



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:24 AM UTC

PDB ID : 6Q84 / pdb_00006q84
Title : Crystal structure of RanGTP-Pdr6-eIF5A export complex
Authors : Aksu, M.; Trakhanov, S.; Vera-Rodriguez, A.; Gorlich, D.
Deposited on : 2018-12-14
Resolution : 3.70 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:

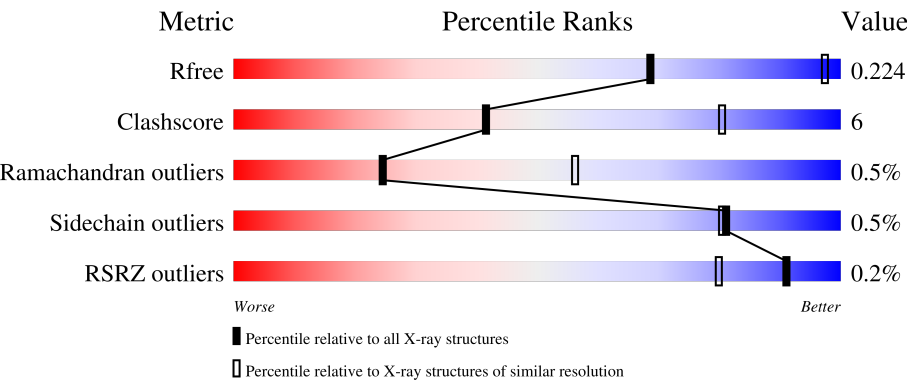
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	1080	78%16%6%
1	D	1080	79%15%6%
2	B	176	%86%11%. .
2	E	176	84%14%. .
3	C	142	73%22%. .

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Mol	Chain	Length	Quality of chain
3	F	142	65% 23% • 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 21207 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 Importin beta-like protein KAP122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	0	0	0
			8177	5270	1313	1549	45			
1	D	1017	Total	C	N	O	S	0	0	0
			8178	5271	1313	1550	44			

- Molecule 2 is a protein called GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1390	904	244	238	4			
2	E	171	Total	C	N	O	S	0	0	0
			1390	904	244	238	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	LEU	GLN	engineered mutation	UNP P62826
E	69	LEU	GLN	engineered mutation	UNP P62826

- Molecule 3 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1044	653	174	208	9			
3	F	126	Total	C	N	O	S	0	0	0
			962	603	155	195	9			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	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

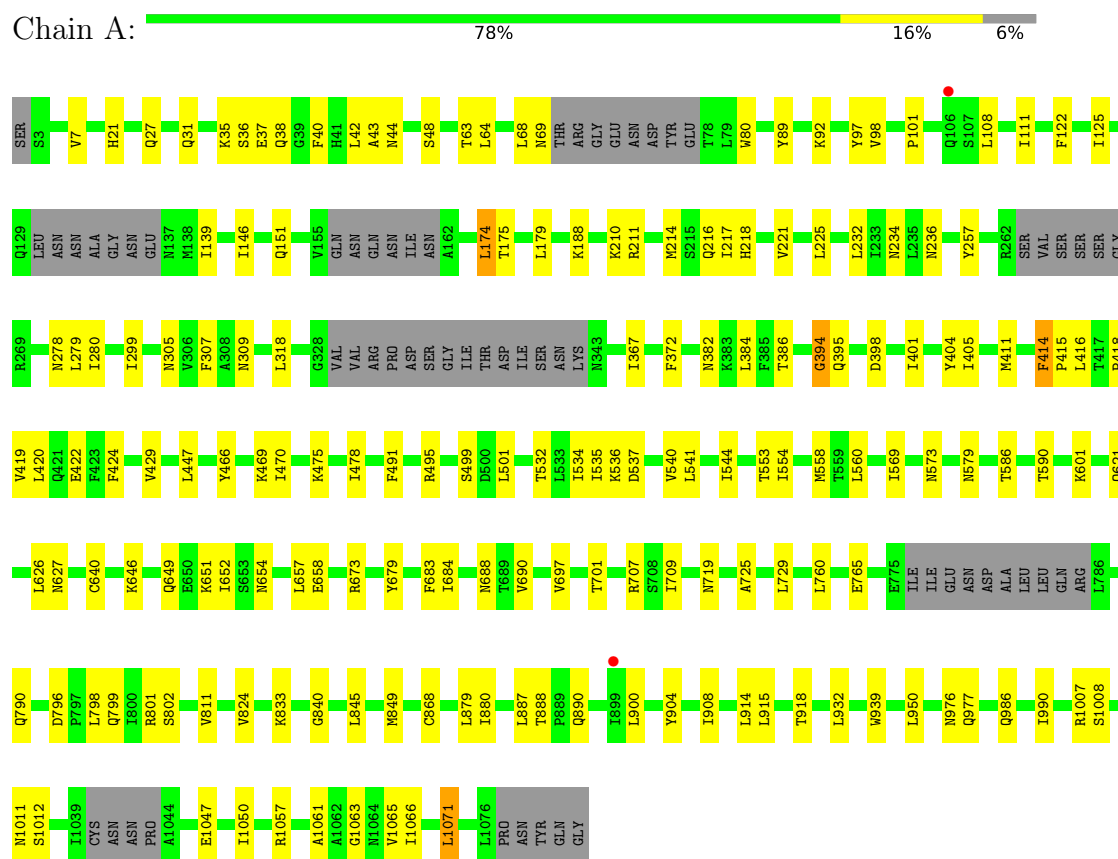
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

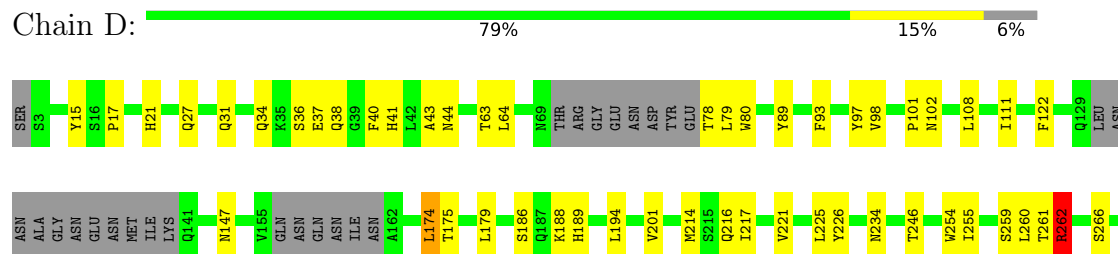
3 Residue-property plots [i](#)

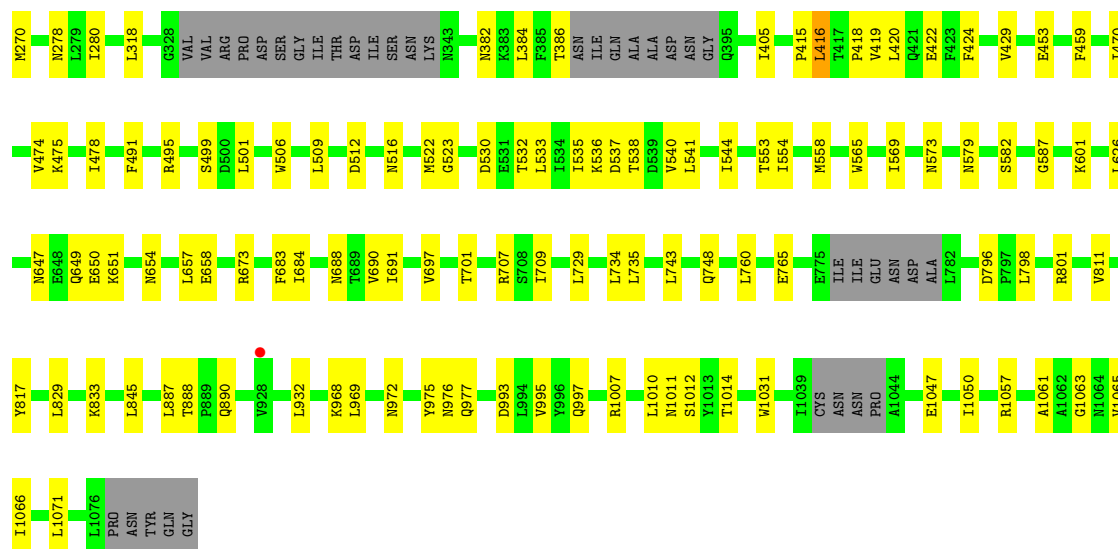
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Importin beta-like protein KAP122

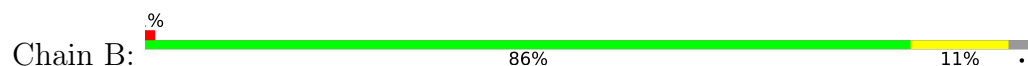


• Molecule 1: Importin beta-like protein KAP122

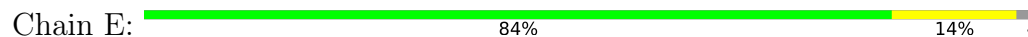




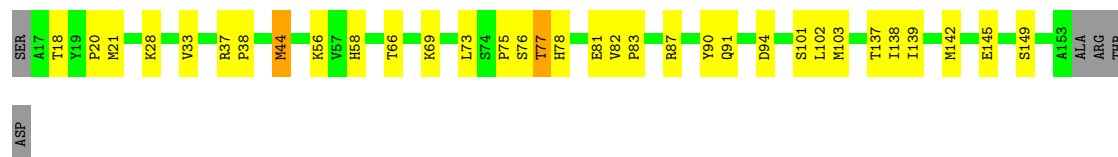
- Molecule 2: GTP-binding nuclear protein Ran



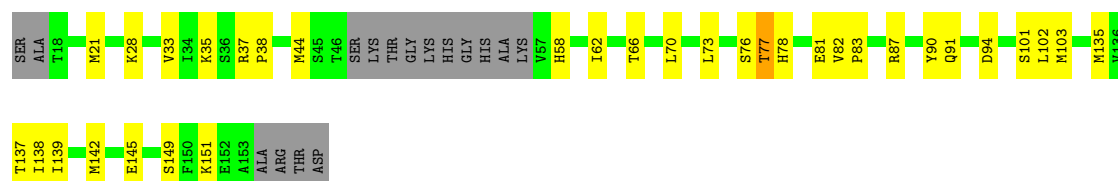
- Molecule 2: GTP-binding nuclear protein Ran



- Molecule 3: Eukaryotic translation initiation factor 5A-1



- Molecule 3: Eukaryotic translation initiation factor 5A-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	139.54Å 139.54Å 346.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.17 – 3.70 49.17 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.17-3.70) 99.9 (49.17-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.206 , 0.247 0.202 , 0.224	Depositor DCC
R_{free} test set	1217 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	174.7	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 346.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.217 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.280 for h,-h-k,-l	Depositor
Outliers	0 of 40554 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21207	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.08	0/8337	0.26	0/11318
1	D	0.08	0/8339	0.27	0/11320
2	B	0.09	0/1424	0.28	0/1923
2	E	0.09	0/1424	0.28	0/1923
3	C	0.08	0/1059	0.26	0/1424
3	F	0.08	0/974	0.26	0/1312
All	All	0.08	0/21557	0.27	0/29220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8177	0	8149	102	0
1	D	8178	0	8160	109	0
2	B	1390	0	1416	14	0
2	E	1390	0	1416	16	0
3	C	1044	0	1045	22	0
3	F	962	0	952	20	0
4	B	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	32	0	12	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	21207	0	21162	270	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 6.

All (270) 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:D:690:VAL:HG13	1:D:697:VAL:HG21	1.69	0.75
1:D:418:PRO:O	1:D:420:LEU:N	2.21	0.73
3:C:78:HIS:HD2	1:D:538:THR:HB	1.55	0.72
1:A:418:PRO:O	1:A:420:LEU:N	2.22	0.72
2:B:141:LYS:HB3	2:B:144:LEU:HB2	1.73	0.71
1:D:418:PRO:HG2	1:D:474:VAL:HG11	1.75	0.68
1:A:101:PRO:HA	1:A:188:LYS:HD2	1.76	0.67
2:E:141:LYS:HB3	2:E:144:LEU:HB2	1.76	0.67
1:A:429:VAL:HG13	1:A:501:LEU:HD12	1.77	0.66
3:F:137:THR:HB	3:F:149:SER:HB2	1.77	0.66
1:A:690:VAL:HG13	1:A:697:VAL:HG21	1.77	0.66
1:D:101:PRO:HA	1:D:188:LYS:HD2	1.78	0.66
1:D:262:ARG:NH2	1:D:270:MET:H	1.95	0.64
1:D:429:VAL:HG13	1:D:501:LEU:HD12	1.79	0.64
1:D:995:VAL:HG11	1:D:1031:TRP:HB3	1.78	0.64
1:D:535:ILE:HD12	1:D:541:LEU:HD13	1.80	0.64
2:E:86:ALA:HB3	2:E:117:ILE:HG12	1.81	0.63
1:D:27:GLN:OE1	1:D:31:GLN:NE2	2.31	0.63
3:C:137:THR:HB	3:C:149:SER:HB2	1.81	0.63
2:B:13:LEU:HD22	2:B:63:VAL:HG13	1.81	0.62
1:D:415:PRO:O	1:D:416:LEU:HB2	1.98	0.62
1:D:569:ILE:O	1:D:573:ASN:ND2	2.31	0.62
3:C:78:HIS:NE2	1:D:537:ASP:OD1	2.29	0.62
3:C:87:ARG:HG2	3:C:139:ILE:HG12	1.82	0.61
3:F:87:ARG:HG2	3:F:139:ILE:HG12	1.81	0.61
1:A:151:GLN:HB2	1:A:174:LEU:HD11	1.82	0.61
1:A:214:MET:HE3	1:A:217:ILE:HG21	1.84	0.60
3:C:28:LYS:HG2	3:C:44:MET:HB3	1.83	0.60
3:F:94:ASP:HB3	3:F:101:SER:HB3	1.82	0.60
1:D:262:ARG:HA	1:D:266:SER:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:HA	1:A:401:ILE:HG22	1.84	0.59
3:C:94:ASP:HB3	3:C:101:SER:HB3	1.84	0.59
1:D:36:SER:O	1:D:38:GLN:N	2.36	0.59
3:C:21:MET:HE2	3:C:82:VAL:HG21	1.83	0.59
3:F:138:ILE:HD11	3:F:145:GLU:HB3	1.83	0.59
1:A:27:GLN:OE1	1:A:31:GLN:NE2	2.36	0.59
3:C:33:VAL:HB	3:C:81:GLU:HB2	1.85	0.59
1:A:569:ILE:O	1:A:573:ASN:ND2	2.34	0.59
1:A:415:PRO:O	1:A:416:LEU:HB2	2.02	0.58
3:C:138:ILE:HD11	3:C:145:GLU:HB3	1.85	0.58
1:A:108:LEU:HA	1:A:111:ILE:HB	1.85	0.58
2:B:86:ALA:HB3	2:B:117:ILE:HG12	1.85	0.58
3:F:58:HIS:HB2	3:F:73:LEU:HD13	1.84	0.58
1:A:36:SER:O	1:A:38:GLN:N	2.36	0.58
1:D:707:ARG:HB2	1:D:765:GLU:HB3	1.86	0.58
1:A:560:LEU:O	1:A:621:GLN:NE2	2.37	0.58
3:F:21:MET:HE2	3:F:82:VAL:HG21	1.86	0.57
1:D:214:MET:HE3	1:D:217:ILE:HG21	1.85	0.57
1:D:262:ARG:HH22	1:D:270:MET:H	1.51	0.57
2:E:13:LEU:HD22	2:E:63:VAL:HG13	1.86	0.57
1:A:684:ILE:O	1:A:688:ASN:ND2	2.38	0.57
1:D:40:PHE:O	1:D:44:ASN:ND2	2.38	0.57
1:D:554:ILE:HG22	1:D:558:MET:HE3	1.87	0.57
1:A:790:GLN:NE2	1:A:840:GLY:O	2.34	0.56
1:A:175:THR:HG21	1:A:179:LEU:HD23	1.88	0.56
1:A:470:ILE:O	1:A:495:ARG:NH1	2.39	0.56
3:C:20:PRO:HB3	1:D:536:LYS:HB3	1.86	0.56
1:D:280:ILE:HD12	1:D:318:LEU:HD12	1.85	0.56
1:A:418:PRO:HG3	1:A:469:LYS:HE3	1.88	0.56
2:E:119:LEU:HB3	2:E:146:TYR:HD1	1.70	0.56
1:A:1063:GLY:HA2	1:A:1066:ILE:HB	1.88	0.56
3:C:91:GLN:HG3	3:C:103:MET:HB3	1.87	0.56
1:A:174:LEU:HD13	1:A:175:THR:H	1.70	0.56
1:A:535:ILE:HD12	1:A:541:LEU:HD13	1.88	0.56
1:A:420:LEU:HG	1:A:478:ILE:HG12	1.86	0.56
1:D:470:ILE:O	1:D:495:ARG:NH1	2.39	0.56
1:A:760:LEU:HD11	1:A:811:VAL:HG11	1.87	0.55
3:C:37:ARG:HH22	3:C:66:THR:HG23	1.71	0.55
1:A:64:LEU:O	1:A:89:TYR:OH	2.25	0.55
1:A:915:LEU:HD21	1:A:950:LEU:HD22	1.89	0.54
1:D:1063:GLY:HA2	1:D:1066:ILE:HB	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:91:GLN:HG3	3:F:103:MET:HB3	1.89	0.54
1:A:707:ARG:HB2	1:A:765:GLU:HB3	1.88	0.54
1:D:234:ASN:ND2	1:D:278:ASN:OD1	2.41	0.54
1:D:683:PHE:HB3	1:D:709:ILE:HD11	1.90	0.54
1:A:211:ARG:HB2	1:A:1071:LEU:HG	1.88	0.54
1:A:7:VAL:HG11	1:A:42:LEU:HD21	1.90	0.53
1:A:422:GLU:OE1	1:A:424:PHE:N	2.42	0.53
1:A:976:ASN:OD1	1:A:977:GLN:N	2.40	0.53
1:D:1050:ILE:HG13	1:D:1065:VAL:HG12	1.89	0.53
1:D:174:LEU:HD13	1:D:175:THR:H	1.73	0.53
1:A:646:LYS:HB3	1:A:651:LYS:HG3	1.91	0.53
1:D:175:THR:HG21	1:D:179:LEU:HD23	1.91	0.53
1:A:796:ASP:OD1	1:A:801:ARG:NH2	2.42	0.53
1:D:530:ASP:H	1:D:536:LYS:HZ1	1.57	0.53
1:A:554:ILE:HG22	1:A:558:MET:HE3	1.90	0.53
1:D:684:ILE:O	1:D:688:ASN:ND2	2.41	0.53
1:D:15:TYR:HB3	2:E:82:GLN:HG3	1.91	0.52
1:D:108:LEU:HA	1:D:111:ILE:HB	1.90	0.52
1:D:651:LYS:HA	1:D:654:ASN:HB3	1.91	0.52
1:D:743:LEU:HD11	1:D:811:VAL:HG22	1.91	0.52
1:A:658:GLU:HG2	1:A:701:THR:HG21	1.90	0.52
1:D:796:ASP:OD1	1:D:801:ARG:NH2	2.42	0.52
1:A:544:ILE:HD11	1:A:579:ASN:HB3	1.92	0.52
1:A:1050:ILE:HG13	1:A:1065:VAL:HG12	1.92	0.52
1:A:40:PHE:O	1:A:44:ASN:ND2	2.43	0.51
1:A:499:SER:HB2	1:A:553:THR:HG21	1.93	0.51
1:D:533:LEU:HB3	1:D:582:SER:HA	1.92	0.51
2:E:129:ARG:NE	2:E:131:VAL:O	2.44	0.51
1:A:1047:GLU:O	1:A:1050:ILE:HG22	2.11	0.50
1:A:280:ILE:HD12	1:A:318:LEU:HD12	1.94	0.50
1:A:232:LEU:O	1:A:236:ASN:ND2	2.41	0.50
1:A:683:PHE:HB3	1:A:709:ILE:HD11	1.93	0.50
1:D:565:TRP:HB2	3:F:58:HIS:CE1	2.47	0.50
2:B:129:ARG:NE	2:B:131:VAL:O	2.44	0.50
3:C:58:HIS:HB2	3:C:73:LEU:HD13	1.93	0.50
1:D:512:ASP:HA	1:D:516:ASN:HB2	1.94	0.50
3:C:90:TYR:HB3	3:C:102:LEU:HB3	1.94	0.50
3:F:37:ARG:HH22	3:F:66:THR:HG23	1.76	0.50
1:A:649:GLN:O	1:A:652:ILE:HG12	2.11	0.50
1:D:97:TYR:CZ	1:D:111:ILE:HG23	2.47	0.49
1:A:908:ILE:HG12	1:A:914:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:GLN:HB3	1:A:802:SER:HB3	1.93	0.49
1:D:658:GLU:HG2	1:D:701:THR:HG21	1.94	0.49
1:D:1047:GLU:O	1:D:1050:ILE:HG22	2.11	0.49
1:D:976:ASN:OD1	1:D:977:GLN:N	2.44	0.49
1:A:888:THR:HG22	1:A:890:GLN:H	1.77	0.49
1:D:64:LEU:O	1:D:89:TYR:OH	2.29	0.49
1:A:601:LYS:HE2	1:A:657:LEU:HD21	1.95	0.49
1:A:904:TYR:HA	1:A:908:ILE:HB	1.95	0.49
1:A:627:ASN:OD1	1:A:679:TYR:OH	2.31	0.49
3:F:90:TYR:HB3	3:F:102:LEU:HB3	1.94	0.49
1:A:97:TYR:CZ	1:A:111:ILE:HG23	2.48	0.49
2:B:141:LYS:HD2	2:B:144:LEU:HD23	1.95	0.48
1:A:939:TRP:NE1	1:A:986:GLN:OE1	2.40	0.48
1:A:234:ASN:ND2	1:A:278:ASN:OD1	2.46	0.48
2:E:162:LEU:HD11	2:E:175:GLU:HA	1.96	0.48
1:D:420:LEU:HD12	1:D:478:ILE:HA	1.95	0.48
1:D:41:HIS:HA	1:D:44:ASN:HD22	1.78	0.48
3:C:18:THR:HG1	1:D:536:LYS:HZ3	1.52	0.48
1:D:522:MET:O	1:D:579:ASN:ND2	2.41	0.48
1:D:888:THR:HG22	1:D:890:GLN:H	1.78	0.48
1:A:221:VAL:HG13	1:A:225:LEU:HD23	1.96	0.48
1:A:801:ARG:HG2	1:A:845:LEU:HD12	1.95	0.48
1:A:586:THR:O	1:A:590:THR:OG1	2.21	0.47
1:D:760:LEU:HD11	1:D:811:VAL:HG11	1.96	0.47
1:D:887:LEU:HB3	1:D:932:LEU:HD21	1.95	0.47
1:D:544:ILE:HD11	1:D:579:ASN:HB3	1.97	0.47
1:A:887:LEU:HB3	1:A:932:LEU:HD21	1.96	0.47
1:A:1011:ASN:OD1	1:A:1012:SER:N	2.48	0.47
1:A:68:LEU:HD23	1:A:68:LEU:H	1.80	0.47
1:A:214:MET:O	1:A:216:GLN:N	2.48	0.47
1:A:384:LEU:HD11	1:A:405:ILE:HG13	1.97	0.47
3:C:56:LYS:HA	3:C:75:PRO:HA	1.97	0.47
1:D:1057:ARG:NE	1:D:1061:ALA:HB3	2.29	0.47
1:A:218:HIS:ND1	1:A:257:TYR:OH	2.31	0.46
1:D:459:PHE:HB2	1:D:509:LEU:HD21	1.98	0.46
2:E:12:LYS:NZ	2:E:81:ILE:O	2.38	0.46
1:A:122:PHE:CE2	1:A:217:ILE:HD11	2.50	0.46
1:D:691:ILE:HD11	1:D:735:LEU:HD23	1.97	0.46
3:F:33:VAL:HG23	3:F:83:PRO:HD3	1.98	0.46
1:A:475:LYS:HB2	1:A:491:PHE:CE2	2.50	0.46
1:A:651:LYS:HA	1:A:654:ASN:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1057:ARG:NE	1:A:1061:ALA:HB3	2.31	0.46
2:B:86:ALA:O	2:B:117:ILE:HA	2.16	0.46
1:A:305:ASN:OD1	1:A:309:ASN:ND2	2.48	0.46
2:B:13:LEU:HB3	2:B:63:VAL:HA	1.98	0.46
1:D:80:TRP:CD1	1:D:80:TRP:H	2.34	0.46
1:D:214:MET:O	1:D:216:GLN:N	2.49	0.46
1:D:1010:LEU:O	1:D:1014:THR:HG23	2.16	0.46
1:A:824:VAL:HG11	1:A:868:CYS:HB3	1.96	0.46
1:D:1057:ARG:HE	1:D:1061:ALA:HB3	1.79	0.45
1:A:719:ASN:HA	1:D:453:GLU:HG2	1.97	0.45
1:D:43:ALA:HB2	1:D:63:THR:HB	1.96	0.45
2:B:124:VAL:HG21	2:B:148:ASP:HB3	1.97	0.45
1:D:1011:ASN:OD1	1:D:1012:SER:N	2.50	0.45
1:D:673:ARG:H	1:D:673:ARG:HG3	1.50	0.45
1:D:174:LEU:HD22	1:D:174:LEU:HA	1.82	0.45
1:A:900:LEU:HD13	1:A:918:THR:HG23	1.99	0.45
1:A:537:ASP:HB3	1:A:540:VAL:HG12	1.99	0.45
3:F:28:LYS:HG2	3:F:44:MET:HB3	1.98	0.45
2:B:119:LEU:HB3	2:B:146:TYR:HD1	1.81	0.44
1:A:125:ILE:HD13	1:A:139:ILE:HD13	1.99	0.44
3:C:81:GLU:HG2	1:D:536:LYS:HB2	1.99	0.44
3:F:38:PRO:HG3	3:F:142:MET:SD	2.57	0.44
1:A:880:ILE:HA	1:A:887:LEU:HD11	2.00	0.44
1:A:411:MET:O	1:A:414:PHE:HB2	2.17	0.44
3:C:76:SER:C	3:C:78:HIS:H	2.26	0.44
1:D:17:PRO:O	2:E:10:GLN:NE2	2.50	0.44
1:D:522:MET:HE3	1:D:544:ILE:HD11	2.00	0.44
1:A:35:LYS:HD2	1:A:69:ASN:HB3	1.99	0.44
1:D:801:ARG:HG2	1:D:845:LEU:HD12	1.98	0.44
1:D:993:ASP:O	1:D:997:GLN:HG2	2.18	0.44
1:A:849:MET:HG3	1:A:879:LEU:HD11	1.99	0.44
3:C:38:PRO:HG3	3:C:142:MET:SD	2.57	0.44
1:A:833:LYS:HA	1:A:833:LYS:HD3	1.82	0.43
3:F:33:VAL:HB	3:F:81:GLU:HB2	1.98	0.43
1:A:534:ILE:HG22	1:A:536:LYS:HG3	2.00	0.43
1:D:147:ASN:HB3	1:D:174:LEU:CB	2.49	0.43
1:D:499:SER:HB2	1:D:553:THR:HG21	2.00	0.43
1:D:691:ILE:HD13	1:D:734:LEU:HG	2.00	0.43
1:D:221:VAL:HG13	1:D:225:LEU:HD23	1.99	0.43
1:A:43:ALA:HB2	1:A:63:THR:HB	2.00	0.43
1:A:48:SER:HB3	1:A:92:LYS:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HG13	1:A:225:LEU:HB3	1.99	0.43
2:E:85:CYS:HB2	2:E:164:LEU:HD22	1.99	0.43
2:B:54:THR:HG21	2:B:174:LEU:HD21	2.00	0.43
1:D:453:GLU:OE1	1:D:453:GLU:N	2.47	0.43
1:D:221:VAL:HG13	1:D:225:LEU:HB3	2.01	0.43
1:D:587:GLY:O	1:D:601:LYS:HG3	2.19	0.43
1:D:1007:ARG:HD2	1:D:1007:ARG:HA	1.82	0.43
1:D:748:GLN:HG3	1:D:817:TYR:HE2	1.84	0.43
2:E:54:THR:HG21	2:E:174:LEU:HD21	2.00	0.43
1:A:1057:ARG:HE	1:A:1061:ALA:HB3	1.83	0.43
1:A:558:MET:HG2	3:C:69:LYS:HD2	2.01	0.42
1:D:122:PHE:CE2	1:D:217:ILE:HD11	2.54	0.42
2:E:101:VAL:HG11	2:E:119:LEU:HD11	2.00	0.42
1:A:673:ARG:H	1:A:673:ARG:HG3	1.55	0.42
1:D:78:THR:OG1	1:D:79:LEU:N	2.52	0.42
1:D:201:VAL:HG11	1:D:254:TRP:HA	2.00	0.42
1:D:97:TYR:CE2	1:D:111:ILE:HG12	2.54	0.42
1:D:255:ILE:O	1:D:259:SER:N	2.51	0.42
1:D:565:TRP:HB2	3:F:58:HIS:HE1	1.84	0.42
2:B:101:VAL:HG11	2:B:119:LEU:HD11	2.01	0.42
1:D:506:TRP:HZ3	3:F:62:ILE:HG12	1.85	0.42
2:E:86:ALA:O	2:E:117:ILE:HA	2.19	0.42
1:D:226:TYR:CE1	1:D:270:MET:HB3	2.54	0.42
1:A:35:LYS:O	1:A:35:LYS:HG2	2.20	0.42
1:A:382:ASN:O	1:A:386:THR:HG22	2.20	0.42
1:A:466:TYR:HA	1:A:469:LYS:HB2	2.01	0.42
3:C:18:THR:HG22	3:C:83:PRO:HA	2.00	0.42
3:F:35:LYS:HD2	3:F:70:LEU:HD22	2.02	0.42
3:F:135:MET:HB2	3:F:151:LYS:HB3	2.00	0.42
1:A:279:LEU:HD22	1:A:299:ILE:HG12	2.01	0.42
1:A:1007:ARG:HH11	1:A:1008:SER:H	1.66	0.42
1:D:98:VAL:O	1:D:101:PRO:HD2	2.20	0.42
1:D:650:GLU:O	1:D:654:ASN:N	2.44	0.42
1:D:384:LEU:HD11	1:D:405:ILE:HG13	2.01	0.42
1:D:475:LYS:HB2	1:D:491:PHE:CE2	2.55	0.42
1:D:601:LYS:HE2	1:D:657:LEU:HD21	2.02	0.42
1:A:394:GLY:HA3	1:A:395:GLN:HA	1.77	0.41
1:D:523:GLY:HA3	1:D:573:ASN:HB3	2.00	0.41
1:A:146:ILE:HD13	1:A:146:ILE:HA	1.97	0.41
1:A:729:LEU:HD22	1:A:798:LEU:HD13	2.02	0.41
2:B:81:ILE:HG22	2:B:82:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:969:LEU:HD12	1:D:975:TYR:OH	2.20	0.41
1:A:214:MET:C	1:A:216:GLN:H	2.29	0.41
1:D:382:ASN:O	1:D:386:THR:HG22	2.20	0.41
3:F:76:SER:O	3:F:77:THR:HG22	2.20	0.41
1:A:80:TRP:CD1	1:A:80:TRP:H	2.38	0.41
1:D:34:GLN:HB3	1:D:63:THR:HG23	2.02	0.41
1:D:262:ARG:NH2	1:D:270:MET:N	2.65	0.41
1:A:210:LYS:HE3	1:A:210:LYS:HB2	1.86	0.41
1:A:307:PHE:CD2	1:A:372:PHE:HB2	2.55	0.41
1:A:401:ILE:HA	1:A:404:TYR:HB3	2.03	0.41
1:A:725:ALA:HB1	1:A:798:LEU:HD12	2.02	0.41
1:D:89:TYR:O	1:D:93:PHE:HB2	2.21	0.41
2:E:71:LYS:H	2:E:71:LYS:HG3	1.70	0.41
1:D:422:GLU:OE1	1:D:424:PHE:N	2.54	0.41
1:A:97:TYR:OH	1:A:111:ILE:HG23	2.21	0.41
1:A:367:ILE:HD12	2:B:140:ARG:HH22	1.86	0.41
1:A:640:CYS:HB2	1:A:654:ASN:OD1	2.21	0.41
2:B:158:GLU:HB3	2:B:176:PHE:CD2	2.56	0.41
1:D:97:TYR:OH	1:D:111:ILE:O	2.36	0.41
1:D:537:ASP:HB3	1:D:540:VAL:HG12	2.03	0.41
1:D:829:LEU:O	1:D:833:LYS:HG2	2.21	0.41
2:E:80:TYR:HB2	2:E:111:VAL:HG21	2.02	0.41
3:F:76:SER:C	3:F:78:HIS:H	2.29	0.41
1:D:647:ASN:C	1:D:649:GLN:H	2.28	0.40
1:D:968:LYS:O	1:D:972:ASN:HB2	2.21	0.40
2:E:81:ILE:HG22	2:E:82:GLN:HG2	2.04	0.40
1:A:990:ILE:H	1:A:990:ILE:HG13	1.79	0.40
1:D:194:LEU:HD23	1:D:246:THR:HB	2.02	0.40
1:D:729:LEU:HD22	1:D:798:LEU:HD13	2.03	0.40
1:D:102:ASN:OD1	1:D:102:ASN:N	2.51	0.40
1:D:186:SER:HB3	1:D:189:HIS:ND1	2.37	0.40
3:C:76:SER:O	3:C:77:THR:HG22	2.20	0.40
1:A:98:VAL:O	1:A:101:PRO:HD2	2.21	0.40
1:D:214:MET:C	1:D:216:GLN:H	2.30	0.40
1:D:262:ARG:CZ	1:D:262:ARG:O	2.69	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	1003/1080 (93%)	936 (93%)	62 (6%)	5 (0%)	24	56
1	D	1001/1080 (93%)	939 (94%)	55 (6%)	7 (1%)	18	50
2	B	169/176 (96%)	161 (95%)	8 (5%)	0	100	100
2	E	169/176 (96%)	161 (95%)	8 (5%)	0	100	100
3	C	135/142 (95%)	129 (96%)	5 (4%)	1 (1%)	18	50
3	F	122/142 (86%)	117 (96%)	4 (3%)	1 (1%)	16	48
All	All	2599/2796 (93%)	2443 (94%)	142 (6%)	14 (0%)	24	56

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	419	VAL
1	D	21	HIS
1	D	262	ARG
1	D	419	VAL
1	A	37	GLU
1	A	394	GLY
1	D	37	GLU
1	D	261	THR
1	D	416	LEU
3	C	77	THR
1	D	260	LEU
3	F	77	THR
1	A	414	PHE

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	936/1000 (94%)	931 (100%)	5 (0%)	81	80
1	D	940/1000 (94%)	935 (100%)	5 (0%)	81	80
2	B	150/154 (97%)	150 (100%)	0	100	100
2	E	150/154 (97%)	150 (100%)	0	100	100
3	C	117/121 (97%)	116 (99%)	1 (1%)	70	75
3	F	109/121 (90%)	109 (100%)	0	100	100
All	All	2402/2550 (94%)	2391 (100%)	11 (0%)	81	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	LEU
1	A	447	LEU
1	A	532	THR
1	A	626	LEU
1	A	1071	LEU
3	C	44	MET
1	D	174	LEU
1	D	262	ARG
1	D	532	THR
1	D	626	LEU
1	D	1071	LEU

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	31	GLN
1	A	44	ASN
1	A	234	ASN
1	A	309	ASN
1	A	320	GLN
1	A	356	ASN
1	A	421	GLN
1	A	621	GLN
1	A	635	GLN
1	A	638	HIS

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Mol	Chain	Res	Type
1	A	642	ASN
1	A	1006	GLN
3	C	54	HIS
3	C	88	ASN
3	C	91	GLN
1	D	27	GLN
1	D	31	GLN
1	D	34	GLN
1	D	44	ASN
1	D	55	ASN
1	D	171	ASN
1	D	234	ASN
1	D	356	ASN
1	D	524	GLN
1	D	621	GLN
1	D	635	GLN
2	E	82	GLN
2	E	145	GLN
3	F	91	GLN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	B	217	5	33,34,34	0.97	1 (3%)	50,54,54	1.57	9 (18%)
4	GTP	E	217	5	33,34,34	0.99	1 (3%)	50,54,54	1.55	9 (18%)

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	B	217	5	-	8/22/38/38	0/3/3/3
4	GTP	E	217	5	-	8/22/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	217	GTP	C2-N3	2.26	1.38	1.33
4	E	217	GTP	C2-N3	2.26	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	217	GTP	C5-C4-N3	-5.23	120.07	128.39
4	B	217	GTP	C5-C4-N3	-5.20	120.11	128.39
4	E	217	GTP	C2-N3-C4	4.53	120.11	112.30
4	B	217	GTP	C2-N3-C4	4.52	120.09	112.30
4	E	217	GTP	N9-C4-N3	3.50	132.96	125.95
4	B	217	GTP	N9-C4-N3	3.49	132.93	125.95
4	E	217	GTP	C2-N1-C6	-2.99	119.69	125.11
4	B	217	GTP	C2-N1-C6	-2.97	119.72	125.11
4	E	217	GTP	O6-C6-C5	-2.65	119.53	126.53
4	B	217	GTP	O6-C6-C5	-2.63	119.58	126.53
4	E	217	GTP	C5-C6-N1	2.40	119.36	113.25
4	B	217	GTP	C5-C6-N1	2.39	119.34	113.25
4	B	217	GTP	N9-C8-N7	-2.38	108.98	113.40
4	B	217	GTP	C8-N7-C5	2.33	108.41	104.26
4	E	217	GTP	C8-N7-C5	2.31	108.38	104.26
4	E	217	GTP	N9-C8-N7	-2.31	109.12	113.40
4	E	217	GTP	C3'-C2'-C1'	2.22	105.66	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	217	GTP	C3'-C2'-C1'	2.10	105.44	101.46

There are no chirality outliers.

All (16) torsion outliers are listed below:

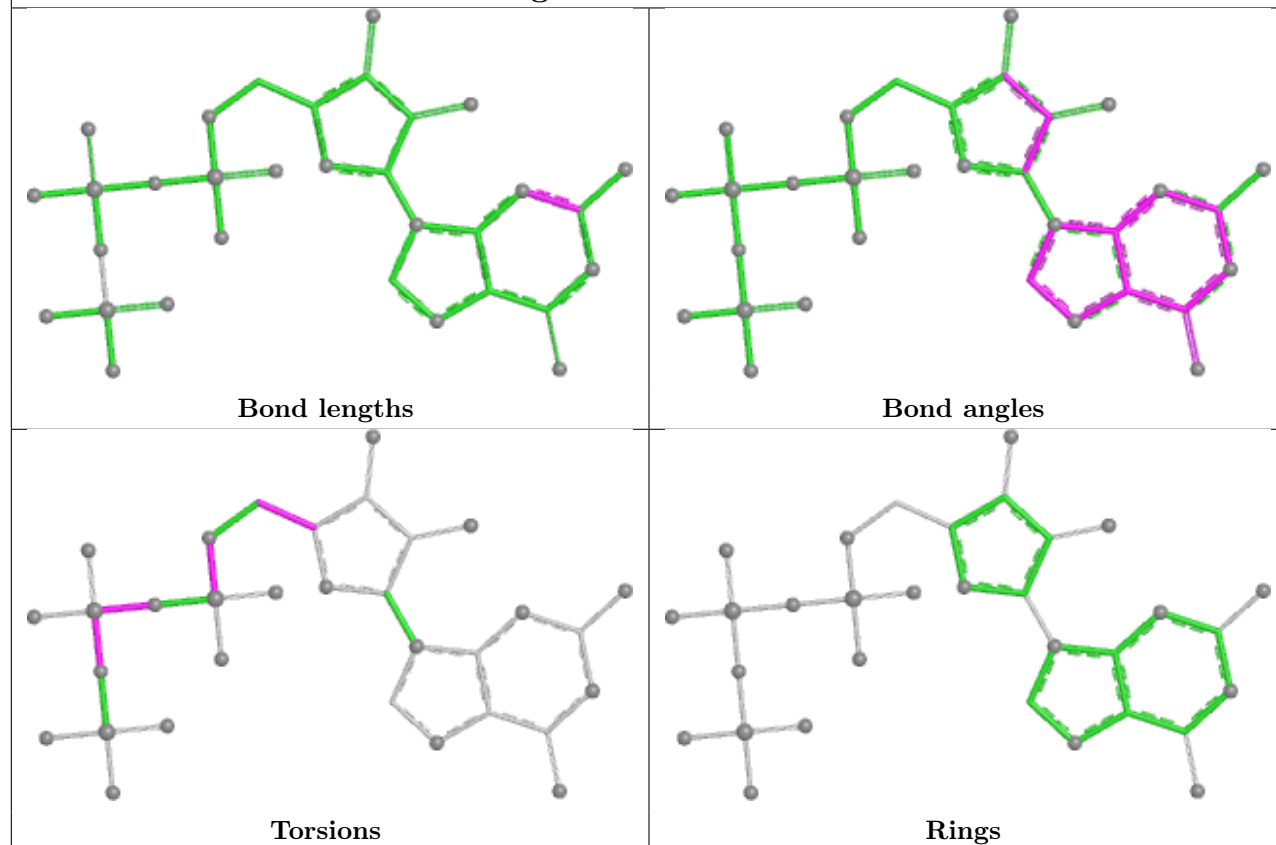
Mol	Chain	Res	Type	Atoms
4	E	217	GTP	C5'-O5'-PA-O2A
4	B	217	GTP	O4'-C4'-C5'-O5'
4	E	217	GTP	O4'-C4'-C5'-O5'
4	E	217	GTP	C3'-C4'-C5'-O5'
4	B	217	GTP	C3'-C4'-C5'-O5'
4	B	217	GTP	PG-O3B-PB-O1B
4	B	217	GTP	PA-O3A-PB-O2B
4	B	217	GTP	C5'-O5'-PA-O3A
4	B	217	GTP	C5'-O5'-PA-O1A
4	B	217	GTP	C5'-O5'-PA-O2A
4	E	217	GTP	C5'-O5'-PA-O3A
4	E	217	GTP	C5'-O5'-PA-O1A
4	E	217	GTP	PA-O3A-PB-O1B
4	B	217	GTP	PG-O3B-PB-O2B
4	E	217	GTP	PG-O3B-PB-O2B
4	E	217	GTP	PA-O3A-PB-O2B

There are no ring outliers.

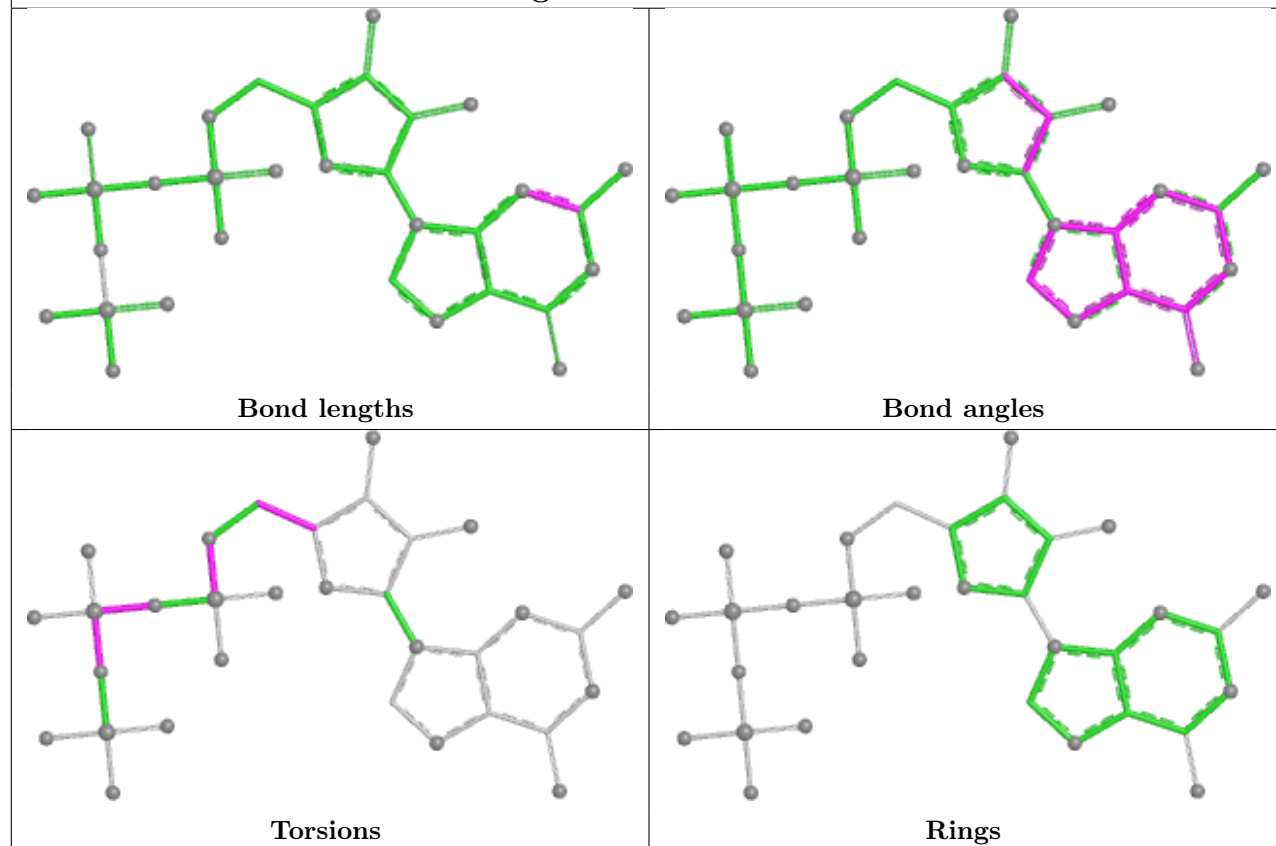
No monomer is involved in short contacts.

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 B 217



Ligand GTP E 217



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1019/1080 (94%)	-0.57	2 (0%) 91 80	135, 203, 251, 286	0
1	D	1017/1080 (94%)	-0.69	1 (0%) 92 86	120, 181, 239, 289	0
2	B	171/176 (97%)	-0.64	1 (0%) 85 66	156, 198, 258, 321	0
2	E	171/176 (97%)	-0.65	0 100 100	133, 189, 250, 286	0
3	C	137/142 (96%)	-0.73	0 100 100	133, 195, 252, 272	0
3	F	126/142 (88%)	-0.26	0 100 100	185, 247, 285, 310	0
All	All	2641/2796 (94%)	-0.62	4 (0%) 91 80	120, 195, 254, 321	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	GLN	3.1
1	D	928	VAL	3.1
2	B	133	ALA	2.1
1	A	899	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

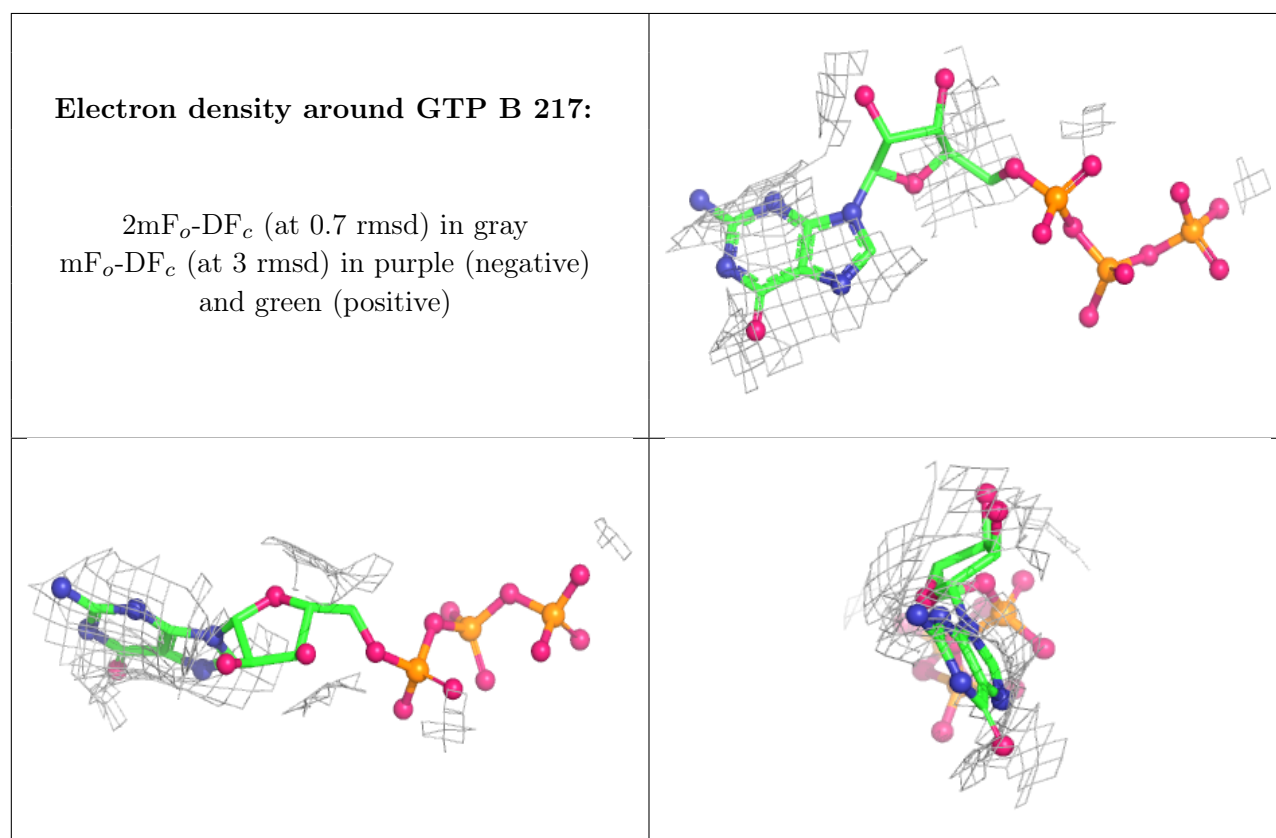
6.4 Ligands [i](#)

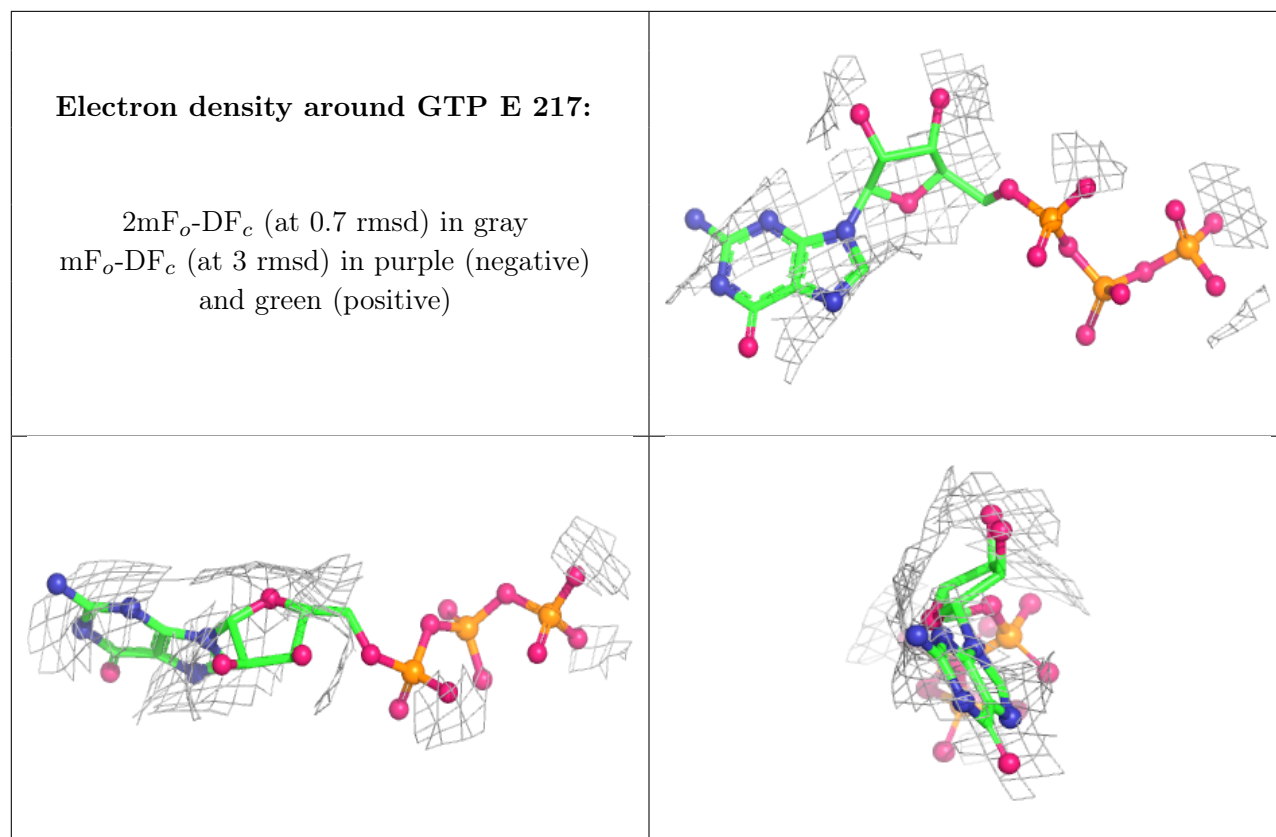
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GTP	B	217	32/32	0.99	0.04	151,178,219,235	0
5	MG	B	218	1/1	0.99	0.05	158,158,158,158	0
4	GTP	E	217	32/32	1.00	0.03	140,174,200,210	0
5	MG	E	218	1/1	1.00	0.02	139,139,139,139	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.