Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:05 AM GMT

PDB ID	:	3KUD
Title	:	Complex of Ras-GDP with RafRBD(A85K)
Authors	:	Filchtinski, D.; Sharabi, O.; Rueppel, A.; Vetter, I.R.; Herrmann, C.; Shifman, J.M.
Deposited on	:	2009-11-27
Resolution	:	2.15 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:

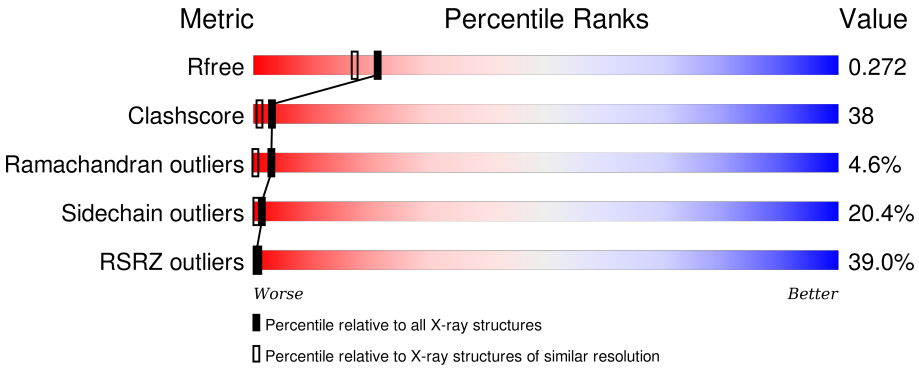
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	166	25% 63% 24% 9%
2	B	81	64% 27% 41% 25% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2005 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 GTPase HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1312	818	225	262	7			

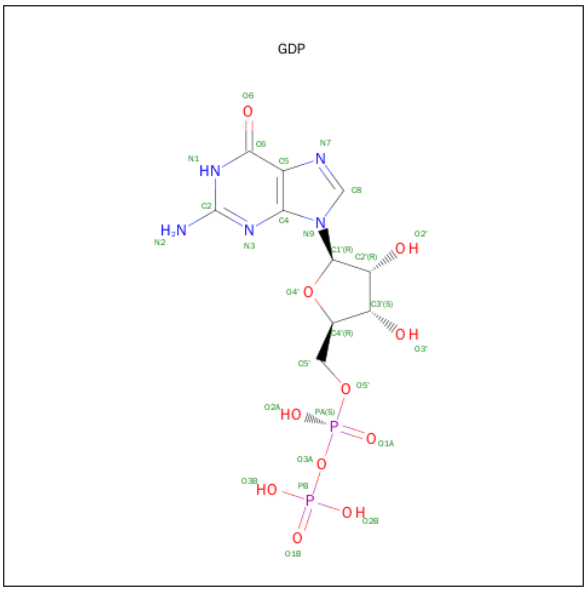
- Molecule 2 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	2	0
			625	395	119	106	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	LYS	ALA	ENGINEERED	UNP P04049

- 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		

- 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		

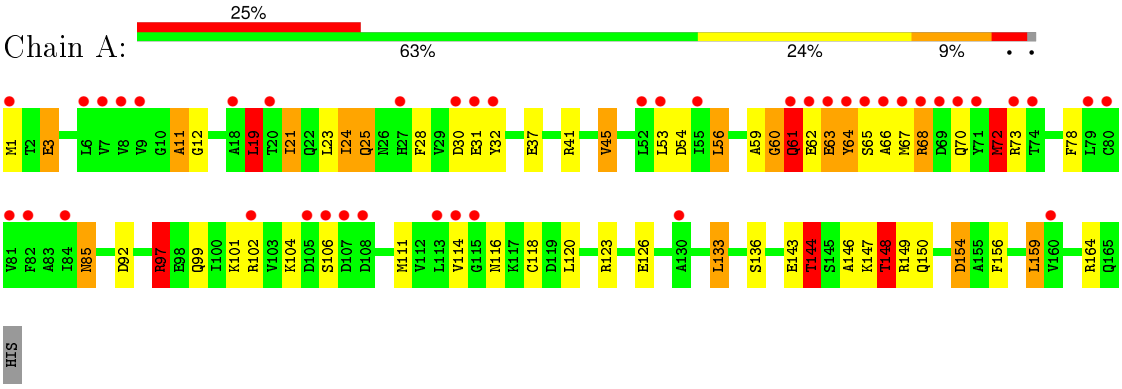
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	13	Total	O	0	0
			13	13		

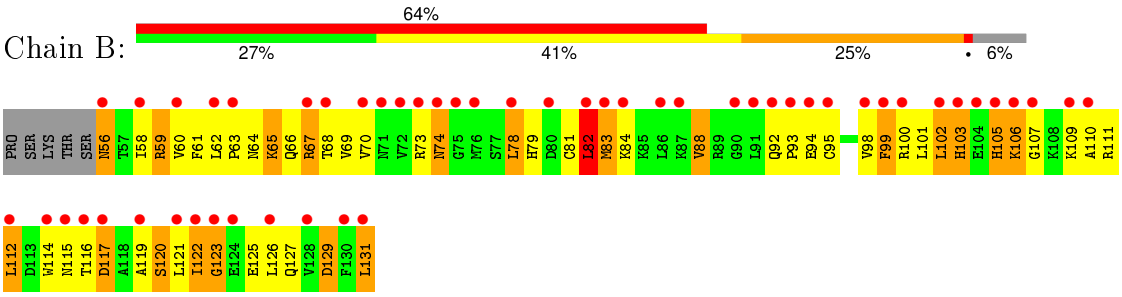
3 Residue-property plots (i)

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: GTPase HRas



- Molecule 2: RAF proto-oncogene serine/threonine-protein kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	91.13Å 91.13Å 277.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.68 – 2.15 19.68 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.68-2.15) 99.8 (19.68-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.264 0.249 , 0.272	Depositor DCC
R_{free} test set	1230 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 64.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 24583 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2005	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% 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	1.37	6/1330 (0.5%)	1.32	16/1795 (0.9%)
2	B	1.10	0/640	1.15	2/857 (0.2%)
All	All	1.29	6/1970 (0.3%)	1.27	18/2652 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	GLN	CG-CD	10.25	1.74	1.51
1	A	126	GLU	CB-CG	6.24	1.64	1.52
1	A	143	GLU	CB-CG	6.11	1.63	1.52
1	A	3	GLU	CG-CD	5.28	1.59	1.51
1	A	114	VAL	CB-CG2	5.16	1.63	1.52
1	A	118	CYS	CB-SG	5.16	1.91	1.82

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ASP	CB-CG-OD1	-8.69	110.48	118.30
1	A	97	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	97	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	64	TYR	N-CA-C	-6.83	92.56	111.00
1	A	123	ARG	NE-CZ-NH1	6.50	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	131	LEU	CA-CB-CG	6.36	129.93	115.30
2	B	82	LEU	CA-CB-CG	-6.20	101.04	115.30
1	A	164	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	97	ARG	CG-CD-NE	5.91	124.21	111.80
1	A	92	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	148	THR	N-CA-CB	-5.56	99.74	110.30
1	A	133	LEU	CB-CG-CD2	5.38	120.14	111.00
1	A	92	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	19	LEU	CB-CG-CD1	5.17	119.80	111.00
1	A	144	THR	N-CA-CB	-5.17	100.48	110.30
1	A	159	LEU	CB-CG-CD2	5.13	119.72	111.00
1	A	45	VAL	CB-CA-C	5.03	120.96	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	GLN	Peptide
1	A	62	GLU	Peptide
1	A	63	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1312	0	1288	51	0
2	B	625	0	660	98	0
3	A	28	0	12	1	0
4	A	1	0	0	0	0
5	A	26	0	0	1	1
5	B	13	0	0	4	0
All	All	2005	0	1960	149	1

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 38.

All (149) 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:25:GLN:CG	1:A:25:GLN:CD	1.74	1.50
1:A:61:GLN:O	1:A:63:GLU:HA	1.25	1.29
2:B:67[A]:ARG:HG2	2:B:67[A]:ARG:NH1	1.50	1.09
2:B:100:ARG:NH2	2:B:116:THR:HG21	1.70	1.06
2:B:67[A]:ARG:CG	2:B:67[A]:ARG:HH11	1.68	1.05
2:B:67[B]:ARG:HH11	2:B:67[B]:ARG:HG3	0.95	1.05
2:B:100:ARG:HH21	2:B:116:THR:HG21	1.24	1.00
2:B:99:PHE:HZ	2:B:129:ASP:HB2	1.26	1.00
2:B:101:LEU:HD21	2:B:109:LYS:HG2	1.46	0.97
2:B:67[B]:ARG:HE	2:B:69:VAL:HG22	1.26	0.97
1:A:148:THR:HG22	1:A:150:GLN:H	1.32	0.94
1:A:61:GLN:O	1:A:63:GLU:CA	2.18	0.91
2:B:100:ARG:NH2	2:B:116:THR:CG2	2.33	0.91
3:A:170:GDP:O3B	5:A:501:HOH:O	1.86	0.91
2:B:67[B]:ARG:HH11	2:B:67[B]:ARG:CG	1.84	0.90
1:A:63:GLU:HB3	1:A:64:TYR:CD2	2.08	0.88
2:B:67[B]:ARG:HG3	2:B:67[B]:ARG:NH1	1.77	0.88
2:B:100:ARG:HG3	2:B:112:LEU:HD21	1.56	0.88
1:A:61:GLN:C	1:A:63:GLU:HA	1.95	0.86
2:B:101:LEU:CD2	2:B:109:LYS:HG2	2.05	0.85
2:B:99:PHE:CZ	2:B:129:ASP:HB2	2.11	0.85
1:A:19:LEU:HD11	1:A:144:THR:HG23	1.58	0.84
2:B:67[A]:ARG:HG2	2:B:67[A]:ARG:HH11	0.74	0.84
2:B:67[B]:ARG:HE	2:B:69:VAL:CG2	1.91	0.83
2:B:100:ARG:HH21	2:B:116:THR:CG2	1.93	0.80
1:A:99:GLN:NE2	1:A:102:ARG:HH22	1.80	0.80
2:B:98:VAL:O	2:B:112:LEU:HB2	1.84	0.77
2:B:64:ASN:O	2:B:65:LYS:HB2	1.84	0.76
1:A:148:THR:CG2	1:A:150:GLN:H	1.97	0.76
1:A:67:MET:SD	1:A:68:ARG:HG3	2.26	0.76
2:B:59:ARG:HH21	2:B:125:GLU:HG3	1.51	0.75
1:A:41:ARG:HD3	1:A:54:ASP:OD1	1.87	0.75
2:B:103:HIS:CE1	5:B:502:HOH:O	2.39	0.74
1:A:99:GLN:HE22	1:A:102:ARG:HH22	1.35	0.74
1:A:19:LEU:HD11	1:A:144:THR:CG2	2.17	0.73
2:B:62:LEU:O	5:B:505:HOH:O	2.06	0.73
1:A:59:ALA:O	1:A:60:GLY:O	2.08	0.72
2:B:101:LEU:CD2	2:B:109:LYS:CG	2.72	0.68
2:B:78[B]:LEU:CD1	2:B:112:LEU:HD12	2.23	0.68
2:B:103:HIS:HA	2:B:107:GLY:H	1.59	0.68
2:B:99:PHE:HB2	5:B:529:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78[A]:LEU:HD21	2:B:121:LEU:HD11	1.77	0.67
2:B:81:CYS:SG	2:B:82:LEU:HD12	2.34	0.67
2:B:67[B]:ARG:NE	2:B:69:VAL:CG2	2.58	0.67
1:A:116:ASN:OD1	1:A:144:THR:CG2	2.42	0.67
2:B:56:ASN:HA	2:B:122:ILE:HG23	1.78	0.66
2:B:60:VAL:HG21	2:B:82:LEU:HD11	1.78	0.65
2:B:78[A]:LEU:HD21	2:B:121:LEU:CD1	2.26	0.65
1:A:19:LEU:HD13	1:A:146:ALA:HB2	1.78	0.65
1:A:37:GLU:OE2	2:B:67[B]:ARG:NH1	2.30	0.65
2:B:101:LEU:HD12	2:B:125:GLU:OE2	1.98	0.64
1:A:73:ARG:HH11	1:A:104:LYS:HZ1	1.45	0.64
2:B:67[B]:ARG:HH21	2:B:69:VAL:HG21	1.62	0.63
1:A:85:ASN:H	1:A:85:ASN:HD22	1.45	0.63
2:B:100:ARG:CG	2:B:112:LEU:HD21	2.28	0.63
1:A:116:ASN:HA	1:A:144:THR:HG22	1.82	0.62
1:A:61:GLN:C	1:A:63:GLU:CA	2.66	0.61
2:B:78[B]:LEU:HD13	2:B:112:LEU:HD12	1.81	0.61
2:B:100:ARG:HB2	2:B:110:ALA:HB3	1.82	0.61
2:B:100:ARG:O	2:B:110:ALA:HB3	2.01	0.60
2:B:112:LEU:N	2:B:112:LEU:HD23	2.16	0.60
2:B:59:ARG:HH11	2:B:59:ARG:HG3	1.67	0.60
2:B:67[B]:ARG:NE	2:B:69:VAL:HG22	2.06	0.60
2:B:59:ARG:NH1	2:B:59:ARG:HG3	2.16	0.59
2:B:122:ILE:CG2	2:B:122:ILE:O	2.49	0.59
2:B:100:ARG:NE	2:B:112:LEU:HD21	2.18	0.58
2:B:79:HIS:O	2:B:83:MET:HB2	2.02	0.58
2:B:58:ILE:HB	2:B:70:VAL:HG23	1.84	0.58
2:B:67[B]:ARG:HH21	2:B:69:VAL:CG2	2.16	0.57
2:B:111:ARG:C	2:B:112:LEU:HD23	2.25	0.57
2:B:100:ARG:HH22	2:B:116:THR:CG2	2.16	0.56
2:B:122:ILE:HG22	2:B:122:ILE:O	2.06	0.56
2:B:102:LEU:HD11	2:B:110:ALA:HB2	1.88	0.56
1:A:116:ASN:OD1	1:A:144:THR:HG23	2.05	0.56
2:B:100:ARG:HG3	2:B:112:LEU:CD2	2.34	0.56
1:A:12:GLY:HA2	1:A:60:GLY:HA3	1.88	0.56
1:A:73:ARG:NH1	1:A:104:LYS:HE3	2.21	0.55
2:B:103:HIS:HB2	2:B:106:LYS:HZ3	1.71	0.54
1:A:11:ALA:HA	1:A:61:GLN:HG3	1.87	0.54
2:B:78[B]:LEU:HD11	2:B:112:LEU:HD12	1.89	0.53
1:A:25:GLN:CG	1:A:25:GLN:NE2	2.68	0.53
2:B:59:ARG:NH2	2:B:125:GLU:HG3	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PHE:O	2:B:127:GLN:HA	2.09	0.53
1:A:116:ASN:OD1	1:A:144:THR:HG22	2.09	0.52
2:B:100:ARG:HE	2:B:112:LEU:HD21	1.74	0.52
2:B:100:ARG:HG2	2:B:126:LEU:CD2	2.40	0.51
1:A:65:SER:O	1:A:67:MET:N	2.40	0.51
1:A:73:ARG:HH11	1:A:104:LYS:NZ	2.09	0.51
2:B:101:LEU:CD2	5:B:529:HOH:O	2.57	0.51
1:A:99:GLN:NE2	1:A:102:ARG:NH2	2.56	0.50
2:B:78[A]:LEU:HD12	2:B:112:LEU:HD12	1.93	0.50
1:A:61:GLN:HA	1:A:63:GLU:O	2.12	0.50
1:A:25:GLN:CD	1:A:25:GLN:CB	2.72	0.50
2:B:100:ARG:CD	2:B:112:LEU:HD21	2.42	0.50
2:B:67[B]:ARG:HD2	2:B:68:THR:N	2.28	0.49
1:A:73:ARG:NH1	1:A:104:LYS:CE	2.76	0.49
1:A:68:ARG:HB2	1:A:72:MET:HE3	1.94	0.48
1:A:23:LEU:HD22	1:A:156:PHE:CG	2.48	0.48
2:B:59:ARG:HD2	2:B:59:ARG:C	2.34	0.48
2:B:127:GLN:NE2	2:B:129:ASP:OD2	2.46	0.48
2:B:63:PRO:O	2:B:64:ASN:HB2	2.14	0.48
2:B:64:ASN:O	2:B:65:LYS:CB	2.58	0.48
2:B:121:LEU:O	2:B:123:GLY:N	2.37	0.48
2:B:67[B]:ARG:NH2	2:B:69:VAL:CG2	2.76	0.48
2:B:67[A]:ARG:NH1	2:B:67[A]:ARG:CG	2.38	0.48
2:B:61:PHE:HB2	2:B:127:GLN:HB2	1.95	0.47
2:B:101:LEU:CD1	2:B:125:GLU:OE2	2.62	0.47
2:B:112:LEU:CD2	2:B:112:LEU:N	2.73	0.47
2:B:84:LYS:O	2:B:88:VAL:HG22	2.14	0.46
2:B:67[B]:ARG:NH2	2:B:69:VAL:HG21	2.30	0.46
2:B:99:PHE:HZ	2:B:129:ASP:CB	2.14	0.46
2:B:83:MET:HG2	2:B:93:PRO:HG3	1.97	0.46
1:A:149:ARG:O	1:A:150:GLN:C	2.53	0.46
2:B:103:HIS:CB	2:B:106:LYS:HZ3	2.28	0.46
1:A:148:THR:HG22	1:A:150:GLN:N	2.15	0.46
2:B:100:ARG:NH2	2:B:116:THR:HG22	2.29	0.45
2:B:103:HIS:HB3	2:B:106:LYS:NZ	2.31	0.45
2:B:100:ARG:HE	2:B:112:LEU:CD2	2.30	0.45
2:B:62:LEU:N	2:B:66:GLN:O	2.31	0.45
2:B:92:GLN:HB2	2:B:95:CYS:HB2	1.98	0.45
1:A:24:ILE:HG22	1:A:25:GLN:HB2	1.99	0.44
1:A:78:PHE:HB2	1:A:111:MET:HE2	1.98	0.44
2:B:56:ASN:HD22	2:B:56:ASN:N	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:HD2	1:A:73:ARG:HA	1.81	0.44
1:A:37:GLU:OE1	1:A:56:LEU:HD21	2.18	0.44
1:A:73:ARG:HH11	1:A:104:LYS:CE	2.30	0.44
1:A:32:TYR:C	1:A:32:TYR:CD1	2.90	0.43
1:A:41:ARG:HD3	1:A:54:ASP:CG	2.39	0.43
2:B:103:HIS:CB	2:B:106:LYS:NZ	2.80	0.43
1:A:97:ARG:O	1:A:101:LYS:HG3	2.19	0.43
2:B:119:ALA:C	2:B:121:LEU:H	2.22	0.43
2:B:103:HIS:HB3	2:B:106:LYS:HZ2	1.84	0.43
1:A:28:PHE:CD1	1:A:147:LYS:HA	2.53	0.43
1:A:21:ILE:HD13	1:A:21:ILE:N	2.33	0.42
2:B:78[B]:LEU:HD21	2:B:98:VAL:HG11	2.01	0.42
2:B:56:ASN:HA	2:B:122:ILE:CG2	2.48	0.42
1:A:63:GLU:OE2	1:A:64:TYR:HD2	2.03	0.42
2:B:56:ASN:CA	2:B:122:ILE:HG23	2.48	0.42
2:B:74:ASN:HA	2:B:74:ASN:HD22	1.71	0.42
2:B:64:ASN:O	2:B:65:LYS:HD3	2.20	0.41
1:A:99:GLN:CD	1:A:102:ARG:NH2	2.74	0.41
2:B:78[B]:LEU:CD2	2:B:114:TRP:HA	2.51	0.41
1:A:59:ALA:H	1:A:67:MET:HE1	1.86	0.41
2:B:59:ARG:HG2	2:B:69:VAL:HG22	2.02	0.41
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.84	0.41
2:B:100:ARG:HG2	2:B:126:LEU:HD22	2.02	0.40
2:B:65:LYS:C	2:B:67[A]:ARG:HH12	2.23	0.40
2:B:92:GLN:HA	2:B:93:PRO:HD2	1.77	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:539:HOH:O	5:A:541:HOH:O[18_444]	1.16	1.04

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	163/166 (98%)	148 (91%)	10 (6%)	5 (3%)	5 1
2	B	76/81 (94%)	59 (78%)	11 (14%)	6 (8%)	1 0
All	All	239/247 (97%)	207 (87%)	21 (9%)	11 (5%)	3 0

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLY
1	A	66	ALA
1	A	72	MET
2	B	65	LYS
2	B	105	HIS
2	B	120	SER
2	B	122	ILE
1	A	11	ALA
1	A	70	GLN
2	B	117	ASP
2	B	123	GLY

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	143/144 (99%)	121 (85%)	22 (15%)	3 1
2	B	70/73 (96%)	47 (67%)	23 (33%)	0 0
All	All	213/217 (98%)	168 (79%)	45 (21%)	1 0

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	21	ILE
1	A	24	ILE
1	A	30	ASP
1	A	31	GLU
1	A	45	VAL
1	A	53	LEU
1	A	56	LEU
1	A	61	GLN
1	A	68	ARG
1	A	72	MET
1	A	85	ASN
1	A	97	ARG
1	A	106	SER
1	A	133	LEU
1	A	136	SER
1	A	144	THR
1	A	148	THR
1	A	154	ASP
1	A	159	LEU
2	B	56	ASN
2	B	59	ARG
2	B	67[A]	ARG
2	B	67[B]	ARG
2	B	73	ARG
2	B	74	ASN
2	B	78[A]	LEU
2	B	78[B]	LEU
2	B	82	LEU
2	B	83	MET
2	B	88	VAL
2	B	94	GLU
2	B	99	PHE
2	B	102	LEU
2	B	103	HIS
2	B	105	HIS
2	B	106	LYS
2	B	112	LEU
2	B	115	ASN
2	B	117	ASP
2	B	120	SER
2	B	129	ASP

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Mol	Chain	Res	Type
2	B	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	99	GLN
1	A	150	GLN
2	B	56	ASN
2	B	71	ASN
2	B	74	ASN
2	B	103	HIS
2	B	115	ASN

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 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	GDP	A	170	-	23,30,30	1.19	2 (8%)	30,47,47	1.92	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	170	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	170	GDP	C5-C4	3.25	1.47	1.40
3	A	170	GDP	C6-C5	3.35	1.48	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	170	GDP	C5-C6-N1	-4.45	117.50	123.59
3	A	170	GDP	C2'-C1'-N9	-4.39	107.59	114.29
3	A	170	GDP	C6-C5-C4	-3.42	116.81	120.90
3	A	170	GDP	O3'-C3'-C2'	-2.88	102.46	111.83
3	A	170	GDP	C4-C5-N7	-2.84	106.87	109.48
3	A	170	GDP	PA-O3A-PB	-2.30	124.94	132.67
3	A	170	GDP	O3B-PB-O1B	-2.25	103.34	110.58
3	A	170	GDP	C6-N1-C2	4.21	121.78	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	A	170	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	165/166 (99%)	1.41	42 (25%)	1	1	18, 29, 64, 82	0
2	B	76/81 (93%)	3.65	52 (68%)	0	0	35, 52, 61, 65	0
All	All	241/247 (97%)	2.12	94 (39%)	0	1	18, 36, 63, 82	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	LEU	16.7
1	A	66	ALA	16.6
2	B	122	ILE	14.7
2	B	102	LEU	12.9
2	B	105	HIS	9.7
2	B	75	GLY	9.2
2	B	78[A]	LEU	8.1
2	B	104	GLU	7.6
2	B	74	ASN	7.4
1	A	105	ASP	7.0
2	B	103	HIS	6.7
1	A	106	SER	6.7
2	B	106	LYS	6.7
2	B	72	VAL	6.4
2	B	130	PHE	6.4
2	B	93	PRO	6.3
1	A	107	ASP	6.0
1	A	1	MET	5.9
2	B	123	GLY	5.4
1	A	32	TYR	5.4
2	B	91	LEU	5.1
2	B	82	LEU	4.9
2	B	73	ARG	4.9
2	B	92	GLN	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	71	TYR	4.9
2	B	116	THR	4.9
1	A	63	GLU	4.8
2	B	76	MET	4.7
2	B	98	VAL	4.7
1	A	62	GLU	4.6
1	A	79	LEU	4.5
1	A	65	SER	4.4
1	A	67	MET	4.3
1	A	8	VAL	4.2
2	B	95	CYS	4.2
2	B	124	GLU	4.1
1	A	108	ASP	4.1
1	A	9	VAL	4.0
2	B	115	ASN	3.8
1	A	114	VAL	3.8
1	A	102	ARG	3.7
1	A	7	VAL	3.7
2	B	60	VAL	3.7
2	B	112	LEU	3.7
2	B	67[A]	ARG	3.6
2	B	126	LEU	3.4
2	B	71	ASN	3.4
1	A	70	GLN	3.4
1	A	81	VAL	3.4
2	B	58	ILE	3.4
1	A	30	ASP	3.4
2	B	90	GLY	3.4
2	B	119	ALA	3.3
1	A	52	LEU	3.3
1	A	69	ASP	3.3
2	B	114	TRP	3.2
1	A	31	GLU	3.2
1	A	74	THR	3.1
2	B	94	GLU	3.1
1	A	80	CYS	3.1
1	A	64	TYR	3.0
1	A	73	ARG	2.9
2	B	70	VAL	2.9
1	A	68	ARG	2.9
2	B	87	LYS	2.8
2	B	128	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	2.8
2	B	63	PRO	2.7
2	B	84	LYS	2.7
1	A	130	ALA	2.7
1	A	113	LEU	2.7
1	A	53	LEU	2.7
2	B	117	ASP	2.6
1	A	18	ALA	2.6
2	B	62	LEU	2.5
1	A	27	HIS	2.5
2	B	86	LEU	2.5
1	A	61	GLN	2.5
1	A	55	ILE	2.4
2	B	121	LEU	2.4
2	B	68	THR	2.4
1	A	20	THR	2.4
2	B	109	LYS	2.3
1	A	115	GLY	2.3
2	B	56	ASN	2.3
2	B	100	ARG	2.3
2	B	107	GLY	2.3
1	A	82	PHE	2.2
2	B	110	ALA	2.2
1	A	160	VAL	2.2
2	B	83	MET	2.1
1	A	84	ILE	2.1
2	B	99	PHE	2.1
2	B	80	ASP	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
4	MG	A	171	1/1	0.68	0.23	0.91	39,39,39,39	0
3	GDP	A	170	28/28	0.98	0.12	-1.08	17,24,29,31	0

6.5 Other polymers (i)

There are no such residues in this entry.