Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 11:08 AM EDT

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)

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

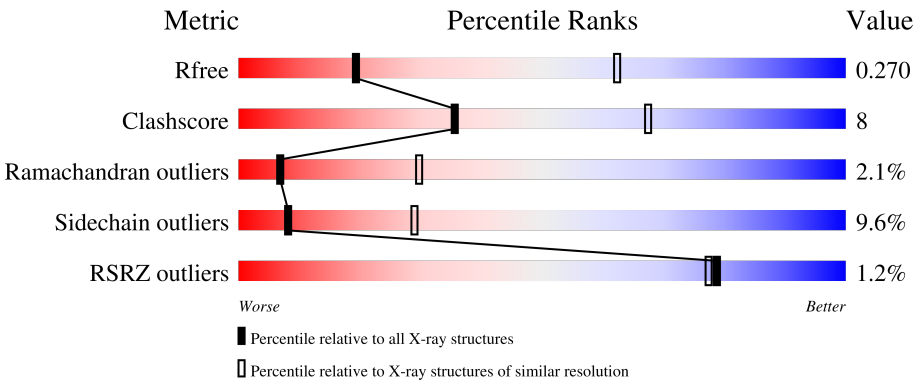
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	341	68% 28% • •
1	B	341	% 74% 23% • •
1	C	341	3% 74% 21% • •
2	D	167	74% 20% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9465 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 Rap1 GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	336	2706	1744	453	498	11	0	0	0
1	B	337	2709	1745	453	500	11	0	0	0
1	C	332	2675	1725	448	491	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 mutation	UNP P47736
B	204	ALA	GLN	engineered mutation	UNP P47736
C	204	ALA	GLN	engineered mutation	UNP P47736

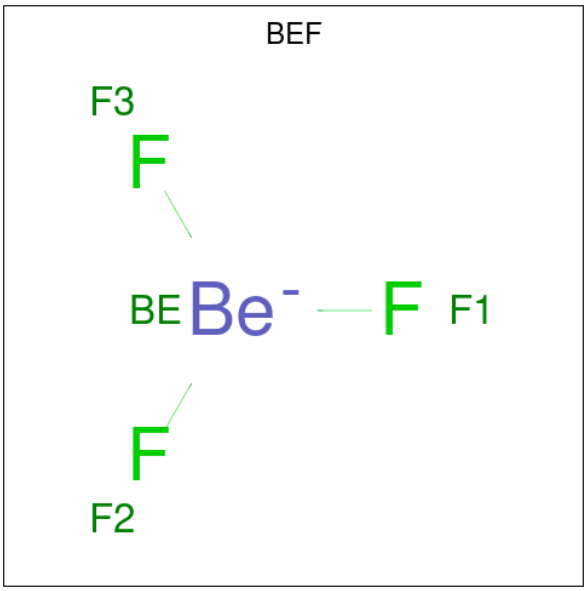
- Molecule 2 is a protein called Ras-related protein Rap-1b.

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

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

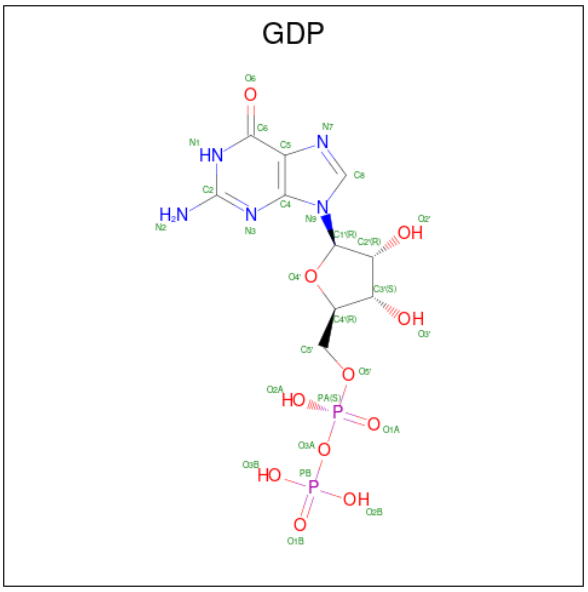
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	D	1	1	1	0	0

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
4	D	1	4	1	3	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
			Total	C	N	O	P		
5	D	1	28	10	5	11	2	0	0

- Molecule 6 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Rap1 GTPase-activating protein 1

Chain A: 68% 28% • •

PRO T76 T77 C83 T86 A87 R88 K92 K97 S104 T107 S115 V120 I121 Q124 E125 H126 L127 R128 L129 L130 L131 R132 T133 K134 C135 R136 T137 Y138 H139 P143 I144 S145 C146 L147 T148 E149 F150 P151 Q155 M156 L159 V166 D167 R168 K176

R179 L180 T183 F184 D185 S190 N191 N192 F193 K194 K201 L202 E215 E216 F220 F226 L227 G228 Q229 K230 V231 K232 L233 R240 L243 D244 V245 T246 G251 T252 E253 N258 K262 E263 I264 M265 F266 H267 K271 L272 P273 Y274 T275 Q280 Q281 L282

Q283 R284 K285 R286 F297 P306 P327 P330 R339 D340 D341 V342 P343 G346 P347 P348 L349 R356 K357 Q362 K368 L369 I370 N371 A372 E373 Y377 E380 K381 K384 R390 E395 E399 L411 GLY GLY ASP GLU

• Molecule 1: Rap1 GTPase-activating protein 1

Chain B: % 74% 23% • •

PRO THR THR K78 V79 K80 L81 Y102 Y103 T107 H111 S115 D119 H126 R132 T133 R136 T137 Y138 P143 I144 L147 T148 E149 F150 M156 L159 D163 V166 D167 R168 F169 Y170 P171 P175 R179 I189 F195 Y199 Q200 K201

L202 G203 A204 E209 P218 A219 F220 V221 F226 L227 V231 F239 R240 G241 V255 Y256 C257 V268 K271 T275 E276 A279 Q280 Q281 I292 V293 F297 Q298 D299 T302 P303 F304 M308 F313 Q321 A322 E323 G324 G325 G326 P327 D328 G329 P330

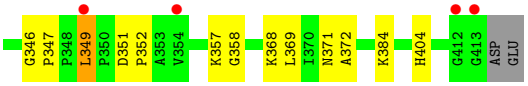
L331 Y332 K333 D341 V342 P343 G346 V354 F355 R356 Q362 E363 K368 N371 E386 L393 L394 E395 Y398 S407 D414 GLU

• Molecule 1: Rap1 GTPase-activating protein 1

Chain C: 3% 74% 21% • •

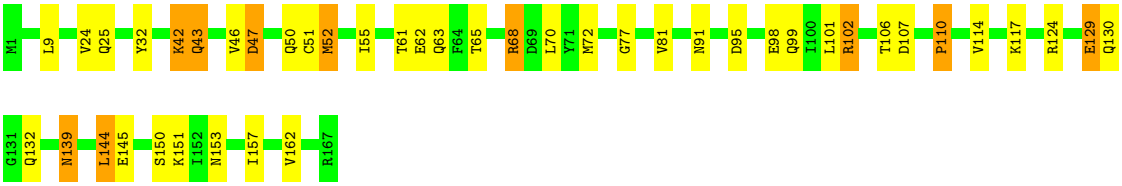
PRO THR THR K78 V79 R91 Y102 Y103 S104 L112 L116 D119 L131 R132 T133 R136 D140 V141 I142 S145 C146 L147 T148 E149 F150 P151 M156 L159 V160 V166 D167 R168 F169 Y170 Y174 E186 F193 G196 V197 I198 L202 G203

E208 E209 L210 F211 S217 P218 A219 F223 K237 H247 G248 Q249 N261 K262 V268 K271 T275 D278 L282 Q283 R284 I288 V296 N301 Y317 V318 V319 E323 G324 G325 GLY PRO ASP GLY P330 L331 Y332 K333 V334 S335 V336 R339 D340 D341



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

Chain D:



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 5.2.0005	Depositor
R, R_{free}	0.234 , 0.280 0.227 , 0.270	Depositor DCC
R_{free} test set	1878 reflections (4.99%)	wwPDB-VP
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 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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 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	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

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 (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C: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:HH11	1:B:136:ARG:HB3	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	Interatomic distance (Å)	Clash overlap (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:A:128:ARG:NH2	2:D:124:ARG:O	2.38	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: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:HG13	1:B:189:ILE:O	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:A:151:PRO:HB2	1:A:156:MET:HG3	1.90	0.54
1:C:148:THR:HG1	1:C:149:GLU:HG2	1.72	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:115:SER:OG	1:A:132:ARG:NH2	2.41	0.53
1:A:133:THR:HG23	1:A:136:ARG:H	1.73	0.53
1:A:395:GLU:O	1:A:399:GLU:HG2	2.09	0.53
1:B:275:THR:H	1:B:281:GLN:HE22	1.58	0.52
1:C:217:SER:HB3	1:C:218:PRO:HD2	1.90	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:A:245:VAL:HG13	1:A:246:THR:HG23	1.93	0.51
1:B:111:HIS:NE2	1:B:395:GLU:HG3	2.26	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:195:PHE:CD1	1:B:293:VAL:HB	2.48	0.49
1:B:203:GLY:HA2	1:B:302:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLY:HA3	1:C:288:ILE:HG23	1.94	0.49
1:C:102:TYR:HB3	1:C:169:PHE:HB3	1.95	0.49
1:C:336:VAL:HG11	1:C:349:LEU:HD22	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:A:120:VAL:HG22	1:A:125:GLU:HG2	1.95	0.48
1:C:150:PHE:HA	1:C:151:PRO:HD2	1.49	0.48
1:A:146:CYS:C	1:A:148:THR:N	2.66	0.48
1:A:77:THR:HG21	1:B:279:ALA:HA	1.95	0.48
1:C:332:TYR:HE2	1:C:357:LYS:HG2	1.77	0.48
1:B:292:ILE:HD11	2:D:63:GLN:HE22	1.78	0.48
2:D:129:GLU:OE2	2:D:129:GLU:HA	2.13	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:140:ASP:HB2	1:C:160:VAL:HG23	1.97	0.47
1:C:147:LEU:HD23	1:C:147:LEU:H	1.79	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:A:346:GLY:HA2	1:A:371:ASN:HD22	1.78	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: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
1:B:102:TYR:HB3	1:B:169:PHE:HB3	1.98	0.46
2:D:144:LEU:HD11	2:D:157:ILE:HD13	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:A:380:GLU:HG3	1:A:381:LYS:N	2.32	0.45
1:B:156:MET:HA	1:B:159:LEU:HD12	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:GLU:O	1:A:377:TYR:HD1	1.99	0.44
1:B:103:TYR:HB2	1:B:398:TYR:CE2	2.53	0.44
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:A:233:LEU:HD21	1:A:243:LEU:HD13	2.00	0.43
1:B:333:LYS:HA	1:B:354:VAL:HG22	1.99	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:130:LEU:HD12	1:A:139:HIS:HB2	2.00	0.43
1:A:136:ARG:O	1:A:390:ARG:NH2	2.52	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:A:194:LYS:HE2	1:A:267:HIS:HE1	1.84	0.42
1:B:268:VAL:HG12	1:B:271:LYS:H	1.83	0.42
1:A:227:LEU:HD21	1:A:266:PHE:CE2	2.55	0.42
2:D:117:LYS:HG2	5:D:171:GDP:C6	2.54	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:A:264:ILE:HD11	1:A:370:ILE:HD11	2.03	0.41
1:B:133:THR:HG21	1:B:138:TYR:CE2	2.55	0.41
1:C:319:VAL:H	1:C:335:SER:HB3	1.85	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
1:A:342:VAL:HA	1:A:343:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:LEU:H	1:C:349:LEU:HD23	1.86	0.40
2:D:102:ARG:HH11	2:D:102:ARG:CG	2.34	0.40
1:A:253:GLU:HG3	1:A:271:LYS:HD2	2.03	0.40
1:B:304:PHE:CD2	1:B:308:MET:HE1	2.56	0.40
2:D:46:VAL:HG23	2:D:46:VAL:O	2.21	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	334/341 (98%)	305 (91%)	23 (7%)	6 (2%)	8 32
1	B	335/341 (98%)	300 (90%)	28 (8%)	7 (2%)	7 30
1	C	328/341 (96%)	282 (86%)	40 (12%)	6 (2%)	8 32
2	D	165/167 (99%)	146 (88%)	14 (8%)	5 (3%)	4 23
All	All	1162/1190 (98%)	1033 (89%)	105 (9%)	24 (2%)	7 30

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

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Mol	Chain	Res	Type
2	D	47	ASP
1	A	215	GLU
2	D	139	ASN
2	D	150	SER
1	B	137	THR
1	B	149	GLU
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 (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	295/300 (98%)	263 (89%)	32 (11%)	6 24
1	B	295/300 (98%)	267 (90%)	28 (10%)	8 29
1	C	291/300 (97%)	269 (92%)	22 (8%)	13 41
2	D	147/147 (100%)	130 (88%)	17 (12%)	5 20
All	All	1028/1047 (98%)	929 (90%)	99 (10%)	8 29

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
2	D	144	LEU

Sometimes 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 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 monosaccharides 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	-	-	-		
5	GDP	D	171	-	24,30,30	0.89	0	30,47,47	1.37	7 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	D	171	-	-	1/12/32/32	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	171	GDP	O6-C6-C5	-2.60	119.30	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	171	GDP	C2-N1-C6	-2.58	120.36	125.10
5	D	171	GDP	C5-C6-N1	2.40	118.19	113.95
5	D	171	GDP	O2B-PB-O1B	2.38	120.00	110.68
5	D	171	GDP	PA-O3A-PB	-2.32	124.85	132.83
5	D	171	GDP	C3'-C2'-C1'	2.07	104.10	100.98
5	D	171	GDP	C8-N7-C5	2.06	106.92	102.99

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	171	GDP	PA-O3A-PB-O2B

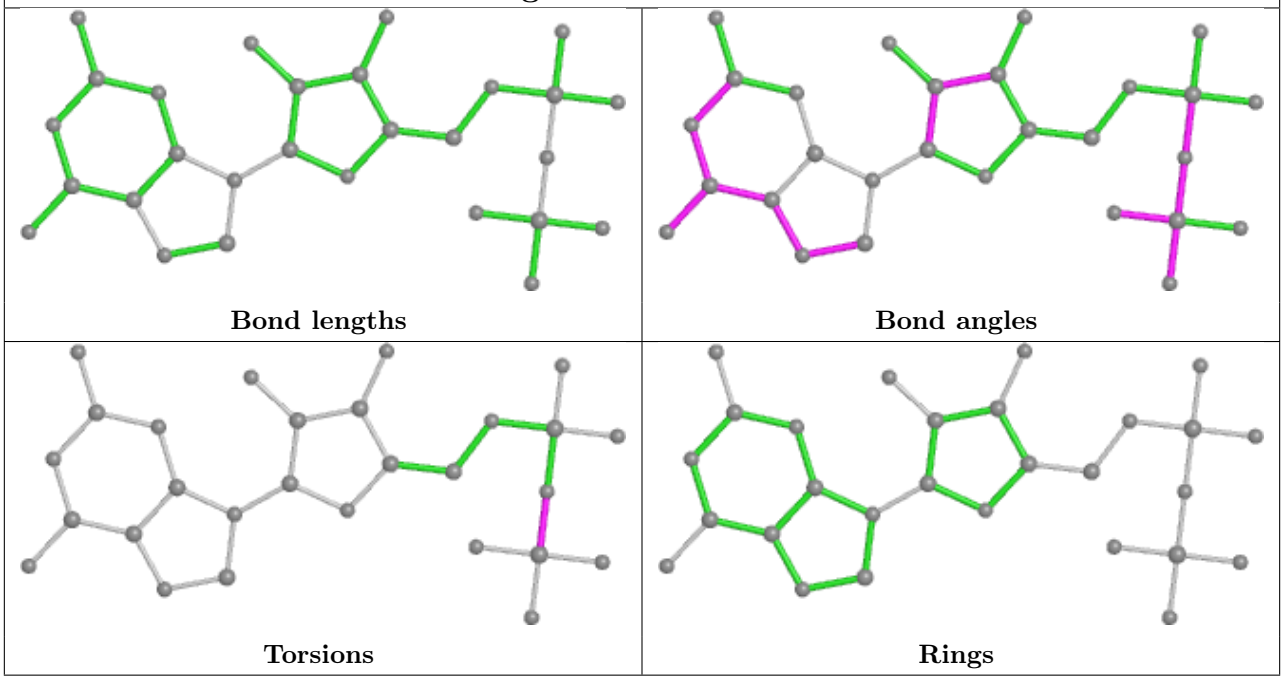
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	171	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP D 171



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.09	1 (0%) 94 93	69, 102, 124, 128	0
1	B	337/341 (98%)	-0.15	3 (0%) 84 83	54, 80, 112, 126	0
1	C	332/341 (97%)	0.14	10 (3%) 50 49	61, 136, 163, 167	0
2	D	167/167 (100%)	-0.19	0 100 100	63, 76, 90, 94	0
All	All	1172/1190 (98%)	-0.06	14 (1%) 79 77	54, 91, 156, 167	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	PRO	3.4
1	B	327	PRO	3.2
1	C	282	LEU	3.1
1	C	296	VAL	3.1
1	C	317	TYR	2.7
1	C	349	LEU	2.6
1	C	413	GLY	2.5
1	C	198	ILE	2.3
1	B	326	GLY	2.3
1	C	334	VAL	2.1
1	C	354	VAL	2.1
1	A	327	PRO	2.0
1	B	325	GLY	2.0
1	C	412	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

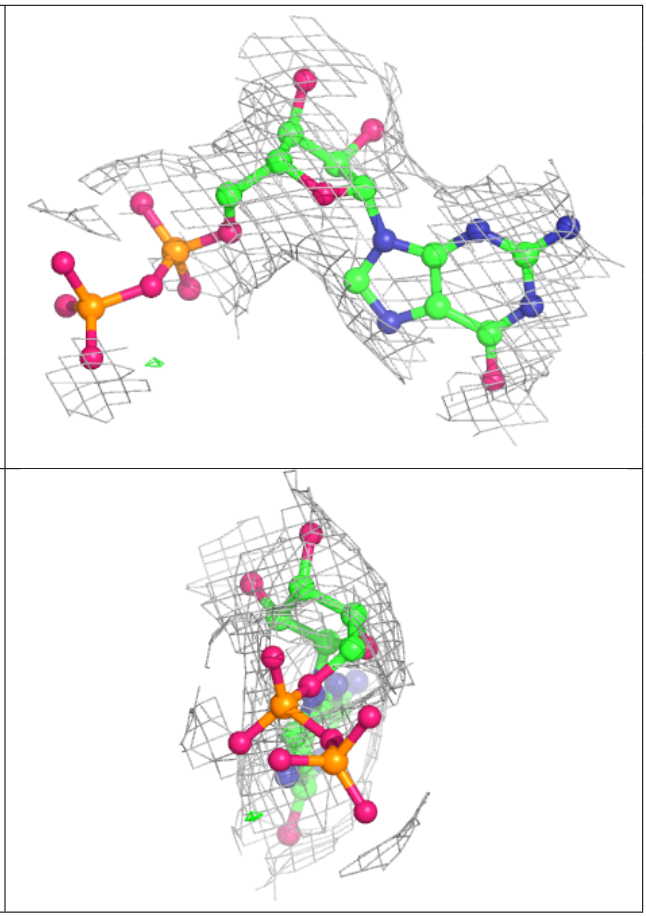
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	D	172	1/1	0.98	0.21	68,68,68,68	0
5	GDP	D	171	28/28	0.98	0.20	62,63,63,64	0
4	BEF	D	170	4/4	0.99	0.20	64,64,64,65	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP D 171:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.