



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:35 PM UTC

PDB ID : 4V0O / pdb_00004v0o
Title : Crystal structure of BBS1N in complex with ARL6DN, soaked with lead
Authors : Mourao, A.; Lorentzen, E.
Deposited on : 2014-09-17
Resolution : 3.35 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:

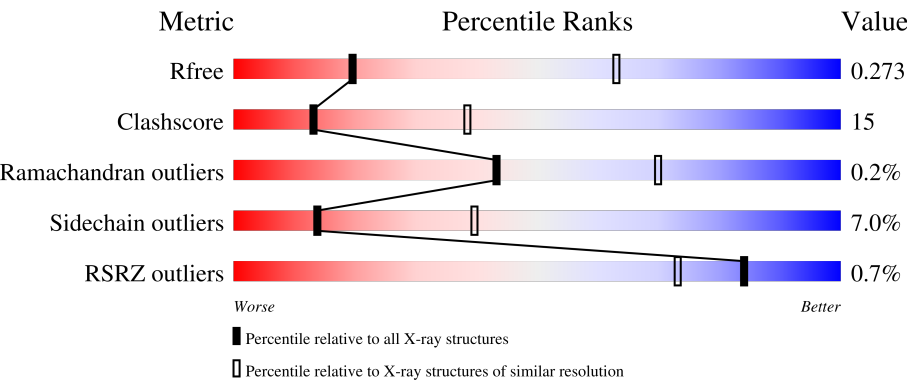
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	76%20%..
1	C	169	% 72%26%..
1	E	169	67%27%...
1	G	169	% 71%23%..
2	B	425	48%28%.22%

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Mol	Chain	Length	Quality of chain
2	D	425	% 44% 26% • 28%
2	F	425	% 46% 24% • 27%
2	H	425	47% 25% • 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14519 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
			1265	809	215	235	6			
1	C	166	Total	C	N	O	S	0	0	0
			1291	823	223	239	6			
1	E	166	Total	C	N	O	S	0	0	0
			1278	816	219	237	6			
1	G	166	Total	C	N	O	S	0	0	0
			1286	822	221	237	6			

There are 16 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
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
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

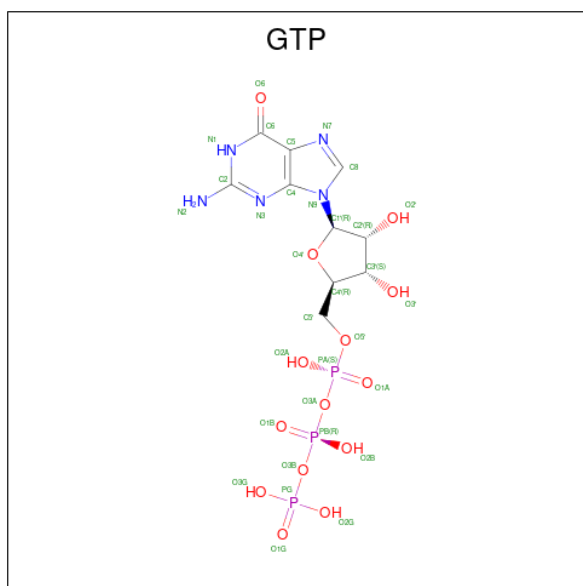
- Molecule 2 is a protein called BARDET-BIEDL SYNDROME 1 PROTEIN.

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	307	Total	C	N	O	S	0	0	0
			2205	1401	387	405	12			
2	F	309	Total	C	N	O	S	0	0	0
			2230	1424	384	409	13			
2	H	325	Total	C	N	O	S	0	0	0
			2386	1525	411	437	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 GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

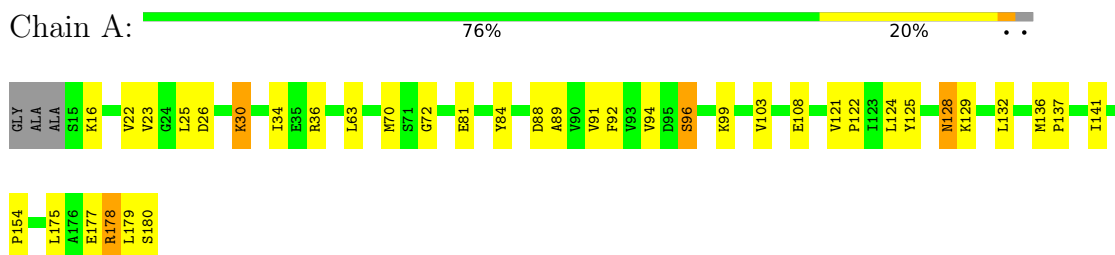
- Molecule 5 is LEAD (II) ION (CCD ID: PB) (formula: Pb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Pb 2	0	0
5	B	4	Total 4	Pb 4	0	0
5	D	3	Total 3	Pb 3	0	0
5	E	1	Total 1	Pb 1	0	0
5	F	3	Total 3	Pb 3	0	0
5	G	1	Total 1	Pb 1	0	0
5	H	4	Total 4	Pb 4	0	0

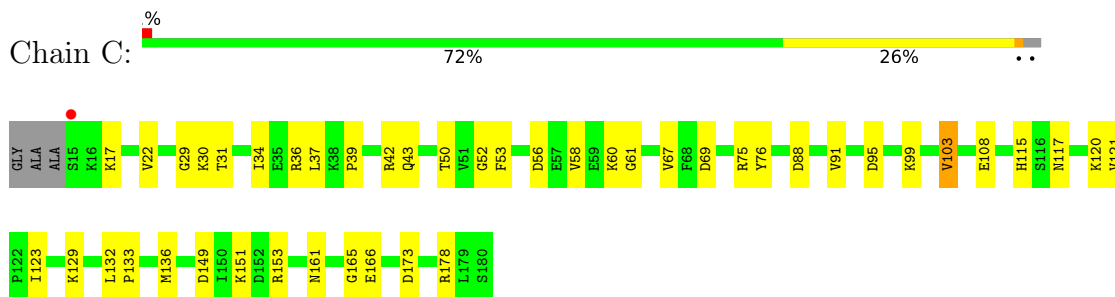
3 Residue-property plots

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

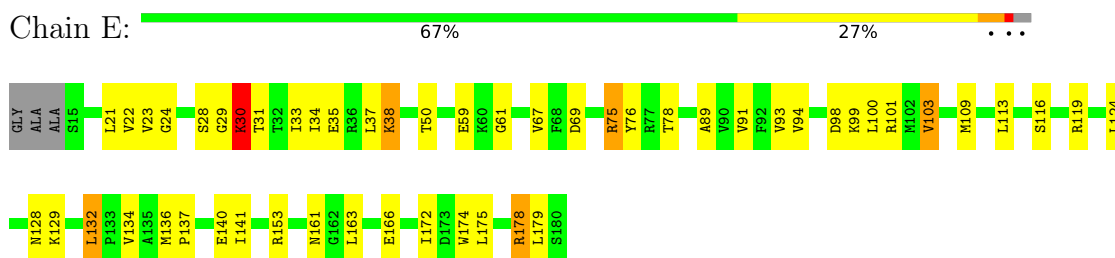
• Molecule 1: ARF-LIKE SMALL GTPASE



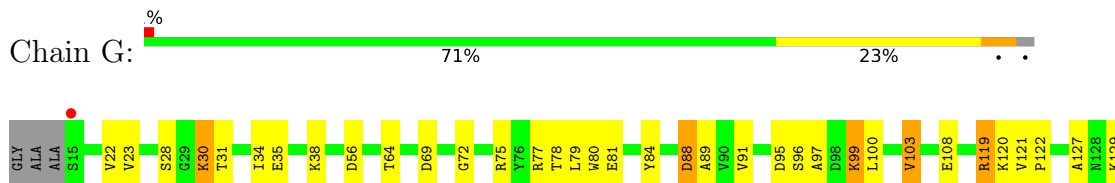
• Molecule 1: ARF-LIKE SMALL GTPASE



• Molecule 1: ARF-LIKE SMALL GTPASE



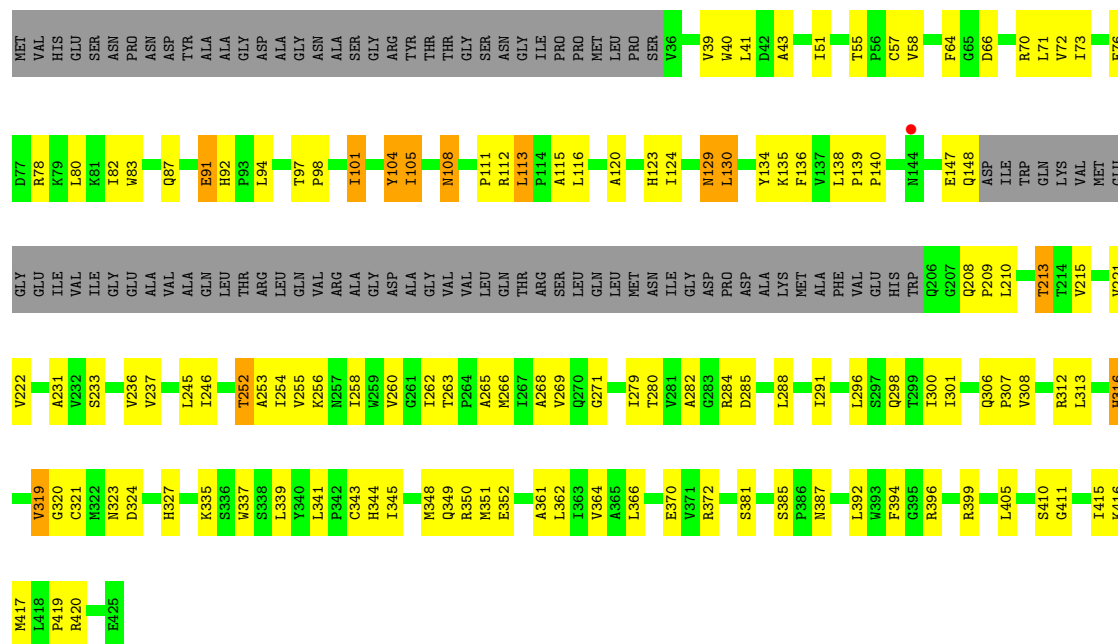
• Molecule 1: ARF-LIKE SMALL GTPASE





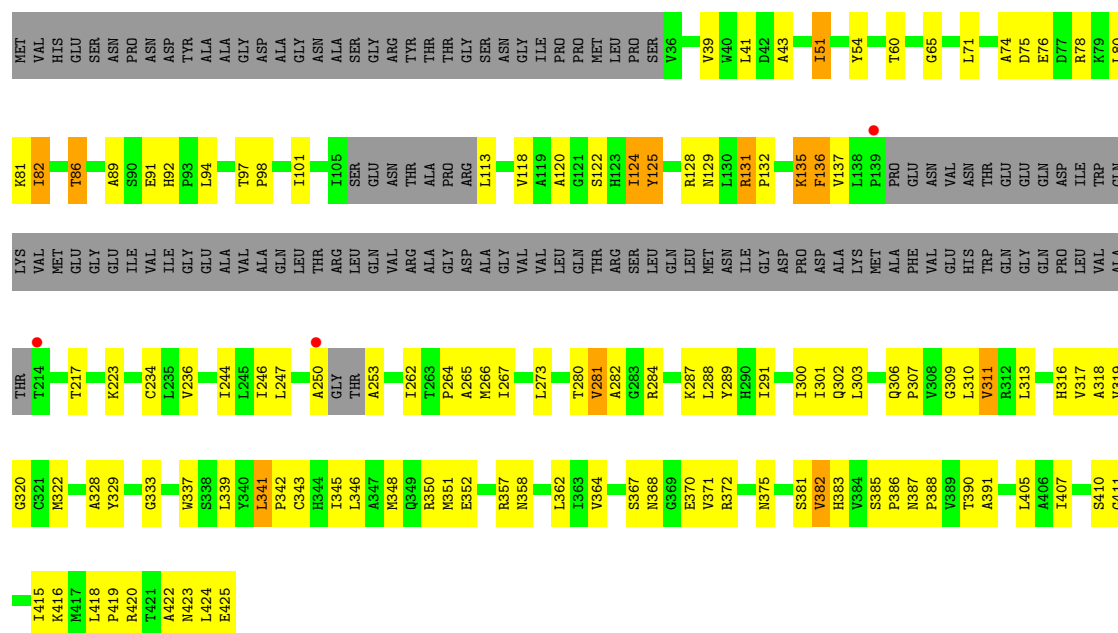
• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

Chain B: 48% 28% 22%

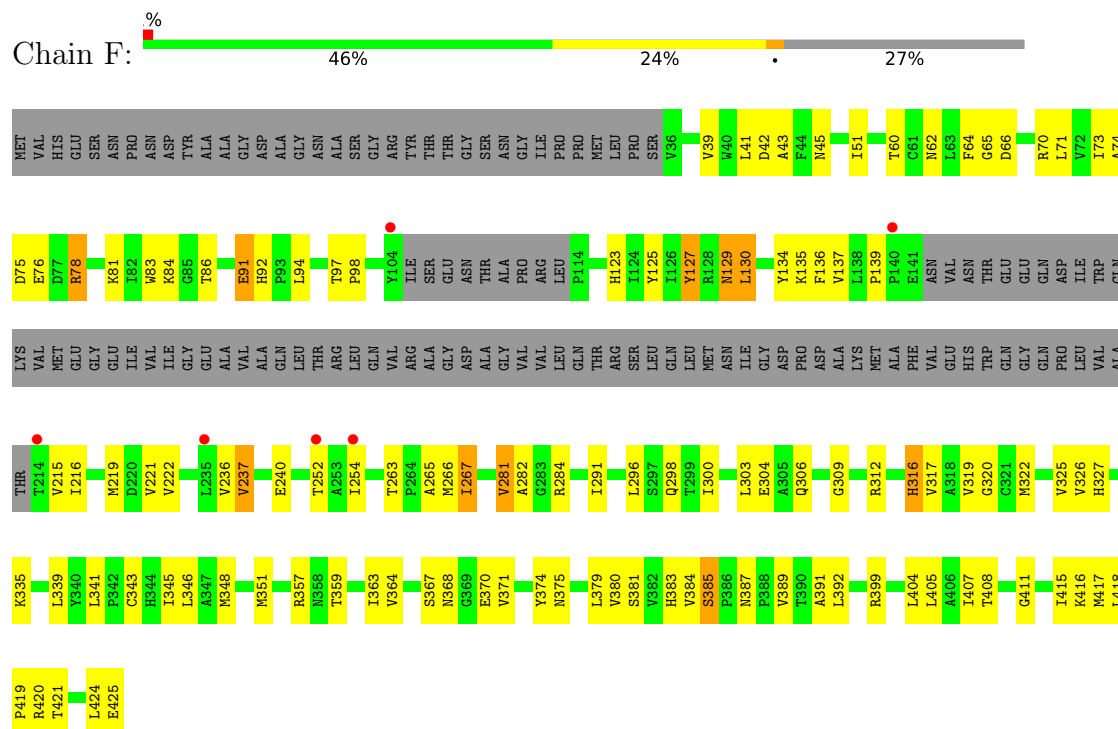


• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN

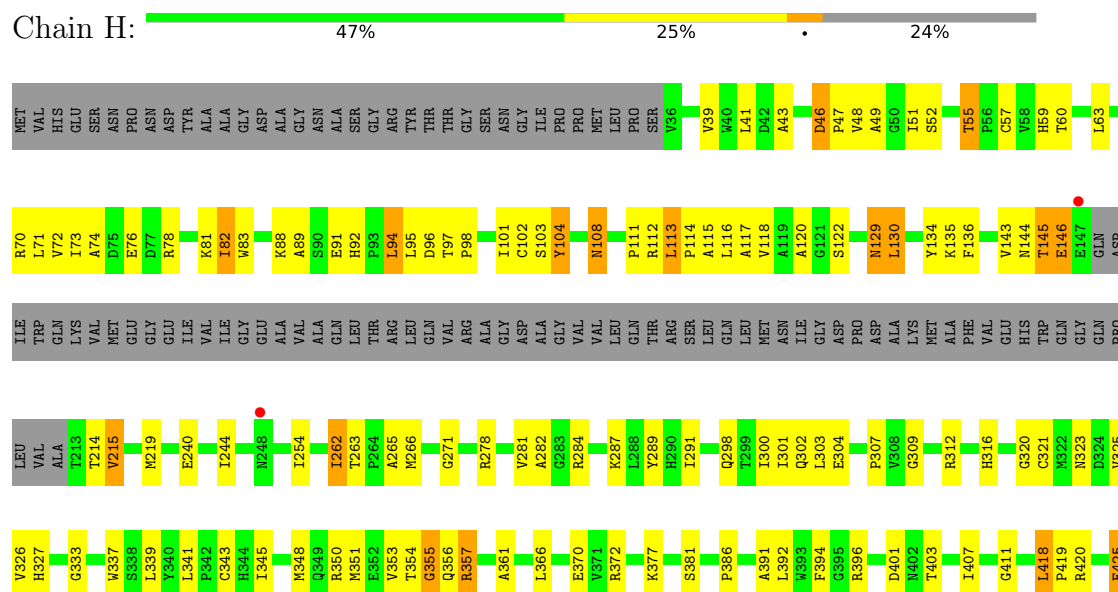
Chain D: 44% 26% 28%



• Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN



● Molecule 2: BARDET-BIEDL SYNDROME 1 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.70Å 123.70Å 439.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	96.27 – 3.35 96.27 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.2 (96.27-3.35) 99.3 (96.27-3.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.221 , 0.268 0.225 , 0.273	Depositor DCC
R_{free} test set	2837 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	114.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14519	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, PB, 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	0.57	0/1291	0.98	1/1758 (0.1%)
1	C	0.84	0/1317	1.14	5/1788 (0.3%)
1	E	0.81	0/1304	1.12	3/1773 (0.2%)
1	G	0.62	0/1312	1.00	5/1781 (0.3%)
2	B	0.80	0/2480	1.15	16/3398 (0.5%)
2	D	0.63	0/2247	1.09	7/3077 (0.2%)
2	F	0.65	0/2276	1.10	16/3118 (0.5%)
2	H	0.78	0/2437	1.19	15/3341 (0.4%)
All	All	0.72	0/14664	1.11	68/20034 (0.3%)

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	H	0	1

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	356	GLN	N-CA-C	-12.77	91.38	110.28
2	D	131	ARG	CA-C-N	9.36	129.42	119.78
2	D	131	ARG	C-N-CA	9.36	129.42	119.78
2	H	129	ASN	N-CA-C	9.12	124.36	113.23
2	H	113	LEU	CA-C-N	-9.06	110.78	120.66
2	H	113	LEU	C-N-CA	-9.06	110.78	120.66
2	H	46	ASP	CA-C-N	8.70	128.41	119.19
2	H	46	ASP	C-N-CA	8.70	128.41	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	129	ASN	N-CA-C	8.52	122.97	112.58
2	B	129	ASN	N-CA-C	8.30	122.70	112.58
2	B	341	LEU	CA-C-N	8.23	128.33	119.28
2	B	341	LEU	C-N-CA	8.23	128.33	119.28
2	B	113	LEU	CA-C-N	-7.53	112.45	120.66
2	B	113	LEU	C-N-CA	-7.53	112.45	120.66
2	H	355	GLY	N-CA-C	-7.45	102.31	112.52
2	H	146	GLU	N-CA-C	7.31	121.28	110.46
2	F	341	LEU	CA-C-N	7.19	127.19	119.28
2	F	341	LEU	C-N-CA	7.19	127.19	119.28
2	F	385	SER	CA-C-N	7.08	128.69	119.84
2	F	385	SER	C-N-CA	7.08	128.69	119.84
2	D	341	LEU	CA-C-N	7.07	127.05	119.28
2	D	341	LEU	C-N-CA	7.07	127.05	119.28
2	B	208	GLN	N-CA-C	6.85	124.95	109.81
1	C	88	ASP	N-CA-C	-6.69	105.03	113.72
2	B	385	SER	CA-C-N	6.48	127.94	119.84
2	B	385	SER	C-N-CA	6.48	127.94	119.84
1	G	137	PRO	CA-C-N	6.17	127.55	119.84
1	G	137	PRO	C-N-CA	6.17	127.55	119.84
2	B	271	GLY	N-CA-C	6.00	119.36	110.60
2	B	308	VAL	N-CA-C	-5.98	107.67	113.53
2	F	127	TYR	N-CA-C	-5.87	102.08	110.59
2	F	139	PRO	CA-C-N	-5.86	112.51	119.84
2	F	139	PRO	C-N-CA	-5.86	112.51	119.84
1	C	61	GLY	CA-C-N	5.86	126.96	120.45
1	C	61	GLY	C-N-CA	5.86	126.96	120.45
2	B	208	GLN	CA-C-N	5.85	127.15	119.84
2	B	208	GLN	C-N-CA	5.85	127.15	119.84
2	H	262	ILE	N-CA-C	5.83	118.15	109.17
1	E	30	LYS	N-CA-C	-5.69	104.99	111.14
2	F	420	ARG	N-CA-C	-5.69	105.16	111.36
2	F	281	VAL	N-CA-C	5.65	116.00	107.75
1	G	88	ASP	N-CA-C	-5.60	106.34	114.12
2	F	91	GLU	N-CA-C	-5.59	101.47	110.14
2	H	271	GLY	N-CA-C	5.57	118.73	110.60
1	G	72	GLY	N-CA-C	-5.47	106.28	115.80
2	B	252	THR	N-CA-C	5.46	118.15	111.82
2	B	253	ALA	N-CA-C	5.41	118.26	109.06
2	F	139	PRO	N-CA-C	5.41	117.30	110.70
2	D	281	VAL	N-CA-C	5.39	115.62	107.75
2	H	418	LEU	CA-C-N	5.38	125.37	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	418	LEU	C-N-CA	5.38	125.37	119.89
2	B	147	GLU	N-CA-C	5.33	117.96	109.65
2	D	113	LEU	CA-C-N	-5.32	113.19	119.84
2	D	113	LEU	C-N-CA	-5.32	113.19	119.84
2	B	319	VAL	CB-CA-C	-5.31	103.62	110.84
1	A	128	ASN	N-CA-C	5.28	117.14	110.33
2	H	355	GLY	CA-C-O	-5.26	117.04	122.25
1	G	99	LYS	N-CA-C	-5.24	105.57	111.28
2	H	144	ASN	N-CA-C	5.23	119.18	109.56
1	E	61	GLY	CA-C-N	5.22	125.92	120.12
1	E	61	GLY	C-N-CA	5.22	125.92	120.12
2	F	237	VAL	N-CA-C	5.17	115.92	108.48
1	C	121	VAL	CA-C-N	5.16	125.16	119.90
1	C	121	VAL	C-N-CA	5.16	125.16	119.90
2	H	215	VAL	N-CA-C	5.06	115.77	108.48
2	F	45	ASN	N-CA-C	5.06	117.64	108.69
2	F	216	ILE	N-CA-C	5.04	115.54	108.89
2	F	78	ARG	N-CA-C	-5.02	105.28	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	355	GLY	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	1265	0	1248	27	0
1	C	1291	0	1297	35	0
1	E	1278	0	1272	40	0
1	G	1286	0	1294	32	0
2	B	2428	0	2359	80	0
2	D	2205	0	2101	75	0
2	F	2230	0	2145	73	0
2	H	2386	0	2329	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	12	4	0
3	C	32	0	12	3	0
3	E	32	0	12	5	0
3	G	32	0	12	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
5	D	3	0	0	0	0
5	E	1	0	0	0	0
5	F	3	0	0	1	0
5	G	1	0	0	0	0
5	H	4	0	0	0	0
All	All	14519	0	14093	427	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 15.

All (427) 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:B:320:GLY:HA3	2:B:348:MET:HE1	1.57	0.86
1:C:129:LYS:HB3	1:C:132:LEU:HD12	1.58	0.84
2:H:345:ILE:HG21	2:H:348:MET:HE2	1.59	0.83
2:B:345:ILE:HG21	2:B:348:MET:HE2	1.63	0.81
2:H:320:GLY:HA3	2:H:348:MET:HE1	1.62	0.81
2:D:82:ILE:HG22	2:D:89:ALA:HB3	1.64	0.80
2:D:74:ALA:HB1	2:D:98:PRO:HG2	1.63	0.79
2:F:39:VAL:HG13	2:F:381:SER:HB2	1.64	0.79
2:F:91:GLU:O	2:F:92:HIS:ND1	2.17	0.78
2:B:350:ARG:NH2	2:B:352:GLU:OE1	2.16	0.78
2:H:112:ARG:N	2:H:113:LEU:HA	1.99	0.77
2:D:345:ILE:HG21	2:D:348:MET:HE2	1.64	0.77
2:D:39:VAL:HG13	2:D:381:SER:HB2	1.66	0.77
1:G:129:LYS:HB3	1:G:132:LEU:HD12	1.67	0.76
2:H:72:VAL:HG11	2:H:116:LEU:HD11	1.67	0.75
1:E:129:LYS:HB3	1:E:132:LEU:HD12	1.70	0.73
2:B:41:LEU:HG	2:B:419:PRO:HG3	1.71	0.73
2:H:136:PHE:HZ	2:H:254:ILE:HG13	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:LYS:O	1:C:34:ILE:HG13	1.89	0.72
1:G:89:ALA:HB2	1:G:179:LEU:HD21	1.72	0.72
2:D:91:GLU:O	2:D:92:HIS:ND1	2.21	0.71
2:H:91:GLU:O	2:H:92:HIS:ND1	2.24	0.71
2:D:311:VAL:HG11	2:D:362:LEU:HD13	1.73	0.70
2:D:94:LEU:HD13	2:D:98:PRO:HG3	1.74	0.70
2:H:94:LEU:HD22	2:H:98:PRO:HG3	1.74	0.69
2:D:346:LEU:HD21	2:D:367:SER:HB3	1.75	0.69
1:A:108:GLU:OE2	2:B:420:ARG:NH1	2.26	0.69
2:H:39:VAL:HG13	2:H:381:SER:HB2	1.75	0.68
2:B:136:PHE:HE2	2:B:138:LEU:HD23	1.57	0.68
2:B:71:LEU:HB3	2:B:83:TRP:HB2	1.75	0.68
2:B:112:ARG:N	2:B:113:LEU:HA	2.08	0.68
1:C:103:VAL:HG11	2:D:43:ALA:HA	1.75	0.68
2:H:108:ASN:OD1	2:H:108:ASN:N	2.26	0.68
2:D:348:MET:HG2	2:D:364:VAL:HG12	1.76	0.68
2:F:296:LEU:HD23	2:F:296:LEU:H	1.59	0.68
2:B:265:ALA:HB2	2:B:284:ARG:HG2	1.76	0.67
2:H:341:LEU:HD23	2:H:366:LEU:HD11	1.77	0.67
2:B:72:VAL:HG11	2:B:116:LEU:HD11	1.77	0.66
2:F:71:LEU:HB3	2:F:83:TRP:HB2	1.77	0.66
2:F:42:ASP:OD1	2:F:416:LYS:NZ	2.27	0.66
1:C:30:LYS:N	3:C:600:GTP:O1B	2.21	0.66
1:A:129:LYS:HB3	1:A:132:LEU:HD12	1.77	0.66
2:H:55:THR:HG23	2:H:392:LEU:H	1.61	0.66
1:A:129:LYS:HG2	3:A:600:GTP:C6	2.30	0.66
2:H:94:LEU:HD21	2:H:118:VAL:HG11	1.78	0.65
2:D:266:MET:HG3	2:D:310:LEU:HB3	1.78	0.65
2:H:130:LEU:O	2:H:130:LEU:HG	1.96	0.65
2:B:51:ILE:HD13	2:B:73:ILE:HD13	1.78	0.65
2:B:321:CYS:HB2	2:B:323:ASN:OD1	1.97	0.65
1:C:39:PRO:HD2	1:C:42:ARG:HD2	1.79	0.65
2:H:51:ILE:HD13	2:H:73:ILE:HD13	1.79	0.65
2:B:288:LEU:HD11	2:B:319:VAL:HG21	1.79	0.64
2:D:265:ALA:HB2	2:D:284:ARG:HG2	1.78	0.64
2:F:346:LEU:HD21	2:F:367:SER:HB3	1.79	0.64
1:E:89:ALA:HB1	1:E:175:LEU:HD11	1.80	0.64
2:F:134:TYR:HD1	2:F:135:LYS:H	1.45	0.63
1:E:30:LYS:N	3:E:600:GTP:O1B	2.21	0.63
1:G:99:LYS:HA	1:G:136:MET:HE1	1.80	0.63
2:B:134:TYR:CZ	2:B:252:THR:HG23	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:ARG:NH2	2:D:352:GLU:OE1	2.32	0.62
1:G:103:VAL:HG11	2:H:43:ALA:HA	1.82	0.61
2:F:304:GLU:OE2	2:F:327:HIS:NE2	2.22	0.61
1:G:178:ARG:N	1:G:178:ARG:HH11	1.99	0.61
1:G:108:GLU:OE1	2:H:420:ARG:NH1	2.34	0.61
2:B:91:GLU:O	2:B:92:HIS:ND1	2.34	0.60
2:B:104:TYR:CE1	2:B:115:ALA:HB3	2.37	0.60
2:F:123:HIS:HA	2:F:137:VAL:HG22	1.82	0.60
2:F:345:ILE:HG21	2:F:348:MET:HE2	1.84	0.60
1:A:22:VAL:HG22	1:A:91:VAL:HB	1.84	0.60
1:A:30:LYS:NZ	1:A:70:MET:O	2.35	0.60
2:H:244:ILE:HD11	2:H:281:VAL:HG21	1.83	0.60
1:G:81:GLU:HA	1:G:84:TYR:CD2	2.37	0.59
2:B:222:VAL:HG23	2:B:236:VAL:HG21	1.84	0.59
2:H:41:LEU:HG	2:H:419:PRO:HG3	1.83	0.59
2:F:134:TYR:HE2	2:F:252:THR:HA	1.66	0.59
2:F:320:GLY:HA3	2:F:348:MET:HE1	1.84	0.59
2:F:74:ALA:HB1	2:F:98:PRO:HG2	1.83	0.59
2:F:418:LEU:HD12	2:F:419:PRO:HD2	1.85	0.59
3:A:600:GTP:C8	3:A:600:GTP:H5'	2.37	0.59
2:D:320:GLY:HA3	2:D:348:MET:HE1	1.84	0.59
2:D:236:VAL:HG22	2:D:246:ILE:HG23	1.84	0.59
2:H:60:THR:HG22	2:H:71:LEU:HA	1.85	0.58
2:F:125:TYR:CD1	2:F:135:LYS:HG2	2.39	0.58
2:D:368:ASN:OD1	2:D:370:GLU:HG2	2.04	0.58
2:B:255:VAL:HG12	2:B:256:LYS:HG2	1.84	0.58
2:B:262:ILE:HG12	2:B:285:ASP:HB3	1.85	0.58
1:A:16:LYS:HB3	1:A:63:LEU:HD23	1.84	0.58
2:B:51:ILE:O	2:B:411:GLY:HA2	2.03	0.58
1:A:96:SER:HB2	1:A:128:ASN:O	2.03	0.57
1:E:103:VAL:HG22	2:F:41:LEU:HD13	1.85	0.57
2:H:266:MET:HE3	2:H:307:PRO:HB2	1.86	0.57
2:H:266:MET:HG2	2:H:282:ALA:HB3	1.86	0.57
2:F:94:LEU:HD13	2:F:98:PRO:HG3	1.85	0.57
2:H:49:ALA:HB1	2:H:51:ILE:HG13	1.85	0.57
1:C:99:LYS:HB3	2:D:86:THR:HG21	1.86	0.57
2:H:104:TYR:CE1	2:H:115:ALA:HB3	2.39	0.57
2:B:108:ASN:OD1	2:B:108:ASN:N	2.28	0.57
2:H:136:PHE:CZ	2:H:254:ILE:HG13	2.38	0.57
1:E:37:LEU:HD21	1:E:172:ILE:HG13	1.86	0.57
2:F:70:ARG:HH11	2:F:84:LYS:CB	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:GLU:C	2:H:78:ARG:H	2.13	0.57
1:C:129:LYS:HG2	3:C:600:GTP:C6	2.40	0.56
1:G:38:LYS:HE2	1:G:56:ASP:OD2	2.05	0.56
1:C:123:ILE:HD11	1:C:153:ARG:HD3	1.86	0.56
2:D:267:ILE:HG22	2:D:281:VAL:HG22	1.88	0.56
1:G:89:ALA:HB1	1:G:175:LEU:HD11	1.87	0.56
2:D:391:ALA:HB3	2:D:407:ILE:HB	1.88	0.56
2:F:368:ASN:OD1	2:F:370:GLU:HG2	2.05	0.56
2:F:222:VAL:HG23	2:F:236:VAL:HG21	1.87	0.56
2:B:98:PRO:HA	2:B:120:ALA:HB2	1.88	0.56
2:D:54:TYR:CD2	2:D:390:THR:HB	2.41	0.56
2:H:63:LEU:HD21	2:H:116:LEU:HD12	1.89	0.55
2:H:122:SER:HB3	2:H:214:THR:O	2.06	0.55
2:D:423:ASN:OD1	2:D:423:ASN:N	2.39	0.55
2:H:370:GLU:OE2	2:H:372:ARG:NE	2.38	0.55
2:F:75:ASP:OD2	2:F:81:LYS:HE3	2.07	0.55
2:F:343:CYS:HB2	2:F:368:ASN:ND2	2.20	0.55
2:B:279:ILE:HB	2:B:291:ILE:HB	1.89	0.55
2:D:250:ALA:O	2:D:253:ALA:N	2.40	0.55
1:E:31:THR:OG1	3:E:600:GTP:O2B	2.24	0.55
1:C:103:VAL:HG22	2:D:41:LEU:HD13	1.89	0.54
2:D:309:GLY:HA3	2:D:348:MET:HE3	1.89	0.54
2:H:51:ILE:O	2:H:411:GLY:HA2	2.08	0.54
2:B:43:ALA:HB1	2:B:417:MET:HE2	1.89	0.54
2:D:357:ARG:NH1	2:D:422:ALA:O	2.34	0.54
2:H:321:CYS:HB2	2:H:323:ASN:OD1	2.06	0.54
3:G:600:GTP:H5'	3:G:600:GTP:H8	1.73	0.54
2:H:101:ILE:HD12	2:H:116:LEU:HD21	1.90	0.54
1:C:120:LYS:HA	1:C:153:ARG:NH1	2.23	0.54
2:F:357:ARG:O	2:F:359:THR:HG23	2.08	0.54
2:H:71:LEU:HB3	2:H:83:TRP:HB2	1.89	0.54
1:C:36:ARG:NH1	1:C:43:GLN:OE1	2.41	0.53
2:H:351:MET:HA	2:H:394:PHE:CD2	2.43	0.53
2:D:125:TYR:CD1	2:D:135:LYS:HD3	2.43	0.53
2:D:41:LEU:HG	2:D:419:PRO:HG3	1.91	0.53
1:E:29:GLY:N	3:E:600:GTP:O1B	2.40	0.53
1:G:22:VAL:HG22	1:G:91:VAL:HB	1.89	0.53
2:F:129:ASN:N	2:F:130:LEU:HA	2.23	0.53
2:B:64:PHE:HB2	2:B:66:ASP:OD1	2.08	0.53
2:F:326:VAL:HB	2:F:339:LEU:HB2	1.90	0.53
2:B:80:LEU:HB2	2:B:94:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:CZ	1:E:76:TYR:HE1	2.22	0.52
2:F:265:ALA:HB2	2:F:284:ARG:HG2	1.92	0.52
2:H:304:GLU:OE2	2:H:327:HIS:NE2	2.42	0.52
1:G:122:PRO:HA	1:G:154:PRO:HG2	1.91	0.52
2:B:351:MET:HG3	2:B:394:PHE:CE2	2.45	0.52
2:B:76:GLU:C	2:B:78:ARG:H	2.17	0.52
1:A:23:VAL:HG23	1:A:92:PHE:CD2	2.45	0.52
2:B:298:GLN:O	2:B:300:ILE:HD12	2.10	0.52
1:A:103:VAL:HG11	2:B:43:ALA:HA	1.91	0.52
2:F:76:GLU:C	2:F:78:ARG:H	2.16	0.52
2:H:309:GLY:HA3	2:H:348:MET:HE3	1.92	0.52
2:B:266:MET:HG2	2:B:282:ALA:HB3	1.91	0.51
2:D:217:THR:OG1	2:D:264:PRO:HG2	2.10	0.51
2:B:39:VAL:HG13	2:B:381:SER:HB2	1.92	0.51
2:B:101:ILE:HD12	2:B:116:LEU:HD21	1.93	0.51
2:D:98:PRO:HA	2:D:120:ALA:HB2	1.91	0.51
2:D:244:ILE:HD11	2:D:281:VAL:HG21	1.93	0.51
1:E:34:ILE:HD13	1:E:67:VAL:HG11	1.91	0.51
2:D:54:TYR:CE2	2:D:390:THR:HB	2.46	0.51
1:A:89:ALA:HB1	1:A:175:LEU:HD11	1.93	0.51
2:H:129:ASN:N	2:H:130:LEU:HA	2.25	0.51
2:H:337:TRP:CE3	2:H:339:LEU:HD13	2.46	0.51
2:B:105:ILE:HG12	2:B:231:ALA:O	2.11	0.51
3:G:600:GTP:H5'	3:G:600:GTP:C8	2.46	0.51
2:D:311:VAL:HG12	2:D:318:ALA:HB3	1.92	0.50
2:D:51:ILE:O	2:D:411:GLY:HA2	2.10	0.50
1:A:89:ALA:HB2	1:A:179:LEU:HD21	1.93	0.50
3:A:600:GTP:H5'	3:A:600:GTP:H8	1.76	0.50
1:E:29:GLY:HA2	3:E:600:GTP:O1A	2.11	0.50
1:E:98:ASP:OD2	1:E:101:ARG:HG3	2.12	0.50
2:D:101:ILE:HG22	2:D:118:VAL:HA	1.93	0.50
2:F:75:ASP:OD1	2:F:76:GLU:N	2.45	0.50
2:F:348:MET:HG2	2:F:364:VAL:HG12	1.94	0.50
2:B:94:LEU:HD23	2:B:98:PRO:HG3	1.94	0.49
2:B:362:LEU:HD22	2:B:364:VAL:HG23	1.93	0.49
2:F:60:THR:HG22	2:F:71:LEU:HA	1.93	0.49
2:F:312:ARG:O	2:F:312:ARG:HG3	2.12	0.49
2:H:278:ARG:HA	2:H:291:ILE:O	2.12	0.49
2:F:371:VAL:HB	2:F:383:HIS:NE2	2.28	0.49
2:B:370:GLU:OE1	2:B:372:ARG:NE	2.44	0.49
1:C:99:LYS:HG3	1:C:136:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:ASN:HB3	1:E:166:GLU:HB3	1.95	0.49
1:E:31:THR:HG23	1:E:69:ASP:OD2	2.11	0.49
1:C:149:ASP:HA	1:C:151:LYS:HE3	1.94	0.49
2:H:74:ALA:HB1	2:H:98:PRO:HG2	1.94	0.49
1:E:30:LYS:O	1:E:34:ILE:HG13	2.13	0.49
1:E:174:TRP:NE1	1:E:178:ARG:HE	2.10	0.49
2:F:43:ALA:HB3	2:F:415:ILE:O	2.12	0.49
1:G:96:SER:O	1:G:136:MET:N	2.43	0.49
2:D:423:ASN:ND2	2:D:425:GLU:OE2	2.46	0.49
2:F:391:ALA:HB3	2:F:407:ILE:HB	1.95	0.49
2:D:75:ASP:OD2	2:D:81:LYS:HE3	2.13	0.49
2:D:371:VAL:HB	2:D:383:HIS:NE2	2.28	0.49
2:D:375:ASN:ND2	2:D:424:LEU:O	2.44	0.49
2:F:327:HIS:CE1	2:F:335:LYS:HE3	2.48	0.49
2:B:266:MET:HE3	2:B:307:PRO:HB2	1.94	0.49
2:H:298:GLN:O	2:H:300:ILE:HD12	2.13	0.49
2:H:396:ARG:NH1	2:H:401:ASP:OD1	2.46	0.49
2:B:136:PHE:CE2	2:B:138:LEU:HD23	2.44	0.48
2:D:287:LYS:HE2	2:D:302:GLN:OE1	2.13	0.48
2:B:260:VAL:HG22	2:B:296:LEU:HG	1.96	0.48
2:F:51:ILE:O	2:F:411:GLY:HA2	2.13	0.48
2:F:266:MET:HG2	2:F:282:ALA:HB3	1.95	0.48
1:A:88:ASP:O	1:A:121:VAL:HB	2.12	0.48
2:B:108:ASN:O	2:B:111:PRO:HD3	2.13	0.48
2:D:136:PHE:CZ	2:D:253:ALA:HA	2.48	0.48
2:D:385:SER:OG	2:D:387:ASN:O	2.31	0.48
2:B:350:ARG:NH2	2:B:352:GLU:HB2	2.28	0.48
2:F:136:PHE:HZ	2:F:254:ILE:HG13	1.77	0.48
1:E:31:THR:OG1	1:E:50:THR:OG1	2.31	0.48
2:H:287:LYS:HE2	2:H:302:GLN:OE1	2.13	0.48
1:A:30:LYS:O	1:A:34:ILE:HG13	2.14	0.48
1:E:24:GLY:O	1:E:30:LYS:HE2	2.14	0.48
1:E:99:LYS:HA	1:E:136:MET:HE1	1.95	0.48
1:G:127:ALA:HB3	1:G:159:PRO:HA	1.96	0.48
2:D:328:ALA:HB3	2:D:337:TRP:H	1.79	0.48
2:H:94:LEU:HD11	2:H:118:VAL:HG21	1.95	0.48
2:B:123:HIS:CE1	2:B:135:LYS:HD3	2.49	0.47
1:G:108:GLU:CD	2:H:420:ARG:HH11	2.22	0.47
2:H:262:ILE:HD12	2:H:263:THR:H	1.79	0.47
1:E:35:GLU:HA	1:E:38:LYS:HD3	1.97	0.47
2:F:375:ASN:ND2	2:F:424:LEU:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:PRO:HB2	2:B:113:LEU:CB	2.44	0.47
1:E:23:VAL:C	1:E:30:LYS:HD3	2.39	0.47
1:G:23:VAL:HB	1:G:80:TRP:CZ3	2.50	0.47
2:D:346:LEU:HD11	2:D:388:PRO:HB2	1.97	0.47
1:G:77:ARG:C	1:G:79:LEU:H	2.23	0.47
2:B:129:ASN:N	2:B:130:LEU:HA	2.29	0.47
2:H:425:GLU:N	2:H:425:GLU:OE1	2.48	0.47
2:B:130:LEU:HG	2:B:130:LEU:O	2.13	0.47
2:D:125:TYR:HD1	2:D:135:LYS:HD3	1.78	0.47
2:F:240:GLU:HG3	2:F:263:THR:HG23	1.96	0.47
1:G:120:LYS:HD2	1:G:152:ASP:HB2	1.97	0.47
2:H:41:LEU:CG	2:H:419:PRO:HG3	2.45	0.47
2:H:351:MET:HG3	2:H:394:PHE:CE2	2.49	0.47
2:F:51:ILE:HD13	2:F:73:ILE:HD13	1.96	0.47
2:H:82:ILE:HG22	2:H:89:ALA:HB3	1.97	0.47
2:B:140:PRO:HB3	2:B:213:THR:HG23	1.97	0.47
2:D:289:TYR:CD1	2:D:300:ILE:HD12	2.49	0.47
1:G:35:GLU:OE1	1:G:38:LYS:HD2	2.14	0.47
1:C:39:PRO:HG2	1:C:42:ARG:CZ	2.45	0.47
1:E:34:ILE:HD13	1:E:67:VAL:CG1	2.45	0.47
2:B:387:ASN:CG	2:B:410:SER:HB3	2.39	0.46
2:F:387:ASN:HB2	2:F:408:THR:HB	1.97	0.46
2:H:394:PHE:HA	2:H:403:THR:O	2.15	0.46
2:D:76:GLU:C	2:D:78:ARG:H	2.22	0.46
2:H:59:HIS:CE1	2:H:103:SER:HB3	2.51	0.46
2:H:391:ALA:HB3	2:H:407:ILE:HB	1.96	0.46
2:F:316:HIS:N	2:F:316:HIS:CD2	2.84	0.46
1:C:29:GLY:HA2	3:C:600:GTP:O1A	2.16	0.46
2:H:101:ILE:HG22	2:H:118:VAL:HG13	1.98	0.46
2:H:304:GLU:OE1	2:H:323:ASN:ND2	2.36	0.46
1:C:75:ARG:CZ	1:C:76:TYR:HE1	2.29	0.46
1:E:109:MET:O	1:E:113:LEU:HD12	2.15	0.46
2:F:320:GLY:HA3	2:F:348:MET:CE	2.45	0.46
2:F:375:ASN:HB2	2:F:380:VAL:HG21	1.97	0.46
2:H:111:PRO:C	2:H:113:LEU:HA	2.40	0.46
2:H:117:ALA:O	2:H:219:MET:HE1	2.16	0.46
2:B:136:PHE:HZ	2:B:254:ILE:HG13	1.81	0.46
1:G:108:GLU:OE2	2:H:420:ARG:HD3	2.15	0.46
1:G:138:PRO:HG3	1:G:159:PRO:HB3	1.98	0.46
1:C:108:GLU:OE1	2:D:420:ARG:NH1	2.49	0.45
2:D:372:ARG:HG2	2:D:382:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:ALA:CB	2:B:417:MET:HE2	2.46	0.45
1:C:34:ILE:HD13	1:C:67:VAL:HG11	1.98	0.45
1:C:132:LEU:HD23	1:C:133:PRO:HD2	1.97	0.45
2:F:125:TYR:HB3	2:F:127:TYR:HE1	1.80	0.45
1:G:88:ASP:O	1:G:121:VAL:HB	2.17	0.45
2:H:326:VAL:HB	2:H:339:LEU:HB2	1.97	0.45
2:B:124:ILE:HD11	2:B:237:VAL:HG21	1.98	0.45
2:F:71:LEU:HD13	2:F:405:LEU:HD13	1.97	0.45
2:F:370:GLU:HB3	2:F:384:VAL:HG22	1.98	0.45
1:G:103:VAL:CG2	2:H:41:LEU:HB3	2.46	0.45
1:A:122:PRO:HG3	1:A:154:PRO:HG2	1.98	0.45
2:F:64:PHE:O	2:F:66:ASP:N	2.50	0.45
1:C:115:HIS:CE1	1:C:117:ASN:HB2	2.52	0.45
2:H:102:CYS:HB3	2:H:103:SER:H	1.62	0.45
1:C:31:THR:OG1	1:C:50:THR:OG1	2.35	0.45
2:D:337:TRP:CE3	2:D:339:LEU:HD13	2.51	0.45
2:B:320:GLY:HA3	2:B:348:MET:CE	2.40	0.45
2:B:351:MET:O	2:B:361:ALA:N	2.43	0.45
1:G:103:VAL:HG21	2:H:41:LEU:HB3	1.98	0.45
2:H:240:GLU:HA	2:H:263:THR:HG23	1.99	0.45
2:B:41:LEU:CG	2:B:419:PRO:HG3	2.46	0.44
2:B:268:ALA:HB3	2:B:280:THR:HB	1.98	0.44
1:G:31:THR:HG23	1:G:69:ASP:OD2	2.18	0.44
1:E:21:LEU:HG	1:E:23:VAL:HG13	1.98	0.44
2:B:324:ASP:OD1	2:B:344:HIS:HA	2.18	0.44
1:A:136:MET:HA	1:A:137:PRO:HD3	1.84	0.44
1:E:100:LEU:HD12	1:E:100:LEU:HA	1.68	0.44
1:E:101:ARG:HD3	2:F:399:ARG:HB2	2.00	0.44
2:F:70:ARG:HG2	2:F:83:TRP:O	2.18	0.44
1:E:136:MET:HA	1:E:137:PRO:HD3	1.75	0.44
2:F:392:LEU:HD22	2:F:404:LEU:HD11	1.98	0.44
1:C:60:LYS:NZ	1:C:173:ASP:OD1	2.47	0.44
2:D:223:LYS:O	2:D:273:LEU:N	2.34	0.44
2:F:306:GLN:HG3	2:F:322:MET:HB2	1.99	0.44
2:F:309:GLY:HA3	2:F:348:MET:HE3	2.00	0.44
2:H:57:CYS:HB3	2:H:74:ALA:HB3	1.99	0.44
1:A:26:ASP:HB3	1:A:72:GLY:C	2.42	0.44
2:D:341:LEU:HA	2:D:342:PRO:HD3	1.79	0.44
2:F:385:SER:OG	2:F:389:VAL:HG23	2.18	0.44
2:H:41:LEU:CD2	2:H:419:PRO:HG3	2.48	0.44
2:H:301:ILE:HD11	2:H:333:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:NH2	1:E:76:TYR:HE1	2.16	0.44
1:G:136:MET:HE3	1:G:136:MET:HB2	1.85	0.44
2:D:74:ALA:HB1	2:D:98:PRO:CG	2.42	0.43
1:E:103:VAL:HG11	2:F:43:ALA:HA	2.00	0.43
1:E:163:LEU:HA	1:E:163:LEU:HD23	1.58	0.43
1:A:92:PHE:HB3	1:A:125:TYR:CD1	2.53	0.43
2:B:57:CYS:HA	2:B:101:ILE:HG23	2.00	0.43
2:D:266:MET:HE3	2:D:307:PRO:HB2	2.00	0.43
2:H:262:ILE:HG21	2:H:289:TYR:CE2	2.52	0.43
2:H:357:ARG:H	2:H:357:ARG:HG3	1.32	0.43
1:C:52:GLY:HA2	1:C:76:TYR:CD2	2.53	0.43
2:D:301:ILE:HG21	2:D:329:TYR:CE1	2.53	0.43
2:D:387:ASN:CG	2:D:410:SER:HB3	2.43	0.43
1:E:75:ARG:H	1:E:75:ARG:HG2	1.33	0.43
1:A:81:GLU:HA	1:A:84:TYR:CD2	2.54	0.43
2:B:43:ALA:HB3	2:B:415:ILE:O	2.18	0.43
2:B:97:THR:HA	2:B:98:PRO:HD3	1.77	0.43
2:B:313:LEU:HB2	2:B:316:HIS:O	2.18	0.43
2:H:244:ILE:HD12	2:H:291:ILE:HD12	2.00	0.43
2:B:140:PRO:HB3	2:B:213:THR:CG2	2.48	0.43
2:D:244:ILE:HD12	2:D:291:ILE:HD12	1.99	0.43
1:A:36:ARG:HA	1:A:36:ARG:HD3	1.88	0.43
1:A:99:LYS:HA	1:A:136:MET:HE1	2.00	0.43
2:D:351:MET:HE3	2:D:418:LEU:HD22	1.99	0.43
2:H:46:ASP:HA	2:H:47:PRO:HD2	1.77	0.43
2:H:111:PRO:HB2	2:H:113:LEU:CB	2.49	0.43
2:H:265:ALA:HB2	2:H:284:ARG:HG2	2.00	0.43
1:A:30:LYS:N	3:A:600:GTP:O1B	2.27	0.43
2:B:221:VAL:CG1	2:B:233:SER:HB2	2.49	0.43
2:B:366:LEU:HD12	2:B:370:GLU:HB2	1.99	0.43
1:C:22:VAL:HG12	1:C:30:LYS:HD2	2.01	0.43
1:E:136:MET:HB3	1:E:141:ILE:HG13	2.01	0.43
2:B:58:VAL:HG22	2:B:73:ILE:HG23	2.01	0.43
1:C:161:ASN:HB3	1:C:166:GLU:HB3	2.01	0.43
1:E:22:VAL:HG22	1:E:91:VAL:HB	2.00	0.43
2:F:267:ILE:HG22	2:F:281:VAL:HA	2.01	0.43
2:F:298:GLN:O	2:F:300:ILE:HD12	2.19	0.43
2:D:289:TYR:HD1	2:D:300:ILE:HD12	1.84	0.43
2:B:222:VAL:HA	2:B:269:VAL:HG11	2.00	0.42
2:B:351:MET:HB3	2:B:361:ALA:HB3	2.01	0.42
2:D:131:ARG:HA	2:D:132:PRO:HD3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:PHE:HE2	2:D:253:ALA:N	2.17	0.42
1:E:129:LYS:HG2	3:E:600:GTP:C6	2.54	0.42
2:F:219:MET:HG3	2:F:237:VAL:HG22	2.01	0.42
1:G:119:ARG:HE	1:G:119:ARG:HB2	1.63	0.42
2:D:234:CYS:HB3	2:D:247:LEU:O	2.20	0.42
1:E:113:LEU:HD23	1:E:153:ARG:CZ	2.50	0.42
2:F:351:MET:HB2	2:F:363:ILE:HD11	2.00	0.42
2:H:76:GLU:C	2:H:78:ARG:N	2.77	0.42
1:C:37:LEU:HB3	1:C:58:VAL:HG11	2.00	0.42
2:F:92:HIS:NE2	2:F:130:LEU:HD11	2.34	0.42
2:F:325:VAL:HG13	5:F:1427:PB:PB	1.63	0.42
2:F:371:VAL:HB	2:F:383:HIS:CD2	2.55	0.42
1:E:101:ARG:HA	2:F:417:MET:HE1	2.02	0.42
1:C:22:VAL:HG22	1:C:91:VAL:HB	2.00	0.42
1:C:31:THR:HG23	1:C:69:ASP:OD2	2.19	0.42
1:C:95:ASP:C	1:C:95:ASP:OD1	2.62	0.42
2:H:98:PRO:HA	2:H:120:ALA:HB2	2.01	0.42
2:B:134:TYR:CE2	2:B:252:THR:HA	2.55	0.42
1:C:161:ASN:O	1:C:165:GLY:N	2.50	0.42
1:A:26:ASP:OD1	2:B:399:ARG:HD2	2.19	0.42
2:D:288:LEU:HG	2:D:303:LEU:HD11	2.01	0.42
2:F:97:THR:HA	2:F:98:PRO:HD3	1.71	0.42
2:F:136:PHE:CZ	2:F:254:ILE:HG13	2.54	0.42
1:A:108:GLU:CD	2:B:420:ARG:NH1	2.77	0.42
2:B:351:MET:HG3	2:B:394:PHE:CD2	2.55	0.42
2:D:97:THR:HA	2:D:98:PRO:HD3	1.66	0.42
1:E:101:ARG:NH1	2:F:399:ARG:HB2	2.34	0.42
2:F:291:ILE:HG12	2:F:296:LEU:HA	2.01	0.42
1:G:97:ALA:HB1	1:G:134:VAL:HG23	2.01	0.42
2:D:280:THR:HG21	2:D:317:VAL:HG21	2.01	0.42
1:E:137:PRO:HD2	1:E:140:GLU:HB3	2.02	0.42
2:F:134:TYR:CD1	2:F:135:LYS:N	2.88	0.42
2:D:71:LEU:HD13	2:D:405:LEU:HD13	2.02	0.41
2:D:301:ILE:HD11	2:D:333:GLY:HA2	2.01	0.41
2:H:134:TYR:CD1	2:H:135:LYS:N	2.88	0.41
2:B:139:PRO:HA	2:B:140:PRO:HD3	1.89	0.41
2:D:122:SER:HB2	2:D:137:VAL:HG13	2.02	0.41
1:A:91:VAL:HG22	1:A:124:LEU:HD23	2.02	0.41
2:B:40:TRP:HB3	2:B:416:LYS:HB3	2.02	0.41
1:A:94:VAL:HG21	1:A:141:ILE:HG21	2.01	0.41
2:H:59:HIS:NE2	2:H:103:SER:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:HIS:CG	2:B:335:LYS:HE3	2.56	0.41
2:B:396:ARG:NH2	2:B:399:ARG:HA	2.35	0.41
1:C:53:PHE:CD1	1:C:53:PHE:C	2.98	0.41
1:C:103:VAL:HG21	2:D:41:LEU:HB3	2.03	0.41
1:E:128:ASN:CG	1:E:129:LYS:H	2.27	0.41
2:H:97:THR:HA	2:H:98:PRO:HD3	1.86	0.41
2:B:258:ILE:HD13	2:B:291:ILE:HD13	2.03	0.41
2:B:337:TRP:CE3	2:B:339:LEU:HD13	2.56	0.41
2:H:370:GLU:OE2	2:H:372:ARG:NH2	2.54	0.41
2:D:118:VAL:O	2:D:124:ILE:HA	2.20	0.41
2:D:358:ASN:CG	1:E:116:SER:HB3	2.45	0.41
1:G:30:LYS:O	1:G:34:ILE:HG13	2.21	0.41
2:B:210:LEU:C	2:B:210:LEU:HD23	2.46	0.41
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.91	0.41
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.86	0.41
1:C:103:VAL:CG1	2:D:43:ALA:HA	2.46	0.41
2:D:43:ALA:HB3	2:D:415:ILE:O	2.20	0.41
2:D:80:LEU:HD23	2:D:94:LEU:HD11	2.02	0.41
2:F:303:LEU:CD2	2:F:319:VAL:HG21	2.51	0.41
2:H:81:LYS:HD3	2:H:88:LYS:NZ	2.36	0.41
2:H:113:LEU:N	2:H:114:PRO:CD	2.83	0.41
2:H:145:THR:HG22	2:H:146:GLU:H	1.86	0.41
2:H:312:ARG:O	2:H:350:ARG:NH1	2.54	0.41
1:C:17:LYS:HE3	1:C:17:LYS:HB3	1.71	0.41
1:G:96:SER:HB3	1:G:136:MET:H	1.86	0.41
2:H:351:MET:HB3	2:H:361:ALA:HB3	2.03	0.41
2:F:370:GLU:HA	2:F:384:VAL:HA	2.03	0.40
2:H:351:MET:HE3	2:H:418:LEU:HD22	2.03	0.40
1:A:177:GLU:OE1	1:A:178:ARG:NH2	2.53	0.40
2:D:266:MET:HG2	2:D:282:ALA:HB3	2.03	0.40
2:D:288:LEU:HD11	2:D:319:VAL:HG11	2.04	0.40
1:E:28:SER:HB2	1:E:93:VAL:HG12	2.03	0.40
1:G:28:SER:HA	1:G:95:ASP:HB2	2.04	0.40
1:G:100:LEU:HA	1:G:100:LEU:HD12	1.87	0.40
2:B:246:ILE:O	2:B:255:VAL:N	2.42	0.40
2:F:374:TYR:CE1	2:F:379:LEU:HB2	2.57	0.40
2:B:349:GLN:NE2	2:B:392:LEU:O	2.48	0.40
1:C:52:GLY:HA2	1:C:76:TYR:CE2	2.56	0.40
2:F:76:GLU:C	2:F:78:ARG:N	2.80	0.40
1:G:77:ARG:C	1:G:79:LEU:N	2.79	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%)	155 (94%)	9 (6%)	0	100	100
1	C	164/169 (97%)	152 (93%)	12 (7%)	0	100	100
1	E	164/169 (97%)	153 (93%)	11 (7%)	0	100	100
1	G	164/169 (97%)	154 (94%)	10 (6%)	0	100	100
2	B	329/425 (77%)	294 (89%)	34 (10%)	1 (0%)	36	63
2	D	299/425 (70%)	267 (89%)	31 (10%)	1 (0%)	36	63
2	F	303/425 (71%)	273 (90%)	29 (10%)	1 (0%)	36	63
2	H	321/425 (76%)	293 (91%)	28 (9%)	0	100	100
All	All	1908/2376 (80%)	1741 (91%)	164 (9%)	3 (0%)	43	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	209	PRO
2	F	65	GLY
2	D	65	GLY

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	132/142 (93%)	128 (97%)	4 (3%)	36	60
1	C	138/142 (97%)	135 (98%)	3 (2%)	45	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	135/142 (95%)	121 (90%)	14 (10%)	7	24
1	G	137/142 (96%)	129 (94%)	8 (6%)	18	45
2	B	243/352 (69%)	223 (92%)	20 (8%)	10	35
2	D	214/352 (61%)	194 (91%)	20 (9%)	8	30
2	F	221/352 (63%)	211 (96%)	10 (4%)	24	51
2	H	243/352 (69%)	219 (90%)	24 (10%)	7	27
All	All	1463/1976 (74%)	1360 (93%)	103 (7%)	14	40

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LYS
1	A	96	SER
1	A	178	ARG
1	A	180	SER
2	B	55	THR
2	B	70	ARG
2	B	82	ILE
2	B	87	GLN
2	B	91	GLU
2	B	101	ILE
2	B	104	TYR
2	B	105	ILE
2	B	108	ASN
2	B	130	LEU
2	B	148	GLN
2	B	213	THR
2	B	215	VAL
2	B	245	LEU
2	B	263	THR
2	B	301	ILE
2	B	306	GLN
2	B	312	ARG
2	B	316	HIS
2	B	343	CYS
1	C	56	ASP
1	C	103	VAL
1	C	178	ARG
2	D	51	ILE
2	D	60	THR

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Mol	Chain	Res	Type
2	D	82	ILE
2	D	86	THR
2	D	124	ILE
2	D	125	TYR
2	D	128	ARG
2	D	129	ASN
2	D	135	LYS
2	D	136	PHE
2	D	262	ILE
2	D	306	GLN
2	D	311	VAL
2	D	313	LEU
2	D	316	HIS
2	D	322	MET
2	D	343	CYS
2	D	382	VAL
2	D	386	PRO
2	D	416	LYS
1	E	30	LYS
1	E	33	ILE
1	E	38	LYS
1	E	59	GLU
1	E	75	ARG
1	E	78	THR
1	E	94	VAL
1	E	103	VAL
1	E	119	ARG
1	E	124	LEU
1	E	132	LEU
1	E	134	VAL
1	E	178	ARG
1	E	179	LEU
2	F	62	ASN
2	F	86	THR
2	F	130	LEU
2	F	215	VAL
2	F	221	VAL
2	F	267	ILE
2	F	316	HIS
2	F	317	VAL
2	F	421	THR
2	F	425	GLU

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Mol	Chain	Res	Type
1	G	30	LYS
1	G	64	THR
1	G	75	ARG
1	G	78	THR
1	G	103	VAL
1	G	119	ARG
1	G	136	MET
1	G	178	ARG
2	H	48	VAL
2	H	52	SER
2	H	55	THR
2	H	70	ARG
2	H	82	ILE
2	H	94	LEU
2	H	95	LEU
2	H	96	ASP
2	H	104	TYR
2	H	108	ASN
2	H	130	LEU
2	H	143	VAL
2	H	145	THR
2	H	215	VAL
2	H	303	LEU
2	H	316	HIS
2	H	325	VAL
2	H	343	CYS
2	H	353	VAL
2	H	354	THR
2	H	357	ARG
2	H	377	LYS
2	H	386	PRO
2	H	425	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	257	ASN
2	B	306	GLN
2	D	356	GLN
2	D	387	ASN
2	F	59	HIS
2	F	334	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 26 ligands modelled in this entry, 22 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$
3	GTP	G	600	4	33,34,34	1.07	3 (9%)	50,54,54	1.57	10 (20%)
3	GTP	C	600	4	33,34,34	1.11	2 (6%)	50,54,54	1.60	12 (24%)
3	GTP	E	600	4	33,34,34	1.24	4 (12%)	50,54,54	1.67	12 (24%)
3	GTP	A	600	4	33,34,34	1.02	3 (9%)	50,54,54	1.60	10 (20%)

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
3	GTP	G	600	4	-	2/22/38/38	0/3/3/3
3	GTP	C	600	4	-	5/22/38/38	0/3/3/3
3	GTP	E	600	4	-	5/22/38/38	0/3/3/3
3	GTP	A	600	4	-	5/22/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	600	GTP	PB-O3B	3.31	1.63	1.59
3	E	600	GTP	PB-O3A	3.17	1.62	1.59
3	E	600	GTP	PA-O3A	3.03	1.62	1.59
3	C	600	GTP	PB-O3A	2.87	1.62	1.59
3	G	600	GTP	PA-O3A	2.60	1.62	1.59
3	C	600	GTP	PA-O3A	2.50	1.62	1.59
3	A	600	GTP	PA-O3A	2.44	1.62	1.59
3	A	600	GTP	C2-N3	2.36	1.38	1.33
3	A	600	GTP	PB-O3B	2.27	1.61	1.59
3	E	600	GTP	C2-N3	2.25	1.38	1.33
3	G	600	GTP	C5-N7	-2.16	1.34	1.39
3	G	600	GTP	PB-O3A	2.13	1.61	1.59

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	GTP	C5-C4-N3	-4.98	120.47	128.39
3	E	600	GTP	C5-C4-N3	-4.73	120.86	128.39
3	G	600	GTP	C5-C4-N3	-4.53	121.19	128.39
3	A	600	GTP	C2-N3-C4	4.42	119.92	112.30
3	G	600	GTP	C2-N3-C4	4.29	119.69	112.30
3	C	600	GTP	C5-C4-N3	-3.91	122.16	128.39
3	E	600	GTP	C2-N3-C4	3.87	118.97	112.30
3	C	600	GTP	C2-N3-C4	3.73	118.72	112.30
3	E	600	GTP	C2'-C3'-C4'	-3.37	96.10	102.61
3	A	600	GTP	N9-C4-N3	3.31	132.57	125.95
3	E	600	GTP	N9-C4-N3	3.21	132.38	125.95
3	E	600	GTP	C2-N1-C6	-3.03	119.62	125.11
3	C	600	GTP	N9-C8-N7	-3.02	107.80	113.40
3	C	600	GTP	C2'-C3'-C4'	-2.99	96.82	102.61
3	C	600	GTP	O6-C6-C5	-2.94	118.77	126.53
3	A	600	GTP	C2-N1-C6	-2.90	119.86	125.11
3	G	600	GTP	C2-N1-C6	-2.88	119.89	125.11
3	E	600	GTP	O2'-C2'-C1'	2.78	119.69	110.10
3	C	600	GTP	N9-C4-N3	2.74	131.44	125.95
3	E	600	GTP	O3'-C3'-C4'	-2.73	103.24	111.08
3	G	600	GTP	N9-C4-N3	2.72	131.39	125.95
3	C	600	GTP	C2-N1-C6	-2.70	120.22	125.11
3	A	600	GTP	N9-C8-N7	-2.67	108.45	113.40
3	G	600	GTP	N9-C8-N7	-2.62	108.54	113.40
3	G	600	GTP	O4'-C1'-N9	-2.57	102.53	108.36
3	G	600	GTP	C5-C6-N1	2.48	119.56	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	GTP	N9-C8-N7	-2.43	108.89	113.40
3	E	600	GTP	O6-C6-C5	-2.43	120.12	126.53
3	A	600	GTP	O2B-PB-O3B	2.42	113.81	107.27
3	A	600	GTP	C8-N7-C5	2.40	108.54	104.26
3	A	600	GTP	C5-C6-N1	2.40	119.36	113.25
3	G	600	GTP	C5'-C4'-C3'	-2.36	106.72	115.21
3	A	600	GTP	O6-C6-C5	-2.28	120.50	126.53
3	C	600	GTP	C8-N7-C5	2.27	108.30	104.26
3	G	600	GTP	O6-C6-C5	-2.26	120.56	126.53
3	E	600	GTP	C5-C6-N1	2.25	118.98	113.25
3	E	600	GTP	C5'-C4'-C3'	-2.22	107.24	115.21
3	C	600	GTP	C5-C6-N1	2.21	118.88	113.25
3	E	600	GTP	C8-N7-C5	2.17	108.12	104.26
3	C	600	GTP	C5'-C4'-C3'	-2.12	107.57	115.21
3	G	600	GTP	C8-N7-C5	2.12	108.04	104.26
3	A	600	GTP	O4'-C1'-N9	-2.10	103.60	108.36
3	C	600	GTP	O2B-PB-O3A	2.09	112.92	107.27
3	C	600	GTP	O3G-PG-O3B	2.06	111.56	104.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

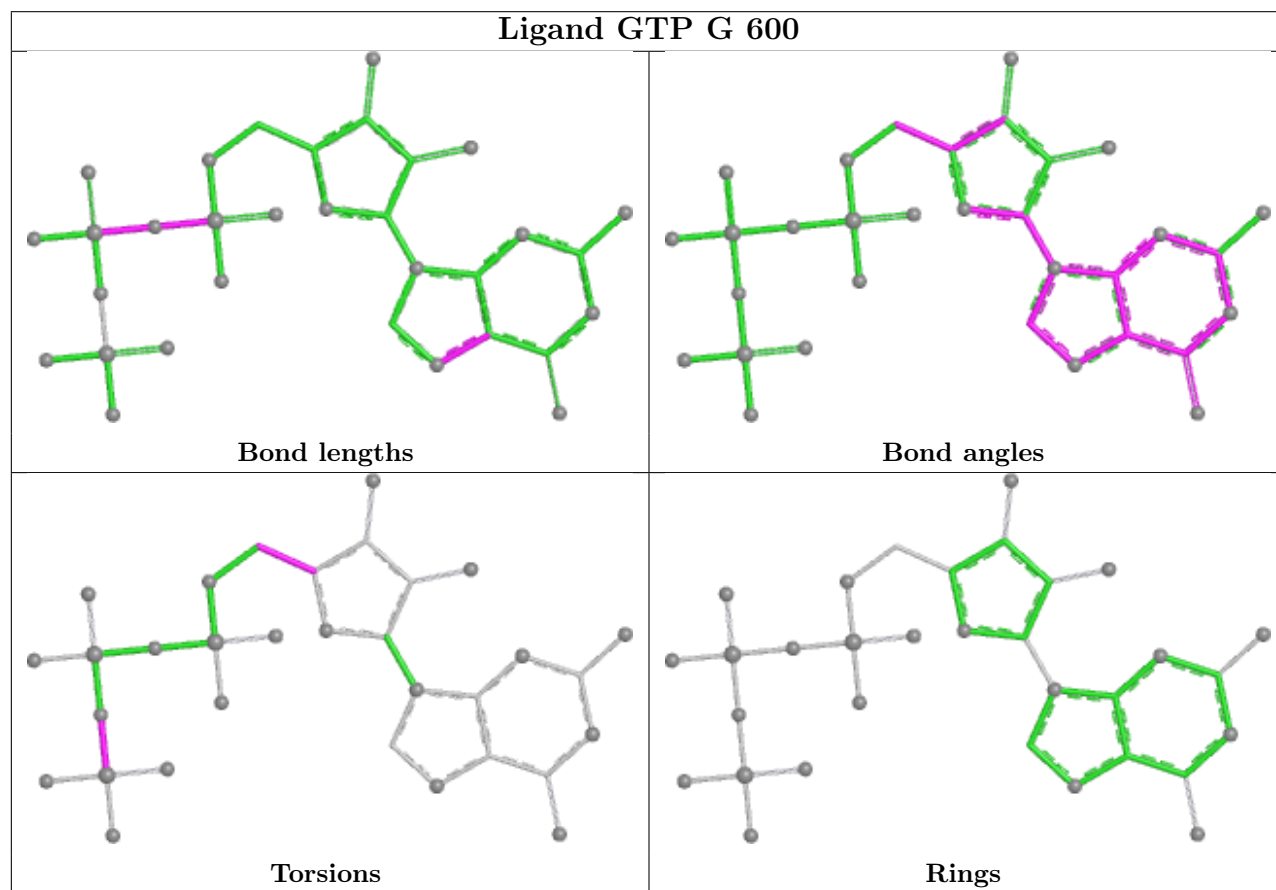
Mol	Chain	Res	Type	Atoms
3	G	600	GTP	PB-O3B-PG-O3G
3	E	600	GTP	O4'-C4'-C5'-O5'
3	C	600	GTP	O4'-C4'-C5'-O5'
3	A	600	GTP	O4'-C4'-C5'-O5'
3	A	600	GTP	PB-O3B-PG-O1G
3	E	600	GTP	C5'-O5'-PA-O1A
3	E	600	GTP	PA-O3A-PB-O2B
3	C	600	GTP	PB-O3B-PG-O1G
3	G	600	GTP	O4'-C4'-C5'-O5'
3	A	600	GTP	PG-O3B-PB-O1B
3	A	600	GTP	PB-O3B-PG-O2G
3	A	600	GTP	PB-O3B-PG-O3G
3	C	600	GTP	PB-O3B-PG-O2G
3	C	600	GTP	PB-O3B-PG-O3G
3	E	600	GTP	PB-O3B-PG-O2G
3	C	600	GTP	PA-O3A-PB-O2B
3	E	600	GTP	PA-O3A-PB-O1B

There are no ring outliers.

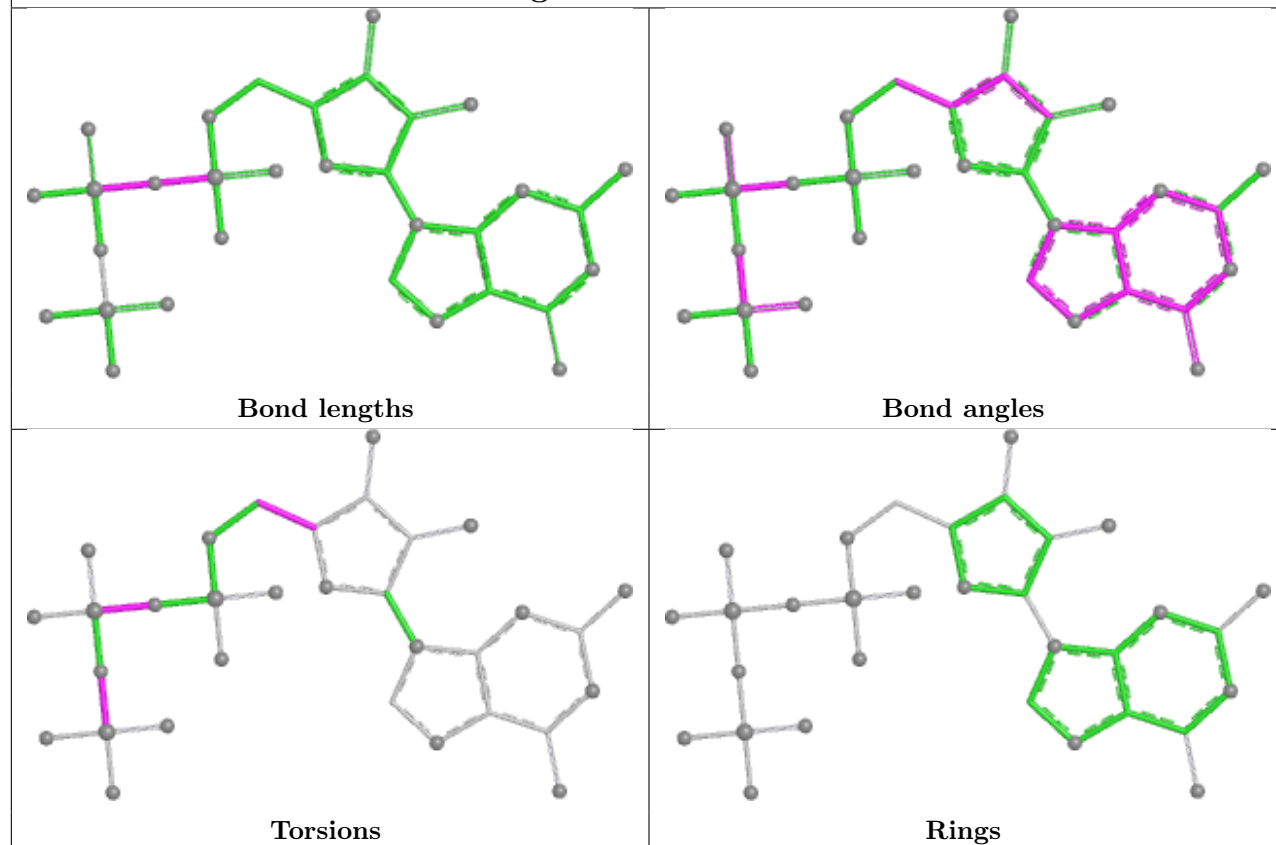
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	600	GTP	2	0
3	C	600	GTP	3	0
3	E	600	GTP	5	0
3	A	600	GTP	4	0

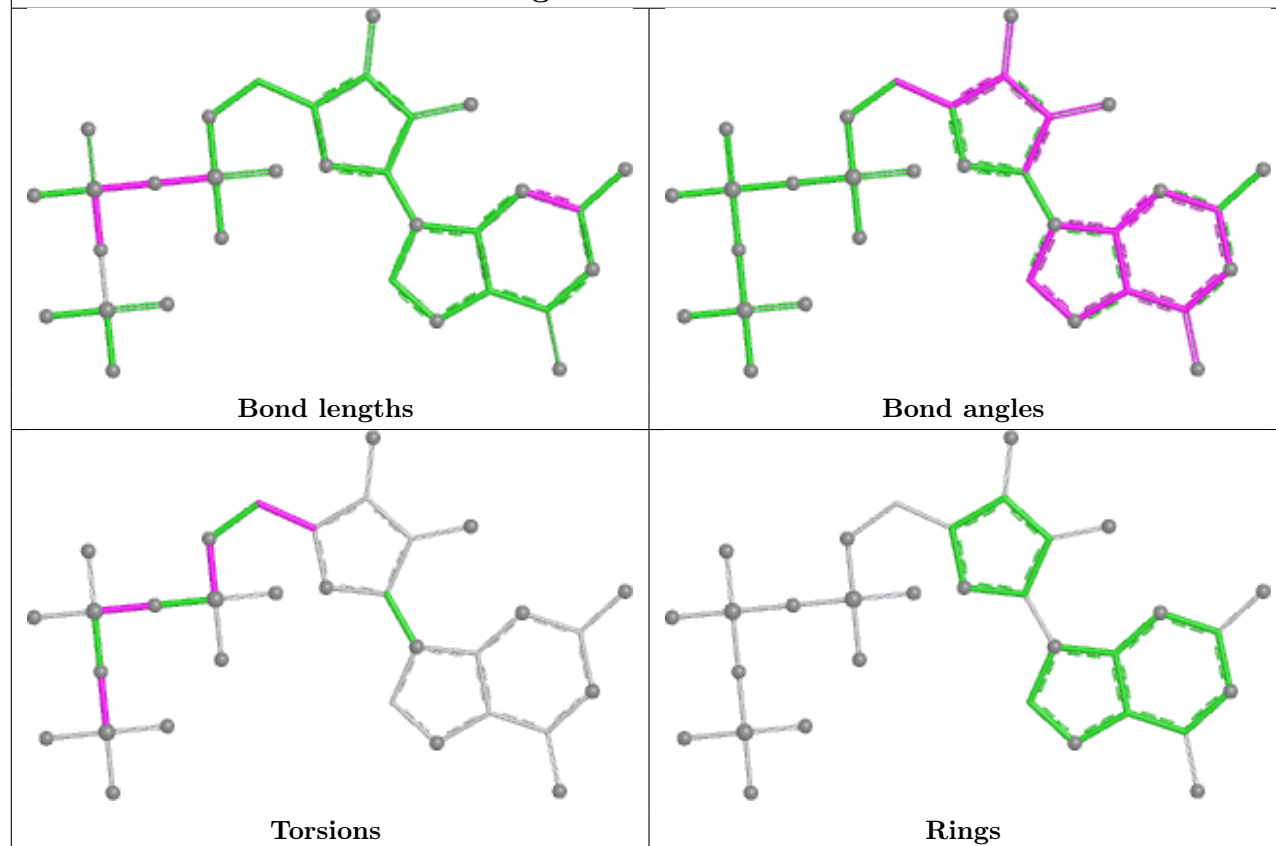
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

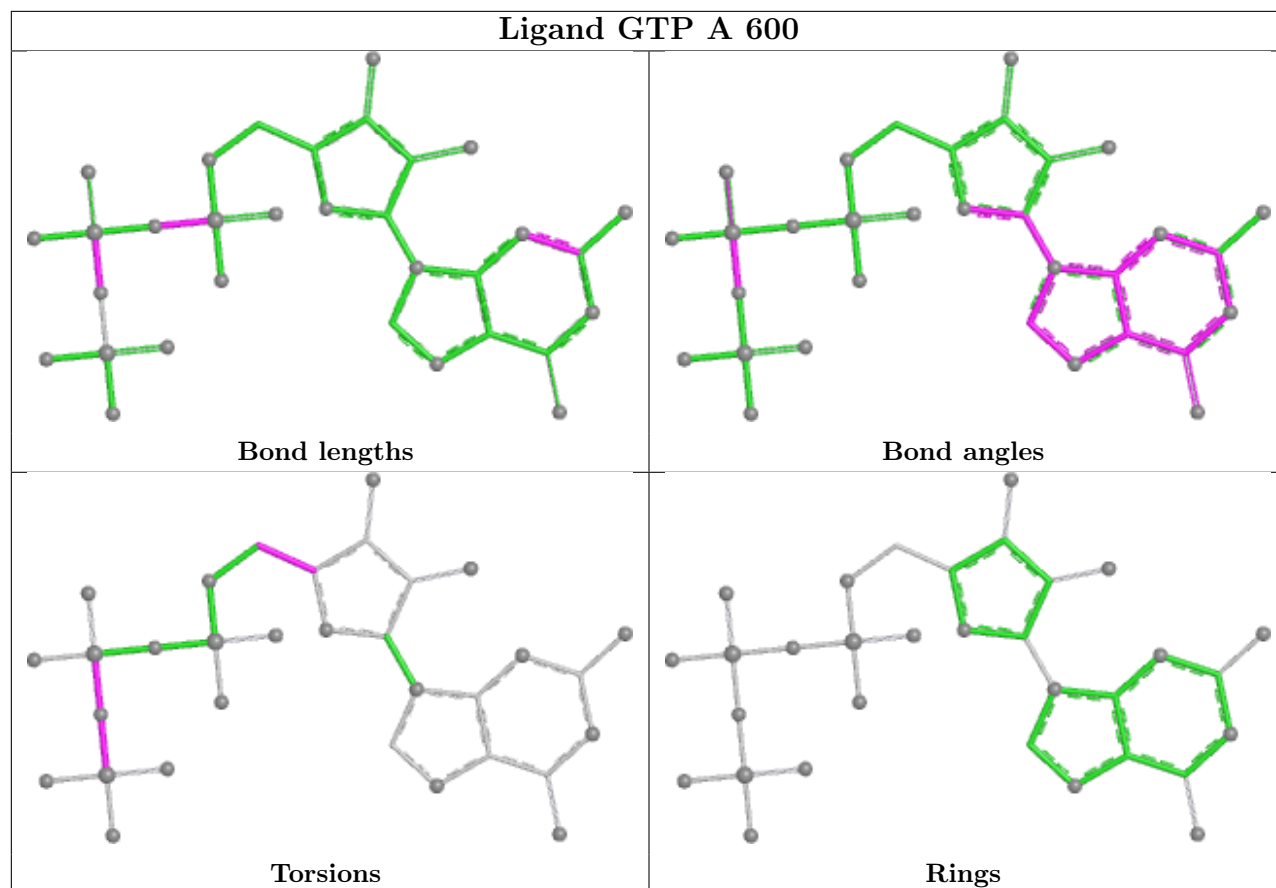


Ligand GTP C 600



Ligand GTP E 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

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	166/169 (98%)	-0.59	0 100 100	9, 35, 61, 85	0
1	C	166/169 (98%)	-0.73	1 (0%) 85 75	1, 4, 33, 48	0
1	E	166/169 (98%)	-0.71	0 100 100	1, 8, 39, 66	0
1	G	166/169 (98%)	-0.65	1 (0%) 85 75	8, 24, 51, 60	0
2	B	333/425 (78%)	-0.61	1 (0%) 90 84	1, 16, 50, 81	0
2	D	307/425 (72%)	-0.32	3 (0%) 79 66	2, 44, 96, 105	0
2	F	309/425 (72%)	-0.31	6 (1%) 66 49	1, 37, 92, 120	0
2	H	325/425 (76%)	-0.64	2 (0%) 85 75	1, 16, 49, 77	0
All	All	1938/2376 (81%)	-0.54	14 (0%) 84 73	1, 21, 83, 120	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	147	GLU	3.7
2	B	144	ASN	3.6
2	F	104	TYR	3.3
2	F	254	ILE	3.1
2	F	140	PRO	2.9
1	G	15	SER	2.9
2	D	139	PRO	2.7
1	C	15	SER	2.5
2	D	214	THR	2.3
2	H	248	ASN	2.3
2	D	250	ALA	2.2
2	F	214	THR	2.1
2	F	252	THR	2.1
2	F	235	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

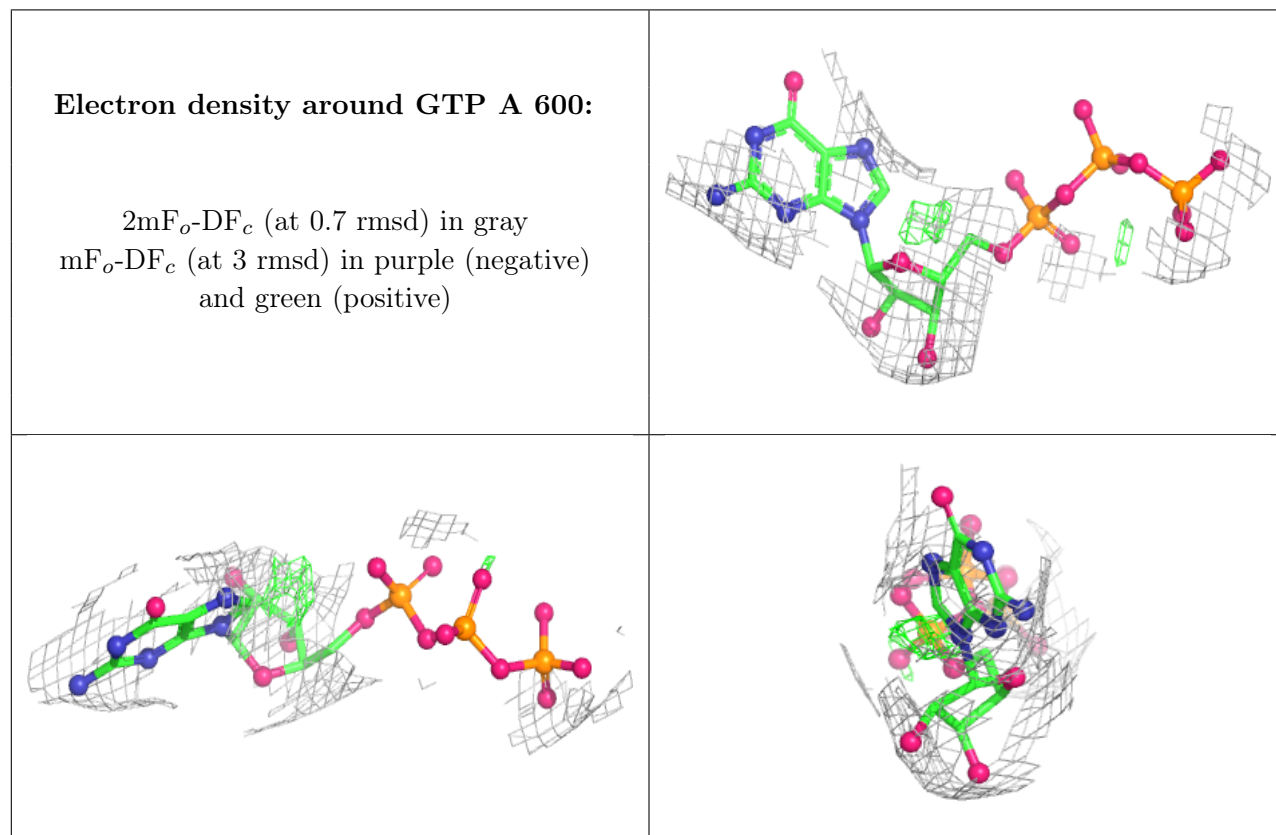
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

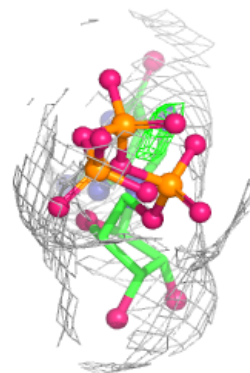
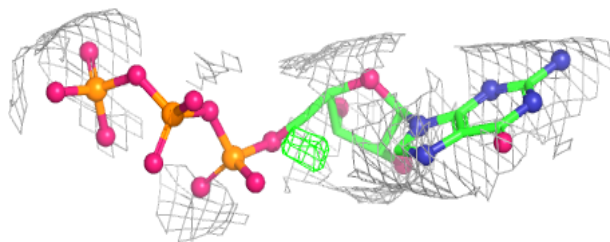
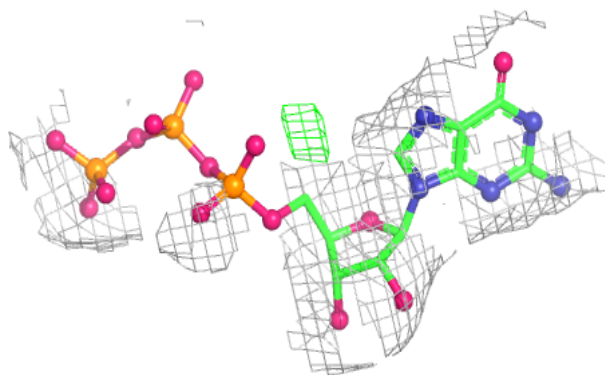
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PB	B	1429	1/1	0.74	0.08	66,66,66,66	1
5	PB	A	1181	1/1	0.83	0.05	170,170,170,170	1
5	PB	H	1429	1/1	0.85	0.05	84,84,84,84	1
5	PB	E	1181	1/1	0.86	0.08	120,120,120,120	1
5	PB	G	1181	1/1	0.86	0.05	106,106,106,106	1
5	PB	B	1427	1/1	0.86	0.06	85,85,85,85	1
5	PB	D	1428	1/1	0.88	0.05	140,140,140,140	1
5	PB	H	1427	1/1	0.90	0.11	16,16,16,16	1
5	PB	H	1428	1/1	0.90	0.06	89,89,89,89	1
5	PB	D	1427	1/1	0.90	0.10	79,79,79,79	1
5	PB	F	1426	1/1	0.92	0.10	83,83,83,83	1
5	PB	F	1428	1/1	0.93	0.07	83,83,83,83	1
5	PB	A	1182	1/1	0.95	0.04	112,112,112,112	1
3	GTP	A	600	32/32	0.96	0.05	29,35,46,48	0
3	GTP	G	600	32/32	0.97	0.05	15,19,25,26	0
5	PB	B	1428	1/1	0.97	0.06	12,12,12,12	1
5	PB	B	1426	1/1	0.97	0.10	33,33,33,33	1
5	PB	D	1426	1/1	0.97	0.07	35,35,35,35	1
5	PB	F	1427	1/1	0.97	0.05	23,23,23,23	1
5	PB	H	1426	1/1	0.98	0.09	35,35,35,35	1
4	MG	C	601	1/1	0.98	0.10	1,1,1,1	0
3	GTP	E	600	32/32	0.98	0.04	5,8,14,17	0
4	MG	A	601	1/1	0.98	0.08	29,29,29,29	0
3	GTP	C	600	32/32	0.99	0.04	1,3,4,4	0
4	MG	E	601	1/1	0.99	0.07	6,6,6,6	0
4	MG	G	601	1/1	1.00	0.07	15,15,15,15	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.

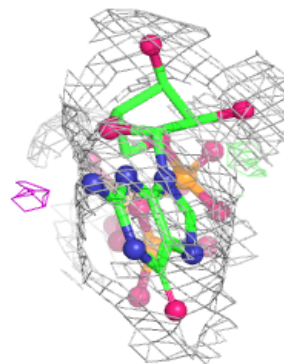
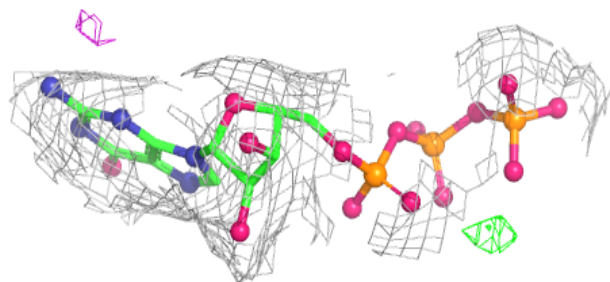
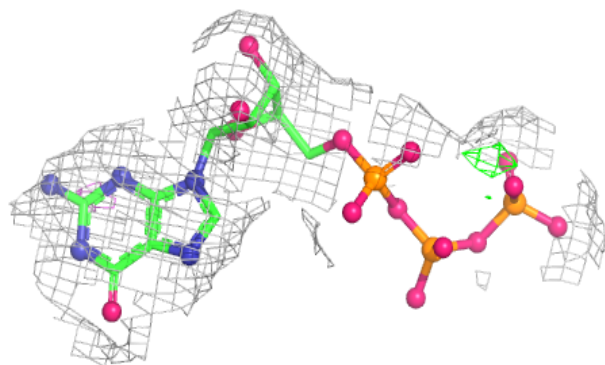


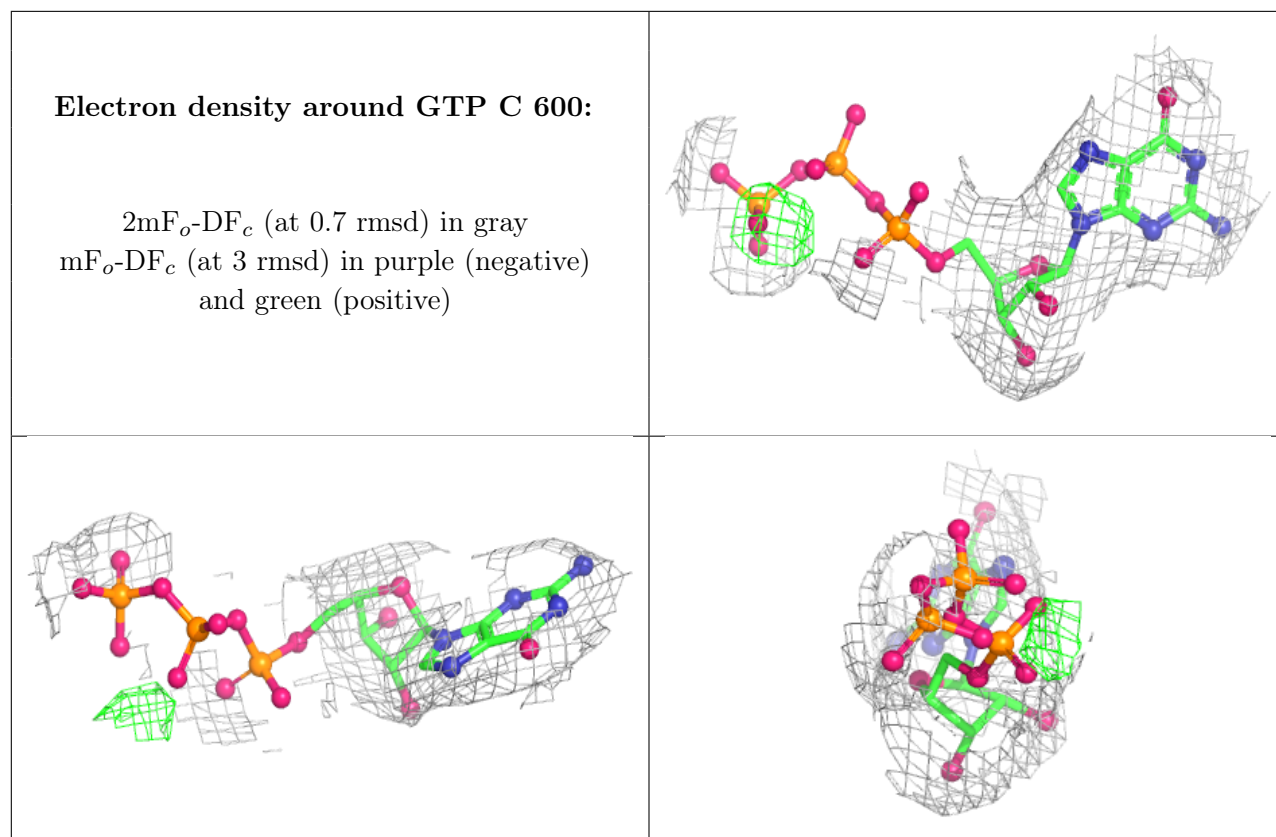
Electron density around GTP G 600:

$2mF_o-DF_c$ (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.