Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:02 PM GMT

PDB ID	:	4K81
Title	:	Crystal structure of the Grb14 RA and PH domains in complex with GTP-loaded H-Ras
Authors	:	Qamra, R.; Hubbard, S.R.
Deposited on	:	2013-04-17
Resolution	:	2.40 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:

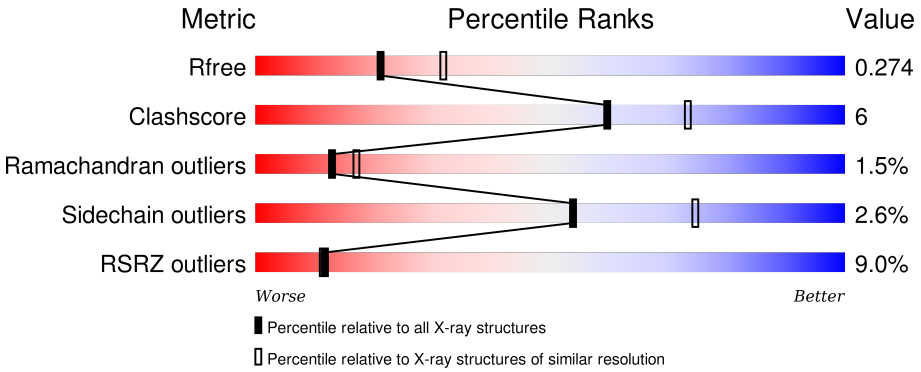
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	258	3% 77% 17% • 5%
1	C	258	6% 76% 17% • 5%
1	E	258	7% 82% 12% • 5%
1	G	258	28% 76% 17% • 5%
2	B	171	4% 89% 10% •

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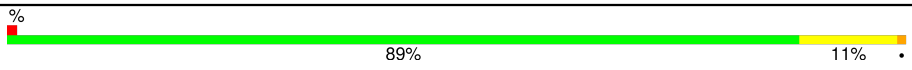
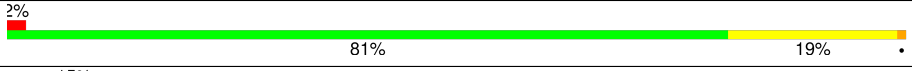
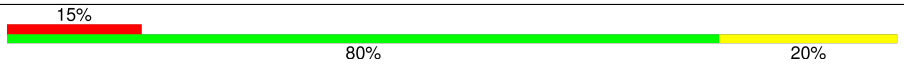
Mol	Chain	Length	Quality of chain
2	D	171	
2	F	171	
2	H	171	

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
3	GOL	A	401	-	-	-	X
3	GOL	A	403	-	-	-	X
3	GOL	C	400	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13867 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 Growth factor receptor-bound protein 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	0	0
			2023	1312	340	361	10			
1	C	244	Total	C	N	O	S	0	0	0
			2023	1312	340	361	10			
1	E	244	Total	C	N	O	S	0	0	0
			2023	1312	340	361	10			
1	G	244	Total	C	N	O	S	0	0	0
			2023	1312	340	361	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLY	-	EXPRESSION TAG	UNP Q14449
A	100	HIS	-	EXPRESSION TAG	UNP Q14449
A	101	MET	-	EXPRESSION TAG	UNP Q14449
A	102	ALA	-	EXPRESSION TAG	UNP Q14449
A	103	SER	-	EXPRESSION TAG	UNP Q14449
A	104	GLY	-	EXPRESSION TAG	UNP Q14449
A	105	SER	-	EXPRESSION TAG	UNP Q14449
A	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
A	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449
C	99	GLY	-	EXPRESSION TAG	UNP Q14449
C	100	HIS	-	EXPRESSION TAG	UNP Q14449
C	101	MET	-	EXPRESSION TAG	UNP Q14449
C	102	ALA	-	EXPRESSION TAG	UNP Q14449
C	103	SER	-	EXPRESSION TAG	UNP Q14449
C	104	GLY	-	EXPRESSION TAG	UNP Q14449
C	105	SER	-	EXPRESSION TAG	UNP Q14449
C	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
C	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449
E	99	GLY	-	EXPRESSION TAG	UNP Q14449
E	100	HIS	-	EXPRESSION TAG	UNP Q14449
E	101	MET	-	EXPRESSION TAG	UNP Q14449

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Chain	Residue	Modelled	Actual	Comment	Reference
E	102	ALA	-	EXPRESSION TAG	UNP Q14449
E	103	SER	-	EXPRESSION TAG	UNP Q14449
E	104	GLY	-	EXPRESSION TAG	UNP Q14449
E	105	SER	-	EXPRESSION TAG	UNP Q14449
E	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
E	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449
G	99	GLY	-	EXPRESSION TAG	UNP Q14449
G	100	HIS	-	EXPRESSION TAG	UNP Q14449
G	101	MET	-	EXPRESSION TAG	UNP Q14449
G	102	ALA	-	EXPRESSION TAG	UNP Q14449
G	103	SER	-	EXPRESSION TAG	UNP Q14449
G	104	GLY	-	EXPRESSION TAG	UNP Q14449
G	105	SER	-	EXPRESSION TAG	UNP Q14449
G	272	ALA	LYS	ENGINEERED MUTATION	UNP Q14449
G	273	ALA	GLU	ENGINEERED MUTATION	UNP Q14449

- Molecule 2 is a protein called GTPase HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			
2	D	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			
2	F	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			
2	H	171	Total	C	N	O	S	0	0	0
			1352	842	233	269	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP P01112
B	-3	ALA	-	EXPRESSION TAG	UNP P01112
B	-2	MET	-	EXPRESSION TAG	UNP P01112
B	-1	GLY	-	EXPRESSION TAG	UNP P01112
B	0	SER	-	EXPRESSION TAG	UNP P01112
B	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112
D	-4	GLY	-	EXPRESSION TAG	UNP P01112
D	-3	ALA	-	EXPRESSION TAG	UNP P01112
D	-2	MET	-	EXPRESSION TAG	UNP P01112
D	-1	GLY	-	EXPRESSION TAG	UNP P01112
D	0	SER	-	EXPRESSION TAG	UNP P01112

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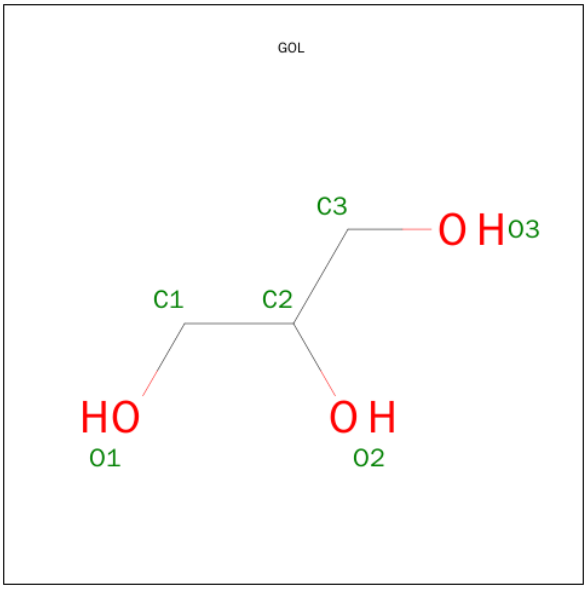
Chain	Residue	Modelled	Actual	Comment	Reference
D	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112
F	-4	GLY	-	EXPRESSION TAG	UNP P01112
F	-3	ALA	-	EXPRESSION TAG	UNP P01112
F	-2	MET	-	EXPRESSION TAG	UNP P01112
F	-1	GLY	-	EXPRESSION TAG	UNP P01112
F	0	SER	-	EXPRESSION TAG	UNP P01112
F	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112
H	-4	GLY	-	EXPRESSION TAG	UNP P01112
H	-3	ALA	-	EXPRESSION TAG	UNP P01112
H	-2	MET	-	EXPRESSION TAG	UNP P01112
H	-1	GLY	-	EXPRESSION TAG	UNP P01112
H	0	SER	-	EXPRESSION TAG	UNP P01112
H	12	VAL	GLY	ENGINEERED MUTATION	UNP P01112

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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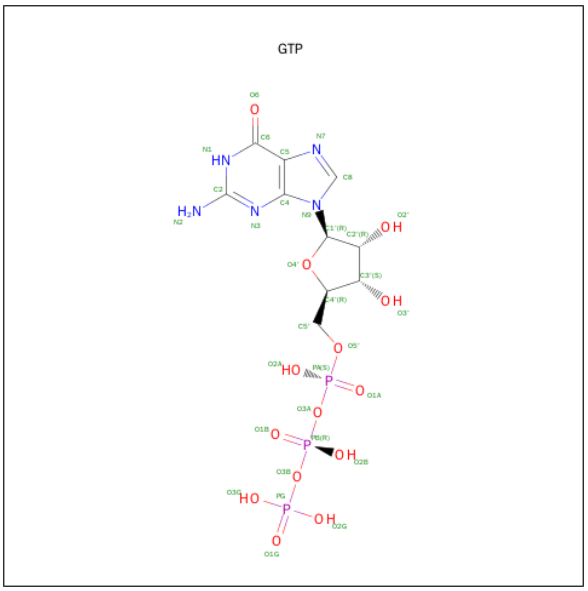
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 32 10 5 14 3	0	0
4	D	1	Total C N O P 32 10 5 14 3	0	0
4	F	1	Total C N O P 32 10 5 14 3	0	0
4	H	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is water.

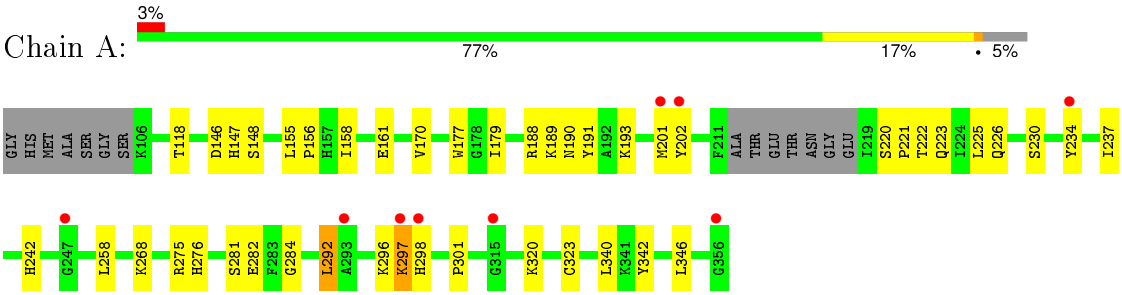
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0
6	B	24	Total O 24 24	0	0
6	C	25	Total O 25 25	0	0
6	D	21	Total O 21 21	0	0
6	E	33	Total O 33 33	0	0
6	F	16	Total O 16 16	0	0
6	G	10	Total O 10 10	0	0
6	H	6	Total O 6 6	0	0

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.

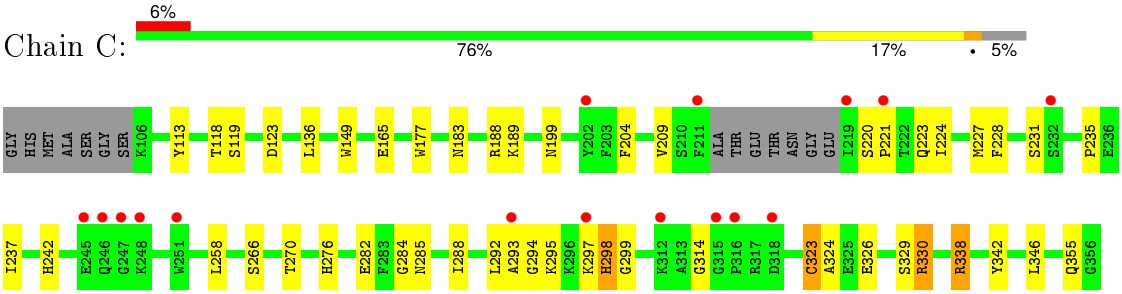
- Molecule 1: Growth factor receptor-bound protein 14

Chain A:



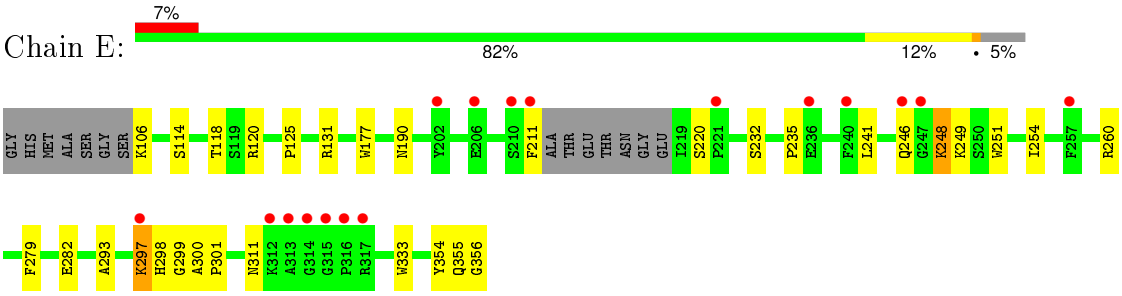
- Molecule 1: Growth factor receptor-bound protein 14

Chain C:



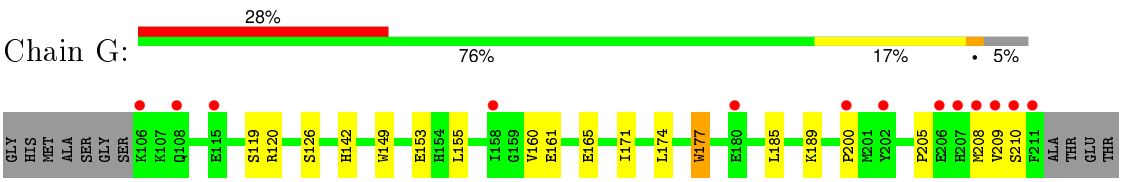
- Molecule 1: Growth factor receptor-bound protein 14

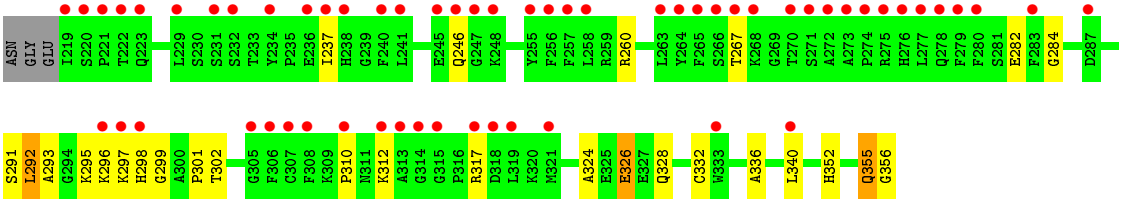
Chain E:



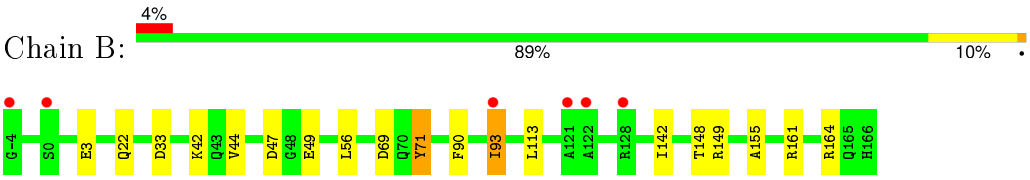
- Molecule 1: Growth factor receptor-bound protein 14

Chain G:

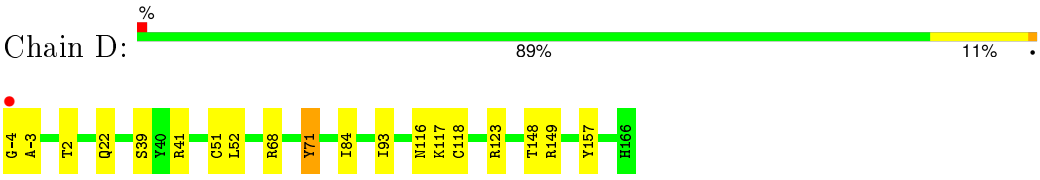




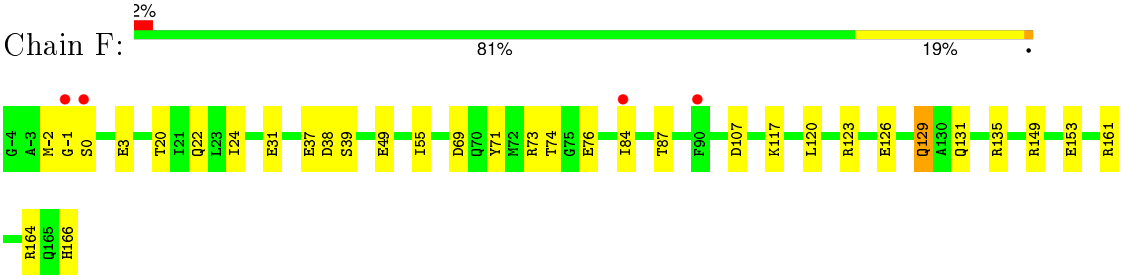
• Molecule 2: GTPase HRas



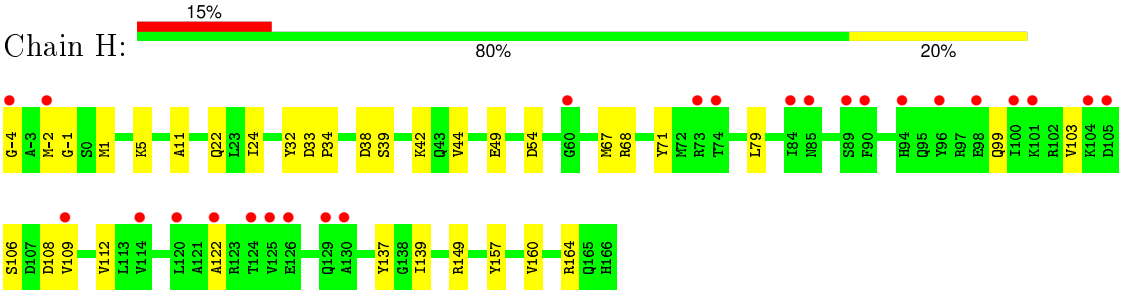
• Molecule 2: GTPase HRas



• Molecule 2: GTPase HRas



• Molecule 2: GTPase HRas



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.73Å 115.59Å 103.11Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 46.81 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.40) 99.6 (46.81-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.219 , 0.277 0.217 , 0.274	Depositor DCC
R_{free} test set	3628 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 71966 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13867	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% 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: GTP, GOL, 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	0.62	0/2083	0.68	0/2808
1	C	0.56	1/2083 (0.0%)	0.64	1/2808 (0.0%)
1	E	0.58	2/2083 (0.1%)	0.64	0/2808
1	G	0.51	1/2083 (0.0%)	0.53	0/2808
2	B	0.48	0/1371	0.63	0/1850
2	D	0.51	0/1371	0.66	0/1850
2	F	0.43	0/1371	0.59	0/1850
2	H	0.36	0/1371	0.53	0/1850
All	All	0.52	4/13816 (0.0%)	0.62	1/18632 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	177	TRP	CD2-CE2	5.25	1.47	1.41
1	G	177	TRP	CD2-CE2	5.23	1.47	1.41
1	C	149	TRP	CD2-CE2	5.22	1.47	1.41
1	E	251	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	338	ARG	NE-CZ-NH2	-5.27	117.67	120.30

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	2023	0	1974	31	0
1	C	2023	0	1974	28	0
1	E	2023	0	1974	15	0
1	G	2023	0	1974	24	0
2	B	1352	0	1326	14	0
2	D	1352	0	1326	16	0
2	F	1352	0	1325	19	0
2	H	1352	0	1326	19	0
3	A	24	0	32	4	0
3	B	6	0	8	1	0
3	C	12	0	16	0	0
3	E	12	0	16	0	0
4	B	32	0	12	0	0
4	D	32	0	12	0	0
4	F	32	0	12	1	0
4	H	32	0	12	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	A	46	0	0	6	0
6	B	24	0	0	2	0
6	C	25	0	0	0	0
6	D	21	0	0	0	0
6	E	33	0	0	1	0
6	F	16	0	0	2	0
6	G	10	0	0	0	0
6	H	6	0	0	1	0
All	All	13867	0	13319	154	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 6.

All (154) 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:342:TYR:HB2	6:A:540:HOH:O	1.56	1.03
1:C:330:ARG:HG2	1:C:330:ARG:HH11	1.28	0.96
1:E:356:GLY:HA2	6:E:507:HOH:O	1.72	0.86
2:D:84:ILE:HD12	2:D:123:ARG:HG2	1.63	0.80
1:A:346:LEU:HG	6:A:540:HOH:O	1.82	0.78
2:B:49:GLU:HB2	2:B:164:ARG:HH22	1.48	0.77
2:D:22:GLN:O	2:D:149:ARG:NH1	2.19	0.75
2:B:3:GLU:O	2:D:-4:GLY:HA3	1.86	0.75
1:E:297:LYS:C	1:E:299:GLY:H	1.91	0.74
2:H:106:SER:HB3	2:H:109:VAL:HG23	1.74	0.69
2:H:137:TYR:HB2	2:H:139:ILE:HG12	1.74	0.69
1:E:120:ARG:HG3	2:F:38:ASP:OD1	1.92	0.69
1:A:275:ARG:HB2	6:A:525:HOH:O	1.92	0.68
2:H:68:ARG:HA	2:H:71:TYR:CE2	2.29	0.67
2:B:93:ILE:HD13	2:B:113:LEU:HD11	1.76	0.67
1:G:237:ILE:HD13	1:G:336:ALA:HB1	1.77	0.65
1:C:118:THR:HB	2:D:39:SER:O	1.97	0.64
6:B:318:HOH:O	1:C:294:GLY:HA2	1.98	0.62
1:C:330:ARG:CG	1:C:330:ARG:HH11	2.09	0.61
1:G:260:ARG:HA	1:G:340:LEU:HD11	1.84	0.60
2:F:0:SER:OG	2:H:-2:MET:HG3	2.02	0.60
2:B:142:ILE:HD12	2:B:155:ALA:HA	1.82	0.60
1:A:220:SER:HB3	1:A:223:GLN:HB2	1.84	0.60
1:G:297:LYS:C	1:G:299:GLY:H	2.05	0.60
2:B:47:ASP:HB3	1:C:295:LYS:HE3	1.86	0.58
1:C:227:MET:O	1:C:235:PRO:HD3	2.03	0.58
2:F:3:GLU:O	2:H:-4:GLY:HA3	2.03	0.58
1:G:352:HIS:O	1:G:355:GLN:NE2	2.37	0.57
1:A:242:HIS:CG	1:A:301:PRO:HG2	2.39	0.57
1:C:165:GLU:OE2	1:C:338:ARG:HD2	2.05	0.56
1:A:268:LYS:HG3	1:A:276:HIS:CD2	2.41	0.56
1:C:330:ARG:HG2	1:C:330:ARG:NH1	2.08	0.56
1:G:174:LEU:O	1:G:177:TRP:HB2	2.06	0.56
2:F:84:ILE:HD13	2:F:123:ARG:HG2	1.89	0.55
2:H:32:TYR:CE1	2:H:34:PRO:HG3	2.41	0.55
2:F:117:LYS:HB3	2:F:120:LEU:HD12	1.89	0.55
1:E:297:LYS:C	1:E:299:GLY:N	2.59	0.54
1:C:242:HIS:HB2	1:C:323:CYS:HB3	1.90	0.53
1:A:190:ASN:HD21	3:A:402:GOL:H11	1.72	0.53
1:G:310:PRO:HG2	1:G:317:ARG:HA	1.90	0.53
2:H:22:GLN:CG	2:H:149:ARG:HG3	2.39	0.52
1:C:266:SER:HA	1:C:276:HIS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:LEU:HD21	1:E:333:TRP:CD1	2.44	0.52
1:A:296:LYS:O	1:A:298:HIS:N	2.37	0.51
1:A:242:HIS:HB2	1:A:323:CYS:HB3	1.93	0.51
1:G:205:PRO:HD2	1:G:208:MET:HG3	1.92	0.51
2:F:131:GLN:O	2:F:135:ARG:HB2	2.10	0.51
2:B:90:PHE:O	2:B:93:ILE:HG13	2.10	0.51
1:E:232:SER:O	1:E:260:ARG:HD3	2.10	0.50
1:E:106:LYS:O	1:E:125:PRO:HA	2.11	0.50
1:C:355:GLN:HA	1:C:355:GLN:OE1	2.12	0.50
4:F:200:GTP:O2G	6:F:310:HOH:O	2.18	0.50
2:D:68:ARG:HA	2:D:71:TYR:CE2	2.47	0.49
1:A:223:GLN:O	1:A:226:GLN:HG2	2.13	0.49
2:H:11:ALA:HB1	6:H:304:HOH:O	2.12	0.49
2:D:84:ILE:HD11	2:D:118:CYS:HA	1.95	0.48
2:B:49:GLU:HB2	2:B:164:ARG:NH2	2.23	0.48
1:C:188:ARG:HG2	1:C:189:LYS:N	2.29	0.48
2:B:148:THR:O	2:B:149:ARG:HB2	2.13	0.48
1:G:153:GLU:O	1:G:161:GLU:HA	2.13	0.48
1:A:146:ASP:HB3	1:A:148:SER:H	1.77	0.48
1:C:123:ASP:O	1:G:356:GLY:HA2	2.14	0.48
1:E:279:PHE:HZ	1:E:282:GLU:HB2	1.79	0.47
1:C:220:SER:HB2	1:C:223:GLN:HB2	1.97	0.47
1:E:131:ARG:NH1	1:E:355:GLN:HG3	2.30	0.47
2:F:20:THR:O	2:F:24:ILE:HG12	2.15	0.47
1:G:155:LEU:HD12	1:G:160:VAL:HG23	1.95	0.47
2:F:149:ARG:NH2	2:F:153:GLU:OE2	2.41	0.47
1:C:342:TYR:HB2	1:C:346:LEU:HG	1.97	0.47
1:A:147:HIS:HA	3:A:401:GOL:H32	1.96	0.47
1:G:119:SER:H	2:H:39:SER:HB3	1.80	0.47
2:D:41:ARG:NH1	2:D:52:LEU:HD21	2.29	0.47
1:A:281:SER:HB2	1:A:320:LYS:HD3	1.96	0.47
2:D:148:THR:O	2:D:149:ARG:HB2	2.15	0.46
1:A:296:LYS:C	1:A:298:HIS:H	2.19	0.46
2:D:157:TYR:N	2:D:157:TYR:CD1	2.83	0.46
3:A:401:GOL:H31	6:A:532:HOH:O	2.15	0.46
2:H:106:SER:CB	2:H:109:VAL:HG23	2.45	0.46
1:G:297:LYS:C	1:G:299:GLY:N	2.68	0.46
2:B:22:GLN:CG	2:B:149:ARG:HG2	2.46	0.46
1:G:326:GLU:HG3	1:G:328:GLN:H	1.81	0.46
1:C:165:GLU:OE1	1:C:342:TYR:CE2	2.68	0.46
1:A:220:SER:O	1:A:223:GLN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:VAL:HG12	1:G:291:SER:HA	1.97	0.45
1:A:161:GLU:OE2	1:A:188:ARG:NH2	2.49	0.45
1:A:201:MET:HB3	1:A:221:PRO:HA	1.98	0.45
2:F:76:GLU:OE2	2:H:-4:GLY:HA2	2.16	0.45
1:A:201:MET:HG3	1:A:202:TYR:CD2	2.52	0.45
1:A:342:TYR:HB2	1:A:346:LEU:HG	1.98	0.45
2:F:22:GLN:O	2:F:149:ARG:NH1	2.47	0.44
1:E:190:ASN:C	1:E:190:ASN:OD1	2.55	0.44
2:F:-2:MET:HA	2:H:1:MET:O	2.17	0.44
1:A:177:TRP:HZ3	3:A:404:GOL:H12	1.82	0.44
2:B:161:ARG:HD2	6:B:321:HOH:O	2.18	0.44
2:F:39:SER:HA	2:F:55:ILE:O	2.16	0.44
2:D:116:ASN:CG	2:D:117:LYS:H	2.21	0.44
1:A:222:THR:HA	1:A:225:LEU:HB3	2.00	0.44
2:D:22:GLN:NE2	2:D:149:ARG:HG3	2.33	0.43
1:A:296:LYS:HG3	1:A:297:LYS:N	2.32	0.43
1:A:193:LYS:CD	6:A:536:HOH:O	2.66	0.43
1:C:284:GLY:O	1:C:285:ASN:HB2	2.17	0.43
1:E:211:PHE:CE1	1:E:235:PRO:HB3	2.52	0.43
2:D:84:ILE:CD1	2:D:118:CYS:HA	2.47	0.43
2:F:84:ILE:HD12	2:F:84:ILE:C	2.39	0.43
2:H:5:LYS:HA	2:H:54:ASP:HB3	2.00	0.43
1:G:149:TRP:CZ2	1:G:189:LYS:HE2	2.54	0.43
2:F:74:THR:HB	6:F:301:HOH:O	2.17	0.43
1:E:248:LYS:HE2	1:E:249:LYS:HE2	2.01	0.43
2:H:44:VAL:HG11	2:H:157:TYR:OH	2.19	0.43
1:G:282:GLU:CD	1:G:284:GLY:H	2.21	0.43
1:A:156:PRO:HD2	6:A:522:HOH:O	2.18	0.43
1:C:227:MET:HG2	1:C:235:PRO:HG3	1.99	0.43
1:G:302:THR:OG1	1:G:324:ALA:O	2.36	0.43
1:A:155:LEU:HD12	1:A:158:ILE:HD11	2.00	0.42
1:C:297:LYS:C	1:C:299:GLY:H	2.22	0.42
1:C:113:TYR:CD1	1:C:119:SER:HB3	2.54	0.42
1:A:237:ILE:HB	1:A:258:LEU:HB3	2.01	0.42
1:G:120:ARG:HG3	2:H:38:ASP:OD1	2.19	0.42
1:G:126:SER:HA	1:G:171:ILE:HG13	2.01	0.42
1:A:282:GLU:HG3	1:A:284:GLY:H	1.85	0.42
1:C:237:ILE:HB	1:C:258:LEU:HB3	2.00	0.42
2:D:41:ARG:HH11	2:D:52:LEU:HD21	1.84	0.42
1:E:300:ALA:HA	1:E:301:PRO:HD3	1.80	0.42
1:C:177:TRP:CD2	1:C:183:ASN:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:ARG:NH2	1:G:296:LYS:HD2	2.35	0.42
1:A:189:LYS:HE2	1:A:191:TYR:OH	2.19	0.42
2:D:22:GLN:HG3	2:D:149:ARG:HG2	2.00	0.42
1:G:174:LEU:HD11	1:G:185:LEU:HD11	2.02	0.42
2:B:33:ASP:OD1	1:E:354:TYR:HE1	2.03	0.42
1:C:165:GLU:HG2	1:C:346:LEU:CD2	2.51	0.41
2:H:160:VAL:O	2:H:164:ARG:HG3	2.20	0.41
2:F:69:ASP:O	2:F:73:ARG:HG3	2.20	0.41
2:B:56:LEU:HD23	2:B:71:TYR:HB2	2.02	0.41
1:G:292:LEU:HB2	1:G:293:ALA:H	1.66	0.41
2:B:49:GLU:CB	2:B:164:ARG:HH22	2.27	0.41
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.20	0.41
2:F:49:GLU:HB3	2:F:164:ARG:NH2	2.36	0.41
2:B:42:LYS:HE3	2:B:44:VAL:HG12	2.02	0.41
2:H:99:GLN:O	2:H:103:VAL:HG23	2.20	0.41
2:D:157:TYR:HD1	2:D:157:TYR:N	2.17	0.41
1:C:295:LYS:HB2	1:C:298:HIS:CD2	2.56	0.41
2:D:116:ASN:CG	2:D:117:LYS:N	2.75	0.41
1:A:234:TYR:CZ	1:A:340:LEU:HB2	2.56	0.41
1:C:324:ALA:HB1	1:C:329:SER:HB3	2.03	0.41
1:G:205:PRO:HD3	1:G:332:CYS:SG	2.61	0.40
1:G:209:VAL:HG12	1:G:210:SER:N	2.36	0.40
1:C:220:SER:HA	1:C:221:PRO:HD3	1.97	0.40
1:E:118:THR:HB	2:F:39:SER:O	2.22	0.40
1:C:204:PHE:HB3	1:C:209:VAL:HG23	2.02	0.40
1:C:224:ILE:O	1:C:228:PHE:HD2	2.04	0.40
2:H:79:LEU:HD12	2:H:112:VAL:HB	2.03	0.40
2:H:24:ILE:CD1	2:H:42:LYS:HB2	2.51	0.40
2:F:126:GLU:N	2:F:129:GLN:OE1	2.33	0.40
1:A:118:THR:HG21	3:B:201:GOL:C1	2.51	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	240/258 (93%)	223 (93%)	15 (6%)	2 (1%)	24 35
1	C	240/258 (93%)	222 (92%)	14 (6%)	4 (2%)	11 14
1	E	240/258 (93%)	222 (92%)	13 (5%)	5 (2%)	9 10
1	G	240/258 (93%)	213 (89%)	19 (8%)	8 (3%)	5 4
2	B	169/171 (99%)	163 (96%)	6 (4%)	0	100 100
2	D	169/171 (99%)	166 (98%)	2 (1%)	1 (1%)	30 43
2	F	169/171 (99%)	161 (95%)	6 (4%)	2 (1%)	16 23
2	H	169/171 (99%)	160 (95%)	7 (4%)	2 (1%)	16 23
All	All	1636/1716 (95%)	1530 (94%)	82 (5%)	24 (2%)	13 17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	293	ALA
1	E	248	LYS
1	C	298	HIS
2	D	-3	ALA
1	E	293	ALA
1	E	298	HIS
1	G	246	GLN
2	H	-1	GLY
2	H	122	ALA
1	C	314	GLY
1	G	295	LYS
1	G	301	PRO
1	G	312	LYS
1	A	292	LEU
1	A	297	LYS
1	E	246	GLN
1	G	200	PRO
1	G	292	LEU
1	G	298	HIS
1	E	297	LYS
2	F	-1	GLY
2	F	37	GLU
1	G	355	GLN
1	C	292	LEU

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	219/228 (96%)	215 (98%)	4 (2%)	66	84
1	C	219/228 (96%)	210 (96%)	9 (4%)	37	57
1	E	219/228 (96%)	215 (98%)	4 (2%)	66	84
1	G	219/228 (96%)	215 (98%)	4 (2%)	66	84
2	B	147/147 (100%)	144 (98%)	3 (2%)	63	81
2	D	147/147 (100%)	143 (97%)	4 (3%)	52	73
2	F	147/147 (100%)	141 (96%)	6 (4%)	37	57
2	H	147/147 (100%)	143 (97%)	4 (3%)	52	73
All	All	1464/1500 (98%)	1426 (97%)	38 (3%)	54	74

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	VAL
1	A	179	ILE
1	A	230	SER
1	A	292	LEU
2	B	69	ASP
2	B	71	TYR
2	B	93	ILE
1	C	136	LEU
1	C	199	ASN
1	C	231	SER
1	C	270	THR
1	C	282	GLU
1	C	288	ILE
1	C	323	CYS
1	C	326	GLU
1	C	330	ARG
2	D	2	THR
2	D	51	CYS
2	D	71	TYR

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Mol	Chain	Res	Type
2	D	93	ILE
1	E	114	SER
1	E	220	SER
1	E	254	ILE
1	E	311	ASN
2	F	31	GLU
2	F	71	TYR
2	F	87	THR
2	F	107	ASP
2	F	129	GLN
2	F	166	HIS
1	G	142	HIS
1	G	165	GLU
1	G	267	THR
1	G	326	GLU
2	H	33	ASP
2	H	49	GLU
2	H	67	MET
2	H	108	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	349	ASN
1	C	298	HIS
1	C	345	GLN
1	C	349	ASN
1	E	207	HIS
1	E	246	GLN
1	E	311	ASN
1	E	345	GLN
1	E	349	ASN
1	E	352	HIS
2	F	61	GLN
2	F	150	GLN
1	G	328	GLN
1	G	349	ASN
1	G	355	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	GOL	A	401	-	5,5,5	0.36	0	5,5,5	0.66	0
3	GOL	A	402	-	5,5,5	0.31	0	5,5,5	0.43	0
3	GOL	A	403	-	5,5,5	0.56	0	5,5,5	0.66	0
3	GOL	A	404	-	5,5,5	0.56	0	5,5,5	0.87	0
3	GOL	B	201	-	5,5,5	0.39	0	5,5,5	0.60	0
4	GTP	B	202	5	25,34,34	1.08	2 (8%)	34,54,54	2.04	12 (35%)
3	GOL	C	400	-	5,5,5	0.36	0	5,5,5	0.58	0
3	GOL	C	401	-	5,5,5	0.23	0	5,5,5	0.49	0
4	GTP	D	200	5	25,34,34	1.17	2 (8%)	34,54,54	1.77	8 (23%)
3	GOL	E	400	-	5,5,5	0.27	0	5,5,5	0.45	0
3	GOL	E	401	-	5,5,5	0.26	0	5,5,5	0.89	0
4	GTP	F	200	5	25,34,34	1.25	2 (8%)	34,54,54	1.94	9 (26%)
4	GTP	H	200	5	25,34,34	1.13	2 (8%)	34,54,54	1.83	8 (23%)

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	GOL	A	401	-	-	0/4/4/4	0/0/0/0
3	GOL	A	402	-	-	0/4/4/4	0/0/0/0
3	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	A	404	-	-	0/4/4/4	0/0/0/0
3	GOL	B	201	-	-	0/4/4/4	0/0/0/0
4	GTP	B	202	5	-	0/18/38/38	0/3/3/3
3	GOL	C	400	-	-	0/4/4/4	0/0/0/0
3	GOL	C	401	-	-	0/4/4/4	0/0/0/0
4	GTP	D	200	5	-	0/18/38/38	0/3/3/3
3	GOL	E	400	-	-	0/4/4/4	0/0/0/0
3	GOL	E	401	-	-	0/4/4/4	0/0/0/0
4	GTP	F	200	5	-	0/18/38/38	0/3/3/3
4	GTP	H	200	5	-	0/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	GTP	C5-C4	3.03	1.47	1.40
4	H	200	GTP	C5-C4	3.17	1.47	1.40
4	F	200	GTP	C5-C4	3.34	1.48	1.40
4	D	200	GTP	C5-C4	3.36	1.48	1.40
4	B	202	GTP	C6-C5	3.59	1.48	1.41
4	H	200	GTP	C6-C5	3.65	1.48	1.41
4	D	200	GTP	C6-C5	3.70	1.48	1.41
4	F	200	GTP	C6-C5	4.11	1.49	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	200	GTP	C5-C6-N1	-4.89	116.91	123.59
4	B	202	GTP	C5-C6-N1	-4.75	117.09	123.59
4	B	202	GTP	C2'-C1'-N9	-4.40	107.57	114.29
4	D	200	GTP	C5-C6-N1	-4.27	117.75	123.59
4	H	200	GTP	C5-C6-N1	-4.00	118.12	123.59
4	F	200	GTP	C4-C5-N7	-3.96	105.83	109.48
4	H	200	GTP	PA-O3A-PB	-3.86	121.89	132.73
4	D	200	GTP	PA-O3A-PB	-3.29	123.48	132.73
4	B	202	GTP	C6-C5-C4	-3.24	117.03	120.90
4	H	200	GTP	N3-C2-N1	-3.24	122.51	127.44
4	H	200	GTP	C6-C5-C4	-3.15	117.13	120.90
4	F	200	GTP	PA-O3A-PB	-3.06	124.14	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	200	GTP	N3-C2-N1	-3.02	122.84	127.44
4	H	200	GTP	C2'-C1'-N9	-2.95	109.78	114.29
4	D	200	GTP	C6-C5-C4	-2.95	117.37	120.90
4	D	200	GTP	N3-C2-N1	-2.93	122.98	127.44
4	D	200	GTP	C4-C5-N7	-2.90	106.81	109.48
4	H	200	GTP	C4-C5-N7	-2.84	106.87	109.48
4	F	200	GTP	C6-C5-C4	-2.83	117.52	120.90
4	B	202	GTP	PA-O3A-PB	-2.77	124.96	132.73
4	B	202	GTP	C4-C5-N7	-2.50	107.18	109.48
4	F	200	GTP	PB-O3B-PG	-2.49	124.33	132.67
4	B	202	GTP	N3-C2-N1	-2.47	123.68	127.44
4	D	200	GTP	PB-O3B-PG	-2.41	124.58	132.67
4	B	202	GTP	C1'-N9-C4	-2.41	123.31	126.94
4	H	200	GTP	PB-O3B-PG	-2.38	124.69	132.67
4	B	202	GTP	O3A-PA-O5'	-2.32	96.79	102.94
4	F	200	GTP	C2'-C1'-N9	-2.24	110.88	114.29
4	B	202	GTP	PB-O3B-PG	-2.23	125.20	132.67
4	F	200	GTP	O3G-PG-O2G	2.18	115.69	107.38
4	B	202	GTP	O3G-PG-O2G	2.37	116.41	107.38
4	D	200	GTP	C4'-O4'-C1'	2.53	112.50	109.72
4	B	202	GTP	O4'-C1'-N9	2.99	114.36	108.10
4	H	200	GTP	C6-N1-C2	4.67	122.42	115.94
4	D	200	GTP	C6-N1-C2	4.76	122.54	115.94
4	F	200	GTP	C6-N1-C2	5.16	123.10	115.94
4	B	202	GTP	C6-N1-C2	5.21	123.18	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	2	0
3	A	402	GOL	1	0
3	A	404	GOL	1	0
3	B	201	GOL	1	0
4	F	200	GTP	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	244/258 (94%)	0.25	9 (3%) 45 46	26, 46, 87, 107	0
1	C	244/258 (94%)	0.39	16 (6%) 22 22	34, 57, 111, 127	0
1	E	244/258 (94%)	0.44	17 (6%) 19 19	29, 55, 95, 136	0
1	G	244/258 (94%)	1.55	72 (29%) 1 1	43, 93, 159, 187	0
2	B	171/171 (100%)	0.18	6 (3%) 48 48	29, 52, 85, 112	0
2	D	171/171 (100%)	0.07	1 (0%) 90 90	29, 47, 73, 103	0
2	F	171/171 (100%)	0.36	4 (2%) 64 63	38, 63, 95, 121	0
2	H	171/171 (100%)	1.15	25 (14%) 3 3	47, 90, 156, 196	0
All	All	1660/1716 (96%)	0.57	150 (9%) 12 11	26, 60, 129, 196	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	257	PHE	9.4
1	G	271	SER	8.8
1	G	297	LYS	8.5
1	G	315	GLY	7.3
1	G	265	PHE	7.1
1	G	246	GLN	7.1
1	G	264	TYR	6.9
1	E	313	ALA	6.8
1	G	207	HIS	6.5
1	G	247	GLY	6.5
1	C	211	PHE	6.3
1	G	266	SER	6.2
1	E	246	GLN	6.2
2	F	-1	GLY	6.1
1	E	316	PRO	6.1
1	E	315	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	211	PHE	5.9
1	G	219	ILE	5.9
1	G	270	THR	5.9
1	G	245	GLU	5.7
1	G	277	LEU	5.6
2	H	130	ALA	5.6
1	G	221	PRO	5.5
1	G	240	PHE	5.5
1	C	246	GLN	5.5
1	G	248	LYS	5.3
1	G	268	LYS	5.3
2	H	90	PHE	5.3
1	E	312	LYS	5.1
2	H	109	VAL	5.1
1	G	272	ALA	5.0
1	G	313	ALA	5.0
1	A	297	LYS	5.0
2	H	96	TYR	4.9
2	H	-2	MET	4.7
2	H	125	VAL	4.7
1	G	276	HIS	4.7
1	G	273	ALA	4.7
1	G	280	PHE	4.6
1	G	333	TRP	4.5
1	E	297	LYS	4.5
1	G	296	LYS	4.4
2	H	126	GLU	4.3
1	E	317	ARG	4.2
1	G	308	PHE	4.2
1	G	209	VAL	4.0
1	G	298	HIS	4.0
2	H	104	LYS	3.9
2	H	100	ILE	3.9
1	C	245	GLU	3.9
1	C	297	LYS	3.8
1	E	314	GLY	3.7
2	H	120	LEU	3.6
2	B	-4	GLY	3.6
1	C	202	TYR	3.5
1	G	220	SER	3.5
1	G	310	PRO	3.5
2	D	-4	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	275	ARG	3.5
2	H	122	ALA	3.4
1	C	221	PRO	3.4
2	H	105	ASP	3.4
1	C	312	LYS	3.4
2	F	90	PHE	3.4
1	G	287	ASP	3.4
1	G	256	PHE	3.4
2	H	60	GLY	3.4
1	G	208	MET	3.3
2	H	129	GLN	3.3
2	H	84	ILE	3.3
1	G	236	GLU	3.3
1	G	267	THR	3.3
1	G	258	LEU	3.2
1	G	210	SER	3.2
1	G	222	THR	3.2
1	A	234	TYR	3.2
1	A	298	HIS	3.2
1	G	106	LYS	3.1
2	B	121	ALA	3.1
1	G	307	CYS	3.1
1	G	229	LEU	3.1
1	G	158	ILE	3.1
1	G	234	TYR	3.1
1	G	202	TYR	3.1
1	A	202	TYR	3.0
2	H	89	SER	3.0
1	G	318	ASP	3.0
1	C	316	PRO	3.0
1	E	240	PHE	3.0
1	A	356	GLY	2.9
1	C	232	SER	2.9
1	G	279	PHE	2.9
1	G	314	GLY	2.9
1	G	317	ARG	2.9
1	G	241	LEU	2.8
1	G	312	LYS	2.8
2	B	128	ARG	2.7
1	A	247	GLY	2.7
1	E	210	SER	2.7
1	C	219	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	237	ILE	2.7
2	H	73	ARG	2.7
2	H	-4	GLY	2.7
1	G	206	GLU	2.6
2	H	101	LYS	2.6
1	C	315	GLY	2.6
1	A	315	GLY	2.6
1	E	206	GLU	2.6
1	G	255	TYR	2.6
1	G	223	GLN	2.6
2	F	0	SER	2.6
1	G	306	PHE	2.6
1	A	293	ALA	2.5
1	G	232	SER	2.5
1	E	247	GLY	2.5
2	H	94	HIS	2.5
1	G	283	PHE	2.5
1	E	202	TYR	2.5
1	G	278	GLN	2.5
2	H	114	VAL	2.4
1	C	247	GLY	2.4
2	H	85	ASN	2.4
1	G	180	GLU	2.4
2	F	84	ILE	2.4
1	C	248	LYS	2.3
1	A	201	MET	2.3
1	G	108	GLN	2.3
1	G	200	PRO	2.3
1	E	236	GLU	2.3
1	G	274	PRO	2.3
1	G	263	LEU	2.3
1	E	221	PRO	2.2
1	G	115	GLU	2.2
2	H	124	THR	2.2
1	C	318	ASP	2.2
1	G	211	PHE	2.2
1	G	319	LEU	2.2
1	G	340	LEU	2.1
1	G	321	MET	2.1
2	B	93	ILE	2.1
1	G	231	SER	2.1
1	G	305	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	238	HIS	2.1
2	H	98	GLU	2.1
2	H	74	THR	2.1
1	C	293	ALA	2.0
1	C	251	TRP	2.0
2	B	0	SER	2.0
2	B	122	ALA	2.0
1	E	257	PHE	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	GOL	A	403	6/6	0.78	0.34	14.12	49,51,55,56	0
3	GOL	C	400	6/6	0.76	0.38	9.45	65,67,68,70	0
3	GOL	A	401	6/6	0.93	0.26	2.38	46,47,48,51	0
3	GOL	E	401	6/6	0.88	0.20	1.88	41,43,44,45	0
3	GOL	B	201	6/6	0.91	0.19	1.01	46,54,55,61	0
5	MG	D	201	1/1	0.90	0.17	0.47	45,45,45,45	0
3	GOL	A	402	6/6	0.92	0.18	0.44	32,34,34,37	0
3	GOL	C	401	6/6	0.91	0.19	0.35	40,43,44,44	0
5	MG	B	203	1/1	0.97	0.16	-0.03	40,40,40,40	0
3	GOL	A	404	6/6	0.85	0.15	-0.11	44,50,54,55	0
4	GTP	F	200	32/32	0.97	0.15	-0.42	39,56,66,66	0
3	GOL	E	400	6/6	0.95	0.14	-0.45	41,43,44,47	0
4	GTP	B	202	32/32	0.97	0.15	-0.49	34,41,52,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GTP	H	200	32/32	0.94	0.18	-1.02	69,80,91,93	0
4	GTP	D	200	32/32	0.98	0.13	-1.28	38,46,50,51	0
5	MG	H	201	1/1	0.85	0.21	-	63,63,63,63	0
5	MG	F	201	1/1	0.97	0.22	-	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.