Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:20 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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

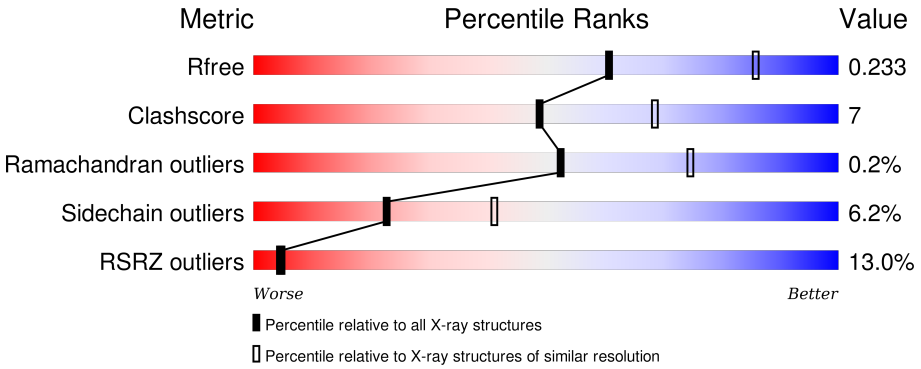
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=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 <=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	216	8% 65% 13% • 19%
1	C	216	17% 69% 9% 22%
2	B	861	8% 83% 15% •
2	D	861	17% 85% 12% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	222	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16428 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 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

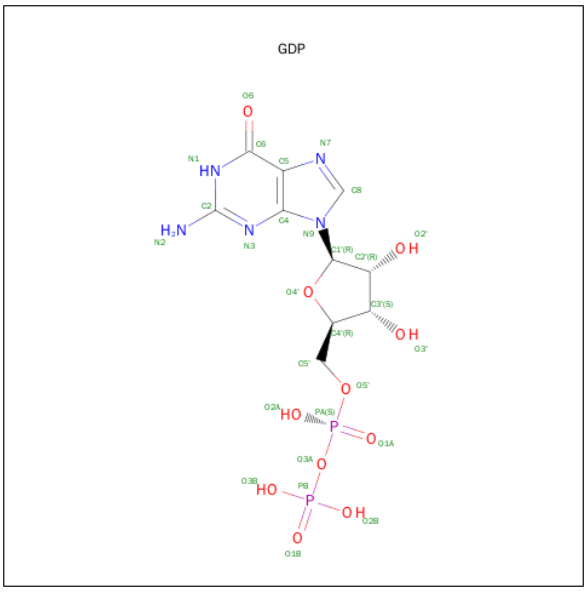
- Molecule 2 is a protein called Importin subunit beta-1.

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: $C_{10}H_{15}N_5O_{11}P_2$).



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.

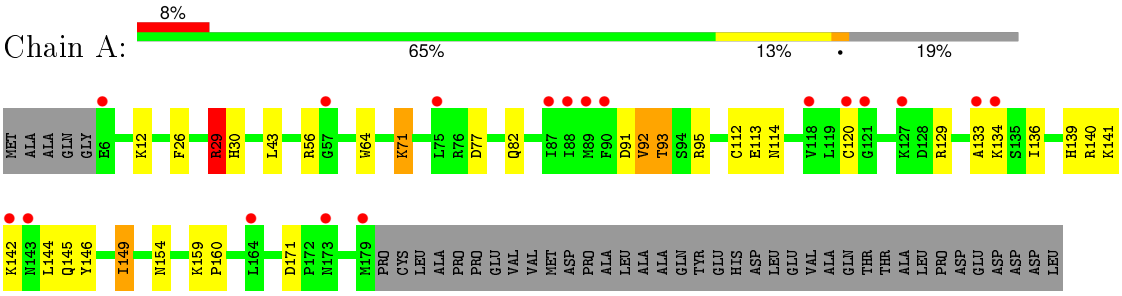
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total	O	0	0
			68	68		
5	B	178	Total	O	0	0
			178	178		
5	C	34	Total	O	0	0
			34	34		
5	D	84	Total	O	0	0
			84	84		

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.

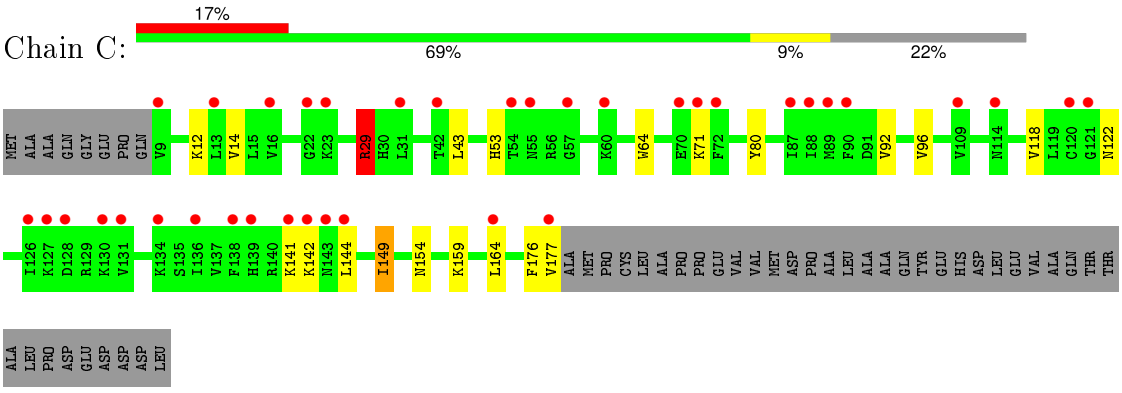
- Molecule 1: GTP-binding nuclear protein Ran

Chain A:



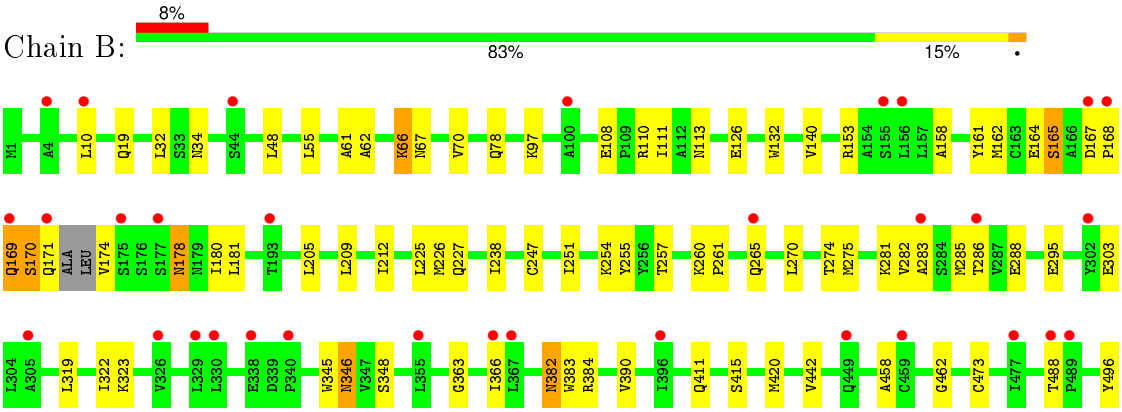
- Molecule 1: GTP-binding nuclear protein Ran

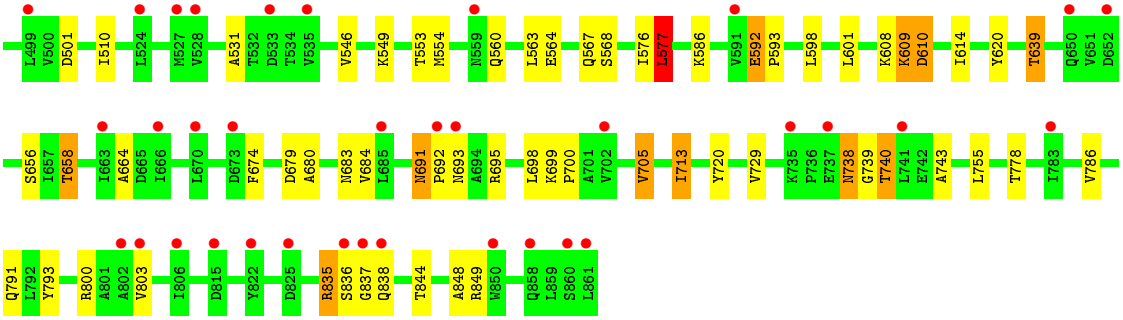
Chain C:



- Molecule 2: Importin subunit beta-1

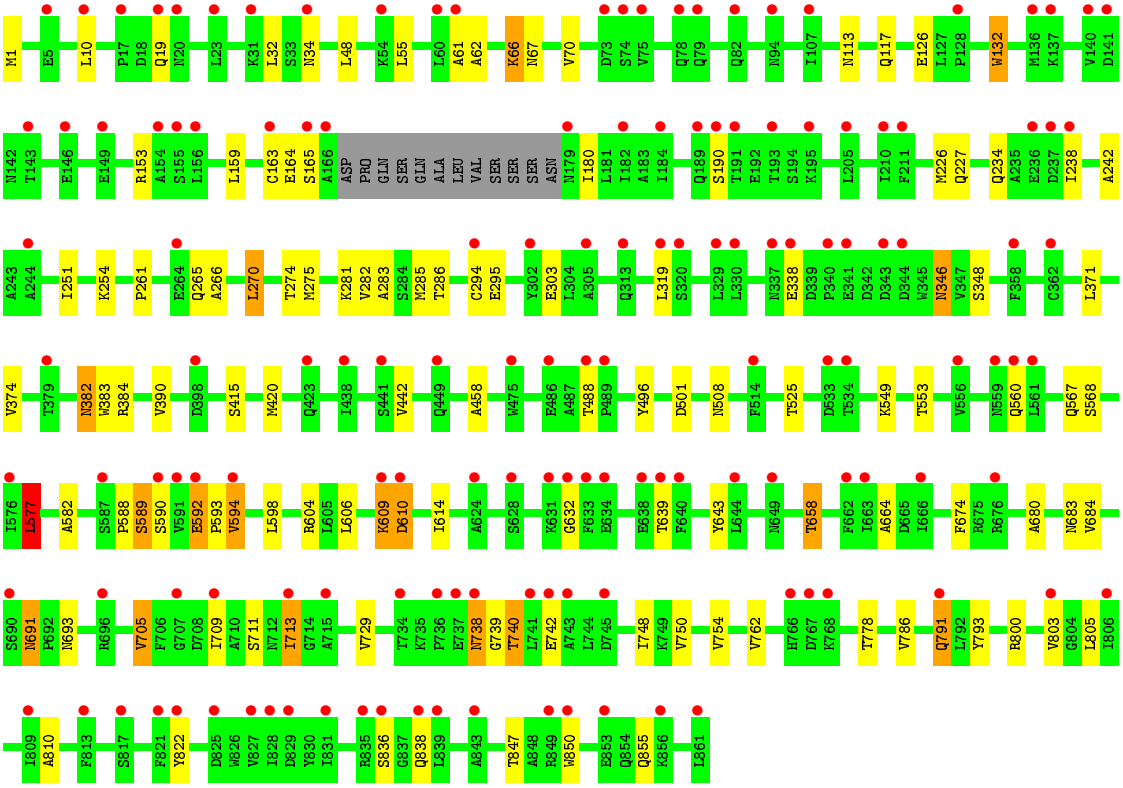
Chain B:





- Molecule 2: Importin subunit beta-1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.78 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.189 , 0.232 0.193 , 0.233	Depositor DCC
R_{free} test set	4240 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 84778 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16428	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 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	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

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 7.

All (231) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:738:ASN:HD22	2:B:739:GLY:N	2.00	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	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%)	39	61
2	D	845/861 (98%)	821 (97%)	22 (3%)	2 (0%)	52	75
All	All	2039/2154 (95%)	1974 (97%)	60 (3%)	5 (0%)	52	75

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 (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	153/186 (82%)	144 (94%)	9 (6%)	24	44
1	C	149/186 (80%)	142 (95%)	7 (5%)	32	56
2	B	725/726 (100%)	680 (94%)	45 (6%)	23	41
2	D	715/726 (98%)	668 (93%)	47 (7%)	21	38
All	All	1742/1824 (96%)	1634 (94%)	108 (6%)	23	41

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
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 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 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	23,30,30	1.00	2 (8%)	30,47,47	1.86	6 (20%)
3	GDP	C	220	4	23,30,30	1.17	2 (8%)	30,47,47	2.15	8 (26%)

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	-	0/12/32/32	0/3/3/3
3	GDP	C	220	4	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	220	GDP	C6-C5	2.24	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	220	GDP	C5-C4	2.64	1.46	1.40
3	C	220	GDP	C5-C4	2.89	1.47	1.40
3	C	220	GDP	C6-C5	3.07	1.47	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	220	GDP	C5-C6-N1	-6.00	115.39	123.59
3	A	220	GDP	C5-C6-N1	-5.60	115.94	123.59
3	C	220	GDP	PA-O3A-PB	-3.73	120.16	132.67
3	C	220	GDP	C4-C5-N7	-3.07	106.65	109.48
3	A	220	GDP	PA-O3A-PB	-2.97	122.71	132.67
3	C	220	GDP	C2'-C1'-N9	-2.75	110.09	114.29
3	A	220	GDP	C6-C5-C4	-2.63	117.75	120.90
3	C	220	GDP	C6-C5-C4	-2.61	117.78	120.90
3	C	220	GDP	N3-C2-N1	-2.53	123.59	127.44
3	C	220	GDP	C1'-N9-C4	-2.29	123.49	126.94
3	A	220	GDP	C4-C5-N7	-2.18	107.47	109.48
3	A	220	GDP	N2-C2-N1	2.22	120.87	117.20
3	A	220	GDP	C6-N1-C2	5.17	123.12	115.94
3	C	220	GDP	C6-N1-C2	5.73	123.89	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	220	GDP	1	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

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^{th} 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	174/216 (80%)	0.62	18 (10%) 9 9	52, 62, 88, 121	0
1	C	169/216 (78%)	1.18	37 (21%) 1 1	55, 65, 93, 111	0
2	B	859/861 (99%)	0.69	67 (7%) 16 17	51, 65, 83, 110	0
2	D	849/861 (98%)	1.07	145 (17%) 2 2	53, 67, 82, 99	0
All	All	2051/2154 (95%)	0.88	267 (13%) 5 4	51, 66, 84, 121	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	LYS	10.2
1	C	138	PHE	8.2
2	B	861	LEU	7.8
1	C	127	LYS	7.2
2	B	488	THR	7.0
2	D	128	PRO	6.6
2	B	692	PRO	6.1
1	C	143	ASN	6.0
2	D	861	LEU	6.0
2	D	639	THR	5.9
1	A	179	MET	5.9
2	D	166	ALA	5.7
1	C	141	LYS	5.6
2	D	591	VAL	5.5
2	D	839	LEU	5.5
2	D	559	ASN	5.3
2	D	587	SER	5.3
2	B	836	SER	5.2
1	C	139	HIS	5.0
2	D	741	LEU	5.0
2	D	140	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	663	ILE	4.7
2	D	156	LEU	4.7
2	D	340	PRO	4.7
2	D	560	GLN	4.7
2	D	149	GLU	4.6
2	D	449	GLN	4.5
2	D	737	GLU	4.5
1	C	134	LYS	4.5
2	D	825	ASP	4.4
2	D	441	SER	4.4
2	B	302	TYR	4.4
2	D	107	ILE	4.3
2	D	191	THR	4.3
2	D	137	LYS	4.2
2	D	488	THR	4.2
1	A	142	LYS	4.1
2	D	320	SER	4.1
2	B	167	ASP	4.1
2	B	168	PRO	4.1
2	B	477	ILE	4.1
2	B	489	PRO	4.1
2	D	236	GLU	4.0
2	D	237	ASP	4.0
2	D	341	GLU	4.0
2	D	94	ASN	4.0
1	C	89	MET	3.9
2	D	767	ASP	3.9
1	C	144	LEU	3.9
2	B	4	ALA	3.9
2	D	338	GLU	3.9
2	B	837	GLY	3.8
1	C	72	PHE	3.8
2	D	210	ILE	3.7
2	B	535	VAL	3.7
1	C	87	ILE	3.7
2	D	75	VAL	3.7
2	D	662	PHE	3.6
2	D	489	PRO	3.6
2	D	486	GLU	3.6
2	D	634	GLU	3.6
1	A	89	MET	3.5
2	D	713	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	61	ALA	3.5
2	D	514	PHE	3.5
1	C	120	CYS	3.5
2	D	184	ILE	3.5
1	C	9	VAL	3.5
2	B	737	GLU	3.4
2	D	330	LEU	3.5
2	B	802	ALA	3.4
1	C	90	PHE	3.4
2	B	783	ILE	3.4
2	D	20	ASN	3.4
2	B	527	MET	3.4
2	D	806	ILE	3.4
1	C	131	VAL	3.4
2	D	768	LYS	3.4
2	D	822	TYR	3.3
1	A	173	ASN	3.3
1	C	114	ASN	3.3
2	D	74	SER	3.3
2	B	838	GLN	3.3
2	D	79	GLN	3.3
2	D	305	ALA	3.3
2	D	745	ASP	3.2
2	D	766	HIS	3.2
2	B	449	GLN	3.2
1	C	136	ILE	3.2
2	D	666	ILE	3.2
2	D	676	ARG	3.2
2	D	638	GLU	3.2
2	B	663	ILE	3.2
2	D	610	ASP	3.2
1	A	164	LEU	3.2
2	D	19	GLN	3.2
2	D	165	SER	3.2
2	D	696	ARG	3.1
2	D	592	GLU	3.1
1	C	164	LEU	3.1
2	D	736	PRO	3.1
2	D	143	THR	3.1
1	C	16	VAL	3.1
2	D	205	LEU	3.1
2	B	693	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	632	GLY	3.1
1	A	90	PHE	3.0
2	D	742	GLU	3.0
2	D	10	LEU	3.0
2	B	803	VAL	3.0
2	B	533	ASP	3.0
1	C	60	LYS	3.0
2	D	423	GLN	3.0
1	A	134	LYS	3.0
1	C	126	ILE	3.0
2	B	650	GLN	2.9
2	D	594	VAL	2.9
2	D	835	ARG	2.9
2	B	175	SER	2.9
2	B	171	GLN	2.9
2	D	640	PHE	2.9
2	D	17	PRO	2.9
2	D	849	ARG	2.8
2	B	193	THR	2.8
2	D	193	THR	2.8
2	D	609	LYS	2.8
2	B	825	ASP	2.8
2	D	163	CYS	2.8
1	A	75	LEU	2.8
2	D	329	LEU	2.8
1	A	133	ALA	2.8
2	D	649	ASN	2.8
2	B	652	ASP	2.8
2	B	815	ASP	2.8
2	B	670	LEU	2.8
2	D	189	GLN	2.8
2	D	179	ASN	2.8
1	C	71	LYS	2.8
2	D	576	ILE	2.8
2	D	154	ALA	2.8
2	D	78	GLN	2.7
2	D	82	GLN	2.7
2	D	238	ILE	2.7
2	D	23	LEU	2.7
2	D	141	ASP	2.7
1	A	118	VAL	2.7
2	D	821	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	6	GLU	2.6
2	B	366	ILE	2.6
2	D	828	ILE	2.6
2	D	302	TYR	2.6
1	A	120	CYS	2.6
2	D	5	GLU	2.6
2	D	438	ILE	2.6
2	D	690	SER	2.6
2	B	559	ASN	2.6
2	D	136	MET	2.6
2	B	265	GLN	2.6
1	C	31	LEU	2.6
1	C	55	ASN	2.6
2	B	326	VAL	2.5
2	B	286	THR	2.5
2	B	44	SER	2.5
2	B	806	ILE	2.5
2	D	533	ASP	2.5
2	D	590	SER	2.5
2	D	264	GLU	2.5
2	D	791	GLN	2.5
1	C	109	VAL	2.5
2	D	734	THR	2.5
2	D	644	LEU	2.4
2	D	344	ASP	2.4
2	D	534	THR	2.4
2	D	155	SER	2.4
1	C	70	GLU	2.4
2	B	340	PRO	2.4
2	D	803	VAL	2.4
1	C	128	ASP	2.4
2	D	343	ASP	2.4
2	D	715	ALA	2.4
1	C	130	LYS	2.4
2	D	631	LYS	2.4
2	B	305	ALA	2.4
2	D	850	TRP	2.4
2	B	338	GLU	2.4
2	D	337	ASN	2.4
2	B	10	LEU	2.4
1	C	88	ILE	2.4
2	D	738	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	146	GLU	2.3
2	D	838	GLN	2.3
2	B	459	CYS	2.3
2	D	556	VAL	2.3
1	C	42	THR	2.3
2	B	330	LEU	2.3
2	D	195	LYS	2.3
2	D	628	SER	2.3
2	D	843	ALA	2.3
2	B	735	LYS	2.3
2	D	853	GLU	2.3
1	A	57	GLY	2.3
2	D	182	ILE	2.3
2	B	355	LEU	2.3
2	B	591	VAL	2.3
2	D	73	ASP	2.3
2	B	396	ILE	2.3
2	B	741	LEU	2.3
2	D	809	ILE	2.2
2	B	524	LEU	2.2
2	B	850	TRP	2.2
2	B	169	GLN	2.2
2	D	817	SER	2.2
2	D	319	LEU	2.2
1	A	88	ILE	2.2
2	D	211	PHE	2.2
2	B	156	LEU	2.2
2	B	367	LEU	2.2
2	D	31	LYS	2.2
2	D	294	CYS	2.2
1	C	22	GLY	2.2
1	C	54	THR	2.2
2	B	283	ALA	2.2
2	D	34	ASN	2.2
2	D	244	ALA	2.2
2	D	362	CYS	2.2
2	D	624	ALA	2.2
2	D	829	ASP	2.2
2	D	475	TRP	2.2
1	C	177	VAL	2.2
2	B	177	SER	2.2
2	D	743	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	831	ILE	2.2
2	D	813	PHE	2.2
1	C	23	LYS	2.2
2	B	528	VAL	2.1
2	B	155	SER	2.1
1	A	87	ILE	2.1
2	B	499	LEU	2.1
2	D	358	PHE	2.1
2	D	561	LEU	2.1
1	C	121	GLY	2.1
2	D	54	LYS	2.1
2	D	707	GLY	2.1
2	B	329	LEU	2.1
1	A	121	GLY	2.1
2	D	379	THR	2.1
1	C	13	LEU	2.1
2	D	190	SER	2.1
2	B	858	GLN	2.1
2	D	827	VAL	2.1
2	B	666	ILE	2.1
2	D	709	ILE	2.1
2	D	856	LYS	2.1
2	B	860	SER	2.1
1	C	57	GLY	2.0
2	B	685	LEU	2.0
2	B	673	ASP	2.0
2	B	100	ALA	2.0
2	B	702	VAL	2.0
2	D	313	GLN	2.0
2	D	398	ASP	2.0
2	D	633	PHE	2.0
2	D	836	SER	2.0
1	A	143	ASN	2.0
2	D	60	LEU	2.0
1	A	127	LYS	2.0
2	B	822	TYR	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^{th} 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
3	GDP	C	220	28/28	0.97	0.14	-1.05	53,58,61,61	0
3	GDP	A	220	28/28	0.98	0.12	-1.35	42,49,53,54	0
4	MG	C	222	1/1	0.98	0.05	-2.20	58,58,58,58	0
4	MG	A	221	1/1	0.97	0.05	-2.62	43,43,43,43	0
4	MG	A	222	1/1	1.00	0.05	-3.39	55,55,55,55	0
4	MG	C	221	1/1	0.94	0.09	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.