



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 AM GMT

PDB ID : 2X19  
Title : CRYSTAL STRUCTURE OF IMPORTIN13 - RANGTP COMPLEX  
Authors : Bono, F.; Cook, A.G.; Gruenwald, M.; Ebert, J.; Conti, E.  
Deposited on : 2009-12-23  
Resolution : 2.80 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](mailto: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.

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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

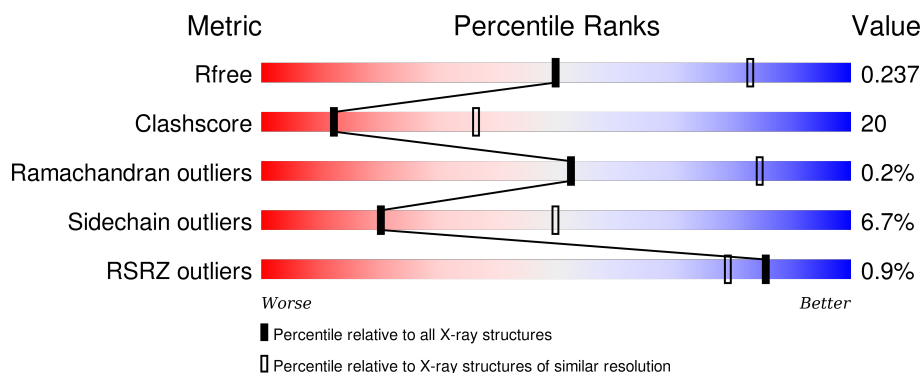
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	172	 66% 28% 5%
2	B	963	 62% 30% 6%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8440 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 GTP-BINDING NUCLEAR PROTEIN GSP1/CNR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1372	892	231	245	4			

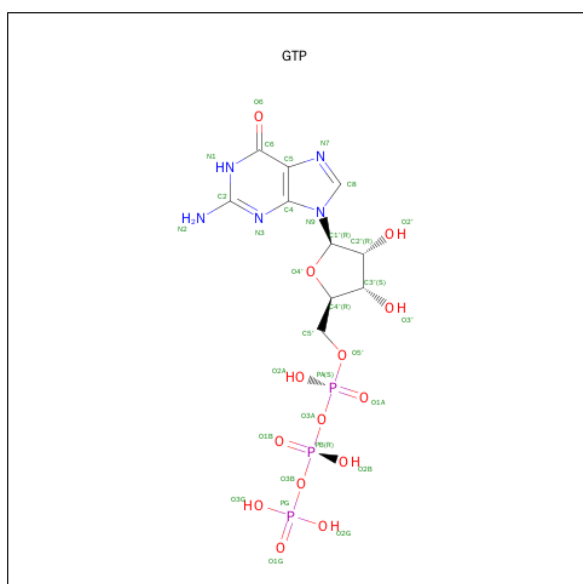
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	GLN	ENGINEERED MUTATION	UNP P32835

- Molecule 2 is a protein called IMPORTIN-13.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	907	Total	C	N	O	S	Se	0	0	1
			6977	4505	1159	1270	21	22			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: 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		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

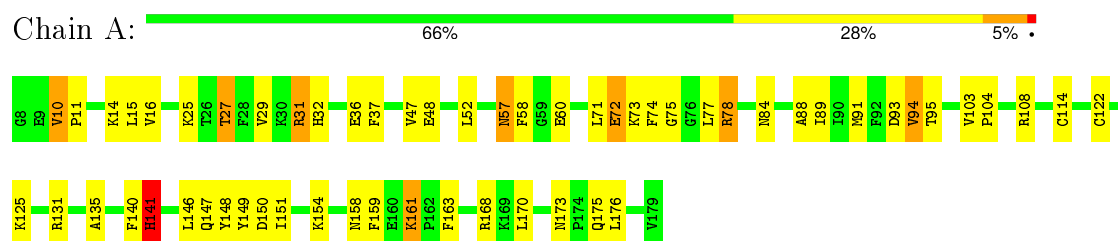
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	42	Total	O	0	0
			42	42		

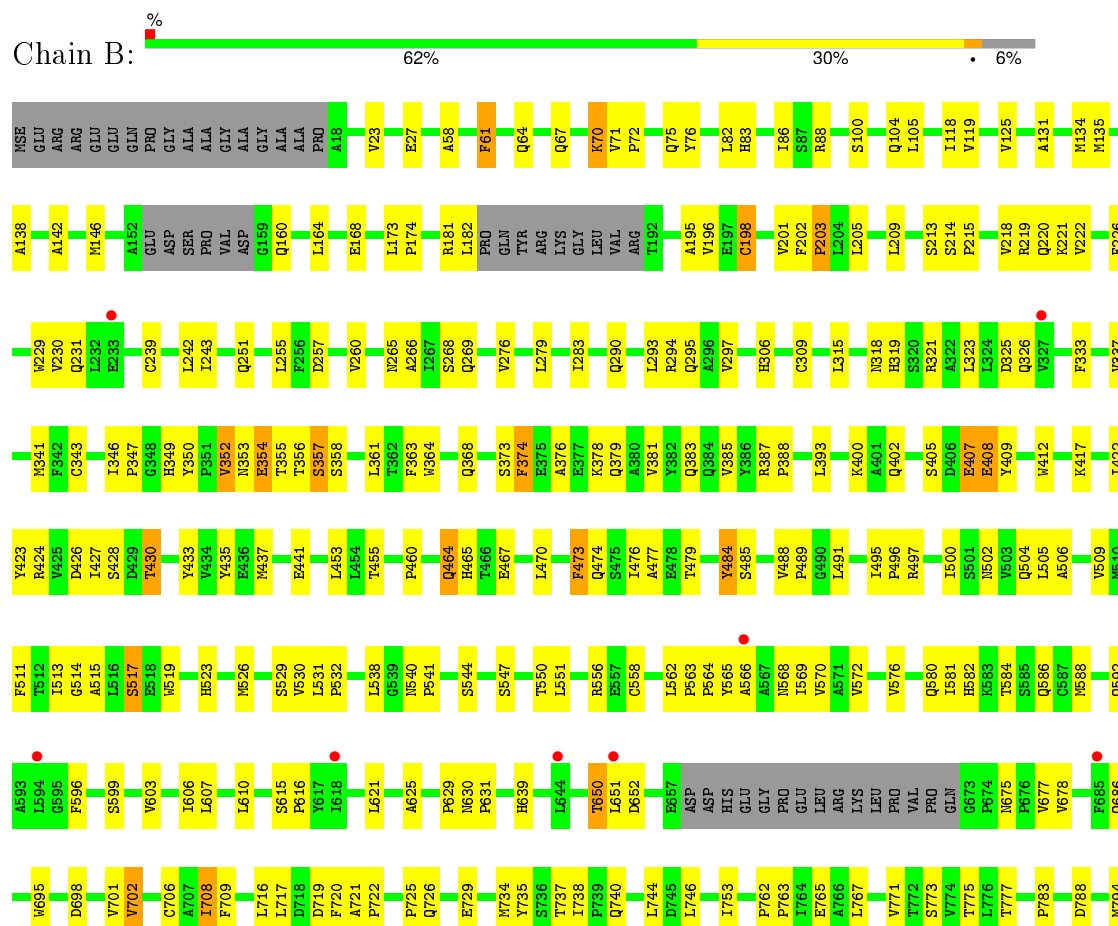
### 3 Residue-property plots

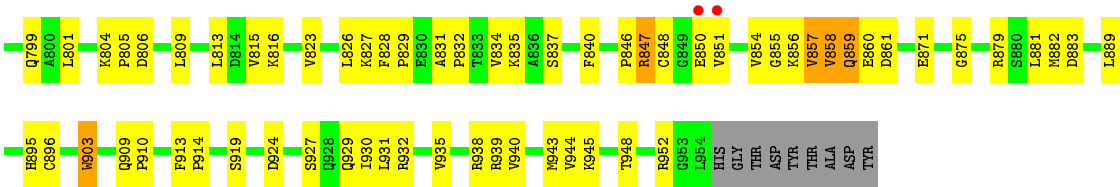
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: GTP-BINDING NUCLEAR PROTEIN GSP1/CNR1



#### • Molecule 2: IMPORTIN-13





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.93Å 99.93Å 276.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 49.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.80) 99.7 (49.97-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.44 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.236 , 0.268 0.232 , 0.237	Depositor DCC
$R_{free}$ test set	2022 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 51.1	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 40301 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.47	0/1407	0.68	0/1906
2	B	0.44	0/7109	0.64	2/9659 (0.0%)
All	All	0.44	0/8516	0.64	2/11565 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	460	PRO	N-CA-CB	6.37	110.94	103.30
2	B	629	PRO	N-CA-CB	5.43	109.81	103.30

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	1372	0	1342	60	0
2	B	6977	0	6839	274	0
3	A	32	0	12	5	0
4	A	1	0	0	0	0
5	A	16	0	0	1	0
5	B	42	0	0	9	0
All	All	8440	0	8193	327	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 20.

All (327) 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:78:ARG:NH2	2:B:88:ARG:HD3	1.66	1.10
2:B:815:VAL:HG21	2:B:854:VAL:HG11	1.35	1.03
1:A:78:ARG:HH22	2:B:88:ARG:HD3	1.17	1.00
2:B:290:GLN:HE21	2:B:294:ARG:HE	1.05	0.95
1:A:78:ARG:HH12	2:B:88:ARG:NH1	1.64	0.94
2:B:368:GLN:HG2	2:B:433:TYR:CE2	2.04	0.93
2:B:513:ILE:HD13	2:B:530:VAL:HG13	1.54	0.90
2:B:464:GLN:HE21	2:B:464:GLN:H	1.16	0.89
2:B:485:SER:O	2:B:489:PRO:HD2	1.74	0.87
1:A:10:VAL:HG12	1:A:11:PRO:HD2	1.55	0.86
1:A:78:ARG:HH22	2:B:88:ARG:CD	1.88	0.86
2:B:854:VAL:O	2:B:857:VAL:HG12	1.76	0.86
2:B:290:GLN:NE2	2:B:294:ARG:HE	1.76	0.82
2:B:794:MSE:CE	2:B:837:SER:HA	2.10	0.82
2:B:354:GLU:CD	2:B:357:SER:HB3	2.00	0.81
1:A:78:ARG:HD3	1:A:78:ARG:H	1.44	0.81
2:B:716:LEU:O	2:B:716:LEU:HD12	1.81	0.80
2:B:488:VAL:HB	2:B:489:PRO:HD3	1.61	0.80
2:B:815:VAL:HG21	2:B:854:VAL:CG1	2.14	0.78
1:A:75:GLY:HA3	1:A:78:ARG:HH11	1.48	0.77
2:B:474:GLN:NE2	2:B:511:PHE:HB3	1.99	0.76
2:B:131:ALA:O	2:B:135:MSE:HB2	1.86	0.75
2:B:290:GLN:HE21	2:B:294:ARG:NE	1.82	0.74
2:B:716:LEU:CD1	2:B:720:PHE:HB2	2.18	0.74
2:B:773:SER:O	2:B:777:THR:HG23	1.87	0.73
2:B:361:LEU:HD22	2:B:430:THR:HG21	1.69	0.72
2:B:257:ASP:O	2:B:260:VAL:HG12	1.89	0.72
2:B:488:VAL:HG11	2:B:519:TRP:CD2	2.24	0.72
2:B:737:THR:HG22	2:B:738:ILE:HG13	1.72	0.71
2:B:783:PRO:O	2:B:828:PHE:CZ	2.44	0.71
1:A:75:GLY:HA3	1:A:78:ARG:NH1	2.05	0.71
2:B:488:VAL:HG11	2:B:519:TRP:CE2	2.26	0.71
1:A:27:THR:OG1	3:A:1181:GTP:H5"	1.91	0.71
2:B:201:VAL:HG21	2:B:229:TRP:CZ2	2.26	0.71
2:B:519:TRP:O	2:B:523:HIS:HD2	1.74	0.71
2:B:455:THR:CB	2:B:497:ARG:HH12	2.04	0.71
2:B:407:GLU:HG2	5:B:2020:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:913:PHE:HB3	2:B:914:PRO:HD3	1.73	0.70
2:B:592:GLN:O	2:B:650:THR:HG21	1.91	0.69
2:B:464:GLN:NE2	2:B:464:GLN:H	1.88	0.69
2:B:502:ASN:HD21	2:B:504:GLN:HB2	1.56	0.69
2:B:815:VAL:HG11	2:B:854:VAL:HG12	1.74	0.69
2:B:829:PRO:HG2	5:B:2033:HOH:O	1.93	0.69
2:B:603:VAL:O	2:B:607:LEU:HG	1.93	0.69
2:B:142:ALA:O	2:B:146:MSE:HG3	1.92	0.69
2:B:794:MSE:HE3	2:B:837:SER:HA	1.74	0.69
2:B:794:MSE:HE2	2:B:837:SER:HA	1.74	0.68
2:B:502:ASN:ND2	2:B:504:GLN:HB2	2.09	0.68
2:B:562:LEU:N	2:B:563:PRO:CD	2.55	0.68
2:B:721:ALA:HB3	2:B:722:PRO:HD3	1.76	0.68
2:B:940:VAL:O	2:B:944:VAL:HG23	1.93	0.68
1:A:47:VAL:HG22	1:A:48:GLU:N	2.08	0.68
2:B:599:SER:HB2	2:B:652:ASP:O	1.93	0.68
2:B:455:THR:CB	2:B:497:ARG:HH22	2.07	0.67
1:A:75:GLY:CA	1:A:78:ARG:HH11	2.07	0.67
2:B:134:MSE:HB2	2:B:138:ALA:HB3	1.77	0.67
2:B:726:GLN:HG3	5:B:2032:HOH:O	1.92	0.67
2:B:376:ALA:HA	2:B:379:GLN:HB3	1.75	0.67
2:B:804:LYS:HE2	2:B:806:ASP:OD1	1.95	0.66
2:B:368:GLN:NE2	2:B:437:MSE:HB2	2.11	0.66
2:B:474:GLN:HE21	2:B:511:PHE:HB3	1.61	0.65
2:B:735:TYR:OH	2:B:775:THR:HG22	1.97	0.65
2:B:426:ASP:O	2:B:430:THR:HG22	1.96	0.65
1:A:31:ARG:HB3	1:A:159:PHE:HZ	1.61	0.65
1:A:78:ARG:NH1	2:B:88:ARG:NH1	2.42	0.64
1:A:57:ASN:HD22	1:A:57:ASN:N	1.94	0.64
2:B:675:ASN:HD22	2:B:678:VAL:H	1.45	0.64
2:B:215:PRO:O	2:B:219:ARG:HG3	1.98	0.64
2:B:239:CYS:O	2:B:243:ILE:HG12	1.98	0.63
2:B:464:GLN:HE21	2:B:464:GLN:N	1.93	0.63
2:B:479:THR:O	2:B:479:THR:HG22	1.99	0.62
2:B:484:TYR:CD2	2:B:484:TYR:N	2.67	0.62
2:B:716:LEU:HD12	2:B:720:PHE:HB2	1.81	0.62
2:B:453:LEU:HD22	2:B:465:HIS:HD2	1.65	0.61
2:B:855:GLY:CA	5:B:2040:HOH:O	2.47	0.61
2:B:58:ALA:HA	2:B:61:PHE:CE2	2.35	0.61
2:B:930:ILE:HB	2:B:943:MSE:HE1	1.82	0.61
2:B:584:THR:O	2:B:588:MSE:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLU:HG2	2:B:354:GLU:O	1.99	0.61
2:B:283:ILE:HD11	2:B:323:LEU:HD22	1.81	0.60
2:B:325:ASP:OD1	2:B:378:LYS:NZ	2.35	0.60
2:B:387:ARG:N	2:B:388:PRO:HD2	2.15	0.60
2:B:794:MSE:HE3	2:B:840:PHE:HB3	1.81	0.60
2:B:855:GLY:HA3	5:B:2040:HOH:O	2.01	0.60
2:B:218:VAL:O	2:B:222:VAL:HG23	2.02	0.60
2:B:435:TYR:HE1	2:B:479:THR:O	1.85	0.60
2:B:799:GLN:NE2	2:B:799:GLN:HA	2.17	0.59
1:A:31:ARG:HB3	1:A:159:PHE:CZ	2.36	0.59
3:A:1181:GTP:O2B	5:A:2016:HOH:O	2.16	0.59
2:B:827:LYS:HZ1	2:B:871:GLU:HB2	1.67	0.59
2:B:514:GLY:O	2:B:517:SER:HB2	2.03	0.59
2:B:349:HIS:HE1	2:B:402:GLN:O	1.85	0.59
1:A:72:GLU:OE2	2:B:88:ARG:HD2	2.04	0.58
1:A:57:ASN:H	1:A:57:ASN:ND2	2.01	0.58
2:B:847:ARG:HD3	2:B:850:GLU:HG2	1.85	0.58
2:B:859:GLN:N	2:B:859:GLN:OE1	2.37	0.58
2:B:71:VAL:O	2:B:75:GLN:HG3	2.04	0.58
2:B:514:GLY:CA	2:B:550:THR:HG23	2.33	0.57
2:B:801:LEU:O	2:B:805:PRO:HG3	2.04	0.57
2:B:556:ARG:HB2	2:B:596:PHE:CE1	2.39	0.57
2:B:226:PHE:O	2:B:230:VAL:HG23	2.05	0.57
2:B:939:ARG:O	2:B:943:MSE:HG2	2.03	0.57
1:A:131:ARG:HH22	1:A:150:ASP:CG	2.08	0.57
2:B:195:ALA:O	2:B:198:CYS:HB3	2.04	0.57
2:B:783:PRO:O	2:B:828:PHE:HZ	1.86	0.57
1:A:10:VAL:HG11	1:A:60:GLU:O	2.04	0.56
1:A:158:ASN:OD1	1:A:161:LYS:HE3	2.04	0.56
2:B:599:SER:HB3	2:B:651:LEU:HD12	1.86	0.56
2:B:215:PRO:HD2	2:B:218:VAL:CG2	2.36	0.56
2:B:268:SER:HA	2:B:318:ASN:ND2	2.20	0.56
2:B:882:MSE:HE2	2:B:882:MSE:HA	1.85	0.56
2:B:354:GLU:OE1	2:B:357:SER:HB3	2.04	0.56
2:B:606:ILE:O	2:B:610:LEU:HB2	2.05	0.56
2:B:368:GLN:NE2	2:B:433:TYR:O	2.38	0.56
2:B:827:LYS:NZ	2:B:871:GLU:HB2	2.20	0.56
2:B:855:GLY:O	2:B:858:VAL:HG23	2.06	0.56
2:B:424:ARG:NH2	2:B:467:GLU:OE1	2.31	0.56
1:A:57:ASN:ND2	1:A:58:PHE:HD2	2.04	0.55
2:B:675:ASN:HD21	2:B:677:VAL:HB	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:PHE:CD2	2:B:491:LEU:HD22	2.41	0.55
1:A:57:ASN:N	1:A:57:ASN:ND2	2.53	0.55
2:B:23:VAL:CG2	2:B:64:GLN:OE1	2.55	0.55
2:B:675:ASN:ND2	2:B:677:VAL:HB	2.22	0.55
2:B:675:ASN:HD22	2:B:678:VAL:HG23	1.71	0.55
2:B:83:HIS:CD2	2:B:125:VAL:HG12	2.43	0.54
2:B:500:ILE:O	2:B:500:ILE:HG22	2.08	0.54
2:B:500:ILE:HG23	2:B:506:ALA:HB2	1.89	0.54
2:B:100:SER:O	2:B:104:GLN:HG3	2.07	0.54
2:B:427:ILE:HA	2:B:430:THR:HG23	1.89	0.54
2:B:805:PRO:HG2	2:B:847:ARG:HD2	1.88	0.54
2:B:513:ILE:HG23	2:B:530:VAL:HG11	1.89	0.54
2:B:909:GLN:N	2:B:910:PRO:HD2	2.22	0.54
2:B:381:VAL:O	2:B:385:VAL:HG23	2.08	0.54
2:B:23:VAL:HG23	2:B:64:GLN:OE1	2.08	0.54
2:B:350:TYR:HB2	2:B:423:TYR:CZ	2.43	0.54
2:B:767:LEU:O	2:B:771:VAL:HG23	2.07	0.54
1:A:57:ASN:HD21	1:A:176:LEU:HA	1.72	0.53
2:B:675:ASN:HB3	2:B:678:VAL:HG23	1.91	0.53
2:B:856:LYS:HD3	2:B:859:GLN:HB2	1.90	0.53
2:B:368:GLN:HG2	2:B:433:TYR:CD2	2.44	0.53
2:B:855:GLY:HA2	5:B:2040:HOH:O	2.09	0.53
2:B:164:LEU:HD22	2:B:221:LYS:HD2	1.90	0.53
2:B:538:LEU:HD12	2:B:547:SER:OG	2.09	0.53
2:B:846:PRO:HA	2:B:895:HIS:ND1	2.23	0.53
2:B:562:LEU:N	2:B:563:PRO:HD3	2.24	0.53
1:A:131:ARG:HH12	1:A:135:ALA:HB2	1.74	0.53
2:B:231:GLN:HA	2:B:269:GLN:HE22	1.73	0.52
2:B:27:GLU:OE2	2:B:70:LYS:HD2	2.09	0.52
2:B:306:HIS:CD2	2:B:355:THR:HG22	2.45	0.52
2:B:346:ILE:HD12	2:B:356:THR:HB	1.90	0.52
2:B:485:SER:O	2:B:489:PRO:CD	2.53	0.52
1:A:10:VAL:CG1	1:A:11:PRO:HD2	2.33	0.52
2:B:201:VAL:HG21	2:B:229:TRP:CE2	2.45	0.52
2:B:455:THR:CA	2:B:497:ARG:HH22	2.23	0.51
1:A:47:VAL:CG2	1:A:48:GLU:N	2.73	0.51
1:A:125:LYS:HG2	3:A:1181:GTP:C6	2.45	0.51
2:B:596:PHE:CD2	2:B:650:THR:HG22	2.45	0.51
2:B:82:LEU:O	2:B:86:ILE:HG13	2.10	0.51
1:A:173:ASN:OD1	1:A:175:GLN:HB2	2.10	0.51
2:B:198:CYS:HB2	2:B:229:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:ILE:HG22	2:B:709:PHE:N	2.25	0.51
1:A:78:ARG:HH12	2:B:88:ARG:HH12	1.54	0.51
2:B:762:PRO:HB2	2:B:763:PRO:HD3	1.92	0.51
2:B:630:ASN:HB2	2:B:631:PRO:HD2	1.92	0.51
2:B:850:GLU:O	2:B:850:GLU:HG3	2.11	0.51
2:B:76:TYR:HA	2:B:119:VAL:HG22	1.93	0.51
1:A:131:ARG:NH1	1:A:135:ALA:H	2.09	0.51
1:A:141:HIS:N	1:A:141:HIS:ND1	2.52	0.50
2:B:805:PRO:CG	2:B:847:ARG:HD2	2.41	0.50
1:A:15:LEU:HD21	1:A:89:ILE:HG13	1.94	0.50
2:B:939:ARG:NH1	2:B:943:MSE:HB3	2.26	0.50
2:B:675:ASN:HB3	2:B:678:VAL:CG2	2.42	0.50
2:B:584:THR:HG22	2:B:639:HIS:CE1	2.47	0.50
2:B:61:PHE:C	2:B:61:PHE:CD1	2.86	0.50
2:B:848:CYS:HB3	2:B:856:LYS:HE3	1.93	0.50
2:B:831:ALA:N	2:B:832:PRO:HD2	2.26	0.50
1:A:140:PHE:CZ	1:A:146:LEU:HD22	2.47	0.49
2:B:615:SER:N	2:B:616:PRO:HD2	2.27	0.49
2:B:788:ASP:HB3	5:B:2034:HOH:O	2.12	0.49
2:B:717:LEU:O	2:B:753:ILE:HG21	2.11	0.49
1:A:75:GLY:C	1:A:78:ARG:HH11	2.16	0.49
2:B:513:ILE:HD13	2:B:530:VAL:CG1	2.34	0.49
2:B:349:HIS:H	2:B:353:ASN:HD22	1.61	0.49
2:B:584:THR:HG22	2:B:639:HIS:ND1	2.27	0.49
2:B:294:ARG:HG2	2:B:294:ARG:HH11	1.77	0.49
2:B:834:VAL:HG11	2:B:881:LEU:HD13	1.95	0.49
1:A:93:ASP:CG	1:A:125:LYS:HD2	2.32	0.49
2:B:306:HIS:CD2	2:B:355:THR:CG2	2.96	0.49
2:B:531:LEU:N	2:B:532:PRO:HD2	2.27	0.49
2:B:562:LEU:H	2:B:563:PRO:HD3	1.78	0.49
2:B:355:THR:O	2:B:355:THR:HG22	2.12	0.49
2:B:857:VAL:CG1	2:B:858:VAL:N	2.76	0.48
1:A:168:ARG:HA	1:A:176:LEU:HD12	1.94	0.48
2:B:294:ARG:HG2	2:B:294:ARG:NH1	2.28	0.48
2:B:168:GLU:OE1	2:B:168:GLU:HA	2.13	0.48
2:B:930:ILE:CA	2:B:943:MSE:HE1	2.42	0.48
2:B:319:HIS:O	2:B:323:LEU:HG	2.14	0.48
2:B:544:SER:OG	2:B:586:GLN:HG2	2.12	0.48
1:A:103:VAL:HB	1:A:104:PRO:HD3	1.96	0.48
2:B:470:LEU:HD21	2:B:509:VAL:HA	1.95	0.48
2:B:544:SER:HB2	2:B:582:HIS:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:ARG:HH22	2:B:373:SER:CB	2.26	0.48
2:B:333:PHE:O	2:B:337:VAL:HG23	2.14	0.48
2:B:354:GLU:CG	2:B:354:GLU:O	2.61	0.48
2:B:276:VAL:HA	2:B:279:LEU:HD12	1.95	0.48
1:A:93:ASP:OD1	1:A:95:THR:OG1	2.29	0.47
2:B:484:TYR:H	2:B:484:TYR:HD2	1.61	0.47
2:B:799:GLN:HE21	2:B:799:GLN:HA	1.78	0.47
2:B:226:PHE:CD1	2:B:242:LEU:HD13	2.49	0.47
2:B:930:ILE:CB	2:B:943:MSE:HE1	2.45	0.47
2:B:835:LYS:HG3	2:B:881:LEU:CD2	2.44	0.47
2:B:181:ARG:O	2:B:182:LEU:CB	2.62	0.47
1:A:73:LYS:HE3	1:A:74:PHE:CE2	2.50	0.47
2:B:686:GLN:CD	2:B:686:GLN:H	2.17	0.47
2:B:474:GLN:NE2	2:B:511:PHE:CB	2.74	0.47
2:B:889:LEU:HD22	2:B:930:ILE:HD11	1.96	0.47
2:B:346:ILE:HG23	2:B:347:PRO:HD2	1.97	0.47
2:B:464:GLN:NE2	2:B:464:GLN:N	2.60	0.46
2:B:848:CYS:SG	2:B:859:GLN:NE2	2.89	0.46
2:B:735:TYR:OH	2:B:775:THR:CG2	2.63	0.46
2:B:576:VAL:HG11	2:B:582:HIS:CE1	2.50	0.46
2:B:581:ILE:HG22	2:B:582:HIS:CD2	2.50	0.46
2:B:321:ARG:NH2	2:B:373:SER:OG	2.48	0.46
2:B:220:GLN:HG3	2:B:255:LEU:HD23	1.98	0.46
2:B:565:TYR:O	2:B:569:ILE:HG13	2.15	0.46
1:A:93:ASP:OD1	1:A:125:LYS:HD2	2.15	0.46
2:B:675:ASN:ND2	2:B:678:VAL:HG23	2.31	0.46
2:B:513:ILE:CG2	2:B:530:VAL:HG11	2.46	0.46
1:A:47:VAL:HG22	1:A:48:GLU:H	1.79	0.46
2:B:505:LEU:O	2:B:509:VAL:HG23	2.16	0.46
2:B:568:ASN:O	2:B:572:VAL:HG23	2.15	0.46
1:A:14:LYS:HD3	1:A:84:ASN:O	2.15	0.46
2:B:815:VAL:HG11	2:B:854:VAL:CG1	2.45	0.46
2:B:744:LEU:HD23	2:B:771:VAL:HG11	1.97	0.46
2:B:309:CYS:HB2	2:B:356:THR:HG23	1.98	0.45
2:B:695:TRP:CE3	2:B:701:VAL:HG21	2.50	0.45
2:B:363:PHE:C	2:B:363:PHE:CD2	2.87	0.45
2:B:341:MSE:HE1	2:B:393:LEU:HB2	1.99	0.45
1:A:16:VAL:HG22	1:A:88:ALA:HB2	1.97	0.45
2:B:854:VAL:O	2:B:858:VAL:HG22	2.17	0.45
1:A:94:VAL:HG21	1:A:131:ARG:HE	1.81	0.45
2:B:231:GLN:HA	2:B:269:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:SER:HB2	5:B:2020:HOH:O	2.16	0.45
2:B:350:TYR:CE1	2:B:358:SER:HB2	2.52	0.45
2:B:71:VAL:HG13	2:B:72:PRO:HD2	1.98	0.45
1:A:108:ARG:HH11	1:A:108:ARG:HG3	1.82	0.45
2:B:702:VAL:HG11	2:B:740:GLN:NE2	2.32	0.45
2:B:488:VAL:CB	2:B:489:PRO:HD3	2.39	0.45
2:B:725:PRO:HG2	5:B:2032:HOH:O	2.17	0.45
2:B:698:ASP:CG	2:B:701:VAL:HG23	2.37	0.45
2:B:827:LYS:HD3	2:B:827:LYS:HA	1.52	0.44
2:B:230:VAL:HG11	2:B:266:ALA:HA	1.98	0.44
1:A:25:LYS:O	1:A:29:VAL:HG23	2.17	0.44
2:B:293:LEU:O	2:B:297:VAL:HG23	2.18	0.44
1:A:91:MET:HE2	1:A:122:CYS:HB2	1.99	0.44
2:B:173:LEU:HB3	2:B:174:PRO:CD	2.47	0.44
2:B:363:PHE:HE2	2:B:364:TRP:CZ3	2.36	0.44
2:B:495:ILE:HB	2:B:496:PRO:HD3	1.99	0.44
2:B:488:VAL:HB	2:B:489:PRO:CD	2.39	0.44
2:B:563:PRO:N	2:B:564:PRO:HD2	2.32	0.44
1:A:158:ASN:CG	1:A:161:LYS:HE3	2.38	0.44
2:B:354:GLU:OE2	2:B:400:LYS:NZ	2.51	0.44
2:B:215:PRO:HD2	2:B:218:VAL:HG21	2.00	0.44
2:B:453:LEU:CD2	2:B:465:HIS:HD2	2.28	0.43
2:B:164:LEU:CD2	2:B:221:LYS:HD2	2.48	0.43
2:B:903:TRP:HA	2:B:903:TRP:HE3	1.83	0.43
2:B:349:HIS:CE1	2:B:402:GLN:O	2.67	0.43
2:B:903:TRP:HA	2:B:903:TRP:CE3	2.53	0.43
2:B:939:ARG:HH12	2:B:943:MSE:HB3	1.83	0.43
1:A:125:LYS:HE2	3:A:1181:GTP:C4	2.54	0.43
1:A:122:CYS:HB3	1:A:151:ILE:HG12	2.00	0.43
2:B:435:TYR:HB2	2:B:476:ILE:HD13	2.01	0.43
2:B:387:ARG:N	2:B:388:PRO:CD	2.78	0.43
2:B:927:SER:O	2:B:931:LEU:HG	2.19	0.43
2:B:725:PRO:O	2:B:729:GLU:HG3	2.19	0.43
2:B:544:SER:CB	2:B:582:HIS:HD2	2.32	0.43
2:B:566:ALA:O	2:B:570:VAL:HG23	2.19	0.43
2:B:857:VAL:O	2:B:860:GLU:HG2	2.18	0.42
2:B:858:VAL:C	2:B:860:GLU:H	2.22	0.42
2:B:621:LEU:O	2:B:625:ALA:N	2.51	0.42
1:A:78:ARG:HH21	2:B:88:ARG:HD3	1.73	0.42
1:A:125:LYS:HG2	3:A:1181:GTP:C5	2.54	0.42
2:B:592:GLN:HA	2:B:650:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:LEU:HD13	2:B:719:ASP:C	2.40	0.42
2:B:580:GLN:HA	2:B:580:GLN:OE1	2.20	0.42
1:A:77:LEU:O	1:A:78:ARG:C	2.56	0.42
2:B:374:PHE:O	2:B:379:GLN:HB2	2.20	0.42
2:B:265:ASN:O	2:B:269:GLN:HG2	2.20	0.42
2:B:363:PHE:HE2	2:B:364:TRP:CE3	2.38	0.42
2:B:409:TYR:CE2	2:B:417:LYS:HE2	2.55	0.42
2:B:596:PHE:CG	2:B:650:THR:HG22	2.55	0.42
2:B:343:CYS:HB3	2:B:356:THR:HG22	2.01	0.42
1:A:71:LEU:HD13	1:A:73:LYS:HE2	2.02	0.42
1:A:148:TYR:CG	1:A:149:TYR:N	2.88	0.42
2:B:540:ASN:HA	2:B:541:PRO:HD2	1.93	0.42
2:B:455:THR:CB	2:B:497:ARG:NH1	2.80	0.41
2:B:945:LYS:O	2:B:948:THR:HG22	2.19	0.41
2:B:794:MSE:HE2	2:B:837:SER:CA	2.44	0.41
2:B:500:ILE:CG2	2:B:506:ALA:HB2	2.50	0.41
2:B:209:LEU:O	2:B:219:ARG:NH2	2.48	0.41
2:B:823:VAL:O	2:B:826:LEU:HB2	2.20	0.41
2:B:526:MSE:HA	2:B:526:MSE:HE2	2.03	0.41
2:B:794:MSE:HE3	2:B:840:PHE:CB	2.48	0.41
2:B:716:LEU:HD11	2:B:720:PHE:HB2	2.01	0.41
2:B:913:PHE:CB	2:B:914:PRO:HD3	2.45	0.41
2:B:64:GLN:HA	2:B:67:GLN:NE2	2.36	0.41
2:B:544:SER:OG	2:B:582:HIS:CD2	2.73	0.41
1:A:37:PHE:CE2	1:A:154:LYS:HG3	2.55	0.41
2:B:706:CYS:SG	2:B:734:MSE:HE1	2.60	0.41
1:A:75:GLY:CA	1:A:78:ARG:NH1	2.75	0.41
2:B:205:LEU:HD22	2:B:222:VAL:HG13	2.02	0.41
2:B:879:ARG:HB3	2:B:879:ARG:HE	1.66	0.41
2:B:352:VAL:HG13	2:B:352:VAL:O	2.20	0.41
2:B:387:ARG:NH2	2:B:441:GLU:OE2	2.44	0.41
2:B:408:GLU:OE1	2:B:412:TRP:NE1	2.52	0.41
2:B:477:ALA:HB3	2:B:515:ALA:HB1	2.02	0.41
2:B:929:GLN:HG2	2:B:932:ARG:NH2	2.36	0.41
1:A:93:ASP:OD2	1:A:125:LYS:HD2	2.21	0.40
2:B:383:GLN:NE2	2:B:387:ARG:HH11	2.18	0.40
2:B:875:GLY:HA2	2:B:952:ARG:CZ	2.51	0.40
1:A:147:GLN:HG3	1:A:148:TYR:N	2.36	0.40
2:B:105:LEU:HA	2:B:105:LEU:HD23	1.77	0.40
2:B:202:PHE:HB2	2:B:203:PRO:HD3	2.03	0.40
2:B:816:LYS:NZ	2:B:861:ASP:OD2	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:CE1	1:A:163:PHE:HE2	2.40	0.40
2:B:771:VAL:O	2:B:775:THR:HG23	2.22	0.40
2:B:118:ILE:HG13	2:B:118:ILE:H	1.65	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	170/172 (99%)	159 (94%)	10 (6%)	1 (1%)	30	65
2	B	899/963 (93%)	850 (94%)	48 (5%)	1 (0%)	56	87
All	All	1069/1135 (94%)	1009 (94%)	58 (5%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
2	B	851	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/150 (95%)	130 (91%)	13 (9%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	738/824 (90%)	692 (94%)	46 (6%)	23	54
All	All	881/974 (90%)	822 (93%)	59 (7%)	20	50

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	27	THR
1	A	31	ARG
1	A	36	GLU
1	A	52	LEU
1	A	57	ASN
1	A	72	GLU
1	A	78	ARG
1	A	94	VAL
1	A	114	CYS
1	A	141	HIS
1	A	161	LYS
1	A	170	LEU
2	B	61	PHE
2	B	70	LYS
2	B	160	GLN
2	B	196	VAL
2	B	198	CYS
2	B	203	PRO
2	B	213	SER
2	B	214	SER
2	B	251	GLN
2	B	295	GLN
2	B	315	LEU
2	B	326	GLN
2	B	352	VAL
2	B	354	GLU
2	B	357	SER
2	B	374	PHE
2	B	407	GLU
2	B	408	GLU
2	B	422	ILE
2	B	428	SER
2	B	430	THR
2	B	464	GLN
2	B	473	PHE

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Mol	Chain	Res	Type
2	B	484	TYR
2	B	517	SER
2	B	529	SER
2	B	551	LEU
2	B	558	CYS
2	B	650	THR
2	B	702	VAL
2	B	708	ILE
2	B	746	LEU
2	B	765	GLU
2	B	809	LEU
2	B	813	LEU
2	B	847	ARG
2	B	857	VAL
2	B	858	VAL
2	B	859	GLN
2	B	883	ASP
2	B	896	CYS
2	B	903	TRP
2	B	919	SER
2	B	924	ASP
2	B	935	VAL
2	B	938	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	57	ASN
1	A	102	ASN
2	B	25	ASN
2	B	67	GLN
2	B	83	HIS
2	B	151	GLN
2	B	211	GLN
2	B	220	GLN
2	B	290	GLN
2	B	292	GLN
2	B	295	GLN
2	B	299	ASN
2	B	349	HIS
2	B	353	ASN

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Mol	Chain	Res	Type
2	B	368	GLN
2	B	383	GLN
2	B	464	GLN
2	B	465	HIS
2	B	474	GLN
2	B	502	ASN
2	B	523	HIS
2	B	582	HIS
2	B	633	ASN
2	B	675	ASN
2	B	740	GLN
2	B	752	HIS
2	B	799	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	A	1181	4	25,34,34	1.52	2 (8%)	34,54,54	2.49	15 (44%)

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	A	1181	4	-	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)
3	A	1181	GTP	C6-N1	2.73	1.38	1.33
3	A	1181	GTP	O4'-C1'	4.09	1.46	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1181	GTP	PB-O3B-PG	-6.71	110.18	132.67
3	A	1181	GTP	PA-O3A-PB	-6.20	115.32	132.73
3	A	1181	GTP	C2'-C1'-N9	-4.63	107.22	114.29
3	A	1181	GTP	N3-C2-N1	-4.20	121.05	127.44
3	A	1181	GTP	C5-C6-N1	-3.69	118.54	123.59
3	A	1181	GTP	C6-C5-C4	-2.94	117.38	120.90
3	A	1181	GTP	C4-C5-N7	-2.46	107.22	109.48
3	A	1181	GTP	C5'-C4'-C3'	-2.33	105.94	115.21
3	A	1181	GTP	C1'-N9-C4	-2.21	123.61	126.94
3	A	1181	GTP	O4'-C4'-C3'	2.11	109.39	105.15
3	A	1181	GTP	C2'-C3'-C4'	2.17	107.07	102.61
3	A	1181	GTP	O2B-PB-O3B	2.27	115.40	105.09
3	A	1181	GTP	O2B-PB-O3A	2.40	115.98	105.09
3	A	1181	GTP	O4'-C1'-N9	2.44	113.21	108.10
3	A	1181	GTP	C6-N1-C2	3.47	120.76	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1181	GTP	5	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	172/172 (100%)	-0.13	0 <span>100</span> <span>100</span>	39, 53, 80, 88	0
2	B	885/963 (91%)	-0.04	10 (1%) <span>82</span> <span>74</span>	38, 69, 96, 110	0
All	All	1057/1135 (93%)	-0.05	10 (0%) <span>85</span> <span>79</span>	38, 67, 95, 110	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	851	VAL	3.6
2	B	651	LEU	2.5
2	B	327	VAL	2.5
2	B	618	ILE	2.5
2	B	850	GLU	2.4
2	B	566	ALA	2.3
2	B	594	LEU	2.2
2	B	685	PHE	2.1
2	B	644	LEU	2.1
2	B	233	GLU	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 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	GTP	A	1181	32/32	0.95	0.24	1.88	48,62,65,69	0
4	MG	A	1182	1/1	0.96	0.23	-	41,41,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.