



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:28 AM UTC

PDB ID : 4V0M / pdb_00004v0m
Title : Crystal structure of BBS1N in complex with ARL6DN
Authors : Mourao, A.; Lorentzen, E.
Deposited on : 2014-09-17
Resolution : 3.45 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

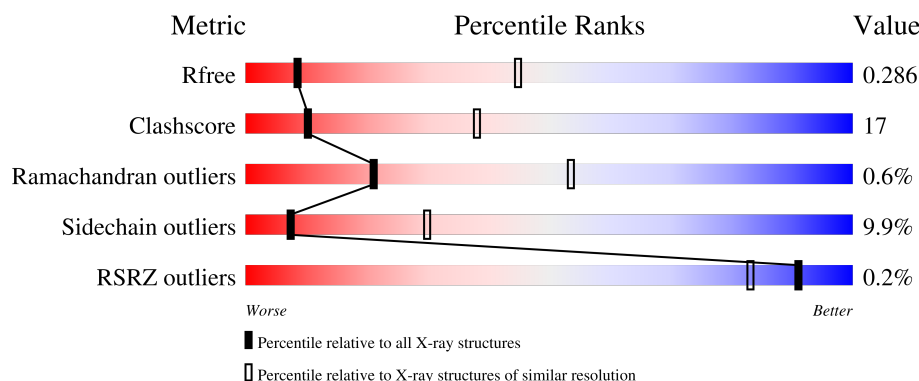
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	169	% 67% 29% ..
1	C	169	66% 28% 5% .
1	G	169	% 69% 25% ..
2	B	425	46% 27% .. 22%
2	D	425	43% 26% . 29%

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Mol	Chain	Length	Quality of chain
2	F	425	47%24%•27%
2	H	425	38%31%7%•24%
3	E	169	65%28%5%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14402 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 ARF-LIKE SMALL GTPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1255	800	214	235	6			
1	C	166	Total	C	N	O	S	0	0	0
			1291	823	223	239	6			
1	G	166	Total	C	N	O	S	0	0	0
			1285	822	221	236	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP A8JF99
A	13	ALA	-	expression tag	UNP A8JF99
A	14	ALA	-	expression tag	UNP A8JF99
A	15	SER	-	expression tag	UNP A8JF99
C	12	GLY	-	expression tag	UNP A8JF99
C	13	ALA	-	expression tag	UNP A8JF99
C	14	ALA	-	expression tag	UNP A8JF99
C	15	SER	-	expression tag	UNP A8JF99
G	12	GLY	-	expression tag	UNP A8JF99
G	13	ALA	-	expression tag	UNP A8JF99
G	14	ALA	-	expression tag	UNP A8JF99
G	15	SER	-	expression tag	UNP A8JF99

- Molecule 2 is a protein called BARDET-BIEDL SYNDROME 1 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	333	Total	C	N	O	S	0	0	0
			2428	1551	422	442	13			
2	D	303	Total	C	N	O	S	0	0	0
			2151	1360	379	400	12			
2	F	309	Total	C	N	O	S	0	0	0
			2198	1396	382	407	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	325	Total	C	N	O	S	0	0	0
			2384	1525	411	435	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	ARG	LYS	conflict	UNP A8JEA1
D	37	ARG	LYS	conflict	UNP A8JEA1
F	37	ARG	LYS	conflict	UNP A8JEA1
H	37	ARG	LYS	conflict	UNP A8JEA1

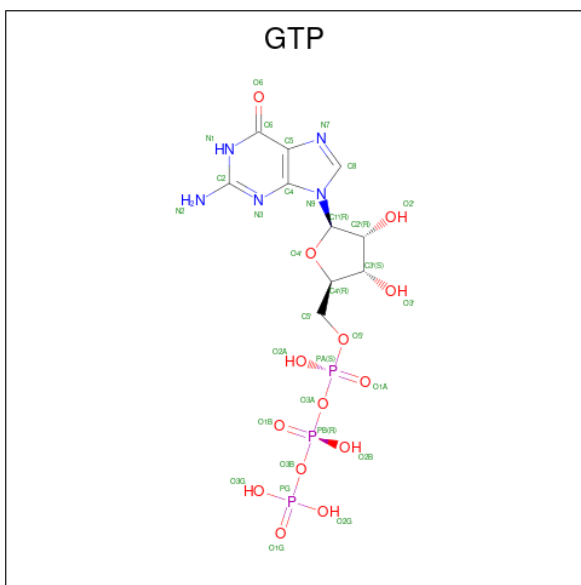
- Molecule 3 is a protein called ARF-LIKE SMALL GTPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1278	816	219	237	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	12	GLY	-	expression tag	UNP A8JF99
E	13	ALA	-	expression tag	UNP A8JF99
E	14	ALA	-	expression tag	UNP A8JF99
E	15	SER	-	expression tag	UNP A8JF99
E	132	ILE	LEU	conflict	UNP A8JF99

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

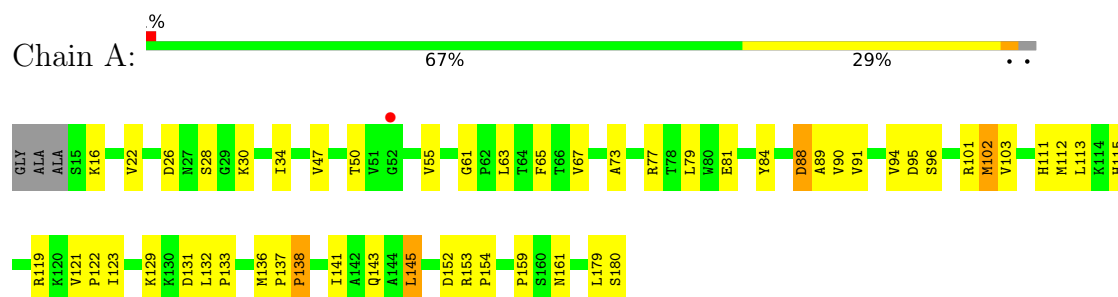
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

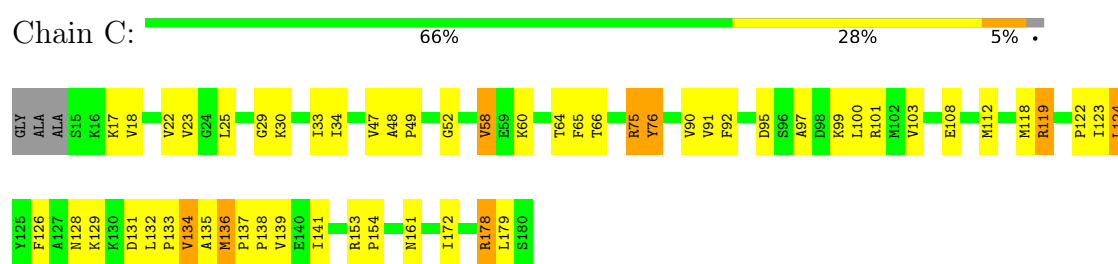
3 Residue-property plots [i](#)

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.

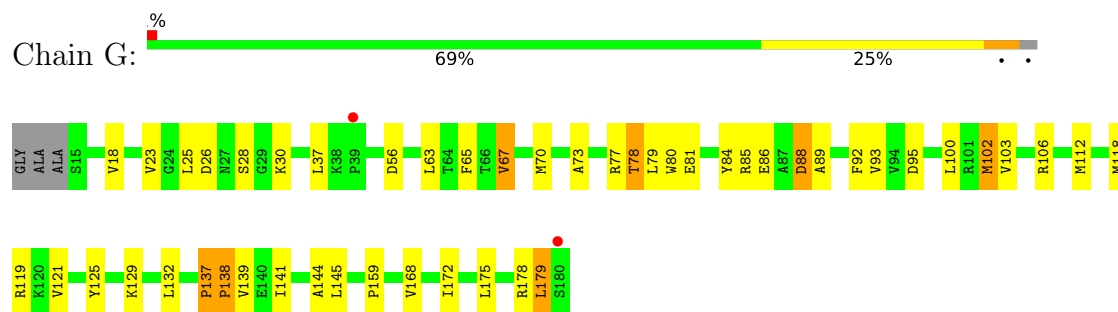
• Molecule 1: ARF-LIKE SMALL GTPASE



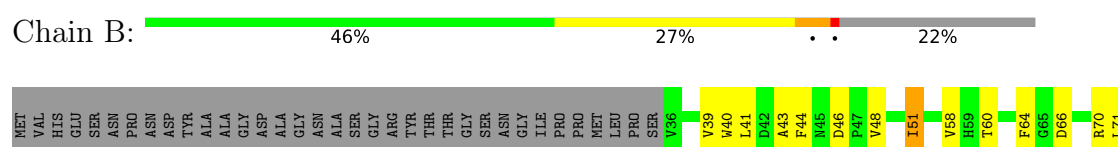
• Molecule 1: ARF-LIKE SMALL GTPASE

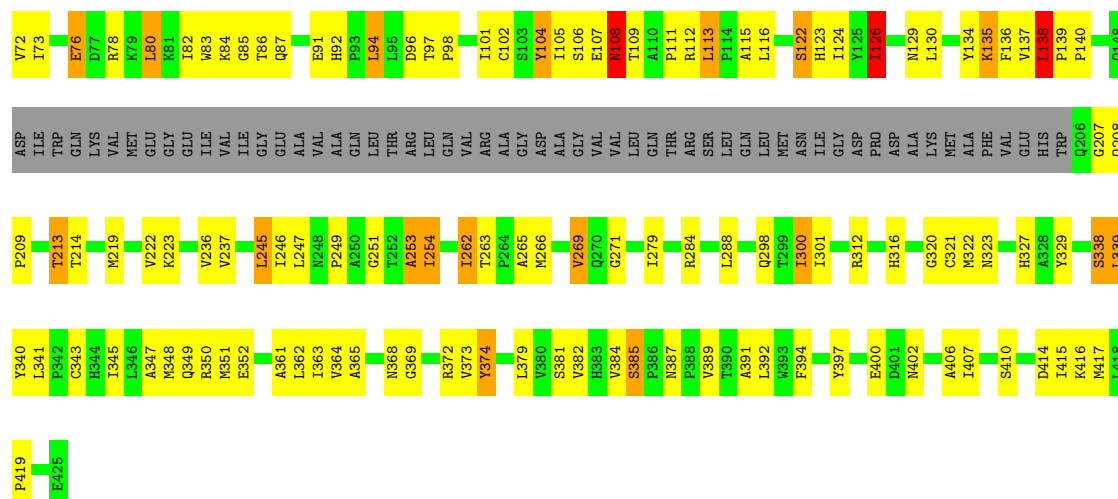


• Molecule 1: ARF-LIKE SMALL GTPASE



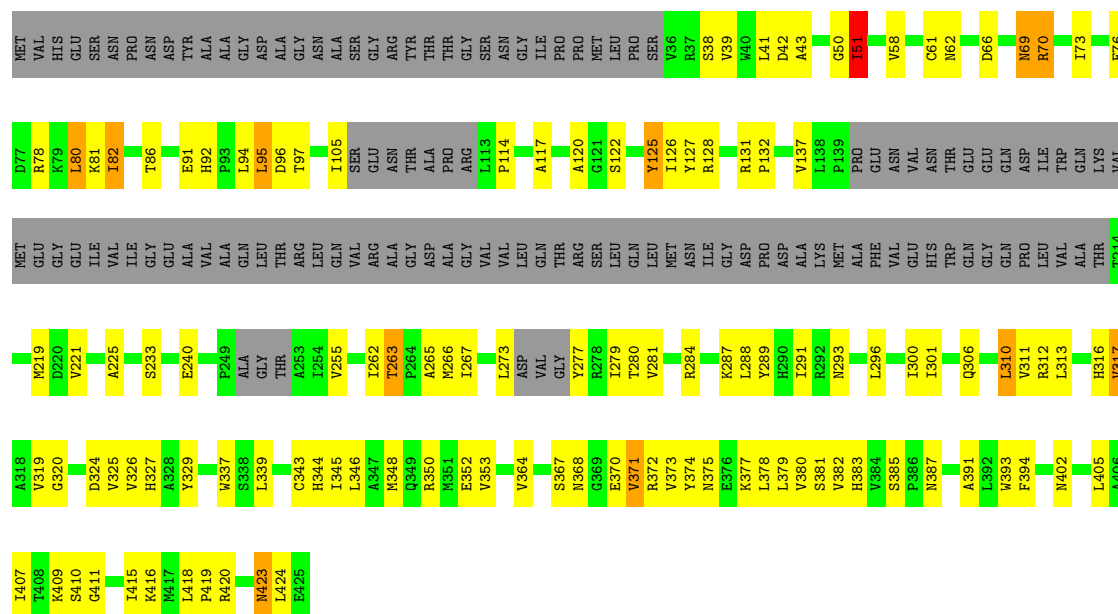
• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN





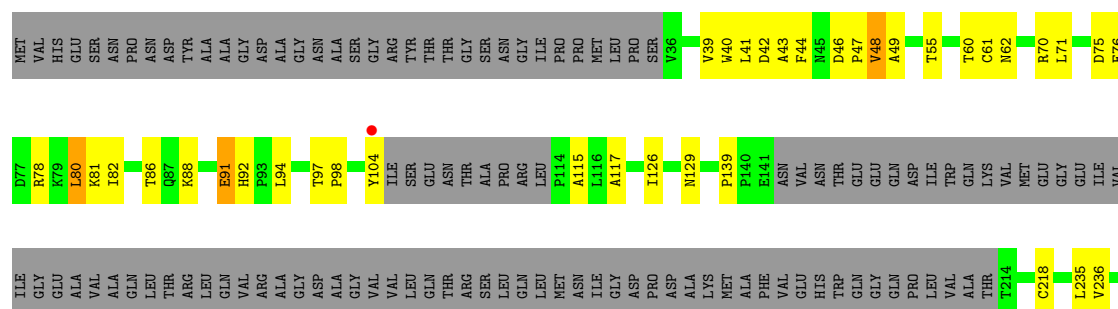
• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

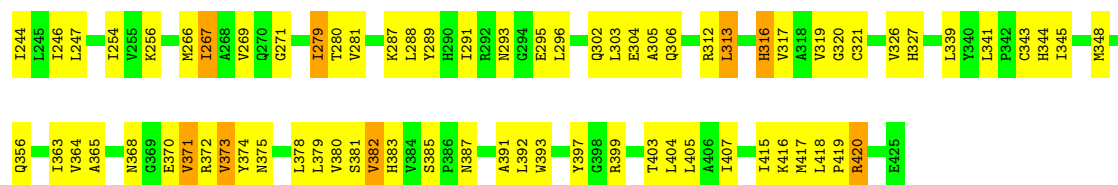
Chain D: 43% 26% • 29%



• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

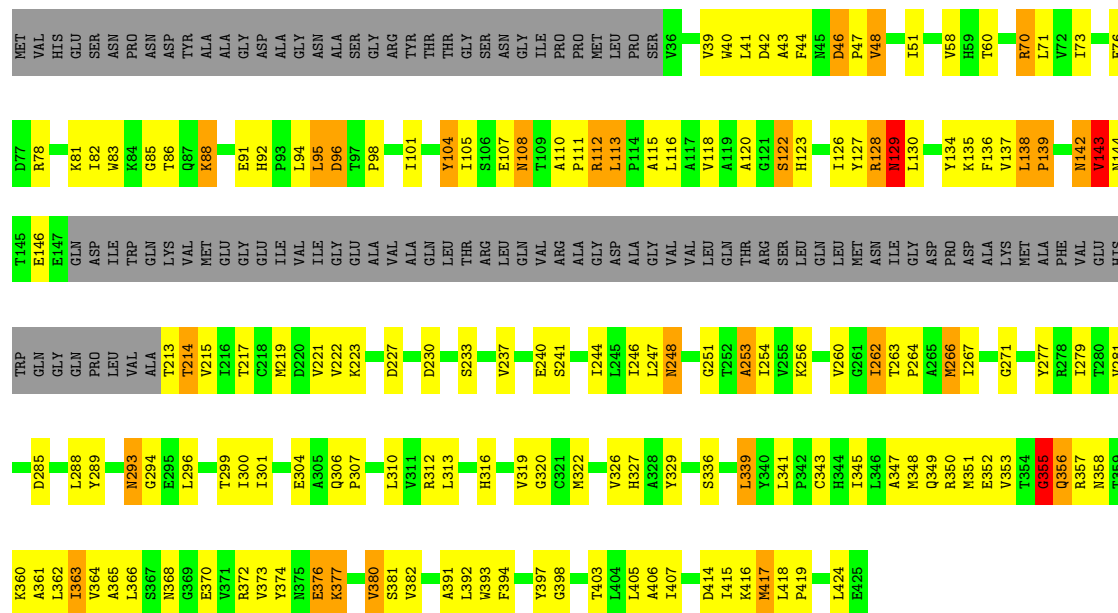
Chain F: 47% 24% • 27%





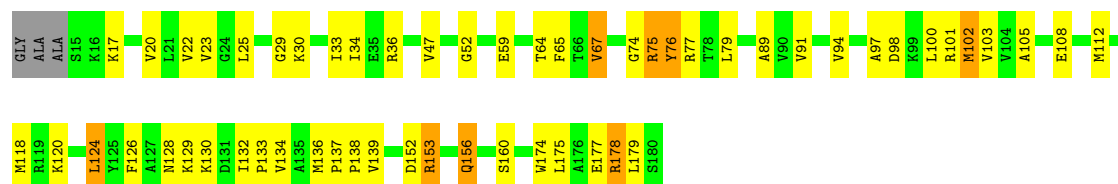
• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

Chain H: 38% 31% 7% 24%



• Molecule 3: ARF-LIKE SMALL GTPASE

Chain E: 65% 28% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.78Å 124.78Å 441.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.13 – 3.45 87.13 – 3.45	Depositor EDS
% Data completeness (in resolution range)	96.2 (87.13-3.45) 96.2 (87.13-3.45)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.41Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.281 0.233 , 0.286	Depositor DCC
R_{free} test set	2652 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	126.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 86.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.073 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14402	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: GTP, MG

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	0.60	0/1280	1.05	5/1745 (0.3%)
1	C	0.73	0/1317	1.17	4/1788 (0.2%)
1	G	0.58	0/1311	0.96	4/1780 (0.2%)
2	B	0.78	0/2480	1.25	21/3398 (0.6%)
2	D	0.68	0/2190	1.13	9/3001 (0.3%)
2	F	0.65	0/2240	1.17	11/3069 (0.4%)
2	H	0.81	0/2435	1.31	28/3337 (0.8%)
3	E	0.70	0/1304	1.13	6/1773 (0.3%)
All	All	0.71	0/14557	1.17	88/19891 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	H	0	2
All	All	0	3

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	127	TYR	N-CA-C	11.03	126.56	112.89
2	B	208	GLN	N-CA-C	10.38	124.40	110.08
1	C	136	MET	CA-C-N	10.29	130.98	120.38
1	C	136	MET	C-N-CA	10.29	130.98	120.38
2	F	139	PRO	CA-C-N	-10.11	109.93	120.85
2	F	139	PRO	C-N-CA	-10.11	109.93	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	208	GLN	CA-C-N	9.11	131.22	119.84
2	B	208	GLN	C-N-CA	9.11	131.22	119.84
2	B	113	LEU	CA-C-N	-9.04	110.80	120.66
2	B	113	LEU	C-N-CA	-9.04	110.80	120.66
2	H	113	LEU	CA-C-N	-8.84	111.30	120.85
2	H	113	LEU	C-N-CA	-8.84	111.30	120.85
2	H	129	ASN	N-CA-C	8.67	121.42	109.54
2	H	271	GLY	N-CA-C	8.29	121.14	110.20
2	B	341	LEU	CA-C-N	8.14	127.81	119.19
2	B	341	LEU	C-N-CA	8.14	127.81	119.19
2	B	271	GLY	N-CA-C	7.43	119.80	110.29
2	H	356	GLN	N-CA-C	-7.33	98.11	109.76
3	E	136	MET	CA-C-N	7.19	127.78	120.38
3	E	136	MET	C-N-CA	7.19	127.78	120.38
1	A	137	PRO	CA-C-N	7.15	128.78	119.84
1	A	137	PRO	C-N-CA	7.15	128.78	119.84
2	H	306	GLN	CA-C-N	7.13	127.69	119.99
2	H	306	GLN	C-N-CA	7.13	127.69	119.99
2	D	380	VAL	CB-CA-C	-6.91	104.14	110.91
2	D	97	THR	CA-C-N	6.89	127.07	120.31
2	D	97	THR	C-N-CA	6.89	127.07	120.31
2	D	51	ILE	N-CA-C	6.87	117.91	108.84
2	D	255	VAL	N-CA-C	6.76	117.62	111.81
1	A	55	VAL	N-CA-C	6.63	117.26	106.72
2	H	380	VAL	N-CA-C	-6.62	107.42	113.71
2	B	46	ASP	CA-C-N	6.55	126.14	119.19
2	B	46	ASP	C-N-CA	6.55	126.14	119.19
2	H	355	GLY	N-CA-C	-6.36	102.79	112.84
2	F	420	ARG	N-CA-C	-6.36	104.45	111.82
2	B	51	ILE	N-CA-C	6.33	116.61	108.12
2	F	40	TRP	N-CA-C	6.17	119.62	110.48
2	F	271	GLY	N-CA-C	6.09	118.24	110.20
2	F	341	LEU	N-CA-C	6.04	117.68	110.07
2	H	46	ASP	CA-C-N	5.97	125.52	119.19
2	H	46	ASP	C-N-CA	5.97	125.52	119.19
2	B	262	ILE	N-CA-C	5.79	117.25	108.80
1	G	88	ASP	N-CA-C	-5.72	106.28	113.72
2	F	97	THR	CA-C-N	5.65	125.85	120.31
2	F	97	THR	C-N-CA	5.65	125.85	120.31
2	H	110	ALA	CA-C-N	5.65	126.90	119.84
2	H	110	ALA	C-N-CA	5.65	126.90	119.84
1	A	61	GLY	CA-C-N	5.64	125.32	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	GLY	C-N-CA	5.64	125.32	119.56
2	H	128	ARG	N-CA-C	5.62	116.85	108.31
2	H	146	GLU	N-CA-C	5.61	118.39	109.81
2	B	126	ILE	N-CA-C	5.60	115.62	108.12
2	D	378	LEU	N-CA-C	5.60	118.61	109.59
1	C	90	VAL	N-CA-C	5.58	115.92	108.11
2	B	76	GLU	N-CA-C	-5.55	106.27	113.16
2	H	248	ASN	N-CA-C	-5.54	102.65	110.29
2	H	253	ALA	N-CA-C	5.52	117.24	108.79
2	B	253	ALA	N-CA-C	5.50	117.21	108.79
2	B	384	VAL	N-CA-C	5.50	115.91	107.77
3	E	67	VAL	N-CA-C	5.48	116.20	108.36
1	G	137	PRO	CA-C-N	5.47	126.68	119.84
1	G	137	PRO	C-N-CA	5.47	126.68	119.84
2	H	254	ILE	N-CA-C	5.43	116.70	109.37
2	F	91	GLU	N-CA-C	-5.42	101.11	109.52
2	H	139	PRO	CA-C-N	5.36	126.64	120.85
2	H	139	PRO	C-N-CA	5.36	126.64	120.85
3	E	160	SER	N-CA-C	5.33	115.58	108.38
2	H	262	ILE	N-CA-C	5.33	117.31	108.99
2	H	51	ILE	N-CA-C	5.33	115.26	108.12
2	B	108	ASN	N-CA-C	-5.32	106.86	113.19
2	F	378	LEU	N-CA-C	5.31	118.46	109.76
2	H	112	ARG	N-CA-C	5.30	122.10	110.80
2	B	126	ILE	CB-CA-C	-5.25	105.63	111.35
2	H	142	ASN	N-CA-C	5.23	117.62	109.52
2	H	214	THR	N-CA-C	5.22	118.08	109.72
2	B	138	LEU	CA-C-N	5.15	125.69	120.38
2	B	138	LEU	C-N-CA	5.15	125.69	120.38
2	F	397	TYR	N-CA-C	-5.13	101.28	109.23
2	H	336	SER	N-CA-C	5.12	116.71	111.03
3	E	137	PRO	CA-C-N	5.11	126.22	119.84
3	E	137	PRO	C-N-CA	5.11	126.22	119.84
2	D	263	THR	CA-C-N	5.09	125.88	120.13
2	D	263	THR	C-N-CA	5.09	125.88	120.13
2	B	254	ILE	N-CA-C	5.07	116.22	109.37
1	C	135	ALA	N-CA-C	5.06	117.37	110.24
2	D	409	LYS	N-CA-C	-5.06	106.21	112.38
2	H	363	ILE	N-CA-C	-5.05	101.14	108.97
1	G	67	VAL	N-CA-C	5.01	115.53	108.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	207	GLY	Peptide
2	H	355	GLY	Peptide
2	H	356	GLN	Peptide

5.2 Too-close contacts [i](#)

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	1255	0	1230	35	0
1	C	1291	0	1297	45	0
1	G	1285	0	1291	37	0
2	B	2428	0	2360	92	0
2	D	2151	0	2018	73	0
2	F	2198	0	2098	70	0
2	H	2384	0	2330	108	0
3	E	1278	0	1273	45	0
4	A	32	0	12	6	0
4	C	32	0	12	4	0
4	E	32	0	12	3	0
4	G	32	0	12	2	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
All	All	14402	0	13945	485	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:HB3	1:C:132:LEU:HD12	1.53	0.90
2:H:349:GLN:NE2	2:H:392:LEU:O	2.08	0.86
2:D:345:ILE:HG21	2:D:348:MET:HE2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:VAL:HG13	2:D:381:SER:HB2	1.58	0.84
2:B:320:GLY:HA3	2:B:348:MET:HE1	1.58	0.84
2:H:320:GLY:HA3	2:H:348:MET:HE1	1.58	0.83
2:F:304:GLU:OE2	2:F:327:HIS:NE2	2.13	0.78
2:H:39:VAL:HG13	2:H:381:SER:HB2	1.63	0.78
1:C:30:LYS:N	4:C:600:GTP:O1B	2.12	0.78
2:B:345:ILE:HG21	2:B:348:MET:HE2	1.65	0.78
2:H:345:ILE:HG21	2:H:348:MET:HE2	1.66	0.78
2:B:41:LEU:HG	2:B:419:PRO:HG3	1.65	0.76
2:F:39:VAL:HG13	2:F:381:SER:HB2	1.66	0.75
2:B:136:PHE:HE2	2:B:253:ALA:HA	1.52	0.75
2:H:312:ARG:O	2:H:350:ARG:NH1	2.19	0.75
2:B:60:THR:HG22	2:B:71:LEU:HA	1.69	0.75
2:B:39:VAL:HG13	2:B:381:SER:HB2	1.67	0.74
2:H:112:ARG:N	2:H:113:LEU:HA	2.01	0.74
1:G:129:LYS:HB3	1:G:132:LEU:HD12	1.69	0.73
2:D:372:ARG:HG2	2:D:382:VAL:HG22	1.69	0.73
2:F:55:THR:HG22	2:F:392:LEU:H	1.54	0.73
1:A:96:SER:HB3	1:A:136:MET:H	1.55	0.72
2:H:136:PHE:HE2	2:H:253:ALA:HA	1.55	0.72
3:E:174:TRP:O	3:E:178:ARG:NH1	2.21	0.72
2:F:372:ARG:HG2	2:F:382:VAL:HG22	1.70	0.72
2:B:71:LEU:HB3	2:B:83:TRP:HB2	1.72	0.71
2:F:91:GLU:O	2:F:92:HIS:ND1	2.23	0.71
1:C:103:VAL:HG11	2:D:43:ALA:HA	1.72	0.71
2:H:108:ASN:OD1	2:H:108:ASN:N	2.23	0.70
1:C:58:VAL:HG12	1:C:65:PHE:HB2	1.73	0.70
2:D:61:CYS:O	2:D:69:ASN:ND2	2.24	0.69
1:C:136:MET:HE2	1:C:141:ILE:HG13	1.73	0.69
2:D:80:LEU:HB2	2:D:94:LEU:HG	1.73	0.69
1:A:129:LYS:HG2	4:A:600:GTP:C6	2.27	0.69
2:B:108:ASN:OD1	2:B:108:ASN:N	2.25	0.68
2:B:112:ARG:N	2:B:113:LEU:HA	2.09	0.67
2:F:326:VAL:HB	2:F:339:LEU:HB2	1.76	0.67
3:E:30:LYS:N	4:E:600:GTP:O1B	2.21	0.67
2:B:94:LEU:HD23	2:B:98:PRO:HG3	1.75	0.67
2:H:111:PRO:C	2:H:113:LEU:HA	2.20	0.66
2:H:391:ALA:HB3	2:H:407:ILE:HB	1.77	0.66
3:E:17:LYS:HG2	3:E:64:THR:HB	1.78	0.65
2:B:379:LEU:HD21	2:B:382:VAL:HG23	1.78	0.65
2:D:393:TRP:HB3	2:D:405:LEU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:95:LEU:H	2:H:95:LEU:HD22	1.62	0.65
2:B:350:ARG:NH2	2:B:352:GLU:OE1	2.29	0.65
2:B:351:MET:HB3	2:B:361:ALA:HB3	1.78	0.65
2:H:76:GLU:C	2:H:78:ARG:H	2.03	0.64
1:G:129:LYS:HG2	4:G:600:GTP:C6	2.33	0.64
2:D:267:ILE:HG22	2:D:281:VAL:HG22	1.79	0.64
2:D:310:LEU:HD12	2:D:319:VAL:HG12	1.80	0.64
1:G:106:ARG:NH1	1:G:144:ALA:O	2.30	0.64
2:H:366:LEU:HD12	2:H:370:GLU:HG3	1.79	0.64
1:A:103:VAL:HG22	2:B:41:LEU:HD13	1.79	0.63
2:D:69:ASN:HD22	2:D:70:ARG:N	1.96	0.63
2:D:423:ASN:OD1	2:D:423:ASN:N	2.31	0.63
3:E:52:GLY:H	3:E:76:TYR:HE2	1.45	0.63
2:H:304:GLU:OE2	2:H:327:HIS:NE2	2.30	0.63
2:H:105:ILE:N	2:H:233:SER:OG	2.22	0.63
1:A:141:ILE:HG23	1:A:145:LEU:HD23	1.79	0.62
2:B:91:GLU:O	2:B:92:HIS:ND1	2.32	0.62
2:F:61:CYS:SG	2:F:62:ASN:N	2.72	0.62
2:H:91:GLU:O	2:H:92:HIS:ND1	2.31	0.62
3:E:120:LYS:HE2	3:E:152:ASP:HB2	1.82	0.62
2:H:47:PRO:HG2	2:H:48:VAL:HG23	1.81	0.62
1:C:103:VAL:HG22	2:D:41:LEU:HD13	1.80	0.62
2:H:104:TYR:CE1	2:H:115:ALA:HB3	2.35	0.62
1:A:30:LYS:N	4:A:600:GTP:O1A	2.33	0.61
2:F:348:MET:HG3	2:F:364:VAL:HG23	1.81	0.61
2:D:122:SER:HB2	2:D:137:VAL:HG13	1.81	0.61
2:B:391:ALA:HB3	2:B:407:ILE:HB	1.81	0.61
2:F:345:ILE:HG21	2:F:348:MET:HE2	1.82	0.60
1:A:131:ASP:OD2	1:A:161:ASN:ND2	2.34	0.60
2:F:55:THR:HG23	2:F:391:ALA:HA	1.81	0.60
2:B:122:SER:HB3	2:B:214:THR:O	2.01	0.60
3:E:120:LYS:HA	3:E:153:ARG:NH1	2.16	0.60
2:D:339:LEU:HD13	2:D:374:TYR:CD2	2.37	0.60
2:D:374:TYR:HE1	2:D:379:LEU:HD12	1.66	0.60
2:F:280:THR:HG21	2:F:317:VAL:HG11	1.83	0.60
2:H:41:LEU:HG	2:H:419:PRO:HG3	1.84	0.60
3:E:132:ILE:HG23	3:E:133:PRO:HD2	1.83	0.60
2:F:81:LYS:HB3	2:F:88:LYS:HE3	1.84	0.60
1:C:124:LEU:HD11	1:C:126:PHE:CE1	2.37	0.59
2:D:91:GLU:O	2:D:92:HIS:ND1	2.34	0.59
2:D:346:LEU:HD21	2:D:367:SER:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:ASP:OD1	2:F:416:LYS:NZ	2.35	0.59
1:C:123:ILE:HD11	1:C:153:ARG:HD3	1.84	0.59
1:G:84:TYR:CZ	1:G:112:MET:HG3	2.39	0.58
3:E:108:GLU:OE1	2:F:420:ARG:NH1	2.36	0.58
2:H:351:MET:HB3	2:H:361:ALA:HB3	1.85	0.58
2:D:312:ARG:O	2:D:350:ARG:NH1	2.36	0.58
2:H:341:LEU:HD22	2:H:366:LEU:HD21	1.87	0.57
1:C:100:LEU:HD11	2:D:415:ILE:HG21	1.85	0.57
2:B:339:LEU:HD13	2:B:374:TYR:CD2	2.40	0.57
2:D:385:SER:OG	2:D:387:ASN:O	2.21	0.57
2:B:85:GLY:O	2:B:397:TYR:OH	2.18	0.57
2:H:40:TRP:HH2	2:H:351:MET:SD	2.28	0.57
1:C:29:GLY:HA2	4:C:600:GTP:O1A	2.04	0.57
1:C:30:LYS:O	1:C:34:ILE:HG13	2.05	0.57
3:E:124:LEU:HD11	3:E:126:PHE:CE1	2.40	0.57
2:F:393:TRP:HB3	2:F:405:LEU:HB2	1.87	0.57
2:H:40:TRP:HB3	2:H:416:LYS:HB3	1.86	0.57
2:F:269:VAL:HA	2:F:279:ILE:HG12	1.86	0.56
2:H:71:LEU:HB3	2:H:83:TRP:HB2	1.87	0.56
2:B:136:PHE:CE2	2:B:253:ALA:HA	2.38	0.56
2:D:339:LEU:HD13	2:D:374:TYR:HD2	1.70	0.56
2:H:83:TRP:CE2	2:H:88:LYS:HG3	2.40	0.56
1:G:103:VAL:HG22	2:H:41:LEU:HD13	1.88	0.56
2:H:266:MET:HE1	2:H:307:PRO:HB2	1.88	0.56
2:F:374:TYR:HE1	2:F:379:LEU:HB2	1.71	0.56
2:D:273:LEU:HA	2:D:277:TYR:CD2	2.40	0.56
3:E:89:ALA:HB2	3:E:179:LEU:HD21	1.88	0.56
1:A:30:LYS:O	1:A:34:ILE:HG13	2.05	0.56
1:G:28:SER:HA	1:G:95:ASP:HB2	1.87	0.56
2:H:370:GLU:OE2	2:H:372:ARG:NH2	2.39	0.56
3:E:100:LEU:HD11	2:F:415:ILE:HG21	1.88	0.56
1:C:99:LYS:HE2	2:D:86:THR:HG21	1.88	0.56
2:H:60:THR:HG22	2:H:71:LEU:HA	1.87	0.56
1:C:95:ASP:OD1	1:C:97:ALA:N	2.29	0.55
1:C:129:LYS:HG2	4:C:600:GTP:C6	2.41	0.55
2:D:61:CYS:C	2:D:69:ASN:HD21	2.15	0.55
1:G:102:MET:HE3	1:G:141:ILE:HG12	1.89	0.55
2:B:43:ALA:HB3	2:B:415:ILE:O	2.07	0.55
1:C:76:TYR:N	1:C:76:TYR:HD1	2.03	0.55
2:H:237:VAL:O	2:H:244:ILE:HA	2.06	0.55
2:B:265:ALA:HB2	2:B:284:ARG:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:128:ASN:HD22	3:E:129:LYS:HG3	1.72	0.54
2:H:122:SER:HB3	2:H:214:THR:O	2.07	0.54
1:C:129:LYS:HG2	4:C:600:GTP:N1	2.22	0.54
1:G:81:GLU:HA	1:G:84:TYR:CD2	2.42	0.54
2:D:51:ILE:O	2:D:411:GLY:HA2	2.06	0.54
2:F:236:VAL:HG22	2:F:246:ILE:HG23	1.89	0.54
2:H:143:VAL:HG12	2:H:144:ASN:H	1.73	0.54
2:H:262:ILE:HG12	2:H:285:ASP:CG	2.32	0.54
2:D:287:LYS:HB2	2:D:289:TYR:CE1	2.43	0.54
3:E:75:ARG:HB2	3:E:76:TYR:CD1	2.42	0.54
2:H:85:GLY:O	2:H:397:TYR:OH	2.26	0.54
2:D:117:ALA:O	2:D:219:MET:HE1	2.08	0.54
3:E:33:ILE:HD13	3:E:126:PHE:CD2	2.43	0.54
3:E:74:GLY:HA2	3:E:77:ARG:HG3	1.89	0.54
1:A:88:ASP:O	1:A:121:VAL:HB	2.08	0.54
2:B:107:GLU:C	2:B:109:THR:H	2.16	0.54
1:G:103:VAL:HG21	2:H:41:LEU:HB3	1.90	0.54
2:B:126:ILE:CD1	2:B:251:GLY:HA3	2.38	0.53
1:G:30:LYS:NZ	1:G:70:MET:O	2.41	0.53
2:H:288:LEU:HD23	2:H:301:ILE:HD12	1.90	0.53
2:F:46:ASP:OD2	2:F:49:ALA:N	2.42	0.53
1:G:26:ASP:HB3	1:G:73:ALA:N	2.23	0.53
4:A:600:GTP:C8	4:A:600:GTP:H5'	2.43	0.53
2:B:288:LEU:HB3	2:B:301:ILE:HD12	1.90	0.53
1:G:84:TYR:CE1	1:G:112:MET:HG3	2.43	0.53
2:H:267:ILE:HG22	2:H:281:VAL:HG22	1.90	0.53
1:A:94:VAL:HG21	1:A:141:ILE:HG21	1.90	0.53
2:B:44:PHE:HD2	2:B:415:ILE:HD12	1.74	0.52
2:F:267:ILE:HG22	2:F:281:VAL:HG22	1.92	0.52
2:H:76:GLU:C	2:H:78:ARG:N	2.66	0.52
2:H:393:TRP:HB3	2:H:405:LEU:HB2	1.91	0.52
2:D:350:ARG:NH2	2:D:352:GLU:OE1	2.42	0.52
1:A:101:ARG:HD2	2:B:400:GLU:HG2	1.91	0.52
2:B:222:VAL:HG22	2:B:269:VAL:HG11	1.91	0.52
2:F:218:CYS:SG	2:F:266:MET:HA	2.49	0.52
2:B:126:ILE:HD11	2:B:251:GLY:HA3	1.91	0.52
3:E:101:ARG:HD2	2:F:399:ARG:H	1.75	0.52
2:F:291:ILE:HG12	2:F:296:LEU:HA	1.89	0.52
1:A:103:VAL:HG11	2:B:43:ALA:HA	1.91	0.52
2:F:80:LEU:HB2	2:F:94:LEU:HG	1.91	0.52
2:B:64:PHE:HB2	2:B:66:ASP:OD1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:129:LYS:HG2	4:E:600:GTP:C6	2.45	0.52
2:D:394:PHE:HZ	2:D:402:ASN:HB3	1.73	0.52
1:G:37:LEU:HD21	1:G:172:ILE:HG13	1.91	0.52
2:B:368:ASN:OD1	2:B:369:GLY:N	2.43	0.52
2:F:247:LEU:HD22	2:F:254:ILE:HA	1.92	0.52
2:H:217:THR:OG1	2:H:264:PRO:HG2	2.09	0.52
3:E:75:ARG:HB2	3:E:76:TYR:HD1	1.74	0.51
2:F:374:TYR:CE1	2:F:379:LEU:HB2	2.45	0.51
1:A:50:THR:N	4:A:600:GTP:O1G	2.41	0.51
2:F:405:LEU:CD2	2:F:415:ILE:HG12	2.40	0.51
2:H:368:ASN:OD1	2:H:370:GLU:HG2	2.10	0.51
2:B:106:SER:HA	2:B:249:PRO:O	2.11	0.51
2:B:123:HIS:CD2	2:B:137:VAL:HG22	2.45	0.51
2:D:81:LYS:O	2:D:82:ILE:HD12	2.10	0.51
1:G:129:LYS:HG2	4:G:600:GTP:N1	2.25	0.51
3:E:77:ARG:HD2	3:E:108:GLU:OE2	2.10	0.51
2:H:105:ILE:HD12	2:H:230:ASP:HA	1.91	0.51
1:C:133:PRO:HG2	1:C:134:VAL:HG22	1.93	0.51
2:F:405:LEU:HD23	2:F:415:ILE:HG12	1.93	0.51
1:A:101:ARG:CD	2:B:400:GLU:HG2	2.40	0.51
2:B:269:VAL:HG22	2:B:279:ILE:HG12	1.91	0.51
2:B:80:LEU:HB2	2:B:94:LEU:HD13	1.92	0.51
2:D:310:LEU:HD12	2:D:319:VAL:CG1	2.40	0.51
1:C:76:TYR:N	1:C:76:TYR:CD1	2.76	0.50
2:D:368:ASN:OD1	2:D:370:GLU:HG2	2.11	0.50
2:H:351:MET:HE3	2:H:418:LEU:HD22	1.93	0.50
2:B:92:HIS:CD2	2:B:130:LEU:HD22	2.47	0.50
2:F:365:ALA:HB2	2:F:371:VAL:HG13	1.92	0.50
2:F:47:PRO:HG2	2:F:48:VAL:HG22	1.94	0.50
2:B:372:ARG:HB2	2:B:374:TYR:HE1	1.75	0.50
2:D:61:CYS:N	2:D:69:ASN:HD21	2.09	0.50
2:D:301:ILE:HG21	2:D:329:TYR:CE1	2.46	0.50
2:D:374:TYR:CE1	2:D:379:LEU:HD12	2.44	0.50
2:F:403:THR:HG23	2:F:417:MET:HG2	1.94	0.50
2:B:349:GLN:NE2	2:B:392:LEU:O	2.36	0.50
2:B:140:PRO:HB3	2:B:213:THR:HA	1.93	0.50
2:D:42:ASP:OD1	2:D:416:LYS:HE2	2.11	0.50
2:B:134:TYR:CD1	2:B:135:LYS:N	2.79	0.50
2:B:78:ARG:NE	2:B:97:THR:HG23	2.27	0.49
2:F:41:LEU:HG	2:F:419:PRO:HG3	1.95	0.49
2:F:55:THR:CG2	2:F:392:LEU:H	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:304:GLU:CD	2:H:327:HIS:HE2	2.18	0.49
2:F:320:GLY:HA3	2:F:348:MET:HE1	1.93	0.49
2:B:76:GLU:C	2:B:78:ARG:H	2.19	0.49
1:A:138:PRO:HG2	1:A:159:PRO:HB3	1.94	0.49
2:D:353:VAL:HG21	2:D:424:LEU:HD11	1.93	0.49
2:F:343:CYS:HB2	2:F:368:ASN:ND2	2.28	0.49
1:G:23:VAL:HG23	1:G:92:PHE:CD2	2.47	0.49
2:H:123:HIS:CD2	2:H:137:VAL:HG22	2.47	0.49
2:F:117:ALA:HA	2:F:126:ILE:HA	1.95	0.49
2:B:245:LEU:HD13	2:B:254:ILE:HD11	1.94	0.49
2:B:298:GLN:C	2:B:300:ILE:HD12	2.38	0.49
2:D:69:ASN:HD22	2:D:70:ARG:H	1.60	0.49
3:E:124:LEU:HD21	3:E:126:PHE:CZ	2.47	0.49
2:B:70:ARG:HD2	2:B:84:LYS:HB2	1.94	0.49
2:F:287:LYS:HB2	2:F:289:TYR:CE1	2.48	0.49
3:E:98:ASP:OD2	3:E:101:ARG:HD3	2.13	0.48
1:A:28:SER:HA	1:A:95:ASP:HB2	1.95	0.48
1:A:132:LEU:HB3	1:A:133:PRO:HD2	1.94	0.48
1:A:22:VAL:HG22	1:A:91:VAL:HB	1.94	0.48
2:B:362:LEU:HD23	2:B:363:ILE:O	2.14	0.48
2:H:326:VAL:HB	2:H:339:LEU:HB2	1.95	0.48
2:B:351:MET:O	2:B:361:ALA:N	2.39	0.48
3:E:77:ARG:C	3:E:79:LEU:H	2.21	0.48
2:D:240:GLU:O	2:D:263:THR:HG22	2.12	0.48
3:E:94:VAL:CG1	3:E:102:MET:HE1	2.43	0.48
2:F:244:ILE:HD11	2:F:281:VAL:HG21	1.96	0.48
2:B:137:VAL:O	2:B:139:PRO:HD3	2.14	0.48
2:B:372:ARG:HG2	2:B:382:VAL:HG22	1.95	0.48
2:F:368:ASN:OD1	2:F:370:GLU:HG2	2.13	0.48
1:C:52:GLY:H	1:C:76:TYR:HE2	1.62	0.48
2:D:38:SER:HB2	2:D:383:HIS:HB3	1.96	0.48
2:D:105:ILE:N	2:D:233:SER:OG	2.46	0.48
2:H:313:LEU:HD22	2:H:361:ALA:O	2.14	0.48
2:D:280:THR:HG21	2:D:317:VAL:HG21	1.95	0.48
2:H:289:TYR:HE1	2:H:300:ILE:HG12	1.78	0.48
2:B:246:ILE:C	2:B:247:LEU:HD23	2.39	0.47
1:C:178:ARG:HB3	1:C:178:ARG:HH11	1.79	0.47
2:H:41:LEU:CG	2:H:419:PRO:HG3	2.43	0.47
2:F:94:LEU:HD13	2:F:98:PRO:HG3	1.96	0.47
2:F:287:LYS:HE2	2:F:302:GLN:OE1	2.14	0.47
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:PHE:HE1	2:H:138:LEU:HD23	1.80	0.47
2:B:351:MET:HG3	2:B:394:PHE:CE2	2.49	0.47
3:E:103:VAL:HG11	2:F:43:ALA:HA	1.97	0.47
2:F:371:VAL:HB	2:F:383:HIS:NE2	2.30	0.47
1:G:119:ARG:O	1:G:121:VAL:N	2.45	0.47
2:D:96:ASP:HB3	2:D:120:ALA:HB1	1.95	0.47
2:F:356:GLN:O	2:F:356:GLN:HG3	2.14	0.47
2:H:380:VAL:HG11	2:H:424:LEU:HA	1.96	0.47
1:C:136:MET:HA	1:C:137:PRO:HD3	1.51	0.47
2:F:391:ALA:HB3	2:F:407:ILE:HB	1.97	0.47
2:H:134:TYR:CD1	2:H:135:LYS:N	2.82	0.47
2:H:262:ILE:HD12	2:H:263:THR:H	1.79	0.47
2:B:92:HIS:NE2	2:B:130:LEU:HD13	2.30	0.47
2:D:277:TYR:CZ	2:D:293:ASN:HA	2.49	0.47
2:D:391:ALA:HB3	2:D:407:ILE:HB	1.95	0.47
2:F:316:HIS:CD2	2:F:316:HIS:N	2.83	0.47
1:G:106:ARG:HG3	1:G:145:LEU:HA	1.97	0.47
2:D:62:ASN:O	2:D:114:PRO:HG3	2.14	0.47
3:E:29:GLY:N	4:E:600:GTP:O1B	2.48	0.47
2:H:351:MET:HG3	2:H:394:PHE:CE2	2.49	0.47
1:A:65:PHE:HB3	1:A:67:VAL:HG23	1.96	0.47
1:C:18:VAL:HG21	1:C:179:LEU:HD13	1.97	0.47
1:G:89:ALA:HB1	1:G:175:LEU:HD11	1.97	0.47
2:H:81:LYS:HD3	2:H:88:LYS:HD3	1.97	0.47
2:B:124:ILE:HD11	2:B:237:VAL:HG21	1.97	0.46
2:D:289:TYR:CD2	2:D:300:ILE:HD12	2.50	0.46
1:C:108:GLU:OE1	2:D:420:ARG:NH1	2.48	0.46
2:D:320:GLY:HA2	2:D:326:VAL:HA	1.97	0.46
2:H:95:LEU:HD22	2:H:95:LEU:N	2.30	0.46
2:H:372:ARG:HD3	2:H:374:TYR:OH	2.14	0.46
2:D:371:VAL:HB	2:D:383:HIS:NE2	2.30	0.46
2:F:348:MET:CG	2:F:364:VAL:HG23	2.45	0.46
2:B:104:TYR:CE1	2:B:115:ALA:HB3	2.50	0.46
2:F:235:LEU:HD12	2:F:235:LEU:H	1.81	0.46
2:F:343:CYS:SG	2:F:344:HIS:N	2.83	0.46
1:C:122:PRO:HG3	1:C:154:PRO:HG2	1.96	0.46
1:G:77:ARG:C	1:G:79:LEU:H	2.23	0.46
2:H:221:VAL:HG12	2:H:222:VAL:N	2.30	0.46
3:E:89:ALA:HB1	3:E:175:LEU:HD11	1.97	0.46
2:B:135:LYS:O	2:B:137:VAL:HG23	2.16	0.46
2:D:41:LEU:HG	2:D:419:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:HG13	2:B:381:SER:CB	2.40	0.45
2:B:406:ALA:HB3	2:B:414:ASP:HB3	1.98	0.45
3:E:36:ARG:HA	3:E:36:ARG:HD3	1.74	0.45
2:B:374:TYR:CD1	2:B:374:TYR:N	2.83	0.45
1:C:25:LEU:HB3	1:C:101:ARG:NH2	2.31	0.45
2:F:313:LEU:HD22	2:F:313:LEU:HA	1.85	0.45
1:G:138:PRO:HG2	1:G:159:PRO:HB3	1.97	0.45
2:H:260:VAL:HG22	2:H:296:LEU:HD13	1.99	0.45
1:C:178:ARG:H	1:C:178:ARG:HG2	1.49	0.45
1:G:103:VAL:HG11	2:H:43:ALA:HA	1.97	0.45
1:A:90:VAL:HG11	1:A:112:MET:HE1	1.97	0.45
1:A:152:ASP:OD2	1:A:153:ARG:NE	2.49	0.45
3:E:30:LYS:O	3:E:34:ILE:HG13	2.16	0.45
2:H:355:GLY:O	2:H:358:ASN:HB2	2.16	0.45
2:H:418:LEU:HD11	2:H:424:LEU:HD21	1.98	0.45
2:B:40:TRP:HH2	2:B:351:MET:SD	2.40	0.45
2:B:222:VAL:HG23	2:B:236:VAL:HG21	1.98	0.45
1:G:95:ASP:CG	1:G:129:LYS:HD2	2.42	0.45
2:H:41:LEU:CD2	2:H:419:PRO:HG3	2.47	0.45
2:H:58:VAL:HG22	2:H:73:ILE:HG23	1.98	0.45
3:E:97:ALA:HB2	3:E:132:ILE:HG21	1.99	0.45
2:B:58:VAL:HG22	2:B:73:ILE:HG23	1.99	0.45
2:D:324:ASP:OD1	2:D:344:HIS:HA	2.17	0.45
2:H:310:LEU:HD12	2:H:319:VAL:HA	1.98	0.45
2:B:387:ASN:CG	2:B:410:SER:HB3	2.41	0.45
2:H:136:PHE:CE2	2:H:253:ALA:HA	2.42	0.45
2:D:265:ALA:HB2	2:D:284:ARG:HG2	1.98	0.45
2:D:374:TYR:HD1	2:D:379:LEU:HA	1.82	0.45
2:D:387:ASN:CG	2:D:410:SER:HB2	2.42	0.45
2:F:43:ALA:HB3	2:F:415:ILE:O	2.17	0.45
2:F:313:LEU:HB2	2:F:316:HIS:O	2.17	0.45
2:D:337:TRP:CB	2:D:377:LYS:HG3	2.47	0.44
1:G:103:VAL:CG2	2:H:41:LEU:HB3	2.47	0.44
2:B:362:LEU:HD22	2:B:364:VAL:HG23	1.99	0.44
2:H:244:ILE:HD11	2:H:281:VAL:HG21	1.99	0.44
2:H:277:TYR:CZ	2:H:293:ASN:HA	2.52	0.44
2:H:372:ARG:NH1	2:H:374:TYR:OH	2.37	0.44
2:B:327:HIS:HB3	2:B:329:TYR:CE1	2.52	0.44
2:F:76:GLU:C	2:F:78:ARG:H	2.25	0.44
2:F:418:LEU:HD12	2:F:419:PRO:HD2	2.00	0.44
2:B:414:ASP:OD2	2:B:416:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:ILE:HG12	2:D:296:LEU:HA	1.99	0.44
2:F:375:ASN:HB2	2:F:380:VAL:HG21	1.99	0.44
2:H:94:LEU:HD13	2:H:98:PRO:HG3	1.99	0.44
2:H:351:MET:HA	2:H:394:PHE:CD2	2.52	0.44
2:B:51:ILE:HG21	2:B:73:ILE:HD13	1.99	0.44
2:B:347:ALA:HB3	2:B:365:ALA:HB3	1.99	0.44
2:H:277:TYR:OH	2:H:294:GLY:N	2.50	0.44
2:B:72:VAL:HG22	2:B:82:ILE:CD1	2.48	0.44
1:C:136:MET:HE2	1:C:136:MET:HB3	1.73	0.44
2:F:280:THR:OG1	2:F:317:VAL:HG21	2.18	0.44
3:E:20:VAL:HG22	3:E:89:ALA:HB3	2.00	0.44
1:A:89:ALA:HB2	1:A:179:LEU:HD21	1.98	0.44
1:A:129:LYS:HE2	4:A:600:GTP:C4	2.53	0.44
2:B:136:PHE:HE1	2:B:138:LEU:HD23	1.83	0.44
2:F:392:LEU:HD22	2:F:404:LEU:HD11	1.99	0.44
2:H:347:ALA:HB3	2:H:365:ALA:HB3	1.98	0.44
2:H:352:GLU:HG3	2:H:360:LYS:HE2	1.99	0.44
1:A:112:MET:HG3	1:A:113:LEU:N	2.31	0.44
3:E:23:VAL:C	3:E:30:LYS:HD3	2.43	0.44
2:H:128:ARG:HB3	2:H:129:ASN:OD1	2.18	0.44
2:D:374:TYR:HE1	2:D:379:LEU:HB2	1.83	0.43
3:E:76:TYR:HD1	3:E:76:TYR:N	2.16	0.43
2:H:95:LEU:H	2:H:95:LEU:CD2	2.29	0.43
2:F:373:VAL:HG23	2:F:381:SER:O	2.17	0.43
1:A:115:HIS:CE1	2:H:355:GLY:HA2	2.53	0.43
2:B:136:PHE:HZ	2:B:254:ILE:HG13	1.83	0.43
2:B:222:VAL:HG12	2:B:223:LYS:O	2.18	0.43
3:E:132:ILE:CG2	3:E:133:PRO:HD2	2.48	0.43
2:H:262:ILE:HG21	2:H:289:TYR:HE2	1.83	0.43
1:C:23:VAL:HG23	1:C:92:PHE:CD2	2.54	0.43
2:D:418:LEU:HA	2:D:419:PRO:HD3	1.84	0.43
3:E:76:TYR:CD1	3:E:76:TYR:N	2.86	0.43
3:E:103:VAL:HG22	2:F:41:LEU:HD13	2.00	0.43
2:H:377:LYS:HB2	2:H:377:LYS:NZ	2.33	0.43
2:B:41:LEU:CG	2:B:419:PRO:HG3	2.43	0.43
2:B:365:ALA:HB1	2:B:389:VAL:HB	2.01	0.43
2:D:58:VAL:HG22	2:D:73:ILE:HG23	1.99	0.43
1:G:118:MET:HB2	1:G:118:MET:HE2	1.82	0.43
2:H:44:PHE:CZ	2:H:46:ASP:HB2	2.53	0.43
2:D:76:GLU:C	2:D:78:ARG:H	2.26	0.43
1:G:30:LYS:HG2	1:G:93:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LEU:HB2	2:B:94:LEU:CD1	2.48	0.43
2:B:219:MET:HB2	2:B:236:VAL:O	2.19	0.43
2:B:385:SER:HB3	2:B:387:ASN:O	2.19	0.43
1:C:112:MET:HG2	1:C:118:MET:HE3	2.00	0.43
1:G:23:VAL:HB	1:G:80:TRP:CZ3	2.54	0.43
2:H:96:ASP:HB3	2:H:120:ALA:HB1	2.00	0.43
4:A:600:GTP:H5'	4:A:600:GTP:H8	1.84	0.43
2:F:287:LYS:HB2	2:F:289:TYR:HE1	1.82	0.43
2:H:60:THR:OG1	2:H:393:TRP:NE1	2.52	0.43
2:D:288:LEU:HD23	2:D:288:LEU:HA	1.84	0.43
3:E:156:GLN:HE21	3:E:174:TRP:CD1	2.37	0.43
2:D:394:PHE:CZ	2:D:402:ASN:HB3	2.53	0.42
1:A:26:ASP:HB3	1:A:73:ALA:N	2.33	0.42
1:C:75:ARG:C	1:C:76:TYR:HD1	2.27	0.42
1:G:100:LEU:HG	2:H:417:MET:HE1	2.01	0.42
2:H:138:LEU:HA	2:H:139:PRO:HD2	1.73	0.42
2:H:362:LEU:HG	2:H:364:VAL:HG23	2.01	0.42
1:C:65:PHE:HE2	1:C:172:ILE:HG23	1.84	0.42
2:D:50:GLY:HA3	2:D:81:LYS:HZ2	1.84	0.42
2:D:348:MET:HG2	2:D:364:VAL:HG12	2.01	0.42
2:H:246:ILE:C	2:H:247:LEU:HD23	2.44	0.42
2:H:391:ALA:O	2:H:406:ALA:HA	2.18	0.42
2:B:321:CYS:HB2	2:B:323:ASN:OD1	2.19	0.42
3:E:59:GLU:CG	3:E:64:THR:HG23	2.50	0.42
2:F:385:SER:OG	2:F:387:ASN:O	2.30	0.42
2:H:351:MET:HB2	2:H:363:ILE:HD11	2.01	0.42
1:A:122:PRO:HA	1:A:154:PRO:HG2	2.00	0.42
1:A:123:ILE:HD11	1:A:153:ARG:HD3	2.00	0.42
2:B:338:SER:HB2	2:B:340:TYR:CE1	2.55	0.42
1:C:25:LEU:HD23	1:C:101:ARG:NE	2.35	0.42
1:C:136:MET:HE2	1:C:141:ILE:CG1	2.45	0.42
3:E:59:GLU:HG2	3:E:64:THR:HG23	2.01	0.42
2:H:43:ALA:HB3	2:H:415:ILE:O	2.20	0.42
2:B:394:PHE:CZ	2:B:402:ASN:HB3	2.55	0.42
2:D:131:ARG:HA	2:D:132:PRO:HD3	1.92	0.42
1:C:22:VAL:HG12	1:C:30:LYS:HD2	2.02	0.42
1:C:33:ILE:HD13	1:C:126:PHE:CD2	2.54	0.42
1:C:128:ASN:ND2	1:C:129:LYS:HG3	2.34	0.42
2:F:75:ASP:OD2	2:F:81:LYS:HE3	2.19	0.42
2:F:383:HIS:ND1	2:F:416:LYS:HE3	2.34	0.42
2:H:46:ASP:HA	2:H:47:PRO:HD2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:THR:HA	2:H:70:ARG:O	2.20	0.42
1:A:81:GLU:OE2	1:G:78:THR:HG21	2.20	0.42
1:C:119:ARG:H	1:C:119:ARG:HG3	1.24	0.42
2:F:303:LEU:CD2	2:F:319:VAL:HG21	2.50	0.42
2:H:414:ASP:OD2	2:H:416:LYS:HE3	2.19	0.42
1:C:17:LYS:HD3	1:C:66:THR:OG1	2.20	0.41
1:C:99:LYS:HG3	1:C:136:MET:SD	2.60	0.41
3:E:34:ILE:HD13	3:E:67:VAL:HG11	2.02	0.41
2:H:376:GLU:HB3	2:H:377:LYS:H	1.69	0.41
2:D:50:GLY:HA3	2:D:81:LYS:NZ	2.35	0.41
2:F:372:ARG:HG2	2:F:382:VAL:CG2	2.44	0.41
1:G:37:LEU:HD21	1:G:168:VAL:HG12	2.02	0.41
2:H:71:LEU:HD13	2:H:405:LEU:HD13	2.02	0.41
2:B:262:ILE:HG13	2:B:263:THR:N	2.36	0.41
1:C:22:VAL:HG22	1:C:91:VAL:HB	2.02	0.41
3:E:34:ILE:HD13	3:E:67:VAL:CG1	2.50	0.41
2:F:60:THR:HG22	2:F:71:LEU:HA	2.01	0.41
2:B:138:LEU:HD23	2:B:138:LEU:HA	1.78	0.41
2:B:322:MET:HE3	2:B:322:MET:HA	2.01	0.41
2:B:372:ARG:CB	2:B:374:TYR:HE1	2.33	0.41
2:D:325:VAL:HG11	2:D:327:HIS:NE2	2.35	0.41
2:H:42:ASP:OD1	2:H:416:LYS:HE2	2.20	0.41
2:B:107:GLU:C	2:B:109:THR:N	2.76	0.41
1:C:103:VAL:CG1	2:D:43:ALA:HA	2.47	0.41
2:H:223:LYS:HD3	2:H:223:LYS:HA	1.66	0.41
1:A:94:VAL:HB	1:A:102:MET:HE1	2.02	0.41
2:D:43:ALA:HB3	2:D:415:ILE:O	2.21	0.41
2:F:293:ASN:C	2:F:295:GLU:H	2.29	0.41
1:G:65:PHE:HB3	1:G:67:VAL:HG23	2.01	0.41
1:G:137:PRO:O	1:G:139:VAL:N	2.54	0.41
2:H:301:ILE:HG21	2:H:329:TYR:CE1	2.55	0.41
2:H:397:TYR:CG	2:H:398:GLY:N	2.88	0.41
2:D:339:LEU:HD22	2:D:374:TYR:CE2	2.55	0.41
1:G:88:ASP:O	1:G:121:VAL:HB	2.20	0.41
2:H:285:ASP:N	2:H:285:ASP:OD1	2.53	0.41
1:A:90:VAL:O	1:A:123:ILE:HA	2.21	0.41
2:B:72:VAL:HA	2:B:82:ILE:HD13	2.02	0.41
1:G:89:ALA:CB	1:G:175:LEU:HD11	2.51	0.41
2:H:299:THR:O	2:H:299:THR:OG1	2.38	0.41
1:A:77:ARG:C	1:A:79:LEU:H	2.28	0.41
2:B:102:CYS:HB2	2:B:219:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASP:HB3	1:C:161:ASN:ND2	2.36	0.41
2:D:95:LEU:HD23	2:D:125:TYR:CE2	2.56	0.41
2:F:305:ALA:HB3	2:F:321:CYS:HB3	2.01	0.41
2:H:101:ILE:HG22	2:H:118:VAL:HA	2.03	0.41
2:H:248:ASN:O	2:H:251:GLY:N	2.40	0.41
2:H:372:ARG:HG2	2:H:382:VAL:HG22	2.03	0.41
2:F:104:TYR:O	2:F:115:ALA:N	2.52	0.41
2:B:362:LEU:CD2	2:B:364:VAL:HG23	2.52	0.40
2:B:374:TYR:HD1	2:B:374:TYR:H	1.69	0.40
1:C:75:ARG:HB2	1:C:76:TYR:CD1	2.56	0.40
3:E:25:LEU:CD1	3:E:105:ALA:HA	2.51	0.40
1:G:25:LEU:HA	1:G:25:LEU:HD23	1.69	0.40
2:B:104:TYR:OH	2:B:251:GLY:N	2.53	0.40
1:C:25:LEU:HD23	1:C:101:ARG:CZ	2.52	0.40
3:E:112:MET:HG2	3:E:118:MET:HE3	2.04	0.40
1:G:18:VAL:HG11	1:G:179:LEU:HD22	2.04	0.40
2:H:58:VAL:CG1	2:H:71:LEU:HD11	2.51	0.40
1:A:81:GLU:HA	1:A:84:TYR:CD2	2.56	0.40
2:B:111:PRO:C	2:B:113:LEU:HA	2.46	0.40
1:C:48:ALA:HA	1:C:49:PRO:HD3	1.96	0.40
3:E:178:ARG:H	3:E:178:ARG:HG2	1.49	0.40
1:G:85:ARG:HB3	1:G:86:GLU:OE2	2.22	0.40
2:H:219:MET:HE2	2:H:219:MET:HB3	1.98	0.40
2:H:394:PHE:HA	2:H:403:THR:O	2.21	0.40
1:A:16:LYS:HB3	1:A:63:LEU:HD23	2.04	0.40
1:A:145:LEU:HD13	1:A:145:LEU:HA	1.95	0.40
2:D:66:ASP:OD1	2:D:66:ASP:N	2.46	0.40
3:E:22:VAL:HG22	3:E:91:VAL:HB	2.03	0.40
3:E:65:PHE:HB3	3:E:67:VAL:HG23	2.02	0.40
1:G:92:PHE:O	1:G:125:TYR:HA	2.22	0.40
2:H:373:VAL:CG2	2:H:381:SER:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	164/169 (97%)	148 (90%)	15 (9%)	1 (1%)	21	53
1	C	164/169 (97%)	148 (90%)	15 (9%)	1 (1%)	21	53
1	G	164/169 (97%)	149 (91%)	14 (8%)	1 (1%)	21	53
2	B	329/425 (77%)	287 (87%)	41 (12%)	1 (0%)	36	67
2	D	293/425 (69%)	258 (88%)	32 (11%)	3 (1%)	12	44
2	F	303/425 (71%)	266 (88%)	36 (12%)	1 (0%)	36	67
2	H	321/425 (76%)	278 (87%)	41 (13%)	2 (1%)	21	53
3	E	164/169 (97%)	148 (90%)	15 (9%)	1 (1%)	21	53
All	All	1902/2376 (80%)	1682 (88%)	209 (11%)	11 (1%)	21	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	209	PRO
2	D	128	ARG
2	F	129	ASN
1	A	138	PRO
2	D	127	TYR
3	E	138	PRO
1	G	138	PRO
2	H	227	ASP
1	C	138	PRO
2	D	225	ALA
2	H	143	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/142 (92%)	122 (94%)	8 (6%)	16	44
1	C	138/142 (97%)	127 (92%)	11 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	136/142 (96%)	130 (96%)	6 (4%)	25	52
2	B	243/352 (69%)	213 (88%)	30 (12%)	4	23
2	D	206/352 (58%)	183 (89%)	23 (11%)	6	26
2	F	215/352 (61%)	197 (92%)	18 (8%)	10	35
2	H	242/352 (69%)	207 (86%)	35 (14%)	3	18
3	E	135/142 (95%)	123 (91%)	12 (9%)	9	33
All	All	1445/1976 (73%)	1302 (90%)	143 (10%)	7	30

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	88	ASP
1	A	102	MET
1	A	111	HIS
1	A	119	ARG
1	A	143	GLN
1	A	145	LEU
1	A	180	SER
2	B	48	VAL
2	B	80	LEU
2	B	86	THR
2	B	87	GLN
2	B	94	LEU
2	B	96	ASP
2	B	101	ILE
2	B	104	TYR
2	B	105	ILE
2	B	108	ASN
2	B	116	LEU
2	B	122	SER
2	B	126	ILE
2	B	129	ASN
2	B	135	LYS
2	B	138	LEU
2	B	213	THR
2	B	245	LEU
2	B	266	MET
2	B	269	VAL
2	B	300	ILE

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Mol	Chain	Res	Type
2	B	312	ARG
2	B	316	HIS
2	B	338	SER
2	B	339	LEU
2	B	343	CYS
2	B	373	VAL
2	B	374	TYR
2	B	385	SER
2	B	417	MET
1	C	47	VAL
1	C	58	VAL
1	C	60	LYS
1	C	64	THR
1	C	75	ARG
1	C	76	TYR
1	C	119	ARG
1	C	124	LEU
1	C	134	VAL
1	C	139	VAL
1	C	178	ARG
2	D	51	ILE
2	D	69	ASN
2	D	70	ARG
2	D	80	LEU
2	D	82	ILE
2	D	95	LEU
2	D	125	TYR
2	D	126	ILE
2	D	221	VAL
2	D	262	ILE
2	D	266	MET
2	D	279	ILE
2	D	306	GLN
2	D	310	LEU
2	D	311	VAL
2	D	313	LEU
2	D	316	HIS
2	D	317	VAL
2	D	343	CYS
2	D	371	VAL
2	D	373	VAL
2	D	375	ASN

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Mol	Chain	Res	Type
2	D	423	ASN
3	E	47	VAL
3	E	75	ARG
3	E	76	TYR
3	E	102	MET
3	E	124	LEU
3	E	130	LYS
3	E	134	VAL
3	E	139	VAL
3	E	153	ARG
3	E	156	GLN
3	E	177	GLU
3	E	178	ARG
2	F	44	PHE
2	F	48	VAL
2	F	70	ARG
2	F	80	LEU
2	F	82	ILE
2	F	86	THR
2	F	256	LYS
2	F	267	ILE
2	F	279	ILE
2	F	288	LEU
2	F	306	GLN
2	F	312	ARG
2	F	313	LEU
2	F	316	HIS
2	F	363	ILE
2	F	371	VAL
2	F	373	VAL
2	F	382	VAL
1	G	56	ASP
1	G	63	LEU
1	G	78	THR
1	G	102	MET
1	G	178	ARG
1	G	179	LEU
2	H	48	VAL
2	H	70	ARG
2	H	82	ILE
2	H	86	THR
2	H	88	LYS

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Mol	Chain	Res	Type
2	H	95	LEU
2	H	96	ASP
2	H	104	TYR
2	H	107	GLU
2	H	108	ASN
2	H	116	LEU
2	H	122	SER
2	H	126	ILE
2	H	129	ASN
2	H	130	LEU
2	H	138	LEU
2	H	142	ASN
2	H	143	VAL
2	H	213	THR
2	H	215	VAL
2	H	240	GLU
2	H	241	SER
2	H	256	LYS
2	H	266	MET
2	H	279	ILE
2	H	293	ASN
2	H	316	HIS
2	H	322	MET
2	H	339	LEU
2	H	343	CYS
2	H	353	VAL
2	H	357	ARG
2	H	376	GLU
2	H	377	LYS
2	H	417	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	43	GLN
2	B	59	HIS
2	B	402	ASN
2	D	69	ASN
2	D	306	GLN
2	D	334	HIS
3	E	156	GLN

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Mol	Chain	Res	Type
2	F	87	GLN
1	G	19	ASN
2	H	257	ASN
2	H	387	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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
4	GTP	A	600	5	33,34,34	1.12	4 (12%)	50,54,54	1.61	11 (22%)
4	GTP	C	600	5	33,34,34	1.06	3 (9%)	50,54,54	1.73	11 (22%)
4	GTP	G	600	5	33,34,34	0.96	1 (3%)	50,54,54	1.68	10 (20%)
4	GTP	E	600	5	33,34,34	1.02	3 (9%)	50,54,54	1.63	8 (16%)

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
4	GTP	A	600	5	-	1/22/38/38	0/3/3/3
4	GTP	C	600	5	-	4/22/38/38	0/3/3/3
4	GTP	G	600	5	-	1/22/38/38	0/3/3/3
4	GTP	E	600	5	-	1/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	PB-O3B	2.99	1.62	1.59
4	C	600	GTP	PB-O3A	2.50	1.62	1.59
4	A	600	GTP	PB-O3A	2.32	1.62	1.59
4	G	600	GTP	C2-N3	2.32	1.38	1.33
4	A	600	GTP	C2-N3	2.32	1.38	1.33
4	E	600	GTP	C2-N3	2.23	1.38	1.33
4	E	600	GTP	PB-O3B	2.20	1.61	1.59
4	A	600	GTP	PA-O3A	2.20	1.61	1.59
4	E	600	GTP	PB-O3A	2.18	1.61	1.59
4	C	600	GTP	C2-N3	2.05	1.38	1.33
4	C	600	GTP	C5-N7	-2.04	1.35	1.39

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	600	GTP	C5-C4-N3	-5.12	120.24	128.39
4	G	600	GTP	C5-C4-N3	-5.11	120.25	128.39
4	G	600	GTP	C2-N3-C4	4.72	120.44	112.30
4	E	600	GTP	C5-C4-N3	-4.71	120.90	128.39
4	A	600	GTP	C5-C4-N3	-4.70	120.92	128.39
4	A	600	GTP	C2-N3-C4	4.22	119.57	112.30
4	C	600	GTP	C2-N3-C4	4.13	119.42	112.30
4	E	600	GTP	C2-N3-C4	4.05	119.28	112.30
4	E	600	GTP	N9-C8-N7	-3.61	106.71	113.40
4	C	600	GTP	N9-C4-N3	3.58	133.11	125.95
4	G	600	GTP	N9-C4-N3	3.48	132.92	125.95
4	C	600	GTP	C2-N1-C6	-3.45	118.86	125.11
4	E	600	GTP	N9-C4-N3	3.41	132.76	125.95
4	G	600	GTP	C2-N1-C6	-3.16	119.38	125.11
4	E	600	GTP	C8-N7-C5	3.12	109.82	104.26
4	A	600	GTP	C2-N1-C6	-3.11	119.47	125.11
4	G	600	GTP	N9-C8-N7	-3.11	107.63	113.40
4	E	600	GTP	C2-N1-C6	-3.05	119.57	125.11
4	C	600	GTP	N9-C8-N7	-2.96	107.91	113.40
4	G	600	GTP	C5-C6-N1	2.78	120.32	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	600	GTP	N9-C4-N3	2.68	131.32	125.95
4	C	600	GTP	O6-C6-C5	-2.68	119.45	126.53
4	G	600	GTP	O4'-C1'-N9	-2.65	102.35	108.36
4	G	600	GTP	C8-N7-C5	2.65	108.98	104.26
4	A	600	GTP	N9-C8-N7	-2.62	108.54	113.40
4	C	600	GTP	C5-C6-N1	2.60	119.87	113.25
4	C	600	GTP	C8-N7-C5	2.54	108.79	104.26
4	C	600	GTP	C2'-C1'-N9	-2.53	106.21	113.25
4	G	600	GTP	O2G-PG-O3B	2.51	113.06	104.64
4	E	600	GTP	C5-C6-N1	2.50	119.61	113.25
4	A	600	GTP	C5-C6-N1	2.44	119.47	113.25
4	A	600	GTP	O4'-C1'-N9	-2.44	102.83	108.36
4	A	600	GTP	C8-N7-C5	2.44	108.60	104.26
4	C	600	GTP	O2B-PB-O3A	2.37	113.69	107.27
4	E	600	GTP	O6-C6-C5	-2.32	120.41	126.53
4	A	600	GTP	C3'-C2'-C1'	2.28	105.77	101.46
4	G	600	GTP	O6-C6-C5	-2.25	120.59	126.53
4	A	600	GTP	O6-C6-C5	-2.22	120.66	126.53
4	A	600	GTP	O3G-PG-O3B	2.18	111.95	104.64
4	C	600	GTP	O3'-C3'-C4'	-2.16	104.88	111.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

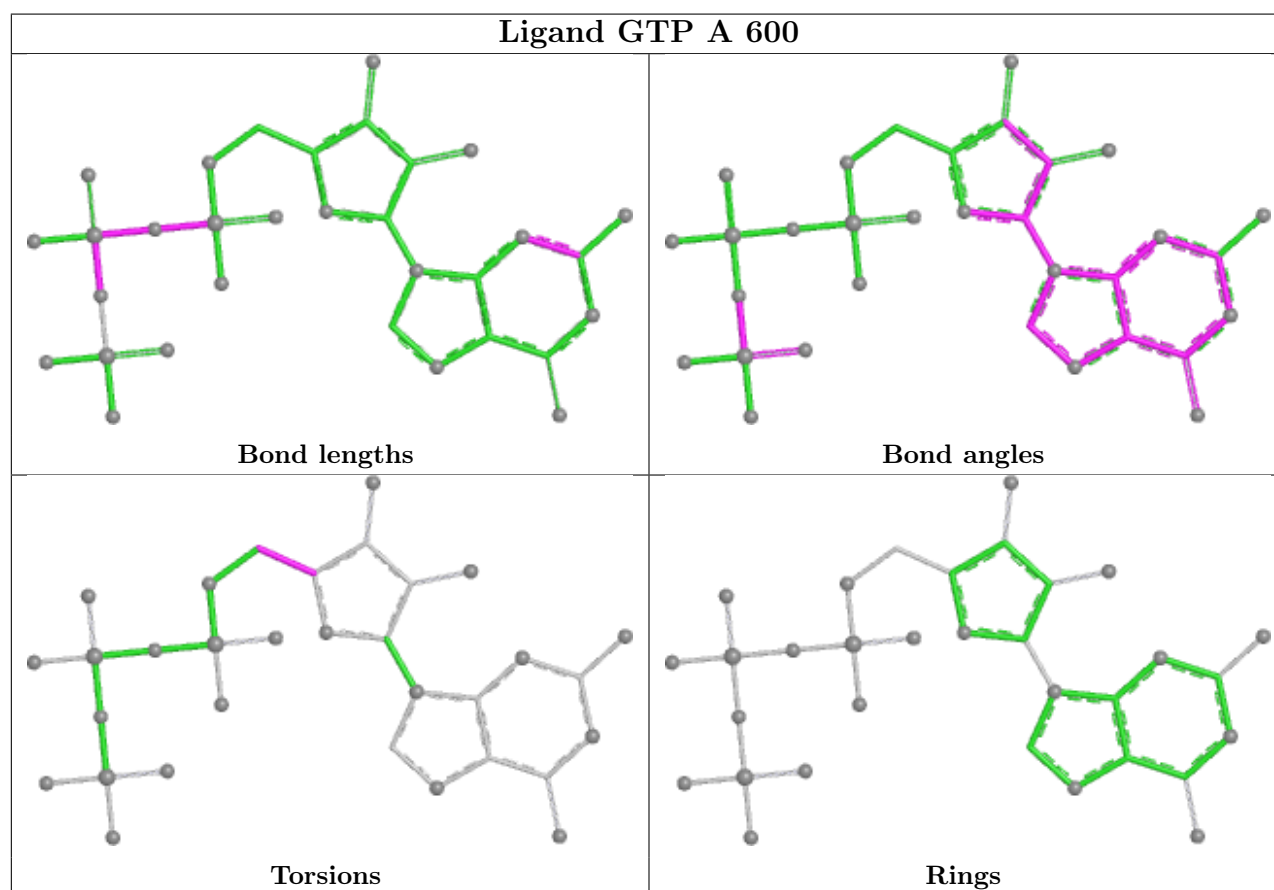
Mol	Chain	Res	Type	Atoms
4	E	600	GTP	PB-O3B-PG-O2G
4	G	600	GTP	PB-O3B-PG-O2G
4	C	600	GTP	O4'-C4'-C5'-O5'
4	A	600	GTP	O4'-C4'-C5'-O5'
4	C	600	GTP	C3'-C4'-C5'-O5'
4	C	600	GTP	PB-O3B-PG-O2G
4	C	600	GTP	PA-O3A-PB-O2B

There are no ring outliers.

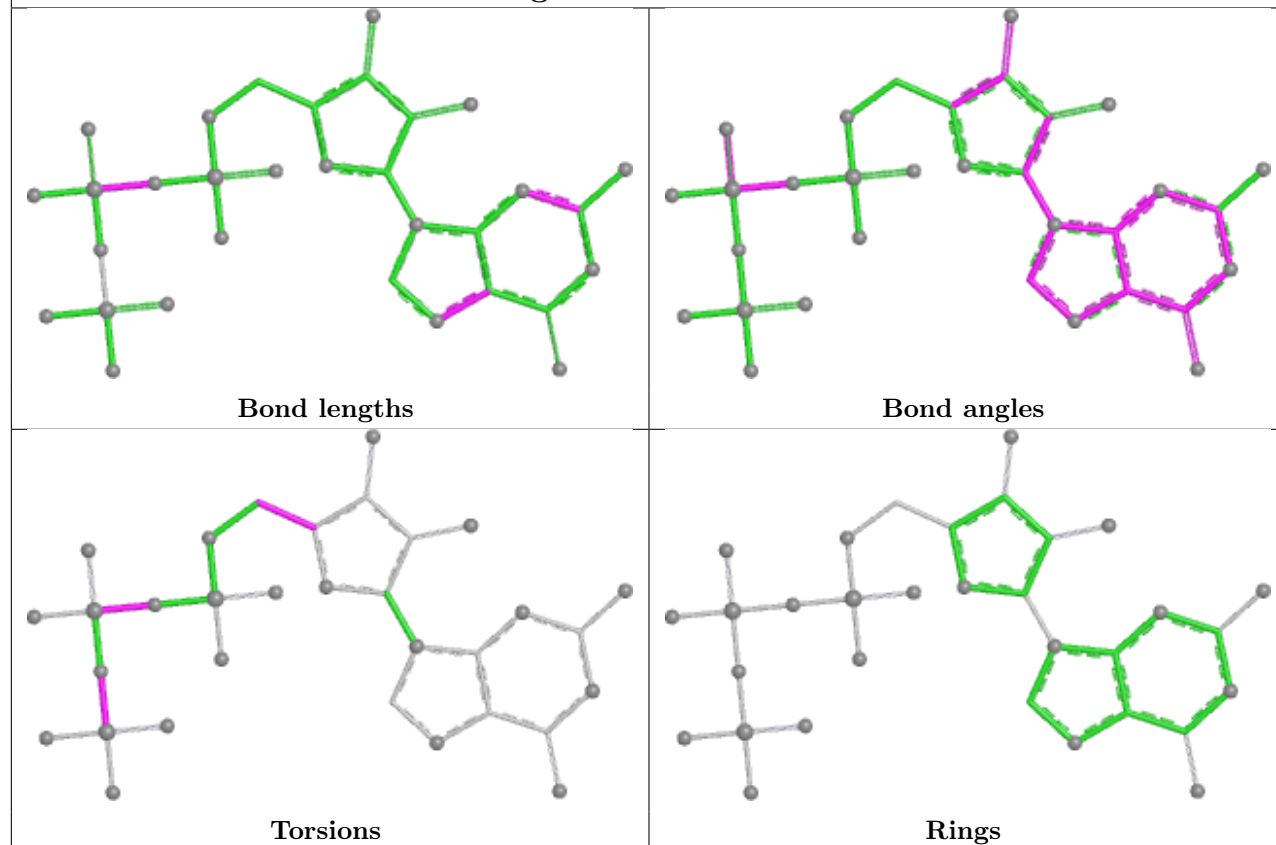
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	6	0
4	C	600	GTP	4	0
4	G	600	GTP	2	0
4	E	600	GTP	3	0

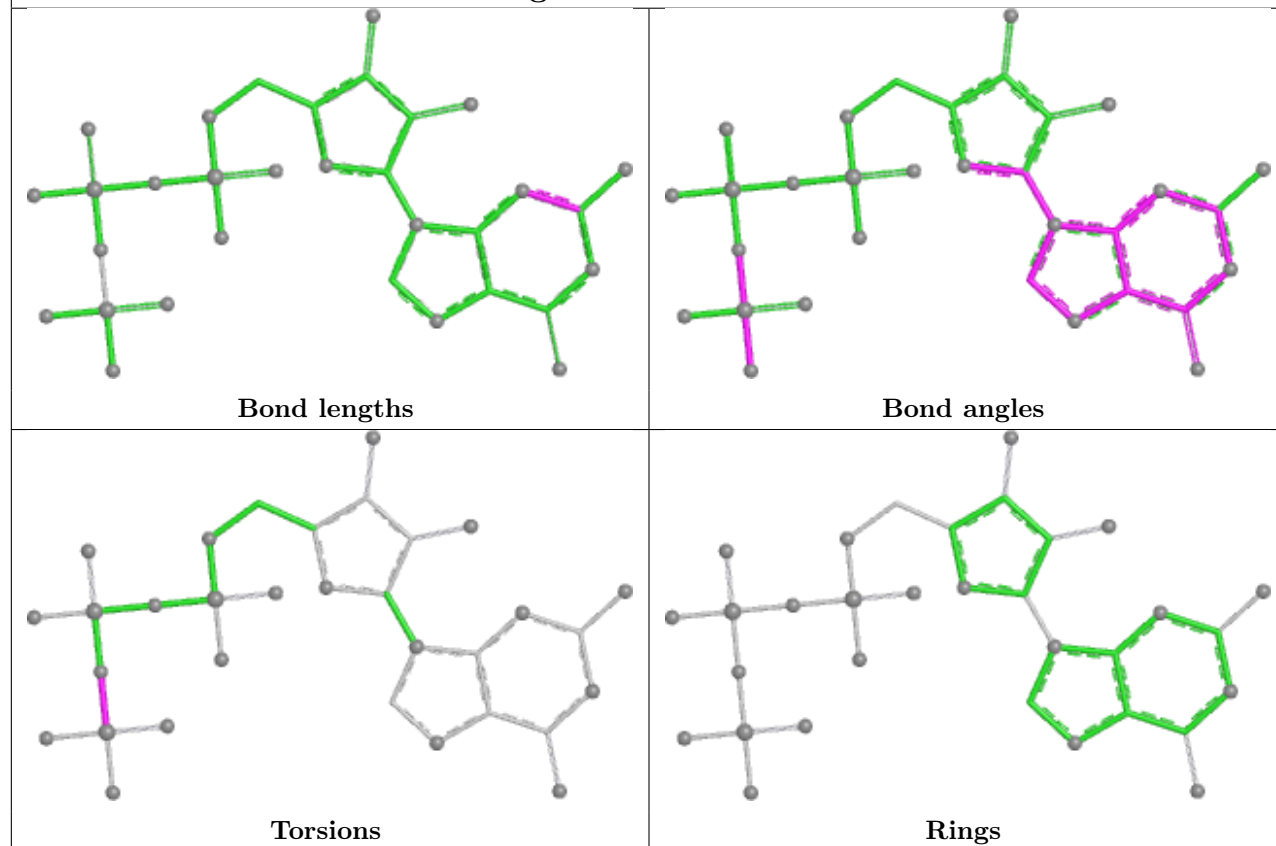
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

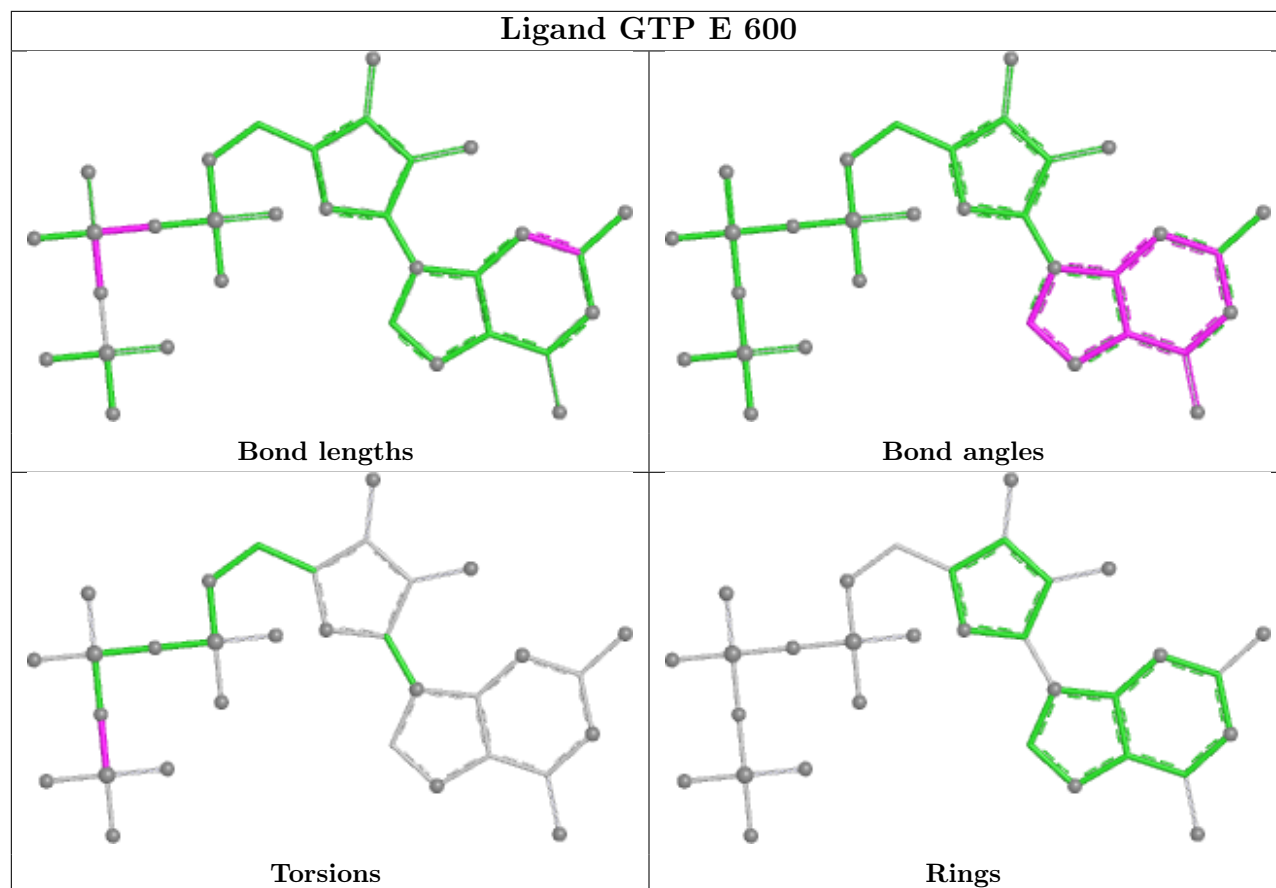


Ligand GTP C 600



Ligand GTP G 600





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	166/169 (98%)	-0.58	1 (0%) 85 66	16, 76, 135, 207	0
1	C	166/169 (98%)	-0.79	0 100 100	1, 33, 90, 129	0
1	G	166/169 (98%)	-0.60	2 (1%) 76 53	20, 68, 124, 159	0
2	B	333/425 (78%)	-0.65	0 100 100	1, 38, 97, 174	0
2	D	303/425 (71%)	-0.49	0 100 100	1, 68, 153, 197	0
2	F	309/425 (72%)	-0.59	1 (0%) 90 77	1, 69, 152, 248	0
2	H	325/425 (76%)	-0.76	0 100 100	2, 40, 90, 128	0
3	E	166/169 (98%)	-0.76	0 100 100	1, 40, 108, 142	0
All	All	1934/2376 (81%)	-0.65	4 (0%) 91 83	1, 51, 132, 248	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	GLY	4.0
2	F	104	TYR	2.4
1	G	39	PRO	2.2
1	G	180	SER	2.2

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](#)

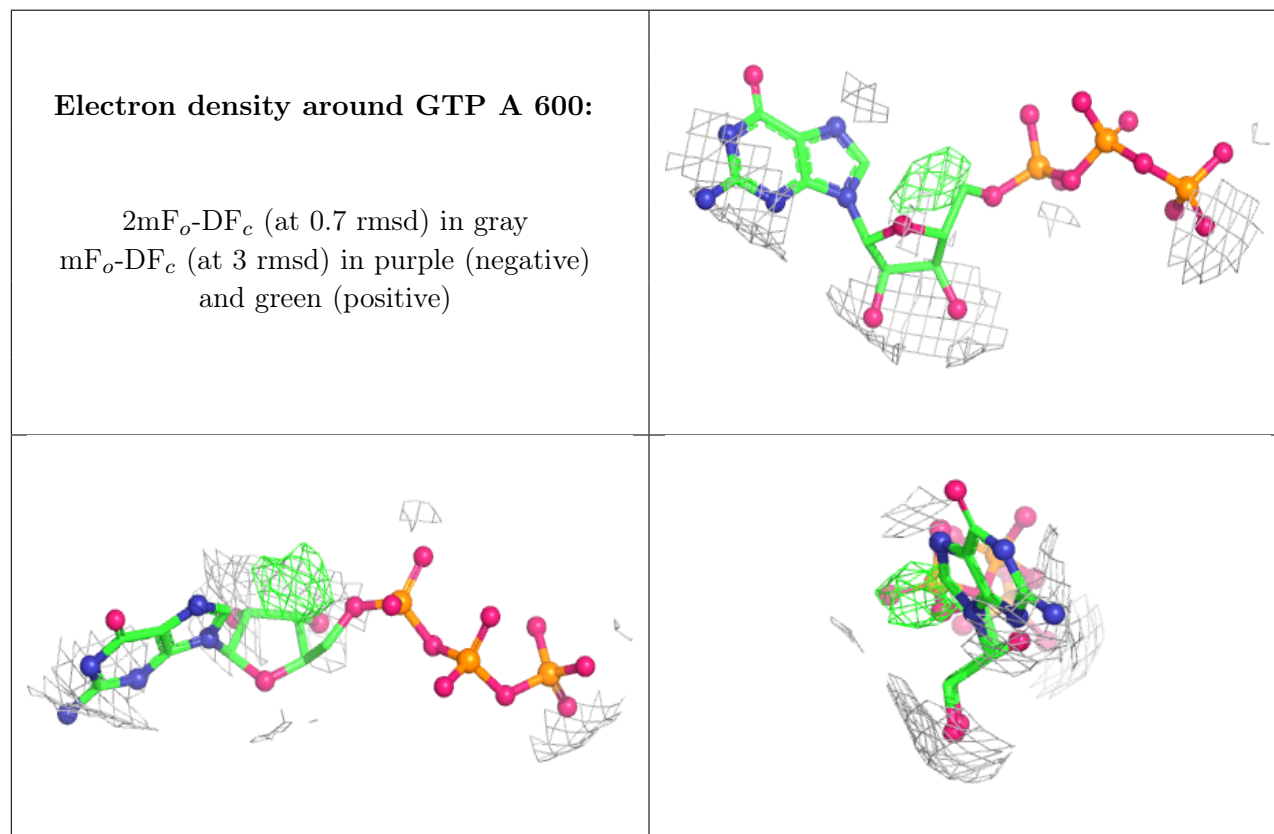
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

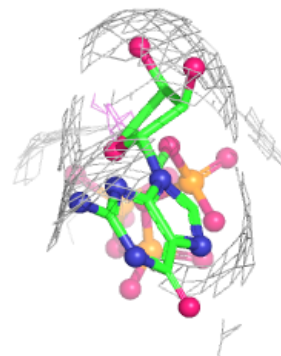
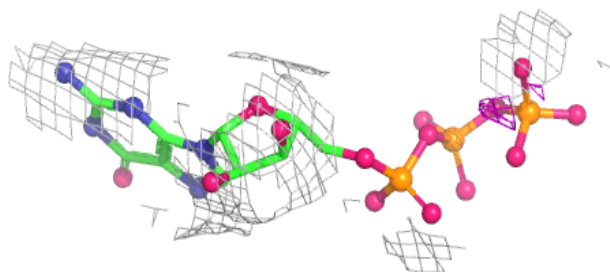
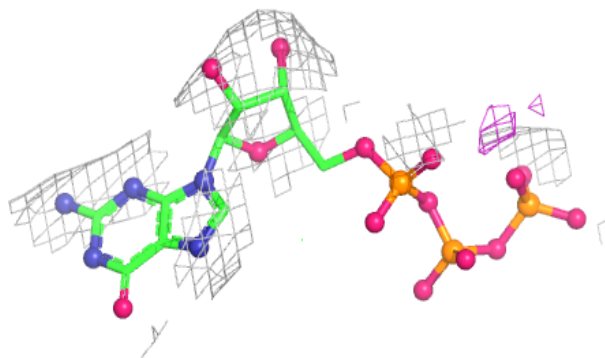
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GTP	A	600	32/32	0.94	0.06	62,71,84,88	0
4	GTP	G	600	32/32	0.96	0.05	51,58,64,70	0
4	GTP	E	600	32/32	0.98	0.04	31,34,40,45	0
4	GTP	C	600	32/32	0.98	0.05	25,31,38,43	0
5	MG	C	601	1/1	0.99	0.10	2,2,2,2	0
5	MG	A	601	1/1	1.00	0.04	16,16,16,16	0
5	MG	E	601	1/1	1.00	0.04	1,1,1,1	0
5	MG	G	601	1/1	1.00	0.03	14,14,14,14	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.

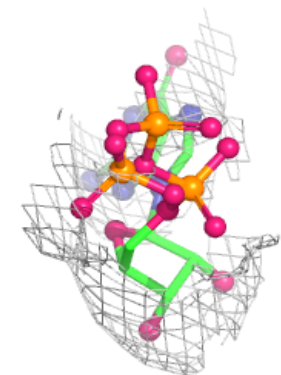
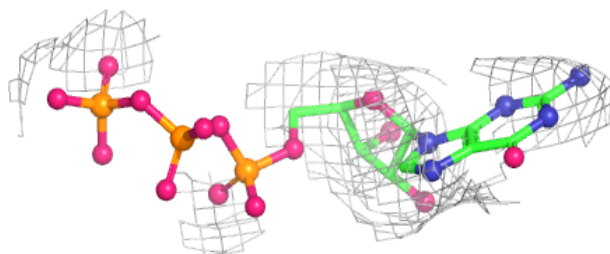
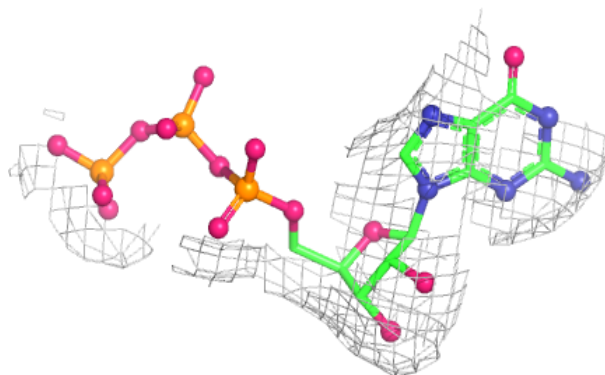


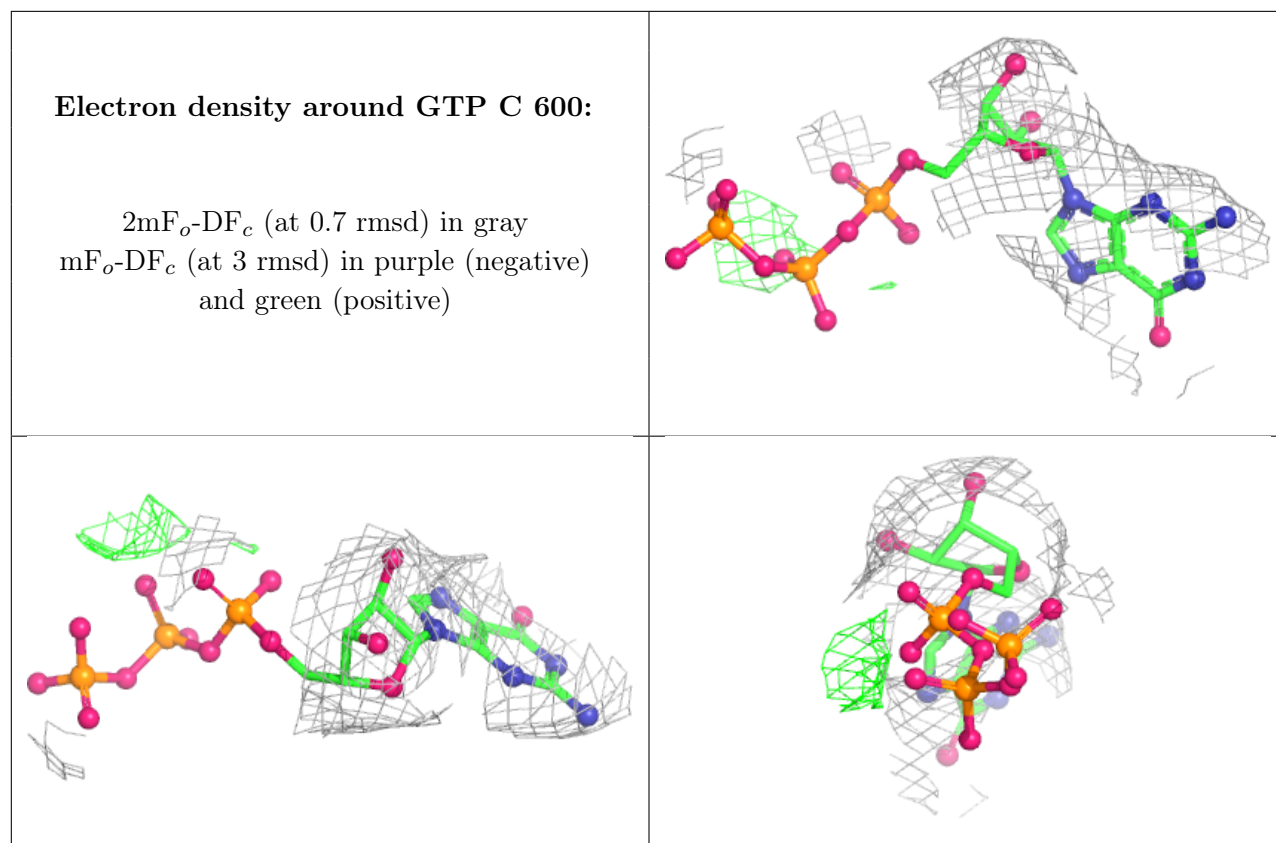
Electron density around GTP G 600:

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

**Electron density around GTP 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.