



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:59 AM UTC

PDB ID : 2OCP / pdb_00002ocp
Title : Crystal Structure of Human Deoxyguanosine Kinase
Authors : Johansson, K.; Ramaswamy, S.; Ljungkrantz, C.; Knecht, W.; Piskur, J.;
Munch-Petersen, B.; Eriksson, S.; Eklund, H.
Deposited on : 2006-12-21
Resolution : 2.80 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

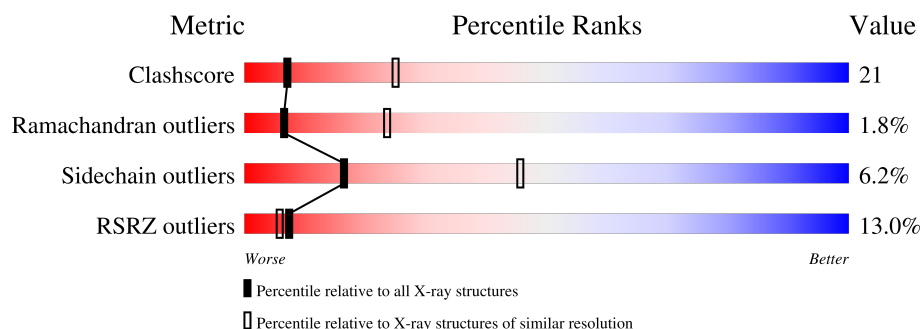
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	241	
1	B	241	
1	C	241	
1	D	241	
1	E	241	
1	F	241	
1	G	241	

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Mol	Chain	Length	Quality of chain
1	H	241	17% 53% 38% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15832 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.

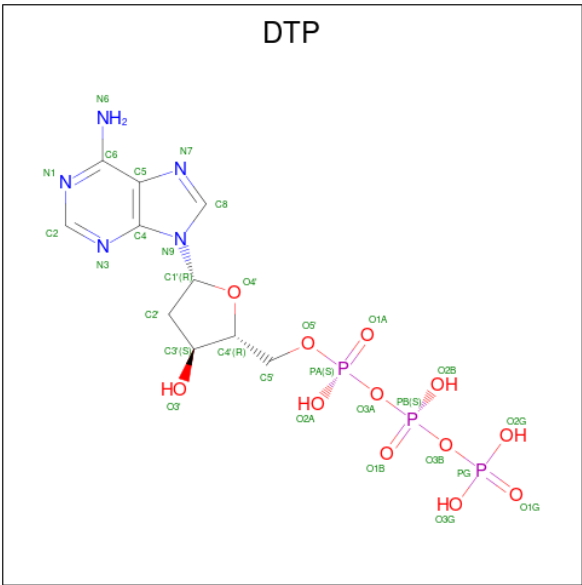
- Molecule 1 is a protein called Deoxyguanosine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	B	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	C	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	D	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	E	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	F	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	G	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	H	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ASN	THR	variant	UNP Q16854
B	83	ASN	THR	variant	UNP Q16854
C	83	ASN	THR	variant	UNP Q16854
D	83	ASN	THR	variant	UNP Q16854
E	83	ASN	THR	variant	UNP Q16854
F	83	ASN	THR	variant	UNP Q16854
G	83	ASN	THR	variant	UNP Q16854
H	83	ASN	THR	variant	UNP Q16854

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	G	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	H	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	25	Total	O	0	0
			25	25		
3	C	25	Total	O	0	0
			25	25		
3	D	25	Total	O	0	0
			25	25		

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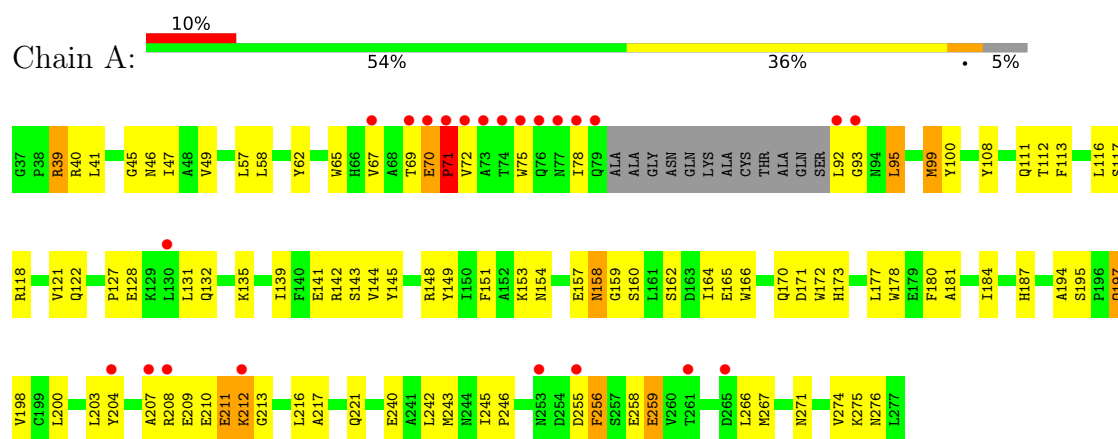
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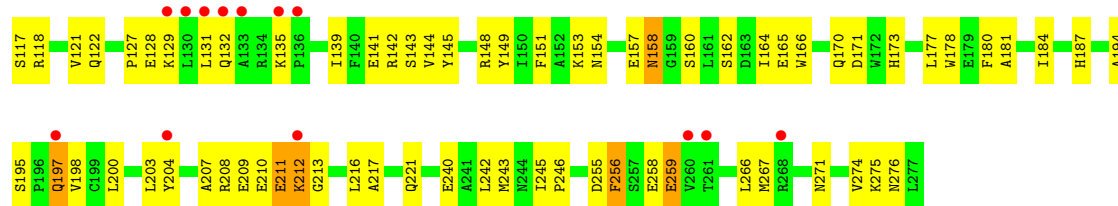
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	25	Total 25	O 25	0	0
3	F	25	Total 25	O 25	0	0
3	G	25	Total 25	O 25	0	0
3	H	25	Total 25	O 25	0	0

3 Residue-property plots [i](#)

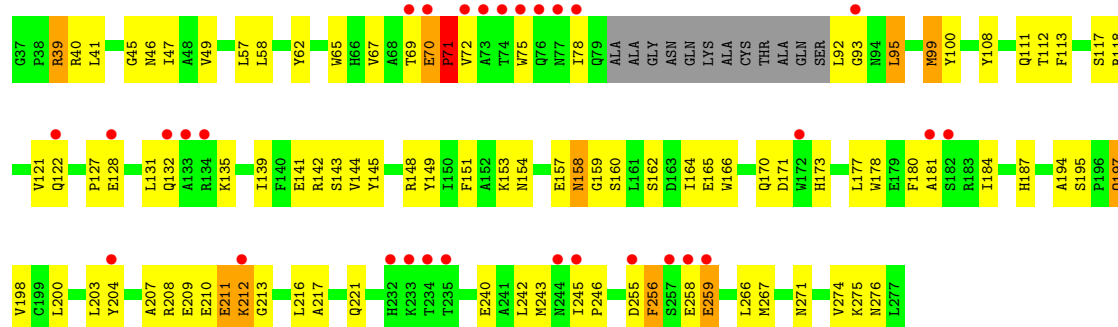
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Deoxyguanosine kinase

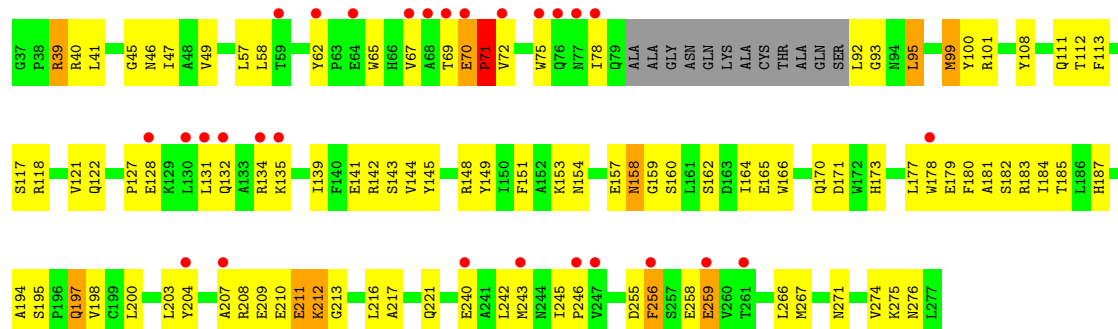




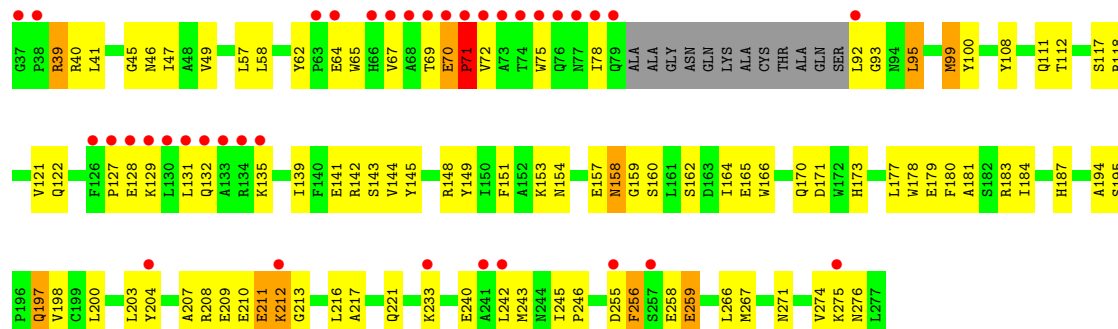
• Molecule 1: Deoxyguanosine kinase



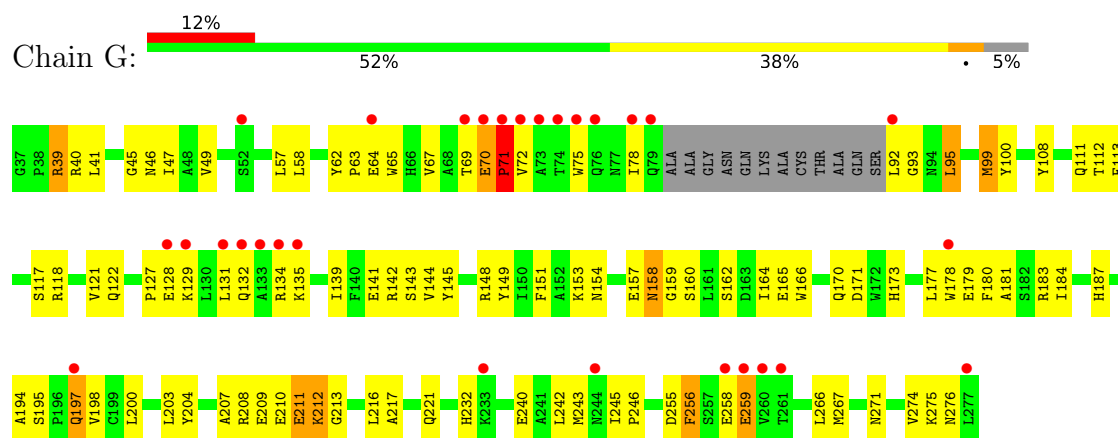
• Molecule 1: Deoxyguanosine kinase



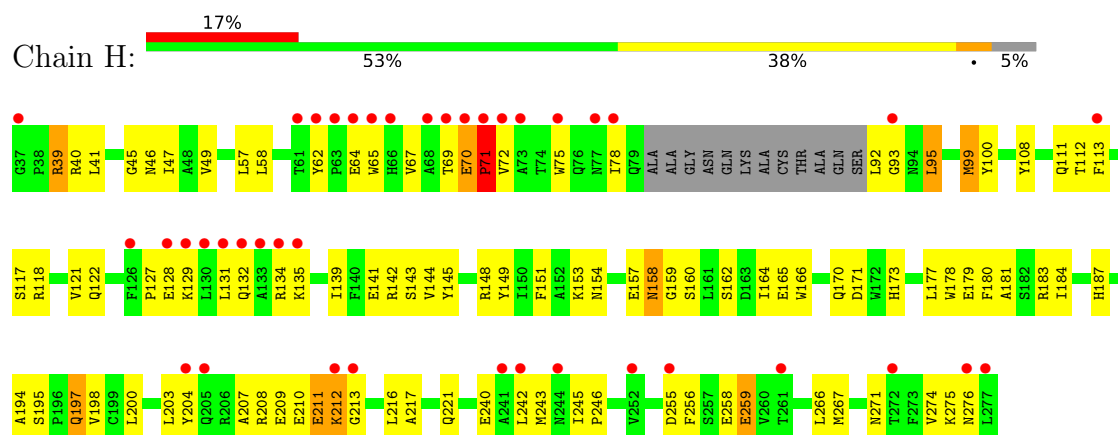
• Molecule 1: Deoxyguanosine kinase



- Molecule 1: Deoxyguanosine kinase



- Molecule 1: Deoxyguanosine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.18Å 120.03Å 154.35Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.80) 97.4 (30.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.265 , 0.277 0.285 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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: DTP

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	0.45	0/1976	0.95	10/2676 (0.4%)
1	B	0.45	0/1976	0.95	10/2676 (0.4%)
1	C	0.45	0/1976	0.95	10/2676 (0.4%)
1	D	0.45	0/1976	0.95	10/2676 (0.4%)
1	E	0.45	0/1976	0.95	10/2676 (0.4%)
1	F	0.45	0/1976	0.95	10/2676 (0.4%)
1	G	0.45	0/1976	0.95	10/2676 (0.4%)
1	H	0.45	0/1976	0.95	9/2676 (0.3%)
All	All	0.45	0/15808	0.95	79/21408 (0.4%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	GLU	CA-C-N	10.84	133.39	119.84
1	H	70	GLU	C-N-CA	10.84	133.39	119.84
1	A	70	GLU	CA-C-N	10.82	133.37	119.84
1	A	70	GLU	C-N-CA	10.82	133.37	119.84
1	B	70	GLU	CA-C-N	10.82	133.36	119.84
1	B	70	GLU	C-N-CA	10.82	133.36	119.84
1	C	70	GLU	CA-C-N	10.81	133.35	119.84
1	C	70	GLU	C-N-CA	10.81	133.35	119.84
1	E	70	GLU	CA-C-N	10.81	133.35	119.84
1	E	70	GLU	C-N-CA	10.81	133.35	119.84
1	G	70	GLU	CA-C-N	10.80	133.34	119.84
1	G	70	GLU	C-N-CA	10.80	133.34	119.84
1	F	70	GLU	CA-C-N	10.79	133.32	119.84
1	F	70	GLU	C-N-CA	10.79	133.32	119.84
1	D	70	GLU	CA-C-N	10.78	133.32	119.84
1	D	70	GLU	C-N-CA	10.78	133.32	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	143	SER	N-CA-C	6.13	117.50	108.86
1	D	143	SER	N-CA-C	6.13	117.50	108.86
1	B	143	SER	N-CA-C	6.12	117.49	108.86
1	F	143	SER	N-CA-C	6.12	117.48	108.86
1	C	143	SER	N-CA-C	6.10	117.46	108.86
1	A	143	SER	N-CA-C	6.10	117.46	108.86
1	H	143	SER	N-CA-C	6.09	117.45	108.86
1	E	143	SER	N-CA-C	6.09	117.44	108.86
1	E	151	PHE	N-CA-C	5.94	118.90	111.24
1	C	151	PHE	N-CA-C	5.93	118.89	111.24
1	G	151	PHE	N-CA-C	5.93	118.89	111.24
1	F	151	PHE	N-CA-C	5.93	118.89	111.24
1	B	151	PHE	N-CA-C	5.92	118.88	111.24
1	A	151	PHE	N-CA-C	5.92	118.88	111.24
1	H	151	PHE	N-CA-C	5.92	118.88	111.24
1	D	151	PHE	N-CA-C	5.90	118.85	111.24
1	E	71	PRO	N-CA-C	5.48	123.77	112.47
1	C	71	PRO	N-CA-C	5.48	123.76	112.47
1	H	71	PRO	N-CA-C	5.48	123.76	112.47
1	D	71	PRO	N-CA-C	5.47	123.74	112.47
1	F	71	PRO	N-CA-C	5.47	123.75	112.47
1	A	71	PRO	N-CA-C	5.47	123.74	112.47
1	B	71	PRO	N-CA-C	5.47	123.74	112.47
1	G	71	PRO	N-CA-C	5.46	123.72	112.47
1	A	69	THR	N-CA-C	5.39	117.69	110.35
1	G	69	THR	N-CA-C	5.39	117.69	110.35
1	F	69	THR	N-CA-C	5.39	117.68	110.35
1	H	69	THR	N-CA-C	5.39	117.69	110.35
1	C	69	THR	N-CA-C	5.39	117.68	110.35
1	D	69	THR	N-CA-C	5.39	117.67	110.35
1	B	69	THR	N-CA-C	5.38	117.67	110.35
1	E	69	THR	N-CA-C	5.38	117.67	110.35
1	C	149	TYR	N-CA-C	5.26	119.55	113.18
1	B	149	TYR	N-CA-C	5.26	119.54	113.18
1	H	149	TYR	N-CA-C	5.22	119.49	113.18
1	A	149	TYR	N-CA-C	5.21	119.49	113.18
1	F	149	TYR	N-CA-C	5.21	119.48	113.18
1	D	149	TYR	N-CA-C	5.19	119.46	113.18
1	G	149	TYR	N-CA-C	5.19	119.47	113.18
1	E	149	TYR	N-CA-C	5.19	119.46	113.18
1	E	132	GLN	N-CA-C	5.18	117.01	109.71
1	D	132	GLN	N-CA-C	5.17	116.99	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	132	GLN	N-CA-C	5.16	116.99	109.71
1	F	132	GLN	N-CA-C	5.16	116.98	109.71
1	A	132	GLN	N-CA-C	5.15	116.97	109.71
1	B	132	GLN	N-CA-C	5.15	116.97	109.71
1	C	132	GLN	N-CA-C	5.14	116.96	109.71
1	G	132	GLN	N-CA-C	5.14	116.96	109.71
1	C	211	GLU	N-CA-C	5.10	118.66	112.23
1	D	211	GLU	N-CA-C	5.08	118.64	112.23
1	B	211	GLU	N-CA-C	5.08	118.64	112.23
1	A	211	GLU	N-CA-C	5.08	118.63	112.23
1	F	211	GLU	N-CA-C	5.08	118.63	112.23
1	E	211	GLU	N-CA-C	5.07	118.62	112.23
1	G	211	GLU	N-CA-C	5.06	118.61	112.23
1	G	256	PHE	N-CA-C	-5.06	107.06	113.18
1	H	211	GLU	N-CA-C	5.05	118.60	112.23
1	E	256	PHE	N-CA-C	-5.05	107.07	113.18
1	B	256	PHE	N-CA-C	-5.05	107.07	113.18
1	A	256	PHE	N-CA-C	-5.04	107.08	113.18
1	D	256	PHE	N-CA-C	-5.04	107.08	113.18
1	C	256	PHE	N-CA-C	-5.01	107.11	113.18
1	F	256	PHE	N-CA-C	-5.00	107.12	113.18

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	1924	0	1899	81	1
1	B	1924	0	1899	91	3
1	C	1924	0	1899	79	10
1	D	1924	0	1899	78	2
1	E	1924	0	1899	89	11
1	F	1924	0	1899	83	3
1	G	1924	0	1899	84	7
1	H	1924	0	1899	83	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	30	0	12	1	0
2	B	30	0	12	3	0
2	C	30	0	12	2	0
2	D	30	0	12	2	0
2	E	30	0	12	1	0
2	F	30	0	12	2	0
2	G	30	0	12	3	0
2	H	30	0	12	3	0
3	A	25	0	0	5	0
3	B	25	0	0	5	0
3	C	25	0	0	5	0
3	D	25	0	0	5	0
3	E	25	0	0	5	0
3	F	25	0	0	5	0
3	G	25	0	0	5	0
3	H	25	0	0	5	0
All	All	15832	0	15288	647	20

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 21.

All (647) 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:B:244:ASN:CB	1:E:134:ARG:HH22	1.36	1.34
1:B:244:ASN:HB3	1:E:134:ARG:NH2	1.58	1.16
1:B:244:ASN:CB	1:E:134:ARG:NH2	2.13	1.08
1:H:40:ARG:H	1:H:187:HIS:HD2	1.01	1.00
1:G:40:ARG:H	1:G:187:HIS:HD2	1.01	1.00
1:B:244:ASN:HB3	1:E:134:ARG:HH22	0.84	0.99
1:E:40:ARG:H	1:E:187:HIS:HD2	1.01	0.99
1:B:40:ARG:H	1:B:187:HIS:HD2	1.01	0.98
1:C:40:ARG:H	1:C:187:HIS:HD2	1.01	0.95
1:B:244:ASN:CG	1:E:134:ARG:HH22	1.75	0.94
1:A:40:ARG:H	1:A:187:HIS:HD2	1.01	0.93
1:F:40:ARG:H	1:F:187:HIS:HD2	1.01	0.93
1:D:40:ARG:H	1:D:187:HIS:HD2	1.01	0.92
1:C:40:ARG:H	1:C:187:HIS:CD2	1.88	0.92
1:A:40:ARG:H	1:A:187:HIS:CD2	1.88	0.92
1:E:40:ARG:H	1:E:187:HIS:CD2	1.88	0.91
1:D:40:ARG:H	1:D:187:HIS:CD2	1.88	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:H	1:B:187:HIS:CD2	1.88	0.91
1:F:40:ARG:H	1:F:187:HIS:CD2	1.88	0.91
1:B:244:ASN:CG	1:E:134:ARG:NH2	2.28	0.91
1:G:40:ARG:H	1:G:187:HIS:CD2	1.88	0.90
1:H:40:ARG:H	1:H:187:HIS:CD2	1.88	0.90
1:B:58:LEU:HD23	1:B:267:MET:HE1	1.57	0.87
1:H:58:LEU:HD23	1:H:267:MET:HE1	1.57	0.87
1:D:58:LEU:HD23	1:D:267:MET:HE1	1.57	0.86
1:E:58:LEU:HD23	1:E:267:MET:HE1	1.57	0.85
1:C:58:LEU:HD23	1:C:267:MET:HE1	1.57	0.85
1:F:58:LEU:HD23	1:F:267:MET:HE1	1.57	0.85
1:A:58:LEU:HD23	1:A:267:MET:HE1	1.57	0.85
1:A:158:ASN:C	1:A:158:ASN:HD22	1.86	0.84
1:F:118:ARG:HH12	2:F:301:DTP:HN61	1.25	0.84
1:G:58:LEU:HD23	1:G:267:MET:HE1	1.57	0.84
1:F:158:ASN:C	1:F:158:ASN:HD22	1.86	0.84
1:D:158:ASN:C	1:D:158:ASN:HD22	1.86	0.84
1:G:158:ASN:C	1:G:158:ASN:HD22	1.86	0.84
1:A:118:ARG:HH12	2:A:301:DTP:HN61	1.26	0.83
1:C:158:ASN:C	1:C:158:ASN:HD22	1.86	0.83
1:G:118:ARG:HH12	2:G:301:DTP:HN61	1.27	0.83
1:B:158:ASN:C	1:B:158:ASN:HD22	1.86	0.82
1:B:118:ARG:HH12	2:B:301:DTP:HN61	1.27	0.82
1:H:158:ASN:C	1:H:158:ASN:HD22	1.86	0.82
1:D:118:ARG:HH12	2:D:301:DTP:HN61	1.23	0.81
1:E:158:ASN:C	1:E:158:ASN:HD22	1.86	0.81
1:E:118:ARG:HH12	2:E:301:DTP:HN61	1.28	0.80
1:C:118:ARG:HH12	2:C:301:DTP:HN61	1.26	0.80
1:B:40:ARG:N	1:B:187:HIS:HD2	1.80	0.80
1:A:58:LEU:HA	1:A:267:MET:HE1	1.65	0.79
1:H:128:GLU:HA	1:H:131:LEU:HD12	1.64	0.79
1:C:40:ARG:N	1:C:187:HIS:HD2	1.79	0.79
1:B:58:LEU:HA	1:B:267:MET:HE1	1.65	0.79
1:F:58:LEU:HA	1:F:267:MET:HE1	1.65	0.79
1:D:128:GLU:HA	1:D:131:LEU:HD12	1.64	0.79
1:E:58:LEU:HA	1:E:267:MET:HE1	1.65	0.79
1:B:128:GLU:HA	1:B:131:LEU:HD12	1.64	0.78
1:H:118:ARG:HH12	2:H:301:DTP:HN61	1.31	0.78
1:H:58:LEU:HA	1:H:267:MET:HE1	1.65	0.78
1:D:58:LEU:HA	1:D:267:MET:HE1	1.65	0.78
1:G:40:ARG:N	1:G:187:HIS:HD2	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PRO:O	1:C:131:LEU:HG	1.84	0.78
1:C:58:LEU:HA	1:C:267:MET:HE1	1.65	0.78
1:A:40:ARG:N	1:A:187:HIS:HD2	1.80	0.77
1:H:127:PRO:O	1:H:131:LEU:HG	1.84	0.77
1:C:128:GLU:HA	1:C:131:LEU:HD12	1.64	0.77
1:F:127:PRO:O	1:F:131:LEU:HG	1.84	0.77
1:E:40:ARG:N	1:E:187:HIS:HD2	1.80	0.77
1:E:128:GLU:HA	1:E:131:LEU:HD12	1.65	0.77
1:H:40:ARG:N	1:H:187:HIS:HD2	1.80	0.77
1:A:127:PRO:O	1:A:131:LEU:HG	1.84	0.77
1:D:127:PRO:O	1:D:131:LEU:HG	1.84	0.77
1:A:128:GLU:HA	1:A:131:LEU:HD12	1.64	0.76
1:D:40:ARG:N	1:D:187:HIS:HD2	1.80	0.76
1:F:128:GLU:HA	1:F:131:LEU:HD12	1.64	0.76
1:G:128:GLU:HA	1:G:131:LEU:HD12	1.64	0.76
1:B:127:PRO:O	1:B:131:LEU:HG	1.84	0.76
1:G:58:LEU:HA	1:G:267:MET:HE1	1.65	0.76
1:F:40:ARG:N	1:F:187:HIS:HD2	1.79	0.76
1:G:127:PRO:O	1:G:131:LEU:HG	1.84	0.76
1:C:78:ILE:HG13	1:D:164:ILE:HD12	1.67	0.75
1:E:127:PRO:O	1:E:131:LEU:HG	1.84	0.75
1:B:78:ILE:HD11	1:B:95:LEU:HB2	1.70	0.73
1:A:78:ILE:HD11	1:A:95:LEU:HB2	1.71	0.73
1:D:78:ILE:HD11	1:D:95:LEU:HB2	1.71	0.73
1:C:78:ILE:HD11	1:C:95:LEU:HB2	1.70	0.73
1:E:78:ILE:HD11	1:E:95:LEU:HB2	1.71	0.73
1:F:78:ILE:HD11	1:F:95:LEU:HB2	1.71	0.72
1:H:78:ILE:HD11	1:H:95:LEU:HB2	1.70	0.72
1:G:78:ILE:HD11	1:G:95:LEU:HB2	1.70	0.71
1:B:40:ARG:HG3	1:B:40:ARG:HH11	1.55	0.71
1:F:40:ARG:HG3	1:F:40:ARG:HH11	1.56	0.71
1:G:128:GLU:HA	1:G:131:LEU:CD1	2.21	0.70
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.55	0.70
1:E:128:GLU:HA	1:E:131:LEU:CD1	2.21	0.70
1:H:178:TRP:HB2	3:H:808:HOH:O	1.92	0.70
1:D:40:ARG:HG3	1:D:40:ARG:HH11	1.55	0.70
1:E:40:ARG:HG3	1:E:40:ARG:HH11	1.56	0.70
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.55	0.70
1:A:128:GLU:HA	1:A:131:LEU:CD1	2.21	0.70
1:F:128:GLU:HA	1:F:131:LEU:CD1	2.21	0.70
1:H:40:ARG:HH11	1:H:40:ARG:HG3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:GLU:HA	1:H:131:LEU:CD1	2.21	0.70
1:D:128:GLU:HA	1:D:131:LEU:CD1	2.21	0.69
1:C:128:GLU:HA	1:C:131:LEU:CD1	2.21	0.69
1:G:178:TRP:HB2	3:G:708:HOH:O	1.92	0.69
1:B:128:GLU:HA	1:B:131:LEU:CD1	2.21	0.69
1:F:178:TRP:HB2	3:F:608:HOH:O	1.92	0.69
1:A:178:TRP:HB2	3:A:307:HOH:O	1.92	0.69
1:G:40:ARG:HG3	1:G:40:ARG:HH11	1.56	0.69
1:B:178:TRP:HB2	3:B:309:HOH:O	1.92	0.68
1:D:178:TRP:HB2	3:D:309:HOH:O	1.92	0.68
1:E:178:TRP:HB2	3:E:508:HOH:O	1.92	0.68
1:C:178:TRP:HB2	3:C:308:HOH:O	1.92	0.67
1:E:57:LEU:HD22	1:E:267:MET:SD	2.35	0.67
1:H:57:LEU:HD22	1:H:267:MET:SD	2.35	0.67
1:B:57:LEU:HD22	1:B:267:MET:SD	2.35	0.67
1:F:57:LEU:HD22	1:F:267:MET:SD	2.35	0.67
1:F:158:ASN:C	1:F:158:ASN:ND2	2.53	0.67
1:A:70:GLU:HB2	1:A:141:GLU:HB2	1.77	0.67
1:G:57:LEU:HD22	1:G:267:MET:SD	2.35	0.67
1:E:99:MET:HG3	1:E:100:TYR:N	2.10	0.66
1:C:70:GLU:HB2	1:C:141:GLU:HB2	1.77	0.66
1:G:99:MET:HG3	1:G:100:TYR:N	2.10	0.66
1:A:57:LEU:HD22	1:A:267:MET:SD	2.35	0.66
1:D:57:LEU:HD22	1:D:267:MET:SD	2.35	0.66
1:B:158:ASN:C	1:B:158:ASN:ND2	2.53	0.66
1:D:70:GLU:HB2	1:D:141:GLU:HB2	1.77	0.66
1:F:70:GLU:HB2	1:F:141:GLU:HB2	1.77	0.66
1:G:70:GLU:HB2	1:G:141:GLU:HB2	1.77	0.66
1:C:57:LEU:HD22	1:C:267:MET:SD	2.35	0.66
1:E:70:GLU:HB2	1:E:141:GLU:HB2	1.77	0.66
1:H:158:ASN:C	1:H:158:ASN:ND2	2.53	0.66
1:B:99:MET:HG3	1:B:100:TYR:N	2.10	0.66
1:F:99:MET:HG3	1:F:100:TYR:N	2.10	0.66
1:G:158:ASN:C	1:G:158:ASN:ND2	2.53	0.66
1:H:99:MET:HG3	1:H:100:TYR:N	2.10	0.65
1:A:158:ASN:C	1:A:158:ASN:ND2	2.53	0.65
1:D:99:MET:HG3	1:D:100:TYR:N	2.10	0.65
1:H:70:GLU:HB2	1:H:141:GLU:HB2	1.77	0.65
1:A:99:MET:HG3	1:A:100:TYR:N	2.10	0.65
1:C:99:MET:HG3	1:C:100:TYR:N	2.10	0.64
1:B:70:GLU:HB2	1:B:141:GLU:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ASN:C	1:C:158:ASN:ND2	2.53	0.63
1:E:158:ASN:C	1:E:158:ASN:ND2	2.53	0.62
1:C:62:TYR:OH	1:C:271:ASN:HB2	2.01	0.61
1:H:62:TYR:OH	1:H:271:ASN:HB2	2.01	0.61
1:A:62:TYR:OH	1:A:271:ASN:HB2	2.01	0.61
1:D:164:ILE:HG12	3:D:308:HOH:O	2.01	0.60
1:E:62:TYR:OH	1:E:271:ASN:HB2	2.01	0.60
1:G:62:TYR:OH	1:G:271:ASN:HB2	2.01	0.60
1:H:164:ILE:HG12	3:H:807:HOH:O	2.01	0.60
1:E:164:ILE:HG12	3:E:507:HOH:O	2.01	0.60
1:B:62:TYR:OH	1:B:271:ASN:HB2	2.01	0.60
1:F:62:TYR:OH	1:F:271:ASN:HB2	2.01	0.60
1:G:164:ILE:HG12	3:G:707:HOH:O	2.01	0.60
1:A:65:TRP:CH2	1:A:274:VAL:HG21	2.37	0.59
1:F:65:TRP:CH2	1:F:274:VAL:HG21	2.37	0.59
1:D:62:TYR:OH	1:D:271:ASN:HB2	2.01	0.59
1:D:65:TRP:CH2	1:D:274:VAL:HG21	2.37	0.59
1:A:164:ILE:HG12	3:A:306:HOH:O	2.01	0.59
1:B:164:ILE:HG12	3:B:308:HOH:O	2.01	0.59
1:C:195:SER:OG	1:C:198:VAL:HG23	2.03	0.59
1:C:65:TRP:CH2	1:C:274:VAL:HG21	2.37	0.59
1:E:65:TRP:CH2	1:E:274:VAL:HG21	2.37	0.59
1:F:164:ILE:HG12	3:F:607:HOH:O	2.01	0.59
1:C:164:ILE:HG12	3:C:307:HOH:O	2.01	0.59
1:G:70:GLU:OE1	1:G:71:PRO:HD2	2.03	0.59
1:G:65:TRP:CH2	1:G:274:VAL:HG21	2.37	0.59
1:E:195:SER:OG	1:E:198:VAL:HG23	2.03	0.58
1:H:65:TRP:CH2	1:H:274:VAL:HG21	2.37	0.58
1:A:70:GLU:OE1	1:A:71:PRO:HD2	2.03	0.58
1:B:78:ILE:HG12	1:B:93:GLY:O	2.03	0.58
1:F:70:GLU:OE1	1:F:71:PRO:HD2	2.03	0.58
1:B:65:TRP:CH2	1:B:274:VAL:HG21	2.37	0.58
1:F:78:ILE:HG12	1:F:93:GLY:O	2.03	0.58
1:F:195:SER:OG	1:F:198:VAL:HG23	2.03	0.58
1:H:70:GLU:OE1	1:H:71:PRO:HD2	2.03	0.58
1:C:70:GLU:OE1	1:C:71:PRO:HD2	2.03	0.58
1:C:78:ILE:HG12	1:C:93:GLY:O	2.03	0.58
1:A:78:ILE:HG12	1:A:93:GLY:O	2.03	0.58
1:B:195:SER:OG	1:B:198:VAL:HG23	2.03	0.58
1:E:70:GLU:OE1	1:E:71:PRO:HD2	2.03	0.58
1:D:78:ILE:HG12	1:D:93:GLY:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:SER:OG	1:D:198:VAL:HG23	2.03	0.58
1:H:78:ILE:HG12	1:H:93:GLY:O	2.03	0.58
1:B:70:GLU:OE1	1:B:71:PRO:HD2	2.03	0.58
1:D:40:ARG:HG3	1:D:40:ARG:NH1	2.19	0.58
1:A:195:SER:OG	1:A:198:VAL:HG23	2.03	0.57
1:E:40:ARG:HG3	1:E:40:ARG:NH1	2.19	0.57
1:G:40:ARG:HG3	1:G:40:ARG:NH1	2.19	0.57
1:G:78:ILE:HG12	1:G:93:GLY:O	2.03	0.57
1:A:40:ARG:HG3	1:A:40:ARG:NH1	2.19	0.57
1:D:70:GLU:OE1	1:D:71:PRO:HD2	2.03	0.57
1:H:195:SER:OG	1:H:198:VAL:HG23	2.03	0.57
1:C:40:ARG:HG3	1:C:40:ARG:NH1	2.19	0.57
1:G:78:ILE:HG13	1:H:164:ILE:HD12	1.86	0.57
1:G:195:SER:OG	1:G:198:VAL:HG23	2.03	0.57
1:E:78:ILE:HG12	1:E:93:GLY:O	2.03	0.57
1:E:166:TRP:O	1:E:170:GLN:HG3	2.05	0.57
1:B:166:TRP:O	1:B:170:GLN:HG3	2.05	0.56
1:C:166:TRP:O	1:C:170:GLN:HG3	2.05	0.56
1:D:158:ASN:C	1:D:158:ASN:ND2	2.53	0.56
1:H:40:ARG:HG3	1:H:40:ARG:NH1	2.19	0.56
1:A:203:LEU:HD23	1:A:203:LEU:C	2.31	0.56
1:E:203:LEU:C	1:E:203:LEU:HD23	2.31	0.56
1:B:203:LEU:C	1:B:203:LEU:HD23	2.31	0.56
1:G:166:TRP:O	1:G:170:GLN:HG3	2.05	0.56
1:D:145:TYR:CD2	1:D:242:LEU:HD22	2.41	0.56
1:G:145:TYR:CD2	1:G:242:LEU:HD22	2.41	0.56
1:A:145:TYR:CD2	1:A:242:LEU:HD22	2.41	0.56
1:A:166:TRP:O	1:A:170:GLN:HG3	2.05	0.56
1:H:166:TRP:O	1:H:170:GLN:HG3	2.05	0.56
1:A:62:TYR:O	1:A:65:TRP:HB2	2.06	0.56
1:F:203:LEU:HD23	1:F:203:LEU:C	2.31	0.56
1:G:62:TYR:O	1:G:65:TRP:HB2	2.06	0.56
1:D:62:TYR:O	1:D:65:TRP:HB2	2.06	0.55
1:D:203:LEU:C	1:D:203:LEU:HD23	2.31	0.55
1:G:203:LEU:C	1:G:203:LEU:HD23	2.31	0.55
1:H:203:LEU:C	1:H:203:LEU:HD23	2.31	0.55
1:B:145:TYR:CD2	1:B:242:LEU:HD22	2.41	0.55
1:F:145:TYR:CD2	1:F:242:LEU:HD22	2.41	0.55
1:B:153:LYS:O	1:B:157:GLU:HG3	2.07	0.55
1:D:166:TRP:O	1:D:170:GLN:HG3	2.05	0.55
1:C:203:LEU:C	1:C:203:LEU:HD23	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:TRP:O	1:F:170:GLN:HG3	2.05	0.55
1:B:62:TYR:O	1:B:65:TRP:HB2	2.06	0.55
1:E:62:TYR:O	1:E:65:TRP:HB2	2.07	0.55
1:E:153:LYS:O	1:E:157:GLU:HG3	2.07	0.55
1:C:145:TYR:CD2	1:C:242:LEU:HD22	2.41	0.55
1:C:153:LYS:O	1:C:157:GLU:HG3	2.07	0.55
1:E:145:TYR:CD2	1:E:242:LEU:HD22	2.41	0.55
1:H:153:LYS:O	1:H:157:GLU:HG3	2.07	0.55
1:G:212:LYS:HG3	1:G:212:LYS:O	2.07	0.55
1:H:145:TYR:CD2	1:H:242:LEU:HD22	2.41	0.55
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.19	0.55
1:D:153:LYS:O	1:D:157:GLU:HG3	2.07	0.55
1:A:212:LYS:O	1:A:212:LYS:HG3	2.07	0.54
1:B:58:LEU:HA	1:B:267:MET:CE	2.37	0.54
1:C:62:TYR:O	1:C:65:TRP:HB2	2.06	0.54
1:H:62:TYR:O	1:H:65:TRP:HB2	2.06	0.54
1:F:153:LYS:O	1:F:157:GLU:HG3	2.07	0.54
1:H:212:LYS:O	1:H:212:LYS:HG3	2.07	0.54
1:F:40:ARG:HG3	1:F:40:ARG:NH1	2.19	0.54
1:E:203:LEU:HD23	1:E:203:LEU:O	2.08	0.54
1:H:58:LEU:HA	1:H:267:MET:CE	2.37	0.54
1:B:212:LYS:HG3	1:B:212:LYS:O	2.07	0.54
1:C:212:LYS:O	1:C:212:LYS:HG3	2.07	0.54
1:E:212:LYS:O	1:E:212:LYS:HG3	2.07	0.54
1:F:212:LYS:O	1:F:212:LYS:HG3	2.07	0.54
1:B:71:PRO:HG2	1:B:117:SER:OG	2.08	0.54
1:F:203:LEU:HD23	1:F:203:LEU:O	2.08	0.54
1:G:183:ARG:NH2	1:H:179:GLU:OE1	2.33	0.54
1:D:212:LYS:HG3	1:D:212:LYS:O	2.07	0.54
1:F:62:TYR:O	1:F:65:TRP:HB2	2.06	0.54
1:A:58:LEU:HA	1:A:267:MET:CE	2.37	0.53
1:A:153:LYS:O	1:A:157:GLU:HG3	2.07	0.53
1:G:67:VAL:HG22	1:G:139:ILE:HB	1.90	0.53
1:C:67:VAL:HG22	1:C:139:ILE:HB	1.90	0.53
1:G:153:LYS:O	1:G:157:GLU:HG3	2.07	0.53
1:G:154:ASN:HD21	1:G:221:GLN:HE21	1.56	0.53
1:G:203:LEU:HD23	1:G:203:LEU:O	2.08	0.53
1:C:148:ARG:HD2	1:C:173:HIS:ND1	2.24	0.53
1:E:71:PRO:HG2	1:E:117:SER:OG	2.08	0.53
1:F:154:ASN:HD21	1:F:221:GLN:HE21	1.56	0.53
1:A:154:ASN:HD21	1:A:221:GLN:HE21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ARG:HD2	1:D:173:HIS:ND1	2.24	0.53
1:E:67:VAL:HG22	1:E:139:ILE:HB	1.90	0.53
1:F:58:LEU:HA	1:F:267:MET:CE	2.37	0.53
1:A:71:PRO:HG2	1:A:117:SER:OG	2.08	0.53
1:A:203:LEU:HD23	1:A:203:LEU:O	2.08	0.53
1:D:71:PRO:HG2	1:D:117:SER:OG	2.08	0.53
1:F:67:VAL:HG22	1:F:139:ILE:HB	1.90	0.53
1:G:148:ARG:HD2	1:G:173:HIS:ND1	2.24	0.53
1:H:203:LEU:HD23	1:H:203:LEU:O	2.08	0.53
1:B:203:LEU:HD23	1:B:203:LEU:O	2.08	0.53
1:A:148:ARG:HD2	1:A:173:HIS:ND1	2.24	0.53
1:D:203:LEU:HD23	1:D:203:LEU:O	2.08	0.53
1:B:148:ARG:HD2	1:B:173:HIS:ND1	2.24	0.53
1:E:148:ARG:HD2	1:E:173:HIS:ND1	2.24	0.53
1:F:148:ARG:HD2	1:F:173:HIS:ND1	2.24	0.53
1:H:67:VAL:HG22	1:H:139:ILE:HB	1.90	0.53
1:H:71:PRO:HG2	1:H:117:SER:OG	2.08	0.53
1:G:71:PRO:HG2	1:G:117:SER:OG	2.08	0.53
1:C:154:ASN:HD21	1:C:221:GLN:HE21	1.56	0.52
1:D:67:VAL:HG22	1:D:139:ILE:HB	1.90	0.52
1:B:67:VAL:HG22	1:B:139:ILE:HB	1.90	0.52
1:C:203:LEU:HD23	1:C:203:LEU:O	2.08	0.52
1:F:39:ARG:HA	1:F:187:HIS:CD2	2.45	0.52
1:F:71:PRO:HG2	1:F:117:SER:OG	2.08	0.52
1:H:148:ARG:HD2	1:H:173:HIS:ND1	2.24	0.52
1:B:39:ARG:HA	1:B:187:HIS:CD2	2.45	0.52
1:E:154:ASN:HD21	1:E:221:GLN:HE21	1.56	0.52
1:H:39:ARG:HA	1:H:187:HIS:CD2	2.45	0.52
1:D:154:ASN:HD21	1:D:221:GLN:HE21	1.56	0.52
1:G:177:LEU:HD22	1:G:184:ILE:HD13	1.92	0.52
1:H:217:ALA:O	1:H:221:GLN:HG3	2.10	0.52
1:D:58:LEU:HA	1:D:267:MET:CE	2.37	0.52
1:D:177:LEU:HD22	1:D:184:ILE:HD13	1.92	0.52
1:D:217:ALA:O	1:D:221:GLN:HG3	2.10	0.52
1:C:71:PRO:HG2	1:C:117:SER:OG	2.08	0.52
1:C:128:GLU:O	1:C:131:LEU:HB2	2.10	0.52
1:F:217:ALA:O	1:F:221:GLN:HG3	2.10	0.52
1:G:128:GLU:O	1:G:131:LEU:HB2	2.10	0.52
1:G:217:ALA:O	1:G:221:GLN:HG3	2.10	0.52
1:B:154:ASN:HD21	1:B:221:GLN:HE21	1.56	0.52
1:C:39:ARG:HA	1:C:187:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ARG:HA	1:D:187:HIS:CD2	2.45	0.52
1:H:128:GLU:O	1:H:131:LEU:HB2	2.10	0.52
1:H:154:ASN:HD21	1:H:221:GLN:HE21	1.56	0.52
1:C:217:ALA:O	1:C:221:GLN:HG3	2.10	0.51
1:A:67:VAL:HG22	1:A:139:ILE:HB	1.90	0.51
1:G:39:ARG:HA	1:G:187:HIS:CD2	2.45	0.51
1:A:39:ARG:HA	1:A:187:HIS:CD2	2.45	0.51
1:E:39:ARG:HA	1:E:187:HIS:CD2	2.45	0.51
1:E:217:ALA:O	1:E:221:GLN:HG3	2.10	0.51
1:A:128:GLU:O	1:A:131:LEU:HB2	2.10	0.51
1:B:128:GLU:O	1:B:131:LEU:HB2	2.10	0.51
1:E:128:GLU:O	1:E:131:LEU:HB2	2.10	0.51
1:B:177:LEU:HD22	1:B:184:ILE:HD13	1.92	0.51
1:B:217:ALA:O	1:B:221:GLN:HG3	2.10	0.51
1:H:142:ARG:HD3	3:H:814:HOH:O	2.11	0.51
1:F:128:GLU:O	1:F:131:LEU:HB2	2.10	0.51
1:B:72:VAL:HA	1:B:75:TRP:CE3	2.46	0.51
1:E:177:LEU:HD22	1:E:184:ILE:HD13	1.92	0.51
1:H:72:VAL:HA	1:H:75:TRP:CE3	2.46	0.51
1:C:177:LEU:HD22	1:C:184:ILE:HD13	1.92	0.50
1:D:128:GLU:O	1:D:131:LEU:HB2	2.10	0.50
1:G:72:VAL:HA	1:G:75:TRP:CE3	2.46	0.50
1:H:177:LEU:HD22	1:H:184:ILE:HD13	1.92	0.50
1:A:177:LEU:HD22	1:A:184:ILE:HD13	1.92	0.50
1:E:72:VAL:HA	1:E:75:TRP:CE3	2.46	0.50
1:C:72:VAL:HA	1:C:75:TRP:CE3	2.46	0.50
1:E:259:GLU:N	1:E:259:GLU:OE1	2.45	0.50
1:H:259:GLU:OE1	1:H:259:GLU:N	2.45	0.50
1:A:72:VAL:HA	1:A:75:TRP:CE3	2.46	0.50
1:A:217:ALA:O	1:A:221:GLN:HG3	2.10	0.50
1:F:210:GLU:CD	1:F:210:GLU:H	2.20	0.50
1:H:49:VAL:HG23	1:H:194:ALA:HB3	1.93	0.50
1:C:58:LEU:HA	1:C:267:MET:CE	2.37	0.50
1:C:210:GLU:H	1:C:210:GLU:CD	2.20	0.50
1:G:49:VAL:HG23	1:G:194:ALA:HB3	1.93	0.50
1:A:210:GLU:CD	1:A:210:GLU:H	2.20	0.50
1:B:211:GLU:O	1:B:213:GLY:N	2.45	0.50
1:B:210:GLU:CD	1:B:210:GLU:H	2.20	0.50
1:B:259:GLU:N	1:B:259:GLU:OE1	2.45	0.50
1:G:259:GLU:N	1:G:259:GLU:OE1	2.45	0.50
1:A:211:GLU:O	1:A:213:GLY:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:GLU:CD	1:E:210:GLU:H	2.20	0.50
1:F:72:VAL:HA	1:F:75:TRP:CE3	2.46	0.50
1:G:210:GLU:CD	1:G:210:GLU:H	2.20	0.50
1:H:210:GLU:H	1:H:210:GLU:CD	2.20	0.50
1:E:211:GLU:O	1:E:213:GLY:N	2.45	0.50
1:A:142:ARG:HD3	3:A:313:HOH:O	2.11	0.49
1:F:177:LEU:HD22	1:F:184:ILE:HD13	1.92	0.49
1:D:72:VAL:HA	1:D:75:TRP:CE3	2.46	0.49
1:D:211:GLU:O	1:D:213:GLY:N	2.45	0.49
1:C:49:VAL:HG23	1:C:194:ALA:HB3	1.93	0.49
1:C:211:GLU:O	1:C:213:GLY:N	2.45	0.49
1:F:142:ARG:HD3	3:F:614:HOH:O	2.11	0.49
1:G:142:ARG:HD3	3:G:714:HOH:O	2.11	0.49
1:G:211:GLU:O	1:G:213:GLY:N	2.45	0.49
1:A:259:GLU:OE1	1:A:259:GLU:N	2.45	0.49
1:B:49:VAL:HG23	1:B:194:ALA:HB3	1.93	0.49
1:G:58:LEU:HA	1:G:267:MET:CE	2.37	0.49
1:C:142:ARG:HD3	3:C:314:HOH:O	2.11	0.49
1:C:259:GLU:N	1:C:259:GLU:OE1	2.45	0.49
1:F:211:GLU:O	1:F:213:GLY:N	2.45	0.49
1:H:211:GLU:O	1:H:213:GLY:N	2.45	0.49
1:D:142:ARG:HD3	3:D:315:HOH:O	2.11	0.49
1:B:142:ARG:HD3	3:B:315:HOH:O	2.11	0.49
1:D:259:GLU:N	1:D:259:GLU:OE1	2.45	0.49
1:F:49:VAL:HG23	1:F:194:ALA:HB3	1.93	0.49
1:F:259:GLU:OE1	1:F:259:GLU:N	2.45	0.49
1:E:49:VAL:HG23	1:E:194:ALA:HB3	1.93	0.49
1:D:49:VAL:HG23	1:D:194:ALA:HB3	1.93	0.49
1:E:164:ILE:HD12	1:F:78:ILE:HG13	1.95	0.49
1:A:49:VAL:HG23	1:A:194:ALA:HB3	1.93	0.48
1:D:210:GLU:CD	1:D:210:GLU:H	2.20	0.48
1:G:164:ILE:HD12	1:H:78:ILE:HG13	1.94	0.48
1:E:142:ARG:HD3	3:E:514:HOH:O	2.11	0.48
1:A:200:LEU:HD11	1:A:204:TYR:CE1	2.49	0.48
1:F:200:LEU:HD22	1:F:216:LEU:HB2	1.96	0.48
1:D:200:LEU:HD22	1:D:216:LEU:HB2	1.96	0.48
1:H:45:GLY:O	1:H:142:ARG:NH1	2.47	0.48
1:B:200:LEU:HD11	1:B:204:TYR:CE1	2.49	0.48
1:D:200:LEU:HD11	1:D:204:TYR:CE1	2.49	0.48
1:B:200:LEU:HD22	1:B:216:LEU:HB2	1.96	0.48
1:D:45:GLY:O	1:D:142:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD11	1:E:204:TYR:CE1	2.49	0.48
1:G:200:LEU:HD22	1:G:216:LEU:HB2	1.96	0.48
1:F:200:LEU:HD11	1:F:204:TYR:CE1	2.49	0.48
1:D:256:PHE:CD1	1:D:256:PHE:C	2.92	0.48
1:G:45:GLY:O	1:G:142:ARG:NH1	2.47	0.48
1:C:45:GLY:O	1:C:142:ARG:NH1	2.47	0.48
1:E:58:LEU:HA	1:E:267:MET:CE	2.37	0.48
1:E:197:GLN:CD	1:E:197:GLN:H	2.22	0.48
1:H:256:PHE:CD1	1:H:256:PHE:C	2.92	0.48
1:B:256:PHE:CD1	1:B:256:PHE:C	2.92	0.47
1:E:45:GLY:O	1:E:142:ARG:NH1	2.47	0.47
1:A:45:GLY:O	1:A:142:ARG:NH1	2.47	0.47
1:B:99:MET:HE2	1:B:99:MET:O	2.14	0.47
1:C:200:LEU:HD11	1:C:204:TYR:CE1	2.49	0.47
1:H:200:LEU:HD11	1:H:204:TYR:CE1	2.49	0.47
1:C:200:LEU:HD22	1:C:216:LEU:HB2	1.96	0.47
1:C:256:PHE:CD1	1:C:256:PHE:C	2.92	0.47
1:D:99:MET:O	1:D:99:MET:HE2	2.15	0.47
1:E:200:LEU:HD22	1:E:216:LEU:HB2	1.96	0.47
1:F:99:MET:O	1:F:99:MET:HE2	2.14	0.47
1:A:197:GLN:CD	1:A:197:GLN:H	2.22	0.47
1:B:45:GLY:O	1:B:142:ARG:NH1	2.47	0.47
1:F:197:GLN:CD	1:F:197:GLN:H	2.22	0.47
1:F:233:LYS:HB2	1:G:232:HIS:CG	2.50	0.47
1:A:256:PHE:CD1	1:A:256:PHE:C	2.92	0.47
1:A:99:MET:HE2	1:A:99:MET:O	2.14	0.47
1:A:128:GLU:CD	1:A:128:GLU:H	2.23	0.47
1:A:200:LEU:HD22	1:A:216:LEU:HB2	1.96	0.47
1:A:209:GLU:O	1:A:212:LYS:HG2	2.15	0.47
1:D:240:GLU:O	1:D:243:MET:HB2	2.15	0.47
1:E:65:TRP:HH2	1:E:274:VAL:HG21	1.80	0.47
1:E:99:MET:HE2	1:E:99:MET:O	2.14	0.47
1:E:209:GLU:O	1:E:212:LYS:HG2	2.15	0.47
1:E:256:PHE:CD1	1:E:256:PHE:C	2.92	0.47
1:G:200:LEU:HD11	1:G:204:TYR:CE1	2.49	0.47
1:H:99:MET:HE2	1:H:99:MET:O	2.15	0.47
1:H:200:LEU:HD22	1:H:216:LEU:HB2	1.96	0.47
1:D:128:GLU:H	1:D:128:GLU:CD	2.23	0.47
1:E:128:GLU:CD	1:E:128:GLU:H	2.23	0.47
1:F:45:GLY:O	1:F:142:ARG:NH1	2.47	0.47
1:F:92:LEU:N	3:F:624:HOH:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HD12	1:B:78:ILE:HG13	1.96	0.47
1:F:209:GLU:O	1:F:212:LYS:HG2	2.15	0.47
1:F:240:GLU:O	1:F:243:MET:HB2	2.15	0.47
1:F:256:PHE:CD1	1:F:256:PHE:C	2.92	0.47
1:G:99:MET:HE2	1:G:99:MET:O	2.14	0.47
1:H:197:GLN:CD	1:H:197:GLN:H	2.22	0.47
1:H:209:GLU:O	1:H:212:LYS:HG2	2.15	0.47
1:B:240:GLU:O	1:B:243:MET:HB2	2.15	0.47
1:D:209:GLU:O	1:D:212:LYS:HG2	2.15	0.47
1:G:41:LEU:HB2	1:G:139:ILE:HD13	1.97	0.47
1:G:128:GLU:CD	1:G:128:GLU:H	2.23	0.47
1:G:256:PHE:CD1	1:G:256:PHE:C	2.92	0.47
1:C:99:MET:HE2	1:C:99:MET:O	2.15	0.46
1:A:78:ILE:HG13	1:B:164:ILE:HD12	1.96	0.46
1:C:209:GLU:O	1:C:212:LYS:HG2	2.15	0.46
1:C:65:TRP:HH2	1:C:274:VAL:HG21	1.80	0.46
1:C:197:GLN:CD	1:C:197:GLN:H	2.22	0.46
1:C:240:GLU:O	1:C:243:MET:HB2	2.15	0.46
1:E:41:LEU:HB2	1:E:139:ILE:HD13	1.97	0.46
1:G:209:GLU:O	1:G:212:LYS:HG2	2.15	0.46
1:H:41:LEU:HB2	1:H:139:ILE:HD13	1.97	0.46
1:H:128:GLU:CD	1:H:128:GLU:H	2.23	0.46
1:A:158:ASN:ND2	1:A:160:SER:H	2.14	0.46
1:A:240:GLU:O	1:A:243:MET:HB2	2.15	0.46
1:G:65:TRP:HH2	1:G:274:VAL:HG21	1.80	0.46
1:H:158:ASN:ND2	1:H:160:SER:H	2.14	0.46
1:A:70:GLU:HB2	1:A:141:GLU:CB	2.45	0.46
1:F:158:ASN:ND2	1:F:160:SER:H	2.14	0.46
1:G:197:GLN:CD	1:G:197:GLN:H	2.22	0.46
1:G:240:GLU:O	1:G:243:MET:HB2	2.15	0.46
1:H:92:LEU:N	3:H:824:HOH:O	2.48	0.46
1:H:240:GLU:O	1:H:243:MET:HB2	2.15	0.46
1:B:41:LEU:HB2	1:B:139:ILE:HD13	1.97	0.46
1:C:128:GLU:CD	1:C:128:GLU:H	2.23	0.46
1:D:197:GLN:H	1:D:197:GLN:CD	2.22	0.46
1:G:92:LEU:N	3:G:724:HOH:O	2.48	0.46
1:B:158:ASN:ND2	1:B:160:SER:H	2.14	0.46
1:B:197:GLN:CD	1:B:197:GLN:H	2.22	0.46
1:B:209:GLU:O	1:B:212:LYS:HG2	2.15	0.46
1:C:92:LEU:N	3:C:324:HOH:O	2.48	0.46
1:D:92:LEU:N	3:D:325:HOH:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:GLU:O	1:E:243:MET:HB2	2.15	0.46
1:F:128:GLU:CD	1:F:128:GLU:H	2.23	0.46
1:D:41:LEU:HB2	1:D:139:ILE:HD13	1.97	0.46
1:G:245:ILE:HG23	1:G:246:PRO:HD2	1.98	0.46
1:C:41:LEU:HB2	1:C:139:ILE:HD13	1.97	0.46
1:F:41:LEU:HB2	1:F:139:ILE:HD13	1.97	0.46
1:A:92:LEU:N	3:A:323:HOH:O	2.48	0.46
1:B:92:LEU:N	3:B:325:HOH:O	2.48	0.46
1:A:245:ILE:HG23	1:A:246:PRO:HD2	1.98	0.45
1:B:128:GLU:CD	1:B:128:GLU:H	2.23	0.45
1:D:158:ASN:ND2	1:D:160:SER:H	2.14	0.45
1:D:200:LEU:HD11	1:D:204:TYR:HE1	1.81	0.45
1:E:245:ILE:HG23	1:E:246:PRO:HD2	1.98	0.45
1:G:200:LEU:HD11	1:G:204:TYR:HE1	1.81	0.45
1:H:70:GLU:HB2	1:H:141:GLU:CB	2.45	0.45
1:E:158:ASN:ND2	1:E:160:SER:H	2.14	0.45
1:C:158:ASN:ND2	1:C:160:SER:H	2.14	0.45
1:E:92:LEU:N	3:E:524:HOH:O	2.48	0.45
1:A:65:TRP:HH2	1:A:274:VAL:HG21	1.80	0.45
1:A:118:ARG:O	1:A:121:VAL:HG12	2.17	0.45
1:B:200:LEU:HD11	1:B:204:TYR:HE1	1.81	0.45
1:D:65:TRP:HH2	1:D:274:VAL:HG21	1.80	0.45
1:C:70:GLU:HB2	1:C:141:GLU:CB	2.46	0.45
1:E:179:GLU:OE1	1:F:183:ARG:NH2	2.34	0.45
1:E:183:ARG:NH2	1:F:179:GLU:OE1	2.40	0.45
1:F:245:ILE:HG23	1:F:246:PRO:HD2	1.98	0.45
1:H:118:ARG:O	1:H:121:VAL:HG12	2.17	0.45
1:A:41:LEU:HB2	1:A:139:ILE:HD13	1.97	0.45
1:G:158:ASN:ND2	1:G:160:SER:H	2.14	0.45
1:E:118:ARG:O	1:E:121:VAL:HG12	2.17	0.45
1:B:245:ILE:HG23	1:B:246:PRO:HD2	1.98	0.45
1:G:118:ARG:O	1:G:121:VAL:HG12	2.17	0.45
1:D:245:ILE:HG23	1:D:246:PRO:HD2	1.98	0.45
1:E:200:LEU:HD11	1:E:204:TYR:HE1	1.81	0.45
1:H:200:LEU:HD11	1:H:204:TYR:HE1	1.82	0.45
1:A:46:ASN:OD1	1:A:47:ILE:N	2.48	0.44
1:C:245:ILE:HG23	1:C:246:PRO:HD2	1.98	0.44
1:F:70:GLU:HB2	1:F:141:GLU:CB	2.45	0.44
1:H:162:SER:OG	1:H:165:GLU:HG3	2.17	0.44
1:F:118:ARG:O	1:F:121:VAL:HG12	2.17	0.44
1:G:162:SER:OG	1:G:165:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:SER:OG	1:C:165:GLU:HG3	2.17	0.44
1:F:65:TRP:HH2	1:F:274:VAL:HG21	1.80	0.44
1:F:162:SER:OG	1:F:165:GLU:HG3	2.17	0.44
1:H:245:ILE:HG23	1:H:246:PRO:HD2	1.98	0.44
1:A:200:LEU:HD11	1:A:204:TYR:HE1	1.81	0.44
1:C:118:ARG:O	1:C:121:VAL:HG12	2.17	0.44
1:E:162:SER:OG	1:E:165:GLU:HG3	2.18	0.44
1:B:118:ARG:O	1:B:121:VAL:HG12	2.17	0.44
1:B:162:SER:OG	1:B:165:GLU:HG3	2.17	0.44
1:F:46:ASN:OD1	1:F:47:ILE:N	2.48	0.44
1:D:118:ARG:O	1:D:121:VAL:HG12	2.17	0.44
1:D:162:SER:OG	1:D:165:GLU:HG3	2.17	0.44
1:A:162:SER:OG	1:A:165:GLU:HG3	2.17	0.44
1:A:172:TRP:CZ2	1:B:116:LEU:HB2	2.53	0.44
1:B:70:GLU:HA	1:B:71:PRO:HD3	1.76	0.44
1:C:46:ASN:OD1	1:C:47:ILE:N	2.48	0.44
1:F:72:VAL:HG21	2:F:301:DTP:O2A	2.17	0.44
1:A:70:GLU:HG2	3:A:321:HOH:O	2.18	0.43
1:D:70:GLU:HB2	1:D:141:GLU:CB	2.45	0.43
1:H:46:ASN:OD1	1:H:47:ILE:N	2.48	0.43
1:D:70:GLU:HG2	3:D:323:HOH:O	2.18	0.43
1:F:70:GLU:HG2	3:F:622:HOH:O	2.18	0.43
1:F:200:LEU:HD11	1:F:204:TYR:HE1	1.81	0.43
1:E:70:GLU:HB2	1:E:141:GLU:CB	2.45	0.43
1:G:179:GLU:OE1	1:H:183:ARG:NH2	2.39	0.43
1:B:209:GLU:O	1:B:210:GLU:C	2.62	0.43
1:E:209:GLU:O	1:E:210:GLU:C	2.62	0.43
1:D:72:VAL:HG21	2:D:301:DTP:O2A	2.19	0.43
1:C:70:GLU:HA	1:C:71:PRO:HD3	1.76	0.43
1:B:65:TRP:HH2	1:B:274:VAL:HG21	1.80	0.43
1:E:46:ASN:OD1	1:E:47:ILE:N	2.48	0.43
1:A:116:LEU:HB2	1:B:172:TRP:CZ2	2.54	0.42
1:G:70:GLU:HA	1:G:71:PRO:HD3	1.76	0.42
1:C:108:TYR:O	1:C:112:THR:HG23	2.20	0.42
1:C:209:GLU:O	1:C:210:GLU:C	2.62	0.42
1:G:70:GLU:HG2	3:G:722:HOH:O	2.18	0.42
1:H:65:TRP:HH2	1:H:274:VAL:HG21	1.80	0.42
1:H:70:GLU:HG2	3:H:822:HOH:O	2.18	0.42
1:H:209:GLU:O	1:H:210:GLU:C	2.62	0.42
1:B:70:GLU:HG2	3:B:323:HOH:O	2.18	0.42
1:B:158:ASN:HD22	1:B:159:GLY:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:PHE:O	1:B:181:ALA:C	2.63	0.42
1:D:135:LYS:HE3	1:D:275:LYS:HE2	2.02	0.42
1:D:276:ASN:HD22	1:D:276:ASN:N	2.17	0.42
1:G:108:TYR:O	1:G:112:THR:HG23	2.20	0.42
1:G:158:ASN:HD22	1:G:159:GLY:N	2.17	0.42
2:H:301:DTP:H2'2	2:H:301:DTP:H5'2	1.81	0.42
1:A:209:GLU:O	1:A:210:GLU:C	2.62	0.42
1:C:70:GLU:HG2	3:C:322:HOH:O	2.18	0.42
1:F:158:ASN:HD22	1:F:159:GLY:N	2.17	0.42
1:F:276:ASN:N	1:F:276:ASN:HD22	2.17	0.42
1:B:70:GLU:HB2	1:B:141:GLU:CB	2.45	0.42
1:C:200:LEU:HD11	1:C:204:TYR:HE1	1.82	0.42
1:G:135:LYS:HE3	1:G:275:LYS:HE2	2.02	0.42
1:G:209:GLU:O	1:G:210:GLU:C	2.62	0.42
1:E:108:TYR:O	1:E:112:THR:HG23	2.20	0.42
1:G:180:PHE:O	1:G:181:ALA:C	2.63	0.42
1:H:180:PHE:O	1:H:181:ALA:C	2.63	0.42
1:E:70:GLU:HG2	3:E:522:HOH:O	2.18	0.42
1:E:135:LYS:HE3	1:E:275:LYS:HE2	2.02	0.42
1:G:72:VAL:HG21	2:G:301:DTP:O2A	2.20	0.42
1:H:108:TYR:O	1:H:112:THR:HG23	2.20	0.42
1:H:276:ASN:N	1:H:276:ASN:HD22	2.17	0.42
1:C:135:LYS:HE3	1:C:275:LYS:HE2	2.02	0.42
1:H:135:LYS:HE3	1:H:275:LYS:HE2	2.01	0.42
1:A:75:TRP:HD1	1:A:113:PHE:HE2	1.68	0.42
1:A:108:TYR:O	1:A:112:THR:HG23	2.20	0.42
1:B:72:VAL:HG21	2:B:301:DTP:O2A	2.20	0.42
1:B:75:TRP:HD1	1:B:113:PHE:HE2	1.68	0.42
1:C:276:ASN:N	1:C:276:ASN:HD22	2.17	0.42
1:E:187:HIS:O	1:E:246:PRO:HD2	2.20	0.42
1:B:108:TYR:O	1:B:112:THR:HG23	2.20	0.42
1:B:244:ASN:CG	1:E:134:ARG:CZ	2.91	0.42
1:D:158:ASN:HD22	1:D:159:GLY:N	2.17	0.42
1:E:180:PHE:O	1:E:181:ALA:C	2.63	0.42
1:F:108:TYR:O	1:F:112:THR:HG23	2.20	0.42
1:F:209:GLU:O	1:F:210:GLU:C	2.62	0.42
1:A:180:PHE:O	1:A:181:ALA:C	2.63	0.41
1:B:187:HIS:O	1:B:246:PRO:HD2	2.20	0.41
1:D:75:TRP:HD1	1:D:113:PHE:HE2	1.68	0.41
1:D:108:TYR:O	1:D:112:THR:HG23	2.20	0.41
1:E:78:ILE:HG13	1:F:164:ILE:HD12	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:ASN:OD1	1:G:47:ILE:N	2.48	0.41
2:G:301:DTP:H2'2	2:G:301:DTP:H5'2	1.83	0.41
1:H:187:HIS:O	1:H:246:PRO:HD2	2.20	0.41
1:A:276:ASN:N	1:A:276:ASN:HD22	2.17	0.41
1:C:187:HIS:O	1:C:246:PRO:HD2	2.20	0.41
1:A:135:LYS:HE3	1:A:275:LYS:HE2	2.02	0.41
1:F:70:GLU:HA	1:F:71:PRO:HD3	1.76	0.41
1:G:276:ASN:N	1:G:276:ASN:HD22	2.17	0.41
1:H:158:ASN:HD22	1:H:159:GLY:N	2.17	0.41
1:B:124:GLU:HA	1:B:125:PRO:HD3	1.91	0.41
1:D:209:GLU:O	1:D:210:GLU:C	2.62	0.41
1:E:276:ASN:N	1:E:276:ASN:HD22	2.17	0.41
1:F:135:LYS:HE3	1:F:275:LYS:HE2	2.02	0.41
1:F:177:LEU:HD22	1:F:184:ILE:CD1	2.51	0.41
1:A:70:GLU:HA	1:A:71:PRO:HD3	1.76	0.41
1:G:187:HIS:O	1:G:246:PRO:HD2	2.20	0.41
1:H:75:TRP:HD1	1:H:113:PHE:HE2	1.68	0.41
1:F:187:HIS:O	1:F:246:PRO:HD2	2.20	0.41
1:G:203:LEU:C	1:G:203:LEU:CD2	2.94	0.41
1:B:46:ASN:OD1	1:B:47:ILE:N	2.48	0.41
1:B:244:ASN:ND2	1:E:134:ARG:NH2	2.68	0.41
2:B:301:DTP:H2'2	2:B:301:DTP:H5'2	1.80	0.41
1:C:203:LEU:C	1:C:203:LEU:CD2	2.94	0.41
1:G:75:TRP:HD1	1:G:113:PHE:HE2	1.68	0.41
1:C:75:TRP:HD1	1:C:113:PHE:HE2	1.68	0.41
1:E:203:LEU:C	1:E:203:LEU:CD2	2.94	0.41
1:H:177:LEU:HD22	1:H:184:ILE:CD1	2.51	0.41
1:A:158:ASN:HD22	1:A:159:GLY:N	2.17	0.41
1:B:135:LYS:HE3	1:B:275:LYS:HE2	2.02	0.41
1:D:187:HIS:O	1:D:246:PRO:HD2	2.20	0.41
1:F:180:PHE:O	1:F:181:ALA:C	2.63	0.41
1:H:64:GLU:O	1:H:129:LYS:HE2	2.21	0.41
1:A:172:TRP:CE2	1:B:116:LEU:HB2	2.56	0.41
1:H:72:VAL:HG21	2:H:301:DTP:O2A	2.21	0.41
1:B:276:ASN:N	1:B:276:ASN:HD22	2.17	0.40
1:C:180:PHE:O	1:C:181:ALA:C	2.63	0.40
1:E:75:TRP:HD1	1:E:113:PHE:HE2	1.68	0.40
1:E:158:ASN:HD22	1:E:159:GLY:N	2.17	0.40
1:A:177:LEU:HD22	1:A:184:ILE:CD1	2.51	0.40
1:G:64:GLU:O	1:G:129:LYS:HE2	2.21	0.40
1:A:187:HIS:O	1:A:246:PRO:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:VAL:HG21	2:C:301:DTP:O2A	2.21	0.40
1:D:180:PHE:O	1:D:181:ALA:C	2.63	0.40
1:E:70:GLU:HA	1:E:71:PRO:HD3	1.76	0.40
1:F:64:GLU:O	1:F:129:LYS:HE2	2.21	0.40
1:G:70:GLU:HB2	1:G:141:GLU:CB	2.45	0.40
1:H:203:LEU:C	1:H:203:LEU:CD2	2.94	0.40
1:B:75:TRP:HD1	1:B:113:PHE:CE2	2.40	0.40
1:C:64:GLU:O	1:C:129:LYS:HE2	2.21	0.40
1:C:177:LEU:HD22	1:C:184:ILE:CD1	2.51	0.40
1:F:233:LYS:HG3	1:G:232:HIS:HB3	2.04	0.40
1:H:128:GLU:HA	1:H:131:LEU:CG	2.52	0.40
1:D:46:ASN:OD1	1:D:47:ILE:N	2.48	0.40
1:D:177:LEU:HD22	1:D:184:ILE:CD1	2.51	0.40
1:D:203:LEU:C	1:D:203:LEU:CD2	2.94	0.40
1:E:177:LEU:HD22	1:E:184:ILE:CD1	2.51	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:CD	1:E:240:GLU:OE1[2_756]	0.72	1.48
1:C:135:LYS:CE	1:E:240:GLU:OE1[2_756]	0.83	1.37
1:C:135:LYS:CE	1:E:240:GLU:CD[2_756]	1.09	1.11
1:F:129:LYS:CB	1:G:63:PRO:CB[1_655]	1.21	0.99
1:B:131:LEU:CD2	1:H:275:LYS:NZ[1_565]	1.48	0.72
1:C:276:ASN:OD1	1:E:185:THR:CG2[2_756]	1.74	0.46
1:C:135:LYS:CD	1:E:240:GLU:CD[2_756]	1.81	0.39
1:F:129:LYS:CD	1:G:63:PRO:O[1_655]	1.85	0.35
1:D:178:TRP:NE1	1:G:134:ARG:NH1[2_656]	1.88	0.32
1:B:123:LEU:O	1:H:134:ARG:CD[1_565]	1.89	0.31
1:C:135:LYS:CE	1:E:240:GLU:OE2[2_756]	1.91	0.29
1:A:135:LYS:NZ	1:G:240:GLU:OE2[1_565]	1.97	0.23
1:C:135:LYS:CG	1:E:240:GLU:OE1[2_756]	1.98	0.22
1:C:135:LYS:NZ	1:E:240:GLU:OE1[2_756]	2.00	0.20
1:D:178:TRP:CD1	1:G:134:ARG:NH1[2_656]	2.05	0.15
1:F:129:LYS:CG	1:G:63:PRO:CB[1_655]	2.08	0.12
1:B:122:GLN:O	1:H:134:ARG:NH1[1_565]	2.15	0.05
1:E:101:ARG:NH2	1:G:92:LEU:CD1[2_656]	2.15	0.05
1:C:135:LYS:NZ	1:E:240:GLU:CD[2_756]	2.18	0.02
1:C:276:ASN:O	1:E:182:SER:CA[2_756]	2.19	0.01

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	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	B	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	C	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	D	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	E	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	F	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	G	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
1	H	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	6	23
All	All	1800/1928 (93%)	1624 (90%)	144 (8%)	32 (2%)	6	23

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	207	ALA
1	B	71	PRO
1	B	207	ALA
1	C	71	PRO
1	C	207	ALA
1	D	71	PRO
1	D	207	ALA
1	E	71	PRO
1	E	207	ALA
1	F	71	PRO
1	F	207	ALA
1	G	71	PRO
1	G	207	ALA
1	H	71	PRO
1	H	207	ALA
1	A	212	LYS

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Mol	Chain	Res	Type
1	A	255	ASP
1	B	212	LYS
1	B	255	ASP
1	C	212	LYS
1	C	255	ASP
1	D	212	LYS
1	D	255	ASP
1	E	212	LYS
1	E	255	ASP
1	F	212	LYS
1	F	255	ASP
1	G	212	LYS
1	G	255	ASP
1	H	212	LYS
1	H	255	ASP

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	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	B	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	C	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	D	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	E	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	F	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	G	209/216 (97%)	196 (94%)	13 (6%)	16	45
1	H	209/216 (97%)	196 (94%)	13 (6%)	16	45
All	All	1672/1728 (97%)	1568 (94%)	104 (6%)	16	45

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	95	LEU
1	A	99	MET
1	A	111	GLN
1	A	122	GLN
1	A	144	VAL
1	A	158	ASN
1	A	171	ASP
1	A	197	GLN
1	A	208	ARG
1	A	258	GLU
1	A	259	GLU
1	A	266	LEU
1	B	39	ARG
1	B	95	LEU
1	B	99	MET
1	B	111	GLN
1	B	122	GLN
1	B	144	VAL
1	B	158	ASN
1	B	171	ASP
1	B	197	GLN
1	B	208	ARG
1	B	258	GLU
1	B	259	GLU
1	B	266	LEU
1	C	39	ARG
1	C	95	LEU
1	C	99	MET
1	C	111	GLN
1	C	122	GLN
1	C	144	VAL
1	C	158	ASN
1	C	171	ASP
1	C	197	GLN
1	C	208	ARG
1	C	258	GLU
1	C	259	GLU
1	C	266	LEU
1	D	39	ARG
1	D	95	LEU
1	D	99	MET
1	D	111	GLN

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Mol	Chain	Res	Type
1	D	122	GLN
1	D	144	VAL
1	D	158	ASN
1	D	171	ASP
1	D	197	GLN
1	D	208	ARG
1	D	258	GLU
1	D	259	GLU
1	D	266	LEU
1	E	39	ARG
1	E	95	LEU
1	E	99	MET
1	E	111	GLN
1	E	122	GLN
1	E	144	VAL
1	E	158	ASN
1	E	171	ASP
1	E	197	GLN
1	E	208	ARG
1	E	258	GLU
1	E	259	GLU
1	E	266	LEU
1	F	39	ARG
1	F	95	LEU
1	F	99	MET
1	F	111	GLN
1	F	122	GLN
1	F	144	VAL
1	F	158	ASN
1	F	171	ASP
1	F	197	GLN
1	F	208	ARG
1	F	258	GLU
1	F	259	GLU
1	F	266	LEU
1	G	39	ARG
1	G	95	LEU
1	G	99	MET
1	G	111	GLN
1	G	122	GLN
1	G	144	VAL
1	G	158	ASN

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Mol	Chain	Res	Type
1	G	171	ASP
1	G	197	GLN
1	G	208	ARG
1	G	258	GLU
1	G	259	GLU
1	G	266	LEU
1	H	39	ARG
1	H	95	LEU
1	H	99	MET
1	H	111	GLN
1	H	122	GLN
1	H	144	VAL
1	H	158	ASN
1	H	171	ASP
1	H	197	GLN
1	H	208	ARG
1	H	258	GLU
1	H	259	GLU
1	H	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	77	ASN
1	A	158	ASN
1	A	187	HIS
1	A	221	GLN
1	A	223	HIS
1	A	271	ASN
1	A	276	ASN
1	B	76	GLN
1	B	77	ASN
1	B	158	ASN
1	B	187	HIS
1	B	221	GLN
1	B	223	HIS
1	B	271	ASN
1	B	276	ASN
1	C	76	GLN
1	C	77	ASN
1	C	158	ASN

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Mol	Chain	Res	Type
1	C	187	HIS
1	C	221	GLN
1	C	223	HIS
1	C	271	ASN
1	C	276	ASN
1	D	76	GLN
1	D	77	ASN
1	D	158	ASN
1	D	187	HIS
1	D	221	GLN
1	D	223	HIS
1	D	271	ASN
1	D	276	ASN
1	E	76	GLN
1	E	77	ASN
1	E	158	ASN
1	E	187	HIS
1	E	221	GLN
1	E	223	HIS
1	E	271	ASN
1	E	276	ASN
1	F	76	GLN
1	F	77	ASN
1	F	158	ASN
1	F	187	HIS
1	F	221	GLN
1	F	223	HIS
1	F	271	ASN
1	F	276	ASN
1	G	76	GLN
1	G	77	ASN
1	G	158	ASN
1	G	187	HIS
1	G	221	GLN
1	G	223	HIS
1	G	271	ASN
1	G	276	ASN
1	H	76	GLN
1	H	77	ASN
1	H	158	ASN
1	H	187	HIS
1	H	221	GLN

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Mol	Chain	Res	Type
1	H	223	HIS
1	H	271	ASN
1	H	276	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	DTP	E	301	-	31,32,32	1.02	1 (3%)	46,50,50	2.08	14 (30%)
2	DTP	H	301	-	31,32,32	0.94	1 (3%)	46,50,50	2.02	12 (26%)
2	DTP	D	301	-	31,32,32	1.05	1 (3%)	46,50,50	2.08	13 (28%)
2	DTP	G	301	-	31,32,32	0.94	0	46,50,50	2.08	12 (26%)
2	DTP	F	301	-	31,32,32	0.97	1 (3%)	46,50,50	2.10	13 (28%)
2	DTP	A	301	-	31,32,32	0.97	1 (3%)	46,50,50	1.98	12 (26%)
2	DTP	B	301	-	31,32,32	0.98	1 (3%)	46,50,50	2.01	12 (26%)
2	DTP	C	301	-	31,32,32	0.91	1 (3%)	46,50,50	2.11	14 (30%)

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	DTP	E	301	-	-	6/22/34/34	0/3/3/3
2	DTP	H	301	-	-	6/22/34/34	0/3/3/3
2	DTP	D	301	-	-	6/22/34/34	0/3/3/3
2	DTP	G	301	-	-	6/22/34/34	0/3/3/3
2	DTP	F	301	-	-	6/22/34/34	0/3/3/3
2	DTP	A	301	-	-	6/22/34/34	0/3/3/3
2	DTP	B	301	-	-	6/22/34/34	0/3/3/3
2	DTP	C	301	-	-	6/22/34/34	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	DTP	PB-O3A	-3.07	1.56	1.59
2	E	301	DTP	PB-O3A	-2.93	1.56	1.59
2	B	301	DTP	PB-O3A	-2.91	1.56	1.59
2	A	301	DTP	PB-O3A	-2.71	1.56	1.59
2	F	301	DTP	PB-O3A	-2.71	1.56	1.59
2	C	301	DTP	PB-O3A	-2.40	1.56	1.59
2	H	301	DTP	C5-N7	-2.02	1.35	1.39

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	DTP	N3-C2-N1	-5.28	120.58	128.58
2	G	301	DTP	N3-C2-N1	-5.15	120.79	128.58
2	H	301	DTP	C5-C4-N3	-5.14	119.64	126.72
2	D	301	DTP	C5-C4-N3	-5.13	119.65	126.72
2	E	301	DTP	C5-C4-N3	-5.10	119.69	126.72
2	H	301	DTP	N3-C2-N1	-5.10	120.86	128.58
2	D	301	DTP	N3-C2-N1	-5.08	120.89	128.58
2	C	301	DTP	C5-C4-N3	-5.03	119.80	126.72
2	G	301	DTP	C5-C4-N3	-5.02	119.80	126.72
2	C	301	DTP	N3-C2-N1	-5.02	120.98	128.58
2	B	301	DTP	N3-C2-N1	-4.97	121.06	128.58
2	F	301	DTP	C5-C4-N3	-4.89	119.99	126.72
2	B	301	DTP	C5-C4-N3	-4.86	120.03	126.72
2	A	301	DTP	N3-C2-N1	-4.78	121.35	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	DTP	N3-C2-N1	-4.77	121.36	128.58
2	A	301	DTP	C5-C4-N3	-4.73	120.20	126.72
2	E	301	DTP	C5'-C4'-C3'	-4.49	89.54	114.64
2	C	301	DTP	N3-C4-N9	4.40	134.66	127.17
2	G	301	DTP	C5'-C4'-C3'	-4.36	90.26	114.64
2	F	301	DTP	N3-C4-N9	4.35	134.57	127.17
2	B	301	DTP	C5'-C4'-C3'	-4.34	90.35	114.64
2	F	301	DTP	C5'-C4'-C3'	-4.30	90.60	114.64
2	A	301	DTP	C5'-C4'-C3'	-4.28	90.69	114.64
2	D	301	DTP	N3-C4-N9	4.28	134.44	127.17
2	D	301	DTP	C5'-C4'-C3'	-4.28	90.72	114.64
2	E	301	DTP	N3-C4-N9	4.27	134.43	127.17
2	C	301	DTP	C5'-C4'-C3'	-4.19	91.19	114.64
2	H	301	DTP	C5'-C4'-C3'	-4.18	91.28	114.64
2	H	301	DTP	N3-C4-N9	4.15	134.22	127.17
2	G	301	DTP	N3-C4-N9	4.14	134.20	127.17
2	H	301	DTP	C2-N3-C4	4.04	121.69	111.83
2	F	301	DTP	C2-N3-C4	3.98	121.54	111.83
2	D	301	DTP	C2-N3-C4	3.94	121.46	111.83
2	A	301	DTP	N3-C4-N9	3.90	133.80	127.17
2	C	301	DTP	C2-N3-C4	3.84	121.21	111.83
2	G	301	DTP	C2-N3-C4	3.83	121.19	111.83
2	B	301	DTP	N3-C4-N9	3.83	133.68	127.17
2	B	301	DTP	C2-N3-C4	3.82	121.17	111.83
2	E	301	DTP	C2-N3-C4	3.78	121.07	111.83
2	G	301	DTP	C5-N7-C8	3.73	109.32	103.45
2	C	301	DTP	C5-N7-C8	3.71	109.28	103.45
2	A	301	DTP	C2-N3-C4	3.64	120.71	111.83
2	E	301	DTP	C5-N7-C8	3.62	109.13	103.45
2	D	301	DTP	C5-N7-C8	3.53	108.99	103.45
2	B	301	DTP	C5-N7-C8	3.47	108.90	103.45
2	F	301	DTP	C5-N7-C8	3.36	108.72	103.45
2	G	301	DTP	N9-C8-N7	-3.25	109.32	113.94
2	F	301	DTP	O5'-C5'-C4'	3.24	120.03	108.99
2	A	301	DTP	C5-N7-C8	3.15	108.39	103.45
2	G	301	DTP	O5'-C5'-C4'	3.13	119.64	108.99
2	H	301	DTP	C5-N7-C8	3.12	108.36	103.45
2	A	301	DTP	O5'-C5'-C4'	3.12	119.62	108.99
2	E	301	DTP	N9-C8-N7	-3.09	109.55	113.94
2	C	301	DTP	O5'-C5'-C4'	3.08	119.47	108.99
2	C	301	DTP	N9-C8-N7	-3.07	109.58	113.94
2	B	301	DTP	O5'-C5'-C4'	3.07	119.44	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	DTP	O5'-C5'-C4'	3.05	119.37	108.99
2	E	301	DTP	O5'-C5'-C4'	2.97	119.10	108.99
2	D	301	DTP	O5'-C5'-C4'	2.96	119.09	108.99
2	D	301	DTP	N9-C8-N7	-2.90	109.82	113.94
2	A	301	DTP	O2B-PB-O3B	2.79	114.82	107.27
2	G	301	DTP	C4-C5-N7	-2.75	107.44	110.58
2	B	301	DTP	O2A-PA-O3A	2.72	114.62	107.27
2	F	301	DTP	O2A-PA-O3A	2.70	114.56	107.27
2	B	301	DTP	N9-C8-N7	-2.68	110.14	113.94
2	B	301	DTP	C4-C5-N7	-2.63	107.58	110.58
2	F	301	DTP	N9-C8-N7	-2.62	110.22	113.94
2	A	301	DTP	N9-C8-N7	-2.61	110.23	113.94
2	C	301	DTP	C4-C5-N7	-2.59	107.62	110.58
2	C	301	DTP	O2B-PB-O3B	2.56	114.18	107.27
2	D	301	DTP	C4-C5-N7	-2.56	107.66	110.58
2	E	301	DTP	C4-C5-N7	-2.54	107.68	110.58
2	H	301	DTP	O2A-PA-O3A	2.51	114.06	107.27
2	E	301	DTP	O2B-PB-O3B	2.45	113.89	107.27
2	F	301	DTP	O2B-PB-O3B	2.43	113.84	107.27
2	D	301	DTP	O2A-PA-O3A	2.41	113.78	107.27
2	H	301	DTP	O2B-PB-O3B	2.38	113.72	107.27
2	D	301	DTP	O2B-PB-O3B	2.38	113.71	107.27
2	G	301	DTP	O2A-PA-O3A	2.38	113.70	107.27
2	G	301	DTP	O2B-PB-O3B	2.37	113.68	107.27
2	H	301	DTP	N9-C8-N7	-2.37	110.57	113.94
2	C	301	DTP	O2A-PA-O3A	2.37	113.67	107.27
2	E	301	DTP	O2A-PA-O3A	2.36	113.66	107.27
2	A	301	DTP	O2A-PA-O3A	2.35	113.64	107.27
2	C	301	DTP	O3'-C3'-C2'	2.27	118.78	110.88
2	H	301	DTP	C4-C5-N7	-2.24	108.02	110.58
2	A	301	DTP	C4-C5-N7	-2.22	108.04	110.58
2	F	301	DTP	C4-C5-N7	-2.21	108.05	110.58
2	A	301	DTP	O3'-C3'-C2'	2.16	118.39	110.88
2	E	301	DTP	O3'-C3'-C2'	2.16	118.39	110.88
2	B	301	DTP	O2B-PB-O3B	2.16	113.11	107.27
2	C	301	DTP	C4-N9-C8	2.12	107.97	105.74
2	E	301	DTP	O4'-C1'-N9	2.08	111.71	107.96
2	B	301	DTP	O3'-C3'-C2'	2.08	118.11	110.88
2	G	301	DTP	C4-N9-C8	2.07	107.92	105.74
2	F	301	DTP	O4'-C1'-N9	2.05	111.65	107.96
2	C	301	DTP	O3G-PG-O3B	2.05	111.52	104.64
2	F	301	DTP	O4'-C1'-C2'	2.03	110.04	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	DTP	O3A-PB-O1B	-2.01	104.66	110.70
2	D	301	DTP	O3'-C3'-C2'	2.01	117.86	110.88
2	H	301	DTP	O3'-C3'-C2'	2.01	117.84	110.88
2	D	301	DTP	O3A-PB-O1B	-2.00	104.69	110.70

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	DTP	PB-O3B-PG-O2G
2	A	301	DTP	C5'-O5'-PA-O1A
2	A	301	DTP	C5'-O5'-PA-O2A
2	B	301	DTP	PB-O3B-PG-O2G
2	B	301	DTP	PB-O3B-PG-O3G
2	B	301	DTP	C5'-O5'-PA-O1A
2	B	301	DTP	C5'-O5'-PA-O2A
2	C	301	DTP	PB-O3B-PG-O2G
2	C	301	DTP	PB-O3B-PG-O3G
2	C	301	DTP	C5'-O5'-PA-O1A
2	C	301	DTP	C5'-O5'-PA-O2A
2	D	301	DTP	PB-O3B-PG-O3G
2	D	301	DTP	C5'-O5'-PA-O1A
2	D	301	DTP	C5'-O5'-PA-O2A
2	E	301	DTP	C5'-O5'-PA-O1A
2	E	301	DTP	C5'-O5'-PA-O2A
2	F	301	DTP	C5'-O5'-PA-O1A
2	F	301	DTP	C5'-O5'-PA-O2A
2	G	301	DTP	PB-O3B-PG-O2G
2	G	301	DTP	PB-O3B-PG-O3G
2	G	301	DTP	C5'-O5'-PA-O1A
2	G	301	DTP	C5'-O5'-PA-O2A
2	H	301	DTP	PB-O3B-PG-O2G
2	H	301	DTP	C5'-O5'-PA-O1A
2	H	301	DTP	C5'-O5'-PA-O2A
2	A	301	DTP	PB-O3B-PG-O3G
2	D	301	DTP	PB-O3B-PG-O2G
2	E	301	DTP	PB-O3B-PG-O2G
2	E	301	DTP	PB-O3B-PG-O3G
2	F	301	DTP	PB-O3B-PG-O2G
2	F	301	DTP	PB-O3B-PG-O3G
2	H	301	DTP	PB-O3B-PG-O3G
2	A	301	DTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	B	301	DTP	C5'-O5'-PA-O3A
2	C	301	DTP	C5'-O5'-PA-O3A
2	D	301	DTP	C5'-O5'-PA-O3A
2	E	301	DTP	C5'-O5'-PA-O3A
2	F	301	DTP	C5'-O5'-PA-O3A
2	G	301	DTP	C5'-O5'-PA-O3A
2	H	301	DTP	C5'-O5'-PA-O3A
2	A	301	DTP	PA-O3A-PB-O1B
2	C	301	DTP	PA-O3A-PB-O1B
2	D	301	DTP	PA-O3A-PB-O1B
2	E	301	DTP	PA-O3A-PB-O1B
2	F	301	DTP	PA-O3A-PB-O1B
2	G	301	DTP	PA-O3A-PB-O1B
2	H	301	DTP	PA-O3A-PB-O1B
2	B	301	DTP	PA-O3A-PB-O1B

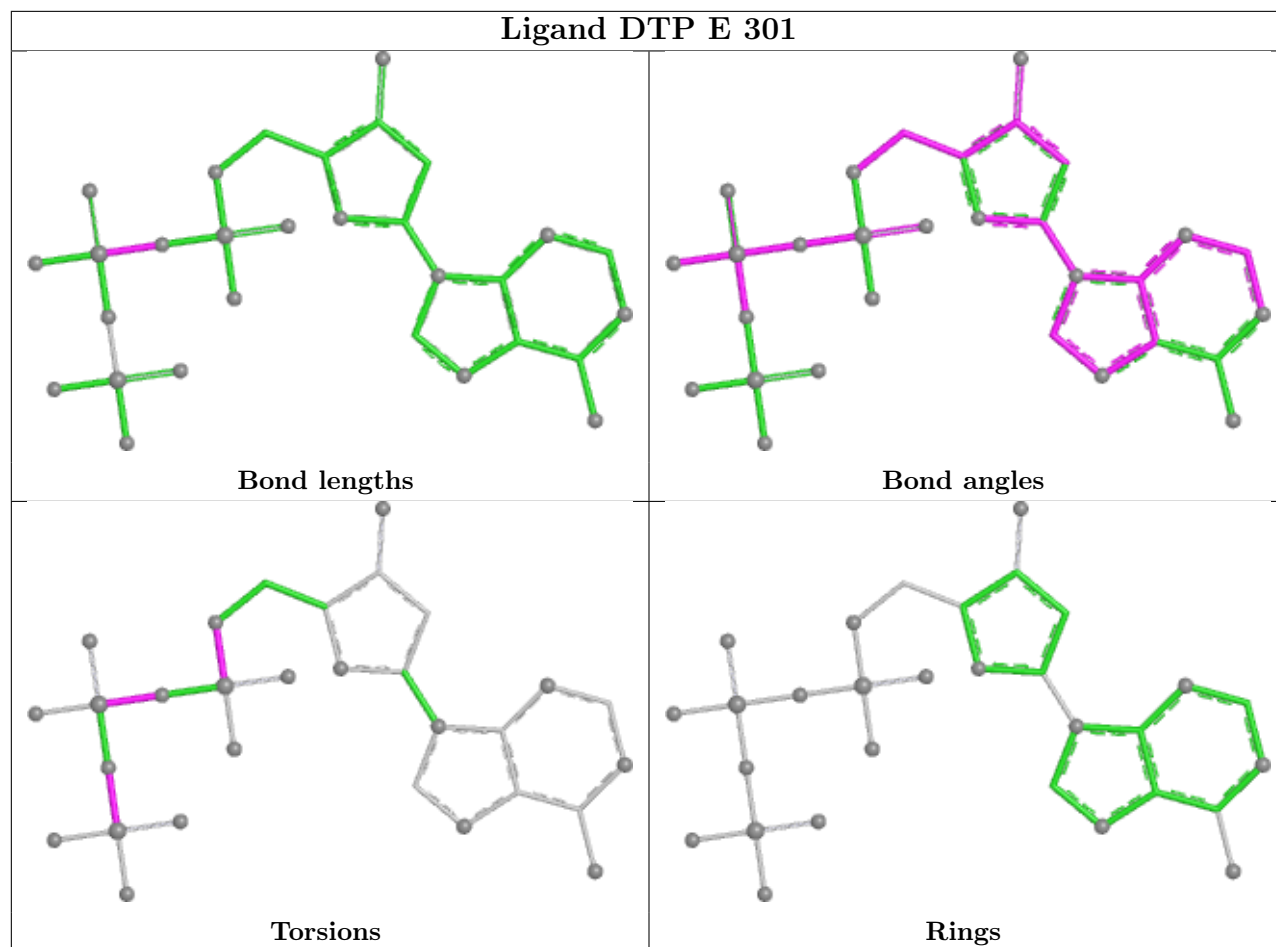
There are no ring outliers.

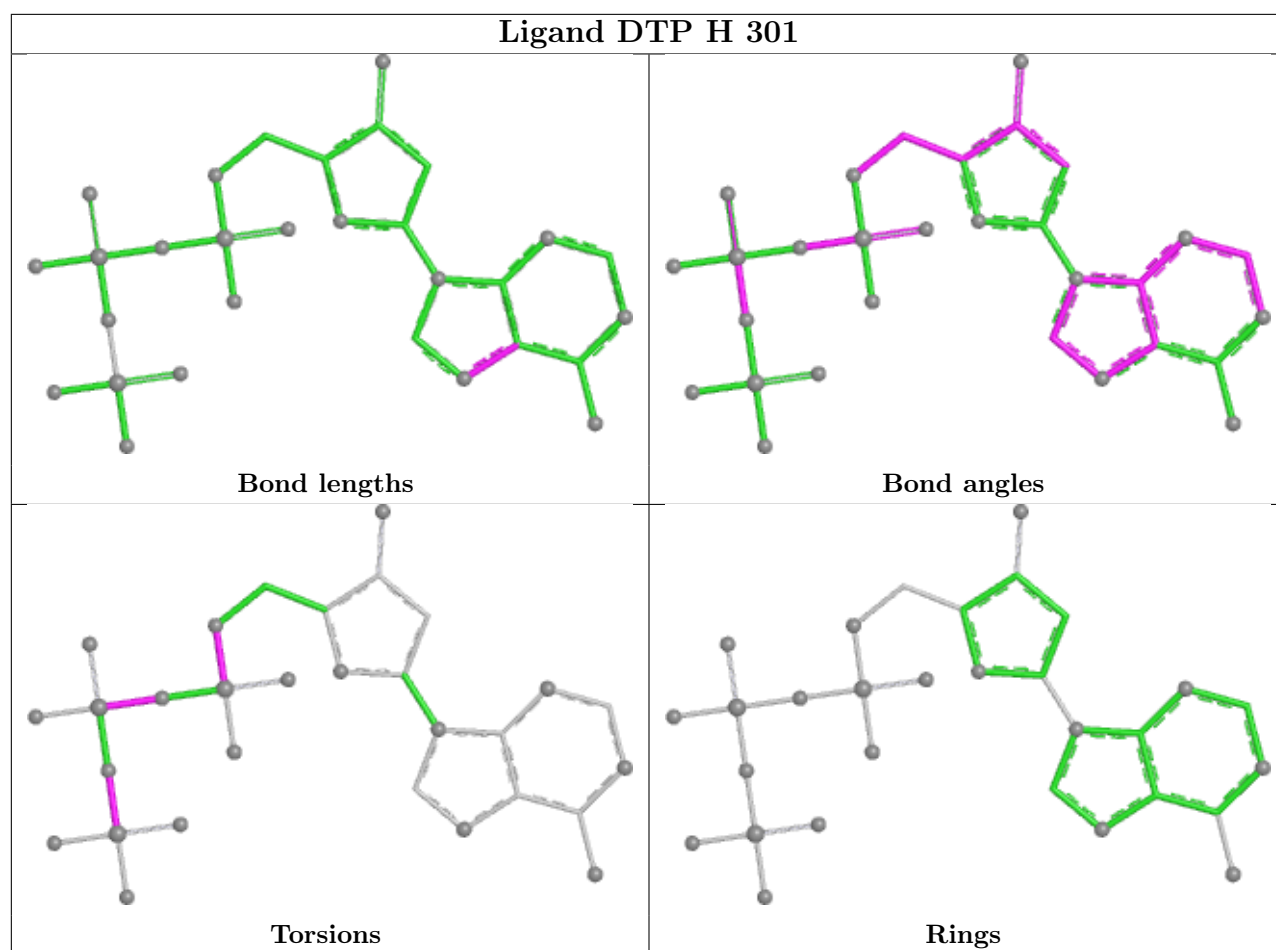
8 monomers are involved in 17 short contacts:

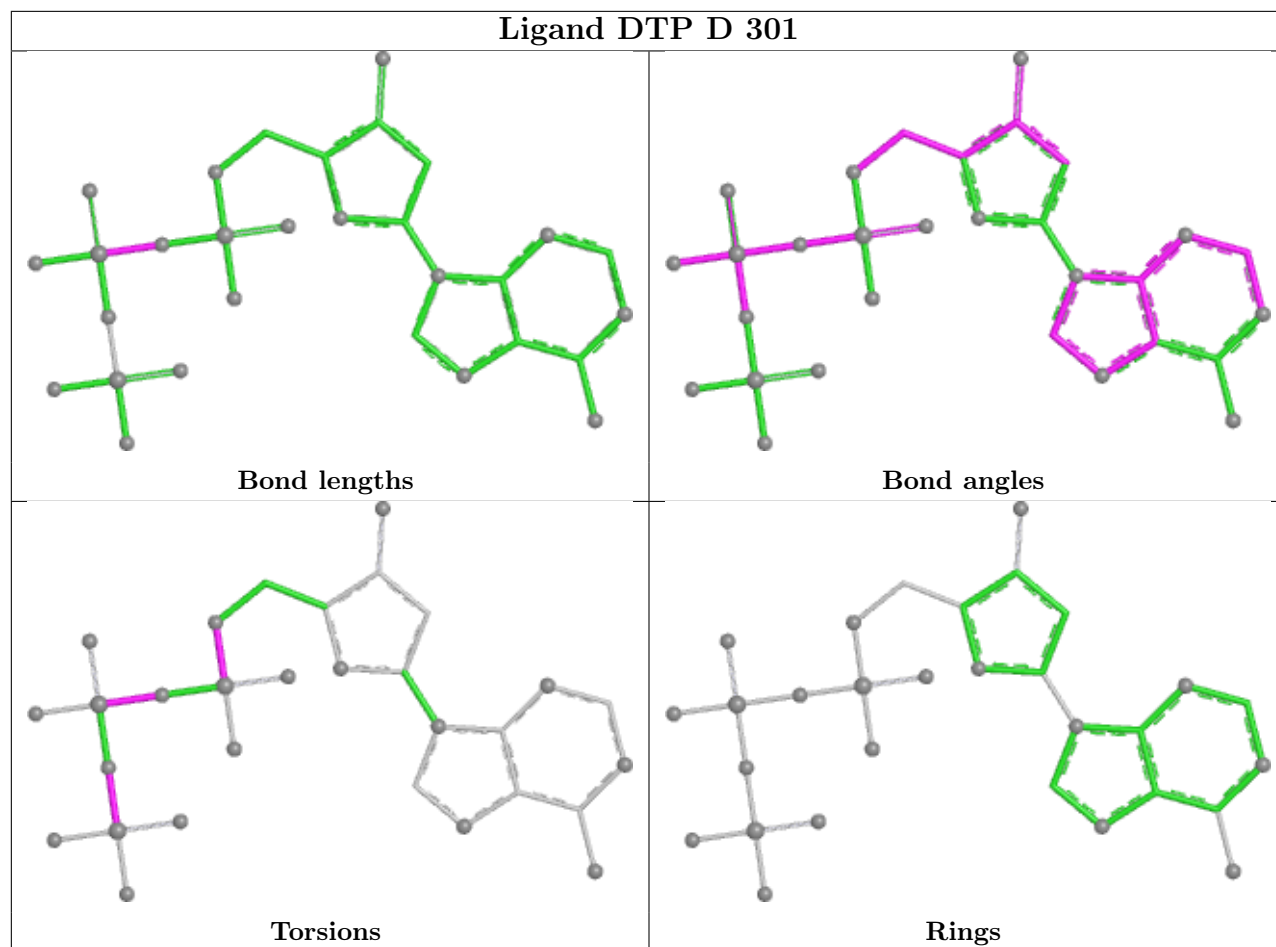
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	DTP	1	0
2	H	301	DTP	3	0
2	D	301	DTP	2	0
2	G	301	DTP	3	0
2	F	301	DTP	2	0
2	A	301	DTP	1	0
2	B	301	DTP	3	0
2	C	301	DTP	2	0

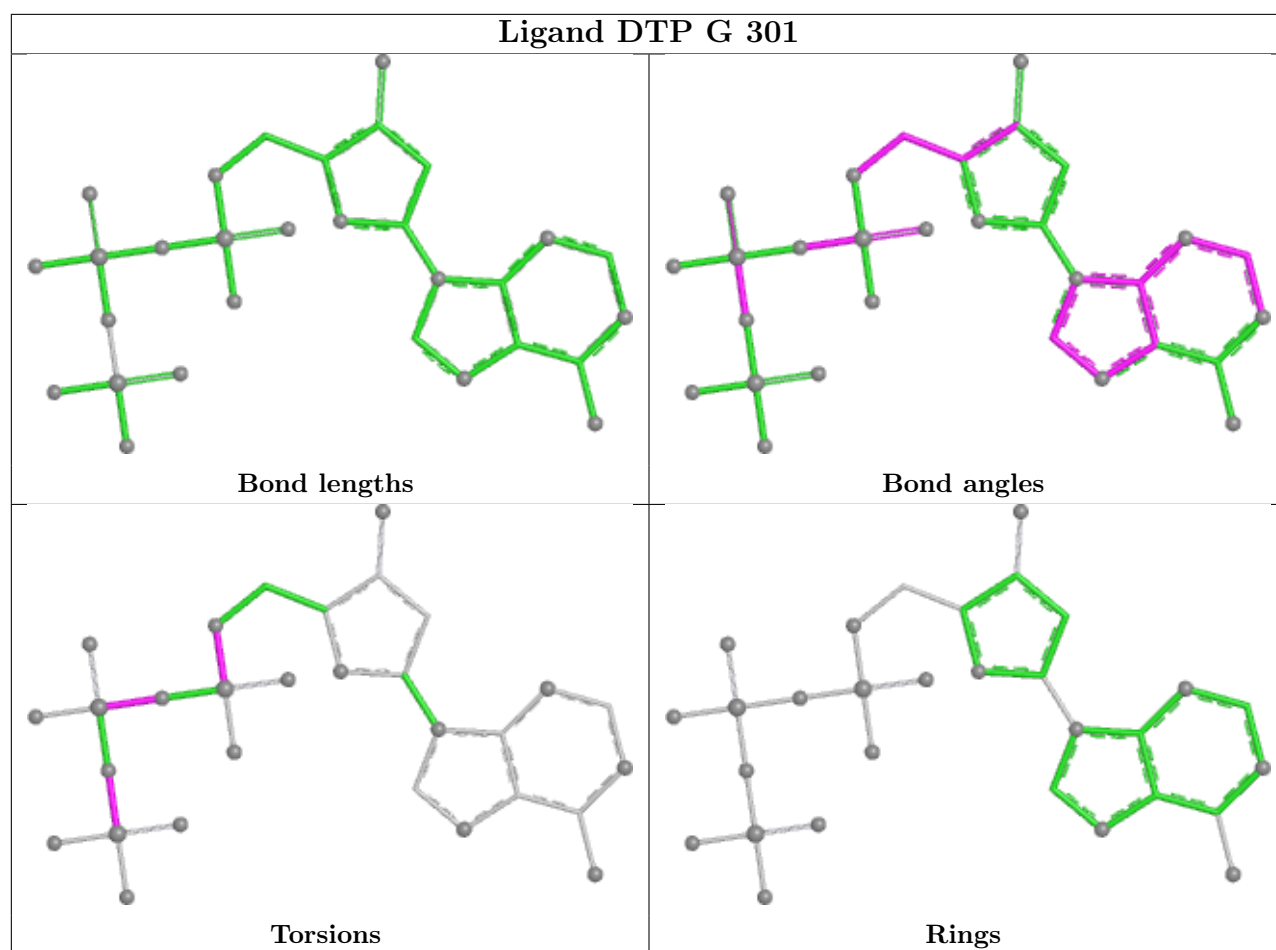
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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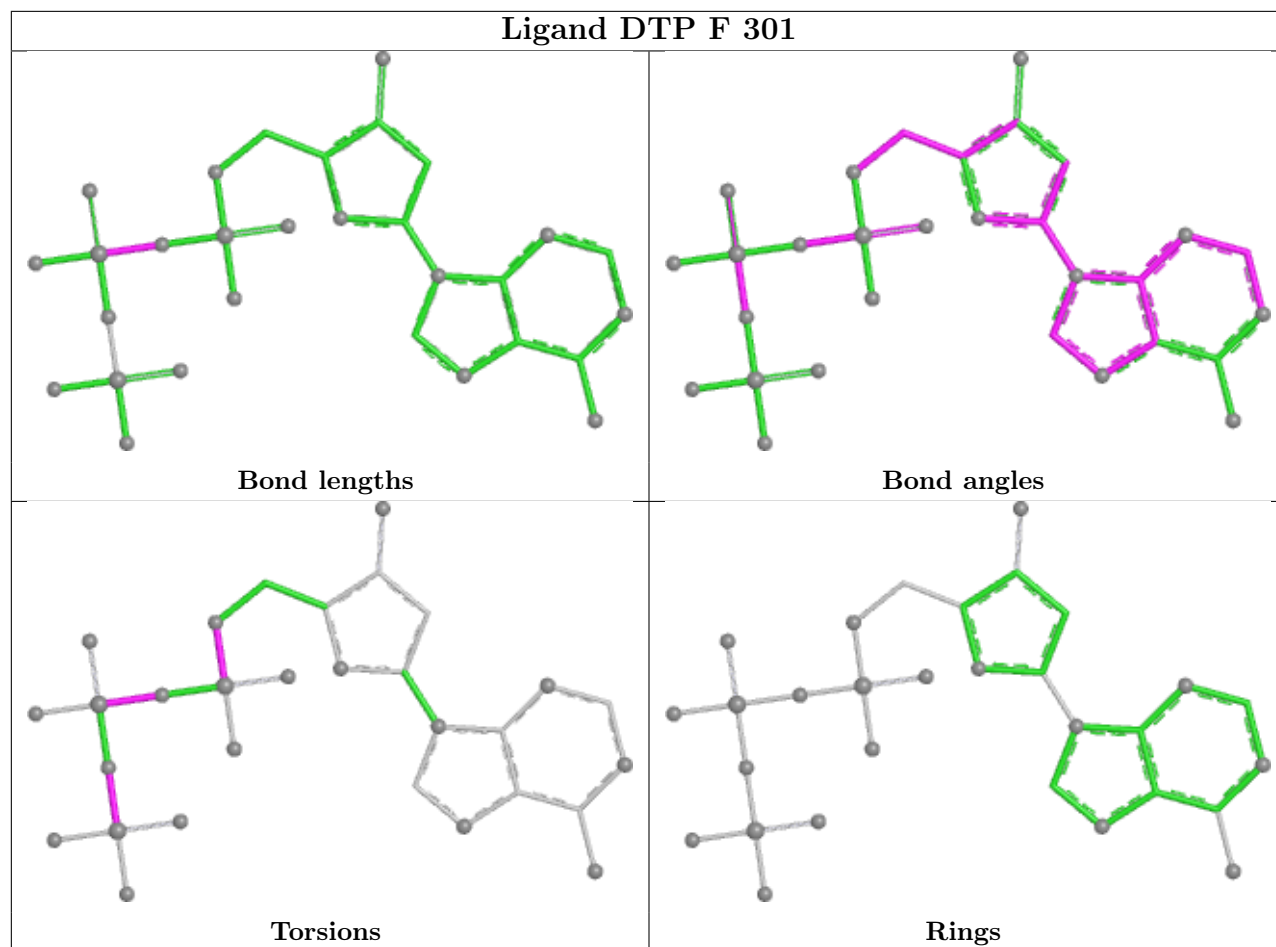


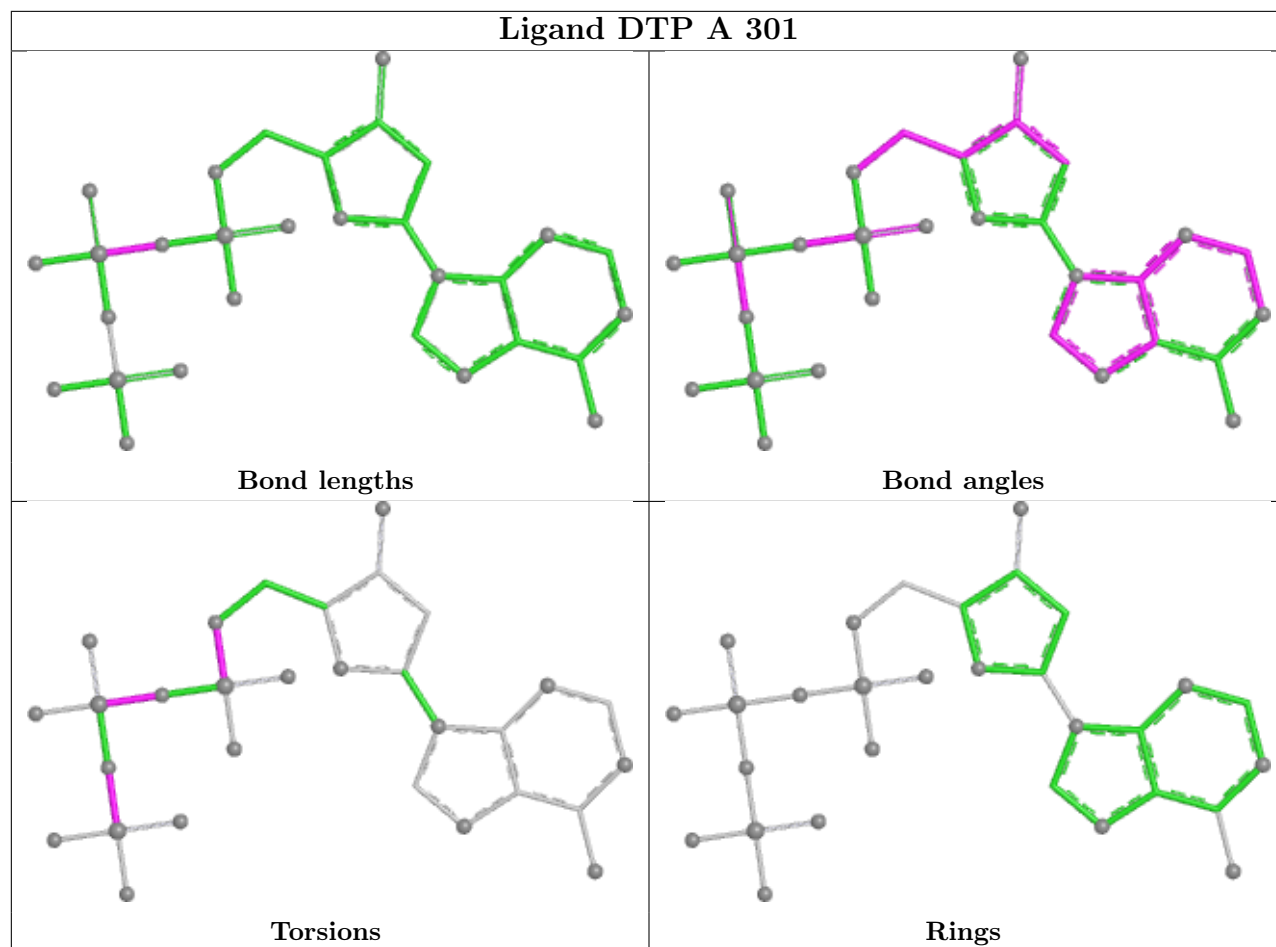


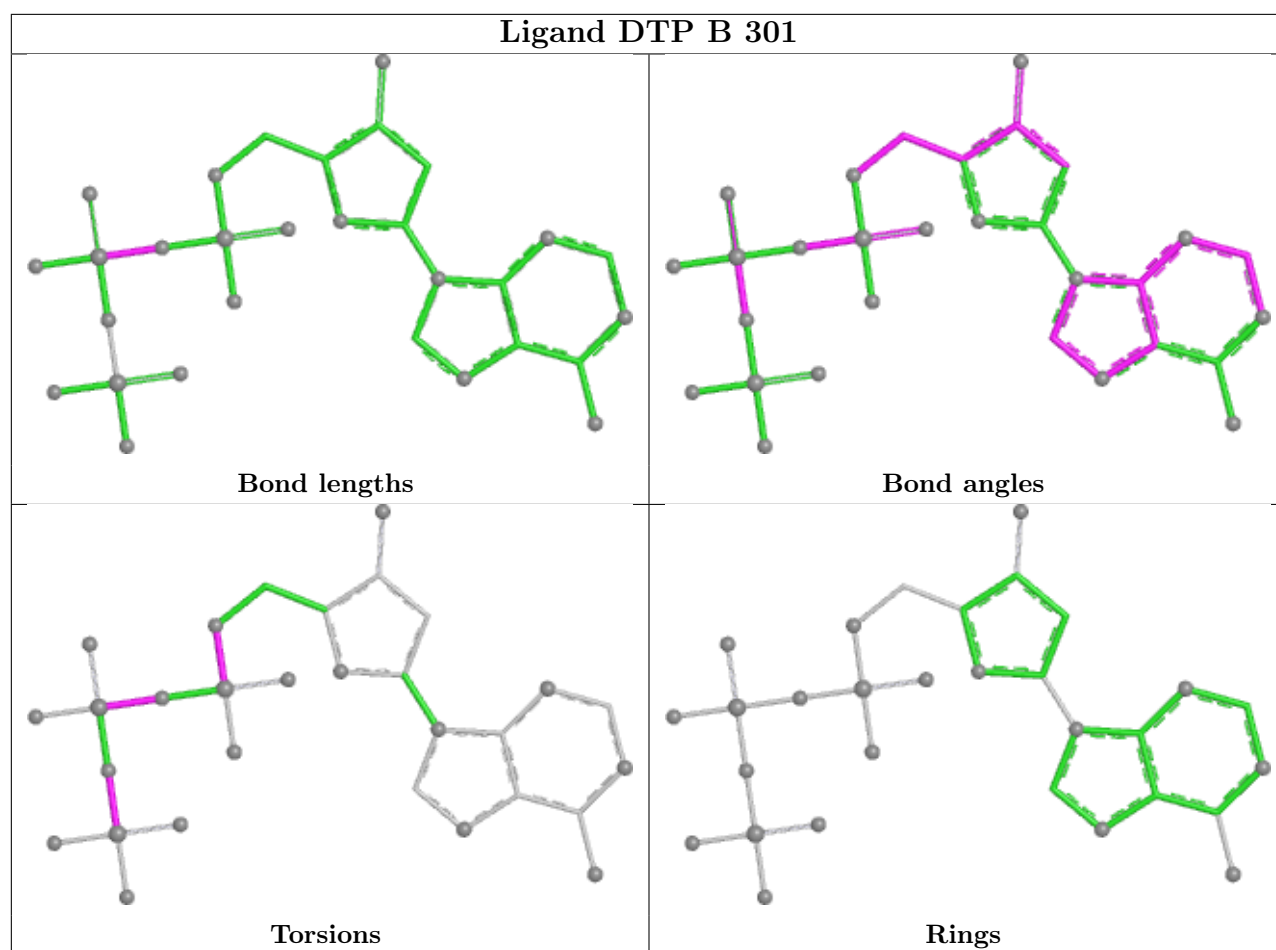


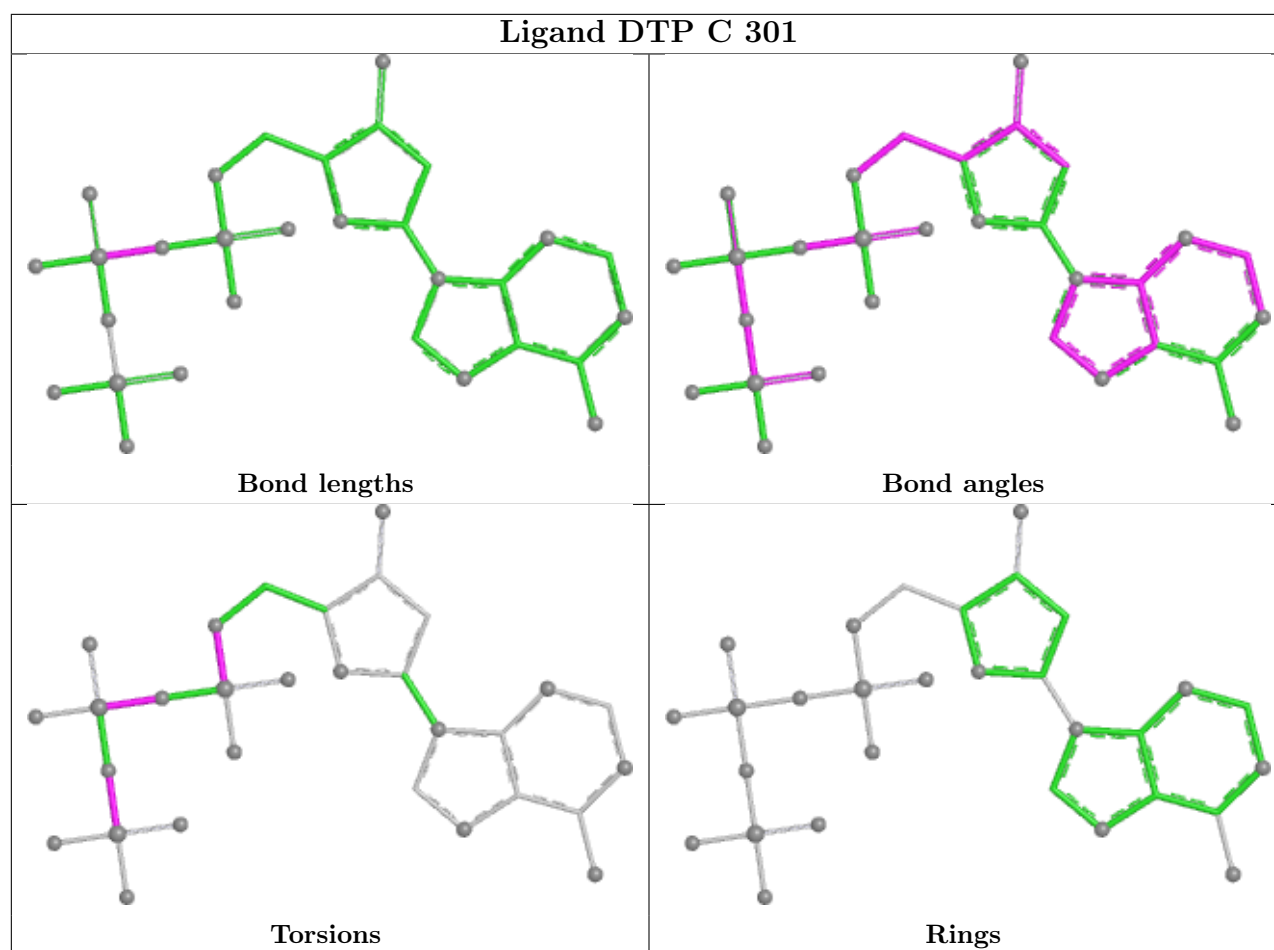


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5.7 Other polymers [i](#)

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	229/241 (95%)	0.82	23 (10%) 12 9	17, 39, 92, 113	0
1	B	229/241 (95%)	0.79	24 (10%) 11 8	16, 41, 85, 104	0
1	C	229/241 (95%)	0.76	27 (11%) 9 7	12, 31, 81, 95	0
1	D	229/241 (95%)	0.68	30 (13%) 7 6	10, 29, 70, 103	0
1	E	229/241 (95%)	0.93	28 (12%) 8 6	19, 44, 91, 109	0
1	F	229/241 (95%)	1.02	37 (16%) 4 4	16, 36, 76, 120	0
1	G	229/241 (95%)	0.82	29 (12%) 8 6	19, 39, 75, 107	0
1	H	229/241 (95%)	1.12	40 (17%) 4 3	20, 46, 90, 107	0
All	All	1832/1928 (95%)	0.87	238 (12%) 7 6	10, 38, 87, 120	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	72	VAL	8.1
1	H	131	LEU	8.0
1	H	133	ALA	7.4
1	F	75	TRP	7.3
1	F	128	GLU	7.2
1	F	129	LYS	6.9
1	F	132	GLN	6.9
1	F	37	GLY	6.8
1	D	244	ASN	6.6
1	F	131	LEU	6.3
1	H	37	GLY	5.8
1	C	130	LEU	5.8
1	H	134	ARG	5.7
1	H	135	LYS	5.5
1	F	69	THR	5.5
1	G	75	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	75	TRP	5.4
1	F	73	ALA	5.4
1	A	75	TRP	5.1
1	H	72	VAL	5.0
1	G	72	VAL	5.0
1	F	126	PHE	5.0
1	G	78	ILE	4.9
1	D	204	TYR	4.8
1	G	132	GLN	4.8
1	G	71	PRO	4.8
1	E	72	VAL	4.7
1	A	78	ILE	4.6
1	H	132	GLN	4.6
1	F	204	TYR	4.6
1	G	128	GLU	4.6
1	D	75	TRP	4.4
1	H	130	LEU	4.4
1	F	74	THR	4.4
1	G	69	THR	4.3
1	H	75	TRP	4.3
1	D	69	THR	4.3
1	G	64	GLU	4.3
1	H	69	THR	4.2
1	E	75	TRP	4.1
1	F	130	LEU	4.1
1	A	72	VAL	4.1
1	A	92	LEU	4.1
1	F	77	ASN	4.0
1	F	78	ILE	4.0
1	B	64	GLU	3.9
1	C	78	ILE	3.9
1	H	204	TYR	3.8
1	B	72	VAL	3.8
1	A	70	GLU	3.8
1	F	70	GLU	3.8
1	A	130	LEU	3.7
1	G	134	ARG	3.7
1	A	212	LYS	3.6
1	C	69	THR	3.6
1	A	76	GLN	3.6
1	E	76	GLN	3.6
1	H	78	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	79	GLN	3.6
1	H	65	TRP	3.6
1	A	204	TYR	3.6
1	E	135	LYS	3.5
1	E	256	PHE	3.5
1	G	70	GLU	3.5
1	A	74	THR	3.5
1	H	126	PHE	3.4
1	C	70	GLU	3.4
1	E	70	GLU	3.4
1	D	72	VAL	3.4
1	H	128	GLU	3.4
1	G	133	ALA	3.4
1	D	74	THR	3.4
1	E	240	GLU	3.4
1	C	131	LEU	3.3
1	D	78	ILE	3.3
1	H	73	ALA	3.3
1	G	129	LYS	3.2
1	E	68	ALA	3.2
1	A	93	GLY	3.2
1	B	69	THR	3.2
1	C	204	TYR	3.2
1	G	76	GLN	3.2
1	C	75	TRP	3.2
1	F	64	GLU	3.2
1	F	63	PRO	3.1
1	F	127	PRO	3.1
1	F	68	ALA	3.1
1	F	71	PRO	3.1
1	B	131	LEU	3.1
1	E	131	LEU	3.1
1	H	129	LYS	3.1
1	D	232	HIS	3.0
1	B	73	ALA	3.0
1	C	72	VAL	3.0
1	B	130	LEU	3.0
1	C	129	LYS	3.0
1	E	204	TYR	3.0
1	D	70	GLU	3.0
1	H	212	LYS	2.9
1	A	79	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	78	ILE	2.9
1	B	71	PRO	2.9
1	D	128	GLU	2.9
1	F	67	VAL	2.9
1	G	74	THR	2.8
1	D	77	ASN	2.8
1	H	77	ASN	2.8
1	E	130	LEU	2.8
1	E	178	TRP	2.8
1	E	78	ILE	2.8
1	H	276	ASN	2.8
1	D	233	LYS	2.7
1	C	64	GLU	2.7
1	H	242	LEU	2.7
1	E	69	THR	2.7
1	B	213	GLY	2.7
1	C	37	GLY	2.7
1	D	182	SER	2.7
1	F	76	GLN	2.7
1	E	67	VAL	2.7
1	H	277	LEU	2.7
1	F	134	ARG	2.7
1	B	128	GLU	2.7
1	C	79	GLN	2.7
1	E	259	GLU	2.7
1	F	133	ALA	2.6
1	F	66	HIS	2.6
1	F	135	LYS	2.6
1	G	259	GLU	2.6
1	C	73	ALA	2.6
1	A	77	ASN	2.6
1	B	197	GLN	2.6
1	D	132	GLN	2.6
1	D	255	ASP	2.6
1	B	207	ALA	2.6
1	D	172	TRP	2.6
1	F	79	GLN	2.6
1	F	255	ASP	2.6
1	D	134	ARG	2.6
1	G	178	TRP	2.6
1	B	67	VAL	2.6
1	H	70	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	131	LEU	2.5
1	A	69	THR	2.5
1	C	68	ALA	2.5
1	G	73	ALA	2.5
1	A	208	ARG	2.5
1	B	277	LEU	2.5
1	A	71	PRO	2.5
1	H	63	PRO	2.5
1	B	70	GLU	2.5
1	H	244	ASN	2.5
1	B	261	THR	2.5
1	H	66	HIS	2.5
1	G	135	LYS	2.4
1	A	261	THR	2.4
1	C	261	THR	2.4
1	E	128	GLU	2.4
1	F	212	LYS	2.4
1	H	62	TYR	2.4
1	D	235	THR	2.4
1	G	261	THR	2.4
1	E	247	VAL	2.4
1	C	76	GLN	2.4
1	C	74	THR	2.4
1	D	245	ILE	2.4
1	C	71	PRO	2.4
1	E	64	GLU	2.4
1	A	73	ALA	2.4
1	H	68	ALA	2.4
1	G	197	GLN	2.4
1	D	234	THR	2.4
1	H	272	THR	2.4
1	A	265	ASP	2.3
1	C	133	ALA	2.3
1	D	181	ALA	2.3
1	B	66	HIS	2.3
1	F	242	LEU	2.3
1	D	73	ALA	2.3
1	F	257	SER	2.3
1	E	59	THR	2.3
1	G	260	VAL	2.3
1	H	93	GLY	2.3
1	D	133	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	241	ALA	2.3
1	B	60	LYS	2.3
1	E	77	ASN	2.3
1	E	132	GLN	2.3
1	E	261	THR	2.3
1	B	127	PRO	2.3
1	B	79	GLN	2.2
1	C	197	GLN	2.2
1	D	76	GLN	2.2
1	G	52	SER	2.2
1	A	253	ASN	2.2
1	C	135	LYS	2.2
1	G	92	LEU	2.2
1	A	67	VAL	2.2
1	D	122	GLN	2.2
1	E	134	ARG	2.2
1	C	136	PRO	2.2
1	E	243	MET	2.2
1	C	212	LYS	2.2
1	D	259	GLU	2.2
1	E	207	ALA	2.2
1	H	64	GLU	2.2
1	H	61	THR	2.2
1	F	233	LYS	2.2
1	F	275	LYS	2.2
1	B	126	PHE	2.2
1	H	241	ALA	2.2
1	F	38	PRO	2.1
1	H	255	ASP	2.1
1	H	213	GLY	2.1
1	H	261	THR	2.1
1	D	257	SER	2.1
1	C	268	ARG	2.1
1	G	258	GLU	2.1
1	H	71	PRO	2.1
1	D	212	LYS	2.1
1	D	93	GLY	2.1
1	C	132	GLN	2.1
1	C	260	VAL	2.1
1	B	68	ALA	2.1
1	C	59	THR	2.1
1	A	207	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	258	GLU	2.1
1	E	62	TYR	2.1
1	H	205	GLN	2.0
1	F	92	LEU	2.0
1	G	277	LEU	2.0
1	A	255	ASP	2.0
1	B	275	LYS	2.0
1	G	233	LYS	2.0
1	E	246	PRO	2.0
1	G	244	ASN	2.0
1	H	113	PHE	2.0
1	H	252	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.

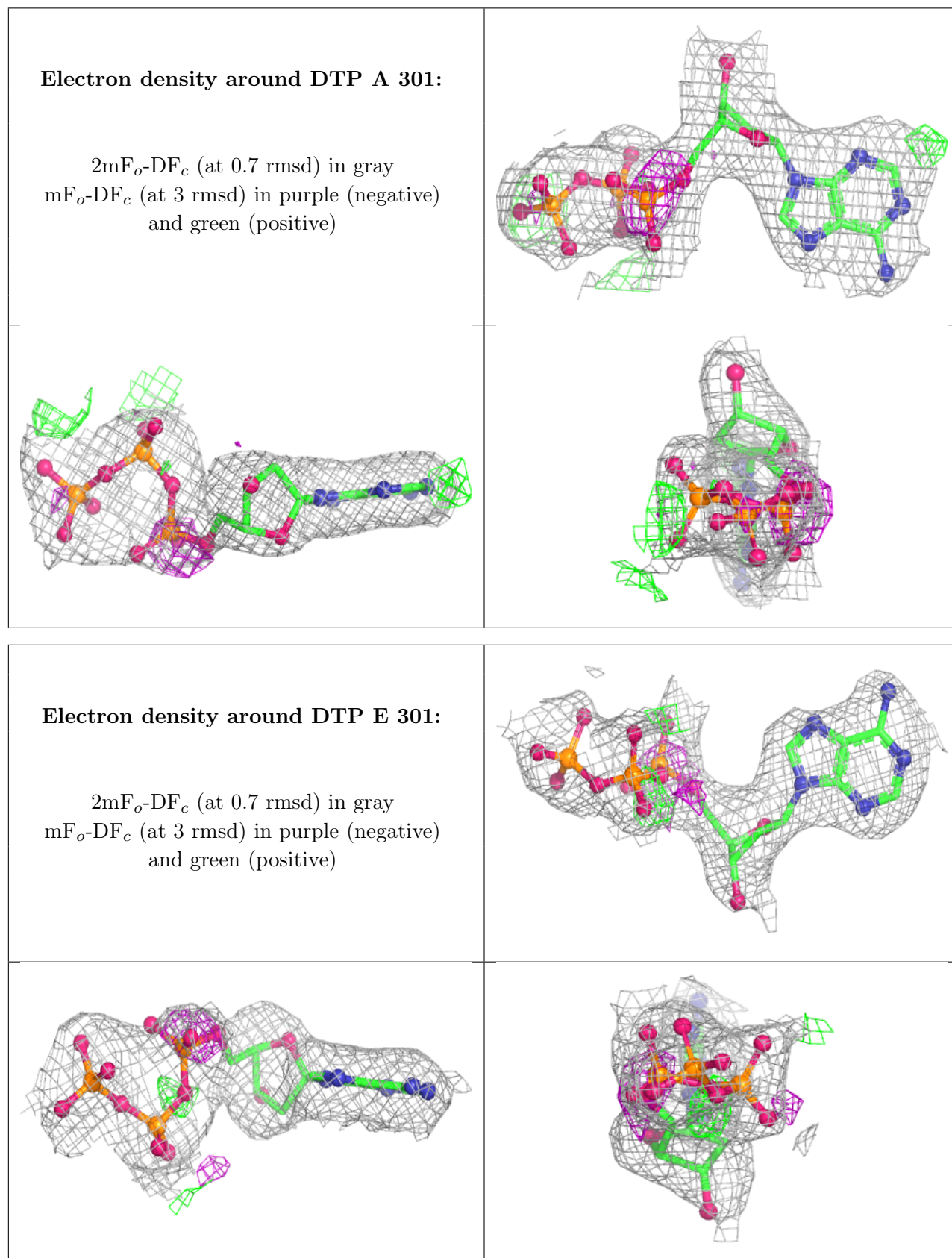
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	DTP	A	301	30/30	0.85	0.14	22,35,55,56	0
2	DTP	E	301	30/30	0.85	0.14	22,36,54,56	0
2	DTP	B	301	30/30	0.86	0.14	21,36,55,55	0
2	DTP	F	301	30/30	0.88	0.13	22,35,54,55	0
2	DTP	H	301	30/30	0.88	0.12	22,36,54,55	0
2	DTP	G	301	30/30	0.89	0.11	22,36,55,56	0
2	DTP	C	301	30/30	0.89	0.13	22,35,54,56	0
2	DTP	D	301	30/30	0.91	0.14	22,35,54,55	0

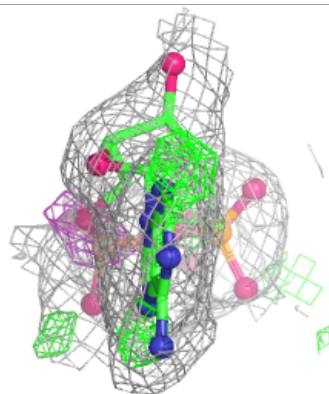
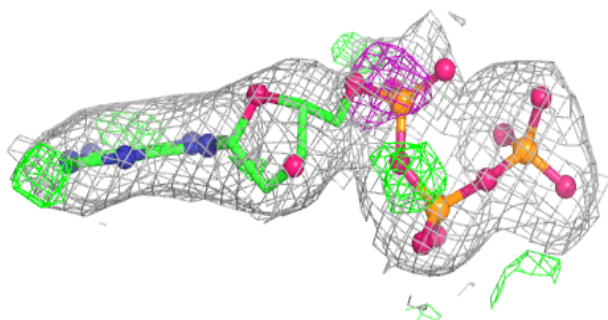
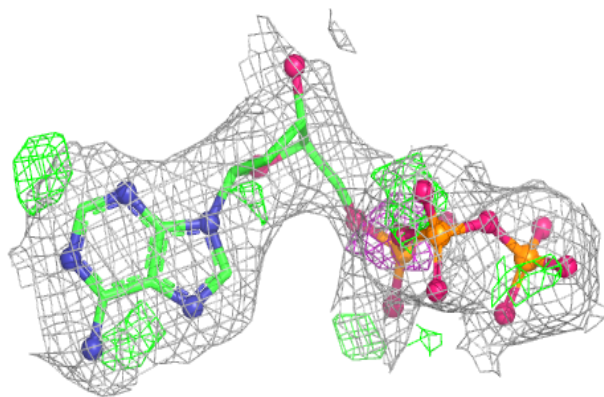
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

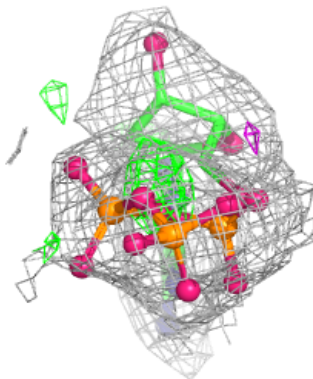
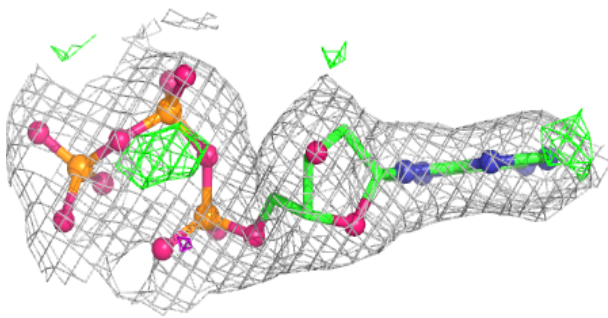
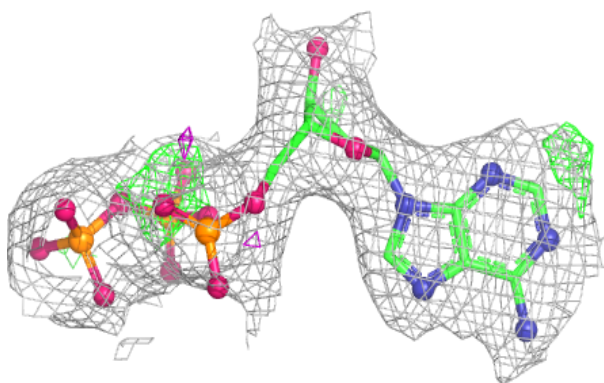


Electron density around DTP B 301:

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

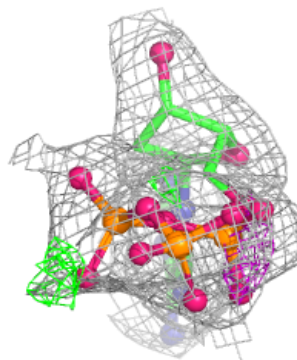
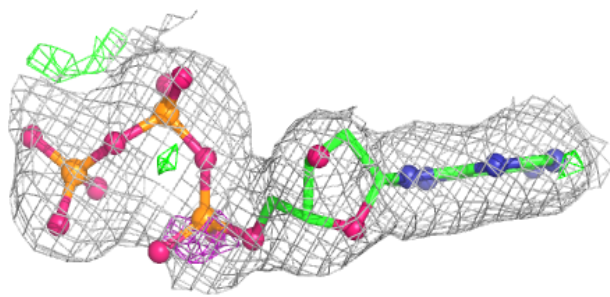
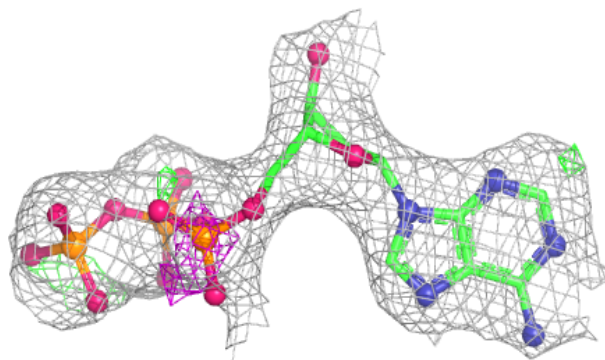
**Electron density around DTP F 301:**

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

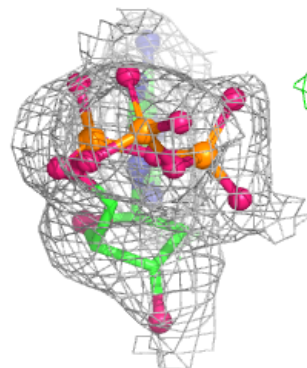
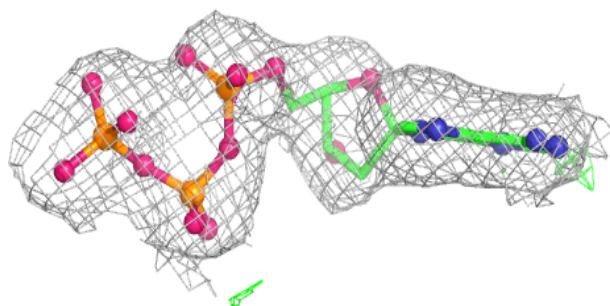
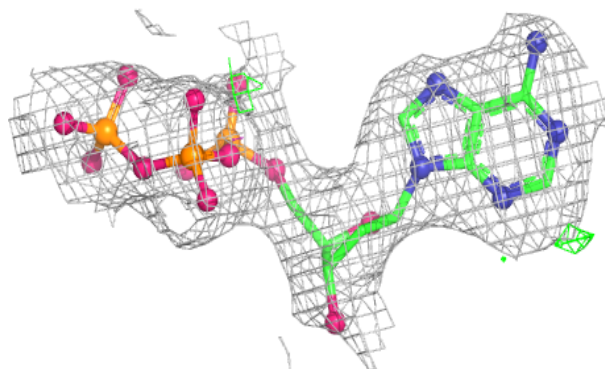


Electron density around DTP H 301:

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

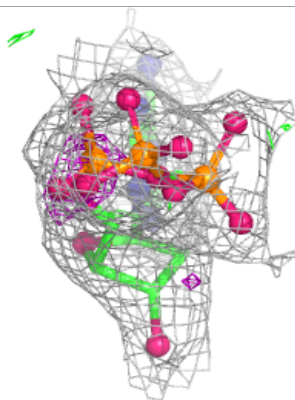
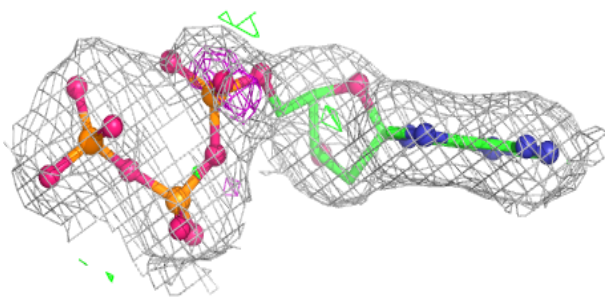
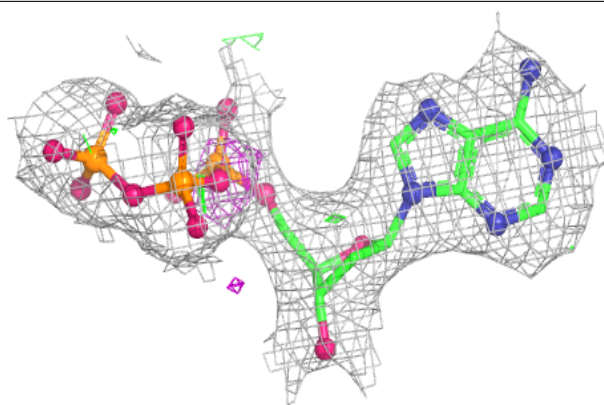
**Electron density around DTP G 301:**

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

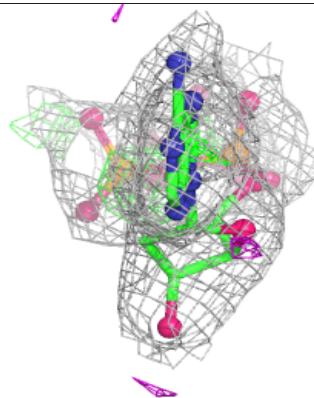
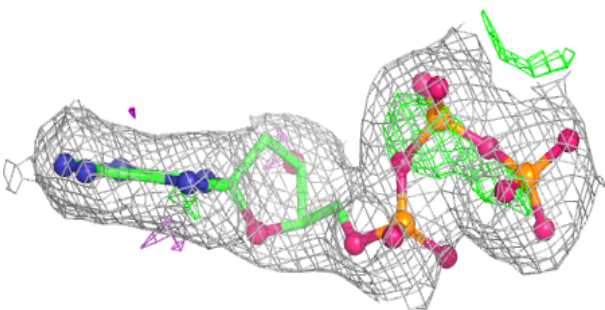
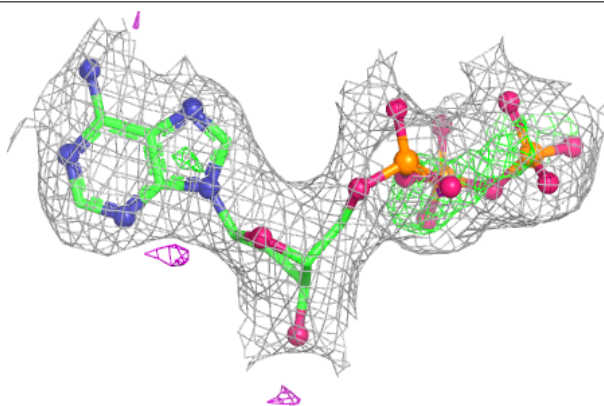


Electron density around DTP C 301:

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

**Electron density around DTP D 301:**

$2mF_o-DF_c$ (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.