



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:24 PM UTC

PDB ID : 4F61 / pdb_00004f61
Title : Tubulin:Stathmin-like domain complex
Authors : Gigant, B.; Mignot, I.; Knossow, M.
Deposited on : 2012-05-14
Resolution : 4.17 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:

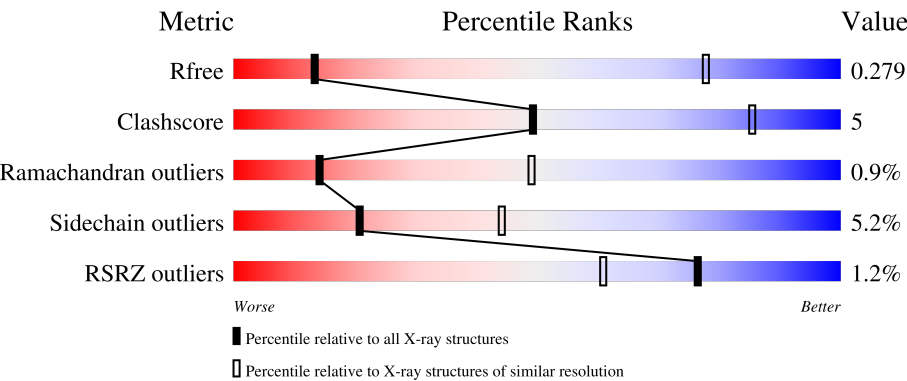
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.17 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1026 (4.50-3.86)
Clashscore	190562	1071 (4.50-3.86)
Ramachandran outliers	187476	1014 (4.52-3.84)
Sidechain outliers	187428	1000 (4.52-3.84)
RSRZ outliers	180081	1023 (4.50-3.86)

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	451	0% 80%15%...
1	C	451	2% 79%14%...
1	E	451	2% 81%13%...
1	G	451	2% 79%15%...
2	B	445	2% 79%16%...

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Mol	Chain	Length	Quality of chain
2	D	445	% 78%18%..
2	F	445	% 77%18%..
2	H	445	76%17%..
3	I	240	51%38%8%..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29129 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3380	2141	574	643	22			
1	C	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			
1	E	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			
1	G	431	Total	C	N	O	S	0	0	0
			3352	2123	570	637	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
E	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
E	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
G	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
G	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	0	0
			3383	2124	576	657	26			
2	D	432	Total	C	N	O	S	0	0	0
			3383	2124	576	657	26			
2	F	432	Total	C	N	O	S	0	0	0
			3383	2124	576	657	26			
2	H	431	Total	C	N	O	S	0	0	0
			3375	2116	579	655	25			

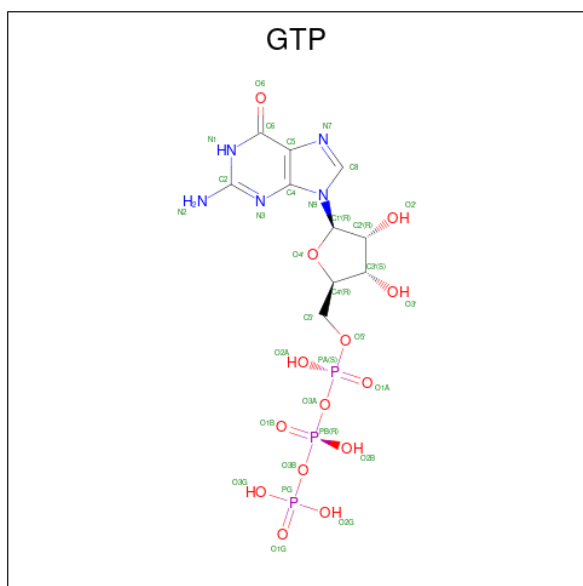
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
F	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
H	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9

- Molecule 3 is a protein called Stathmin-like domain R4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	234	Total	C	N	O	S	0	0	0
			1925	1185	362	369	9			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

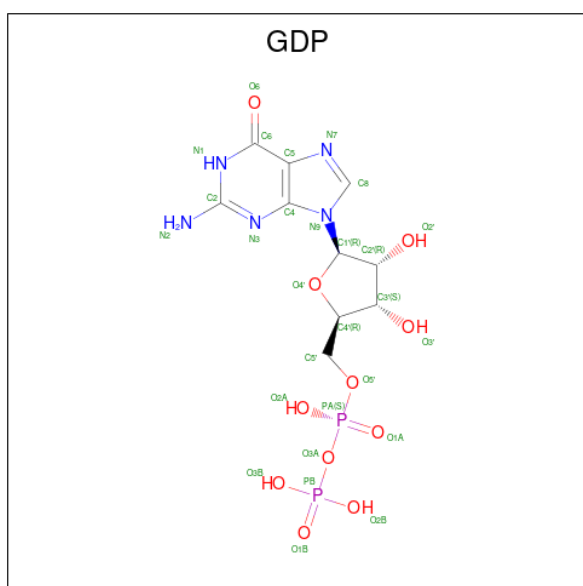


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	G	1	Total Mg 1 1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

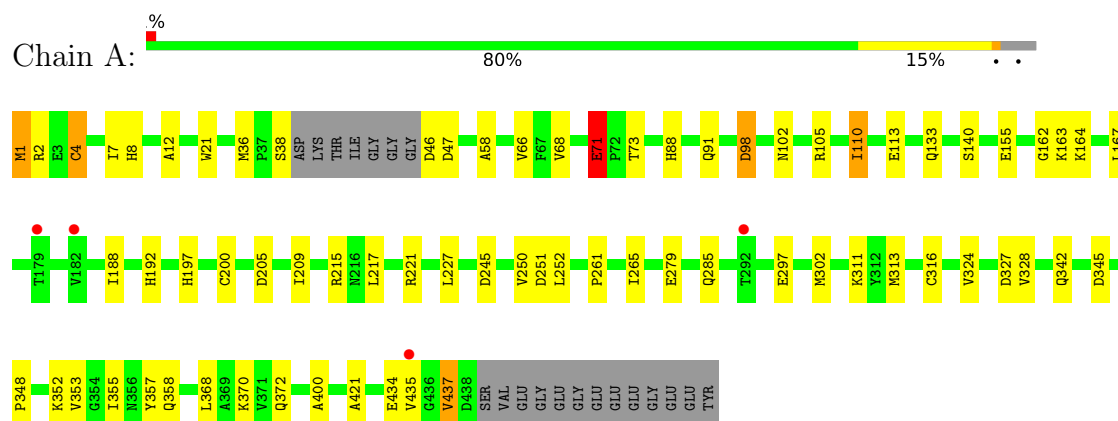


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P 28 10 5 11 2	0	0
6	D	1	Total C N O P 28 10 5 11 2	0	0
6	F	1	Total C N O P 28 10 5 11 2	0	0
6	H	1	Total C N O P 28 10 5 11 2	0	0

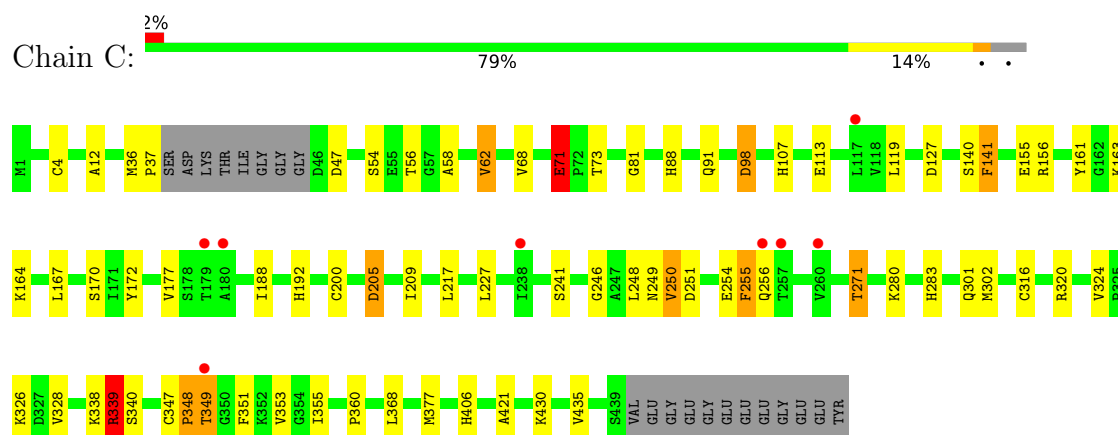
3 Residue-property plots [i](#)

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.

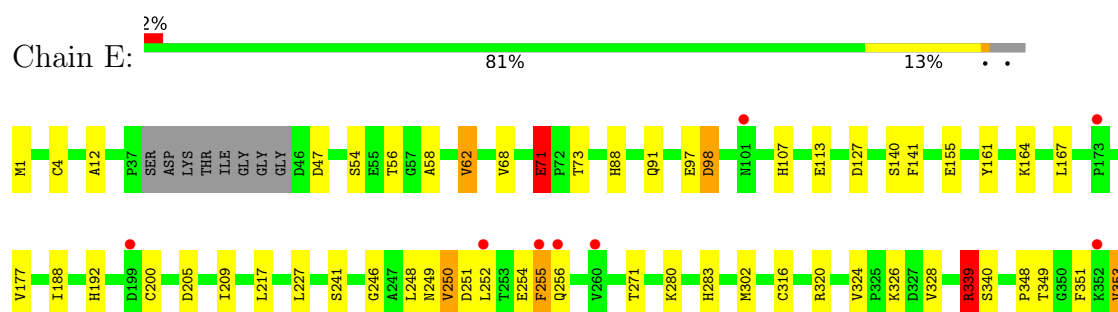
• Molecule 1: Tubulin alpha chain

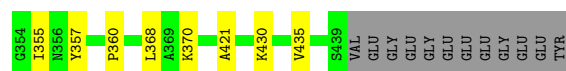


• Molecule 1: Tubulin alpha chain

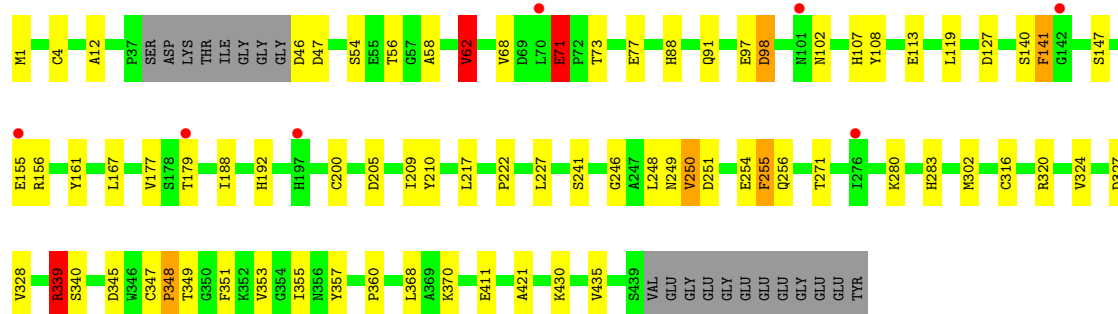
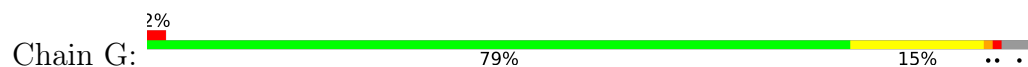


• Molecule 1: Tubulin alpha chain

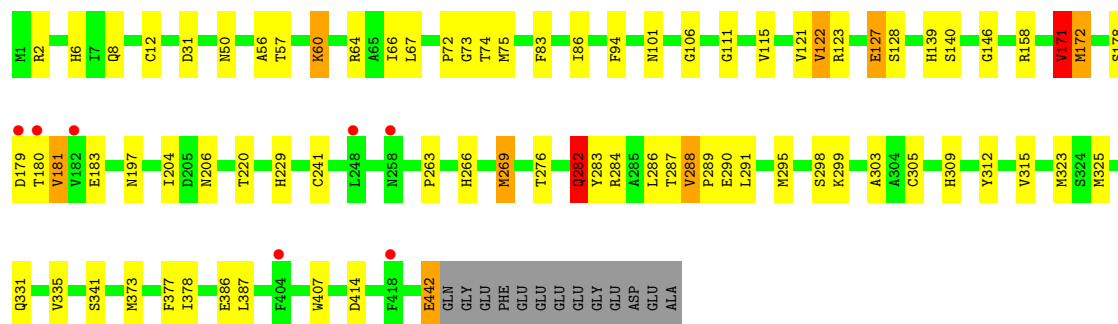




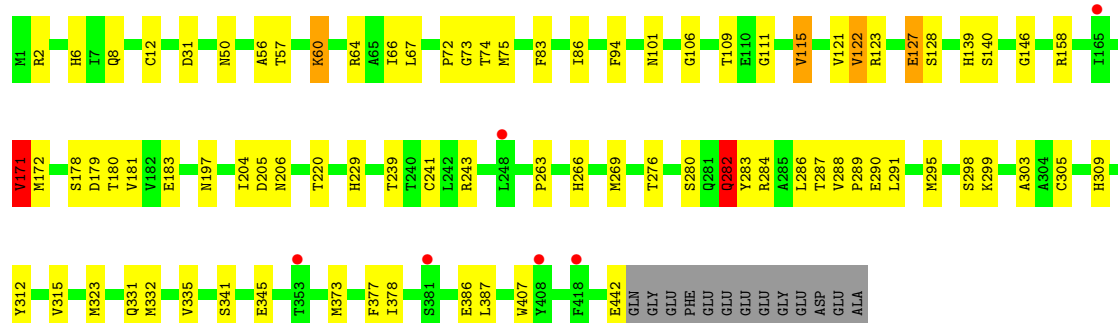
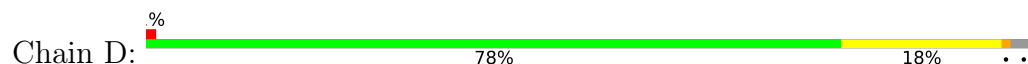
• Molecule 1: Tubulin alpha chain



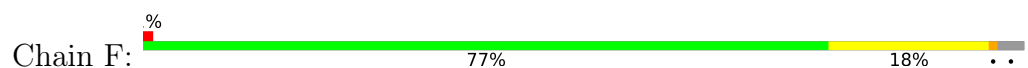
• Molecule 2: Tubulin beta chain

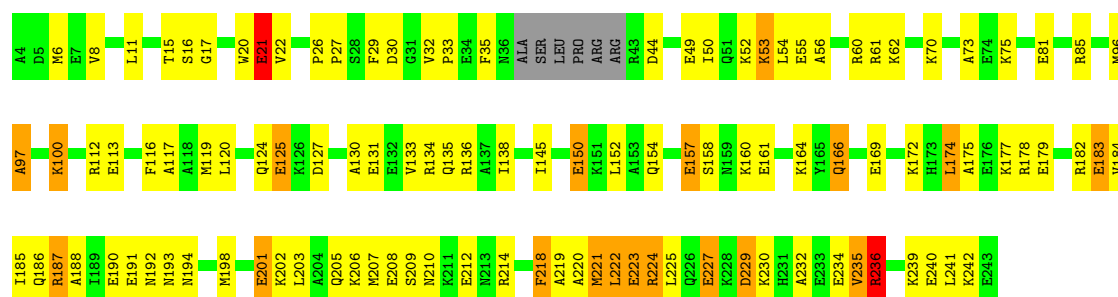


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	639.74Å 66.10Å 128.13Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	49.04 – 4.17 49.04 – 4.17	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.04-4.17) 98.6 (49.04-4.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 4.14Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.241 , 0.261 0.257 , 0.279	Depositor DCC
R_{free} test set	2024 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	150.8	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 225.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29129	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: MG, GTP, GDP

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	0.82	2/3457 (0.1%)	1.35	12/4693 (0.3%)
1	C	0.77	1/3427 (0.0%)	1.35	19/4655 (0.4%)
1	E	0.80	2/3427 (0.1%)	1.37	20/4655 (0.4%)
1	G	0.84	3/3427 (0.1%)	1.39	21/4655 (0.5%)
2	B	0.79	2/3458 (0.1%)	1.33	19/4686 (0.4%)
2	D	0.75	0/3458	1.33	20/4686 (0.4%)
2	F	0.78	1/3458 (0.0%)	1.36	20/4686 (0.4%)
2	H	0.97	3/3449 (0.1%)	1.50	43/4673 (0.9%)
3	I	0.96	1/1947 (0.1%)	1.73	44/2592 (1.7%)
All	All	0.83	15/29508 (0.1%)	1.40	218/39981 (0.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	MET	SD-CE	8.84	2.01	1.79
2	F	172	MET	SD-CE	8.37	2.00	1.79
2	B	172	MET	SD-CE	7.67	1.98	1.79
1	G	177	VAL	CA-C	7.25	1.59	1.52
1	A	1	MET	SD-CE	6.93	1.96	1.79
1	E	177	VAL	CA-C	6.13	1.58	1.52
2	H	178	SER	CA-C	-5.72	1.45	1.52
2	H	179	ASP	C-N	5.62	1.41	1.33
2	B	269	MET	SD-CE	-5.50	1.65	1.79
1	C	177	VAL	CA-C	5.45	1.57	1.52
3	I	16	SER	CA-C	5.45	1.59	1.52
1	G	179	THR	CA-C	5.38	1.59	1.52
1	G	179	THR	CA-CB	5.33	1.62	1.54
1	A	110	ILE	CG1-CD1	-5.22	1.31	1.51
1	E	251	ASP	C-N	5.09	1.40	1.33

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	SER	N-CA-C	10.65	126.06	113.18
3	I	169	GLU	N-CA-C	-10.36	100.07	111.36
2	H	179	ASP	CA-C-N	-10.28	106.56	120.95
2	H	179	ASP	C-N-CA	-10.28	106.56	120.95
1	C	255	PHE	CA-CB-CG	9.02	122.82	113.80
1	E	255	PHE	CA-CB-CG	8.96	122.76	113.80
3	I	183	GLU	N-CA-C	-8.56	102.97	113.50
1	G	255	PHE	CA-CB-CG	8.46	122.26	113.80
3	I	219	ALA	N-CA-C	-8.42	101.13	111.40
2	H	197	ASN	N-CA-C	8.10	123.35	113.38
2	H	281	GLN	CA-C-N	8.08	136.25	121.70
2	H	281	GLN	C-N-CA	8.08	136.25	121.70
3	I	209	SER	N-CA-C	-7.89	103.79	113.50
2	D	179	ASP	CA-CB-CG	7.79	120.39	112.60
2	H	120	ASP	CA-CB-CG	7.76	120.36	112.60
2	F	179	ASP	CA-CB-CG	7.72	120.33	112.60
1	G	77	GLU	CB-CG-CD	7.69	125.67	112.60
2	H	180	THR	N-CA-CB	7.67	121.28	109.85
2	H	280	SER	CA-C-N	7.46	131.33	120.82
2	H	280	SER	C-N-CA	7.46	131.33	120.82
2	B	127	GLU	CB-CG-CD	7.40	125.18	112.60
1	G	351	PHE	N-CA-C	7.27	120.63	108.20
3	I	26	PRO	N-CA-C	7.26	119.56	110.70
3	I	117	ALA	N-CA-C	-7.22	103.02	111.03
2	D	171	VAL	N-CA-CB	7.21	119.22	111.00
2	B	179	ASP	CA-CB-CG	7.13	119.73	112.60
3	I	224	ARG	N-CA-C	-7.13	103.20	110.97
1	C	351	PHE	N-CA-C	7.02	120.21	108.20
2	B	171	VAL	N-CA-CB	7.02	119.00	111.00
2	H	127	GLU	CB-CG-CD	7.00	124.51	112.60
1	E	351	PHE	N-CA-C	6.99	120.16	108.20
3	I	175	ALA	N-CA-C	-6.98	102.24	111.24
2	F	171	VAL	N-CA-CB	6.95	118.92	111.00
2	D	127	GLU	CB-CG-CD	6.89	124.31	112.60
2	F	197	ASN	N-CA-C	6.88	122.67	113.72
1	E	205	ASP	CA-CB-CG	6.83	119.43	112.60
2	H	378	ILE	CA-C-N	-6.82	117.35	122.33
2	H	378	ILE	C-N-CA	-6.82	117.35	122.33
2	H	371	LEU	CD1-CG-CD2	-6.78	95.88	110.80
3	I	187	ARG	N-CA-C	-6.78	103.97	111.36
2	B	197	ASN	N-CA-C	6.70	122.43	113.72
2	H	177	VAL	CA-C-N	-6.70	112.17	122.62
2	H	177	VAL	C-N-CA	-6.70	112.17	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ASP	CA-CB-CG	6.70	119.30	112.60
3	I	157	GLU	N-CA-C	-6.70	103.91	111.14
2	F	127	GLU	CB-CG-CD	6.69	123.98	112.60
3	I	21	GLU	CB-CG-CD	6.67	123.93	112.60
1	G	177	VAL	CB-CA-C	6.63	117.27	110.70
3	I	62	LYS	N-CA-C	6.62	118.50	111.28
1	G	205	ASP	CA-CB-CG	6.58	119.18	112.60
3	I	73	ALA	N-CA-C	-6.56	104.31	112.90
2	H	171	VAL	N-CA-CB	6.55	118.47	111.00
2	B	122	VAL	N-CA-CB	6.53	120.37	110.58
2	H	57	THR	CB-CA-C	6.52	119.12	110.06
2	B	282	GLN	CA-C-N	6.46	133.33	121.70
2	B	282	GLN	C-N-CA	6.46	133.33	121.70
3	I	212	GLU	N-CA-C	-6.46	104.16	111.14
2	D	197	ASN	N-CA-C	6.45	122.10	113.72
2	D	282	GLN	CA-C-N	6.44	133.29	121.70
2	D	282	GLN	C-N-CA	6.44	133.29	121.70
2	H	73	GLY	N-CA-C	6.43	120.42	112.64
3	I	235	VAL	CB-CA-C	6.41	116.70	111.06
2	F	282	GLN	CA-C-N	6.38	133.19	121.70
2	F	282	GLN	C-N-CA	6.38	133.19	121.70
1	A	205	ASP	CA-CB-CG	6.34	118.94	112.60
1	E	255	PHE	CA-C-N	6.31	129.06	120.54
1	E	255	PHE	C-N-CA	6.31	129.06	120.54
3	I	218	PHE	N-CA-C	-6.28	104.19	113.61
2	F	378	ILE	CA-C-N	-6.26	117.76	122.33
2	F	378	ILE	C-N-CA	-6.26	117.76	122.33
2	B	57	THR	CB-CA-C	6.25	118.75	110.06
3	I	230	LYS	N-CA-C	-6.21	104.59	111.36
1	C	113	GLU	CB-CG-CD	6.20	123.14	112.60
2	H	177	VAL	CB-CA-C	6.15	117.27	110.62
1	G	71	GLU	CB-CG-CD	6.14	123.04	112.60
2	H	74	THR	CA-C-N	6.10	128.45	120.28
2	H	74	THR	C-N-CA	6.10	128.45	120.28
2	F	122	VAL	N-CA-CB	6.08	119.69	110.58
2	D	122	VAL	N-CA-CB	6.07	119.69	110.58
3	I	125	GLU	N-CA-C	-6.07	105.72	113.01
3	I	127	ASP	N-CA-C	-6.07	106.51	114.04
1	G	255	PHE	CA-C-N	6.06	128.72	120.54
1	G	255	PHE	C-N-CA	6.06	128.72	120.54
1	A	437	VAL	N-CA-C	5.98	121.77	109.34
3	I	17	GLY	N-CA-C	5.97	119.86	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	191	GLU	N-CA-C	-5.92	103.51	112.04
3	I	205	GLN	CA-C-N	5.91	129.68	120.82
3	I	205	GLN	C-N-CA	5.91	129.68	120.82
2	H	122	VAL	N-CA-CB	5.90	119.43	110.58
2	H	179	ASP	CA-CB-CG	5.88	118.48	112.60
1	E	71	GLU	CB-CG-CD	5.88	122.59	112.60
2	H	441	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	251	ASP	CA-CB-CG	5.84	118.44	112.60
3	I	135	GLN	CA-C-N	5.80	128.63	120.28
3	I	135	GLN	C-N-CA	5.80	128.63	120.28
3	I	131	GLU	N-CA-C	-5.78	103.72	112.04
2	B	60	LYS	N-CA-C	5.78	119.33	110.20
1	G	339	ARG	CA-C-N	5.78	132.57	121.54
1	G	339	ARG	C-N-CA	5.78	132.57	121.54
1	C	71	GLU	CB-CG-CD	5.76	122.39	112.60
1	C	255	PHE	CA-C-N	5.73	128.28	120.54
1	C	255	PHE	C-N-CA	5.73	128.28	120.54
1	E	339	ARG	CA-C-N	5.73	132.48	121.54
1	E	339	ARG	C-N-CA	5.73	132.48	121.54
1	G	113	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	279	GLU	CB-CG-CD	5.72	122.33	112.60
2	B	74	THR	CA-C-N	5.70	127.92	120.28
2	B	74	THR	C-N-CA	5.70	127.92	120.28
1	E	177	VAL	CB-CA-C	5.69	116.34	110.70
2	F	74	THR	CA-C-N	5.69	127.90	120.28
2	F	74	THR	C-N-CA	5.69	127.90	120.28
1	G	161	TYR	N-CA-C	5.66	120.19	112.88
1	G	357	TYR	N-CA-C	5.66	118.99	111.75
2	H	178	SER	N-CA-C	5.65	118.43	109.50
2	H	31	ASP	CA-CB-CG	5.64	118.25	112.60
2	D	60	LYS	N-CA-C	5.63	119.10	110.20
1	G	141	PHE	CA-CB-CG	5.63	119.43	113.80
3	I	135	GLN	N-CA-C	-5.63	105.06	111.14
1	C	339	ARG	CA-C-N	5.61	132.26	121.54
1	C	339	ARG	C-N-CA	5.61	132.26	121.54
1	G	98	ASP	CA-CB-CG	5.60	118.20	112.60
3	I	183	GLU	CA-C-N	5.58	129.28	122.63
3	I	183	GLU	C-N-CA	5.58	129.28	122.63
2	D	378	ILE	CA-C-N	-5.58	118.26	122.33
2	D	378	ILE	C-N-CA	-5.58	118.26	122.33
1	E	161	TYR	N-CA-C	5.57	120.07	112.88
1	A	71	GLU	CB-CG-CD	5.57	122.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74	THR	CA-C-N	5.56	127.73	120.28
2	D	74	THR	C-N-CA	5.56	127.73	120.28
1	G	102	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	327	ASP	CA-CB-CG	5.51	118.11	112.60
2	H	175	PRO	CA-C-N	5.49	128.19	120.28
2	H	175	PRO	C-N-CA	5.49	128.19	120.28
1	E	357	TYR	N-CA-C	5.49	118.78	111.75
2	F	115	VAL	N-CA-C	5.49	116.88	110.62
2	F	72	PRO	CA-C-N	5.48	126.18	119.99
2	F	72	PRO	C-N-CA	5.48	126.18	119.99
2	D	57	THR	CB-CA-C	5.47	117.67	110.06
2	H	60	LYS	N-CA-C	5.46	119.14	109.96
1	G	251	ASP	CA-CB-CG	5.44	118.04	112.60
3	I	223	GLU	CB-CG-CD	5.44	121.85	112.60
2	H	286	LEU	N-CA-C	5.43	122.37	110.80
3	I	124	GLN	N-CA-C	-5.42	106.60	113.43
3	I	138	ILE	CB-CA-C	5.41	117.60	110.84
2	D	31	ASP	CA-CB-CG	5.40	118.00	112.60
3	I	17	GLY	CA-C-N	5.40	131.85	121.54
3	I	17	GLY	C-N-CA	5.40	131.85	121.54
1	A	265	ILE	CB-CG1-CD1	5.39	125.12	113.80
2	F	73	GLY	N-CA-C	5.36	119.13	112.64
2	F	31	ASP	CA-CB-CG	5.36	117.96	112.60
1	G	345	ASP	CA-CB-CG	5.35	117.95	112.60
2	F	205	ASP	CA-CB-CG	5.34	117.94	112.60
1	G	349	THR	CB-CA-C	5.34	121.04	110.42
3	I	81	GLU	CB-CG-CD	5.32	121.65	112.60
2	D	171	VAL	CB-CA-C	5.32	117.40	110.96
1	A	297	GLU	CB-CG-CD	5.32	121.64	112.60
1	E	98	ASP	CA-CB-CG	5.30	117.90	112.60
3	I	55	GLU	N-CA-C	-5.30	106.08	112.54
2	F	171	VAL	CB-CA-C	5.29	117.37	110.96
3	I	112	ARG	N-CA-C	-5.29	107.48	114.04
2	F	60	LYS	N-CA-C	5.29	118.84	109.96
2	H	276	THR	CB-CA-C	-5.29	98.92	109.33
1	E	251	ASP	CA-CB-CG	5.27	117.87	112.60
3	I	210	ASN	N-CA-C	-5.27	105.19	111.03
1	C	349	THR	CB-CA-C	5.26	120.89	110.42
2	H	115	VAL	N-CA-C	5.26	116.61	110.62
1	C	141	PHE	CA-CB-CG	5.24	119.04	113.80
2	H	113	GLU	CB-CG-CD	5.24	121.51	112.60
2	H	177	VAL	N-CA-C	5.24	118.76	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	PRO	CA-C-N	5.22	125.89	119.99
2	B	72	PRO	C-N-CA	5.22	125.89	119.99
2	D	205	ASP	CA-CB-CG	5.21	117.81	112.60
3	I	70	LYS	N-CA-C	-5.21	105.25	111.03
2	B	73	GLY	N-CA-C	5.20	118.94	112.64
2	H	72	PRO	CA-C-N	5.20	125.87	119.99
2	H	72	PRO	C-N-CA	5.20	125.87	119.99
2	D	73	GLY	N-CA-C	5.19	119.16	112.83
2	F	57	THR	CB-CA-C	5.19	117.27	110.06
2	H	288	VAL	N-CA-CB	5.19	114.50	110.45
1	A	102	ASN	CA-CB-CG	5.16	117.76	112.60
1	G	327	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	98	ASP	CA-CB-CG	5.15	117.75	112.60
1	E	353	VAL	CA-C-N	5.14	125.15	121.65
1	E	353	VAL	C-N-CA	5.14	125.15	121.65
2	B	31	ASP	CA-CB-CG	5.14	117.74	112.60
3	I	222	LEU	N-CA-C	5.12	118.68	112.23
3	I	166	GLN	CA-C-N	5.12	129.57	121.18
3	I	166	GLN	C-N-CA	5.12	129.57	121.18
1	G	62	VAL	N-CA-C	5.11	113.46	107.89
1	E	113	GLU	CB-CG-CD	5.11	121.29	112.60
2	H	171	VAL	CB-CA-C	5.11	117.14	110.96
2	H	147	SER	CA-C-N	5.10	125.50	119.94
2	H	147	SER	C-N-CA	5.10	125.50	119.94
2	B	288	VAL	N-CA-CB	5.09	114.42	110.45
2	D	72	PRO	CA-C-N	5.09	125.73	120.03
2	D	72	PRO	C-N-CA	5.09	125.73	120.03
1	C	163	LYS	N-CA-CB	5.08	118.08	110.11
3	I	201	GLU	N-CA-C	5.07	116.89	111.36
1	E	252	LEU	CA-C-N	5.07	127.49	120.29
1	E	252	LEU	C-N-CA	5.07	127.49	120.29
3	I	236	ARG	N-CA-C	-5.07	105.94	111.82
1	E	349	THR	CB-CA-C	5.06	120.49	110.42
1	E	141	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	357	TYR	N-CA-C	5.03	118.52	112.38
2	H	147	SER	N-CA-C	5.03	116.61	111.03
2	B	171	VAL	CB-CA-C	5.03	117.04	110.96
2	D	115	VAL	N-CA-C	5.02	116.35	110.62
1	C	338	LYS	CA-C-N	5.02	131.13	121.54
1	C	338	LYS	C-N-CA	5.02	131.13	121.54
2	H	147	SER	CA-CB-OG	5.02	121.13	111.10
1	A	162	GLY	CA-C-N	5.01	129.53	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLY	C-N-CA	5.01	129.53	122.46
1	C	81	GLY	CA-C-N	5.01	126.99	120.28
1	C	81	GLY	C-N-CA	5.01	126.99	120.28
1	C	161	TYR	N-CA-C	5.01	119.34	112.88
1	A	98	ASP	CA-CB-CG	5.00	117.60	112.60
2	B	378	ILE	CA-C-N	-5.00	118.68	122.33
2	B	378	ILE	C-N-CA	-5.00	118.68	122.33

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	3380	0	3290	28	1
1	C	3352	0	3253	32	0
1	E	3352	0	3253	24	0
1	G	3352	0	3253	28	0
2	B	3383	0	3246	44	0
2	D	3383	0	3246	43	0
2	F	3383	0	3246	44	0
2	H	3375	0	3246	49	1
3	I	1925	0	1912	41	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
4	E	32	0	12	0	0
4	G	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	1	0
6	F	28	0	12	1	0
6	H	28	0	12	1	0
All	All	29129	0	28041	306	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 5.

All (306) 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)
2:H:1:MET:SD	2:H:1:MET:CE	2.01	1.48
1:G:250:VAL:HG23	1:G:254:GLU:HB3	1.36	1.07
1:E:250:VAL:HG23	1:E:254:GLU:HB3	1.40	1.03
1:C:250:VAL:HG23	1:C:254:GLU:HB3	1.39	1.01
2:H:286:LEU:HD12	2:H:291:LEU:HD23	1.44	0.97
2:H:295:MET:SD	2:H:377:PHE:HB2	2.09	0.92
2:H:325:MET:HE2	2:H:355:VAL:HG11	1.59	0.83
1:A:36:MET:HE2	1:A:38:SER:HB3	1.64	0.80
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.66	0.78
2:H:292:THR:HG22	2:H:335:VAL:HG21	1.62	0.78
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.67	0.76
1:G:71:GLU:HB3	1:G:98:ASP:HB3	1.67	0.75
2:H:206:ASN:HD21	6:H:600:GDP:HN22	1.34	0.75
1:E:250:VAL:HG22	1:E:255:PHE:CD1	2.22	0.74
2:F:206:ASN:HD21	6:F:600:GDP:HN22	1.34	0.74
1:E:71:GLU:HB3	1:E:98:ASP:HB3	1.70	0.73
2:B:206:ASN:HD21	6:B:600:GDP:HN22	1.33	0.72
1:C:250:VAL:HG22	1:C:255:PHE:CD1	2.24	0.72
1:G:250:VAL:HG22	1:G:255:PHE:CD1	2.25	0.71
2:D:206:ASN:HD21	6:D:600:GDP:HN22	1.40	0.69
3:I:192:ASN:C	3:I:194:ASN:H	2.01	0.68
1:A:245:ASP:HB3	3:I:15:THR:HB	1.77	0.66
2:D:263:PRO:O	2:D:266:HIS:HD2	1.80	0.65
3:I:198:MET:SD	3:I:202:LYS:HD2	2.36	0.65
3:I:11:LEU:HG	3:I:20:TRP:HA	1.79	0.65
1:E:328:VAL:HG11	1:E:353:VAL:HG11	1.80	0.64
2:B:407:TRP:CH2	1:C:256:GLN:HB3	2.32	0.64
2:H:133:GLN:HE22	2:H:252:LEU:H	1.43	0.64
2:B:263:PRO:O	2:B:266:HIS:HD2	1.81	0.63
2:F:263:PRO:O	2:F:266:HIS:HD2	1.81	0.63
2:H:263:PRO:O	2:H:266:HIS:HD2	1.82	0.63
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.80	0.62
2:H:92:PHE:HD2	2:H:94:PHE:HE2	1.47	0.62
2:D:50:ASN:O	2:D:64:ARG:NH2	2.34	0.60
1:G:328:VAL:HG11	1:G:353:VAL:HG11	1.82	0.60
2:H:322:ARG:HH22	2:H:359:PRO:HD3	1.67	0.60
2:D:229:HIS:HE1	2:D:276:THR:HG23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:HE1	2:B:8:GLN:HG3	1.67	0.59
2:H:6:HIS:HE1	2:H:8:GLN:HG3	1.67	0.59
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.83	0.59
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.68	0.58
2:D:6:HIS:HE1	2:D:8:GLN:HG3	1.68	0.58
2:F:309:HIS:HD2	2:F:386:GLU:OE1	1.86	0.58
2:F:172:MET:HG3	2:F:387:LEU:HD11	1.86	0.58
2:F:180:THR:HG23	2:F:183:GLU:HG3	1.86	0.57
1:G:248:LEU:HB2	1:G:355:ILE:H	1.69	0.57
2:F:6:HIS:HE1	2:F:8:GLN:HG3	1.70	0.57
2:B:229:HIS:HE1	2:B:276:THR:HG23	1.70	0.57
2:F:229:HIS:HE1	2:F:276:THR:HG23	1.69	0.57
2:F:269:MET:HE3	2:F:305:CYS:HB2	1.86	0.56
1:G:88:HIS:HB2	1:G:91:GLN:HE21	1.70	0.56
2:B:180:THR:HG23	2:B:183:GLU:HG3	1.87	0.56
1:C:56:THR:HG23	1:C:58:ALA:H	1.71	0.56
2:D:180:THR:HG23	2:D:183:GLU:HG3	1.87	0.56
2:F:159:GLU:HA	3:I:174:LEU:HD13	1.88	0.56
3:I:52:LYS:O	3:I:56:ALA:HB2	2.04	0.56
1:G:56:THR:HG23	1:G:58:ALA:H	1.69	0.56
3:I:8:VAL:HG22	3:I:22:VAL:HG22	1.86	0.56
2:H:56:ALA:HB3	2:H:60:LYS:HG3	1.87	0.56
2:F:56:ALA:HB3	2:F:60:LYS:HG3	1.88	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.87	0.55
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.88	0.55
2:B:309:HIS:HD2	2:B:386:GLU:OE1	1.89	0.55
1:E:88:HIS:HB2	1:E:91:GLN:HE21	1.71	0.55
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.55	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.55
1:A:105:ARG:HB3	1:A:110:ILE:CD1	2.37	0.55
2:B:286:LEU:HD12	2:B:291:LEU:HD23	1.89	0.55
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.53	0.55
3:I:52:LYS:HE2	3:I:53:LYS:HG3	1.89	0.55
1:E:56:THR:HG23	1:E:58:ALA:H	1.72	0.54
3:I:232:ALA:O	3:I:236:ARG:HD3	2.07	0.54
2:H:286:LEU:HD12	2:H:291:LEU:CD2	2.29	0.54
2:B:282:GLN:CB	2:B:283:TYR:HA	2.37	0.54
2:H:75:MET:CB	2:H:94:PHE:CE2	2.90	0.54
2:D:309:HIS:HD2	2:D:386:GLU:OE1	1.90	0.54
2:H:295:MET:HG3	2:H:377:PHE:CD1	2.42	0.54
2:D:75:MET:HE2	2:D:94:PHE:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:HIS:HE1	2:F:8:GLN:HE21	1.55	0.54
1:A:348:PRO:HB3	3:I:27:PRO:HD3	1.89	0.54
2:D:269:MET:HE3	2:D:305:CYS:HB2	1.89	0.54
2:F:287:THR:HG23	2:F:289:PRO:HD2	1.89	0.54
2:H:50:ASN:O	2:H:64:ARG:NH2	2.37	0.53
2:D:286:LEU:HD12	2:D:291:LEU:HD23	1.90	0.53
2:B:50:ASN:O	2:B:64:ARG:NH2	2.36	0.53
1:E:248:LEU:HB2	1:E:355:ILE:H	1.71	0.53
2:F:286:LEU:HD12	2:F:291:LEU:HD23	1.90	0.53
2:H:6:HIS:HE1	2:H:8:GLN:HE21	1.55	0.53
2:B:269:MET:HE3	2:B:305:CYS:HB2	1.90	0.52
1:C:54:SER:OG	1:C:62:VAL:HG13	2.08	0.52
1:G:246:GLY:H	1:G:249:ASN:HD21	1.58	0.52
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.09	0.52
2:B:56:ALA:HB3	2:B:60:LYS:HG3	1.91	0.52
2:D:139:HIS:HD2	2:D:146:GLY:O	1.93	0.52
2:H:6:HIS:CE1	2:H:8:GLN:HG3	2.44	0.52
2:B:6:HIS:CE1	2:B:8:GLN:HG3	2.43	0.52
2:D:56:ALA:HB3	2:D:60:LYS:HG3	1.91	0.52
2:D:109:THR:HG23	3:I:134:ARG:NH2	2.25	0.52
2:F:269:MET:CE	2:F:305:CYS:HB2	2.39	0.52
1:G:97:GLU:HG3	2:H:1:MET:HG2	1.92	0.52
2:F:75:MET:HE2	2:F:94:PHE:HB3	1.92	0.52
1:G:54:SER:OG	1:G:62:VAL:HG13	2.09	0.52
1:G:108:TYR:HA	3:I:207:MET:HE1	1.92	0.52
1:C:246:GLY:H	1:C:249:ASN:HD21	1.57	0.52
1:C:248:LEU:HB2	1:C:355:ILE:H	1.74	0.52
2:B:269:MET:CE	2:B:305:CYS:HB2	2.40	0.52
2:H:180:THR:HG23	2:H:183:GLU:HG3	1.92	0.51
1:A:105:ARG:HB3	1:A:110:ILE:HD12	1.93	0.51
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.93	0.51
2:F:139:HIS:HD2	2:F:146:GLY:O	1.94	0.51
2:H:274:PRO:HB3	2:H:286:LEU:HG	1.92	0.51
3:I:160:LYS:HE2	3:I:164:LYS:HD2	1.90	0.51
3:I:185:ILE:O	3:I:188:ALA:HB3	2.10	0.51
1:E:54:SER:OG	1:E:62:VAL:HG13	2.10	0.51
2:D:282:GLN:CB	2:D:283:TYR:HA	2.40	0.51
3:I:227:GLU:C	3:I:229:ASP:H	2.19	0.51
2:B:139:HIS:HD2	2:B:146:GLY:O	1.93	0.51
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.92	0.51
2:D:6:HIS:CE1	2:D:8:GLN:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.75	0.51
2:D:269:MET:CE	2:D:305:CYS:HB2	2.41	0.51
2:H:106:GLY:O	2:H:111:GLY:HA3	2.11	0.50
2:F:50:ASN:O	2:F:64:ARG:NH2	2.38	0.50
2:H:139:HIS:HD2	2:H:146:GLY:O	1.94	0.50
2:F:6:HIS:CE1	2:F:8:GLN:HG3	2.46	0.50
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.46	0.50
2:F:282:GLN:CB	2:F:283:TYR:HA	2.41	0.50
2:F:407:TRP:CH2	1:G:256:GLN:HB3	2.47	0.50
1:A:221:ARG:CG	2:B:325:MET:HE2	2.42	0.49
2:D:331:GLN:O	2:D:335:VAL:HG23	2.12	0.49
2:F:106:GLY:O	2:F:111:GLY:HA3	2.11	0.49
3:I:116:PHE:HA	3:I:119:MET:HB2	1.94	0.49
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.49
2:D:106:GLY:O	2:D:111:GLY:HA3	2.11	0.49
1:A:221:ARG:HG2	2:B:325:MET:HE2	1.94	0.49
1:G:107:HIS:HE1	1:G:155:GLU:OE2	1.95	0.49
2:B:331:GLN:O	2:B:335:VAL:HG23	2.13	0.49
1:G:411:GLU:C	3:I:214:ARG:HG3	2.37	0.49
1:E:107:HIS:HE1	1:E:155:GLU:OE2	1.95	0.49
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.94	0.49
2:B:101:ASN:HB3	2:B:180:THR:HG21	1.95	0.49
1:E:246:GLY:H	1:E:249:ASN:HD21	1.61	0.49
1:G:209:ILE:HD11	1:G:302:MET:CE	2.43	0.49
2:F:323:MET:HE3	2:F:373:MET:HE3	1.95	0.49
2:F:331:GLN:O	2:F:335:VAL:HG23	2.12	0.49
3:I:179:GLU:O	3:I:183:GLU:HB2	2.11	0.49
2:H:133:GLN:NE2	2:H:252:LEU:H	2.10	0.49
2:B:414:ASP:HB2	3:I:85:ARG:HH22	1.78	0.48
2:H:69:ASP:HB3	2:H:94:PHE:HD1	1.78	0.48
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.31	0.48
1:A:400:ALA:HB2	2:B:442:GLU:HG2	1.96	0.48
1:A:105:ARG:NE	1:A:110:ILE:HD11	2.27	0.48
3:I:150:GLU:O	3:I:154:GLN:HB2	2.12	0.48
2:D:101:ASN:HB3	2:D:180:THR:HG21	1.95	0.48
2:B:288:VAL:HG22	2:B:323:MET:HE3	1.96	0.48
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.32	0.48
2:H:325:MET:HE2	2:H:355:VAL:CG1	2.39	0.48
2:F:101:ASN:HB3	2:F:180:THR:HG21	1.96	0.47
2:H:178:SER:HB3	2:H:183:GLU:OE2	2.14	0.47
2:D:323:MET:HE3	2:D:373:MET:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG23	1:A:66:VAL:HG13	1.96	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.47
2:F:156:LYS:HE2	3:I:178:ARG:HD2	1.96	0.47
2:H:101:ASN:HB3	2:H:180:THR:HG21	1.96	0.47
2:H:323:MET:HE3	2:H:373:MET:HE3	1.95	0.47
3:I:192:ASN:C	3:I:194:ASN:N	2.71	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.97	0.47
2:F:6:HIS:CE1	2:F:8:GLN:HE21	2.33	0.47
2:H:88:ARG:NH1	2:H:90:ASP:OD1	2.47	0.47
2:H:288:VAL:HG22	2:H:323:MET:HE3	1.97	0.47
3:I:97:ALA:HA	3:I:100:LYS:HB2	1.97	0.47
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.33	0.47
3:I:133:VAL:HG12	3:I:136:ARG:HH11	1.80	0.47
2:H:411:GLU:HA	3:I:239:LYS:HD3	1.97	0.46
2:B:295:MET:HE2	2:B:315:VAL:HG11	1.96	0.46
2:F:123:ARG:O	2:F:127:GLU:HG2	2.15	0.46
2:D:286:LEU:HD13	2:D:290:GLU:HB3	1.97	0.46
1:A:352:LYS:HG2	3:I:21:GLU:HG3	1.98	0.46
2:F:67:LEU:O	2:F:75:MET:HE1	2.16	0.46
2:F:295:MET:HE2	2:F:315:VAL:HG11	1.96	0.46
2:H:92:PHE:CD2	2:H:94:PHE:HE2	2.30	0.46
2:H:385:GLN:HE22	2:H:433:GLN:HE21	1.63	0.46
3:I:182:ARG:HA	3:I:185:ILE:HB	1.97	0.46
1:G:167:LEU:HG	1:G:200:CYS:HB3	1.98	0.46
2:H:2:ARG:NH2	2:H:3:GLU:OE1	2.46	0.46
2:H:123:ARG:O	2:H:127:GLU:HG2	2.16	0.46
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.97	0.45
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.30	0.45
2:D:123:ARG:O	2:D:127:GLU:HG2	2.17	0.45
2:D:288:VAL:HG22	2:D:323:MET:HE3	1.98	0.45
2:H:6:HIS:CE1	2:H:8:GLN:HE21	2.32	0.45
1:G:192:HIS:CG	1:G:421:ALA:HA	2.52	0.45
3:I:192:ASN:O	3:I:194:ASN:N	2.49	0.45
2:H:331:GLN:O	2:H:335:VAL:HG23	2.17	0.45
1:A:261:PRO:HG3	1:A:313:MET:HG3	1.98	0.45
1:A:285:GLN:NE2	1:A:372:GLN:H	2.14	0.45
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.32	0.45
1:G:209:ILE:HD11	1:G:302:MET:SD	2.57	0.45
1:G:107:HIS:NE2	3:I:206:LYS:HE3	2.32	0.45
3:I:56:ALA:HB1	3:I:60:ARG:NH1	2.31	0.45
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ILE:HG22	1:G:227:LEU:HD22	1.99	0.44
2:F:83:PHE:O	2:F:86:ILE:HG22	2.17	0.44
2:F:345:GLU:H	2:F:345:GLU:HG2	1.55	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.44
1:E:167:LEU:HG	1:E:200:CYS:HB3	1.98	0.44
1:E:209:ILE:HG22	1:E:227:LEU:HD22	1.99	0.44
2:F:312:TYR:CE2	2:F:377:PHE:HZ	2.35	0.44
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.44
2:D:407:TRP:CH2	1:E:256:GLN:HB3	2.53	0.44
1:E:209:ILE:HD11	1:E:302:MET:SD	2.58	0.44
2:B:67:LEU:O	2:B:75:MET:HE1	2.19	0.43
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.99	0.43
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.43
2:B:286:LEU:HD13	2:B:290:GLU:HB3	2.00	0.43
2:D:229:HIS:CE1	2:D:276:THR:HG23	2.51	0.43
2:D:295:MET:HE2	2:D:315:VAL:HG11	2.00	0.43
2:F:12:CYS:HB3	2:F:140:SER:HB3	2.00	0.43
2:F:295:MET:HE1	2:F:332:MET:HE1	2.01	0.43
3:I:220:ALA:O	3:I:224:ARG:HD3	2.18	0.43
2:B:407:TRP:CZ2	1:C:256:GLN:HB3	2.53	0.43
1:C:209:ILE:HD11	1:C:302:MET:CE	2.49	0.43
2:D:2:ARG:HB2	2:D:2:ARG:NH1	2.33	0.43
2:F:288:VAL:HG22	2:F:323:MET:HE3	2.01	0.43
3:I:218:PHE:HA	3:I:221:MET:HB3	2.01	0.43
1:C:217:LEU:HD21	1:C:368:LEU:HD23	2.00	0.43
2:F:66:ILE:HG12	2:F:121:VAL:HG12	2.01	0.43
2:B:323:MET:HE3	2:B:373:MET:HE3	2.00	0.43
1:G:88:HIS:O	1:G:91:GLN:HG2	2.18	0.43
2:B:123:ARG:O	2:B:127:GLU:HG2	2.18	0.43
1:E:88:HIS:O	1:E:91:GLN:HG2	2.18	0.43
1:E:209:ILE:HD11	1:E:302:MET:CE	2.49	0.43
1:G:217:LEU:HD21	1:G:368:LEU:HD23	2.00	0.43
2:D:67:LEU:O	2:D:75:MET:HE1	2.18	0.43
1:E:97:GLU:HG3	2:F:1:MET:HG2	2.01	0.43
2:H:292:THR:CG2	2:H:335:VAL:HG21	2.41	0.43
3:I:182:ARG:O	3:I:186:GLN:HG3	2.17	0.43
3:I:130:ALA:O	3:I:134:ARG:HB2	2.19	0.42
2:D:83:PHE:O	2:D:86:ILE:HG22	2.19	0.42
1:E:217:LEU:HD21	1:E:368:LEU:HD23	2.00	0.42
2:H:171:VAL:HA	2:H:204:ILE:O	2.19	0.42
2:F:286:LEU:HD13	2:F:290:GLU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:312:TYR:CE2	2:H:377:PHE:HZ	2.37	0.42
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:C:12:ALA:CB	1:C:140:SER:HB3	2.50	0.42
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.42
2:H:133:GLN:HE21	2:H:133:GLN:HB3	1.31	0.42
2:D:239:THR:O	2:D:243:ARG:HG2	2.20	0.42
1:E:192:HIS:CG	1:E:421:ALA:HA	2.55	0.42
1:A:311:LYS:HG2	1:A:342:GLN:HG2	2.02	0.42
2:B:414:ASP:HB2	3:I:85:ARG:NH2	2.34	0.42
2:H:92:PHE:HD2	2:H:94:PHE:CE2	2.34	0.42
2:H:269:MET:HG3	2:H:303:ALA:HB3	2.00	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.42
1:G:12:ALA:CB	1:G:140:SER:HB3	2.49	0.42
2:H:83:PHE:O	2:H:86:ILE:HG22	2.19	0.42
1:C:141:PHE:CE2	1:C:170:SER:HB3	2.55	0.42
1:G:141:PHE:O	1:G:147:SER:HB3	2.20	0.42
3:I:32:VAL:HB	3:I:33:PRO:HD2	2.00	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:F:2:ARG:NH1	2:F:2:ARG:HB2	2.34	0.42
2:F:385:GLN:HE22	2:F:433:GLN:HE21	1.67	0.42
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.54	0.42
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.42
3:I:134:ARG:HD2	3:I:134:ARG:HA	1.91	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.41
2:D:220:THR:HB	1:E:326:LYS:HE3	2.02	0.41
1:C:88:HIS:H	1:C:91:GLN:NE2	2.19	0.41
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.01	0.41
1:E:12:ALA:CB	1:E:140:SER:HB3	2.50	0.41
1:C:36:MET:HA	1:C:37:PRO:HD3	1.97	0.41
1:E:88:HIS:H	1:E:91:GLN:NE2	2.18	0.41
1:E:250:VAL:CG2	1:E:255:PHE:CD1	2.99	0.41
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.03	0.41
2:F:171:VAL:HA	2:F:204:ILE:O	2.20	0.41
2:F:412:GLY:O	3:I:187:ARG:NH1	2.53	0.41
2:B:66:ILE:HG12	2:B:121:VAL:HG12	2.03	0.41
1:C:347:CYS:HA	1:C:348:PRO:HD3	1.94	0.41
2:B:181:VAL:HA	1:C:349:THR:CG2	2.50	0.41
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.02	0.41
1:C:271:THR:HG22	1:C:301:GLN:HA	2.03	0.41
3:I:157:GLU:HG3	3:I:161:GLU:OE1	2.20	0.41
1:E:320:ARG:HG3	1:E:360:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:CYS:HB3	2:H:140:SER:HB3	2.02	0.41
2:B:83:PHE:O	2:B:86:ILE:HG22	2.20	0.41
2:B:220:THR:HB	1:C:326:LYS:HE3	2.02	0.41
1:C:271:THR:OG1	1:C:377:MET:HB3	2.21	0.41
2:D:295:MET:HE1	2:D:332:MET:HE1	2.03	0.41
2:H:66:ILE:HG12	2:H:121:VAL:HG12	2.01	0.41
3:I:6:MET:SD	3:I:22:VAL:HG13	2.61	0.41
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.68	0.40
1:A:12:ALA:CB	1:A:140:SER:HB3	2.52	0.40
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.40
1:G:320:ARG:HG3	1:G:360:PRO:HD3	2.03	0.40
1:C:88:HIS:O	1:C:91:GLN:HG2	2.22	0.40
2:D:345:GLU:H	2:D:345:GLU:HG2	1.58	0.40
2:F:239:THR:O	2:F:243:ARG:HG2	2.22	0.40
2:H:239:THR:O	2:H:243:ARG:HG2	2.21	0.40
2:F:79:ARG:HH22	2:F:94:PHE:HE2	1.69	0.40
1:G:119:LEU:HD11	1:G:156:ARG:HB3	2.02	0.40
1:G:347:CYS:HA	1:G:348:PRO:HD3	1.94	0.40
1:A:209:ILE:HD11	1:A:302:MET:CE	2.51	0.40
2:H:295:MET:HG3	2:H:377:PHE:HD1	1.86	0.40
1:A:355:ILE:HD11	3:I:20:TRP:HH2	1.87	0.40
1:C:320:ARG:HG3	1:C:360:PRO:HD3	2.03	0.40
1:G:210:TYR:CZ	1:G:222:PRO:HD2	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:58:ALA:CB	2:H:89:PRO:O[2_556]	2.04	0.16

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	427/451 (95%)	410 (96%)	15 (4%)	2 (0%)	24	62
1	C	427/451 (95%)	405 (95%)	17 (4%)	5 (1%)	10	43
1	E	427/451 (95%)	406 (95%)	16 (4%)	5 (1%)	10	43
1	G	427/451 (95%)	405 (95%)	17 (4%)	5 (1%)	10	43
2	B	430/445 (97%)	413 (96%)	15 (4%)	2 (0%)	24	62
2	D	430/445 (97%)	413 (96%)	14 (3%)	3 (1%)	18	55
2	F	430/445 (97%)	412 (96%)	15 (4%)	3 (1%)	18	55
2	H	429/445 (96%)	412 (96%)	14 (3%)	3 (1%)	18	55
3	I	230/240 (96%)	192 (84%)	32 (14%)	6 (3%)	4	26
All	All	3657/3824 (96%)	3468 (95%)	155 (4%)	34 (1%)	14	49

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	282	GLN
1	C	348	PRO
2	D	282	GLN
1	E	348	PRO
2	F	282	GLN
1	G	348	PRO
1	A	47	ASP
1	A	437	VAL
1	C	47	ASP
1	C	339	ARG
1	E	47	ASP
1	E	339	ARG
1	G	47	ASP
1	G	339	ARG
2	H	98	GLY
3	I	193	ASN
1	C	280	LYS
1	E	280	LYS
1	G	280	LYS
2	H	280	SER
1	C	283	HIS
2	D	280	SER
2	D	284	ARG
1	E	283	HIS
1	G	283	HIS
3	I	35	PHE

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Mol	Chain	Res	Type
2	B	284	ARG
2	F	280	SER
2	F	284	ARG
2	H	278	ARG
3	I	30	ASP
3	I	96	MET
3	I	97	ALA
3	I	44	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/379 (96%)	345 (94%)	20 (6%)	19	43
1	C	359/379 (95%)	342 (95%)	17 (5%)	23	46
1	E	359/379 (95%)	340 (95%)	19 (5%)	20	44
1	G	359/379 (95%)	340 (95%)	19 (5%)	20	44
2	B	369/383 (96%)	357 (97%)	12 (3%)	33	55
2	D	369/383 (96%)	357 (97%)	12 (3%)	33	55
2	F	369/383 (96%)	356 (96%)	13 (4%)	32	54
2	H	369/383 (96%)	355 (96%)	14 (4%)	29	51
3	I	198/212 (93%)	161 (81%)	37 (19%)	1	10
All	All	3116/3260 (96%)	2953 (95%)	163 (5%)	21	44

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	4	CYS
1	A	46	ASP
1	A	68	VAL
1	A	71	GLU

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Mol	Chain	Res	Type
1	A	73	THR
1	A	113	GLU
1	A	163	LYS
1	A	164	LYS
1	A	188	ILE
1	A	215	ARG
1	A	250	VAL
1	A	316	CYS
1	A	324	VAL
1	A	345	ASP
1	A	358	GLN
1	A	370	LYS
1	A	434	GLU
1	A	435	VAL
2	B	115	VAL
2	B	122	VAL
2	B	128	SER
2	B	158	ARG
2	B	171	VAL
2	B	178	SER
2	B	181	VAL
2	B	241	CYS
2	B	298	SER
2	B	299	LYS
2	B	341	SER
2	B	442	GLU
1	C	4	CYS
1	C	62	VAL
1	C	68	VAL
1	C	71	GLU
1	C	73	THR
1	C	127	ASP
1	C	164	LYS
1	C	188	ILE
1	C	241	SER
1	C	250	VAL
1	C	271	THR
1	C	316	CYS
1	C	324	VAL
1	C	339	ARG
1	C	340	SER
1	C	430	LYS

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Mol	Chain	Res	Type
1	C	435	VAL
2	D	115	VAL
2	D	122	VAL
2	D	128	SER
2	D	158	ARG
2	D	171	VAL
2	D	178	SER
2	D	181	VAL
2	D	241	CYS
2	D	298	SER
2	D	299	LYS
2	D	341	SER
2	D	442	GLU
1	E	1	MET
1	E	4	CYS
1	E	62	VAL
1	E	68	VAL
1	E	71	GLU
1	E	73	THR
1	E	127	ASP
1	E	164	LYS
1	E	188	ILE
1	E	241	SER
1	E	250	VAL
1	E	271	THR
1	E	316	CYS
1	E	324	VAL
1	E	339	ARG
1	E	340	SER
1	E	370	LYS
1	E	430	LYS
1	E	435	VAL
2	F	115	VAL
2	F	122	VAL
2	F	128	SER
2	F	158	ARG
2	F	171	VAL
2	F	178	SER
2	F	181	VAL
2	F	241	CYS
2	F	298	SER
2	F	299	LYS

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Mol	Chain	Res	Type
2	F	325	MET
2	F	341	SER
2	F	442	GLU
1	G	1	MET
1	G	4	CYS
1	G	46	ASP
1	G	62	VAL
1	G	68	VAL
1	G	71	GLU
1	G	73	THR
1	G	127	ASP
1	G	188	ILE
1	G	241	SER
1	G	250	VAL
1	G	271	THR
1	G	316	CYS
1	G	324	VAL
1	G	339	ARG
1	G	340	SER
1	G	370	LYS
1	G	430	LYS
1	G	435	VAL
2	H	115	VAL
2	H	122	VAL
2	H	128	SER
2	H	147	SER
2	H	158	ARG
2	H	171	VAL
2	H	241	CYS
2	H	276	THR
2	H	286	LEU
2	H	295	MET
2	H	299	LYS
2	H	325	MET
2	H	341	SER
2	H	406	HIS
3	I	21	GLU
3	I	29	PHE
3	I	49	GLU
3	I	50	ILE
3	I	53	LYS
3	I	54	LEU

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Mol	Chain	Res	Type
3	I	61	ARG
3	I	75	LYS
3	I	100	LYS
3	I	113	GLU
3	I	120	LEU
3	I	125	GLU
3	I	145	ILE
3	I	150	GLU
3	I	152	LEU
3	I	158	SER
3	I	166	GLN
3	I	172	LYS
3	I	174	LEU
3	I	177	LYS
3	I	184	VAL
3	I	190	GLU
3	I	201	GLU
3	I	203	LEU
3	I	208	GLU
3	I	221	MET
3	I	222	LEU
3	I	223	GLU
3	I	225	LEU
3	I	227	GLU
3	I	229	ASP
3	I	234	GLU
3	I	235	VAL
3	I	236	ARG
3	I	240	GLU
3	I	241	LEU
3	I	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
1	A	256	GLN

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Mol	Chain	Res	Type
1	A	258	ASN
1	A	285	GLN
1	A	301	GLN
1	A	329	ASN
1	A	372	GLN
1	A	393	HIS
2	B	6	HIS
2	B	14	ASN
2	B	50	ASN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	300	ASN
2	B	309	HIS
2	B	334	ASN
2	B	385	GLN
2	B	433	GLN
2	B	436	GLN
1	C	8	HIS
1	C	35	GLN
1	C	50	ASN
1	C	91	GLN
1	C	133	GLN
1	C	139	HIS
1	C	197	HIS
1	C	249	ASN
1	C	256	GLN
1	C	301	GLN
1	C	342	GLN
1	C	393	HIS
2	D	6	HIS
2	D	14	ASN
2	D	50	ASN
2	D	101	ASN
2	D	139	HIS
2	D	206	ASN
2	D	229	HIS
2	D	266	HIS
2	D	300	ASN
2	D	309	HIS
2	D	334	ASN

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Mol	Chain	Res	Type
2	D	349	ASN
2	D	385	GLN
2	D	433	GLN
2	D	436	GLN
1	E	8	HIS
1	E	11	GLN
1	E	35	GLN
1	E	50	ASN
1	E	91	GLN
1	E	107	HIS
1	E	133	GLN
1	E	139	HIS
1	E	197	HIS
1	E	249	ASN
1	E	301	GLN
1	E	393	HIS
2	F	6	HIS
2	F	14	ASN
2	F	50	ASN
2	F	101	ASN
2	F	139	HIS
2	F	206	ASN
2	F	229	HIS
2	F	266	HIS
2	F	300	ASN
2	F	309	HIS
2	F	385	GLN
2	F	433	GLN
2	F	436	GLN
1	G	8	HIS
1	G	35	GLN
1	G	50	ASN
1	G	91	GLN
1	G	133	GLN
1	G	139	HIS
1	G	197	HIS
1	G	249	ASN
1	G	256	GLN
1	G	301	GLN
1	G	329	ASN
1	G	393	HIS
2	H	6	HIS

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Mol	Chain	Res	Type
2	H	14	ASN
2	H	50	ASN
2	H	101	ASN
2	H	133	GLN
2	H	139	HIS
2	H	206	ASN
2	H	247	GLN
2	H	266	HIS
2	H	294	GLN
2	H	300	ASN
2	H	334	ASN
2	H	385	GLN
2	H	433	GLN
3	I	91	ASN
3	I	111	ASN
3	I	162	ASN
3	I	205	GLN
3	I	213	ASN
3	I	231	HIS

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 ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
6	GDP	D	600	-	29,30,30	0.71	1 (3%)	45,47,47	0.64	0
4	GTP	C	600	5	33,34,34	2.02	2 (6%)	50,54,54	0.54	0
6	GDP	B	600	-	29,30,30	0.51	1 (3%)	45,47,47	0.59	0
4	GTP	A	600	5	33,34,34	1.95	3 (9%)	50,54,54	0.51	0
4	GTP	E	600	5	33,34,34	2.14	2 (6%)	50,54,54	0.52	0
6	GDP	F	600	-	29,30,30	0.47	0	45,47,47	0.65	0
4	GTP	G	600	5	33,34,34	1.99	3 (9%)	50,54,54	0.58	0
6	GDP	H	600	-	29,30,30	0.59	1 (3%)	45,47,47	0.68	0

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
6	GDP	D	600	-	-	5/16/32/32	0/3/3/3
4	GTP	C	600	5	-	6/22/38/38	0/3/3/3
6	GDP	B	600	-	-	5/16/32/32	0/3/3/3
4	GTP	A	600	5	-	6/22/38/38	0/3/3/3
4	GTP	E	600	5	-	6/22/38/38	0/3/3/3
6	GDP	F	600	-	-	5/16/32/32	0/3/3/3
4	GTP	G	600	5	-	6/22/38/38	0/3/3/3
6	GDP	H	600	-	-	5/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	600	GTP	PB-O3B	-8.65	1.50	1.59
4	G	600	GTP	PB-O3B	-8.60	1.50	1.59
4	C	600	GTP	PB-O3B	-8.37	1.50	1.59
4	E	600	GTP	PA-O3A	-8.16	1.50	1.59
4	A	600	GTP	PB-O3B	-7.69	1.51	1.59
4	C	600	GTP	PA-O3A	-7.43	1.51	1.59
4	A	600	GTP	PA-O3A	-7.40	1.51	1.59
4	G	600	GTP	PA-O3A	-6.69	1.52	1.59
6	D	600	GDP	PB-O1B	3.31	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	600	GDP	PB-O2B	2.22	1.63	1.54
4	G	600	GTP	PB-O3A	2.12	1.61	1.59
4	A	600	GTP	PB-O3A	2.05	1.61	1.59
6	B	600	GDP	PB-O1B	2.04	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O1A
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
4	E	600	GTP	PB-O3B-PG-O3G
4	E	600	GTP	C5'-O5'-PA-O3A
4	E	600	GTP	C5'-O5'-PA-O1A
4	E	600	GTP	C5'-O5'-PA-O2A
4	G	600	GTP	PB-O3B-PG-O3G
4	G	600	GTP	C5'-O5'-PA-O3A
4	G	600	GTP	C5'-O5'-PA-O1A
4	G	600	GTP	C5'-O5'-PA-O2A
6	B	600	GDP	C5'-O5'-PA-O3A
6	B	600	GDP	C5'-O5'-PA-O1A
6	B	600	GDP	C5'-O5'-PA-O2A
6	D	600	GDP	C5'-O5'-PA-O3A
6	D	600	GDP	C5'-O5'-PA-O1A
6	D	600	GDP	C5'-O5'-PA-O2A
6	F	600	GDP	C5'-O5'-PA-O3A
6	F	600	GDP	C5'-O5'-PA-O1A
6	F	600	GDP	C5'-O5'-PA-O2A
6	H	600	GDP	C5'-O5'-PA-O3A
6	H	600	GDP	C5'-O5'-PA-O1A
6	H	600	GDP	C5'-O5'-PA-O2A
4	A	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	PB-O3B-PG-O3G
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
4	E	600	GTP	PB-O3A-PA-O2A

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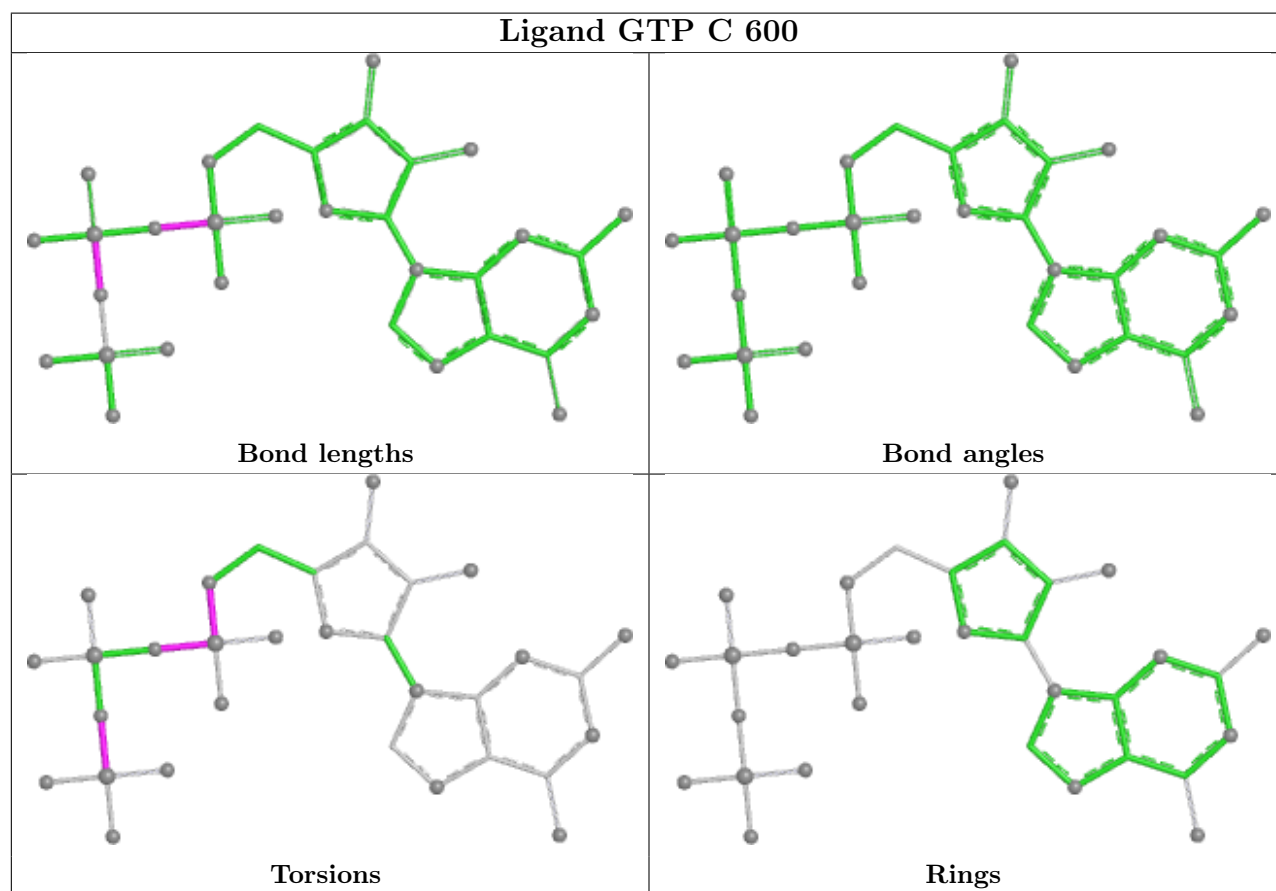
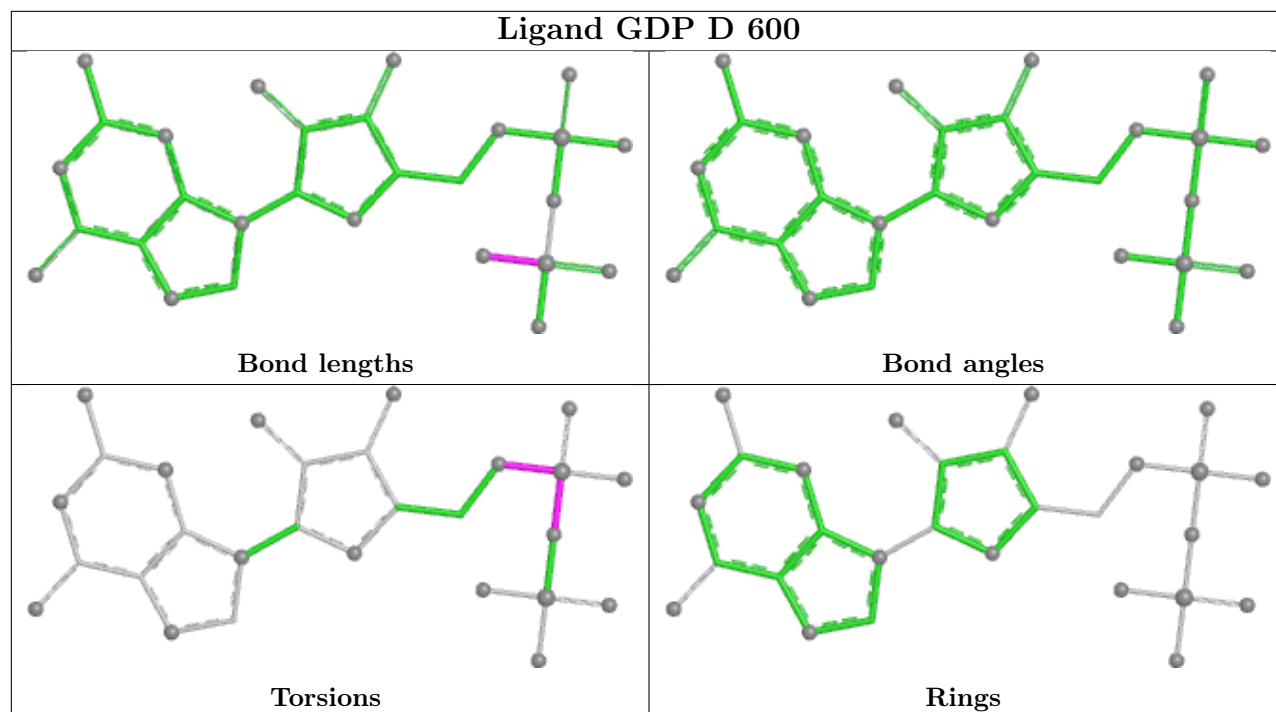
Mol	Chain	Res	Type	Atoms
4	G	600	GTP	PB-O3A-PA-O2A
6	H	600	GDP	PB-O3A-PA-O2A
6	B	600	GDP	PB-O3A-PA-O2A
6	F	600	GDP	PB-O3A-PA-O2A
4	A	600	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O1A
6	B	600	GDP	PB-O3A-PA-O1A
6	D	600	GDP	PB-O3A-PA-O1A
6	D	600	GDP	PB-O3A-PA-O2A
4	E	600	GTP	PB-O3A-PA-O1A
4	G	600	GTP	PB-O3A-PA-O1A
6	F	600	GDP	PB-O3A-PA-O1A
6	H	600	GDP	PB-O3A-PA-O1A

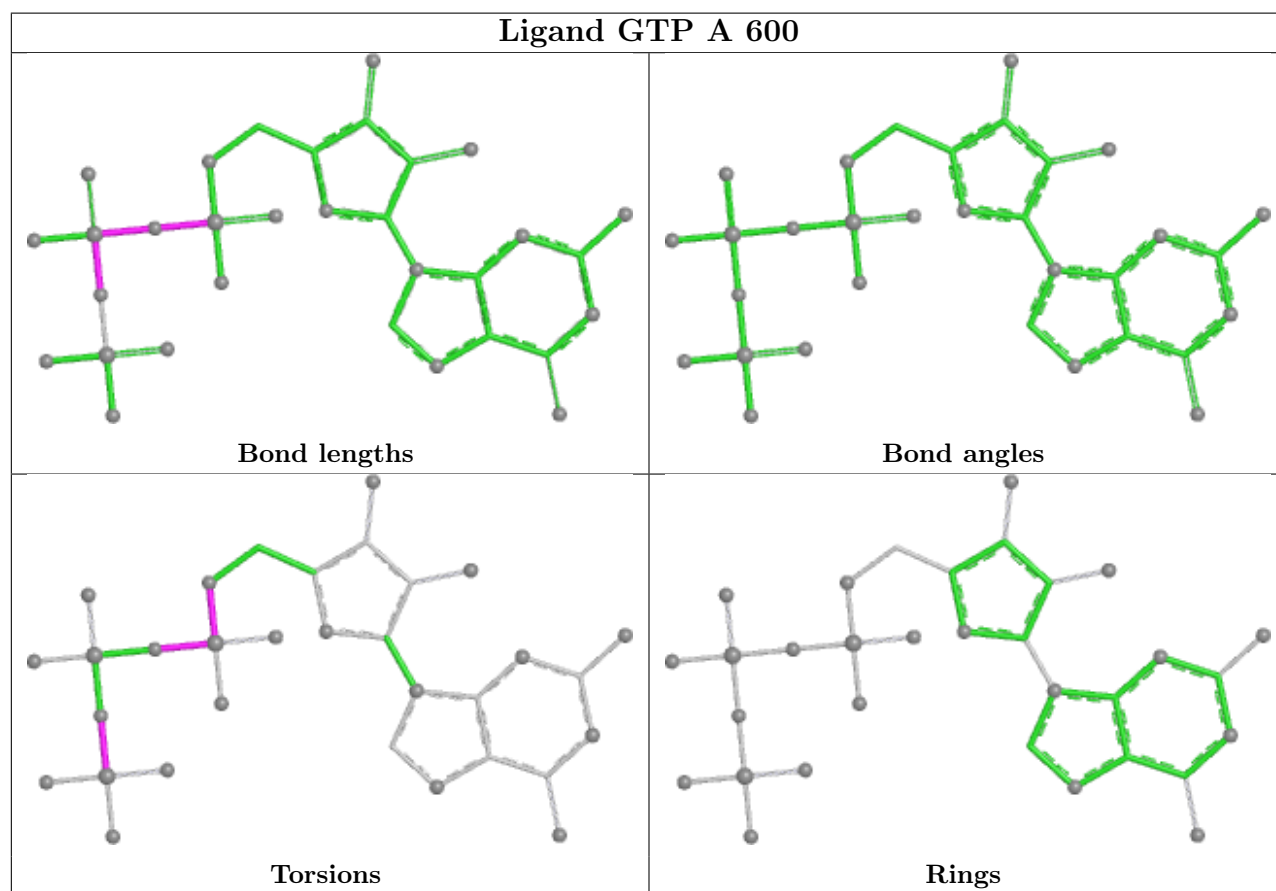
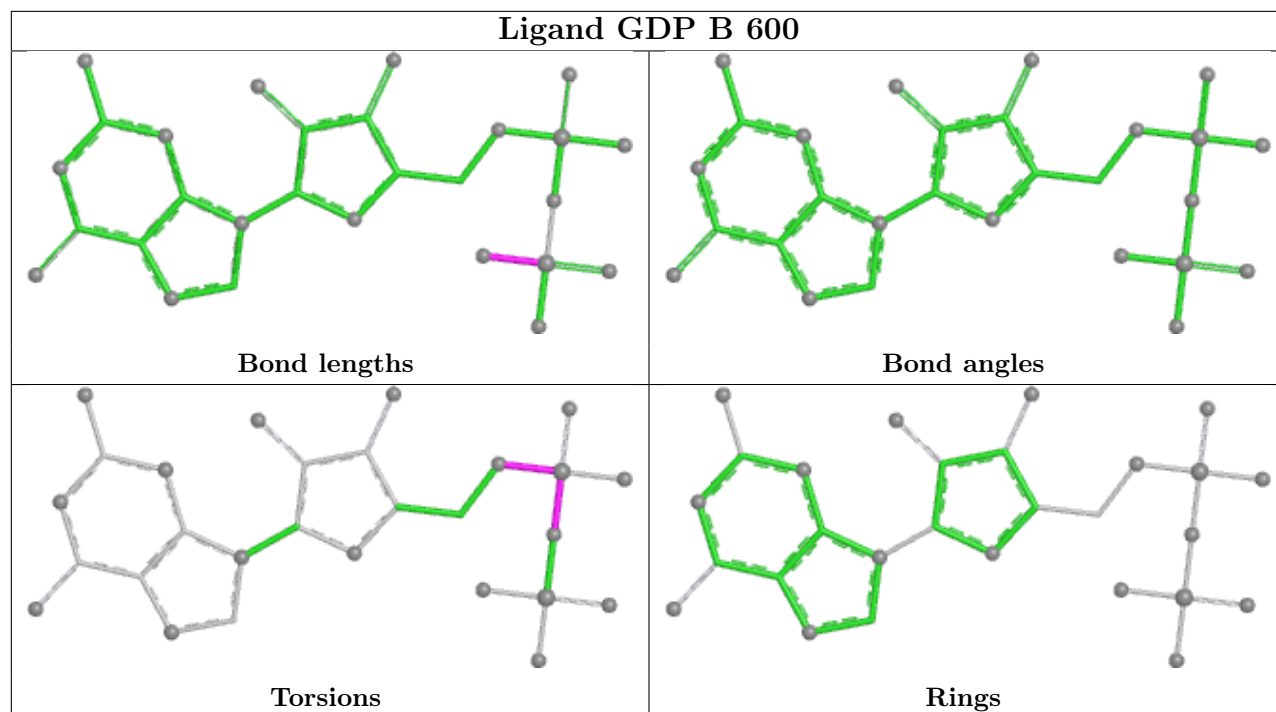
There are no ring outliers.

4 monomers are involved in 4 short contacts:

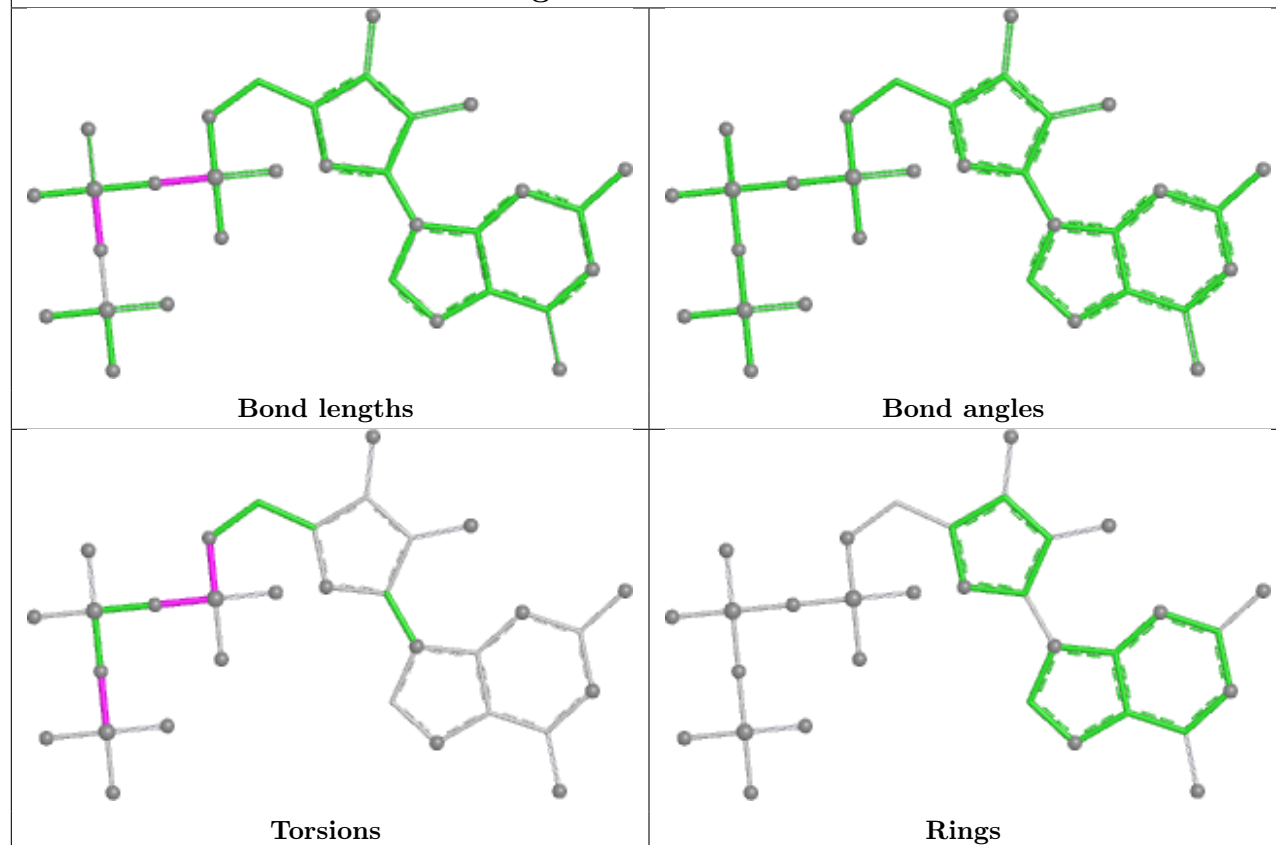
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	600	GDP	1	0
6	B	600	GDP	1	0
6	F	600	GDP	1	0
6	H	600	GDP	1	0

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.

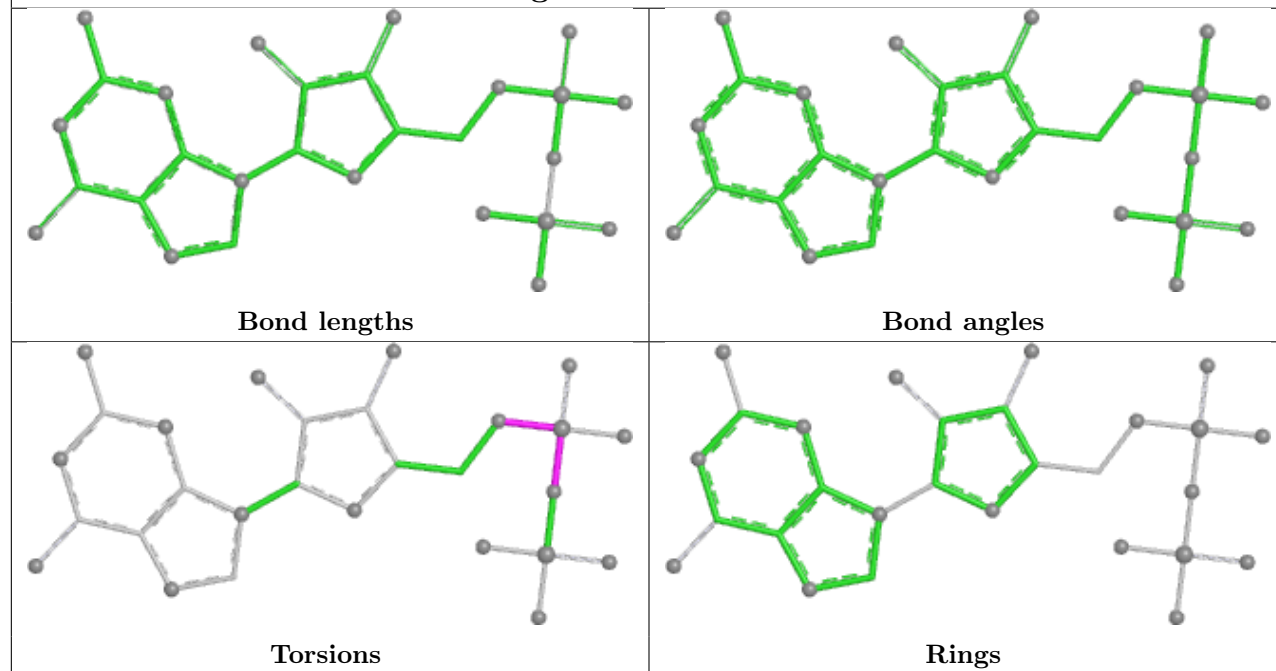


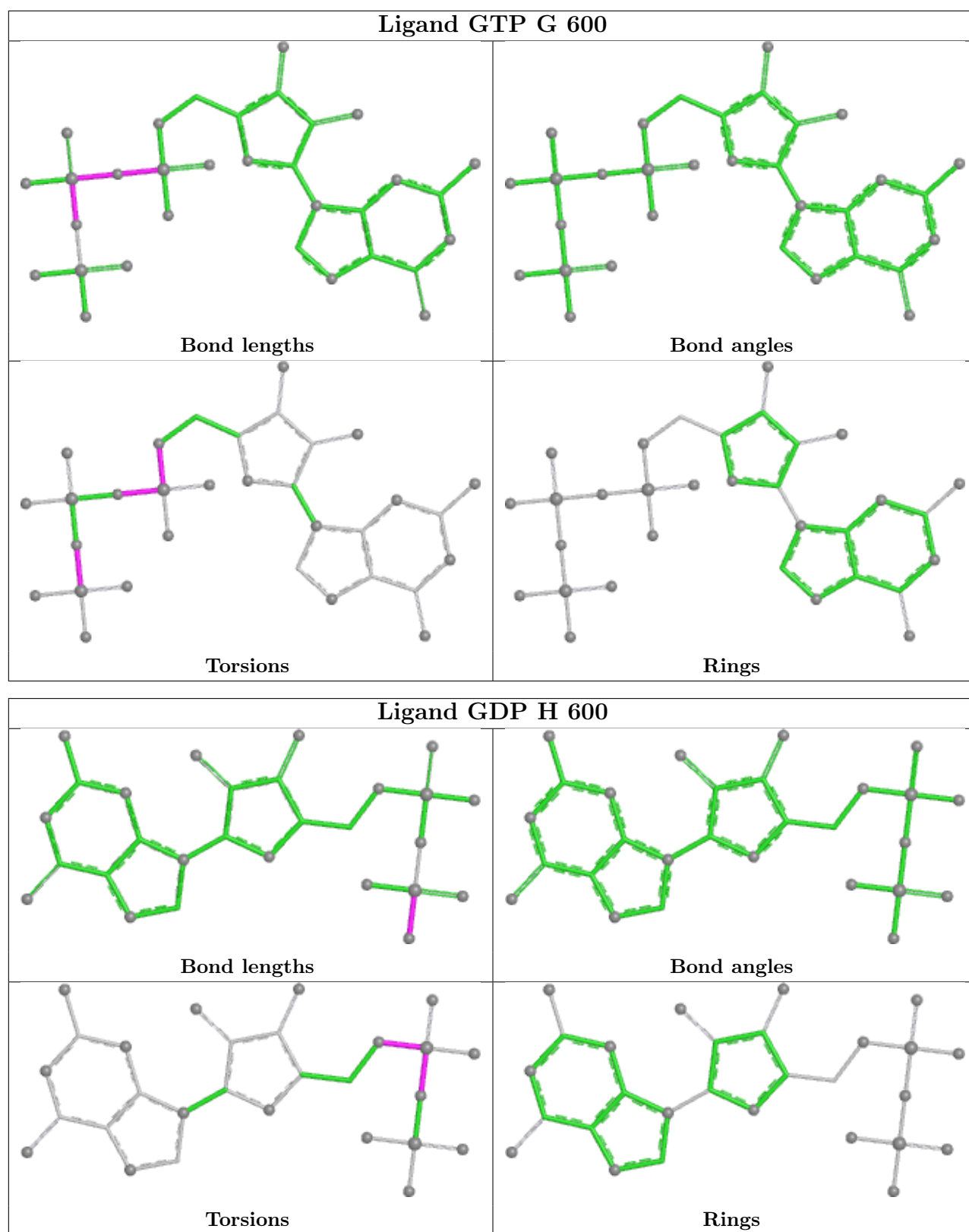


Ligand GTP E 600



Ligand GDP F 600





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	431/451 (95%)	-0.08	4 (0%) 81 66	95, 145, 234, 287	0
1	C	431/451 (95%)	-0.03	8 (1%) 66 51	154, 217, 276, 289	0
1	E	431/451 (95%)	-0.13	8 (1%) 66 51	164, 208, 281, 287	0
1	G	431/451 (95%)	0.01	7 (1%) 70 54	99, 149, 278, 291	0
2	B	432/445 (97%)	-0.09	7 (1%) 70 54	95, 150, 261, 300	0
2	D	432/445 (97%)	-0.15	6 (1%) 73 57	158, 211, 281, 284	0
2	F	432/445 (97%)	-0.18	4 (0%) 81 66	147, 187, 282, 291	0
2	H	431/445 (96%)	-0.11	0 100 100	71, 116, 178, 274	0
3	I	234/240 (97%)	-0.32	0 100 100	108, 193, 273, 291	0
All	All	3685/3824 (96%)	-0.11	44 (1%) 76 61	71, 178, 278, 300	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	180	ALA	5.8
1	C	179	THR	5.7
1	A	179	THR	4.5
1	G	276	ILE	3.8
2	B	180	THR	3.6
1	G	70	LEU	3.3
1	E	256	GLN	3.2
1	G	155	GLU	3.2
2	B	248	LEU	3.2
1	G	179	THR	3.1
2	D	408	TYR	3.0
2	D	381	SER	2.9
2	D	248	LEU	2.8
1	C	260	VAL	2.8
1	C	238	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	182	VAL	2.7
1	C	256	GLN	2.7
2	D	418	PHE	2.6
1	G	101	ASN	2.5
1	A	182	VAL	2.5
2	F	154	ILE	2.5
1	E	101	ASN	2.5
1	E	199	ASP	2.5
1	C	257	THR	2.4
1	C	349	THR	2.4
1	E	255	PHE	2.4
2	F	257	VAL	2.4
2	B	404	PHE	2.3
2	F	258	ASN	2.3
2	F	18	ALA	2.3
1	A	435	VAL	2.3
1	A	292	THR	2.2
1	C	117	LEU	2.2
1	E	252	LEU	2.2
1	G	142	GLY	2.2
1	E	173	PRO	2.1
2	B	418	PHE	2.1
1	E	260	VAL	2.1
2	B	258	ASN	2.1
2	D	353	THR	2.1
2	D	165	ILE	2.0
1	G	197	HIS	2.0
2	B	179	ASP	2.0
1	E	352	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

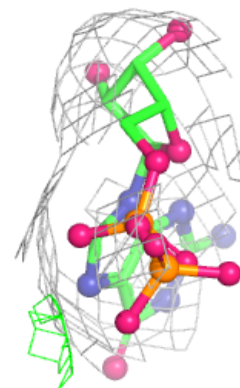
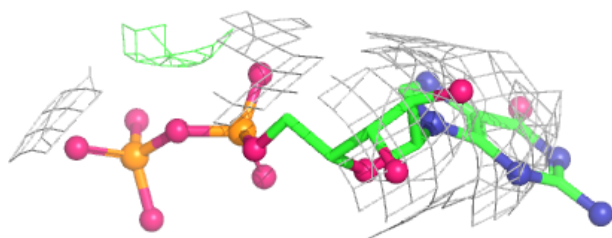
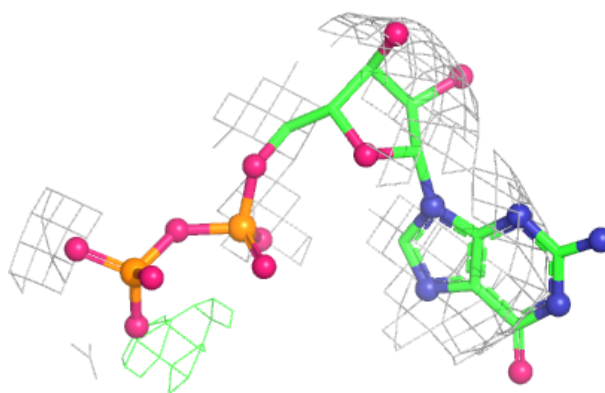
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	G	601	1/1	0.70	0.20	105,105,105,105	0
5	MG	C	601	1/1	0.73	0.19	181,181,181,181	0
6	GDP	D	600	28/28	0.77	0.11	175,181,190,195	0
5	MG	A	601	1/1	0.80	0.17	102,102,102,102	0
6	GDP	B	600	28/28	0.86	0.09	117,126,131,134	0
6	GDP	F	600	28/28	0.89	0.09	153,157,163,165	0
6	GDP	H	600	28/28	0.89	0.10	85,92,96,99	0
5	MG	E	601	1/1	0.91	0.10	175,175,175,175	0
4	GTP	A	600	32/32	0.91	0.08	99,105,112,115	0
4	GTP	G	600	32/32	0.91	0.09	100,104,115,116	0
4	GTP	C	600	32/32	0.92	0.10	169,176,188,193	0
4	GTP	E	600	32/32	0.96	0.06	168,174,185,188	0

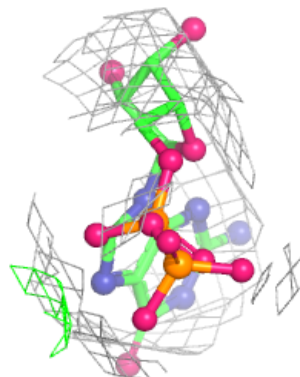
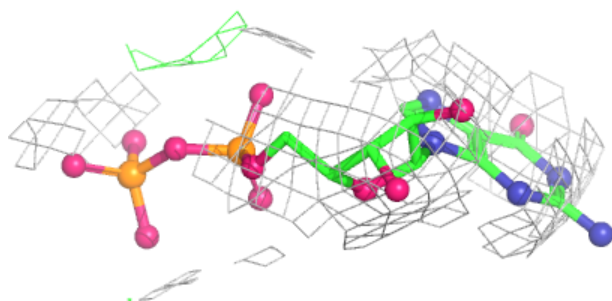
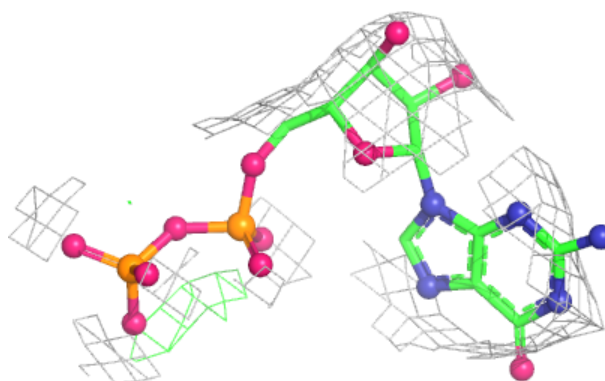
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP D 600:

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

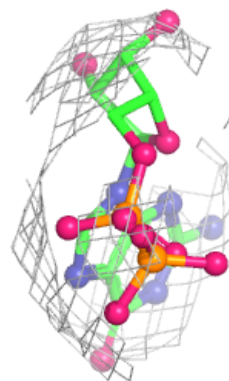
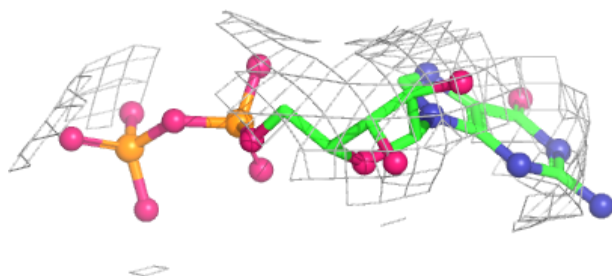
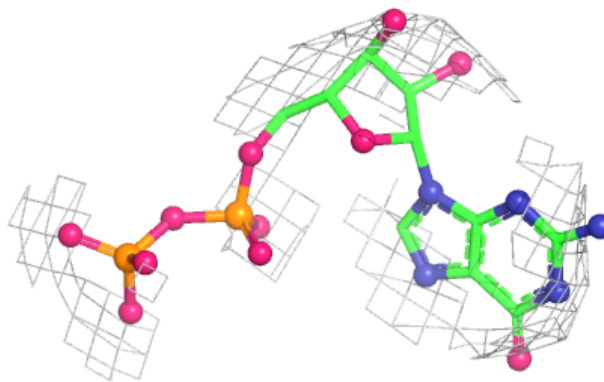
**Electron density around GDP B 600:**

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



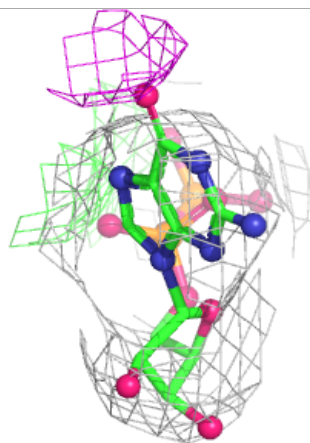
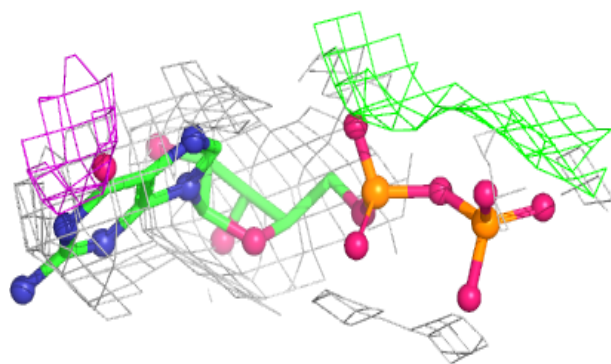
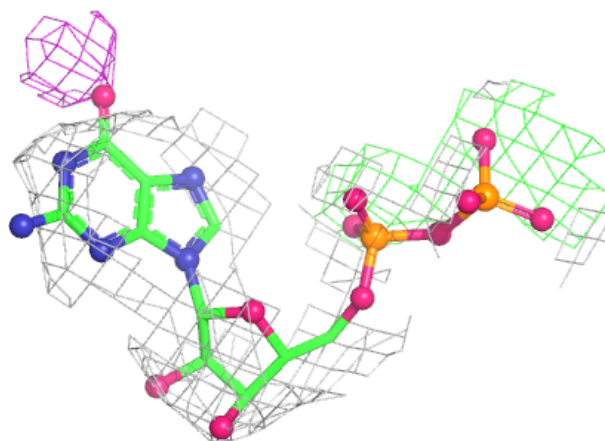
Electron density around GDP F 600:

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



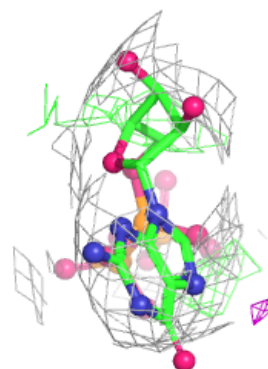
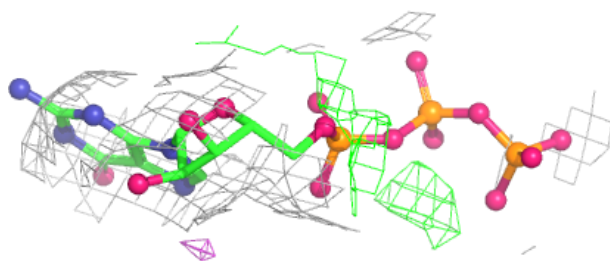
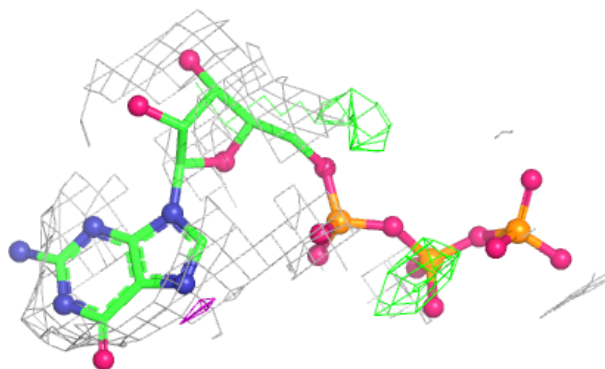
Electron density around GDP H 600:

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

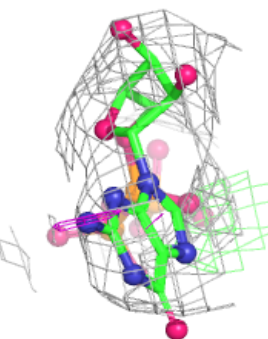
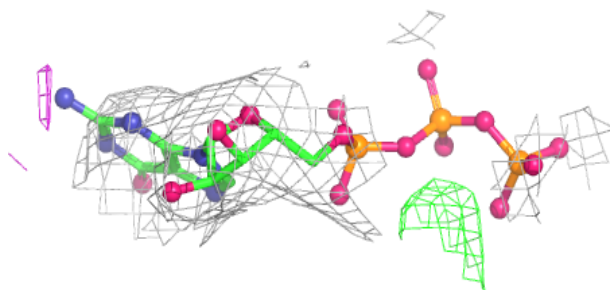
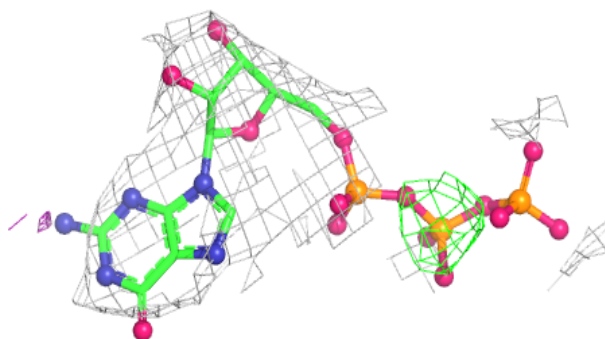


Electron density around GTP A 600:

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

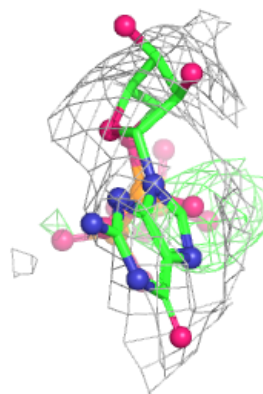
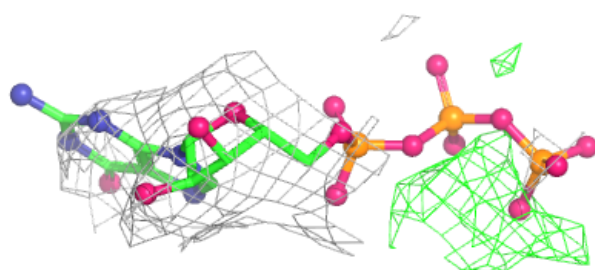
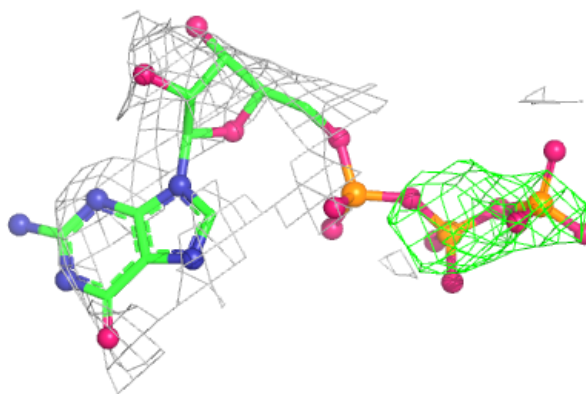
**Electron density around GTP G 600:**

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

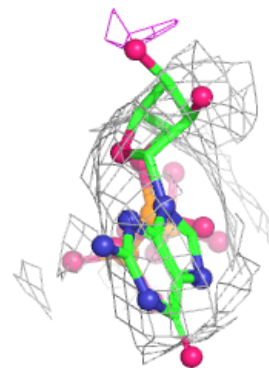
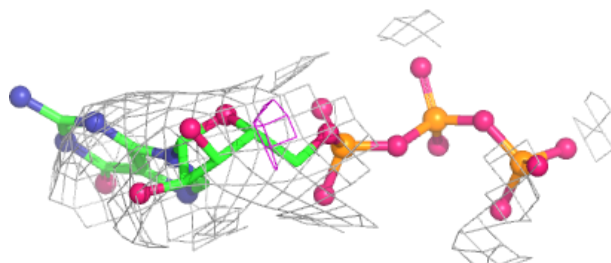
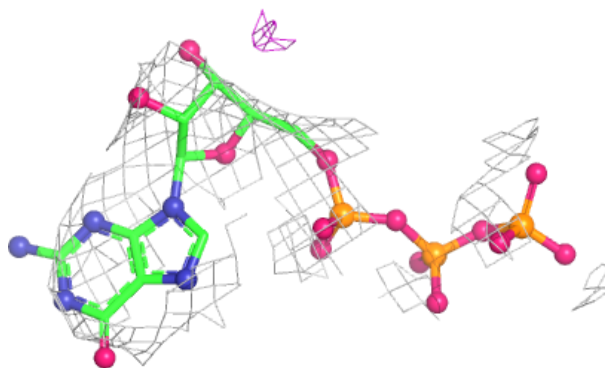


Electron density around GTP C 600:

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

**Electron density around GTP E 600:**

$2mF_o-DF_c$ (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.