WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2014 – 03:23 PM GMT

PDB ID	:	3BRW
Title	:	Structure of the Rap-RapGAP complex
Authors	:	Scrima, A.; Thomas, C.; Deaconescu, D.; Wittinghofer, A.
Deposited on	:	2007-12-21
Resolution	:	3.40 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.269
Clashscore		8
Ramachandran outliers		2.1%
Sidechain outliers		9.6%
RSRZ outliers		0

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
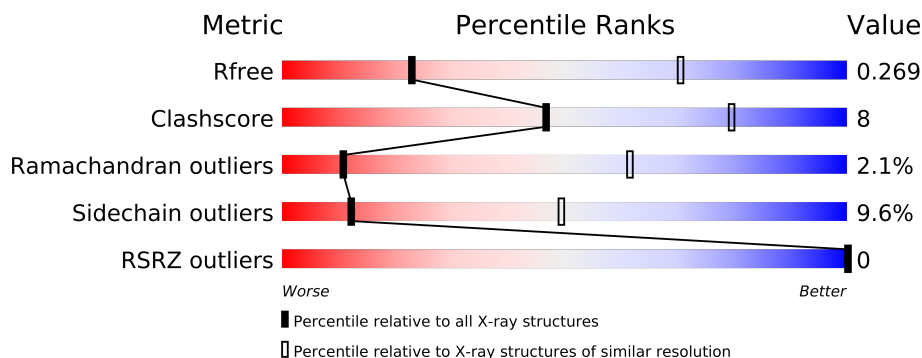
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1017 (3.52-3.28)
Clashscore	79885	1214 (3.50-3.30)
Ramachandran outliers	78287	1177 (3.50-3.30)
Sidechain outliers	78261	1177 (3.50-3.30)
RSRZ outliers	66119	1017 (3.52-3.28)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	
1	C	341	
2	D	167	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9465 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Rap1 GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total 2706	C 1744	N 453	O 498	S 11	0	0	0
1	B	337	Total 2709	C 1745	N 453	O 500	S 11	0	0	0
1	C	332	Total 2675	C 1725	N 448	O 491	S 11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	ALA	GLN	ENGINEERED	UNP P47736
B	204	ALA	GLN	ENGINEERED	UNP P47736
C	204	ALA	GLN	ENGINEERED	UNP P47736

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	167	Total 1332	C 833	N 228	O 263	S 8	0	0	0

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

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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF$_3$).
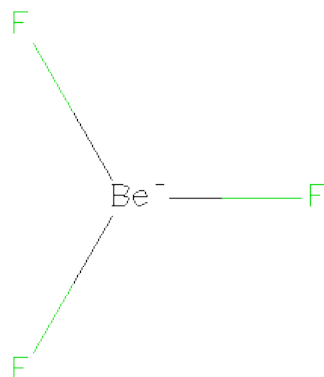
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
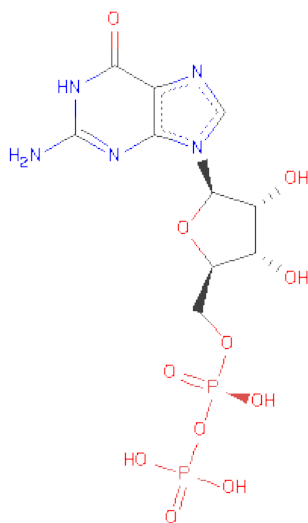
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	B	1	Total 1	O 1	0	0
6	C	3	Total 3	O 3	0	0
6	D	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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: Rap1 GTPase-activating protein 1

Chain A:
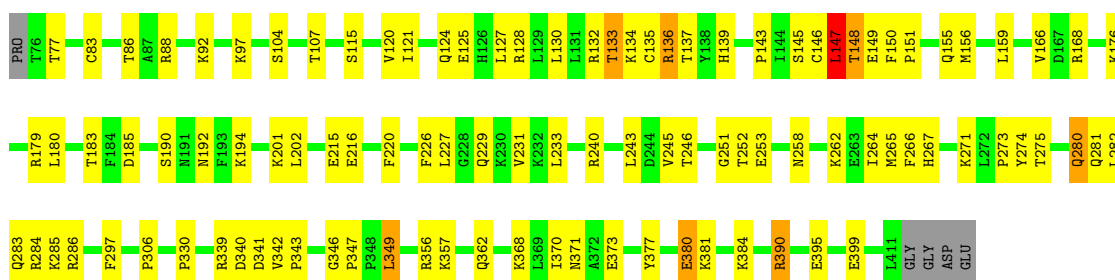
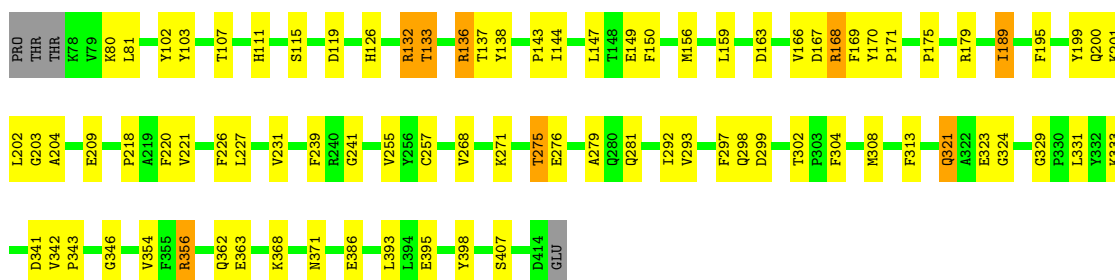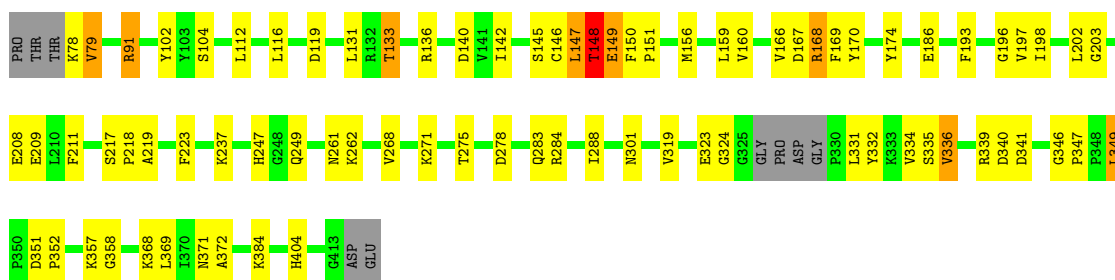- Molecule 1: Rap1 GTPase-activating protein 1

Chain B:

- Molecule 1: Rap1 GTPase-activating protein 1

Chain C:

- Molecule 2: Ras-related protein Rap-1b

Chain D:

M1 L9 V24 Q25 Y32 K42 Q43 V46 D47 Q50 C51 M52 I55 T61 E62 Q63 F64 T65 R68 D69 L70 Y71 M72 G77 V81 N91 D95 E98 Q99 I100 L101 R102 T106 D107 P110 V114 K117 R124 E129 Q130

G131 Q132 N139 L144 E145 S150 K151 I152 N153 I157 V162 R167
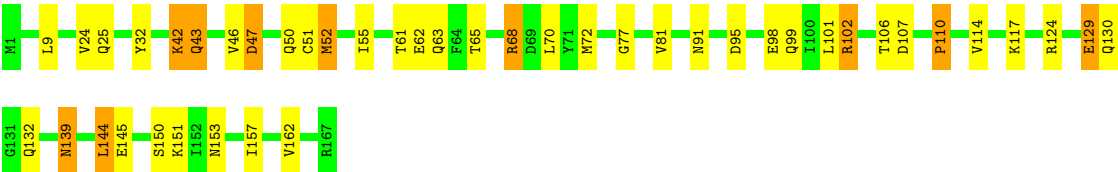
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	209.72Å 209.72Å 108.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 – 3.40 48.08 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.08-3.40) 99.2 (48.08-3.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.234 , 0.280 0.228 , 0.269	Depositor DCC
R_{free} test set	1878 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 26.1	EDS
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
L-test for twinning	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Outliers	0 of 37639 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9465	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

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	0.39	0/2774	0.54	0/3756
1	B	0.40	0/2777	0.55	0/3760
1	C	0.40	0/2741	0.52	0/3708
2	D	0.38	0/1348	0.61	0/1814
All	All	0.40	0/9640	0.55	0/13038

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	148	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2706	0	2659	50	0
1	B	2709	0	2658	39	0
1	C	2675	0	2628	44	0
2	D	1332	0	1320	25	0
3	D	1	0	0	0	0
4	D	4	0	0	0	0
5	D	28	0	12	2	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	4	0	0	0	0
All	All	9465	0	9277	151	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (151) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:148:THR:HB	1:C:149:GLU:HA	1.23	1.18
1:C:148:THR:CB	1:C:149:GLU:HA	1.98	0.94
1:C:148:THR:HB	1:C:149:GLU:CA	2.04	0.86
1:C:319:VAL:HB	1:C:335:SER:CB	2.18	0.73
1:C:319:VAL:HB	1:C:335:SER:HB3	1.70	0.72
1:B:346:GLY:HA2	1:B:371:ASN:HD22	1.54	0.72
1:B:346:GLY:HA3	1:B:368:LYS:HD2	1.74	0.70
1:C:147:LEU:O	1:C:149:GLU:HG2	1.94	0.68
2:D:62:GLU:O	2:D:62:GLU:HG2	1.93	0.67
1:A:339:ARG:C	1:A:341:ASP:H	2.00	0.65
2:D:24:VAL:HA	2:D:42:LYS:HD2	1.79	0.65
1:C:219:ALA:O	1:C:223:PHE:HB2	1.98	0.64
1:C:116:LEU:HD22	1:C:156:MET:HE1	1.79	0.64
1:C:346:GLY:HA2	1:C:371:ASN:HD22	1.63	0.64
1:B:204:ALA:HB1	1:B:209:GLU:HB3	1.81	0.63
2:D:102:ARG:HB3	2:D:102:ARG:NH1	2.13	0.62
1:A:220:PHE:HD1	1:A:297:PHE:CD2	2.18	0.62
1:B:119:ASP:HB3	1:B:126:HIS:CE1	2.36	0.61
1:B:136:ARG:HB3	1:B:136:ARG:HH11	1.67	0.60
1:C:346:GLY:HA3	1:C:368:LYS:HD2	1.84	0.60
1:B:144:ILE:HD11	1:B:147:LEU:HD13	1.83	0.59
2:D:43:GLN:HG2	2:D:52:MET:HG2	1.84	0.59
1:B:199:TYR:CE1	1:B:201:LYS:HD2	2.38	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:133:THR:HG23	1:C:136:ARG:H	1.68	0.58
1:B:220:PHE:HD1	1:B:297:PHE:CD2	2.20	0.58
1:A:146:CYS:C	1:A:148:THR:H	2.07	0.57
1:B:199:TYR:HE1	1:B:201:LYS:HD2	1.69	0.57
2:D:101:LEU:HD22	2:D:107:ASP:HA	1.85	0.57
1:A:128:ARG:NH2	2:D:124:ARG:O	2.38	0.57
1:A:133:THR:C	1:A:135:CYS:H	2.07	0.57
1:A:147:LEU:O	1:A:149:GLU:N	2.37	0.56
1:C:104:SER:OG	1:C:166:VAL:HG21	2.06	0.56
1:A:136:ARG:HD3	1:A:137:THR:H	1.71	0.56
1:B:175:PRO:HG2	1:C:150:PHE:CE1	2.40	0.55
1:C:339:ARG:O	1:C:341:ASP:N	2.40	0.55
1:B:189:ILE:O	1:B:189:ILE:HG13	2.05	0.55
1:A:275:THR:H	1:A:281:GLN:HE22	1.54	0.54
1:A:143:PRO:HG3	2:D:130:GLN:HG2	1.89	0.54
1:C:148:THR:HG1	1:C:149:GLU:HG2	1.72	0.54
1:A:151:PRO:HB2	1:A:156:MET:HG3	1.90	0.54
2:D:46:VAL:HG22	2:D:51:CYS:SG	2.48	0.54
1:A:349:LEU:H	1:A:349:LEU:HD12	1.73	0.53
1:B:321:GLN:HB3	1:B:333:LYS:HB2	1.91	0.53
2:D:46:VAL:HG21	2:D:162:VAL:HG11	1.91	0.53
1:A:306:PRO:HB2	1:A:339:ARG:HE	1.74	0.53
1:A:133:THR:HG23	1:A:136:ARG:H	1.73	0.53
1:A:115:SER:OG	1:A:132:ARG:NH2	2.41	0.53
1:A:395:GLU:O	1:A:399:GLU:HG2	2.09	0.53
1:C:217:SER:HB3	1:C:218:PRO:HD2	1.90	0.52
1:B:275:THR:H	1:B:281:GLN:HE22	1.58	0.52
1:C:197:VAL:HB	1:C:268:VAL:HA	1.93	0.51
1:B:126:HIS:HA	1:B:143:PRO:HA	1.93	0.51
2:D:144:LEU:HD13	2:D:153:ASN:HB3	1.91	0.51
1:A:240:ARG:O	1:A:265:MET:HG2	2.11	0.51
1:B:111:HIS:NE2	1:B:395:GLU:HG3	2.26	0.51
1:A:245:VAL:HG13	1:A:246:THR:HG23	1.93	0.51
1:A:330:PRO:HD2	1:A:357:LYS:HG3	1.91	0.50
1:A:83:CYS:SG	1:A:88:ARG:NH1	2.84	0.50
1:A:251:GLY:N	1:A:273:PRO:HD3	2.26	0.50
1:B:119:ASP:HB3	1:B:126:HIS:NE2	2.27	0.50
1:B:136:ARG:HB3	1:B:136:ARG:NH1	2.25	0.50
2:D:32:TYR:CD1	5:D:171:GDP:H5"	2.46	0.50
1:B:203:GLY:HA2	1:B:302:THR:OG1	2.13	0.49
1:B:195:PHE:CD1	1:B:293:VAL:HB	2.48	0.49
1:C:196:GLY:HA3	1:C:288:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:336:VAL:HG11	1:C:349:LEU:HD22	1.95	0.49
1:C:102:TYR:HB3	1:C:169:PHE:HB3	1.95	0.49
1:A:339:ARG:O	1:A:341:ASP:N	2.42	0.49
1:C:323:GLU:HG3	1:C:324:GLY:H	1.76	0.48
1:C:150:PHE:HA	1:C:151:PRO:HD2	1.49	0.48
1:A:120:VAL:HG22	1:A:125:GLU:HG2	1.95	0.48
1:A:146:CYS:C	1:A:148:THR:N	2.66	0.48
1:C:332:TYR:HE2	1:C:357:LYS:HG2	1.77	0.48
1:A:77:THR:HG21	1:B:279:ALA:HA	1.95	0.48
2:D:129:GLU:HA	2:D:129:GLU:OE2	2.13	0.48
1:B:292:ILE:HD11	2:D:63:GLN:HE22	1.78	0.48
2:D:24:VAL:HG23	2:D:25:GLN:HG3	1.96	0.48
1:C:156:MET:HA	1:C:159:LEU:HD12	1.96	0.48
2:D:124:ARG:HH22	2:D:145:GLU:CD	2.17	0.48
1:B:218:PRO:HA	1:B:221:VAL:HG12	1.95	0.47
1:C:147:LEU:H	1:C:147:LEU:HD23	1.79	0.47
1:C:140:ASP:HB2	1:C:160:VAL:HG23	1.97	0.47
1:A:273:PRO:HG2	1:A:283:GLN:HE21	1.78	0.47
1:C:247:HIS:HB3	1:C:249:GLN:HE21	1.79	0.47
1:C:334:VAL:HG12	1:C:335:SER:N	2.30	0.47
1:C:357:LYS:HD3	1:C:358:GLY:H	1.78	0.47
1:A:346:GLY:HA2	1:A:371:ASN:HD22	1.78	0.47
1:A:155:GLN:O	1:A:159:LEU:HG	2.14	0.47
1:C:91:ARG:NH2	1:C:186:GLU:OE1	2.47	0.47
1:C:211:PHE:O	1:C:284:ARG:NH1	2.48	0.47
1:B:200:GLN:HB3	1:B:298:GLN:HG2	1.97	0.47
2:D:95:ASP:HA	2:D:98:GLU:HB2	1.97	0.47
1:A:132:ARG:NH1	1:A:185:ASP:OD2	2.48	0.46
1:A:274:TYR:HB2	1:A:284:ARG:HH21	1.80	0.46
2:D:144:LEU:HD11	2:D:157:ILE:HD13	1.98	0.46
1:B:102:TYR:HB3	1:B:169:PHE:HB3	1.98	0.46
1:A:280:GLN:H	1:A:280:GLN:HE21	1.64	0.46
1:C:78:LYS:O	1:C:79:VAL:HB	2.16	0.46
1:B:133:THR:HG23	1:B:136:ARG:H	1.81	0.46
1:B:156:MET:HA	1:B:159:LEU:HD12	1.97	0.45
1:A:380:GLU:HG3	1:A:381:LYS:N	2.32	0.45
1:A:145:SER:C	1:A:147:LEU:H	2.20	0.45
1:B:115:SER:OG	1:B:132:ARG:NH2	2.50	0.44
1:A:346:GLY:HA3	1:A:368:LYS:HD2	1.98	0.44
1:B:175:PRO:HB2	1:C:150:PHE:CZ	2.52	0.44
1:B:103:TYR:HB2	1:B:398:TYR:CE2	2.53	0.44
1:A:373:GLU:O	1:A:377:TYR:HD1	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:339:ARG:C	1:A:341:ASP:N	2.70	0.44
2:D:77:GLY:HA2	2:D:110:PRO:HB2	2.00	0.44
1:B:170:TYR:HA	1:B:171:PRO:HD3	1.82	0.44
2:D:61:THR:HG23	2:D:63:GLN:H	1.82	0.44
1:B:333:LYS:HA	1:B:354:VAL:HG22	1.99	0.43
1:A:233:LEU:HD21	1:A:243:LEU:HD13	2.00	0.43
1:A:127:LEU:HD21	1:A:156:MET:SD	2.59	0.43
2:D:81:VAL:HG22	2:D:114:VAL:HB	2.00	0.43
1:C:174:TYR:CD1	1:C:404:HIS:HB3	2.53	0.43
1:A:136:ARG:O	1:A:390:ARG:NH2	2.52	0.43
1:A:130:LEU:HD12	1:A:139:HIS:HB2	2.00	0.43
1:C:79:VAL:HG21	1:C:347:PRO:HB3	2.00	0.43
1:C:369:LEU:O	1:C:372:ALA:HB3	2.19	0.43
1:B:268:VAL:HG12	1:B:271:LYS:H	1.83	0.42
1:A:194:LYS:HE2	1:A:267:HIS:HE1	1.84	0.42
2:D:117:LYS:HG2	5:D:171:GDP:C6	2.54	0.42
1:A:227:LEU:HD21	1:A:266:PHE:CE2	2.55	0.42
1:A:132:ARG:HD3	1:A:185:ASP:OD1	2.20	0.42
1:C:112:LEU:HD22	1:C:131:LEU:HD21	2.01	0.42
1:C:193:PHE:HE2	1:C:262:LYS:HG2	1.84	0.42
1:C:275:THR:HB	1:C:278:ASP:HB2	2.02	0.42
1:A:104:SER:OG	1:A:166:VAL:HG11	2.19	0.42
1:A:124:GLN:HE22	2:D:91:ASN:HD21	1.68	0.42
1:A:280:GLN:H	1:A:280:GLN:NE2	2.18	0.42
1:B:331:LEU:HD13	1:B:356:ARG:HG3	2.02	0.42
1:C:168:ARG:HD3	1:C:170:TYR:CZ	2.55	0.42
1:C:217:SER:HB3	1:C:218:PRO:CD	2.49	0.41
1:B:239:PHE:CZ	1:B:241:GLY:HA2	2.55	0.41
1:B:167:ASP:OD1	1:B:168:ARG:NH1	2.54	0.41
1:A:190:SER:O	1:A:262:LYS:HE3	2.20	0.41
1:B:268:VAL:HG11	1:B:271:LYS:HD2	2.03	0.41
1:C:319:VAL:H	1:C:335:SER:HB3	1.85	0.41
1:B:133:THR:HG21	1:B:138:TYR:CE2	2.55	0.41
1:A:264:ILE:HD11	1:A:370:ILE:HD11	2.03	0.41
1:A:347:PRO:HD3	1:A:371:ASN:HD22	1.86	0.41
1:C:351:ASP:HB2	1:C:352:PRO:HD3	2.03	0.41
2:D:68:ARG:O	2:D:72:MET:HE1	2.20	0.41
1:B:342:VAL:HA	1:B:343:PRO:HD3	1.87	0.40
2:D:102:ARG:HH11	2:D:102:ARG:CG	2.34	0.40
1:C:349:LEU:HD23	1:C:349:LEU:H	1.86	0.40
1:A:342:VAL:HA	1:A:343:PRO:HD3	1.90	0.40
1:A:253:GLU:HG3	1:A:271:LYS:HD2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:46:VAL:HG23	2:D:46:VAL:O	2.21	0.40
1:B:304:PHE:CD2	1:B:308:MET:HE1	2.56	0.40

There are no symmetry-related clashes.

5.3   Torsion angles

5.3.1   Protein backbone ⓘ

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	334/341 (98%)	305 (91%)	23 (7%)	6 (2%)	13	65
1	B	335/341 (98%)	300 (90%)	28 (8%)	7 (2%)	11	61
1	C	328/341 (96%)	282 (86%)	40 (12%)	6 (2%)	13	65
2	D	165/167 (99%)	146 (88%)	14 (8%)	5 (3%)	7	53
All	All	1162/1190 (98%)	1033 (89%)	105 (9%)	24 (2%)	11	61

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	329	GLY
1	C	79	VAL
1	C	340	ASP
2	D	151	LYS
1	A	134	LYS
1	A	148	THR
1	A	202	LEU
1	A	340	ASP
1	C	148	THR
1	C	301	ASN
2	D	47	ASP
1	A	215	GLU
2	D	139	ASN
2	D	150	SER
1	B	137	THR
1	B	149	GLU

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Mol	Chain	Res	Type
1	B	407	SER
1	A	147	LEU
1	B	80	LYS
1	B	324	GLY
1	C	145	SER
1	B	202	LEU
1	C	203	GLY
2	D	110	PRO

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	295/300 (98%)	263 (89%)	32 (11%)	9	42
1	B	295/300 (98%)	267 (90%)	28 (10%)	12	50
1	C	291/300 (97%)	269 (92%)	22 (8%)	19	64
2	D	147/147 (100%)	130 (88%)	17 (12%)	8	37
All	All	1028/1047 (98%)	929 (90%)	99 (10%)	12	49

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	THR
1	A	92	LYS
1	A	97	LYS
1	A	107	THR
1	A	121	ILE
1	A	133	THR
1	A	136	ARG
1	A	147	LEU
1	A	150	PHE
1	A	168	ARG
1	A	176	LYS
1	A	179	ARG
1	A	180	LEU
1	A	183	THR

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Mol	Chain	Res	Type
1	A	192	ASN
1	A	201	LYS
1	A	216	GLU
1	A	226	PHE
1	A	229	GLN
1	A	231	VAL
1	A	252	THR
1	A	258	ASN
1	A	280	GLN
1	A	282	LEU
1	A	285	LYS
1	A	286	ARG
1	A	349	LEU
1	A	356	ARG
1	A	362	GLN
1	A	380	GLU
1	A	384	LYS
1	A	390	ARG
1	B	81	LEU
1	B	107	THR
1	B	132	ARG
1	B	133	THR
1	B	136	ARG
1	B	150	PHE
1	B	163	ASP
1	B	166	VAL
1	B	168	ARG
1	B	179	ARG
1	B	189	ILE
1	B	226	PHE
1	B	227	LEU
1	B	231	VAL
1	B	255	VAL
1	B	257	CYS
1	B	275	THR
1	B	276	GLU
1	B	299	ASP
1	B	313	PHE
1	B	321	GLN
1	B	323	GLU
1	B	341	ASP
1	B	356	ARG

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Mol	Chain	Res	Type
1	B	362	GLN
1	B	363	GLU
1	B	386	GLU
1	B	393	LEU
1	C	91	ARG
1	C	119	ASP
1	C	133	THR
1	C	142	ILE
1	C	146	CYS
1	C	147	LEU
1	C	148	THR
1	C	149	GLU
1	C	167	ASP
1	C	168	ARG
1	C	198	ILE
1	C	202	LEU
1	C	208	GLU
1	C	209	GLU
1	C	237	LYS
1	C	261	ASN
1	C	271	LYS
1	C	283	GLN
1	C	331	LEU
1	C	336	VAL
1	C	349	LEU
1	C	384	LYS
2	D	9	LEU
2	D	42	LYS
2	D	43	GLN
2	D	47	ASP
2	D	50	GLN
2	D	52	MET
2	D	55	ILE
2	D	65	THR
2	D	68	ARG
2	D	70	LEU
2	D	99	GLN
2	D	102	ARG
2	D	106	THR
2	D	129	GLU
2	D	132	GLN
2	D	139	ASN

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Mol	Chain	Res	Type
2	D	144	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	165	ASN
1	A	214	ASN
1	A	229	GLN
1	A	234	GLN
1	A	280	GLN
1	A	281	GLN
1	A	283	GLN
1	A	301	ASN
1	A	321	GLN
1	B	234	GLN
1	B	281	GLN
1	B	301	ASN
1	B	321	GLN
1	B	362	GLN
1	B	371	ASN
1	B	402	HIS
1	B	404	HIS
1	C	249	GLN
1	C	261	ASN
1	C	283	GLN
1	C	301	ASN
1	C	362	GLN
1	C	402	HIS
2	D	43	GLN
2	D	50	GLN
2	D	63	GLN
2	D	137	GLN
2	D	139	ASN

5.3.3 RNA (i)

There are no RNA chains 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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
4	BEF	D	170	-	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	D	171	-	30,30,30	1.40	3 (10%)	44,47,47	1.73	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEF	D	170	-	-	0/0/0/0	0/0/0/0
5	GDP	D	171	-	-	0/16/32/32	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	171	GDP	C6-C5	4.35	1.48	1.41
5	D	171	GDP	C4-N9	-3.44	1.32	1.37
5	D	171	GDP	C2-N2	2.53	1.36	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	171	GDP	C6-C5-N7	-5.06	133.46	134.14
5	D	171	GDP	C2-N3-C4	4.58	121.52	115.09
5	D	171	GDP	C5-C4-N3	-4.14	119.94	125.94
5	D	171	GDP	N3-C4-N9	4.03	132.81	126.91
5	D	171	GDP	O2B-PB-O1B	2.92	120.00	110.44
5	D	171	GDP	C8-N9-C4	2.42	108.75	106.90
5	D	171	GDP	PA-O3A-PB	-2.33	124.85	131.68
5	D	171	GDP	N2-C2-N1	2.20	120.28	117.86
5	D	171	GDP	C3'-C2'-C1'	2.04	104.10	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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	336/341 (98%)	-0.13	0	100	100	69, 102, 124, 128	0
1	B	337/341 (98%)	-0.14	0	100	100	54, 80, 112, 126	0
1	C	332/341 (97%)	0.03	0	100	100	61, 136, 163, 167	0
2	D	167/167 (100%)	-0.17	0	100	100	63, 76, 90, 94	0
All	All	1172/1190 (98%)	-0.09	0	100	100	54, 91, 156, 167	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	BEF	D	170	4/4	0.20	0.11	64,64,64,65	0
3	MG	D	172	1/1	0.19	0.08	68,68,68,68	0
5	GDP	D	171	28/28	0.19	-0.46	62,63,63,64	0

6.5 Other polymers (i)

There are no such residues in this entry.