



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:46 pm GMT

PDB ID : 2BME  
Title : high resolution structure of GppNHp-bound human Rab4a  
Authors : Scheidig, A.J.; Huber, S.K.  
Deposited on : 2005-03-13  
Resolution : 1.57 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

<https://www.wwpdb.org/validation/2017/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:

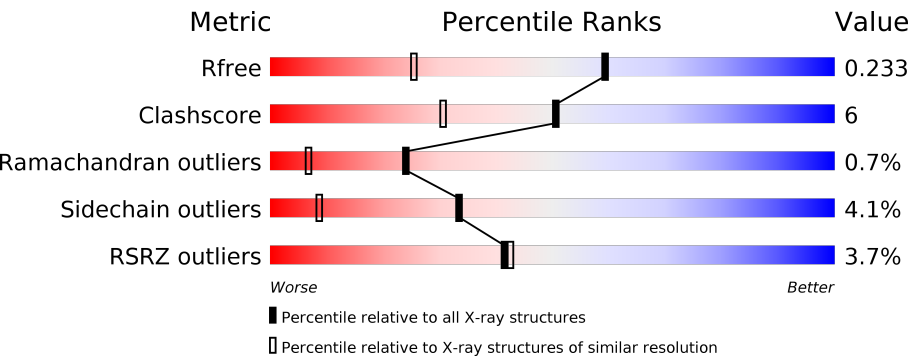
MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

# 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 1.57 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))
$R_{free}$	111664	4679 (1.60-1.56)
Clashscore	122126	4976 (1.60-1.56)
Ramachandran outliers	120053	4851 (1.60-1.56)
Sidechain outliers	120020	4848 (1.60-1.56)
RSRZ outliers	108989	4581 (1.60-1.56)

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	186	<div><div>3%</div><div><div></div><div>80%</div><div>12%</div><div>•• 5%</div></div></div>
1	B	186	<div><div>%</div><div><div></div><div>82%</div><div>10%</div><div>• 7%</div></div></div>
1	C	186	<div><div>4%</div><div><div></div><div>84%</div><div>8%</div><div>• 6%</div></div></div>
1	D	186	<div><div>7%</div><div><div></div><div>81%</div><div>7%</div><div>•• 6%</div></div></div>

2 Entry composition ⓘ

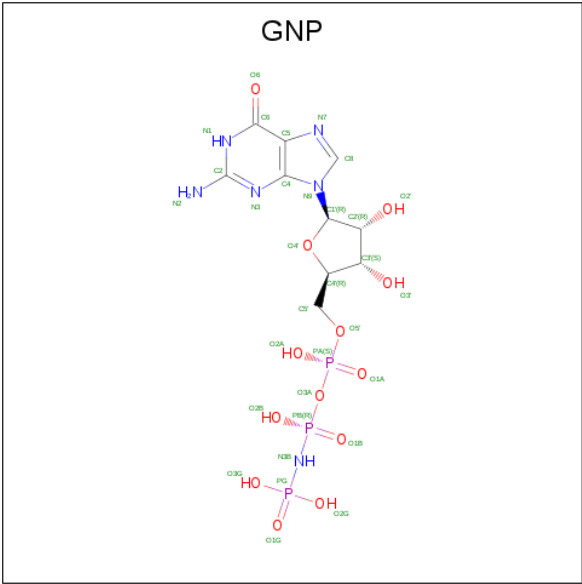
There are 6 unique types of molecules in this entry. The entry contains 6403 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RAB4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	2	0
			1401	889	238	268	6			
1	B	173	Total	C	N	O	S	0	2	0
			1383	878	236	264	5			
1	C	174	Total	C	N	O	S	0	1	0
			1386	880	235	266	5			
1	D	174	Total	C	N	O	S	0	0	0
			1377	874	235	263	5			

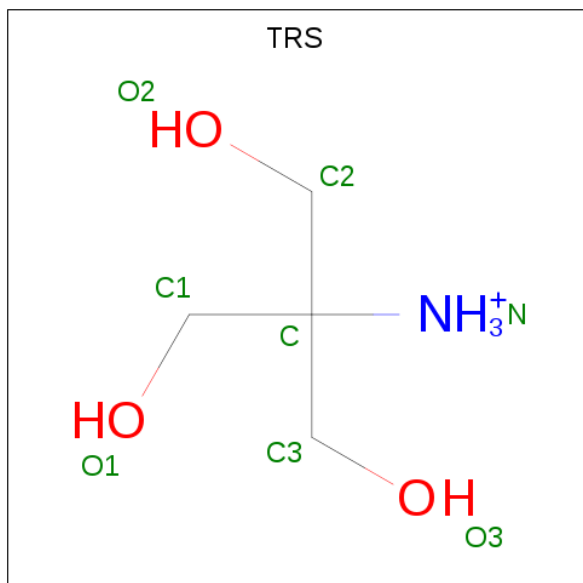
- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	C	1	Total	C	N	O	0	0
			8	4	1	3		
3	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	C	1	Total	C	O	S	0	0
			4	2	1	1		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total	O	0	0
			162	162		
6	B	213	Total	O	0	0
			213	213		
6	C	170	Total	O	0	0
			170	170		

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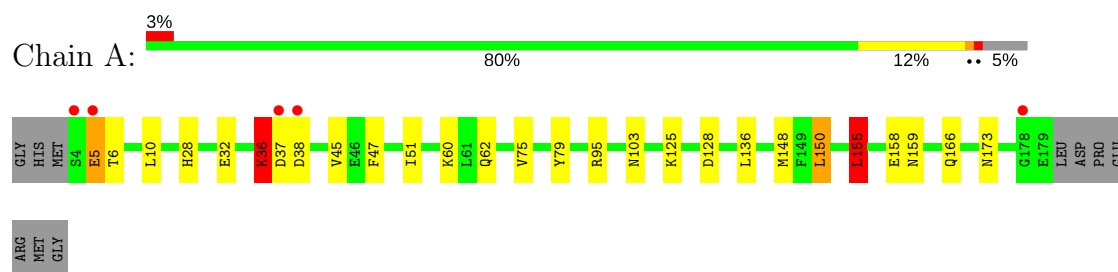
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	139	Total 139	O 139	0	0

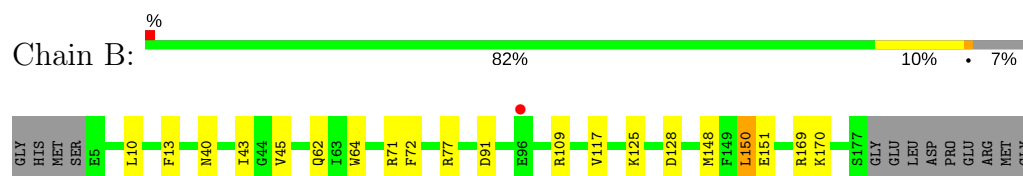
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

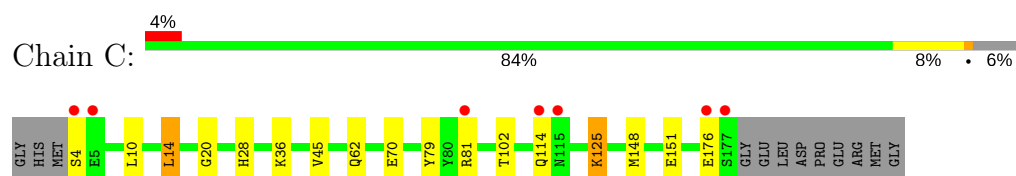
#### • Molecule 1: RAS-RELATED PROTEIN RAB4A



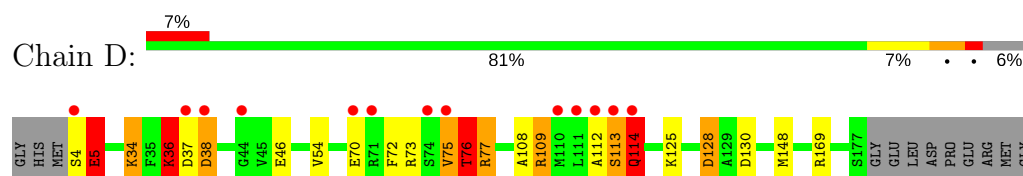
#### • Molecule 1: RAS-RELATED PROTEIN RAB4A



#### • Molecule 1: RAS-RELATED PROTEIN RAB4A



#### • Molecule 1: RAS-RELATED PROTEIN RAB4A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.79Å 99.79Å 95.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.54 – 1.57 19.54 – 1.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.54-1.57) 98.0 (19.54-1.57)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 1.56Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.192 , 0.229 0.204 , 0.233	Depositor DCC
$R_{free}$ test set	6441 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.2	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 36.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.064 for -h,-l,-k 0.064 for -h,l,k 0.065 for l,-k,h 0.066 for -l,-k,-h 0.264 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6403	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5675e-03.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: TRS, MG, GNP, BME

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	0.83	1/1432 (0.1%)	1.34	6/1927 (0.3%)
1	B	0.86	0/1417	1.01	8/1907 (0.4%)
1	C	0.88	0/1413	0.93	2/1903 (0.1%)
1	D	0.88	3/1399 (0.2%)	1.24	10/1882 (0.5%)
All	All	0.86	4/5661 (0.1%)	1.14	26/7619 (0.3%)

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	2
1	D	0	4
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	36	LYS	C-N	-13.24	1.03	1.34
1	A	36	LYS	C-N	8.19	1.52	1.34
1	D	114	GLN	C-N	-6.92	1.18	1.34
1	D	75	VAL	C-N	-6.77	1.18	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LYS	O-C-N	-40.72	57.56	122.70
1	D	36	LYS	O-C-N	-27.41	78.85	122.70
1	D	36	LYS	CA-C-N	15.20	150.65	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	LYS	CA-C-N	11.28	142.01	117.20
1	D	114	GLN	O-C-N	-10.96	105.17	122.70
1	B	77	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	150	LEU	CA-CB-CG	7.17	131.79	115.30
1	D	75	VAL	C-N-CA	6.97	139.13	121.70
1	B	169	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	155	LEU	CA-CB-CG	6.38	129.96	115.30
1	D	75	VAL	O-C-N	-6.25	112.71	122.70
1	D	114	GLN	CA-C-N	6.17	130.78	117.20
1	B	77	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	A	150	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	13	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	C	125	LYS	CD-CE-NZ	-5.77	98.44	111.70
1	B	91	ASP	N-CA-CB	-5.47	100.75	110.60
1	B	150	LEU	CB-CG-CD1	5.46	120.28	111.00
1	A	38	ASP	CB-CG-OD2	5.34	123.11	118.30
1	D	130	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	14	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	169	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	128	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	128	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	114	GLN	C-N-CA	5.08	134.41	121.70
1	B	128	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	LYS	Mainchain,Peptide
1	D	109	ARG	Mainchain
1	D	114	GLN	Mainchain,Peptide
1	D	36	LYS	Mainchain

## 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	1401	0	1386	25	0
1	B	1383	0	1370	13	0
1	C	1386	0	1375	18	0
1	D	1377	0	1358	15	0
2	A	32	0	13	0	0
2	B	32	0	13	0	0
2	C	32	0	13	1	0
2	D	32	0	13	0	0
3	A	16	0	22	9	0
3	C	8	0	12	5	0
3	D	8	0	11	2	0
4	A	4	0	6	0	0
4	C	4	0	6	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	162	0	0	7	0
6	B	213	0	0	3	0
6	C	170	0	0	2	0
6	D	139	0	0	4	0
All	All	6403	0	5598	70	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 (70) 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:159:ASN:HD21	3:A:1181:TRS:H11	0.98	1.08
1:A:159:ASN:ND2	3:A:1181:TRS:H11	1.78	0.96
1:C:70:GLU:H	4:C:1180:BME:H21	1.27	0.95
1:B:125[A]:LYS:HE3	1:B:151:GLU:CB	2.11	0.81
1:C:10:LEU:HD11	1:C:62:GLN:OE1	1.81	0.80
1:A:60:LYS:HZ1	3:A:1182:TRS:H12	1.47	0.79
1:D:37:ASP:CA	6:D:2033:HOH:O	2.29	0.78
1:A:37:ASP:HA	6:A:2027:HOH:O	1.84	0.78
1:D:72:PHE:O	1:D:76:THR:HB	1.89	0.73
1:A:45:VAL:HG12	1:B:45:VAL:HG12	1.73	0.70
1:B:125[A]:LYS:HE3	1:B:151:GLU:HB2	1.73	0.69
1:C:70:GLU:N	4:C:1180:BME:H21	2.06	0.68
1:A:159:ASN:HD21	3:A:1181:TRS:C1	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:SER:O	1:D:5:GLU:HB2	1.95	0.66
1:D:109:ARG:HB3	1:D:114:GLN:HG3	1.76	0.65
1:B:125[A]:LYS:HE3	1:B:151:GLU:HB3	1.78	0.64
1:D:46:GLU:HG3	6:D:2042:HOH:O	1.97	0.64
1:C:125:LYS:HE3	3:C:1179:TRS:O1	1.97	0.64
1:C:125:LYS:HE3	3:C:1179:TRS:C1	2.29	0.61
1:B:125[A]:LYS:CE	1:B:151:GLU:HB2	2.29	0.61
1:C:125:LYS:HE2	1:C:151:GLU:OE1	2.03	0.58
1:B:43:ILE:HD11	6:B:2042:HOH:O	2.02	0.57
1:A:6:THR:HG23	6:A:2006:HOH:O	2.03	0.57
1:A:5:GLU:CG	1:A:51:ILE:HD12	2.34	0.57
1:A:37:ASP:C	6:A:2027:HOH:O	2.43	0.55
1:C:102[A]:THR:HG23	6:C:2100:HOH:O	2.07	0.54
1:D:112:ALA:O	1:D:113:SER:CB	2.56	0.53
1:A:5:GLU:HG2	1:A:51:ILE:HD12	1.89	0.53
1:D:73:ARG:HG3	1:D:77:ARG:HD2	1.91	0.53
1:A:47:PHE:HE2	3:A:1182:TRS:HN3	1.55	0.53
1:C:45:VAL:HG21	1:C:79:TYR:CZ	2.44	0.52
1:A:155:LEU:HD13	6:A:2136:HOH:O	2.09	0.52
1:A:148:MET:CE	1:A:166[A]:GLN:HG2	2.40	0.51
1:A:103:ASN:HB2	6:A:2074:HOH:O	2.09	0.51
1:D:125:LYS:NZ	3:D:1178:TRS:H12	2.26	0.51
1:A:10:LEU:HD11	1:A:62:GLN:HG3	1.93	0.51
1:C:125:LYS:HE3	3:C:1179:TRS:H12	1.92	0.51
3:A:1181:TRS:H12	1:C:62:GLN:OE1	2.11	0.51
1:B:43:ILE:HG23	1:B:72:PHE:HZ	1.77	0.50
1:A:148:MET:HE3	1:A:166[A]:GLN:HG2	1.94	0.50
1:D:128:ASP:HB2	6:D:2093:HOH:O	2.11	0.50
1:A:28:HIS:CD2	1:A:36:LYS:HB3	2.46	0.50
1:D:125:LYS:HZ1	3:D:1178:TRS:C1	2.25	0.49
1:C:10:LEU:HD13	1:C:10:LEU:C	2.34	0.48
1:A:37:ASP:CA	6:A:2027:HOH:O	2.51	0.48
1:D:37:ASP:O	1:D:38:ASP:HB2	2.14	0.48
1:A:125:LYS:HD3	1:A:158:GLU:OE1	2.14	0.48
1:A:75:VAL:HG21	1:B:64:TRP:HH2	1.79	0.48
1:C:125:LYS:CE	3:C:1179:TRS:H12	2.44	0.48
1:C:70:GLU:H	4:C:1180:BME:C2	2.13	0.45
1:B:10:LEU:HD11	1:B:62:GLN:HG3	1.98	0.45
1:A:45:VAL:HG11	1:A:79:TYR:OH	2.17	0.45
1:B:43:ILE:HG23	1:B:72:PHE:CZ	2.53	0.44
1:A:60:LYS:HE2	3:A:1182:TRS:O2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:NZ	3:A:1182:TRS:H12	2.26	0.43
1:A:36:LYS:HE2	1:A:36:LYS:HB2	1.72	0.43
1:C:10:LEU:HD11	1:C:62:GLN:CD	2.38	0.43
1:B:109:ARG:NH1	6:B:2138:HOH:O	2.52	0.43
1:D:109:ARG:C	1:D:114:GLN:HE21	2.23	0.43
1:B:43:ILE:CD1	6:B:2042:HOH:O	2.65	0.42
3:A:1181:TRS:N	1:C:10:LEU:HD12	2.35	0.42
1:A:95:ARG:HD3	6:A:2095:HOH:O	2.19	0.42
3:C:1179:TRS:H11	6:C:2168:HOH:O	2.19	0.42
1:C:114:GLN:H	1:C:114:GLN:HG2	1.49	0.41
1:D:109:ARG:CB	1:D:114:GLN:HG3	2.47	0.41
1:D:34:LYS:NZ	6:D:2032:HOH:O	2.52	0.41
1:D:108:ALA:O	1:D:112:ALA:HB3	2.21	0.41
1:C:20:GLY:H	2:C:1178:GNP:HNB3	1.67	0.40
1:B:117:VAL:HG11	1:B:170:LYS:HB2	2.03	0.40
1:C:28:HIS:CD2	1:C:36:LYS:HB2	2.56	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	176/186 (95%)	172 (98%)	4 (2%)	0	100	100
1	B	173/186 (93%)	171 (99%)	2 (1%)	0	100	100
1	C	173/186 (93%)	172 (99%)	1 (1%)	0	100	100
1	D	172/186 (92%)	163 (95%)	4 (2%)	5 (3%)	5	0
All	All	694/744 (93%)	678 (98%)	11 (2%)	5 (1%)	24	7

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	38	ASP
1	D	5	GLU
1	D	76	THR
1	D	113	SER
1	D	75	VAL

### 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	150/157 (96%)	143 (95%)	7 (5%)	29	6
1	B	149/157 (95%)	144 (97%)	5 (3%)	40	13
1	C	149/157 (95%)	144 (97%)	5 (3%)	40	13
1	D	146/157 (93%)	138 (94%)	8 (6%)	24	4
All	All	594/628 (95%)	569 (96%)	25 (4%)	33	8

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	32	GLU
1	A	36	LYS
1	A	136	LEU
1	A	150	LEU
1	A	155	LEU
1	A	173	ASN
1	B	40[A]	ASN
1	B	40[B]	ASN
1	B	71	ARG
1	B	148	MET
1	B	150	LEU
1	C	4	SER
1	C	14	LEU
1	C	81	ARG
1	C	148	MET
1	C	176	GLU

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Mol	Chain	Res	Type
1	D	5	GLU
1	D	34	LYS
1	D	36	LYS
1	D	54	VAL
1	D	70	GLU
1	D	76	THR
1	D	77	ARG
1	D	148	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	B	62	GLN
1	B	103	ASN
1	B	173	ASN
1	C	69	GLN
1	C	103	ASN
1	C	173	ASN
1	D	40	ASN
1	D	62	GLN
1	D	114	GLN
1	D	115	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	GNP	A	1180	5	27,34,34	2.74	10 (37%)	30,54,54	2.17	9 (30%)
3	TRS	A	1181	-	7,7,7	2.09	1 (14%)	9,9,9	2.06	3 (33%)
3	TRS	A	1182	-	7,7,7	2.28	2 (28%)	9,9,9	2.12	3 (33%)
4	BME	A	1183	-	3,3,3	0.31	0	1,2,2	0.29	0
2	GNP	B	1178	5	27,34,34	3.23	11 (40%)	30,54,54	2.46	9 (30%)
2	GNP	C	1178	5	27,34,34	2.96	11 (40%)	30,54,54	2.26	8 (26%)
3	TRS	C	1179	-	7,7,7	1.69	3 (42%)	9,9,9	3.75	6 (66%)
4	BME	C	1180	-	3,3,3	0.33	0	1,2,2	0.15	0
3	TRS	D	1178	-	7,7,7	1.53	2 (28%)	9,9,9	3.59	4 (44%)
2	GNP	D	1179	5	27,34,34	3.38	10 (37%)	30,54,54	2.20	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
2	GNP	A	1180	5	-	1/16/38/38	0/3/3/3
3	TRS	A	1181	-	-	0/9/9/9	0/0/0/0
3	TRS	A	1182	-	-	0/9/9/9	0/0/0/0
4	BME	A	1183	-	-	0/1/1/1	0/0/0/0
2	GNP	B	1178	5	-	0/16/38/38	0/3/3/3
2	GNP	C	1178	5	-	1/16/38/38	0/3/3/3
3	TRS	C	1179	-	-	0/9/9/9	0/0/0/0
4	BME	C	1180	-	-	0/1/1/1	0/0/0/0
3	TRS	D	1178	-	-	0/9/9/9	0/0/0/0
2	GNP	D	1179	5	-	0/16/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1179	GNP	C4-N9	-8.81	1.36	1.47
2	C	1178	GNP	C4-N9	-6.54	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1180	GNP	C4-N9	-6.42	1.39	1.47
2	D	1179	GNP	C5-C6	-6.06	1.42	1.52
2	B	1178	GNP	C4-N9	-6.00	1.39	1.47
2	C	1178	GNP	C5-C6	-5.95	1.42	1.52
2	B	1178	GNP	C5-C6	-5.72	1.42	1.52
3	A	1182	TRS	C2-C	-5.42	1.39	1.52
2	A	1180	GNP	C5-C6	-5.37	1.43	1.52
3	A	1181	TRS	C2-C	-4.82	1.41	1.52
2	D	1179	GNP	PG-O3G	-4.58	1.44	1.56
2	C	1178	GNP	PG-O2G	-4.56	1.44	1.56
2	B	1178	GNP	PG-O2G	-4.41	1.44	1.56
2	A	1180	GNP	PG-O2G	-4.38	1.44	1.56
2	D	1179	GNP	PG-O2G	-3.94	1.45	1.56
2	C	1178	GNP	PB-O2B	-3.67	1.46	1.56
2	B	1178	GNP	PG-O3G	-3.43	1.47	1.56
2	B	1178	GNP	PB-O2B	-3.11	1.48	1.56
2	B	1178	GNP	C8-N9	-2.81	1.38	1.46
2	D	1179	GNP	PB-O2B	-2.79	1.49	1.56
3	D	1178	TRS	C2-C	-2.77	1.46	1.52
2	C	1178	GNP	C5-C4	-2.72	1.35	1.52
2	D	1179	GNP	C8-N9	-2.68	1.39	1.46
2	C	1178	GNP	PG-O3G	-2.50	1.49	1.56
2	B	1178	GNP	C5-C4	-2.44	1.37	1.52
2	A	1180	GNP	C8-N9	-2.38	1.39	1.46
2	A	1180	GNP	C5-C4	-2.28	1.38	1.52
3	C	1179	TRS	C2-C	-2.22	1.47	1.52
3	A	1182	TRS	O1-C1	-2.21	1.35	1.42
2	C	1178	GNP	C2-N1	-2.20	1.35	1.44
2	A	1180	GNP	PB-O2B	-2.16	1.50	1.56
2	A	1180	GNP	PG-O3G	-2.13	1.50	1.56
2	D	1179	GNP	C5-C4	-2.07	1.39	1.52
2	C	1178	GNP	C8-N9	-2.04	1.40	1.46
3	D	1178	TRS	O1-C1	-2.01	1.35	1.42
2	B	1178	GNP	O4'-C4'	2.12	1.49	1.45
2	D	1179	GNP	PB-O1B	2.12	1.48	1.46
3	C	1179	TRS	O2-C2	2.25	1.49	1.42
3	C	1179	TRS	C1-C	2.70	1.59	1.52
2	B	1178	GNP	C6-N1	4.07	1.40	1.33
2	A	1180	GNP	C6-N1	4.18	1.40	1.33
2	A	1180	GNP	PB-O1B	4.23	1.50	1.46
2	C	1178	GNP	C6-N1	4.50	1.40	1.33
2	C	1178	GNP	PB-O1B	4.55	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1179	GNP	C6-N1	4.67	1.41	1.33
2	B	1178	GNP	PB-O1B	5.62	1.52	1.46
2	A	1180	GNP	PG-O1G	6.82	1.53	1.46
2	C	1178	GNP	PG-O1G	6.95	1.54	1.46
2	B	1178	GNP	PG-O1G	9.54	1.56	1.46
2	D	1179	GNP	PG-O1G	10.16	1.57	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1179	GNP	O1G-PG-N3B	-6.47	102.12	111.79
2	A	1180	GNP	O6-C6-N1	-5.14	115.88	122.71
2	B	1178	GNP	C5-C6-N1	-4.95	112.38	118.27
2	C	1178	GNP	C5-C6-N1	-4.81	112.54	118.27
2	B	1178	GNP	O1G-PG-N3B	-4.74	104.71	111.79
2	B	1178	GNP	O6-C6-N1	-4.68	116.50	122.71
2	C	1178	GNP	O6-C6-N1	-4.46	116.79	122.71
2	A	1180	GNP	C5-C6-N1	-3.97	113.54	118.27
2	C	1178	GNP	O1G-PG-N3B	-3.73	106.21	111.79
3	D	1178	TRS	C3-C-C1	-3.55	101.00	111.06
2	D	1179	GNP	O6-C6-N1	-3.54	118.01	122.71
2	D	1179	GNP	C5-C6-N1	-3.27	114.38	118.27
2	D	1179	GNP	O2G-PG-O1G	-3.03	105.72	113.43
2	A	1180	GNP	O3G-PG-O1G	-2.73	106.49	113.43
3	C	1179	TRS	C1-C-N	-2.72	101.94	107.73
3	C	1179	TRS	C3-C-C1	-2.60	103.71	111.06
2	B	1178	GNP	O3G-PG-O1G	-2.52	107.03	113.43
2	B	1178	GNP	O3'-C3'-C4'	-2.45	103.97	111.06
2	C	1178	GNP	O1B-PB-N3B	-2.34	108.29	111.79
2	A	1180	GNP	O1G-PG-N3B	-2.32	108.32	111.79
2	A	1180	GNP	O1B-PB-N3B	-2.25	108.43	111.79
3	A	1182	TRS	C2-C-N	2.03	112.04	107.73
3	A	1181	TRS	O2-C2-C	2.11	116.59	110.47
2	D	1179	GNP	C2'-C1'-N9	2.24	119.05	113.34
3	A	1182	TRS	O2-C2-C	2.77	118.50	110.47
2	A	1180	GNP	O2B-PB-O1B	2.80	115.66	109.88
3	C	1179	TRS	C3-C-C2	2.80	118.99	111.06
3	D	1178	TRS	C3-C-C2	2.91	119.31	111.06
3	C	1179	TRS	O1-C1-C	3.03	119.25	110.47
2	C	1178	GNP	O3G-PG-O2G	3.03	115.86	107.61
2	A	1180	GNP	O3G-PG-O2G	3.14	116.14	107.61
2	D	1179	GNP	O3G-PG-O2G	3.18	116.24	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1178	GNP	O2B-PB-O1B	3.24	116.57	109.88
2	B	1178	GNP	O2B-PB-O1B	3.26	116.62	109.88
3	A	1181	TRS	O3-C3-C	3.44	120.43	110.47
2	D	1179	GNP	O6-C6-C5	3.69	127.44	119.82
2	B	1178	GNP	O3G-PG-O2G	4.09	118.71	107.61
3	A	1182	TRS	O3-C3-C	4.33	122.99	110.47
3	A	1181	TRS	O1-C1-C	4.57	123.71	110.47
2	A	1180	GNP	C4-C5-N7	5.05	109.15	102.46
2	A	1180	GNP	O6-C6-C5	5.22	130.58	119.82
2	C	1178	GNP	O6-C6-C5	5.26	130.67	119.82
3	D	1178	TRS	O3-C3-C	5.47	126.30	110.47
2	B	1178	GNP	O6-C6-C5	5.48	131.12	119.82
2	D	1179	GNP	C4-C5-N7	5.53	109.79	102.46
2	C	1178	GNP	C4-C5-N7	5.71	110.02	102.46
2	B	1178	GNP	C4-C5-N7	5.74	110.06	102.46
3	C	1179	TRS	O3-C3-C	6.08	128.08	110.47
3	C	1179	TRS	O2-C2-C	7.44	131.99	110.47
3	D	1178	TRS	O2-C2-C	7.78	133.00	110.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1180	GNP	O1B-PB-N3B-PG
2	C	1178	GNP	O1B-PB-N3B-PG

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1181	TRS	5	0
3	A	1182	TRS	4	0
2	C	1178	GNP	1	0
3	C	1179	TRS	5	0
4	C	1180	BME	3	0
3	D	1178	TRS	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	75:VAL	C	76:THR	N	1.18
1	D	114:GLN	C	115:ASN	N	1.18
1	D	36:LYS	C	37:ASP	N	1.03

## 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	176/186 (94%)	0.18	5 (2%) 53 54	14, 23, 41, 51	0
1	B	173/186 (93%)	-0.14	1 (0%) 89 90	13, 20, 33, 44	1 (0%)
1	C	174/186 (93%)	0.06	7 (4%) 38 39	14, 22, 36, 50	0
1	D	174/186 (93%)	0.32	13 (7%) 14 14	17, 26, 47, 60	0
All	All	697/744 (93%)	0.11	26 (3%) 41 42	13, 23, 42, 60	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	7.4
1	D	4	SER	7.1
1	D	75	VAL	6.0
1	D	114	GLN	5.7
1	A	178	GLY	4.7
1	D	37	ASP	4.3
1	C	114	GLN	3.8
1	C	4	SER	3.8
1	D	38	ASP	3.7
1	D	110	MET	3.7
1	D	113	SER	3.7
1	D	112	ALA	3.6
1	A	4	SER	3.4
1	D	111	LEU	3.3
1	A	5	GLU	2.8
1	D	70	GLU	2.6
1	C	177	SER	2.6
1	C	5	GLU	2.5
1	D	71	ARG	2.5
1	C	115	ASN	2.4
1	D	74	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	81	ARG	2.2
1	A	38	ASP	2.1
1	C	176	GLU	2.1
1	D	44	GLY	2.1
1	B	96	GLU	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TRS	A	1182	8/8	0.74	0.29	47,48,48,48	0
4	BME	C	1180	4/4	0.75	0.15	35,41,44,53	0
3	TRS	D	1178	8/8	0.79	0.26	31,40,40,40	0
3	TRS	A	1181	8/8	0.81	0.26	29,36,37,38	0
3	TRS	C	1179	8/8	0.85	0.15	24,33,34,34	0
4	BME	A	1183	4/4	0.87	0.09	29,33,36,44	0
5	MG	D	1180	1/1	0.97	0.08	22,22,22,22	0
5	MG	C	1181	1/1	0.98	0.06	17,17,17,17	0
2	GNP	D	1179	32/32	0.98	0.06	18,21,25,30	0
2	GNP	A	1180	32/32	0.98	0.06	18,22,27,27	0
2	GNP	B	1178	32/32	0.99	0.07	14,16,19,23	0
5	MG	A	1184	1/1	0.99	0.06	19,19,19,19	0
2	GNP	C	1178	32/32	0.99	0.06	15,17,20,22	0
5	MG	B	1179	1/1	0.99	0.05	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.