Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:14 PM GMT

PDB ID	:	4HLQ
Title	:	Crystal structure of human rab1b bound to GDP and BEF3 in complex with the GAP domain of TBC1D20 from homo sapiens
Authors	:	Gazdag, E.M.; Gavriljuk, K.; Itzen, A.; Koetting, C.; Gerwert, K.; Goody, R.S.
Deposited on	:	2012-10-17
Resolution	:	3.30 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:

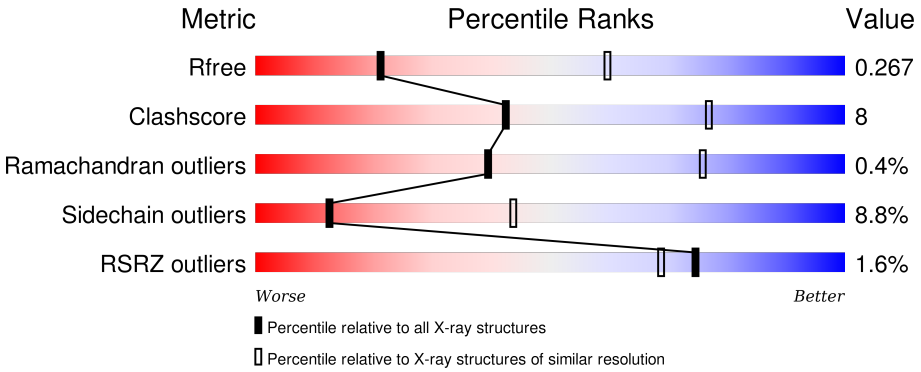
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	305	74% 16% • 8%
1	C	305	69% 21% • 8%
1	E	305	72% 18% • 8%
1	G	305	71% 18% • 8%
1	I	305	70% 21% • 8%

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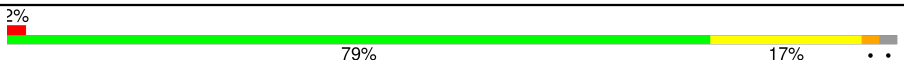
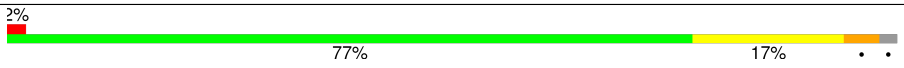
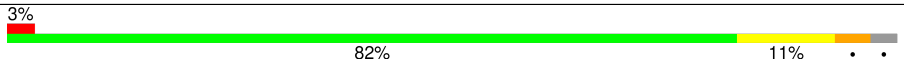
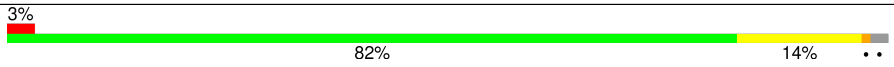
Mol	Chain	Length	Quality of chain
2	B	175	
2	D	175	
2	F	175	
2	H	175	
2	J	175	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17765 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 TBC1 domain family member 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	4	0	0
			2242	1442	391	397	12			
1	C	281	Total	C	N	O	S	0	0	0
			2240	1439	388	401	12			
1	E	281	Total	C	N	O	S	0	0	0
			2246	1442	389	403	12			
1	G	281	Total	C	N	O	S	0	0	0
			2118	1361	365	382	10			
1	I	281	Total	C	N	O	S	0	0	0
			2237	1439	387	399	12			

- Molecule 2 is a protein called Ras-related protein Rab-1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1332	845	218	265	4			
2	D	170	Total	C	N	O	S	0	0	0
			1327	845	217	261	4			
2	F	172	Total	C	N	O	S	0	0	0
			1321	839	219	260	3			
2	H	170	Total	C	N	O	S	4	0	0
			1202	752	203	245	2			
2	J	171	Total	C	N	O	S	0	0	0
			1259	799	205	251	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	EXPRESSION TAG	UNP Q9H0U4
B	1	HIS	-	EXPRESSION TAG	UNP Q9H0U4
B	2	MET	-	EXPRESSION TAG	UNP Q9H0U4
D	0	GLY	-	EXPRESSION TAG	UNP Q9H0U4
D	1	HIS	-	EXPRESSION TAG	UNP Q9H0U4

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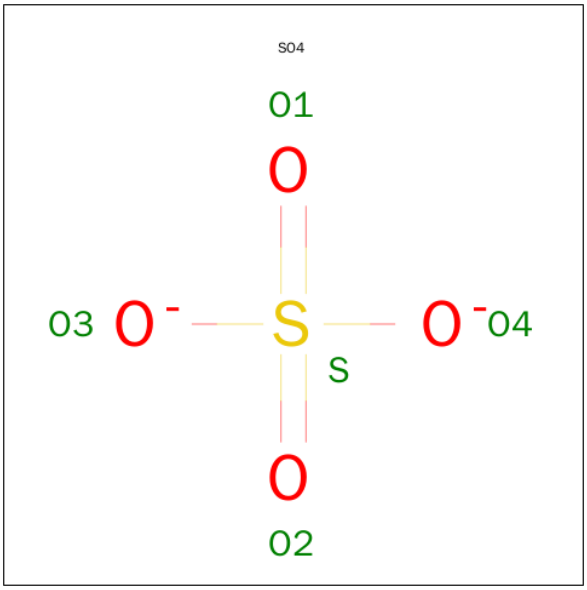
Chain	Residue	Modelled	Actual	Comment	Reference
D	2	MET	-	EXPRESSION TAG	UNP Q9H0U4
F	0	GLY	-	EXPRESSION TAG	UNP Q9H0U4
F	1	HIS	-	EXPRESSION TAG	UNP Q9H0U4
F	2	MET	-	EXPRESSION TAG	UNP Q9H0U4
H	0	GLY	-	EXPRESSION TAG	UNP Q9H0U4
H	1	HIS	-	EXPRESSION TAG	UNP Q9H0U4
H	2	MET	-	EXPRESSION TAG	UNP Q9H0U4
J	0	GLY	-	EXPRESSION TAG	UNP Q9H0U4
J	1	HIS	-	EXPRESSION TAG	UNP Q9H0U4
J	2	MET	-	EXPRESSION TAG	UNP Q9H0U4

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

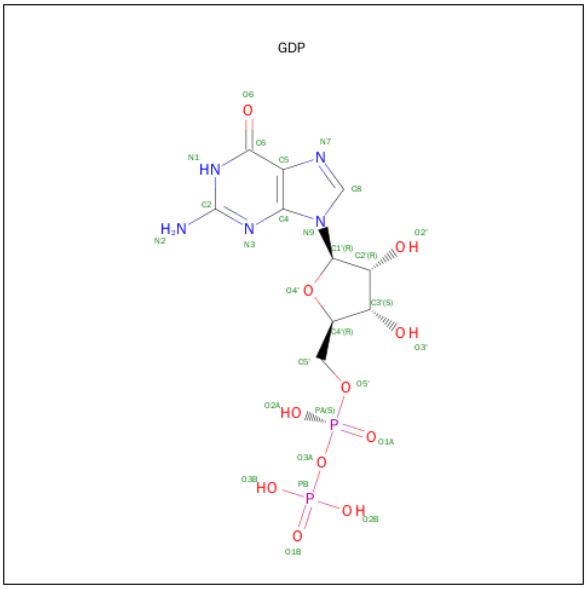


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	I	1	Total O S 5 4 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

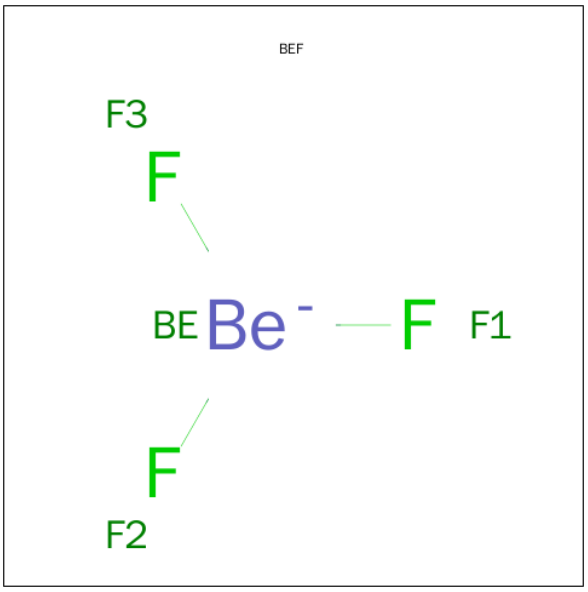
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

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



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

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Be F 4 1 3	0	0
6	D	1	Total Be F 4 1 3	0	0
6	F	1	Total Be F 4 1 3	0	0
6	H	1	Total Be F 4 1 3	0	0
6	J	1	Total Be F 4 1 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	9	Total O 9 9	0	0
7	B	4	Total O 4 4	0	0
7	C	7	Total O 7 7	0	0
7	D	4	Total O 4 4	0	0
7	E	8	Total O 8 8	0	0
7	F	4	Total O 4 4	0	0
7	G	4	Total O 4 4	0	0

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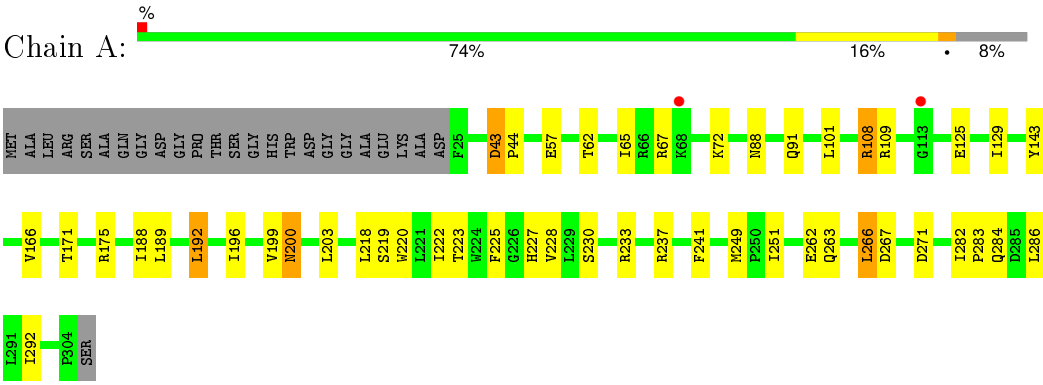
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	2	Total O 2 2	0	0
7	I	7	Total O 7 7	0	0
7	J	2	Total O 2 2	0	0

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.

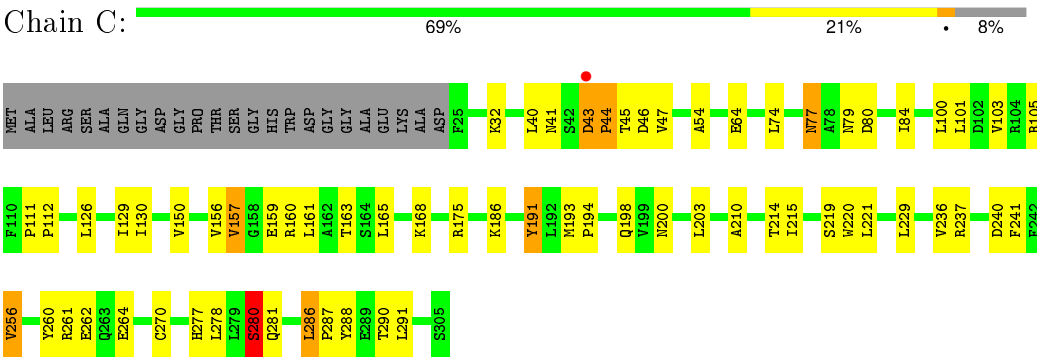
- Molecule 1: TBC1 domain family member 20

Chain A:



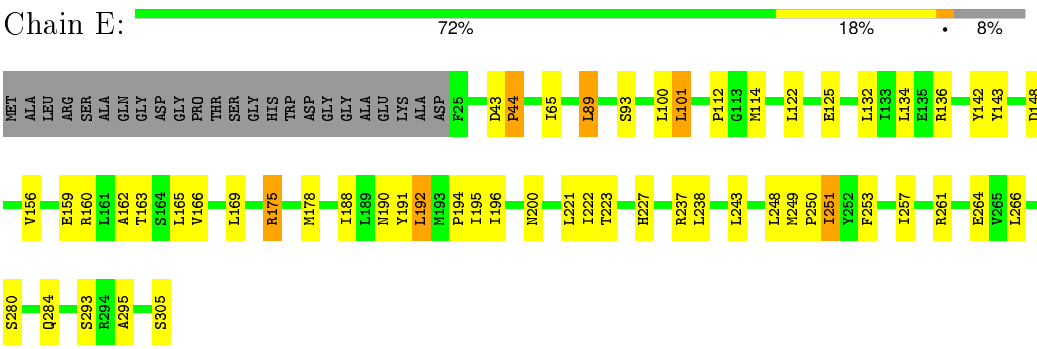
- Molecule 1: TBC1 domain family member 20

Chain C:



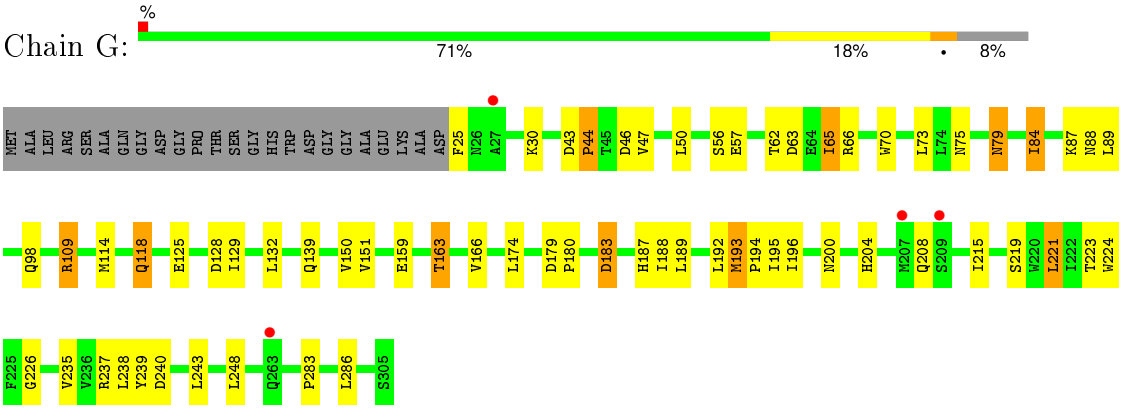
- Molecule 1: TBC1 domain family member 20

Chain E:



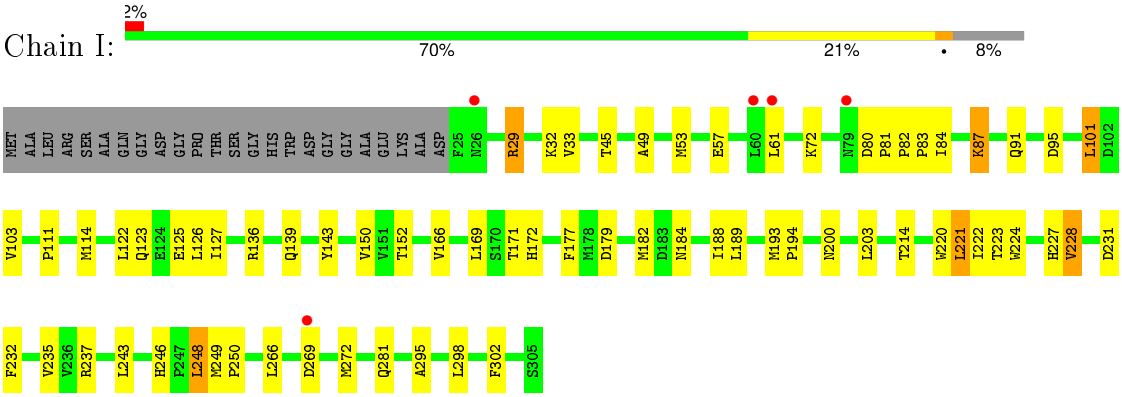
• Molecule 1: TBC1 domain family member 20

Chain G:



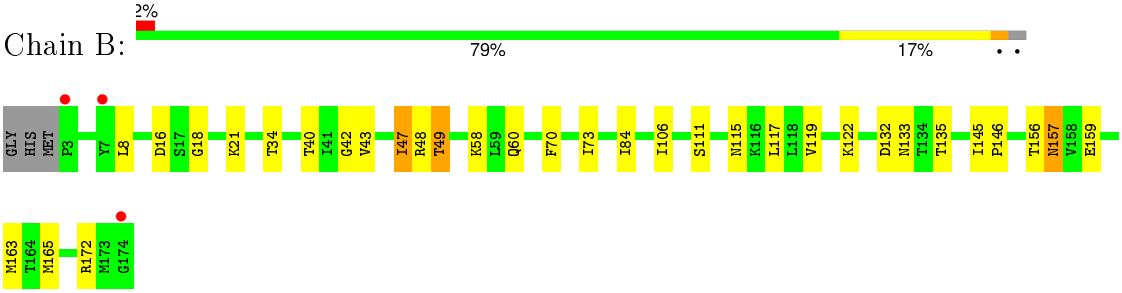
• Molecule 1: TBC1 domain family member 20

Chain I:



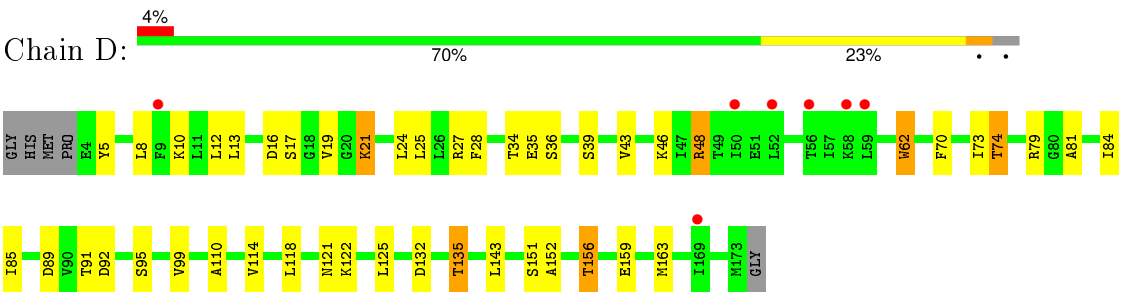
• Molecule 2: Ras-related protein Rab-1B

Chain B:



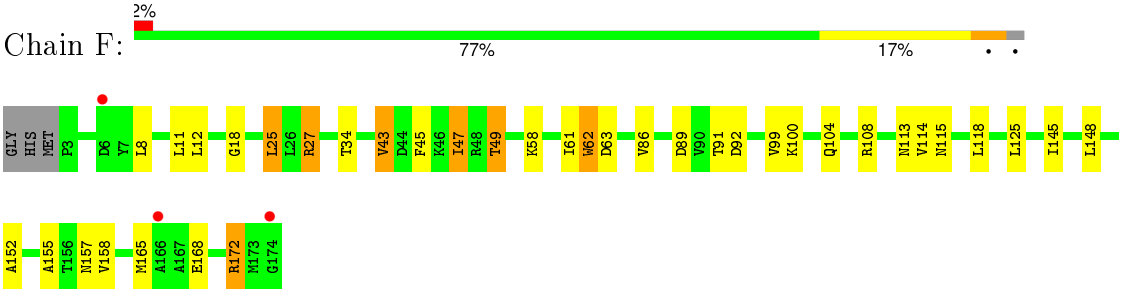
• Molecule 2: Ras-related protein Rab-1B

Chain D:



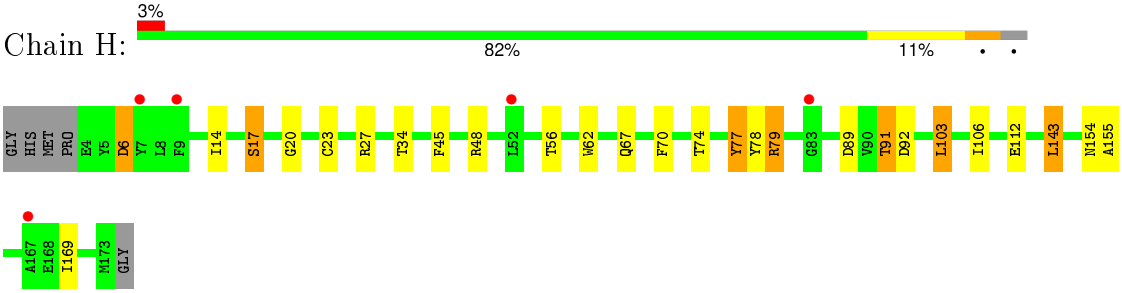
• Molecule 2: Ras-related protein Rab-1B

Chain F:



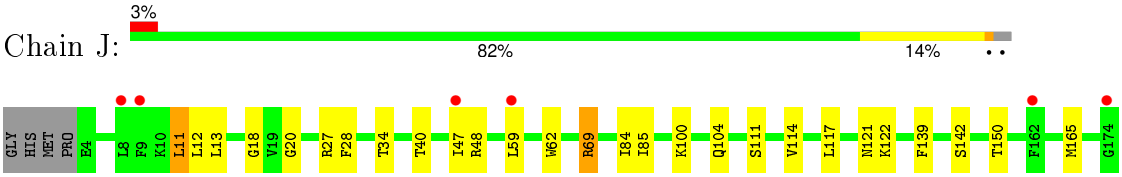
• Molecule 2: Ras-related protein Rab-1B

Chain H:



• Molecule 2: Ras-related protein Rab-1B

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.17Å 118.64Å 290.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.22 – 3.30 48.52 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-3.30) 100.0 (48.52-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.206 , 0.274 0.202 , 0.267	Depositor DCC
R_{free} test set	2334 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	79.9	Xtriage
Anisotropy	0.497	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 77.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 46665 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17765	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, BEF, SO4

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	0.35	0/2298	0.53	0/3130
1	C	0.36	0/2296	0.56	1/3129 (0.0%)
1	E	0.34	0/2302	0.53	0/3137
1	G	0.34	0/2172	0.52	0/2975
1	I	0.34	0/2293	0.54	0/3125
2	B	0.36	0/1353	0.54	0/1832
2	D	0.37	0/1348	0.55	0/1825
2	F	0.35	0/1342	0.54	0/1818
2	H	0.66	1/1221 (0.1%)	0.59	2/1667 (0.1%)
2	J	0.36	0/1280	0.52	0/1744
All	All	0.38	1/17905 (0.0%)	0.54	3/24382 (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	2
1	C	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	79	ARG	CD-NE	-19.54	1.13	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	79	ARG	CG-CD-NE	11.20	135.32	111.80
2	H	79	ARG	CD-NE-CZ	-5.31	116.16	123.60
1	C	280	SER	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ARG	Sidechain
1	A	43	ASP	Peptide
1	C	280	SER	Peptide
1	C	43	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2242	0	2195	40	0
1	C	2240	0	2190	42	0
1	E	2246	0	2195	39	0
1	G	2118	0	1943	35	0
1	I	2237	0	2189	44	0
2	B	1332	0	1278	20	0
2	D	1327	0	1300	25	0
2	F	1321	0	1268	19	0
2	H	1202	0	1014	19	0
2	J	1259	0	1123	13	0
3	A	5	0	0	1	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	I	5	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
5	B	28	0	12	2	0
5	D	28	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	28	0	12	1	0
5	H	28	0	12	7	0
5	J	28	0	12	3	0
6	B	4	0	0	0	0
6	D	4	0	0	0	0
6	F	4	0	0	0	0
6	H	4	0	0	1	0
6	J	4	0	0	1	0
7	A	9	0	0	1	0
7	B	4	0	0	0	0
7	C	7	0	0	0	0
7	D	4	0	0	0	0
7	E	8	0	0	0	0
7	F	4	0	0	0	0
7	G	4	0	0	1	0
7	H	2	0	0	0	0
7	I	7	0	0	0	0
7	J	2	0	0	0	0
All	All	17765	0	16755	287	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 8.

All (287) 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:G:79:ASN:HD22	1:G:79:ASN:H	1.06	0.96
1:E:175:ARG:O	1:E:175:ARG:HD3	1.77	0.83
1:G:98:GLN:HG2	2:H:67:GLN:HE21	1.41	0.83
1:I:177:PHE:HZ	1:I:221:LEU:HD22	1.47	0.80
2:H:45:PHE:HB3	2:H:62:TRP:CD1	2.19	0.77
1:G:109:ARG:HG2	1:G:151:VAL:HG11	1.65	0.77
2:B:49:THR:HG22	2:B:58:LYS:HD3	1.67	0.76
1:I:87:LYS:HD2	1:I:87:LYS:H	1.51	0.76
1:E:143:TYR:CE1	1:E:222:ILE:HG23	2.22	0.75
2:H:20:GLY:HA2	5:H:202:GDP:H5"	1.70	0.74
1:E:101:LEU:HD21	2:F:18:GLY:HA3	1.70	0.72
1:G:79:ASN:ND2	1:G:79:ASN:H	1.86	0.71
1:A:228:VAL:CG1	1:A:282:ILE:HG21	2.20	0.71
2:H:20:GLY:HA2	5:H:202:GDP:C5'	2.22	0.70
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ARG:C	1:E:175:ARG:HD3	2.08	0.69
1:I:80:ASP:HB2	1:I:81:PRO:HD2	1.75	0.69
1:I:177:PHE:CZ	1:I:221:LEU:HD22	2.27	0.68
1:E:175:ARG:HH11	1:E:175:ARG:HG3	1.57	0.68
1:A:62:THR:OG1	1:A:65:ILE:HD13	1.93	0.68
2:H:14:ILE:HG21	2:H:78:TYR:OH	1.94	0.68
2:D:5:TYR:OH	2:D:8:LEU:HD12	1.94	0.67
1:A:143:TYR:CE1	1:A:222:ILE:HG23	2.29	0.67
1:I:143:TYR:CE1	1:I:222:ILE:HG23	2.30	0.67
1:I:179:ASP:O	2:J:69:ARG:NH2	2.28	0.67
1:G:159:GLU:O	1:G:163:THR:HG22	1.95	0.66
1:A:203:LEU:HD12	1:A:262:GLU:HG3	1.77	0.66
1:G:79:ASN:HD22	1:G:79:ASN:N	1.83	0.66
1:I:246:HIS:HE1	1:I:248:LEU:HD12	1.60	0.66
2:H:6:ASP:HB2	2:H:56:THR:O	1.96	0.65
1:G:125:GLU:O	1:G:129:ILE:HG12	1.97	0.65
1:A:241:PHE:HZ	1:A:249:MET:CE	2.09	0.64
1:A:241:PHE:HZ	1:A:249:MET:HE3	1.63	0.64
1:A:230:SER:H	1:A:284:GLN:HE22	1.47	0.62
2:D:151:SER:HB3	2:D:156:THR:HG23	1.82	0.62
5:H:202:GDP:H5'	5:H:202:GDP:C8	2.35	0.61
1:A:241:PHE:CZ	1:A:249:MET:HE2	2.36	0.61
1:C:74:LEU:O	1:C:168:LYS:HD3	2.00	0.61
1:I:224:TRP:HZ3	1:I:243:LEU:HD22	1.64	0.61
5:H:202:GDP:H5'	5:H:202:GDP:H8	1.66	0.61
1:A:125:GLU:O	1:A:129:ILE:HD12	2.00	0.61
1:I:29:ARG:HD2	1:I:61:LEU:HD22	1.82	0.61
1:A:67:ARG:NH1	3:A:401:SO4:O2	2.33	0.61
2:B:21:LYS:N	5:B:202:GDP:O3B	2.33	0.61
2:B:132:ASP:HB3	2:B:135:THR:OG1	2.01	0.60
2:D:70:PHE:O	2:D:73:ILE:HG22	2.01	0.60
1:C:43:ASP:HB3	1:C:44:PRO:HD3	1.84	0.60
2:H:45:PHE:HB3	2:H:62:TRP:HD1	1.63	0.60
1:E:143:TYR:HE1	1:E:222:ILE:HG23	1.63	0.60
2:B:48:ARG:NH2	2:B:159:GLU:OE1	2.35	0.60
1:A:241:PHE:CZ	1:A:249:MET:CE	2.85	0.60
1:A:150:VAL:HG22	1:A:166:VAL:HG11	1.84	0.59
1:E:238:LEU:HD21	1:E:253:PHE:CE2	2.37	0.59
1:G:150:VAL:HG22	1:G:166:VAL:HG11	1.83	0.59
1:A:192:LEU:O	1:A:196:ILE:HG12	2.02	0.58
1:A:57:GLU:HG3	1:A:289:GLU:HG2	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLU:HG2	1:E:159:GLU:HG3	1.85	0.58
1:A:188:ILE:O	1:A:251:ILE:HD13	2.04	0.58
1:E:114:MET:CE	1:E:122:LEU:HD12	2.34	0.57
2:F:27:ARG:HB3	2:F:158:VAL:HG11	1.86	0.57
1:E:150:VAL:HG22	1:E:166:VAL:HG11	1.85	0.57
2:F:89:ASP:OD1	2:F:91:THR:HG22	2.04	0.57
2:B:115:ASN:HD21	2:B:172:ARG:HD3	1.70	0.57
1:E:162:ALA:O	1:E:166:VAL:HG23	2.04	0.56
1:C:107:LEU:C	1:C:109:ARG:H	2.08	0.56
1:C:157:VAL:HG13	1:C:161:LEU:CB	2.35	0.56
1:C:129:ILE:HD11	1:C:159:GLU:HG3	1.86	0.56
1:I:111:PRO:HG2	1:I:114:MET:HB2	1.88	0.56
1:C:54:ALA:O	1:C:237:ARG:NH1	2.39	0.56
2:J:121:ASN:HA	2:J:150:THR:O	2.06	0.56
1:E:112:PRO:HB2	1:I:302:PHE:HZ	1.71	0.55
2:D:43:VAL:HG13	2:D:62:TRP:HD1	1.70	0.55
1:I:45:THR:HG21	1:I:72:LYS:HD2	1.89	0.55
2:H:14:ILE:HD11	2:H:106:ILE:HD11	1.87	0.55
1:A:143:TYR:HE1	1:A:222:ILE:HG23	1.70	0.55
1:C:77:ASN:HD22	1:C:79:ASN:H	1.53	0.55
1:A:287:PRO:HB2	1:A:290:THR:HB	1.89	0.55
1:C:157:VAL:CG1	1:C:161:LEU:HB3	2.36	0.54
1:G:63:ASP:HA	1:G:66:ARG:HG3	1.87	0.54
1:E:249:MET:HE1	1:E:295:ALA:HB1	1.87	0.54
1:E:175:ARG:CG	1:E:175:ARG:HH11	2.20	0.54
1:G:235:VAL:HA	1:G:238:LEU:HD23	1.88	0.54
2:F:125:LEU:HD11	5:F:202:GDP:N2	2.22	0.54
2:J:85:ILE:HG12	2:J:117:LEU:HD23	1.90	0.54
1:I:171:THR:HG23	1:I:172:HIS:ND1	2.23	0.54
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.73	0.54
1:E:188:ILE:O	1:E:191:TYR:HB2	2.08	0.54
1:C:157:VAL:HG13	1:C:161:LEU:HB3	1.91	0.53
1:G:129:ILE:HG23	1:G:163:THR:HB	1.91	0.53
1:C:229:LEU:HD21	1:C:286:LEU:HD12	1.91	0.53
1:G:239:TYR:O	1:G:243:LEU:HB2	2.08	0.53
1:G:183:ASP:O	1:G:187:HIS:ND1	2.42	0.53
1:C:156:VAL:CG2	1:C:236:VAL:HG11	2.39	0.52
1:A:189:LEU:HA	1:A:251:ILE:HD11	1.92	0.52
2:D:132:ASP:HB2	2:D:135:THR:HG23	1.90	0.52
1:C:256:VAL:CG1	1:C:291:LEU:HD22	2.40	0.52
1:C:77:ASN:C	1:C:77:ASN:HD22	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:193:MET:HB3	1:I:194:PRO:CD	2.40	0.52
2:B:156:THR:HG22	2:B:157:ASN:HB2	1.92	0.52
1:E:114:MET:HE1	1:E:122:LEU:HD12	1.91	0.52
1:I:188:ILE:HG23	1:I:248:LEU:HD23	1.92	0.52
1:G:139:GLN:NE2	7:G:404:HOH:O	2.43	0.52
1:C:193:MET:CE	1:C:214:THR:HG22	2.39	0.52
1:A:262:GLU:HG2	1:A:266:LEU:CD1	2.39	0.51
1:A:218:LEU:HD23	2:B:42:GLY:HA2	1.92	0.51
1:A:188:ILE:O	1:A:251:ILE:CD1	2.58	0.51
1:C:237:ARG:O	1:C:237:ARG:HD2	2.10	0.51
1:I:249:MET:CE	1:I:295:ALA:HB1	2.41	0.51
1:A:228:VAL:HG12	1:A:282:ILE:HG21	1.93	0.51
1:I:32:LYS:HE3	1:I:61:LEU:HD11	1.93	0.51
1:E:223:THR:HG21	1:E:227:HIS:HB2	1.93	0.51
1:I:87:LYS:N	1:I:87:LYS:HD2	2.25	0.51
2:D:70:PHE:O	2:D:74:THR:HG23	2.10	0.51
2:B:117:LEU:HD23	2:B:119:VAL:HG23	1.93	0.51
1:E:248:LEU:O	1:E:251:ILE:HG13	2.10	0.51
2:J:139:PHE:O	2:J:142:SER:HB3	2.10	0.51
1:I:83:PRO:HB3	1:I:136:ARG:HH21	1.76	0.51
2:J:20:GLY:HA3	2:J:121:ASN:HD22	1.76	0.50
5:H:202:GDP:C5'	5:H:202:GDP:H8	2.24	0.50
2:D:159:GLU:O	2:D:163:MET:HG2	2.11	0.50
1:E:192:LEU:HD23	1:E:196:ILE:HD11	1.94	0.50
1:C:77:ASN:HB3	1:C:80:ASP:OD2	2.12	0.50
1:A:286:LEU:HD12	1:A:286:LEU:H	1.77	0.50
1:E:277:HIS:HB2	2:F:45:PHE:CE1	2.47	0.50
1:C:191:TYR:O	1:C:194:PRO:HD2	2.12	0.50
1:C:286:LEU:HD23	1:C:287:PRO:HD2	1.93	0.50
1:G:192:LEU:O	1:G:196:ILE:HG12	2.12	0.50
2:B:84:ILE:HD12	2:B:106:ILE:HG23	1.93	0.50
2:D:19:VAL:HG23	2:D:21:LYS:HG3	1.93	0.49
2:B:117:LEU:CD2	2:B:119:VAL:HG23	2.42	0.49
2:F:148:LEU:HD23	2:F:157:ASN:HB3	1.95	0.49
1:I:231:ASP:O	1:I:235:VAL:HG23	2.11	0.49
1:I:184:ASN:O	1:I:188:ILE:HG12	2.12	0.49
2:H:17:SER:HA	6:H:203:BEF:F3	2.02	0.49
1:A:230:SER:HB3	1:A:284:GLN:NE2	2.28	0.49
1:A:189:LEU:HD11	1:A:218:LEU:HD13	1.93	0.49
2:F:113:ASN:HB3	2:F:172:ARG:HE	1.78	0.49
1:E:132:LEU:O	1:E:136:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:VAL:HG12	1:C:157:VAL:HG23	1.94	0.49
1:C:256:VAL:HG13	1:C:291:LEU:HD22	1.95	0.49
2:D:21:LYS:HB2	2:D:21:LYS:NZ	2.27	0.49
2:B:47:ILE:HG12	2:B:58:LYS:HD2	1.93	0.48
2:H:70:PHE:O	2:H:74:THR:HG22	2.13	0.48
1:G:66:ARG:NH1	1:G:240:ASP:OD2	2.47	0.48
2:D:24:LEU:HD23	2:D:152:ALA:HB2	1.96	0.48
1:I:189:LEU:HB3	1:I:214:THR:HB	1.95	0.48
1:I:101:LEU:HD11	2:J:18:GLY:HA3	1.95	0.48
2:D:43:VAL:HG13	2:D:62:TRP:CD1	2.49	0.48
2:F:104:GLN:HB3	2:F:108:ARG:NH1	2.29	0.48
2:F:47:ILE:HG21	2:F:58:LYS:HE2	1.96	0.48
1:I:61:LEU:H	1:I:61:LEU:HD12	1.78	0.48
1:I:32:LYS:HE2	1:I:57:GLU:O	2.14	0.47
2:J:20:GLY:HA2	5:J:202:GDP:O1A	2.14	0.47
1:G:193:MET:HB3	1:G:194:PRO:HD3	1.95	0.47
1:I:223:THR:HG21	1:I:227:HIS:HB2	1.97	0.47
1:C:193:MET:HE3	1:C:214:THR:HG22	1.97	0.47
2:D:24:LEU:HD21	2:D:121:ASN:HD21	1.79	0.47
1:A:237:ARG:NH2	1:A:292:ILE:HD13	2.29	0.47
2:B:70:PHE:O	2:B:73:ILE:HG22	2.14	0.47
1:E:89:LEU:O	1:E:93:SER:HB2	2.15	0.47
1:E:148:ASP:OD2	1:E:227:HIS:CD2	2.68	0.47
1:E:192:LEU:CD2	1:E:196:ILE:HD11	2.44	0.47
1:C:277:HIS:O	1:C:281:GLN:CB	2.63	0.46
1:C:237:ARG:O	1:C:240:ASP:HB2	2.15	0.46
2:B:117:LEU:HD12	2:B:146:PRO:HB2	1.97	0.46
1:E:160:ARG:O	1:E:163:THR:HG22	2.15	0.46
1:G:204:HIS:CE1	1:G:208:GLN:HE21	2.33	0.46
1:G:84:ILE:HD13	1:G:84:ILE:H	1.79	0.46
1:G:98:GLN:HG2	2:H:67:GLN:NE2	2.20	0.46
1:I:188:ILE:HG23	1:I:248:LEU:CD2	2.46	0.46
1:A:228:VAL:HG13	1:A:282:ILE:HG21	1.96	0.46
1:I:29:ARG:O	1:I:33:VAL:HG23	2.15	0.46
1:G:223:THR:H	1:G:224:TRP:HA	1.80	0.46
1:A:263:GLN:O	1:A:267:ASP:HB3	2.15	0.46
1:G:43:ASP:CB	1:G:44:PRO:HD3	2.45	0.46
2:H:89:ASP:OD2	2:H:91:THR:HG22	2.15	0.46
2:F:11:LEU:HD12	2:F:61:ILE:HG12	1.97	0.46
1:A:43:ASP:CB	1:A:44:PRO:HD3	2.46	0.46
1:C:77:ASN:ND2	1:C:79:ASN:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:220:TRP:CD1	1:I:228:VAL:HG21	2.51	0.46
1:I:169:LEU:HD11	1:I:224:TRP:CH2	2.51	0.45
1:C:43:ASP:HB3	1:C:44:PRO:CD	2.47	0.45
2:J:20:GLY:CA	5:J:202:GDP:O1A	2.64	0.45
1:I:81:PRO:HA	1:I:82:PRO:HD3	1.84	0.45
1:E:143:TYR:CE2	1:E:178:MET:HG2	2.51	0.45
1:C:157:VAL:CG1	1:C:161:LEU:CB	2.95	0.45
2:F:115:ASN:ND2	2:F:172:ARG:NH2	2.64	0.45
5:H:202:GDP:C5'	5:H:202:GDP:C8	3.00	0.45
2:F:43:VAL:HG13	2:F:62:TRP:CD1	2.51	0.45
2:F:43:VAL:HG13	2:F:62:TRP:HD1	1.81	0.45
2:D:122:LYS:HB3	2:D:125:LEU:HD12	1.99	0.45
2:F:27:ARG:HG3	2:F:152:ALA:HA	1.99	0.45
2:H:77:TYR:CD1	2:H:77:TYR:N	2.85	0.45
2:J:28:PHE:CE2	2:J:48:ARG:HG2	2.52	0.45
2:J:12:LEU:HD23	2:J:84:ILE:HG12	1.99	0.45
1:E:261:ARG:NH1	1:E:264:GLU:OE1	2.50	0.44
2:F:49:THR:HG22	2:F:58:LYS:HG3	1.99	0.44
1:E:43:ASP:CB	1:E:44:PRO:HD3	2.48	0.44
2:B:115:ASN:ND2	2:B:172:ARG:HH21	2.15	0.44
2:D:19:VAL:HA	2:D:89:ASP:HB2	1.99	0.44
1:C:241:PHE:CZ	1:C:249:MET:HE2	2.53	0.44
1:A:200:ASN:HD22	1:A:200:ASN:C	2.20	0.44
2:D:12:LEU:HB3	2:D:84:ILE:HG12	1.99	0.44
1:I:246:HIS:CE1	1:I:248:LEU:HD12	2.47	0.44
2:D:13:LEU:HD23	2:D:85:ILE:HB	1.99	0.44
1:I:49:ALA:O	1:I:53:MET:HG2	2.18	0.44
1:C:210:ALA:HB2	1:C:270:CYS:SG	2.58	0.44
1:C:220:TRP:CD1	1:C:220:TRP:N	2.86	0.44
1:G:189:LEU:HG	1:G:221:LEU:HD12	2.00	0.44
1:A:88:ASN:HB3	1:A:91:GLN:HB3	2.00	0.44
2:J:111:SER:HB3	2:J:114:VAL:HB	1.99	0.44
1:C:280:SER:H	1:C:281:GLN:CB	2.31	0.43
2:D:92:ASP:HB3	2:D:95:SER:OG	2.17	0.43
1:G:87:LYS:HA	1:G:88:ASN:HA	1.51	0.43
2:H:77:TYR:N	2:H:77:TYR:HD1	2.16	0.43
1:E:175:ARG:C	1:E:175:ARG:CD	2.82	0.43
1:E:114:MET:HE3	1:E:122:LEU:HD12	2.00	0.43
2:D:132:ASP:HB2	2:D:135:THR:CG2	2.48	0.43
1:C:160:ARG:O	1:C:163:THR:HG22	2.18	0.43
1:I:122:LEU:O	1:I:125:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:25:LEU:HD12	2:F:63:ASP:HB2	2.01	0.43
1:G:179:ASP:HB3	1:G:180:PRO:HD2	2.01	0.43
1:C:229:LEU:HD21	1:C:286:LEU:CD1	2.47	0.43
2:H:103:LEU:HD21	2:H:143:LEU:HD11	2.00	0.43
1:A:108:ARG:HH11	1:A:108:ARG:CG	2.26	0.43
2:B:122:LYS:HG2	5:B:202:GDP:C6	2.53	0.43
1:E:249:MET:N	1:E:250:PRO:CD	2.82	0.43
1:G:226:GLY:HA2	1:G:235:VAL:HG21	1.99	0.43
1:E:305:SER:HA	2:H:92:ASP:HB2	2.00	0.43
1:C:130:ILE:HG12	1:C:150:VAL:HG21	2.01	0.43
1:E:152:THR:O	1:E:156:VAL:HG23	2.18	0.43
1:C:261:ARG:NH2	1:C:278:LEU:O	2.52	0.43
2:D:10:LYS:HG2	2:D:81:ALA:HA	2.01	0.43
1:I:222:ILE:HA	1:I:222:ILE:HD13	1.89	0.42
2:F:27:ARG:HD2	2:F:155:ALA:HB2	2.01	0.42
1:C:161:LEU:O	1:C:165:LEU:HG	2.19	0.42
1:I:150:VAL:HG22	1:I:166:VAL:HG11	2.01	0.42
2:F:89:ASP:HB3	2:F:92:ASP:HB3	2.01	0.42
1:C:105:ARG:CZ	2:D:39:SER:HB3	2.49	0.42
2:J:11:LEU:HD21	2:J:59:LEU:HD23	2.00	0.42
1:I:224:TRP:CZ3	1:I:243:LEU:HD22	2.48	0.42
1:G:223:THR:N	1:G:224:TRP:HA	2.34	0.42
1:G:47:VAL:HA	1:G:50:LEU:HD12	2.02	0.42
2:B:8:LEU:HD12	2:B:58:LYS:HG2	2.01	0.42
1:G:114:MET:HG3	1:G:118:GLN:HG2	2.02	0.42
1:C:157:VAL:HG13	1:C:161:LEU:HB2	2.02	0.42
1:C:156:VAL:HG21	1:C:236:VAL:CG1	2.49	0.42
2:B:60:GLN:HG3	2:B:60:GLN:O	2.20	0.42
2:D:48:ARG:NH2	2:D:159:GLU:OE1	2.53	0.42
2:D:110:ALA:HB1	2:D:114:VAL:HG11	2.02	0.42
2:D:28:PHE:CE2	2:D:48:ARG:HG2	2.55	0.41
1:A:101:LEU:HD21	2:B:18:GLY:HA3	2.02	0.41
1:G:215:ILE:H	1:G:215:ILE:HD12	1.85	0.41
1:C:103:VAL:HG13	1:C:126:LEU:HD23	2.01	0.41
2:D:16:ASP:O	2:D:19:VAL:HG22	2.20	0.41
1:C:111:PRO:HA	1:C:112:PRO:HD3	1.90	0.41
1:I:221:LEU:HD23	1:I:250:PRO:HB2	2.02	0.41
1:I:103:VAL:HG13	1:I:126:LEU:HD23	2.01	0.41
1:I:152:THR:HG23	1:I:232:PHE:CE1	2.55	0.41
1:I:249:MET:N	1:I:250:PRO:CD	2.83	0.41
1:G:66:ARG:O	1:G:70:TRP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:CYS:HB2	5:H:202:GDP:O5'	2.19	0.41
1:G:65:ILE:HG22	1:G:66:ARG:N	2.35	0.41
1:E:148:ASP:OD2	1:E:227:HIS:HD2	2.04	0.41
1:C:44:PRO:O	1:C:45:THR:C	2.59	0.41
2:B:159:GLU:O	2:B:163:MET:HG2	2.20	0.41
1:I:220:TRP:HD1	1:I:228:VAL:HG21	1.86	0.41
1:E:165:LEU:O	1:E:169:LEU:HD12	2.20	0.41
1:A:72:LYS:NZ	7:A:501:HOH:O	2.54	0.41
5:J:202:GDP:O3B	6:J:203:BEF:F2	2.28	0.41
1:I:123:GLN:O	1:I:127:ILE:HG13	2.21	0.41
1:E:191:TYR:O	1:E:195:ILE:HG13	2.21	0.41
1:E:134:LEU:HD11	1:E:142:TYR:HB2	2.03	0.41
1:A:220:TRP:HB3	1:A:225:PHE:CE2	2.56	0.41
1:G:188:ILE:HG23	1:G:248:LEU:HD22	2.03	0.41
1:A:223:THR:HG21	1:A:227:HIS:HB2	2.02	0.41
2:B:42:GLY:O	2:B:43:VAL:HG23	2.21	0.41
1:C:107:LEU:HD22	2:D:36:SER:HB2	2.02	0.41
1:A:282:ILE:HG13	1:A:283:PRO:HD2	2.03	0.40
1:A:162:ALA:O	1:A:166:VAL:HG23	2.21	0.40
1:E:305:SER:HA	2:H:92:ASP:CG	2.42	0.40
1:E:190:ASN:O	1:E:194:PRO:HD2	2.22	0.40
1:G:73:LEU:HA	1:G:73:LEU:HD23	1.97	0.40
2:H:169:ILE:HD13	2:H:169:ILE:HA	2.00	0.40
1:I:182:MET:HG3	2:J:69:ARG:O	2.21	0.40
1:G:235:VAL:O	1:G:238:LEU:HB2	2.21	0.40
2:F:86:VAL:HG11	2:F:99:VAL:HG13	2.04	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	278/305 (91%)	264 (95%)	14 (5%)	0	100	100
1	C	279/305 (92%)	266 (95%)	11 (4%)	2 (1%)	26	66
1	E	279/305 (92%)	267 (96%)	11 (4%)	1 (0%)	39	76
1	G	279/305 (92%)	266 (95%)	9 (3%)	4 (1%)	14	50
1	I	279/305 (92%)	276 (99%)	3 (1%)	0	100	100
2	B	170/175 (97%)	161 (95%)	9 (5%)	0	100	100
2	D	168/175 (96%)	163 (97%)	5 (3%)	0	100	100
2	F	170/175 (97%)	159 (94%)	10 (6%)	1 (1%)	30	68
2	H	168/175 (96%)	156 (93%)	11 (6%)	1 (1%)	30	68
2	J	169/175 (97%)	161 (95%)	7 (4%)	1 (1%)	30	68
All	All	2239/2400 (93%)	2139 (96%)	90 (4%)	10 (0%)	39	76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	56	SER
2	H	155	ALA
2	F	114	VAL
1	E	44	PRO
1	G	46	ASP
1	G	283	PRO
2	J	122	LYS
1	G	44	PRO
1	C	44	PRO
1	C	47	VAL

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	239/271 (88%)	230 (96%)	9 (4%)	40	75
1	C	241/271 (89%)	214 (89%)	27 (11%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	242/271 (89%)	225 (93%)	17 (7%)	19 56
1	G	206/271 (76%)	183 (89%)	23 (11%)	7 30
1	I	240/271 (89%)	222 (92%)	18 (8%)	17 52
2	B	138/151 (91%)	128 (93%)	10 (7%)	18 54
2	D	141/151 (93%)	124 (88%)	17 (12%)	6 26
2	F	135/151 (89%)	120 (89%)	15 (11%)	8 31
2	H	103/151 (68%)	91 (88%)	12 (12%)	7 28
2	J	117/151 (78%)	106 (91%)	11 (9%)	11 39
All	All	1802/2110 (85%)	1643 (91%)	159 (9%)	12 44

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	171	THR
1	A	175	ARG
1	A	192	LEU
1	A	199	VAL
1	A	200	ASN
1	A	219	SER
1	A	266	LEU
1	A	271	ASP
2	B	16	ASP
2	B	34	THR
2	B	40	THR
2	B	47	ILE
2	B	49	THR
2	B	111	SER
2	B	133	ASN
2	B	145	ILE
2	B	157	ASN
2	B	165	MET
1	C	32	LYS
1	C	40	LEU
1	C	41	ASN
1	C	46	ASP
1	C	64	GLU
1	C	77	ASN
1	C	84	ILE

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Mol	Chain	Res	Type
1	C	100	LEU
1	C	101	LEU
1	C	157	VAL
1	C	175	ARG
1	C	186	LYS
1	C	191	TYR
1	C	198	GLN
1	C	200	ASN
1	C	203	LEU
1	C	215	ILE
1	C	219	SER
1	C	221	LEU
1	C	243	LEU
1	C	256	VAL
1	C	260	TYR
1	C	262	GLU
1	C	264	GLU
1	C	286	LEU
1	C	288	TYR
1	C	290	THR
2	D	17	SER
2	D	21	LYS
2	D	25	LEU
2	D	27	ARG
2	D	34	THR
2	D	35	GLU
2	D	46	LYS
2	D	48	ARG
2	D	62	TRP
2	D	74	THR
2	D	79	ARG
2	D	91	THR
2	D	99	VAL
2	D	118	LEU
2	D	135	THR
2	D	143	LEU
2	D	156	THR
1	E	65	ILE
1	E	89	LEU
1	E	100	LEU
1	E	101	LEU
1	E	175	ARG

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Mol	Chain	Res	Type
1	E	192	LEU
1	E	200	ASN
1	E	221	LEU
1	E	237	ARG
1	E	243	LEU
1	E	251	ILE
1	E	257	ILE
1	E	266	LEU
1	E	272	MET
1	E	280	SER
1	E	284	GLN
1	E	293	SER
2	F	8	LEU
2	F	12	LEU
2	F	25	LEU
2	F	27	ARG
2	F	34	THR
2	F	43	VAL
2	F	47	ILE
2	F	49	THR
2	F	62	TRP
2	F	100	LYS
2	F	118	LEU
2	F	145	ILE
2	F	165	MET
2	F	168	GLU
2	F	172	ARG
1	G	25	PHE
1	G	30	LYS
1	G	57	GLU
1	G	62	THR
1	G	65	ILE
1	G	75	ASN
1	G	79	ASN
1	G	84	ILE
1	G	89	LEU
1	G	109	ARG
1	G	118	GLN
1	G	128	ASP
1	G	132	LEU
1	G	163	THR
1	G	174	LEU

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Mol	Chain	Res	Type
1	G	183	ASP
1	G	193	MET
1	G	195	ILE
1	G	200	ASN
1	G	219	SER
1	G	221	LEU
1	G	237	ARG
1	G	286	LEU
2	H	6	ASP
2	H	17	SER
2	H	27	ARG
2	H	34	THR
2	H	48	ARG
2	H	77	TYR
2	H	79	ARG
2	H	91	THR
2	H	103	LEU
2	H	112	GLU
2	H	143	LEU
2	H	154	ASN
1	I	29	ARG
1	I	84	ILE
1	I	87	LYS
1	I	91	GLN
1	I	95	ASP
1	I	101	LEU
1	I	139	GLN
1	I	200	ASN
1	I	203	LEU
1	I	221	LEU
1	I	228	VAL
1	I	237	ARG
1	I	248	LEU
1	I	266	LEU
1	I	269	ASP
1	I	272	MET
1	I	281	GLN
1	I	298	LEU
2	J	11	LEU
2	J	13	LEU
2	J	27	ARG
2	J	34	THR

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Mol	Chain	Res	Type
2	J	40	THR
2	J	47	ILE
2	J	62	TRP
2	J	69	ARG
2	J	100	LYS
2	J	104	GLN
2	J	165	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	79	ASN
1	A	91	GLN
1	A	144	GLN
1	A	200	ASN
1	A	284	GLN
2	B	115	ASN
1	C	37	HIS
1	C	38	GLN
1	C	77	ASN
1	C	88	ASN
1	C	91	GLN
1	C	98	GLN
1	C	141	HIS
1	C	144	GLN
1	C	198	GLN
1	C	200	ASN
1	C	227	HIS
1	C	277	HIS
2	D	101	GLN
2	D	115	ASN
2	D	121	ASN
2	D	157	ASN
2	D	160	GLN
1	E	144	GLN
1	E	200	ASN
1	E	227	HIS
1	E	281	GLN
2	F	60	GLN
2	F	115	ASN
2	F	133	ASN

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Mol	Chain	Res	Type
2	F	154	ASN
1	G	26	ASN
1	G	75	ASN
1	G	77	ASN
1	G	79	ASN
1	G	91	GLN
1	G	139	GLN
1	G	200	ASN
1	G	208	GLN
2	H	121	ASN
1	I	41	ASN
1	I	77	ASN
1	I	98	GLN
1	I	137	ASN
1	I	200	ASN
1	I	284	GLN
2	J	104	GLN
2	J	115	ASN
2	J	121	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 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 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	SO4	A	401	-	4,4,4	0.19	0	6,6,6	0.19	0
5	GDP	B	202	4,6	23,30,30	1.92	6 (26%)	30,47,47	1.66	5 (16%)
6	BEF	B	203	5	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	C	401	-	4,4,4	0.17	0	6,6,6	0.08	0
5	GDP	D	202	6	23,30,30	1.82	6 (26%)	30,47,47	1.62	4 (13%)
6	BEF	D	203	5	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	E	401	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	E	402	-	4,4,4	0.16	0	6,6,6	0.13	0
5	GDP	F	202	4,6	23,30,30	1.73	6 (26%)	30,47,47	1.67	5 (16%)
6	BEF	F	203	5	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	H	202	4,6	23,30,30	1.84	5 (21%)	30,47,47	1.84	5 (16%)
6	BEF	H	203	5	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	I	401	-	4,4,4	0.19	0	6,6,6	0.15	0
5	GDP	J	202	4,6	23,30,30	1.86	5 (21%)	30,47,47	1.76	4 (13%)
6	BEF	J	203	5	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	401	-	-	0/0/0/0	0/0/0/0
5	GDP	B	202	4,6	-	0/12/32/32	0/3/3/3
6	BEF	B	203	5	-	0/0/0/0	0/0/0/0
3	SO4	C	401	-	-	0/0/0/0	0/0/0/0
5	GDP	D	202	6	-	0/12/32/32	0/3/3/3
6	BEF	D	203	5	-	0/0/0/0	0/0/0/0
3	SO4	E	401	-	-	0/0/0/0	0/0/0/0
3	SO4	E	402	-	-	0/0/0/0	0/0/0/0
5	GDP	F	202	4,6	-	0/12/32/32	0/3/3/3
6	BEF	F	203	5	-	0/0/0/0	0/0/0/0
5	GDP	H	202	4,6	-	0/12/32/32	0/3/3/3
6	BEF	H	203	5	-	0/0/0/0	0/0/0/0
3	SO4	I	401	-	-	0/0/0/0	0/0/0/0
5	GDP	J	202	4,6	-	0/12/32/32	0/3/3/3
6	BEF	J	203	5	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	202	GDP	C6-C5	-3.87	1.33	1.41
5	B	202	GDP	C6-C5	-3.67	1.33	1.41
5	H	202	GDP	C6-C5	-3.40	1.34	1.41
5	J	202	GDP	C6-C5	-3.39	1.34	1.41
5	F	202	GDP	C6-C5	-3.20	1.34	1.41
5	D	202	GDP	C5-C4	-2.70	1.34	1.40
5	F	202	GDP	C5-C4	-2.68	1.34	1.40
5	J	202	GDP	C5-C4	-2.62	1.34	1.40
5	B	202	GDP	C5-C4	-2.58	1.34	1.40
5	B	202	GDP	PB-O3B	-2.50	1.45	1.54
5	H	202	GDP	C5-C4	-2.50	1.34	1.40
5	F	202	GDP	PB-O3B	-2.10	1.47	1.54
5	D	202	GDP	PB-O3B	-2.01	1.47	1.54
5	F	202	GDP	C2-N1	2.73	1.40	1.35
5	J	202	GDP	C2-N1	2.73	1.40	1.35
5	D	202	GDP	C2-N1	2.84	1.40	1.35
5	B	202	GDP	C2-N1	2.84	1.40	1.35
5	H	202	GDP	C2-N1	3.07	1.40	1.35
5	F	202	GDP	O4'-C1'	3.19	1.45	1.41
5	D	202	GDP	O4'-C1'	3.61	1.45	1.41
5	J	202	GDP	C6-N1	4.00	1.40	1.33
5	D	202	GDP	C6-N1	4.10	1.40	1.33
5	H	202	GDP	C6-N1	4.21	1.40	1.33
5	F	202	GDP	C6-N1	4.23	1.41	1.33
5	B	202	GDP	C6-N1	4.30	1.41	1.33
5	H	202	GDP	O4'-C1'	4.45	1.46	1.41
5	B	202	GDP	O4'-C1'	4.61	1.47	1.41
5	J	202	GDP	O4'-C1'	4.71	1.47	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	202	GDP	N3-C2-N1	-5.54	119.00	127.44
5	F	202	GDP	N3-C2-N1	-5.41	119.21	127.44
5	H	202	GDP	N3-C2-N1	-5.39	119.23	127.44
5	D	202	GDP	N3-C2-N1	-5.21	119.51	127.44
5	B	202	GDP	N3-C2-N1	-5.03	119.78	127.44
5	J	202	GDP	PA-O3A-PB	-4.29	118.29	132.67
5	H	202	GDP	PA-O3A-PB	-4.13	118.83	132.67
5	B	202	GDP	PA-O3A-PB	-3.63	120.50	132.67
5	B	202	GDP	C5-C6-N1	-3.44	118.88	123.59
5	F	202	GDP	C5-C6-N1	-3.19	119.22	123.59
5	F	202	GDP	PA-O3A-PB	-3.15	122.10	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	202	GDP	PA-O3A-PB	-3.15	122.12	132.67
5	H	202	GDP	C5-C6-N1	-3.02	119.46	123.59
5	D	202	GDP	C4'-O4'-C1'	-3.00	106.42	109.72
5	J	202	GDP	C5-C6-N1	-2.81	119.74	123.59
5	D	202	GDP	C5-C6-N1	-2.71	119.89	123.59
5	B	202	GDP	C5'-C4'-C3'	-2.33	105.97	115.21
5	F	202	GDP	C4'-O4'-C1'	-2.19	107.31	109.72
5	H	202	GDP	C1'-N9-C4	-2.11	123.76	126.94
5	F	202	GDP	C4-C5-N7	-2.09	107.55	109.48
5	J	202	GDP	N2-C2-N1	2.01	120.53	117.20
5	B	202	GDP	O3B-PB-O2B	2.16	115.61	107.38
5	H	202	GDP	O4'-C1'-N9	3.48	115.37	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SO4	1	0
5	B	202	GDP	2	0
5	F	202	GDP	1	0
5	H	202	GDP	7	0
6	H	203	BEF	1	0
5	J	202	GDP	3	0
6	J	203	BEF	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	280/305 (91%)	-0.22	2 (0%) 89 86	46, 62, 90, 109	1 (0%)
1	C	281/305 (92%)	-0.19	1 (0%) 93 92	51, 66, 86, 110	0
1	E	281/305 (92%)	-0.13	0 100 100	51, 71, 100, 118	0
1	G	281/305 (92%)	0.04	4 (1%) 78 73	74, 96, 128, 157	0
1	I	281/305 (92%)	-0.06	5 (1%) 71 65	57, 74, 104, 117	0
2	B	172/175 (98%)	0.03	3 (1%) 73 67	51, 68, 97, 118	0
2	D	170/175 (97%)	0.16	7 (4%) 41 34	59, 76, 101, 116	0
2	F	172/175 (98%)	0.07	3 (1%) 73 67	57, 72, 100, 120	0
2	H	170/175 (97%)	0.20	5 (2%) 55 49	79, 102, 141, 163	1 (0%)
2	J	171/175 (97%)	0.19	6 (3%) 48 40	71, 90, 118, 131	0
All	All	2259/2400 (94%)	-0.02	36 (1%) 74 69	46, 75, 114, 163	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	52	LEU	3.5
2	D	169	ILE	3.3
2	D	9	PHE	3.2
2	B	3	PRO	2.8
1	G	27	ALA	2.8
2	F	174	GLY	2.8
1	G	207	MET	2.8
1	G	209	SER	2.6
2	H	83	GLY	2.6
1	C	43	ASP	2.6
2	J	162	PHE	2.5
2	H	9	PHE	2.5
2	D	59	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	26	ASN	2.4
1	A	113	GLY	2.4
2	H	167	ALA	2.4
2	B	7	TYR	2.4
2	F	166	ALA	2.3
2	D	56	THR	2.2
1	G	263	GLN	2.2
1	I	61	LEU	2.2
2	J	9	PHE	2.2
2	J	174	GLY	2.2
2	F	6	ASP	2.2
1	A	68	LYS	2.1
1	I	60	LEU	2.1
2	J	8	LEU	2.1
2	J	59	LEU	2.1
2	B	174	GLY	2.1
1	I	79	ASN	2.1
2	D	50	ILE	2.1
2	H	7	TYR	2.1
2	D	58	LYS	2.0
2	H	52	LEU	2.0
2	J	47	ILE	2.0
1	I	269	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	BEF	F	203	4/4	0.97	0.24	1.04	70,70,70,71	0
4	MG	F	201	1/1	0.94	0.22	0.67	61,61,61,61	0
3	SO4	C	401	5/5	0.89	0.21	0.67	124,124,124,124	0
4	MG	J	201	1/1	0.96	0.20	0.61	61,61,61,61	0
6	BEF	B	203	4/4	0.97	0.23	0.56	64,64,64,64	0
4	MG	D	201	1/1	0.95	0.24	0.47	55,55,55,55	0
6	BEF	J	203	4/4	0.96	0.20	0.38	95,96,96,96	0
3	SO4	I	401	5/5	0.93	0.22	-0.22	107,107,107,107	0
5	GDP	J	202	28/28	0.94	0.18	-0.27	84,90,92,93	0
6	BEF	H	203	4/4	0.95	0.18	-0.34	103,104,104,104	0
4	MG	H	201	1/1	0.96	0.19	-0.58	61,61,61,61	0
5	GDP	B	202	28/28	0.96	0.18	-0.66	51,56,57,58	0
5	GDP	F	202	28/28	0.96	0.17	-0.91	54,59,64,64	0
5	GDP	D	202	28/28	0.96	0.16	-1.04	63,64,67,68	0
5	GDP	H	202	28/28	0.95	0.15	-1.09	64,70,80,80	0
6	BEF	D	203	4/4	0.97	0.16	-1.54	75,75,76,76	0
3	SO4	E	402	5/5	0.95	0.22	-	105,105,105,105	0
3	SO4	E	401	5/5	0.91	0.14	-	106,106,107,107	0
3	SO4	A	401	5/5	0.91	0.17	-	101,101,102,102	0
4	MG	B	201	1/1	0.95	0.23	-	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.