



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:08 AM GMT

PDB ID : 3EA5  
Title : Kap95p Binding Induces the Switch Loops of RanGDP to adopt the GTP-bound Conformation: Implications for Nuclear Import Complex Assembly Dynamics  
Authors : Forwood, J.K.; Lonhienne, J.K.; Guncar, G.; Stewart, M.; Marfori, M.; Kobe, B.  
Deposited on : 2008-08-24  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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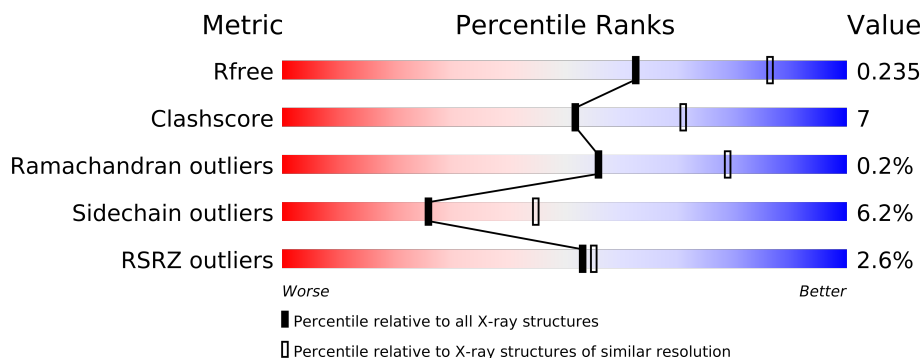
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	216	
1	C	216	
2	B	861	
2	D	861	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16428 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1415	918	248	244	5			
1	C	169	Total	C	N	O	S	0	0	0
			1377	895	242	236	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	ALA	ENGINEERED	UNP P62826
C	181	CYS	ALA	ENGINEERED	UNP P62826

- Molecule 2 is a protein called Importin subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	859	Total	C	N	O	S	0	0	0
			6642	4197	1099	1310	36			
2	D	849	Total	C	N	O	S	0	0	0
			6570	4157	1086	1291	36			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	254	LYS	LEU	ENGINEERED	UNP Q06142
D	254	LYS	LEU	ENGINEERED	UNP Q06142

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
3	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

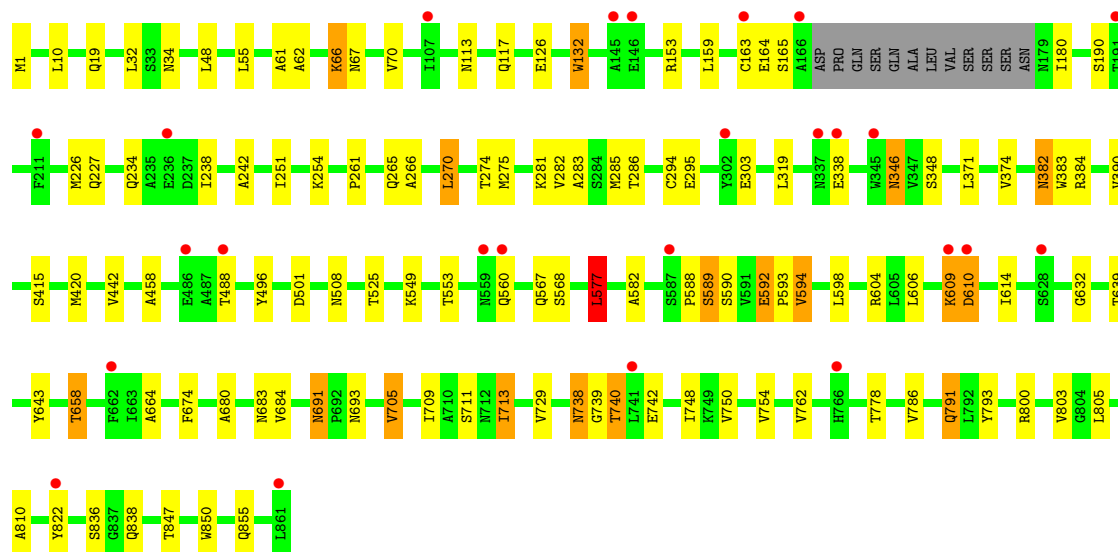
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	B	178	Total	O	0	0
			178	178		
5	C	34	Total	O	0	0
			34	34		
5	D	84	Total	O	0	0
			84	84		



● Molecule 2: Importin subunit beta-1

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.85Å 127.81Å 171.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 100.0 (19.99-2.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.189 , 0.232 0.194 , 0.235	Depositor DCC
$R_{free}$ test set	4240 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 68.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 84778 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 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	0.72	0/1450	0.84	2/1958 (0.1%)
1	C	0.56	0/1411	0.72	2/1905 (0.1%)
2	B	0.61	1/6755 (0.0%)	0.67	1/9179 (0.0%)
2	D	0.52	0/6682	0.63	2/9079 (0.0%)
All	All	0.58	1/16298 (0.0%)	0.68	7/22121 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	247	CYS	CB-SG	-5.86	1.72	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	ARG	NE-CZ-NH2	-11.25	114.67	120.30
1	A	29	ARG	NE-CZ-NH1	10.12	125.36	120.30
2	D	577	LEU	CA-CB-CG	-6.73	99.81	115.30
2	B	577	LEU	CA-CB-CG	-6.28	100.87	115.30
1	C	29	ARG	NE-CZ-NH2	-5.98	117.31	120.30
2	D	800	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	29	ARG	NE-CZ-NH1	5.18	122.89	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens



added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1415	0	1435	32	0
1	C	1377	0	1400	19	0
2	B	6642	0	6592	116	0
2	D	6570	0	6530	85	0
3	A	28	0	12	0	0
3	C	28	0	12	1	0
4	A	2	0	0	2	0
4	C	2	0	0	1	0
5	A	68	0	0	4	0
5	B	178	0	0	15	0
5	C	34	0	0	2	0
5	D	84	0	0	15	0
All	All	16428	0	15981	231	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (231) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:594:VAL:HG23	5:D:885:HOH:O	1.39	1.18
2:D:226:MET:HE1	2:D:251:ILE:HG21	1.19	1.14
2:B:226:MET:HE1	2:B:251:ILE:HG21	1.14	1.14
2:B:169:GLN:HE21	2:B:174:VAL:HG21	1.23	1.04
2:D:226:MET:CE	2:D:251:ILE:HG21	1.90	1.00
2:B:167:ASP:O	2:B:169:GLN:N	2.03	0.92
1:C:154:ASN:HD21	2:D:567:GLN:HE21	1.18	0.87
1:C:142:LYS:HE2	2:D:281:LYS:HZ3	1.40	0.86
2:D:371:LEU:O	5:D:926:HOH:O	1.93	0.85
1:C:29:ARG:HH11	2:D:567:GLN:HE22	1.21	0.85
2:B:257:THR:HG22	5:D:865:HOH:O	1.76	0.84
2:B:169:GLN:NE2	2:B:174:VAL:HG21	1.93	0.82
2:B:620:TYR:HE2	2:B:658:THR:HG21	1.46	0.81
2:B:639:THR:HG22	5:B:878:HOH:O	1.80	0.80
2:B:169:GLN:HE21	2:B:174:VAL:CG2	1.93	0.80
2:B:411:GLN:HG2	5:B:1000:HOH:O	1.82	0.79
2:D:742:GLU:HG2	5:D:921:HOH:O	1.83	0.79
2:B:140:VAL:HG21	2:B:178:ASN:HB3	1.64	0.79
4:A:222:MG:MG	5:A:224:HOH:O	1.27	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:169:GLN:NE2	2:B:174:VAL:HG11	1.99	0.78
5:B:863:HOH:O	2:D:838:GLN:HG3	1.84	0.77
1:C:141:LYS:HB2	1:C:144:LEU:HD12	1.66	0.76
2:B:169:GLN:HA	5:B:935:HOH:O	1.86	0.76
2:B:226:MET:CE	2:B:251:ILE:HG21	2.07	0.75
2:B:113:ASN:HD21	2:B:153:ARG:HH12	1.35	0.75
4:C:222:MG:MG	5:C:223:HOH:O	1.30	0.74
2:D:226:MET:HE1	2:D:251:ILE:HD13	1.69	0.74
2:D:374:VAL:HB	5:D:926:HOH:O	1.90	0.72
2:B:609:LYS:HD3	5:B:933:HOH:O	1.89	0.71
2:B:261:PRO:O	2:B:265:GLN:HG2	1.92	0.70
1:A:149:ILE:HD11	1:A:160:PRO:HG3	1.74	0.69
2:D:338:GLU:HG2	2:D:384:ARG:HH21	1.57	0.68
1:C:29:ARG:HH11	2:D:567:GLN:NE2	1.92	0.68
2:D:604:ARG:HD2	5:D:869:HOH:O	1.93	0.68
1:A:82:GLN:NE2	2:B:110:ARG:HH22	1.92	0.68
2:B:674:PHE:HB3	2:B:713:ILE:HD11	1.76	0.68
2:B:680:ALA:O	2:B:684:VAL:HG23	1.94	0.67
2:D:374:VAL:N	5:D:926:HOH:O	2.27	0.67
2:D:338:GLU:HG2	2:D:384:ARG:NH2	2.09	0.67
2:B:169:GLN:HG2	2:B:174:VAL:HG21	1.77	0.66
2:B:608:LYS:O	5:B:961:HOH:O	2.14	0.66
2:D:226:MET:HE1	2:D:251:ILE:CG2	2.11	0.66
2:D:508:ASN:OD1	2:D:549:LYS:NZ	2.28	0.65
2:D:691:ASN:HD22	2:D:693:ASN:H	1.44	0.65
4:A:222:MG:MG	5:A:223:HOH:O	1.40	0.64
2:B:169:GLN:HE21	2:B:174:VAL:HG11	1.62	0.64
2:D:113:ASN:HD21	2:D:153:ARG:HH12	1.45	0.64
2:B:577:LEU:HD13	2:B:614:ILE:HD11	1.78	0.64
1:A:154:ASN:HD21	2:B:567:GLN:HE21	1.44	0.64
2:B:729:VAL:HG22	2:B:778:THR:HG21	1.78	0.64
1:C:154:ASN:HD21	2:D:567:GLN:NE2	1.94	0.64
1:A:149:ILE:HD11	1:A:160:PRO:CG	2.28	0.64
3:C:220:GDP:O1B	5:C:223:HOH:O	2.15	0.63
2:D:371:LEU:C	5:D:926:HOH:O	2.35	0.63
2:D:588:PRO:C	2:D:590:SER:H	1.99	0.63
1:A:159:LYS:NZ	5:A:281:HOH:O	2.31	0.62
2:B:108:GLU:HG3	5:B:905:HOH:O	1.99	0.61
2:D:658:THR:HG22	5:D:890:HOH:O	2.00	0.61
2:D:66:LYS:HE3	2:D:67:ASN:OD1	2.00	0.61
2:D:1:MET:N	5:D:872:HOH:O	2.34	0.60
2:B:738:ASN:HD22	2:B:739:GLY:N	2.00	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:281:LYS:O	2:B:285:MET:HG3	2.02	0.60
2:D:691:ASN:ND2	2:D:693:ASN:H	2.00	0.59
1:A:29:ARG:HH11	2:B:567:GLN:HE22	1.49	0.59
2:B:729:VAL:HG22	2:B:778:THR:CG2	2.33	0.59
2:B:420:MET:HG3	2:B:458:ALA:HB1	1.83	0.59
2:B:226:MET:CE	2:B:251:ILE:HD13	2.33	0.59
2:B:346:ASN:ND2	2:B:348:SER:OG	2.35	0.59
2:B:786:VAL:O	2:B:793:TYR:HB3	2.03	0.59
2:D:281:LYS:O	2:D:285:MET:HG3	2.03	0.58
2:B:66:LYS:HE3	2:B:67:ASN:OD1	2.02	0.58
2:D:261:PRO:O	2:D:265:GLN:HG2	2.04	0.58
2:D:738:ASN:HD22	2:D:739:GLY:N	2.00	0.57
2:D:346:ASN:ND2	2:D:348:SER:OG	2.37	0.57
1:A:136:ILE:HD13	1:A:146:TYR:CZ	2.39	0.57
2:B:609:LYS:O	2:B:610:ASP:HB2	2.03	0.57
2:B:691:ASN:ND2	2:B:693:ASN:H	2.02	0.57
2:D:226:MET:CE	2:D:251:ILE:HD13	2.35	0.57
1:C:142:LYS:HE2	2:D:281:LYS:NZ	2.18	0.56
1:A:91:ASP:OD1	1:A:93:THR:HB	2.06	0.56
2:D:275:MET:HA	2:D:286:THR:HG21	1.88	0.56
2:B:275:MET:HA	2:B:286:THR:HG21	1.88	0.56
2:B:283:ALA:O	2:B:286:THR:HG22	2.05	0.55
2:D:577:LEU:HD13	2:D:614:ILE:HD11	1.88	0.55
2:D:609:LYS:O	2:D:610:ASP:HB2	2.06	0.55
2:B:169:GLN:CG	2:B:174:VAL:HG21	2.36	0.55
2:D:786:VAL:O	2:D:793:TYR:HB3	2.06	0.55
2:B:169:GLN:HE21	2:B:174:VAL:CG1	2.20	0.55
2:B:691:ASN:C	2:B:691:ASN:HD22	2.10	0.55
1:C:53:HIS:O	1:C:176:PHE:O	2.25	0.54
2:D:382:ASN:HD22	2:D:383:TRP:N	2.05	0.54
2:D:163:CYS:SG	2:D:180:ILE:HG21	2.48	0.54
2:D:803:VAL:HG12	2:D:847:THR:HG22	1.89	0.53
2:B:169:GLN:HE21	2:B:174:VAL:CB	2.21	0.53
1:A:77:ASP:OD2	2:B:66:LYS:NZ	2.41	0.53
2:B:382:ASN:HD22	2:B:383:TRP:N	2.06	0.53
2:D:234:GLN:NE2	2:D:270:LEU:HD13	2.23	0.53
2:B:729:VAL:CG2	2:B:778:THR:HG21	2.39	0.53
1:A:142:LYS:CE	2:B:281:LYS:HD3	2.39	0.53
1:A:56:ARG:NH1	1:A:171:ASP:OD2	2.42	0.53
2:B:554:MET:CE	2:B:601:LEU:HD22	2.38	0.53
2:B:664:ALA:HB2	2:B:705:VAL:HG23	1.91	0.53
1:C:142:LYS:CE	2:D:281:LYS:HZ3	2.17	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:620:TYR:CE2	2:B:658:THR:HG21	2.35	0.52
2:D:632:GLY:N	5:D:877:HOH:O	2.42	0.52
2:B:738:ASN:ND2	2:B:740:THR:OG1	2.42	0.52
2:B:837:GLY:N	5:B:996:HOH:O	2.39	0.52
1:A:71:LYS:HZ3	1:A:71:LYS:HB3	1.75	0.52
2:B:78:GLN:NE2	5:B:1013:HOH:O	2.18	0.52
1:A:142:LYS:HE2	2:B:281:LYS:HD3	1.92	0.52
1:A:71:LYS:NZ	1:A:71:LYS:CB	2.73	0.51
2:B:288:GLU:OE1	5:B:906:HOH:O	2.19	0.51
2:B:546:VAL:HB	2:B:576:ILE:HG23	1.92	0.51
2:D:680:ALA:O	2:D:684:VAL:HG23	2.10	0.51
2:D:420:MET:HG3	2:D:458:ALA:HB1	1.93	0.51
1:A:133:ALA:HA	1:A:136:ILE:HD12	1.93	0.51
1:A:82:GLN:NE2	2:B:110:ARG:NH2	2.58	0.50
1:A:12:LYS:HE3	1:A:64:TRP:CE2	2.47	0.50
2:B:531:ALA:O	2:B:586:LYS:HE2	2.11	0.50
2:B:691:ASN:HD22	2:B:693:ASN:H	1.58	0.50
2:D:691:ASN:C	2:D:691:ASN:HD22	2.15	0.50
2:B:382:ASN:ND2	2:B:384:ARG:H	2.09	0.50
2:D:664:ALA:HB2	2:D:705:VAL:HG23	1.94	0.50
2:B:171:GLN:O	2:B:174:VAL:N	2.45	0.49
2:D:48:LEU:HD13	2:D:62:ALA:HB2	1.94	0.49
2:B:803:VAL:HG11	2:B:848:ALA:HA	1.94	0.49
2:B:205:LEU:HD11	2:B:225:LEU:HD11	1.93	0.49
2:B:549:LYS:O	2:B:553:THR:HG23	2.12	0.49
1:A:154:ASN:HD21	2:B:567:GLN:NE2	2.10	0.49
2:B:303:GLU:OE2	2:D:303:GLU:OE2	2.30	0.49
2:D:283:ALA:O	2:D:286:THR:HG22	2.13	0.48
1:C:12:LYS:HE3	1:C:64:TRP:CE2	2.48	0.48
2:B:161:TYR:O	2:B:165:SER:HB2	2.13	0.48
1:A:71:LYS:NZ	1:A:71:LYS:HB3	2.28	0.48
2:B:411:GLN:CG	5:B:1000:HOH:O	2.49	0.48
2:D:346:ASN:HD22	2:D:348:SER:H	1.59	0.48
2:D:738:ASN:ND2	2:D:740:THR:OG1	2.45	0.48
1:A:26:PHE:CE1	1:A:30:HIS:HE1	2.31	0.48
2:B:226:MET:HE1	2:B:251:ILE:HD13	1.96	0.48
2:B:108:GLU:HB3	2:B:111:ILE:HD12	1.96	0.48
1:A:112:CYS:O	1:A:113:GLU:C	2.51	0.48
2:B:679:ASP:HB3	5:B:899:HOH:O	2.14	0.48
1:C:176:PHE:O	1:C:177:VAL:C	2.51	0.47
1:C:118:VAL:HG23	1:C:164:LEU:HD21	1.96	0.47
1:A:120:CYS:SG	1:A:149:ILE:HD13	2.54	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:LYS:HB2	1:A:144:LEU:HD12	1.96	0.47
2:B:592:GLU:N	2:B:593:PRO:HD2	2.28	0.47
1:A:120:CYS:SG	1:A:149:ILE:CD1	3.02	0.47
2:D:658:THR:CG2	5:D:890:HOH:O	2.62	0.47
2:B:346:ASN:HD22	2:B:348:SER:H	1.61	0.47
2:B:275:MET:CA	2:B:286:THR:HG21	2.45	0.47
2:B:656:SER:OG	2:B:698:LEU:HD21	2.15	0.47
2:D:592:GLU:N	2:D:593:PRO:HD2	2.29	0.47
2:D:159:LEU:HD22	2:D:180:ILE:HG23	1.98	0.46
2:D:729:VAL:HG22	2:D:778:THR:HG21	1.97	0.46
2:B:226:MET:HE2	2:B:251:ILE:HD13	1.97	0.46
2:B:382:ASN:HD22	2:B:382:ASN:C	2.19	0.46
2:D:674:PHE:HB3	2:D:713:ILE:HD11	1.96	0.46
1:C:141:LYS:HB2	1:C:144:LEU:CD1	2.40	0.46
2:D:274:THR:HG23	2:D:282:VAL:CG1	2.45	0.46
1:C:142:LYS:HZ1	2:D:281:LYS:HD3	1.80	0.46
1:A:92:VAL:HG13	1:A:129:ARG:HB3	1.97	0.46
1:C:142:LYS:NZ	2:D:281:LYS:NZ	2.64	0.46
1:C:14:VAL:HG11	1:C:80:TYR:HA	1.98	0.45
2:B:837:GLY:CA	5:B:996:HOH:O	2.63	0.45
2:D:374:VAL:CA	5:D:926:HOH:O	2.64	0.45
2:D:126:GLU:OE1	2:D:132:TRP:HB2	2.17	0.45
1:A:82:GLN:HE21	2:B:110:ARG:HH12	1.65	0.44
2:D:606:LEU:HB3	2:D:643:TYR:CZ	2.52	0.44
2:B:674:PHE:HB3	2:B:713:ILE:CD1	2.46	0.44
2:B:363:GLY:O	2:B:366:ILE:HG22	2.17	0.44
2:B:180:ILE:HD12	5:B:980:HOH:O	2.15	0.44
1:A:29:ARG:HH11	2:B:567:GLN:NE2	2.14	0.44
1:A:136:ILE:HD13	1:A:146:TYR:CE2	2.52	0.44
2:B:803:VAL:CG1	2:B:848:ALA:HA	2.46	0.44
1:A:140:ARG:HG2	2:B:345:TRP:NE1	2.33	0.44
2:B:260:LYS:HB3	2:B:261:PRO:HD3	1.99	0.44
2:B:510:ILE:HG22	2:B:510:ILE:O	2.16	0.44
2:D:275:MET:CA	2:D:286:THR:HG21	2.48	0.44
2:D:762:VAL:HG21	2:D:805:LEU:HD22	2.00	0.44
2:B:274:THR:HG23	2:B:282:VAL:HG12	1.99	0.44
1:C:142:LYS:CE	2:D:281:LYS:NZ	2.78	0.43
2:B:48:LEU:HD13	2:B:62:ALA:HB2	2.00	0.43
2:B:800:ARG:HD3	2:B:844:THR:HA	1.99	0.43
2:D:382:ASN:C	2:D:382:ASN:HD22	2.21	0.43
2:D:117:GLN:NE2	5:D:912:HOH:O	2.49	0.43
2:D:606:LEU:HB3	2:D:643:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:462:GLY:HA3	2:B:473:CYS:SG	2.58	0.43
2:B:169:GLN:O	2:B:170:SER:CB	2.66	0.43
2:B:170:SER:HA	5:B:1023:HOH:O	2.19	0.43
2:D:729:VAL:HG22	2:D:778:THR:CG2	2.49	0.43
2:B:181:LEU:HD23	2:B:181:LEU:C	2.39	0.42
2:B:167:ASP:O	2:B:169:GLN:CA	2.65	0.42
2:B:346:ASN:HD22	2:B:348:SER:N	2.17	0.42
2:D:346:ASN:HD22	2:D:348:SER:N	2.16	0.42
1:A:139:HIS:HB2	1:A:145:GLN:HA	2.01	0.42
1:A:82:GLN:HE22	2:B:110:ARG:NH2	2.17	0.42
2:D:10:LEU:HD13	2:D:61:ALA:HB2	2.00	0.42
2:B:835:ARG:NH1	2:B:849:ARG:HG3	2.33	0.42
1:C:122:ASN:OD1	1:C:149:ILE:HG22	2.19	0.42
2:D:577:LEU:HD13	2:D:614:ILE:CD1	2.49	0.42
2:B:738:ASN:ND2	2:B:743:ALA:CB	2.82	0.42
2:B:209:LEU:O	2:B:255:TYR:OH	2.30	0.42
2:B:592:GLU:HG3	2:B:593:PRO:CD	2.50	0.42
2:D:588:PRO:C	2:D:590:SER:N	2.69	0.42
2:D:374:VAL:CB	5:D:926:HOH:O	2.60	0.42
2:D:549:LYS:O	2:D:553:THR:HG23	2.20	0.42
1:A:142:LYS:NZ	2:B:281:LYS:HD3	2.35	0.42
2:D:592:GLU:HG3	2:D:593:PRO:CD	2.50	0.42
2:B:274:THR:HG23	2:B:282:VAL:CG1	2.50	0.42
2:B:10:LEU:HD13	2:B:61:ALA:HB2	2.01	0.42
2:D:748:ILE:HD13	2:D:791:GLN:HG2	2.02	0.41
2:B:695:ARG:HG2	2:B:698:LEU:HD23	2.02	0.41
2:B:181:LEU:HD12	2:B:212:ILE:HD12	2.01	0.41
2:B:97:LYS:CE	2:B:126:GLU:OE1	2.69	0.41
2:D:242:ALA:HA	2:D:285:MET:SD	2.60	0.41
2:D:750:VAL:O	2:D:754:VAL:HG23	2.21	0.41
2:D:810:ALA:HB2	2:D:822:TYR:CZ	2.55	0.41
2:B:691:ASN:HD22	2:B:692:PRO:N	2.19	0.41
2:B:592:GLU:HG3	2:B:593:PRO:HD3	2.02	0.41
2:D:709:ILE:O	2:D:713:ILE:HB	2.21	0.41
2:B:554:MET:CE	2:B:601:LEU:CD2	2.99	0.41
5:A:254:HOH:O	2:B:563:LEU:HD22	2.20	0.41
2:D:525:THR:HG23	2:D:582:ALA:HB2	2.01	0.41
2:B:679:ASP:CG	2:B:720:TYR:HH	2.24	0.40
2:B:699:LYS:HB3	2:B:700:PRO:CD	2.51	0.40
2:D:66:LYS:HB3	2:D:66:LYS:HE2	1.94	0.40
2:B:322:ILE:O	2:B:323:LYS:C	2.60	0.40
2:B:158:ALA:O	2:B:162:MET:HB2	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:142:LYS:NZ	2:D:281:LYS:HZ2	2.20	0.40
2:B:698:LEU:HD13	2:B:698:LEU:HA	1.88	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	172/216 (80%)	166 (96%)	6 (4%)	0	100	100
1	C	167/216 (77%)	160 (96%)	7 (4%)	0	100	100
2	B	855/861 (99%)	827 (97%)	25 (3%)	3 (0%)	43	66
2	D	845/861 (98%)	821 (97%)	22 (3%)	2 (0%)	56	79
All	All	2039/2154 (95%)	1974 (97%)	60 (3%)	5 (0%)	56	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	168	PRO
2	B	169	GLN
2	B	170	SER
2	D	266	ALA
2	D	589	SER

### 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	153/186 (82%)	144 (94%)	9 (6%)	28	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	149/186 (80%)	142 (95%)	7 (5%)	36	61
2	B	725/726 (100%)	680 (94%)	45 (6%)	26	45
2	D	715/726 (98%)	668 (93%)	47 (7%)	24	41
All	All	1742/1824 (96%)	1634 (94%)	108 (6%)	26	45

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	43	LEU
1	A	71	LYS
1	A	92	VAL
1	A	93	THR
1	A	95	ARG
1	A	114	ASN
1	A	134	LYS
1	A	149	ILE
2	B	19	GLN
2	B	32	LEU
2	B	34	ASN
2	B	55	LEU
2	B	66	LYS
2	B	70	VAL
2	B	132	TRP
2	B	164	GLU
2	B	165	SER
2	B	178	ASN
2	B	227	GLN
2	B	238	ILE
2	B	254	LYS
2	B	270	LEU
2	B	295	GLU
2	B	319	LEU
2	B	346	ASN
2	B	382	ASN
2	B	390	VAL
2	B	415	SER
2	B	442	VAL
2	B	488	THR
2	B	496	TYR
2	B	501	ASP

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Mol	Chain	Res	Type
2	B	560	GLN
2	B	564	GLU
2	B	568	SER
2	B	577	LEU
2	B	592	GLU
2	B	598	LEU
2	B	609	LYS
2	B	610	ASP
2	B	639	THR
2	B	658	THR
2	B	683	ASN
2	B	691	ASN
2	B	705	VAL
2	B	713	ILE
2	B	738	ASN
2	B	740	THR
2	B	755	LEU
2	B	791	GLN
2	B	835	ARG
2	B	836	SER
2	B	838	GLN
1	C	29	ARG
1	C	43	LEU
1	C	71	LYS
1	C	92	VAL
1	C	96	VAL
1	C	149	ILE
1	C	159	LYS
2	D	19	GLN
2	D	32	LEU
2	D	34	ASN
2	D	55	LEU
2	D	66	LYS
2	D	70	VAL
2	D	132	TRP
2	D	164	GLU
2	D	165	SER
2	D	190	SER
2	D	227	GLN
2	D	238	ILE
2	D	254	LYS
2	D	270	LEU

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Mol	Chain	Res	Type
2	D	294	CYS
2	D	295	GLU
2	D	319	LEU
2	D	346	ASN
2	D	382	ASN
2	D	390	VAL
2	D	415	SER
2	D	442	VAL
2	D	488	THR
2	D	496	TYR
2	D	501	ASP
2	D	560	GLN
2	D	568	SER
2	D	577	LEU
2	D	589	SER
2	D	592	GLU
2	D	594	VAL
2	D	598	LEU
2	D	609	LYS
2	D	610	ASP
2	D	639	THR
2	D	658	THR
2	D	683	ASN
2	D	691	ASN
2	D	705	VAL
2	D	711	SER
2	D	713	ILE
2	D	738	ASN
2	D	740	THR
2	D	791	GLN
2	D	836	SER
2	D	850	TRP
2	D	855	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	82	GLN
1	A	100	ASN
1	A	114	ASN
2	B	79	GLN

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Mol	Chain	Res	Type
2	B	113	ASN
2	B	169	GLN
2	B	215	ASN
2	B	306	GLN
2	B	346	ASN
2	B	376	GLN
2	B	382	ASN
2	B	385	ASN
2	B	423	GLN
2	B	567	GLN
2	B	649	ASN
2	B	691	ASN
2	B	712	ASN
2	B	738	ASN
2	B	785	GLN
2	B	838	GLN
1	C	82	GLN
1	C	100	ASN
2	D	79	GLN
2	D	113	ASN
2	D	215	ASN
2	D	234	GLN
2	D	346	ASN
2	D	376	GLN
2	D	382	ASN
2	D	385	ASN
2	D	423	GLN
2	D	567	GLN
2	D	649	ASN
2	D	691	ASN
2	D	712	ASN
2	D	738	ASN
2	D	785	GLN
2	D	838	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
3	GDP	A	220	4	30,30,30	1.34	4 (13%)	44,47,47	1.75	11 (25%)
3	GDP	C	220	4	30,30,30	1.49	5 (16%)	44,47,47	2.30	10 (22%)

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	GDP	A	220	4	-	0/16/32/32	0/1/3/3
3	GDP	C	220	4	-	0/16/32/32	0/1/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	220	GDP	C4-N9	-4.06	1.31	1.37
3	C	220	GDP	C6-C5	3.77	1.47	1.41
3	A	220	GDP	C4-N9	-3.75	1.32	1.37
3	C	220	GDP	C5-C4	2.89	1.47	1.40
3	A	220	GDP	C6-C5	2.76	1.45	1.41
3	A	220	GDP	C6-N1	-2.70	1.32	1.37
3	A	220	GDP	C5-C4	2.64	1.46	1.40
3	C	220	GDP	C2-N2	2.08	1.35	1.32
3	C	220	GDP	C6-N1	-2.02	1.33	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	220	GDP	C6-C5-N7	10.59	135.57	134.14
3	A	220	GDP	C6-C5-N7	4.74	134.78	134.14
3	A	220	GDP	N3-C4-N9	4.42	133.39	126.91
3	A	220	GDP	N2-C2-N3	-4.32	114.44	120.30
3	C	220	GDP	N3-C4-N9	3.99	132.76	126.91
3	C	220	GDP	PA-O3A-PB	-3.93	120.16	131.68
3	A	220	GDP	C5-C4-N3	-3.73	120.53	125.94
3	C	220	GDP	C5-C4-N3	-3.38	121.04	125.94
3	C	220	GDP	C4-C5-N7	-3.35	106.65	109.52
3	C	220	GDP	O4'-C1'-N9	3.23	111.45	108.44
3	A	220	GDP	PA-O3A-PB	-3.06	122.71	131.68
3	C	220	GDP	C8-N9-C4	2.95	109.15	106.90
3	C	220	GDP	N2-C2-N3	-2.80	116.50	120.30
3	A	220	GDP	N2-C2-N1	2.73	120.87	117.86
3	C	220	GDP	C6-N1-C2	2.50	123.89	119.51
3	A	220	GDP	C4-C5-N7	-2.39	107.47	109.52
3	A	220	GDP	C8-N9-C4	2.38	108.72	106.90
3	C	220	GDP	C2-N3-C4	2.28	118.29	115.09
3	A	220	GDP	N1-C2-N3	2.07	124.68	121.78
3	A	220	GDP	C6-N1-C2	2.06	123.12	119.51
3	A	220	GDP	C2-N3-C4	2.05	117.97	115.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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, 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	174/216 (80%)	-0.37	3 (1%) 67 69	52, 62, 88, 121	0
1	C	169/216 (78%)	0.03	8 (4%) 30 31	55, 65, 93, 111	0
2	B	859/861 (99%)	-0.23	17 (1%) 62 64	51, 65, 83, 110	0
2	D	849/861 (98%)	0.03	25 (2%) 49 51	53, 67, 82, 99	0
All	All	2051/2154 (95%)	-0.11	53 (2%) 53 55	51, 66, 84, 121	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LYS	7.8
1	C	127	LYS	4.6
2	D	488	THR	4.6
2	D	861	LEU	4.4
2	B	488	THR	4.1
2	D	166	ALA	4.0
1	C	143	ASN	3.9
2	D	560	GLN	3.8
2	B	693	ASN	3.8
2	D	302	TYR	3.7
2	D	486	GLU	3.5
2	D	587	SER	3.3
1	A	142	LYS	3.3
2	B	861	LEU	3.2
2	D	741	LEU	3.2
2	B	737	GLU	3.0
2	B	302	TYR	3.0
2	B	168	PRO	2.9
1	A	179	MET	2.9
1	C	133	ALA	2.7
1	C	141	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	177	SER	2.6
2	B	692	PRO	2.6
2	B	533	ASP	2.6
2	D	338	GLU	2.6
2	D	610	ASP	2.5
2	B	850	TRP	2.5
2	D	145	ALA	2.5
2	D	345	TRP	2.5
2	B	696	ARG	2.4
2	D	191	THR	2.4
2	D	337	ASN	2.4
2	D	766	HIS	2.4
1	A	178	ALA	2.4
2	D	662	PHE	2.4
2	D	628	SER	2.4
1	C	9	VAL	2.4
2	D	559	ASN	2.4
1	C	134	LYS	2.3
2	D	236	GLU	2.3
2	B	838	GLN	2.2
2	D	146	GLU	2.2
2	D	211	PHE	2.2
2	B	176	SER	2.1
2	B	839	LEU	2.1
2	D	107	ILE	2.1
2	D	609	LYS	2.1
1	C	113	GLU	2.1
2	B	167	ASP	2.1
2	B	175	SER	2.1
2	D	822	TYR	2.0
2	D	163	CYS	2.0
2	B	265	GLN	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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	C	221	1/1	0.14	0.31	55,55,55,55	0
4	MG	A	222	1/1	0.08	-0.47	55,55,55,55	0
3	GDP	A	220	28/28	0.09	-0.59	42,49,53,54	0
4	MG	A	221	1/1	0.07	-0.77	43,43,43,43	0
3	GDP	C	220	28/28	0.10	-0.77	53,58,61,61	0
4	MG	C	222	1/1	0.06	-1.92	58,58,58,58	0

## 6.5 Other polymers

There are no such residues in this entry.