



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:16 PM GMT

PDB ID : 4C0Q
Title : Transportin 3 in complex with Ran(Q69L)GTP
Authors : Maertens, G.; Hare, S.; Cherepanov, P.
Deposited on : 2013-08-06
Resolution : 3.42 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

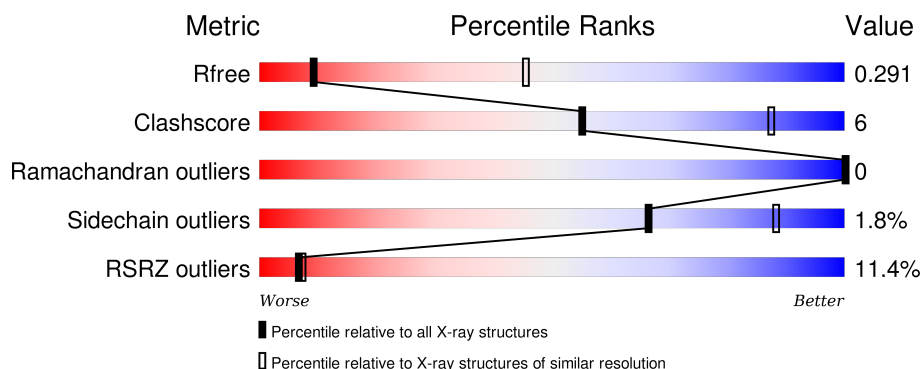
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	923	
1	B	923	
2	C	215	
2	D	215	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15766 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 TRANSPORTIN-3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	Se	0	0	0
			6927	4420	1177	1277	31	22			
1	B	749	Total	C	N	O	S	Se	0	0	0
			5979	3838	1007	1088	26	20			

- Molecule 2 is a protein called GTP-BINDING NUCLEAR PROTEIN RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	169	Total	C	N	O	S	0	0	0
			1376	896	241	235	4			
2	D	175	Total	C	N	O	S	0	0	0
			1418	923	247	243	5			

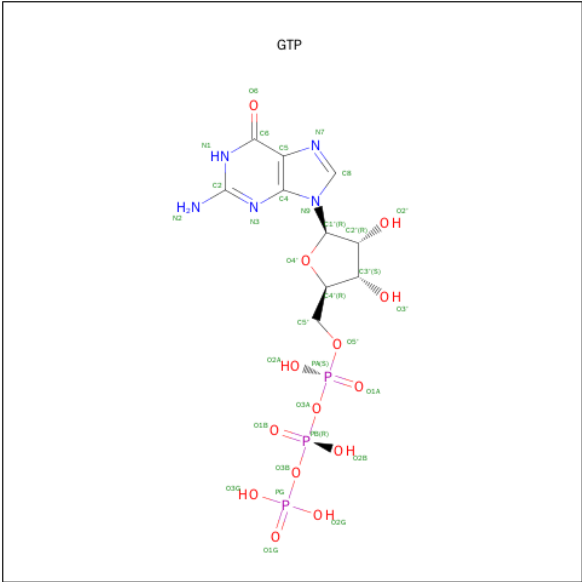
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	69	LEU	GLN	ENGINEERED MUTATION	UNP P62826
D	69	LEU	GLN	ENGINEERED MUTATION	UNP P62826

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

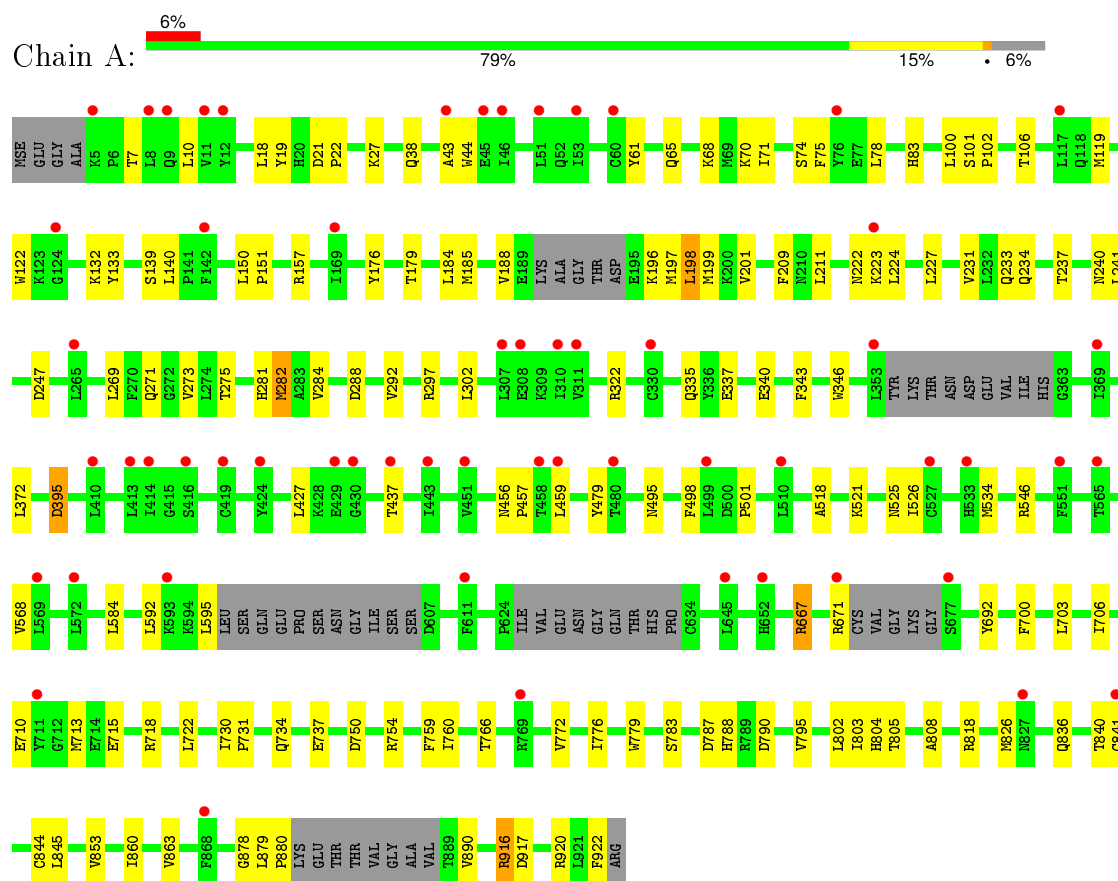
- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

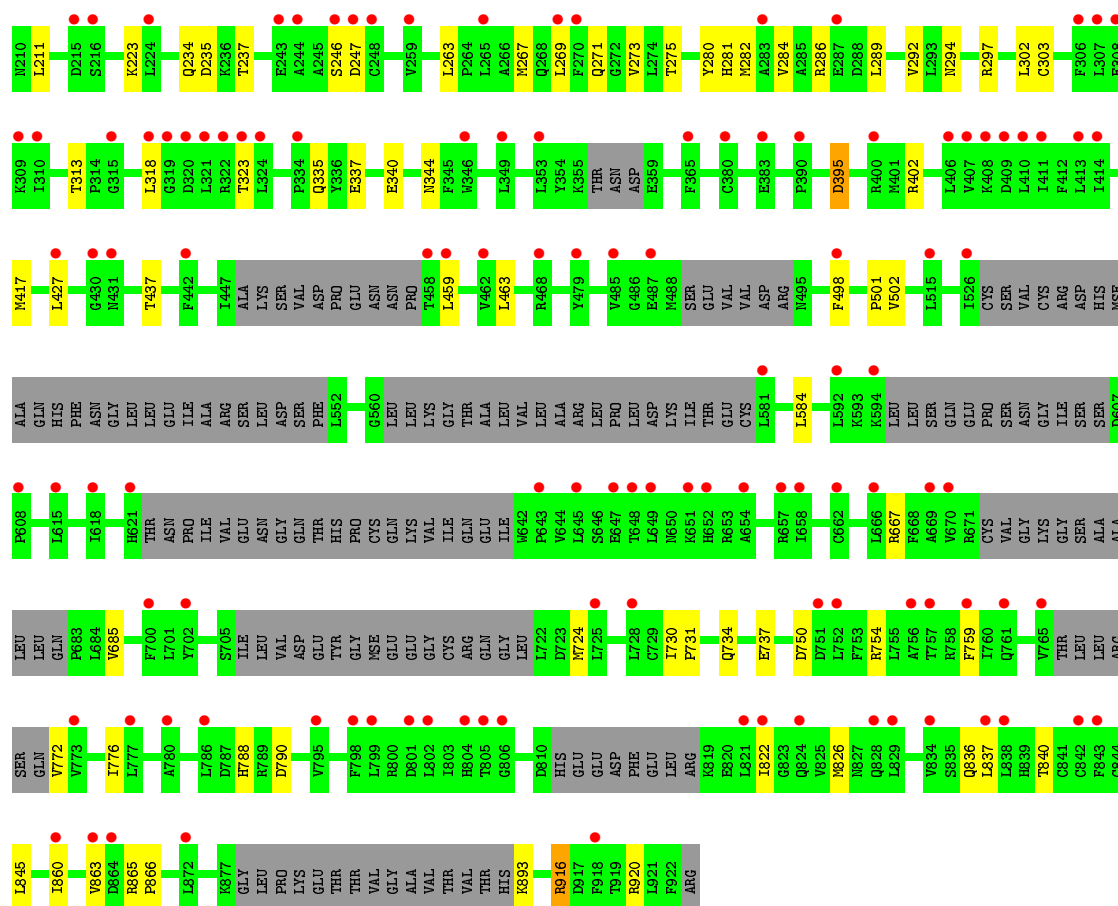


3 Residue-property plots [i](#)

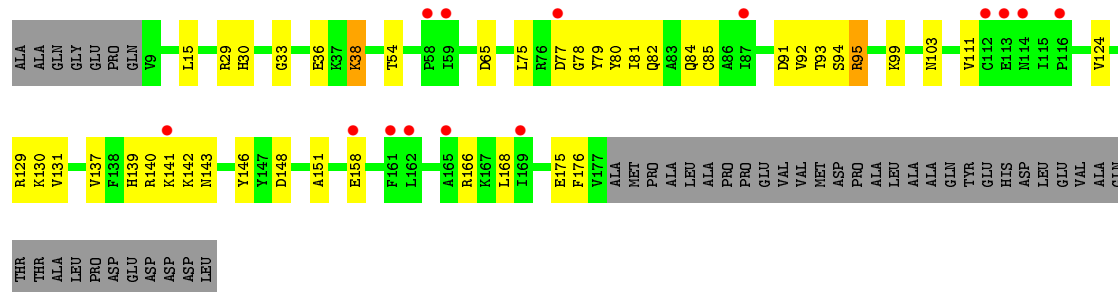
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: TRANSPORTIN-3

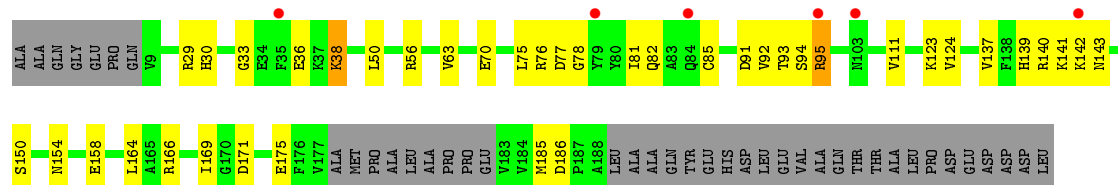




• Molecule 2: GTP-BINDING NUCLEAR PROTEIN RAN



• Molecule 2: GTP-BINDING NUCLEAR PROTEIN RAN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.95Å 93.51Å 104.71Å 78.43° 68.29° 68.28°	Depositor
Resolution (Å)	39.95 – 3.42 39.94 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.95-3.42) 96.8 (39.94-3.42)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.268 , 0.290 0.279 , 0.291	Depositor DCC
R_{free} test set	1765 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	135.4	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 34990 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15766	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	0/7040	0.41	0/9520
1	B	0.22	0/6074	0.41	0/8200
2	C	0.23	0/1410	0.41	0/1904
2	D	0.24	0/1452	0.42	0/1961
All	All	0.22	0/15976	0.41	0/21585

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

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	6927	0	6962	93	0
1	B	5979	0	6006	62	0
2	C	1376	0	1403	29	0
2	D	1418	0	1445	31	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	C	32	0	12	1	0
4	D	32	0	12	2	0
All	All	15766	0	15840	200	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 (200) 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:A:671:ARG:NH1	1:A:710:GLU:OE2	2.09	0.85
1:A:917:ASP:OD1	2:D:56:ARG:NH2	2.11	0.84
1:A:68:LYS:NZ	2:C:77:ASP:OD2	2.21	0.74
1:A:196:LYS:HA	1:A:199:MSE:HE2	1.70	0.73
2:C:142:LYS:HA	2:C:142:LYS:NZ	2.03	0.73
1:A:184:LEU:HG	1:A:201:VAL:HG13	1.72	0.72
2:D:142:LYS:HA	2:D:142:LYS:NZ	2.06	0.71
1:A:427:LEU:HD11	1:A:437:THR:HA	1.72	0.70
1:B:184:LEU:HG	1:B:201:VAL:HG13	1.74	0.69
1:B:68:LYS:NZ	2:D:77:ASP:OD2	2.25	0.69
1:B:340:GLU:OE1	1:B:402:ARG:NH2	2.26	0.66
2:C:29:ARG:NH2	2:C:33:GLY:O	2.27	0.66
1:A:273:VAL:HG11	1:A:302:LEU:HD13	1.77	0.66
1:A:157:ARG:NH1	2:C:103:ASN:OD1	2.27	0.65
1:B:427:LEU:HD11	1:B:437:THR:HA	1.79	0.64
1:A:826:MSE:HE1	1:A:860:ILE:HG23	1.79	0.63
1:A:826:MSE:HG3	1:A:863:VAL:HG11	1.82	0.61
2:D:56:ARG:NH1	2:D:171:ASP:OD2	2.34	0.60
2:D:91:ASP:HB3	2:D:94:SER:HB3	1.84	0.60
2:D:29:ARG:NH1	2:D:154:ASN:OD1	2.35	0.59
2:D:70:GLU:OE2	2:D:76:ARG:NH2	2.34	0.59
1:A:140:LEU:HB3	1:A:197:MSE:HE1	1.85	0.58
1:B:281:HIS:HA	1:B:284:VAL:HG12	1.84	0.58
1:B:133:TYR:HB3	1:B:139:SER:HB3	1.85	0.58
2:D:166:ARG:NH2	2:D:175:GLU:OE2	2.36	0.58
1:B:263:LEU:HD22	1:B:267:MSE:HE3	1.85	0.57
1:A:788:HIS:CE1	1:A:790:ASP:HB2	2.39	0.57
1:A:456:ASN:ND2	1:A:495:ASN:OD1	2.38	0.57
1:B:734:GLN:O	1:B:737:GLU:HG2	2.04	0.57
1:A:151:PRO:HB3	1:A:211:LEU:HD22	1.87	0.57
1:A:734:GLN:O	1:A:737:GLU:HG2	2.04	0.57
2:C:142:LYS:HZ2	2:C:142:LYS:HA	1.70	0.56
1:A:788:HIS:HE1	1:A:790:ASP:HB2	1.70	0.56
1:A:133:TYR:HB3	1:A:139:SER:HB3	1.88	0.55
2:C:92:VAL:HG21	2:C:124:VAL:HG12	1.89	0.55
1:B:38:GLN:HG2	1:B:66:THR:HG23	1.89	0.54
1:A:521:LYS:O	1:A:525:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:ARG:HD3	1:A:706:ILE:HD13	1.90	0.54
2:D:29:ARG:NH2	2:D:33:GLY:O	2.38	0.54
1:A:38:GLN:OE1	2:C:75:LEU:HD23	2.08	0.54
1:A:427:LEU:HD21	1:A:437:THR:HG23	1.91	0.53
1:B:38:GLN:O	1:B:70:LYS:HE3	2.09	0.53
1:B:836:GLN:O	1:B:840:THR:HG23	2.08	0.53
1:A:760:ILE:HG12	1:A:802:LEU:HA	1.90	0.53
2:C:146:TYR:OH	2:C:148:ASP:OD1	2.17	0.53
1:B:822:ILE:O	1:B:826:MSE:HG2	2.09	0.52
1:A:176:TYR:O	1:A:179:THR:OG1	2.26	0.52
1:B:235:ASP:OD2	1:B:286:ARG:NH2	2.42	0.52
2:C:36:GLU:HG3	2:C:38:LYS:HG3	1.91	0.52
1:B:185:MSE:HE3	1:B:223:LYS:HD3	1.90	0.52
1:B:289:LEU:HA	1:B:292:VAL:HG12	1.90	0.52
1:A:395:ASP:N	1:A:395:ASP:OD1	2.42	0.52
2:D:142:LYS:HZ2	2:D:142:LYS:HA	1.75	0.52
1:B:18:LEU:O	1:B:27:LYS:HD2	2.10	0.51
2:D:142:LYS:HA	2:D:142:LYS:HZ3	1.74	0.51
1:A:269:LEU:O	1:A:273:VAL:HG12	2.10	0.51
1:A:836:GLN:O	1:A:840:THR:HG23	2.10	0.51
1:A:713:MSE:SE	1:A:713:MSE:H	2.44	0.51
1:B:119:MSE:SE	1:B:122:TRP:HB2	2.60	0.51
1:A:7:THR:HG22	1:A:10:LEU:HB2	1.93	0.50
2:D:142:LYS:O	2:D:143:ASN:HB3	2.11	0.50
2:C:142:LYS:HA	2:C:142:LYS:HZ1	1.74	0.50
1:B:463:LEU:HD11	1:B:502:VAL:HG22	1.94	0.50
1:B:151:PRO:HB3	1:B:211:LEU:HD22	1.93	0.50
1:B:826:MSE:HG3	1:B:863:VAL:HG11	1.92	0.50
1:A:44:TRP:CE2	1:A:70:LYS:HD2	2.47	0.50
2:D:36:GLU:HG3	2:D:38:LYS:HG3	1.94	0.49
1:B:788:HIS:CE1	1:B:790:ASP:HB2	2.47	0.49
1:A:750:ASP:O	1:A:754:ARG:HG3	2.12	0.49
1:A:715:GLU:HG3	1:A:718:ARG:HD2	1.95	0.49
2:C:142:LYS:O	2:C:143:ASN:HB3	2.13	0.49
1:B:269:LEU:O	1:B:273:VAL:HG12	2.13	0.49
1:A:119:MSE:SE	1:A:122:TRP:HB2	2.63	0.49
1:A:233:GLN:NE2	1:A:275:THR:OG1	2.45	0.49
1:A:43:ALA:HB3	1:A:70:LYS:HE3	1.95	0.49
2:D:95:ARG:NE	2:D:95:ARG:H	2.10	0.49
1:A:805:THR:O	1:A:818:ARG:NH1	2.45	0.49
1:A:730:ILE:HB	1:A:731:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:ILE:HG22	2:C:82:GLN:HG3	1.95	0.48
1:B:730:ILE:HB	1:B:731:PRO:HD3	1.94	0.48
1:A:783:SER:HB3	1:A:795:VAL:HG21	1.94	0.48
1:B:395:ASP:OD1	1:B:395:ASP:N	2.46	0.48
1:B:61:TYR:CD2	2:D:81:ILE:HD11	2.48	0.48
1:B:176:TYR:O	1:B:179:THR:OG1	2.29	0.48
1:A:7:THR:HG23	1:A:10:LEU:H	1.79	0.47
1:B:282:MSE:HA	1:B:282:MSE:HE2	1.95	0.47
1:A:44:TRP:CZ2	1:A:78:LEU:HD21	2.49	0.47
1:B:335:GLN:HG3	1:B:337:GLU:OE1	2.14	0.47
1:A:916:ARG:O	1:A:920:ARG:HD3	2.14	0.47
1:A:282:MSE:HE2	1:A:282:MSE:HA	1.96	0.47
1:A:150:LEU:HB3	1:A:151:PRO:HD3	1.97	0.47
1:B:61:TYR:HE2	2:D:78:GLY:HA2	1.79	0.47
1:B:417:MSE:HE1	1:B:459:LEU:HD11	1.97	0.47
1:A:83:HIS:HB3	1:A:119:MSE:HE2	1.97	0.47
1:A:19:TYR:CZ	2:C:81:ILE:HD12	2.50	0.47
2:D:169:ILE:HD12	2:D:185:MET:HE1	1.97	0.47
2:C:95:ARG:HD3	2:C:130:LYS:HE3	1.96	0.46
1:A:18:LEU:O	1:A:27:LYS:HD2	2.15	0.46
1:B:826:MSE:HE1	1:B:860:ILE:HG23	1.97	0.46
1:A:247:ASP:OD1	1:A:297:ARG:NH2	2.38	0.46
2:D:30:HIS:HE1	2:D:158:GLU:HG2	1.79	0.46
2:C:166:ARG:NH2	2:C:175:GLU:OE2	2.48	0.46
1:A:102:PRO:O	1:A:106:THR:HG23	2.15	0.46
2:D:50:LEU:HD12	2:D:63:VAL:HG21	1.97	0.46
1:A:271:GLN:O	1:A:275:THR:HG23	2.15	0.46
1:A:70:LYS:HD3	1:A:74:SER:HB2	1.98	0.46
1:A:841:CYS:SG	1:A:853:VAL:HG11	2.55	0.46
2:D:81:ILE:HG22	2:D:82:GLN:HG3	1.98	0.46
1:B:196:LYS:HA	1:B:199:MSE:HE2	1.97	0.46
2:D:124:VAL:HG22	2:D:150:SER:HB2	1.98	0.46
2:D:137:VAL:HG13	2:D:140:ARG:CZ	2.46	0.46
1:A:715:GLU:HA	1:A:718:ARG:HG3	1.97	0.45
1:A:456:ASN:N	1:A:457:PRO:HD2	2.31	0.45
1:B:38:GLN:OE1	2:D:75:LEU:HD23	2.16	0.45
2:C:84:GLN:HB3	2:C:168:LEU:HD11	1.99	0.45
2:C:30:HIS:HE1	2:C:158:GLU:HG2	1.82	0.45
1:A:526:ILE:HG22	1:A:534:MSE:HE1	1.99	0.45
2:C:85:CYS:HB3	2:C:168:LEU:HD21	1.99	0.45
1:B:150:LEU:HB3	1:B:151:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TYR:CD2	2:C:81:ILE:HD11	2.53	0.44
1:B:788:HIS:HE1	1:B:790:ASP:HB2	1.82	0.44
1:A:692:TYR:HD1	1:A:700:PHE:HD2	1.66	0.44
1:B:101:SER:HB3	1:B:104:ILE:HD13	1.98	0.44
1:B:280:TYR:CE1	1:B:292:VAL:HG23	2.52	0.44
1:A:71:ILE:O	1:A:75:PHE:HB2	2.17	0.44
1:A:890:VAL:HG21	1:A:922:PHE:CZ	2.53	0.44
1:B:102:PRO:O	1:B:106:THR:HG23	2.17	0.44
1:A:346:TRP:CD2	1:A:372:LEU:HD22	2.52	0.44
2:C:15:LEU:HB3	2:C:65:ASP:HA	2.00	0.44
1:A:234:GLN:HB2	1:A:237:THR:HG23	2.00	0.44
1:B:750:ASP:O	1:B:754:ARG:HG3	2.18	0.44
1:A:787:ASP:HA	1:A:845:LEU:HD22	2.00	0.44
1:A:185:MSE:HE3	1:A:223:LYS:HD3	1.98	0.44
1:B:19:TYR:CZ	2:D:81:ILE:HD12	2.53	0.44
1:B:685:VAL:HG13	1:B:724:MSE:SE	2.68	0.44
1:A:703:LEU:HA	1:A:706:ILE:HD12	2.00	0.43
2:C:151:ALA:N	4:C:1179:GTP:O6	2.51	0.43
1:B:234:GLN:HB2	1:B:237:THR:HG23	1.99	0.43
1:B:267:MSE:HG2	1:B:318:LEU:HD21	1.99	0.43
1:A:132:LYS:HD3	1:A:133:TYR:CE2	2.53	0.43
1:A:44:TRP:NE1	1:A:70:LYS:HD2	2.34	0.43
1:A:281:HIS:HA	1:A:284:VAL:HG12	2.00	0.43
2:C:91:ASP:HB3	2:C:94:SER:HB3	1.99	0.43
1:B:100:LEU:HG	1:B:101:SER:H	1.84	0.43
1:A:479:TYR:CE1	1:A:518:ALA:HB2	2.54	0.43
2:C:75:LEU:HD12	2:C:79:TYR:CE1	2.53	0.43
1:B:498:PHE:C	1:B:501:PRO:HD2	2.39	0.43
1:A:227:LEU:O	1:A:231:VAL:HG13	2.18	0.43
2:C:80:TYR:HB2	2:C:111:VAL:HG11	2.01	0.43
2:C:137:VAL:HG13	2:C:140:ARG:CZ	2.48	0.43
2:D:123:LYS:HG2	4:D:1190:GTP:C5	2.54	0.43
1:A:197:MSE:O	1:A:201:VAL:HG23	2.19	0.42
1:B:271:GLN:O	1:B:275:THR:HG23	2.18	0.42
1:B:34:LEU:HD22	1:B:62:PHE:CZ	2.54	0.42
1:A:667:ARG:O	1:A:671:ARG:HG2	2.19	0.42
1:A:288:ASP:O	1:A:292:VAL:HG13	2.19	0.42
1:B:246:SER:OG	1:B:294:ASN:HB3	2.19	0.42
1:B:772:VAL:O	1:B:776:ILE:HG13	2.20	0.42
1:A:21:ASP:HA	1:A:22:PRO:HD3	1.88	0.42
1:A:199:MSE:SE	1:A:240:ASN:HB3	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:MSE:HG2	1:A:568:VAL:HG11	2.00	0.42
1:A:804:HIS:CD2	1:A:808:ALA:HB2	2.54	0.42
1:B:273:VAL:HG11	1:B:302:LEU:HD13	2.01	0.42
2:D:123:LYS:HE2	4:D:1190:GTP:C8	2.54	0.42
1:A:772:VAL:O	1:A:776:ILE:HG12	2.19	0.42
1:B:313:THR:O	1:B:313:THR:OG1	2.32	0.42
1:B:247:ASP:OD1	1:B:297:ARG:NH2	2.35	0.42
1:A:803:ILE:HD13	1:A:860:ILE:HG12	2.01	0.42
1:A:592:LEU:HA	1:A:595:LEU:HD12	2.02	0.42
1:B:303:CYS:SG	1:B:323:THR:HB	2.59	0.42
1:A:198:LEU:HB3	1:A:241:LEU:HD13	2.02	0.42
1:A:878:GLY:O	1:A:879:LEU:HD12	2.20	0.42
2:D:85:CYS:HB2	2:D:164:LEU:HD22	2.01	0.41
1:B:54:ARG:NH1	1:B:96:ASN:HB3	2.35	0.41
1:A:840:THR:HA	1:A:844:CYS:HB2	2.01	0.41
1:A:61:TYR:HE2	2:C:78:GLY:HA2	1.83	0.41
1:A:335:GLN:HG3	1:A:337:GLU:OE1	2.20	0.41
1:A:779:TRP:O	1:A:783:SER:N	2.53	0.41
1:A:322:ARG:HD2	1:A:322:ARG:HA	1.90	0.41
1:B:103:VAL:HG23	2:D:111:VAL:HA	2.03	0.41
1:A:100:LEU:HG	1:A:101:SER:H	1.86	0.41
1:B:71:ILE:O	1:B:75:PHE:HB2	2.21	0.41
2:D:76:ARG:HB2	2:D:77:ASP:H	1.70	0.41
1:A:157:ARG:NH2	2:C:99:LYS:HE3	2.35	0.41
1:B:840:THR:HB	1:B:845:LEU:HG	2.03	0.41
1:A:188:VAL:HG12	1:A:198:LEU:HD12	2.02	0.41
1:A:879:LEU:HA	1:A:880:PRO:HD3	1.84	0.41
2:C:54:THR:HG22	2:C:176:PHE:CD1	2.56	0.41
1:A:222:ASN:OD1	1:A:224:LEU:HB2	2.21	0.41
1:A:340:GLU:HA	1:A:343:PHE:CD1	2.56	0.41
1:B:916:ARG:O	1:B:920:ARG:HD3	2.21	0.40
1:A:498:PHE:C	1:A:501:PRO:HD2	2.40	0.40
2:C:129:ARG:NE	2:C:131:VAL:O	2.52	0.40
1:B:865:ARG:N	1:B:866:PRO:HD2	2.37	0.40
1:B:130:VAL:HA	1:B:143:LEU:HD21	2.04	0.40
2:D:92:VAL:HG21	2:D:124:VAL:HG12	2.03	0.40
1:A:722:LEU:HD22	1:A:766:THR:HG22	2.03	0.40
1:B:21:ASP:HA	1:B:22:PRO:HD3	1.88	0.40
1:B:344:ASN:HB2	2:D:140:ARG:HH11	1.87	0.40
1:A:805:THR:HG22	1:A:818:ARG:HD2	2.03	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	857/923 (93%)	834 (97%)	23 (3%)	0	100	100
1	B	717/923 (78%)	701 (98%)	16 (2%)	0	100	100
2	C	167/215 (78%)	163 (98%)	4 (2%)	0	100	100
2	D	171/215 (80%)	166 (97%)	5 (3%)	0	100	100
All	All	1912/2276 (84%)	1864 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	779/798 (98%)	768 (99%)	11 (1%)	74	90
1	B	671/798 (84%)	661 (98%)	10 (2%)	72	90
2	C	149/184 (81%)	144 (97%)	5 (3%)	44	79
2	D	154/184 (84%)	148 (96%)	6 (4%)	39	76
All	All	1753/1964 (89%)	1721 (98%)	32 (2%)	66	88

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	209	PHE
1	A	282	MSE
1	A	395	ASP
1	A	459	LEU
1	A	546	ARG
1	A	584	LEU
1	A	667	ARG
1	A	759	PHE
1	A	916	ARG
1	B	65	GLN
1	B	198	LEU
1	B	209	PHE
1	B	395	ASP
1	B	584	LEU
1	B	667	ARG
1	B	759	PHE
1	B	837	LEU
1	B	893	LYS
1	B	916	ARG
2	C	38	LYS
2	C	93	THR
2	C	95	ARG
2	C	139	HIS
2	C	141	LYS
2	D	38	LYS
2	D	93	THR
2	D	95	ARG
2	D	139	HIS
2	D	141	LYS
2	D	186	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	C	1179	3	25,34,34	0.92	1 (4%)	34,54,54	1.83	7 (20%)
4	GTP	D	1190	3	25,34,34	0.94	1 (4%)	34,54,54	1.99	7 (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
4	GTP	C	1179	3	-	0/18/38/38	0/3/3/3
4	GTP	D	1190	3	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1179	GTP	C6-N1	2.76	1.38	1.33
4	D	1190	GTP	C6-N1	2.79	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1190	GTP	PA-O3A-PB	-5.86	116.27	132.73
4	C	1179	GTP	PA-O3A-PB	-4.92	118.90	132.73
4	D	1190	GTP	N3-C2-N1	-4.73	120.24	127.44
4	C	1179	GTP	N3-C2-N1	-4.69	120.31	127.44
4	D	1190	GTP	PB-O3B-PG	-4.07	119.02	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1179	GTP	PB-O3B-PG	-3.97	119.37	132.67
4	D	1190	GTP	C2'-C1'-N9	-3.59	108.81	114.29
4	D	1190	GTP	C5-C6-N1	-2.93	119.58	123.59
4	C	1179	GTP	C5-C6-N1	-2.85	119.69	123.59
4	C	1179	GTP	C2'-C1'-N9	-2.62	110.30	114.29
4	C	1179	GTP	C6-N1-C2	2.69	119.67	115.94
4	C	1179	GTP	C4'-O4'-C1'	2.72	112.70	109.72
4	D	1190	GTP	C4'-O4'-C1'	2.74	112.73	109.72
4	D	1190	GTP	C6-N1-C2	2.80	119.82	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1179	GTP	1	0
4	D	1190	GTP	2	0

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	849/923 (91%)	0.53	58 (6%) 20 19	59, 130, 186, 206	0
1	B	729/923 (78%)	1.01	142 (19%) 1 2	92, 172, 210, 232	0
2	C	169/215 (78%)	0.70	14 (8%) 14 14	62, 104, 148, 158	0
2	D	175/215 (81%)	0.43	6 (3%) 49 44	65, 89, 119, 134	0
All	All	1922/2276 (84%)	0.72	220 (11%) 7 7	59, 139, 200, 232	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	662	CYS	7.2
1	B	431	ASN	6.4
1	B	765	VAL	6.1
1	B	670	VAL	5.5
1	B	863	VAL	5.3
1	B	702	TYR	5.3
1	B	918	PHE	5.3
2	C	161	PHE	5.3
1	B	414	ILE	5.0
1	B	47	SER	4.9
1	B	615	LEU	4.8
1	B	269	LEU	4.8
1	B	459	LEU	4.7
1	B	215	ASP	4.7
1	B	648	THR	4.7
1	B	751	ASP	4.6
1	A	11	VAL	4.6
1	B	842	CYS	4.6
1	B	498	PHE	4.5
1	B	310	ILE	4.5
1	A	310	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	318	LEU	4.4
1	B	458	THR	4.4
1	B	322	ARG	4.3
1	B	44	TRP	4.3
1	B	306	PHE	4.3
1	B	365	PHE	4.3
1	B	658	ILE	4.2
1	B	184	LEU	4.2
1	B	410	LEU	4.2
2	C	158	GLU	4.2
1	A	419	CYS	4.1
1	B	828	GLN	4.1
1	B	804	HIS	4.0
1	B	802	LEU	4.0
1	A	652	HIS	4.0
1	B	5	LYS	3.9
1	B	860	ILE	3.9
1	B	78	LEU	3.9
1	A	430	GLY	3.9
1	B	806	GLY	3.9
1	B	824	GLN	3.9
1	B	843	PHE	3.8
1	B	308	GLU	3.8
1	B	75	PHE	3.8
1	A	572	LEU	3.7
1	B	315	GLY	3.7
1	A	459	LEU	3.7
1	B	411	ILE	3.6
1	B	777	LEU	3.6
1	B	838	LEU	3.6
1	A	769	ARG	3.5
1	B	666	LEU	3.5
2	C	169	ILE	3.5
1	B	822	ILE	3.5
1	B	786	LEU	3.5
1	A	8	LEU	3.5
1	B	647	GLU	3.5
1	B	799	LEU	3.5
1	B	324	LEU	3.4
2	C	162	LEU	3.4
1	B	320	ASP	3.4
1	B	752	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	485	VAL	3.3
1	B	187	CYS	3.3
1	B	645	LEU	3.3
1	A	60	CYS	3.3
1	B	621	HIS	3.3
2	C	59	ILE	3.3
1	A	5	LYS	3.2
1	B	216	SER	3.2
1	B	487	GLU	3.2
1	A	410	LEU	3.2
1	B	11	VAL	3.2
2	C	165	ALA	3.2
1	B	323	THR	3.2
1	B	864	ASP	3.1
1	B	265	LEU	3.1
1	B	608	PRO	3.1
1	B	759	PHE	3.1
1	B	168	GLU	3.0
1	B	65	GLN	3.0
1	A	53	ILE	3.0
1	B	725	LEU	3.0
1	B	97	LEU	3.0
1	B	592	LEU	2.9
1	B	346	TRP	2.9
1	A	46	ILE	2.9
1	A	533	HIS	2.9
1	B	669	ALA	2.9
1	A	414	ILE	2.9
1	B	700	PHE	2.9
1	B	834	VAL	2.9
1	B	6	PRO	2.9
1	B	141	PRO	2.9
1	B	204	CYS	2.9
1	B	413	LEU	2.9
1	B	837	LEU	2.9
1	A	711	TYR	2.9
1	A	565	THR	2.8
2	C	112	CYS	2.8
1	B	152	GLU	2.8
1	A	311	VAL	2.8
1	B	201	VAL	2.8
1	B	74	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	413	LEU	2.8
1	B	581	LEU	2.8
1	B	259	VAL	2.8
1	B	321	LEU	2.7
1	B	757	THR	2.7
1	B	427	LEU	2.7
1	B	248	CYS	2.7
1	B	468	ARG	2.7
1	A	43	ALA	2.7
1	B	353	LEU	2.7
1	B	462	VAL	2.7
2	C	58	PRO	2.6
1	A	142	PHE	2.6
1	A	330	CYS	2.6
1	B	479	TYR	2.6
1	B	649	LEU	2.6
1	B	380	CYS	2.6
1	A	429	GLU	2.6
1	A	12	TYR	2.6
1	B	407	VAL	2.5
1	B	208	TRP	2.5
1	B	657	ARG	2.5
1	B	821	LEU	2.5
1	B	115	LEU	2.5
1	A	9	GLN	2.5
1	B	773	VAL	2.5
1	B	515	LEU	2.5
2	D	84	GLN	2.5
2	D	142	LYS	2.5
1	B	198	LEU	2.4
1	A	265	LEU	2.4
1	B	652	HIS	2.4
1	B	409	ASP	2.4
1	A	424	TYR	2.4
1	A	353	LEU	2.4
1	B	829	LEU	2.4
2	D	35	PHE	2.4
1	B	408	LYS	2.4
1	A	308	GLU	2.4
1	B	618	ILE	2.4
1	A	443	ILE	2.4
1	A	458	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	270	PHE	2.4
1	B	728	LEU	2.4
1	A	307	LEU	2.4
1	A	645	LEU	2.4
1	B	406	LEU	2.4
1	B	801	ASP	2.4
1	B	349	LEU	2.4
1	B	872	LEU	2.4
1	A	45	GLU	2.3
1	A	169	ILE	2.3
2	C	87	ILE	2.3
1	B	651	LYS	2.3
1	B	442	PHE	2.3
1	B	307	LEU	2.3
1	B	805	THR	2.3
1	B	643	PRO	2.3
1	B	526	ILE	2.3
1	B	430	GLY	2.3
2	C	116	PRO	2.3
1	B	287	GLU	2.3
2	D	95	ARG	2.3
1	B	383	GLU	2.3
1	A	527	CYS	2.3
1	B	246	SER	2.3
1	A	499	LEU	2.2
1	B	209	PHE	2.2
1	B	224	LEU	2.2
1	A	51	LEU	2.2
1	B	594	LYS	2.2
1	B	795	VAL	2.2
1	A	117	LEU	2.2
1	B	798	PHE	2.2
1	B	761	GLN	2.2
1	B	319	GLY	2.2
1	B	756	ALA	2.2
2	C	141	LYS	2.2
1	A	677	SER	2.2
1	B	244	ALA	2.2
1	B	654	ALA	2.2
1	B	50	LEU	2.2
1	A	841	CYS	2.2
1	B	400	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	416	SER	2.2
1	B	780	ALA	2.2
1	A	551	PHE	2.2
1	B	390	PRO	2.1
2	C	113	GLU	2.1
1	A	569	LEU	2.1
1	B	118	GLN	2.1
1	B	309	LYS	2.1
1	A	76	TYR	2.1
1	A	437	THR	2.1
1	A	480	THR	2.1
2	D	103	ASN	2.1
2	D	79	TYR	2.1
1	A	510	LEU	2.1
1	B	334	PRO	2.1
1	A	451	VAL	2.1
1	A	223	LYS	2.1
1	A	124	GLY	2.1
1	B	243	GLU	2.1
1	B	283	ALA	2.1
2	C	77	ASP	2.1
1	A	611	PHE	2.1
1	A	868	PHE	2.0
1	B	51	LEU	2.0
1	A	827	ASN	2.0
1	B	158	SER	2.0
2	C	114	ASN	2.0
1	B	247	ASP	2.0
1	A	369	ILE	2.0
1	A	593	LYS	2.0
1	A	671	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	GTP	C	1179	32/32	0.94	0.27	0.47	66,80,93,95	0
4	GTP	D	1190	32/32	0.93	0.24	-0.36	63,73,86,87	0
3	MG	D	1189	1/1	0.96	0.21	-0.55	68,68,68,68	0
3	MG	C	1178	1/1	0.89	0.39	-	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.