	123.99	112.44
2	D	217	T5A	O2C-PC-O3C	-2.47	100.59	107.27
2	F	217	T5A	C5B-C6B-N1B	-2.45	120.65	123.31
2	B	217	T5A	O2B-C2B-N1B	-2.44	119.61	122.80
2	F	217	T5A	O3A-PB-O1B	-2.43	103.39	110.70
2	F	217	T5A	C3F-C2F-C1F	2.43	106.05	101.46
2	H	217	T5A	O2C-PC-O3B	-2.43	100.72	107.27
2	A	217	T5A	C7B-C5B-C6B	-2.42	119.58	122.85
2	D	217	T5A	O1D-PD-O3C	2.42	113.80	107.27
2	D	217	T5A	O3B-PB-O1B	-2.41	103.45	110.70
2	B	217	T5A	C2F-C3F-C4F	-2.39	97.99	102.61
2	B	217	T5A	C5B-C6B-N1B	-2.37	120.74	123.31
2	D	217	T5A	C6B-C5B-C4B	2.36	119.97	118.02
2	H	217	T5A	C5B-C4B-N3B	-2.34	113.29	115.32
2	E	217	T5A	O2F-C2F-C1F	2.34	118.17	110.10
2	F	217	T5A	C6B-C5B-C4B	2.34	119.95	118.02
2	E	217	T5A	C5B-C6B-N1B	-2.33	120.79	123.31
2	H	217	T5A	O1E-PE-O5F	2.32	118.08	107.57
2	A	217	T5A	C6B-C5B-C4B	2.32	119.93	118.02
2	D	217	T5A	C4B-N3B-C2B	-2.29	124.33	127.34
2	C	217	T5A	O3B-PB-O1B	-2.27	103.87	110.70
2	F	217	T5A	C1E-N1B-C2B	-2.27	113.22	117.66
2	F	217	T5A	O4F-C1F-N9A	2.25	112.40	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	217	T5A	O4F-C1F-N9A	2.23	112.38	108.09
2	C	217	T5A	O2C-PC-O3B	2.18	113.17	107.27
2	D	217	T5A	O4E-C4E-C3E	2.17	110.59	105.65
2	C	217	T5A	O2B-C2B-N3B	2.16	125.47	121.49
2	C	217	T5A	C3F-C2F-C1F	2.15	105.54	101.46
2	E	217	T5A	N6A-C6A-N1A	2.15	123.16	118.38
2	G	217	T5A	O3A-PB-O1B	-2.14	104.25	110.70
2	B	217	T5A	O1A-PA-O3A	2.14	113.05	107.27
2	E	217	T5A	O3A-PA-O2A	-2.13	104.30	110.70
2	G	217	T5A	O1D-PD-O2D	2.13	122.34	112.44
2	G	217	T5A	O2C-PC-O1C	2.12	122.31	112.44
2	A	217	T5A	O1D-PD-O2D	2.12	122.30	112.44
2	G	217	T5A	N3A-C4A-N9A	2.10	130.75	127.17
2	E	217	T5A	C4E-O4E-C1E	-2.10	104.53	109.51
2	D	217	T5A	C2F-C1F-N9A	2.09	118.50	113.30
2	B	217	T5A	O2C-PC-O1C	2.07	122.09	112.44
2	E	217	T5A	C7B-C5B-C6B	-2.07	120.05	122.85
2	F	217	T5A	O3D-PE-O2E	-2.07	104.48	110.70
2	C	217	T5A	O4B-C4B-N3B	2.06	123.99	120.11
2	A	217	T5A	O2X-PB-O3A	-2.06	101.72	107.27
2	D	217	T5A	C4A-N9A-C1F	-2.05	121.84	126.63
2	A	217	T5A	O2F-C2F-C1F	2.05	117.15	110.10
2	G	217	T5A	O2B-C2B-N3B	2.02	125.21	121.49
2	B	217	T5A	N6A-C6A-N1A	2.01	122.85	118.38
2	H	217	T5A	O3F-C3F-C2F	2.01	118.25	111.82
2	A	217	T5A	O2C-PC-O1C	2.00	121.75	112.44

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	217	T5A	C2F-C1F-N9A-C8A
2	F	217	T5A	C2F-C1F-N9A-C8A
2	A	217	T5A	PE-O3D-PD-O2D
2	B	217	T5A	PD-O3C-PC-O1C
2	D	217	T5A	PE-O3D-PD-O2D
2	E	217	T5A	PE-O3D-PD-O2D
2	G	217	T5A	PE-O3D-PD-O2D
2	H	217	T5A	PE-O3D-PD-O2D
2	A	217	T5A	PC-O3B-PB-O3A
2	G	217	T5A	PC-O3B-PB-O3A
2	B	217	T5A	C2F-C1F-N9A-C8A

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Mol	Chain	Res	Type	Atoms
2	A	217	T5A	C2F-C1F-N9A-C8A
2	G	217	T5A	C2F-C1F-N9A-C8A
2	B	217	T5A	PE-O3D-PD-O2D
2	E	217	T5A	PD-O3C-PC-O2C
2	E	217	T5A	PE-O3D-PD-O1D
2	F	217	T5A	PE-O3D-PD-O1D
2	A	217	T5A	PD-O3C-PC-O2C
2	A	217	T5A	PE-O3D-PD-O1D
2	C	217	T5A	PE-O3D-PD-O1D
2	G	217	T5A	PA-O3A-PB-O2X
2	G	217	T5A	PE-O3D-PD-O1D
2	H	217	T5A	PD-O3C-PC-O1C
2	H	217	T5A	PD-O3C-PC-O2C
2	H	217	T5A	PE-O3D-PD-O1D
2	C	217	T5A	C2F-C1F-N9A-C4A
2	G	217	T5A	C2F-C1F-N9A-C4A
2	E	217	T5A	C2F-C1F-N9A-C8A
2	A	217	T5A	PA-O3A-PB-O2X
2	B	217	T5A	PE-O3D-PD-O1D
2	H	217	T5A	PA-O3A-PB-O2X
2	B	217	T5A	O4F-C1F-N9A-C8A
2	D	217	T5A	O4F-C1F-N9A-C8A
2	F	217	T5A	O4F-C1F-N9A-C8A
2	A	217	T5A	PA-O3A-PB-O1B
2	B	217	T5A	PA-O3A-PB-O2X
2	B	217	T5A	PD-O3C-PC-O2C
2	C	217	T5A	PB-O3B-PC-O2C
2	D	217	T5A	PA-O3A-PB-O2X
2	D	217	T5A	PE-O3D-PD-O1D
2	E	217	T5A	PA-O3A-PB-O1B
2	E	217	T5A	PA-O3A-PB-O2X
2	E	217	T5A	PC-O3B-PB-O1B
2	F	217	T5A	PD-O3C-PC-O2C
2	F	217	T5A	PE-O3D-PD-O2D
2	G	217	T5A	PA-O3A-PB-O1B
2	G	217	T5A	PD-O3C-PC-O2C
2	C	217	T5A	O4F-C1F-N9A-C8A
2	A	217	T5A	O4F-C1F-N9A-C8A
2	D	217	T5A	C2F-C1F-N9A-C8A
2	A	217	T5A	PB-O3B-PC-O1C
2	C	217	T5A	PA-O3A-PB-O1B
2	E	217	T5A	PD-O3C-PC-O1C

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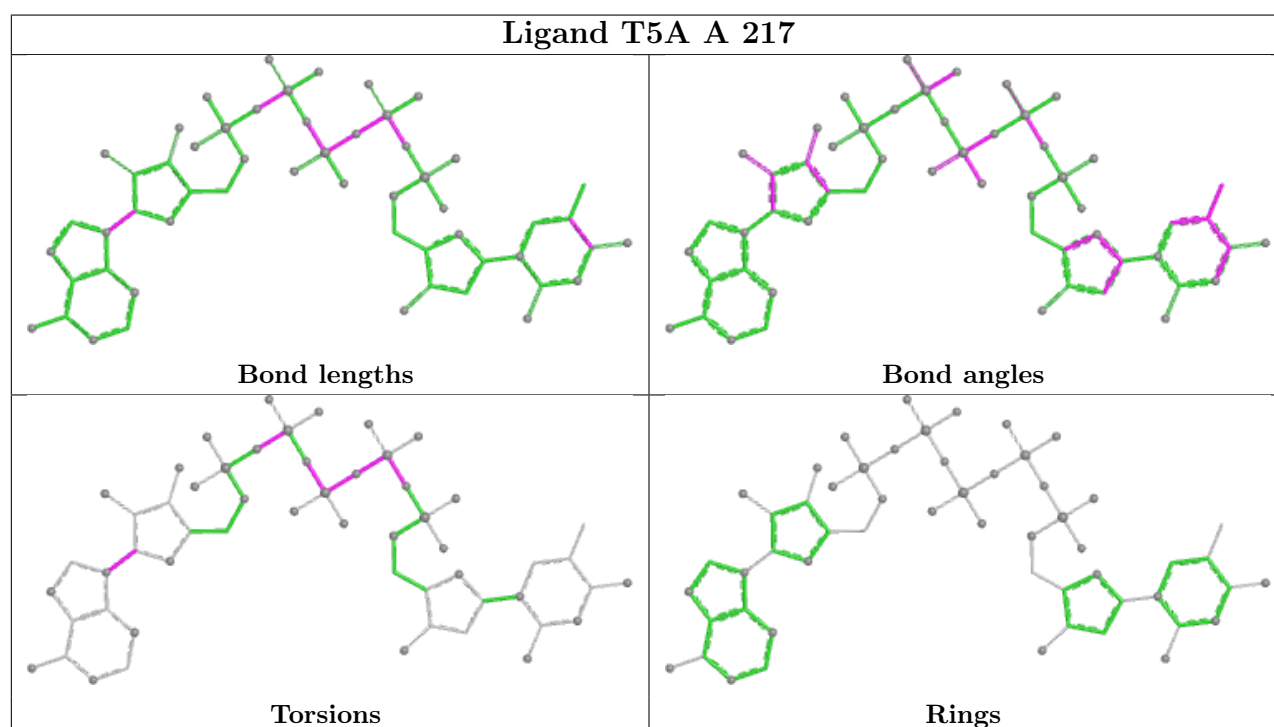
Mol	Chain	Res	Type	Atoms
2	F	217	T5A	PA-O3A-PB-O2X

There are no ring outliers.

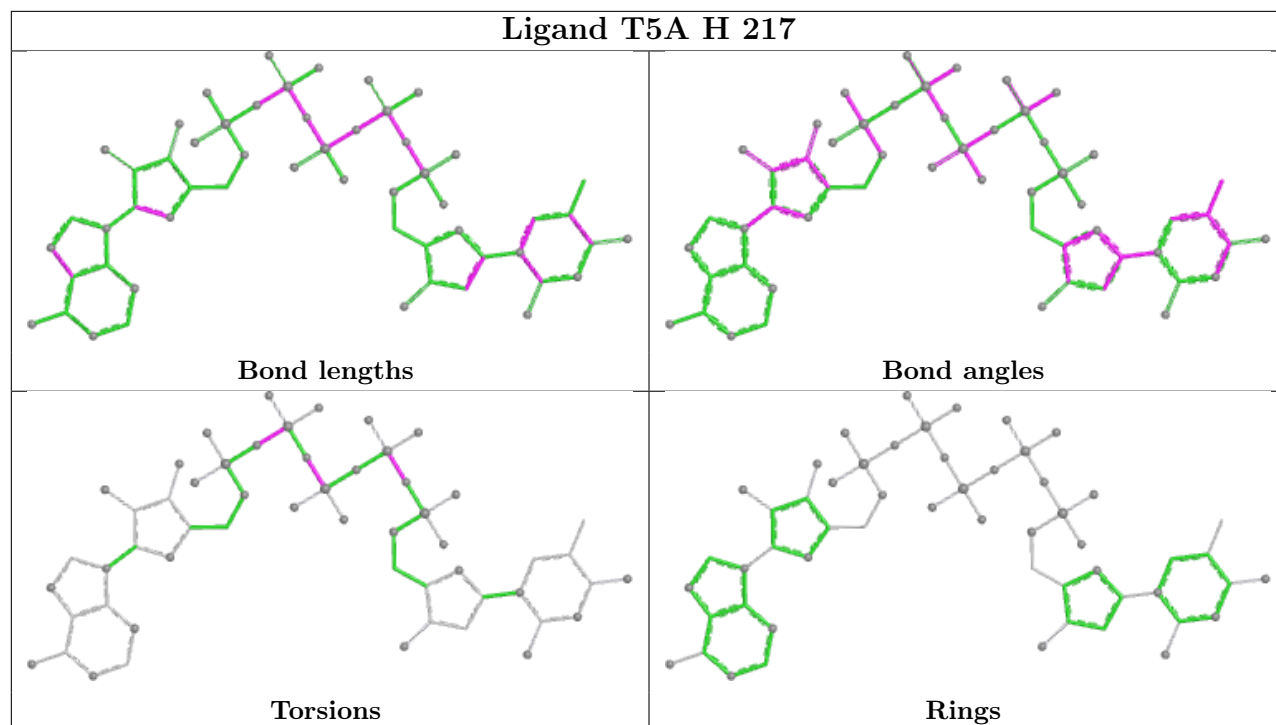
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	217	T5A	1	0
2	C	217	T5A	2	0
2	E	217	T5A	1	0
2	B	217	T5A	1	0

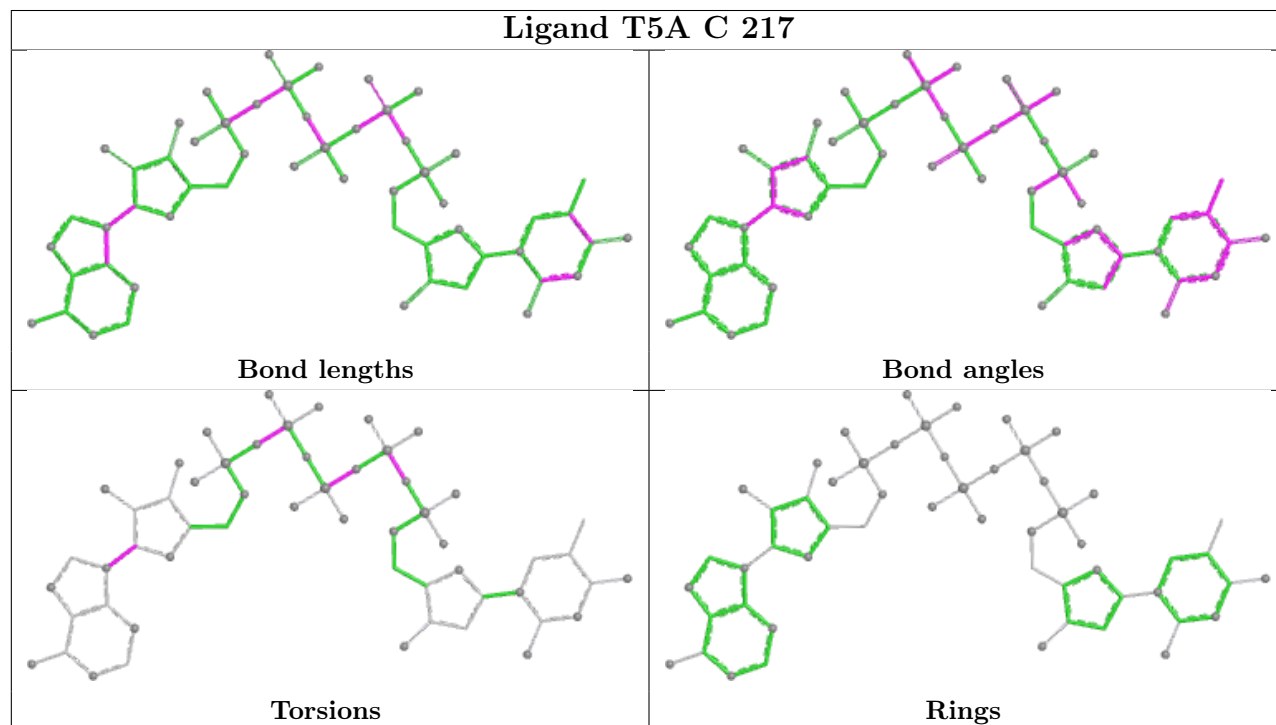
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



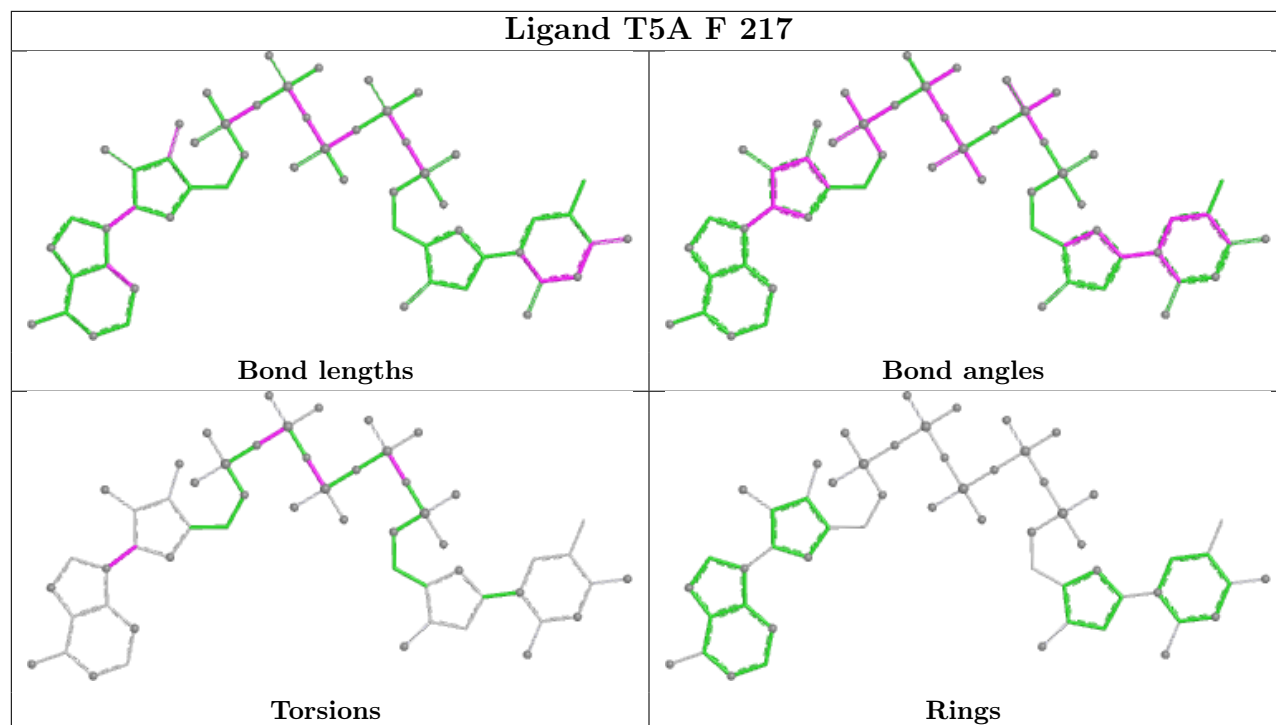
Ligand T5A H 217



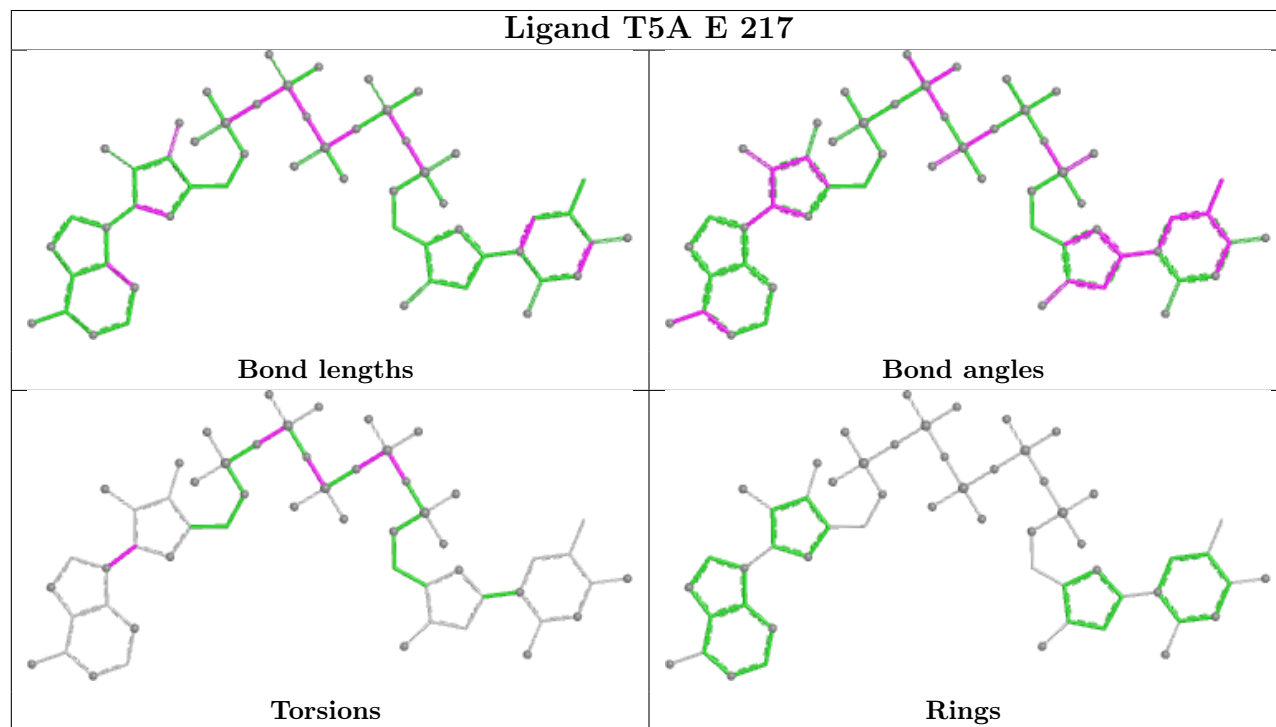
Ligand T5A C 217



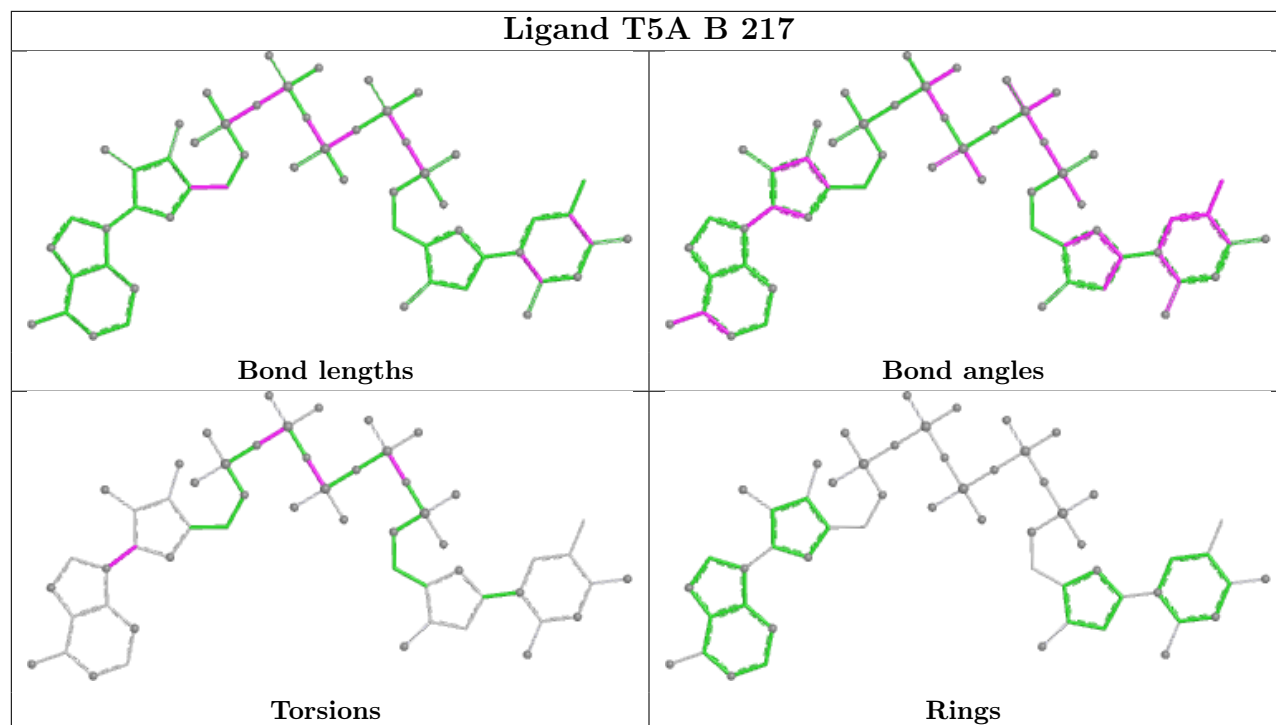
Ligand T5A F 217



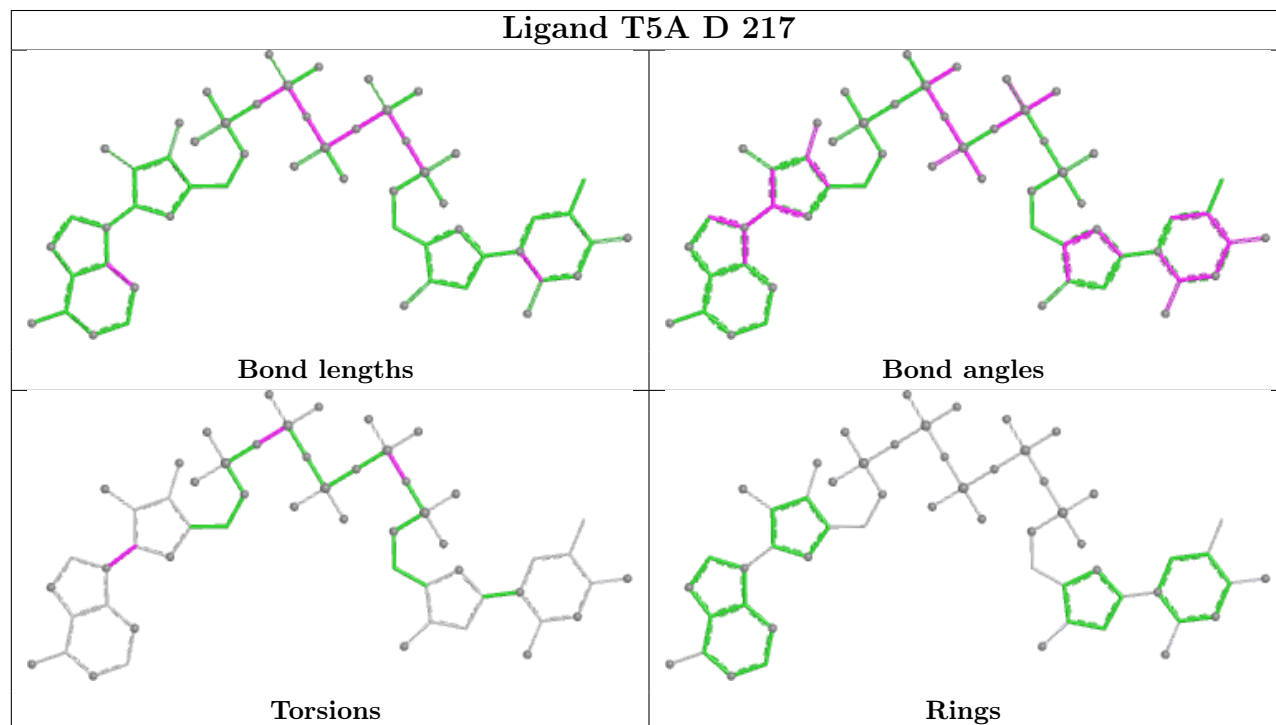
Ligand T5A E 217

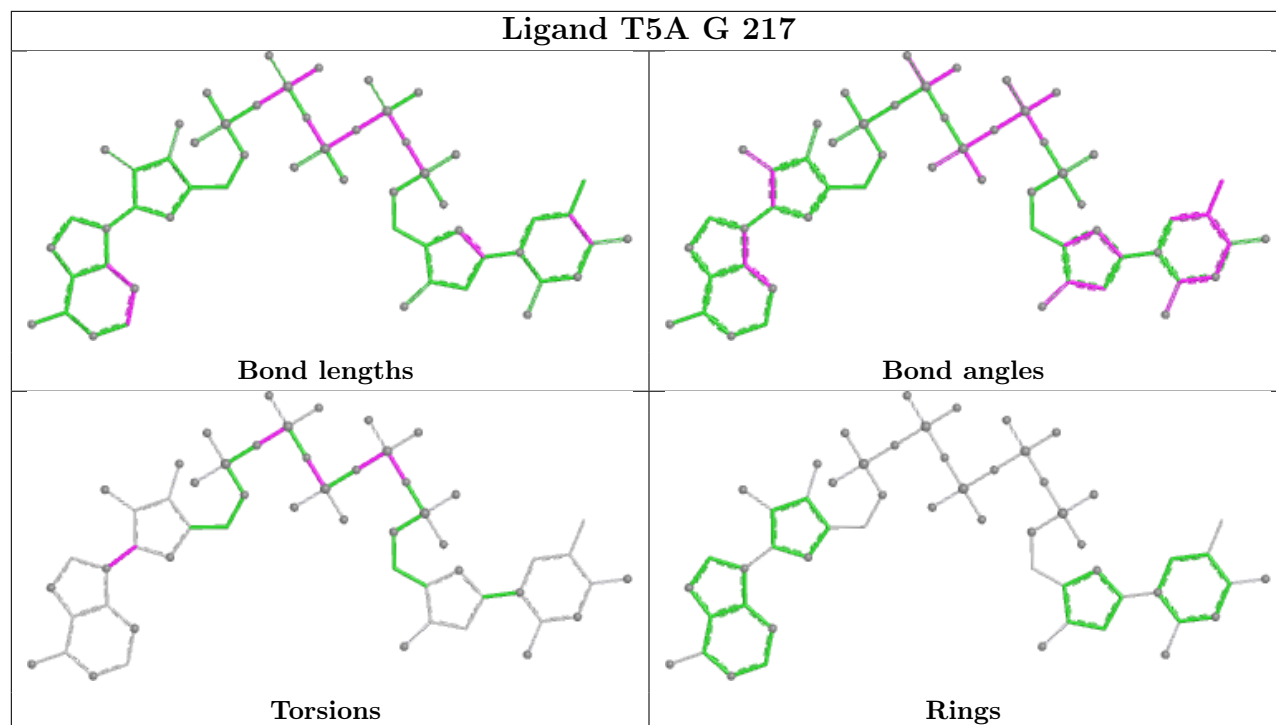


Ligand T5A B 217



Ligand T5A D 217





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	216/216 (100%)	0.24	13 (6%) 27 26	8, 19, 42, 56	0
1	B	216/216 (100%)	0.01	8 (3%) 45 44	8, 17, 42, 49	0
1	C	205/216 (94%)	0.19	10 (4%) 35 34	8, 18, 38, 49	0
1	D	214/216 (99%)	-0.05	7 (3%) 49 48	8, 17, 36, 45	0
1	E	215/216 (99%)	0.24	13 (6%) 27 26	7, 20, 45, 49	0
1	F	216/216 (100%)	-0.01	4 (1%) 66 66	8, 17, 36, 49	0
1	G	215/216 (99%)	0.17	11 (5%) 33 32	7, 19, 41, 47	0
1	H	214/216 (99%)	0.01	11 (5%) 33 32	7, 17, 41, 50	0
All	All	1711/1728 (99%)	0.10	77 (4%) 38 37	7, 18, 41, 56	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	9.2
1	F	141	ALA	4.7
1	H	211	ASP	4.5
1	C	153	THR	4.5
1	E	141	ALA	4.2
1	B	137	VAL	4.0
1	G	146	PHE	4.0
1	A	2	MET	4.0
1	B	208	ILE	3.9
1	F	137	VAL	3.8
1	B	141	ALA	3.8
1	A	145	GLY	3.8
1	A	1	MET	3.7
1	A	137	VAL	3.7
1	F	140	ASN	3.7
1	D	210	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	3	GLY	3.6
1	C	152	GLU	3.6
1	H	141	ALA	3.6
1	E	147	GLY	3.6
1	A	3	GLY	3.5
1	G	145	GLY	3.4
1	B	140	ASN	3.4
1	H	137	VAL	3.4
1	A	139	ASN	3.3
1	A	146	PHE	3.2
1	C	154	VAL	3.1
1	G	147	GLY	3.1
1	G	173	ARG	3.1
1	A	147	GLY	3.1
1	E	146	PHE	3.1
1	H	210	HIS	3.1
1	A	144	SER	3.1
1	D	137	VAL	3.0
1	E	210	HIS	3.0
1	H	143	LYS	3.0
1	E	2	MET	2.9
1	H	140	ASN	2.9
1	E	208	ILE	2.8
1	F	139	ASN	2.8
1	A	135	GLN	2.7
1	B	209	ASP	2.7
1	A	148	ASP	2.7
1	E	57	SER	2.6
1	G	140	ASN	2.6
1	E	142	GLU	2.5
1	G	139	ASN	2.5
1	G	208	ILE	2.5
1	H	3	GLY	2.5
1	D	211	ASP	2.4
1	G	144	SER	2.4
1	B	207	HIS	2.4
1	B	139	ASN	2.4
1	C	172	ILE	2.4
1	E	145	GLY	2.3
1	E	209	ASP	2.3
1	D	208	ILE	2.3
1	H	144	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	139	ASN	2.3
1	D	140	ASN	2.2
1	E	173	ARG	2.2
1	A	138	ASP	2.2
1	E	148	ASP	2.2
1	C	173	ARG	2.2
1	G	136	ASP	2.2
1	H	147	GLY	2.2
1	C	2	MET	2.2
1	E	175	GLY	2.1
1	B	32	ASN	2.1
1	H	186	ASN	2.1
1	D	206	THR	2.1
1	A	208	ILE	2.1
1	G	148	ASP	2.0
1	C	186	ASN	2.0
1	C	162	GLN	2.0
1	C	136	ASP	2.0
1	G	211	ASP	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($\text{\AA}^2$)	Q<0.9
2	T5A	F	217	55/55	0.97	0.06	3,18,28,29	0
2	T5A	B	217	55/55	0.98	0.06	7,16,25,26	0
2	T5A	C	217	55/55	0.98	0.06	6,14,26,27	0
2	T5A	D	217	55/55	0.98	0.05	2,13,24,26	0

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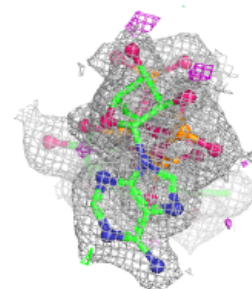
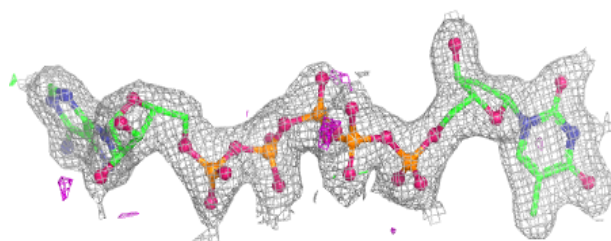
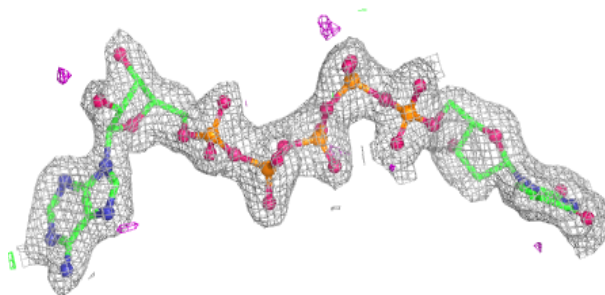
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	T5A	E	217	55/55	0.98	0.06	4,15,27,28	0
2	T5A	A	217	55/55	0.98	0.06	7,15,26,28	0
2	T5A	G	217	55/55	0.98	0.05	4,12,23,26	0
2	T5A	H	217	55/55	0.98	0.06	2,16,25,26	0

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.

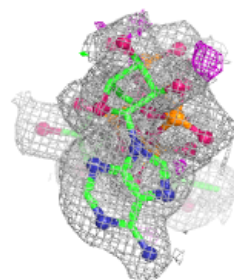
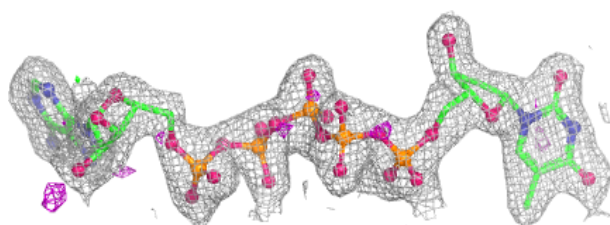
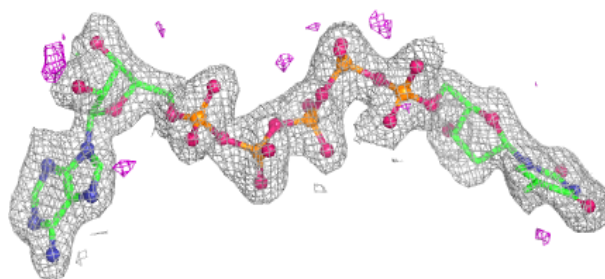
Electron density around T5A F 217:

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

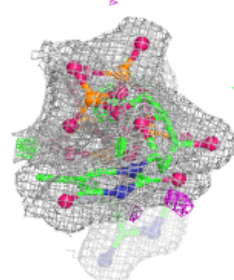
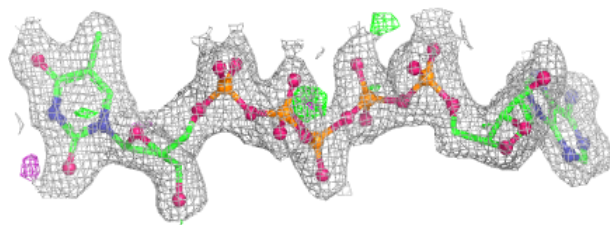
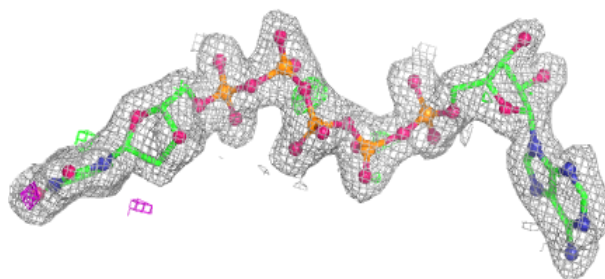


Electron density around T5A B 217:

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

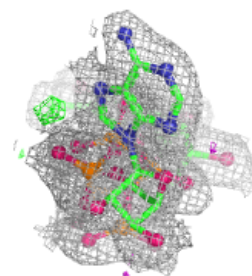
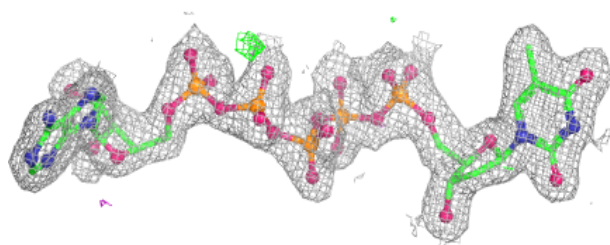
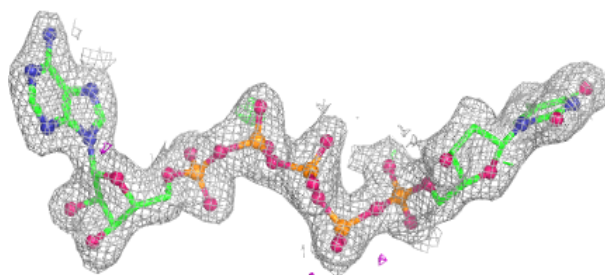
**Electron density around T5A C 217:**

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

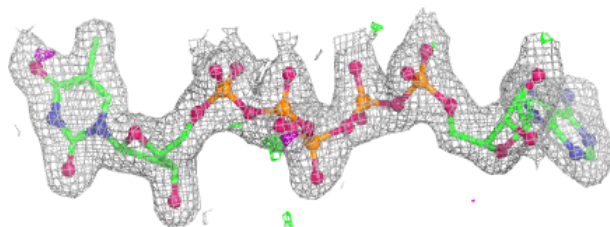
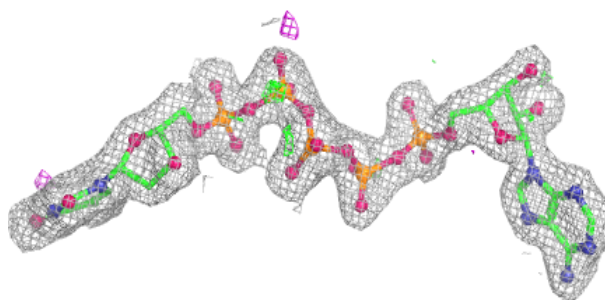


Electron density around T5A D 217:

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

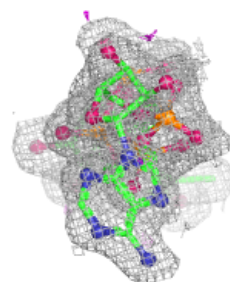
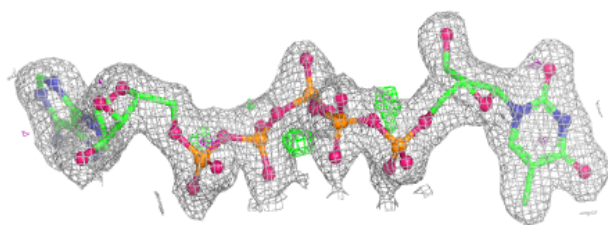
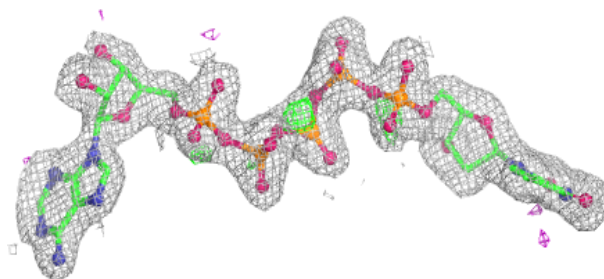
**Electron density around T5A E 217:**

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

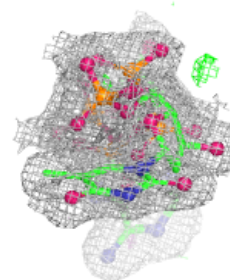
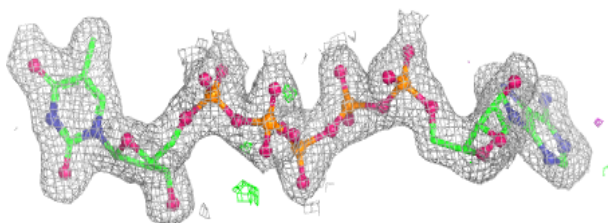
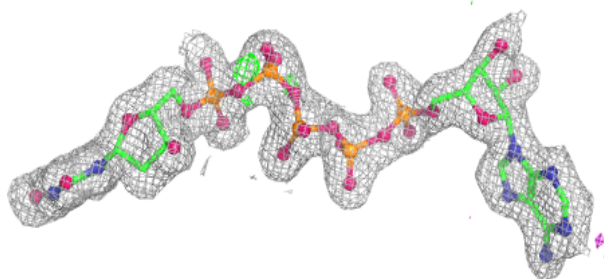


Electron density around T5A A 217:

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

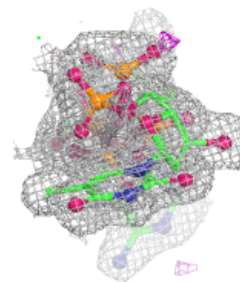
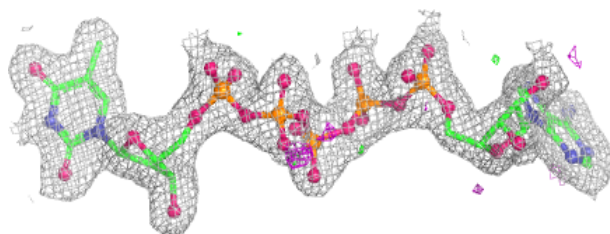
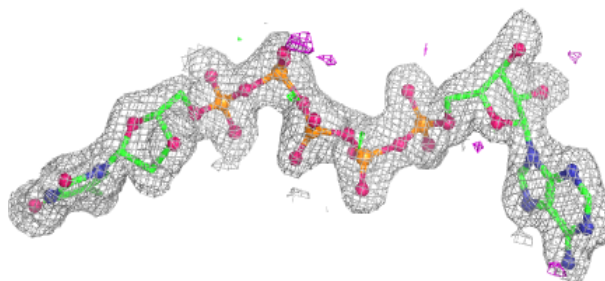
**Electron density around T5A G 217:**

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



Electron density around T5A H 217:

$2mF_o-DF_c$ (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.