Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:13 AM GMT

PDB ID	:	2G77
Title	:	Crystal Structure of Gyp1 TBC domain in complex with Rab33 GTPase bound to GDP and AlF3
Authors	:	Pan, X.; Eathiraj, S.; Munson, M.; Lambright, D.G.
Deposited on	:	2006-02-27
Resolution	:	2.26 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:

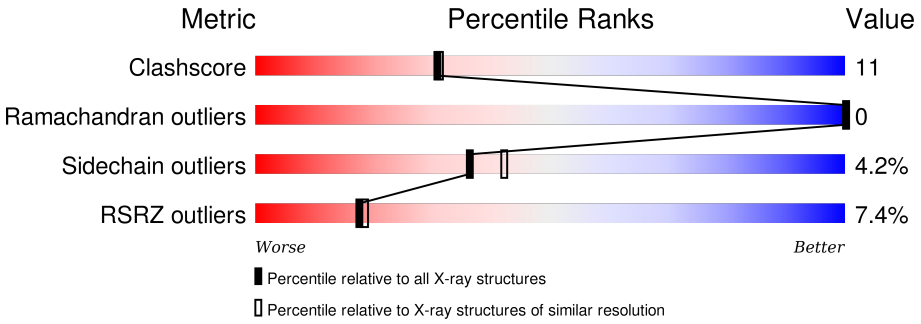
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.26 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	410	4% 68% 12% • 19%
2	B	198	11% 61% 22% 5% 13%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AF3	B	502	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4590 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-activating protein GYP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2767	1786	466	504	11			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	MET	-	CLONING ARTIFACT	UNP Q08484
A	229	GLY	-	CLONING ARTIFACT	UNP Q08484
A	230	HIS	-	CLONING ARTIFACT	UNP Q08484
A	231	HIS	-	CLONING ARTIFACT	UNP Q08484
A	232	HIS	-	CLONING ARTIFACT	UNP Q08484
A	233	HIS	-	CLONING ARTIFACT	UNP Q08484
A	234	HIS	-	CLONING ARTIFACT	UNP Q08484
A	235	HIS	-	CLONING ARTIFACT	UNP Q08484
A	236	GLY	-	CLONING ARTIFACT	UNP Q08484
A	237	SER	-	CLONING ARTIFACT	UNP Q08484
A	238	LEU	-	CLONING ARTIFACT	UNP Q08484
A	239	VAL	-	CLONING ARTIFACT	UNP Q08484
A	240	PRO	-	CLONING ARTIFACT	UNP Q08484
A	241	ARG	-	CLONING ARTIFACT	UNP Q08484
A	242	GLY	-	CLONING ARTIFACT	UNP Q08484
A	243	SER	-	CLONING ARTIFACT	UNP Q08484
A	405	LYS	GLU	ENGINEERED	UNP Q08484

- Molecule 2 is a protein called Ras-related protein Rab-33B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	Se	0	0	0
			1374	869	248	249	4	4			

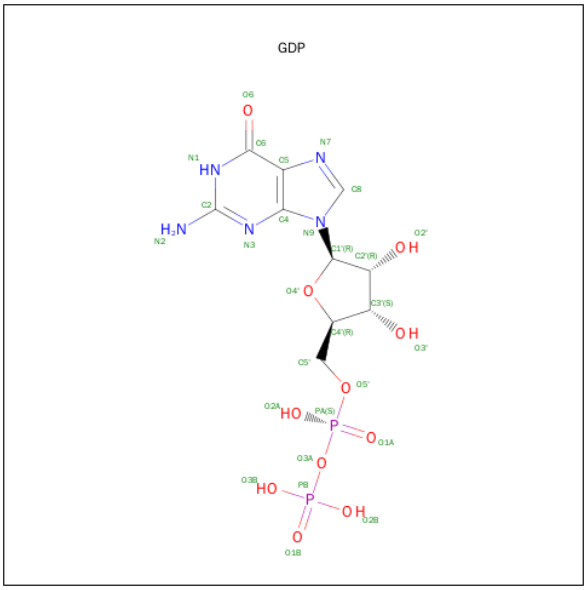
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	MET	-	CLONING ARTIFACT	UNP O35963
B	6	GLY	-	CLONING ARTIFACT	UNP O35963
B	7	HIS	-	CLONING ARTIFACT	UNP O35963
B	8	HIS	-	CLONING ARTIFACT	UNP O35963
B	9	HIS	-	CLONING ARTIFACT	UNP O35963
B	10	HIS	-	CLONING ARTIFACT	UNP O35963
B	11	HIS	-	CLONING ARTIFACT	UNP O35963
B	12	HIS	-	CLONING ARTIFACT	UNP O35963
B	13	GLY	-	CLONING ARTIFACT	UNP O35963
B	116	MSE	MET	MODIFIED RESIDUE	UNP O35963
B	119	MSE	MET	MODIFIED RESIDUE	UNP O35963
B	172	MSE	MET	MODIFIED RESIDUE	UNP O35963
B	193	MSE	MET	MODIFIED RESIDUE	UNP O35963

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

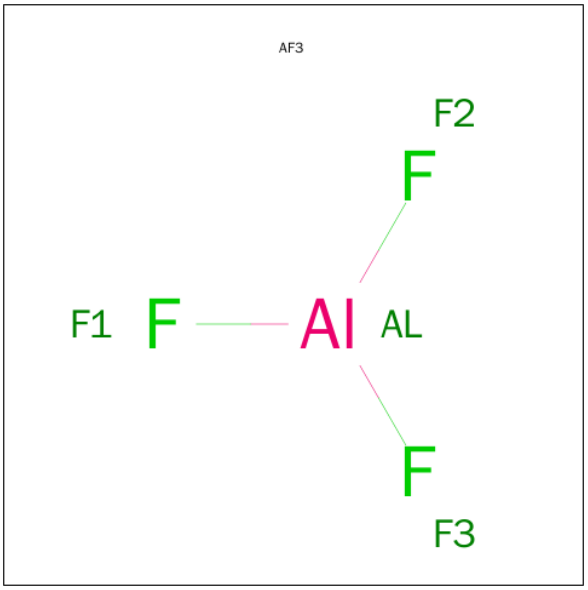
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Al F 4 1 3	0	0

- Molecule 6 is water.

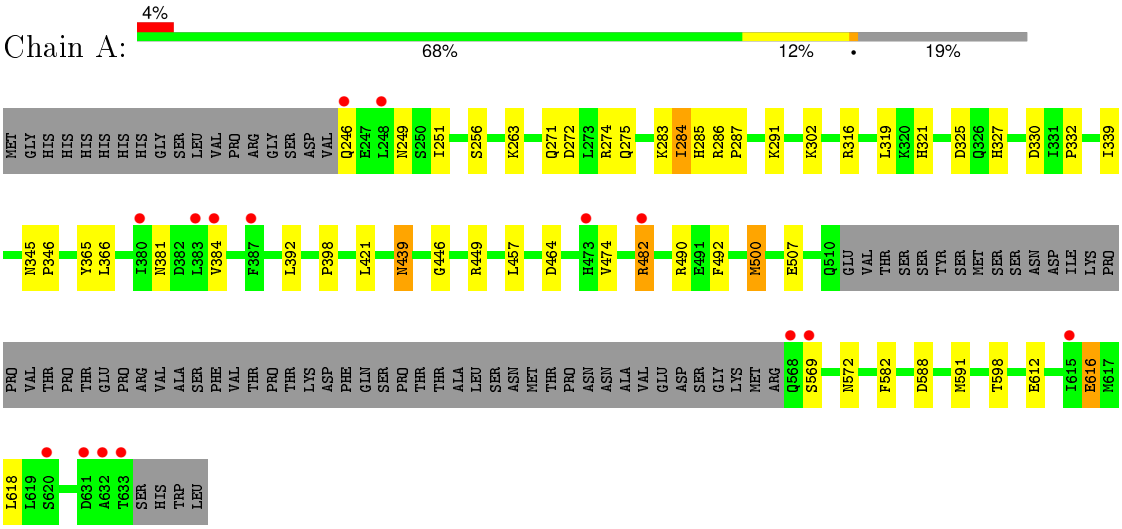
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	284	Total O 284 284	0	0
6	B	132	Total O 132 132	0	0

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.

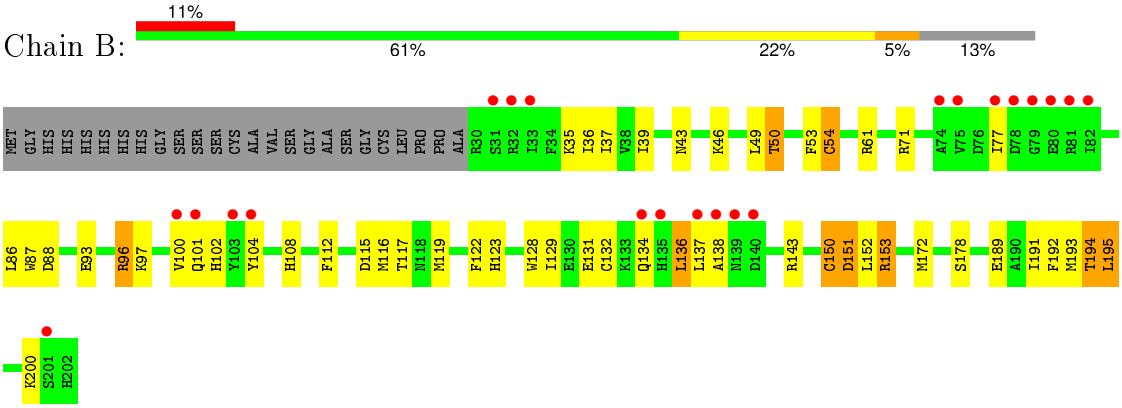
- Molecule 1: GTPase-activating protein GYP1

Chain A:



- Molecule 2: Ras-related protein Rab-33B

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.20Å 94.53Å 102.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.26 47.26 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.7 (8.00-2.26) 98.5 (47.26-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.10 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.244 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.957	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 32968 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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, AF3

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	1.03	4/2840 (0.1%)	0.88	7/3857 (0.2%)
2	B	0.91	4/1400 (0.3%)	0.87	3/1887 (0.2%)
All	All	0.99	8/4240 (0.2%)	0.88	10/5744 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	150	CYS	CB-SG	-7.25	1.70	1.82
1	A	612	GLU	CB-CG	6.63	1.64	1.52
2	B	54	CYS	CB-SG	-6.16	1.71	1.82
1	A	616	GLU	CG-CD	5.72	1.60	1.51
2	B	150	CYS	C-N	-5.60	1.21	1.34
1	A	612	GLU	CD-OE2	5.26	1.31	1.25
1	A	612	GLU	CG-CD	5.12	1.59	1.51
2	B	189	GLU	CG-CD	5.05	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	A	482	ARG	NE-CZ-NH1	9.47	125.03	120.30
2	B	153	ARG	NE-CZ-NH1	-9.35	115.63	120.30
1	A	286	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	272	ASP	CB-CG-OD1	6.07	123.76	118.30
2	B	115	ASP	CB-CG-OD1	5.59	123.33	118.30
2	B	151	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	316	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	272	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	392	LEU	CB-CG-CD1	-5.24	102.10	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2767	0	2704	37	0
2	B	1374	0	1341	54	0
3	B	1	0	0	0	0
4	B	28	0	12	0	0
5	B	4	0	0	0	0
6	A	284	0	0	12	0
6	B	132	0	0	8	0
All	All	4590	0	4057	90	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 11.

All (90) 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:B:136:LEU:HD21	2:B:138:ALA:O	1.45	1.17
2:B:150:CYS:HB2	6:B:614:HOH:O	1.50	1.11
2:B:77:ILE:HB	2:B:200:LYS:HD2	1.43	0.99
1:A:366:LEU:HB2	6:A:920:HOH:O	1.64	0.97
2:B:35:LYS:H	2:B:108:HIS:HD2	1.12	0.96
2:B:77:ILE:O	2:B:200:LYS:HE3	1.64	0.96
1:A:284:ILE:HD11	1:A:398:PRO:HB3	1.47	0.93
1:A:325:ASP:HB2	6:A:705:HOH:O	1.68	0.92
1:A:616:GLU:HG3	6:A:827:HOH:O	1.69	0.91
2:B:119:MSE:CE	2:B:122:PHE:HD2	1.85	0.89
2:B:119:MSE:HE3	2:B:122:PHE:HD2	1.36	0.88
2:B:46:LYS:O	2:B:50:THR:HG23	1.75	0.84
2:B:136:LEU:CD2	2:B:138:ALA:O	2.28	0.80
2:B:119:MSE:CE	2:B:122:PHE:CD2	2.65	0.79
2:B:119:MSE:HE2	2:B:123:HIS:NE2	1.99	0.78
2:B:35:LYS:H	2:B:108:HIS:CD2	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:LEU:HG	2:B:137:LEU:H	1.50	0.75
1:A:327:HIS:HE1	1:A:365:TYR:OH	1.69	0.75
1:A:482:ARG:HD3	1:A:490:ARG:HB2	1.70	0.74
1:A:275:GLN:HG3	6:A:918:HOH:O	1.90	0.71
2:B:93:GLU:OE2	2:B:97:LYS:NZ	2.24	0.70
2:B:119:MSE:HE3	2:B:122:PHE:CD2	2.22	0.70
2:B:119:MSE:HE1	2:B:122:PHE:CD2	2.27	0.70
1:A:285:HIS:HD2	6:A:856:HOH:O	1.75	0.70
2:B:193:MSE:HA	2:B:193:MSE:HE2	1.73	0.70
2:B:136:LEU:HG	2:B:137:LEU:N	2.08	0.69
2:B:136:LEU:CD2	2:B:138:ALA:H	2.07	0.67
1:A:482:ARG:HD3	1:A:490:ARG:CB	2.25	0.67
1:A:464:ASP:HB3	1:A:591:MET:HE1	1.77	0.66
2:B:77:ILE:CB	2:B:200:LYS:HD2	2.22	0.65
2:B:101:GLN:OE1	2:B:102:HIS:HD2	1.79	0.65
2:B:131:GLU:HG2	6:B:635:HOH:O	1.98	0.63
2:B:53:PHE:CD1	2:B:192:PHE:HB2	2.35	0.62
2:B:194:THR:HG23	6:B:572:HOH:O	2.00	0.61
1:A:271:GLN:HE22	1:A:274:ARG:HH11	1.51	0.59
2:B:191:ILE:O	2:B:194:THR:HG22	2.03	0.59
2:B:96:ARG:HG3	2:B:128:TRP:CH2	2.38	0.58
1:A:572:ASN:ND2	6:A:888:HOH:O	2.36	0.58
2:B:116:MSE:SE	2:B:150:CYS:HB3	2.56	0.56
1:A:284:ILE:HD11	1:A:398:PRO:CB	2.29	0.56
2:B:150:CYS:CB	6:B:614:HOH:O	2.28	0.55
2:B:36:ILE:HD13	2:B:195:LEU:HD13	1.88	0.55
2:B:117:THR:HG21	2:B:152:LEU:HB2	1.89	0.55
2:B:36:ILE:HB	2:B:86:LEU:HD23	1.89	0.55
1:A:464:ASP:C	1:A:591:MET:HE1	2.28	0.53
2:B:192:PHE:CD2	2:B:193:MSE:HE3	2.43	0.53
2:B:96:ARG:O	2:B:100:VAL:HG12	2.08	0.53
2:B:131:GLU:HB3	6:B:635:HOH:O	2.09	0.53
1:A:263:LYS:HE2	6:A:882:HOH:O	2.09	0.52
2:B:104:TYR:HE2	2:B:132:CYS:SG	2.33	0.51
1:A:439:ASN:HD22	1:A:446:GLY:HA3	1.76	0.51
1:A:246:GLN:CB	1:A:249:ASN:HB3	2.40	0.50
1:A:339:ILE:HD12	2:B:43:ASN:HB2	1.94	0.50
1:A:284:ILE:CD1	1:A:398:PRO:HB3	2.31	0.50
2:B:136:LEU:HD21	2:B:138:ALA:H	1.77	0.49
2:B:61:ARG:HD2	6:B:531:HOH:O	2.12	0.49
1:A:327:HIS:CE1	1:A:365:TYR:OH	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TYR:HE2	2:B:132:CYS:HG	1.60	0.49
1:A:275:GLN:CG	6:A:918:HOH:O	2.56	0.47
2:B:119:MSE:HE2	2:B:123:HIS:CD2	2.51	0.46
2:B:102:HIS:HB2	6:B:622:HOH:O	2.15	0.46
1:A:492:PHE:CE2	1:A:500:MET:HE1	2.51	0.46
2:B:39:ILE:HD11	2:B:112:PHE:CE2	2.51	0.46
1:A:449:ARG:NH1	6:A:898:HOH:O	2.48	0.45
1:A:582:PHE:HA	1:A:618:LEU:HD11	1.98	0.45
1:A:287:PRO:O	1:A:291:LYS:HG3	2.16	0.45
1:A:321:HIS:HD2	6:A:666:HOH:O	1.98	0.45
2:B:50:THR:HG21	2:B:88:ASP:HB2	1.98	0.45
2:B:192:PHE:CD2	2:B:193:MSE:CE	3.00	0.45
1:A:474:VAL:HG21	1:A:598:THR:HG21	1.99	0.45
1:A:345:ASN:N	1:A:346:PRO:HD3	2.33	0.44
1:A:464:ASP:CB	1:A:591:MET:HE1	2.45	0.44
1:A:492:PHE:CD2	1:A:500:MET:HE1	2.53	0.43
2:B:129:ILE:HD11	2:B:172:MSE:HE1	2.01	0.43
1:A:482:ARG:NH2	6:A:853:HOH:O	2.40	0.43
2:B:136:LEU:CG	2:B:137:LEU:N	2.79	0.42
1:A:330:ASP:OD1	1:A:332:PRO:HD2	2.20	0.42
2:B:136:LEU:HD21	2:B:138:ALA:C	2.31	0.41
2:B:151:ASP:OD1	2:B:178:SER:OG	2.33	0.41
1:A:381:ASN:O	1:A:384:VAL:HG12	2.20	0.41
2:B:77:ILE:CG2	2:B:200:LYS:HD2	2.50	0.41
1:A:582:PHE:CA	1:A:618:LEU:HD11	2.51	0.41
2:B:96:ARG:HD2	2:B:131:GLU:OE1	2.21	0.41
2:B:54:CYS:SG	2:B:86:LEU:HD12	2.60	0.41
2:B:117:THR:CG2	2:B:152:LEU:HB2	2.50	0.41
1:A:507:GLU:OE2	1:A:569:SER:HB3	2.21	0.41
2:B:153:ARG:HB2	6:B:608:HOH:O	2.20	0.41
2:B:37:ILE:HG22	2:B:87:TRP:HB2	2.02	0.41
1:A:271:GLN:HE22	1:A:274:ARG:NH1	2.17	0.40
1:A:283:LYS:HE3	6:A:813:HOH:O	2.21	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	327/410 (80%)	319 (98%)	8 (2%)	0	100	100
2	B	171/198 (86%)	162 (95%)	9 (5%)	0	100	100
All	All	498/608 (82%)	481 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	308/386 (80%)	298 (97%)	10 (3%)	46	57
2	B	146/166 (88%)	137 (94%)	9 (6%)	23	22
All	All	454/552 (82%)	435 (96%)	19 (4%)	36	42

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	ILE
1	A	256	SER
1	A	284	ILE
1	A	302	LYS
1	A	319	LEU
1	A	421	LEU
1	A	439	ASN
1	A	457	LEU

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Mol	Chain	Res	Type
1	A	500	MET
1	A	588	ASP
2	B	49	LEU
2	B	50	THR
2	B	71	ARG
2	B	96	ARG
2	B	134	GLN
2	B	136	LEU
2	B	143	ARG
2	B	194	THR
2	B	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	271	GLN
1	A	321	HIS
1	A	327	HIS
1	A	439	ASN
1	A	450	GLN
1	A	453	ASN
1	A	467	ASN
1	A	471	ASN
2	B	102	HIS
2	B	108	HIS
2	B	183	ASN
2	B	197	HIS

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 (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GDP	B	501	3,5	23,30,30	1.42	4 (17%)	30,47,47	2.22	9 (30%)
5	AF3	B	502	3,4,6	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	B	501	3,5	-	0/12/32/32	0/3/3/3
5	AF3	B	502	3,4,6	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	GDP	PB-O3B	-2.07	1.47	1.54
4	B	501	GDP	C5-C4	2.03	1.45	1.40
4	B	501	GDP	O4'-C1'	2.75	1.44	1.41
4	B	501	GDP	C6-C5	4.58	1.50	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	GDP	C4-C5-N7	-5.10	104.78	109.48
4	B	501	GDP	C5-C6-N1	-4.72	117.14	123.59
4	B	501	GDP	C1'-N9-C4	-3.82	121.17	126.94
4	B	501	GDP	N3-C2-N1	-3.29	122.44	127.44
4	B	501	GDP	PA-O3A-PB	-3.14	122.14	132.67
4	B	501	GDP	C6-C5-C4	-2.63	117.76	120.90
4	B	501	GDP	O3B-PB-O1B	2.22	117.72	110.58
4	B	501	GDP	O2A-PA-O3A	2.78	117.71	105.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	501	GDP	C6-N1-C2	5.51	123.58	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	331/410 (80%)	0.05	15 (4%) 37 41	14, 34, 53, 79	5 (1%)
2	B	169/198 (85%)	0.47	22 (13%) 5 4	26, 45, 81, 92	0
All	All	500/608 (82%)	0.19	37 (7%) 17 18	14, 37, 73, 92	5 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	137	LEU	10.5
2	B	79	GLY	8.7
1	A	633	THR	7.1
1	A	482	ARG	6.3
1	A	615	ILE	6.0
2	B	78	ASP	5.4
2	B	135	HIS	4.8
2	B	100	VAL	4.7
1	A	620	SER	4.3
2	B	134	GLN	4.3
1	A	568	GLN	4.1
1	A	569	SER	4.0
2	B	139	ASN	3.9
2	B	81	ARG	3.9
2	B	138	ALA	3.7
2	B	75	VAL	3.3
2	B	77	ILE	3.2
2	B	82	ILE	3.2
1	A	631	ASP	3.2
1	A	246	GLN	3.1
2	B	31	SER	3.1
1	A	632	ALA	2.9
2	B	140	ASP	2.9
1	A	473	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	248	LEU	2.7
1	A	383	LEU	2.6
2	B	101	GLN	2.5
2	B	80	GLU	2.5
1	A	384	VAL	2.4
2	B	104	TYR	2.4
2	B	32	ARG	2.4
1	A	380	ILE	2.2
2	B	103	TYR	2.2
2	B	201	SER	2.1
2	B	33	ILE	2.1
1	A	387	PHE	2.0
2	B	74	ALA	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
5	AF3	B	502	4/4	0.90	0.20	2.81	33,33,41,44	0
4	GDP	B	501	28/28	0.99	0.10	-0.52	22,30,33,34	0
3	MG	B	503	1/1	0.65	0.09	-3.55	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.