



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:24 PM GMT

PDB ID : 4LHV  
Title : Crystal structure of Rab8 in its inactive GDP-bound form  
Authors : Guo, Z.; Hou, X.M.; Goody, R.S.; Itzen, A.  
Deposited on : 2013-07-01  
Resolution : 1.95 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

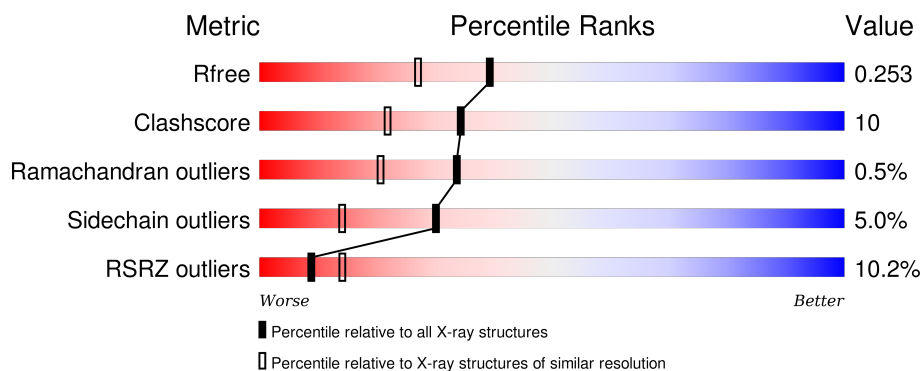
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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	174	<div> <div>4%</div> <div>75% 19% • 5%</div> </div>
1	B	174	<div> <div>8%</div> <div>76% 16% • 7%</div> </div>
1	C	174	<div> <div>8%</div> <div>71% 17% • • 8%</div> </div>
1	D	174	<div> <div>10%</div> <div>74% 16% • 9%</div> </div>
1	E	174	<div> <div>16%</div> <div>71% 13% • 15%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6901 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 Ras-related protein Rab-8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	5	3	0
			1324	844	223	250	7			
1	B	161	Total	C	N	O	S	0	1	0
			1284	823	216	238	7			
1	C	160	Total	C	N	O	S	0	1	0
			1279	817	214	241	7			
1	D	158	Total	C	N	O	S	0	0	0
			1246	793	212	234	7			
1	E	148	Total	C	N	O	S	0	1	0
			1170	745	198	220	7			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	EXPRESSION TAG	UNP P61006
A	4	SER	-	EXPRESSION TAG	UNP P61006
A	5	HIS	-	EXPRESSION TAG	UNP P61006
B	3	GLY	-	EXPRESSION TAG	UNP P61006
B	4	SER	-	EXPRESSION TAG	UNP P61006
B	5	HIS	-	EXPRESSION TAG	UNP P61006
C	3	GLY	-	EXPRESSION TAG	UNP P61006
C	4	SER	-	EXPRESSION TAG	UNP P61006
C	5	HIS	-	EXPRESSION TAG	UNP P61006
D	3	GLY	-	EXPRESSION TAG	UNP P61006
D	4	SER	-	EXPRESSION TAG	UNP P61006
D	5	HIS	-	EXPRESSION TAG	UNP P61006
E	3	GLY	-	EXPRESSION TAG	UNP P61006
E	4	SER	-	EXPRESSION TAG	UNP P61006
E	5	HIS	-	EXPRESSION TAG	UNP P61006

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



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

- 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
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

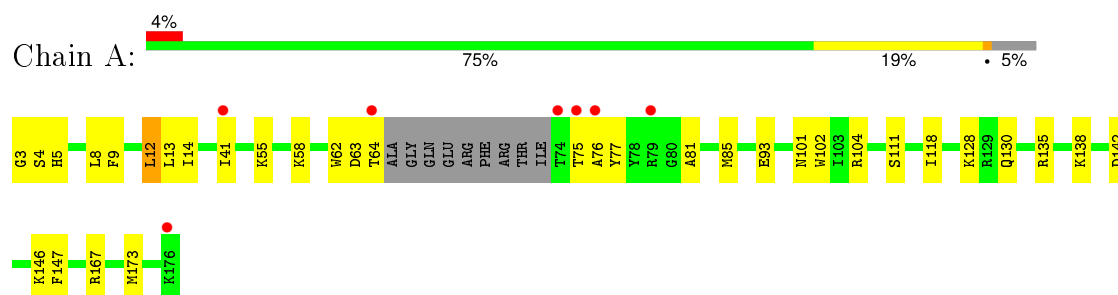
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total 134	O 134	0	0
4	B	94	Total 94	O 94	0	0
4	C	94	Total 94	O 94	0	0
4	D	84	Total 84	O 84	0	0
4	E	47	Total 47	O 47	0	0

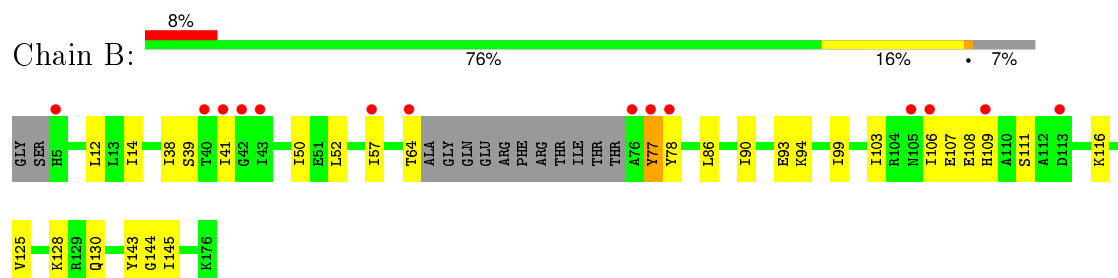
### 3 Residue-property plots [i](#)

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.

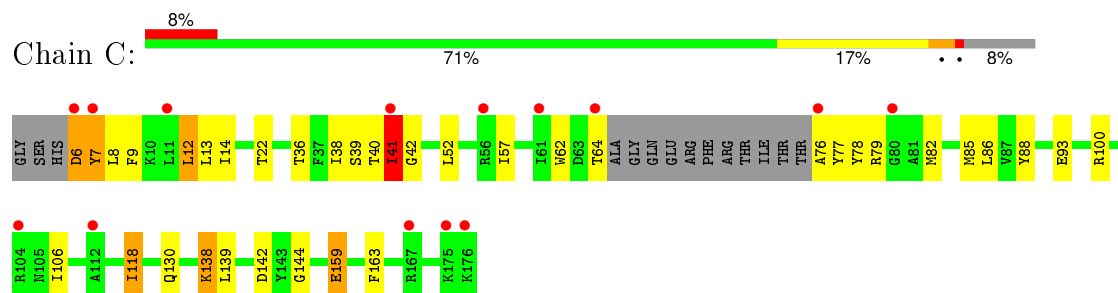
- Molecule 1: Ras-related protein Rab-8A



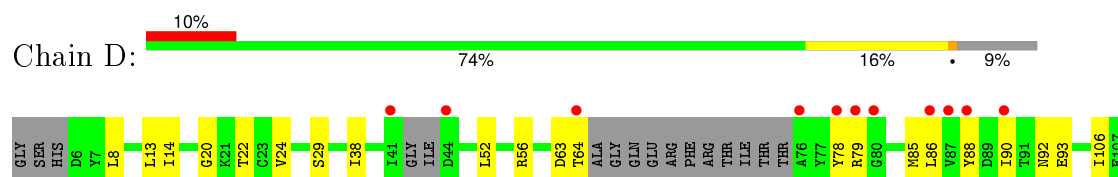
- Molecule 1: Ras-related protein Rab-8A

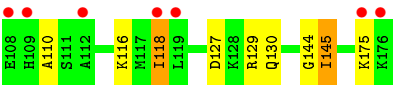


- Molecule 1: Ras-related protein Rab-8A

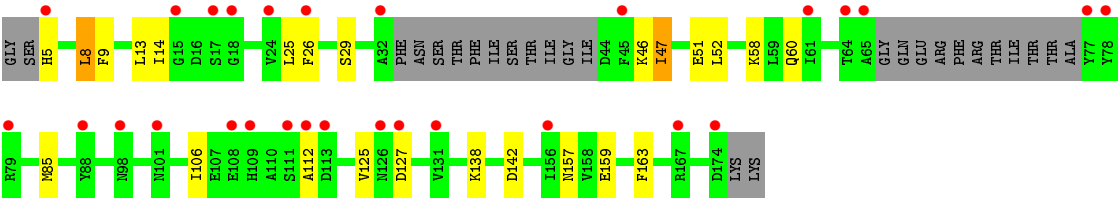


- Molecule 1: Ras-related protein Rab-8A





● Molecule 1: Ras-related protein Rab-8A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.84Å 75.95Å 106.62Å 90.00° 98.44° 90.00°	Depositor
Resolution (Å)	19.96 – 1.95 19.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.96-1.95) 99.3 (19.76-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.95 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.202 , 0.244 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	3413 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.5	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67345 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6901	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.64	0/1351	0.73	0/1811
1	B	0.63	0/1306	0.69	0/1751
1	C	0.58	0/1300	0.69	1/1744 (0.1%)
1	D	0.50	0/1262	0.63	0/1691
1	E	0.50	1/1189 (0.1%)	0.58	0/1596
All	All	0.57	1/6408 (0.0%)	0.67	1/8593 (0.0%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	157	ASN	C-N	-5.63	1.21	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	42	GLY	N-CA-C	-5.74	98.75	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	ILE	Peptide
1	B	39	SER	Peptide
1	C	41	ILE	Peptide

## 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	1324	0	1333	25	1
1	B	1284	0	1280	35	1
1	C	1279	0	1274	39	0
1	D	1246	0	1222	19	0
1	E	1170	0	1143	16	0
2	A	28	0	12	0	0
2	B	28	0	12	0	0
2	C	28	0	12	0	0
2	D	28	0	12	0	0
2	E	28	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	134	0	0	5	1
4	B	94	0	0	3	0
4	C	94	0	0	5	0
4	D	84	0	0	2	0
4	E	47	0	0	2	1
All	All	6901	0	6312	127	3

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 10.

All (127) 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:C:76:ALA:HB1	4:C:358:HOH:O	1.32	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:HD23	1:B:57:ILE:HG13	1.40	1.03
1:B:78:TYR:CD1	1:B:109:HIS:HB2	1.94	1.00
1:E:14:ILE:HD11	1:E:106:ILE:HD11	1.44	0.96
1:B:86:LEU:HD21	1:B:106:ILE:CD1	1.97	0.95
1:B:144:GLY:O	4:B:389:HOH:O	1.86	0.94
1:D:14:ILE:HD11	1:D:106:ILE:HD11	1.54	0.89
1:C:14:ILE:HD11	1:C:106:ILE:HD11	1.55	0.88
1:B:78:TYR:HD1	1:B:109:HIS:HB2	1.37	0.86
1:B:86:LEU:HD21	1:B:106:ILE:HD11	1.57	0.85
1:B:77:TYR:HD2	1:B:78:TYR:H	1.30	0.78
1:B:78:TYR:CE1	1:B:109:HIS:HB2	2.20	0.76
1:D:144:GLY:O	4:D:314:HOH:O	2.07	0.73
1:B:78:TYR:HD1	1:B:109:HIS:CB	2.03	0.70
1:A:138:LYS:HG3	4:A:348:HOH:O	1.89	0.70
1:B:14[A]:ILE:HD11	1:B:86:LEU:CD2	2.22	0.69
1:B:64:THR:HG23	4:B:338:HOH:O	1.93	0.69
1:E:14:ILE:CD1	1:E:106:ILE:HD11	2.23	0.69
1:D:175:LYS:CB	1:E:112:ALA:HB2	2.24	0.68
1:B:77:TYR:HD2	1:B:78:TYR:N	1.90	0.68
1:B:14[A]:ILE:HD11	1:B:86:LEU:HD23	1.75	0.68
1:B:14[A]:ILE:HD11	1:B:106:ILE:HD11	1.75	0.68
1:C:86:LEU:HD21	1:C:106:ILE:HD11	1.76	0.67
1:C:88:TYR:HE1	1:C:118[A]:ILE:HD11	1.58	0.67
1:C:62:TRP:CE3	1:C:76:ALA:HB2	2.29	0.67
1:A:64:THR:HA	4:A:360:HOH:O	1.94	0.66
1:A:93:GLU:H	1:A:130:GLN:HE21	1.42	0.66
1:B:86:LEU:CD2	1:B:106:ILE:HD11	2.25	0.66
1:E:13:LEU:HD23	1:E:85:MET:HB2	1.79	0.65
1:C:6:ASP:OD2	1:C:6:ASP:N	2.30	0.64
1:B:125:VAL:O	1:B:125:VAL:HG12	1.98	0.63
1:C:36:THR:CG2	1:D:29:SER:O	2.46	0.62
1:A:12:LEU:HD22	1:A:81:ALA:CB	2.30	0.62
1:E:125:VAL:HG12	1:E:125:VAL:O	2.00	0.61
1:A:12:LEU:HD22	1:A:81:ALA:HB2	1.82	0.60
1:E:58:LYS:CB	4:E:334:HOH:O	2.49	0.60
1:D:13:LEU:HD23	1:D:85:MET:HB2	1.83	0.60
1:C:13:LEU:HD23	1:C:85:MET:HB2	1.84	0.60
1:B:50:ILE:CD1	1:B:52:LEU:HD21	2.32	0.60
1:C:36:THR:HG21	1:D:29:SER:O	2.02	0.59
1:D:22:THR:OG1	1:D:63:ASP:OD2	2.18	0.59
1:E:47:ILE:HG23	4:E:326:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HD11	1:B:52:LEU:HD21	1.85	0.58
1:C:86:LEU:HD21	1:C:106:ILE:CD1	2.33	0.58
1:E:138:LYS:HE2	1:E:142:ASP:OD2	2.04	0.57
1:A:93:GLU:H	1:A:130:GLN:NE2	2.02	0.56
1:C:22:THR:CG2	1:C:40:THR:HG23	2.36	0.55
1:C:64:THR:N	4:C:311:HOH:O	2.40	0.55
1:A:75:THR:O	1:A:77:TYR:N	2.39	0.54
1:C:88:TYR:HE1	1:C:118[A]:ILE:CD1	2.20	0.54
1:D:116:LYS:HZ3	1:D:145:ILE:HG21	1.73	0.54
1:B:77:TYR:CE2	1:B:109:HIS:HB3	2.43	0.53
1:C:144:GLY:O	4:C:307:HOH:O	2.17	0.53
1:E:29:SER:OG	1:E:46:LYS:HG2	2.09	0.53
1:C:22:THR:HG21	1:C:40:THR:HG23	1.91	0.53
1:A:75:THR:C	1:A:77:TYR:H	2.11	0.52
1:A:8:LEU:HD12	1:A:58:LYS:HB3	1.91	0.52
1:A:12:LEU:HD12	1:A:62:TRP:HB2	1.91	0.52
1:E:8:LEU:HD12	1:E:9:PHE:N	2.24	0.52
1:D:88:TYR:HE1	1:D:118:ILE:HD11	1.74	0.52
1:C:14:ILE:HG13	1:C:86:LEU:HD23	1.93	0.51
1:C:64:THR:C	4:C:316:HOH:O	2.48	0.51
1:D:14:ILE:HG22	1:D:64:THR:OG1	2.11	0.51
1:C:14:ILE:CG1	1:C:86:LEU:HD23	2.41	0.51
1:B:52:LEU:HD23	1:B:57:ILE:CG1	2.27	0.50
1:B:38:ILE:HD11	1:C:159:GLU:HG2	1.94	0.50
1:E:138:LYS:CE	1:E:142:ASP:OD2	2.60	0.50
1:B:38:ILE:HD11	1:C:159:GLU:HB3	1.93	0.50
1:E:8:LEU:HD11	1:E:60:GLN:HB2	1.94	0.50
1:A:118[A]:ILE:HG22	1:A:146:LYS:O	2.13	0.49
1:E:52:LEU:HD11	1:E:163:PHE:CD2	2.48	0.49
1:A:63:ASP:O	1:A:64:THR:C	2.50	0.49
1:A:13:LEU:HD23	1:A:85:MET:HB2	1.95	0.49
1:A:101:ASN:OD1	1:A:104:ARG:NH2	2.46	0.49
1:C:36:THR:HG23	1:D:29:SER:O	2.13	0.49
1:E:51:GLU:O	1:E:52:LEU:HD12	2.13	0.49
1:B:77:TYR:CD2	1:B:78:TYR:N	2.72	0.48
1:C:88:TYR:CE1	1:C:118[A]:ILE:CD1	2.95	0.48
1:A:14:ILE:HD13	1:A:102:TRP:CE3	2.48	0.48
1:D:78:TYR:O	1:D:79:ARG:C	2.52	0.48
1:B:106:ILE:C	1:B:108:GLU:H	2.17	0.48
1:B:103:ILE:HG21	1:B:143:TYR:CD1	2.48	0.48
1:A:14:ILE:HD12	1:A:14:ILE:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118[A]:ILE:HG23	1:A:147:PHE:HD1	1.79	0.47
1:D:78:TYR:CD2	1:D:110:ALA:HB2	2.49	0.47
1:C:93:GLU:H	1:C:130:GLN:NE2	2.12	0.47
1:D:56:ARG:NH2	4:D:334:HOH:O	2.47	0.47
1:B:86:LEU:CD2	1:B:106:ILE:CD1	2.82	0.47
1:B:86:LEU:HD21	1:B:106:ILE:HD12	1.93	0.46
1:A:3:GLY:HA3	1:A:4:SER:HA	1.46	0.46
1:B:106:ILE:HG21	1:B:116:LYS:HD3	1.98	0.46
1:B:14[A]:ILE:CD1	1:B:86:LEU:HD23	2.44	0.46
1:A:167:ARG:NH2	4:A:370:HOH:O	2.28	0.46
1:D:90:ILE:HD12	1:D:129:ARG:HG3	1.97	0.46
1:C:138:LYS:NZ	1:C:142:ASP:OD1	2.28	0.46
1:A:9:PHE:CE1	1:A:173:MET:HE1	2.51	0.45
1:A:93:GLU:OE1	1:A:135:ARG:NH1	2.50	0.45
1:A:173:MET:HB2	1:A:173:MET:HE3	1.72	0.45
1:C:7:TYR:CD2	1:C:57:ILE:HD13	2.51	0.45
1:C:22:THR:HG21	1:C:40:THR:CG2	2.47	0.45
1:E:8:LEU:C	1:E:8:LEU:HD12	2.38	0.44
1:C:40:THR:CG2	1:C:40:THR:O	2.66	0.44
1:E:25:LEU:O	1:E:25:LEU:HD12	2.17	0.44
1:C:76:ALA:CB	4:C:358:HOH:O	2.18	0.44
1:A:3:GLY:HA2	1:A:55:LYS:HE2	2.00	0.43
1:C:100:ARG:NH1	1:C:139:LEU:HD23	2.33	0.43
1:C:14:ILE:HD11	1:C:86:LEU:HD21	2.02	0.42
1:D:93:GLU:H	1:D:130:GLN:NE2	2.17	0.42
1:C:39:SER:OG	1:C:41:ILE:HD13	2.19	0.42
1:C:12:LEU:HD12	1:C:62:TRP:HB2	2.01	0.42
1:A:128:LYS:NZ	4:A:381:HOH:O	2.52	0.42
1:B:38:ILE:HG21	1:C:163:PHE:CE2	2.54	0.42
1:C:9:PHE:CD1	1:C:82:MET:HE2	2.55	0.42
1:C:88:TYR:CE1	1:C:118[A]:ILE:HD11	2.45	0.41
1:C:14:ILE:HD11	1:C:86:LEU:CD2	2.50	0.41
1:B:128:LYS:NZ	4:B:346:HOH:O	2.53	0.41
1:B:106:ILE:O	1:B:108:GLU:N	2.45	0.41
1:B:93:GLU:H	1:B:130:GLN:HE21	1.67	0.41
1:B:14[A]:ILE:CG1	1:B:86:LEU:HD23	2.50	0.41
1:D:93:GLU:H	1:D:130:GLN:HE21	1.69	0.41
1:C:77:TYR:CD2	1:C:78:TYR:N	2.88	0.41
1:D:86:LEU:HD21	1:D:106:ILE:HD12	2.03	0.41
1:C:138:LYS:NZ	1:C:138:LYS:O	2.46	0.41
1:C:7:TYR:HB3	1:C:9:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:GLY:O	1:D:24:VAL:HG23	2.21	0.41
1:A:167:ARG:NE	4:A:370:HOH:O	2.49	0.40
1:B:99:ILE:HA	1:B:99:ILE:HD13	1.95	0.40

All (3) 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)
1:A:58:LYS:CE	1:A:58:LYS:NZ[2_556]	1.97	0.23
1:B:109:HIS:NE2	4:E:344:HOH:O[3_545]	2.16	0.04
4:A:415:HOH:O	4:A:418:HOH:O[2_556]	2.19	0.01

## 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	164/174 (94%)	160 (98%)	3 (2%)	1 (1%)	30	16
1	B	158/174 (91%)	149 (94%)	7 (4%)	2 (1%)	15	4
1	C	157/174 (90%)	152 (97%)	4 (2%)	1 (1%)	30	16
1	D	152/174 (87%)	145 (95%)	7 (5%)	0	100	100
1	E	143/174 (82%)	139 (97%)	4 (3%)	0	100	100
All	All	774/870 (89%)	745 (96%)	25 (3%)	4 (0%)	34	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	B	107	GLU
1	C	79	ARG
1	B	41	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	143/150 (95%)	139 (97%)	4 (3%)	51	39
1	B	135/150 (90%)	129 (96%)	6 (4%)	35	19
1	C	136/150 (91%)	125 (92%)	11 (8%)	15	4
1	D	129/150 (86%)	122 (95%)	7 (5%)	27	12
1	E	121/150 (81%)	115 (95%)	6 (5%)	30	14
All	All	664/750 (88%)	630 (95%)	34 (5%)	30	13

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	12	LEU
1	A	111	SER
1	A	142	ASP
1	B	12	LEU
1	B	77	TYR
1	B	90	ILE
1	B	94	LYS
1	B	111	SER
1	B	145	ILE
1	C	6	ASP
1	C	7	TYR
1	C	8	LEU
1	C	12	LEU
1	C	38	ILE
1	C	41	ILE
1	C	52	LEU
1	C	118[A]	ILE
1	C	118[B]	ILE
1	C	138	LYS
1	C	159	GLU
1	D	8	LEU
1	D	38	ILE

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Mol	Chain	Res	Type
1	D	52	LEU
1	D	92	ASN
1	D	118	ILE
1	D	127	ASP
1	D	145	ILE
1	E	5	HIS
1	E	8	LEU
1	E	26	PHE
1	E	47	ILE
1	E	127	ASP
1	E	159	GLU

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	34	ASN
1	A	130	GLN
1	B	34	ASN
1	B	101	ASN
1	B	130	GLN
1	C	34	ASN
1	C	130	GLN
1	D	92	ASN
1	D	101	ASN
1	D	130	GLN
1	E	60	GLN
1	E	130	GLN
1	E	157	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 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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$
2	GDP	A	201	3	23,30,30	1.03	2 (8%)	30,47,47	1.81	6 (20%)
2	GDP	B	201	3	23,30,30	1.17	3 (13%)	30,47,47	1.77	5 (16%)
2	GDP	C	201	3	23,30,30	1.08	3 (13%)	30,47,47	1.93	8 (26%)
2	GDP	D	201	3	23,30,30	1.29	3 (13%)	30,47,47	1.84	6 (20%)
2	GDP	E	201	3	23,30,30	1.22	2 (8%)	30,47,47	1.98	7 (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
2	GDP	A	201	3	-	0/12/32/32	0/3/3/3
2	GDP	B	201	3	-	0/12/32/32	0/3/3/3
2	GDP	C	201	3	-	0/12/32/32	0/3/3/3
2	GDP	D	201	3	-	0/12/32/32	0/3/3/3
2	GDP	E	201	3	-	0/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	GDP	O4'-C1'	2.06	1.43	1.41
2	B	201	GDP	O4'-C1'	2.06	1.43	1.41
2	C	201	GDP	C5-C4	2.41	1.45	1.40
2	A	201	GDP	C6-C5	2.58	1.46	1.41
2	C	201	GDP	C6-C5	2.64	1.46	1.41
2	A	201	GDP	C5-C4	2.78	1.46	1.40
2	B	201	GDP	C6-C5	2.95	1.47	1.41
2	E	201	GDP	C5-C4	3.08	1.47	1.40
2	D	201	GDP	C6-C5	3.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	GDP	C5-C4	3.31	1.48	1.40
2	D	201	GDP	O4'-C1'	3.37	1.45	1.41
2	B	201	GDP	C5-C4	3.43	1.48	1.40
2	E	201	GDP	C6-C5	4.03	1.49	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	GDP	C5-C6-N1	-5.04	116.70	123.59
2	B	201	GDP	C5-C6-N1	-4.62	117.27	123.59
2	E	201	GDP	C5-C6-N1	-4.47	117.48	123.59
2	A	201	GDP	C5-C6-N1	-4.40	117.57	123.59
2	C	201	GDP	C6-C5-C4	-4.40	115.64	120.90
2	A	201	GDP	C6-C5-C4	-4.19	115.89	120.90
2	C	201	GDP	C5-C6-N1	-4.07	118.02	123.59
2	E	201	GDP	C6-C5-C4	-3.82	116.33	120.90
2	E	201	GDP	PA-O3A-PB	-3.68	120.33	132.67
2	E	201	GDP	C4-C5-N7	-3.63	106.14	109.48
2	D	201	GDP	C6-C5-C4	-3.33	116.92	120.90
2	B	201	GDP	C6-C5-C4	-3.16	117.12	120.90
2	D	201	GDP	C4-C5-N7	-3.10	106.62	109.48
2	C	201	GDP	C4-C5-N7	-3.04	106.69	109.48
2	E	201	GDP	N3-C2-N1	-2.96	122.93	127.44
2	B	201	GDP	C4-C5-N7	-2.96	106.76	109.48
2	C	201	GDP	N3-C2-N1	-2.79	123.19	127.44
2	C	201	GDP	C1'-N9-C4	-2.77	122.76	126.94
2	B	201	GDP	N3-C2-N1	-2.74	123.27	127.44
2	E	201	GDP	C1'-N9-C4	-2.71	122.86	126.94
2	D	201	GDP	N3-C2-N1	-2.62	123.46	127.44
2	C	201	GDP	C2'-C1'-N9	-2.08	111.11	114.29
2	A	201	GDP	N3-C2-N1	-2.07	124.30	127.44
2	D	201	GDP	C1'-N9-C4	-2.03	123.89	126.94
2	A	201	GDP	C4'-O4'-C1'	2.09	112.02	109.72
2	A	201	GDP	O3B-PB-O1B	2.52	118.71	110.58
2	C	201	GDP	N2-C2-N1	2.68	121.63	117.20
2	C	201	GDP	C6-N1-C2	4.72	122.49	115.94
2	E	201	GDP	C6-N1-C2	4.85	122.67	115.94
2	B	201	GDP	C6-N1-C2	4.90	122.75	115.94
2	A	201	GDP	C6-N1-C2	5.00	122.87	115.94
2	D	201	GDP	C6-N1-C2	5.31	123.30	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	165/174 (94%)	0.30	7 (4%) 40 51	24, 36, 56, 70	0
1	B	161/174 (92%)	0.61	14 (8%) 13 20	25, 42, 70, 78	0
1	C	160/174 (91%)	0.61	14 (8%) 12 20	26, 43, 68, 79	0
1	D	158/174 (90%)	0.75	18 (11%) 7 11	26, 47, 72, 79	0
1	E	148/174 (85%)	1.07	28 (18%) 2 2	26, 57, 76, 88	0
All	All	792/870 (91%)	0.66	81 (10%) 9 14	24, 44, 71, 88	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	6	ASP	7.7
1	E	65	ALA	6.4
1	B	109	HIS	6.1
1	D	112	ALA	6.0
1	E	17	SER	5.9
1	B	43	ILE	5.6
1	B	113	ASP	5.5
1	B	5	HIS	5.3
1	C	176	LYS	5.3
1	B	76	ALA	5.1
1	D	176	LYS	5.1
1	A	75	THR	4.9
1	A	79	ARG	4.7
1	D	44	ASP	4.6
1	C	64	THR	4.3
1	D	41	ILE	4.3
1	D	79	ARG	4.3
1	D	64	THR	4.2
1	E	77	TYR	4.2
1	E	113	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	26	PHE	3.9
1	E	127	ASP	3.9
1	E	174	ASP	3.8
1	E	112	ALA	3.8
1	E	101	ASN	3.8
1	B	40	THR	3.7
1	D	118	ILE	3.6
1	C	175	LYS	3.6
1	D	87	VAL	3.6
1	B	42	GLY	3.5
1	E	18	GLY	3.5
1	A	76	ALA	3.4
1	E	32	ALA	3.4
1	B	106	ILE	3.3
1	E	79	ARG	3.3
1	B	41	ILE	3.2
1	C	11	LEU	3.2
1	C	41	ILE	3.2
1	E	24	VAL	3.1
1	E	64	THR	3.1
1	E	111	SER	3.1
1	E	167	ARG	3.1
1	E	78	TYR	3.0
1	B	64	THR	3.0
1	D	119	LEU	2.9
1	E	61	ILE	2.8
1	C	76	ALA	2.8
1	E	108	GLU	2.8
1	B	105	ASN	2.7
1	A	176	LYS	2.7
1	A	74	THR	2.7
1	B	77	TYR	2.7
1	B	78	TYR	2.7
1	E	109	HIS	2.6
1	D	108	GLU	2.6
1	D	109	HIS	2.5
1	C	56	ARG	2.5
1	E	15	GLY	2.4
1	C	7	TYR	2.4
1	D	175	LYS	2.4
1	E	156	ILE	2.4
1	E	88	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	5	HIS	2.3
1	E	131	VAL	2.2
1	D	78	TYR	2.2
1	A	64	THR	2.2
1	C	61	ILE	2.2
1	D	88	TYR	2.2
1	C	104	ARG	2.2
1	E	45	PHE	2.2
1	A	41	ILE	2.2
1	E	98	ASN	2.2
1	D	90	ILE	2.1
1	D	86	LEU	2.1
1	C	112	ALA	2.1
1	C	80	GLY	2.1
1	E	126	ASN	2.1
1	C	167	ARG	2.1
1	D	76	ALA	2.0
1	D	80	GLY	2.0
1	B	57	ILE	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GDP	E	201	28/28	0.87	0.17	-0.12	61,63,65,66	0
2	GDP	C	201	28/28	0.98	0.10	-0.40	27,31,35,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GDP	A	201	28/28	0.97	0.10	-0.52	27,29,31,35	0
2	GDP	B	201	28/28	0.98	0.07	-0.94	28,33,36,37	0
2	GDP	D	201	28/28	0.96	0.08	-1.52	37,38,43,44	0
3	MG	D	202	1/1	0.98	0.03	-	43,43,43,43	0
3	MG	B	202	1/1	0.99	0.04	-	35,35,35,35	0
3	MG	E	202	1/1	0.79	0.08	-	71,71,71,71	0
3	MG	C	202	1/1	0.99	0.03	-	33,33,33,33	0
3	MG	A	202	1/1	0.99	0.02	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.