Full wwPDB X-ray Structure Validation Report ⓘ

Mar 21, 2022 – 06:15 pm GMT

PDB ID	:	7Z01
Title	:	Z-SBTubA4 photoswitch bound to tubulin-DARPin D1 complex
Authors	:	Wranik, M.; Weinert, T.; Standfuss, J.; Steinmetz, M.
Deposited on	:	2022-02-21
Resolution	:	1.82 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 ⓘ symbol.

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

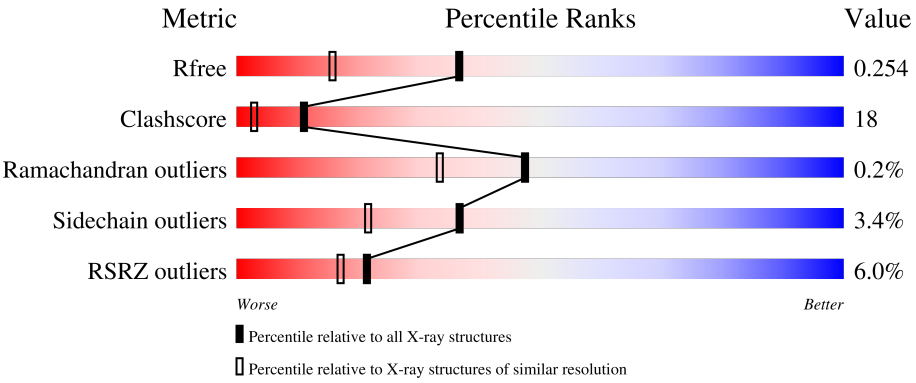
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	451	6% 64% 33%
2	B	445	8% 60% 34%
3	F	169	% 62% 29% 8%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8287 atoms, of which 19 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	437	3431	2173	584	651	23	0	5	0

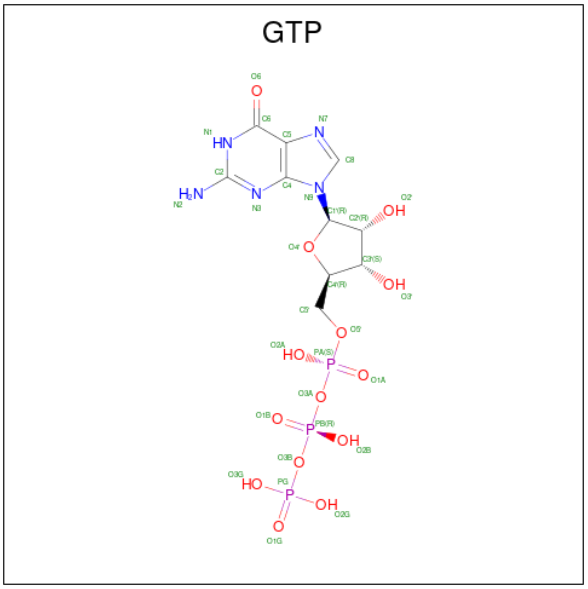
- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	3390	2131	576	654	29	7	6	0

- Molecule 3 is a protein called Designed Ankyrin Repeat Protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	F	155	1159	730	199	227	3	0	1	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

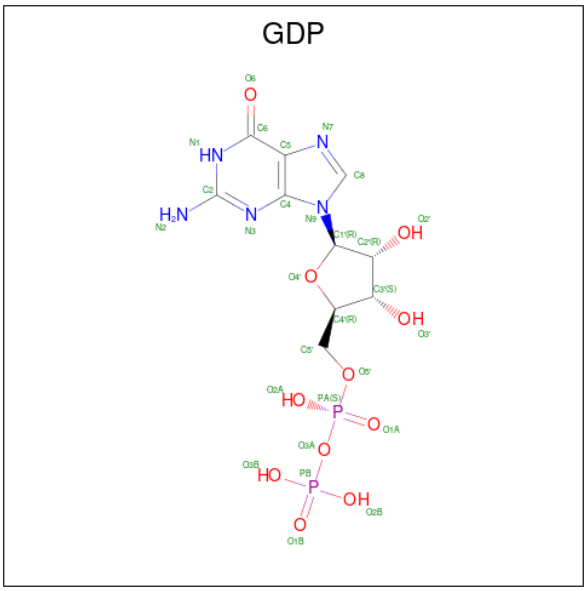
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

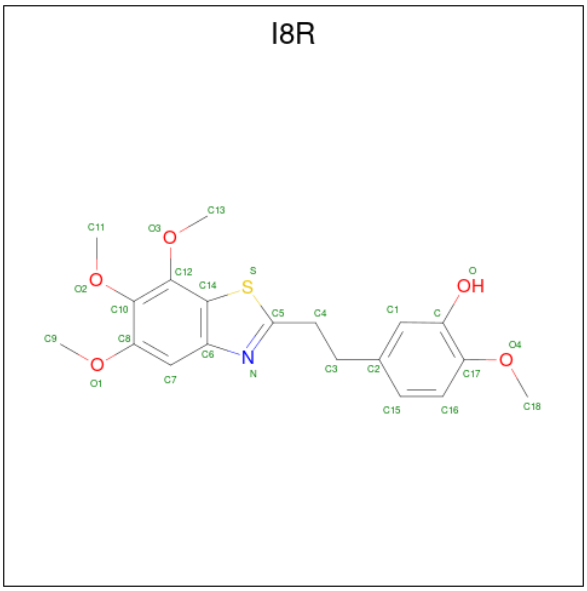
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	1	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 8 is 2-methoxy-5-[2-(5,6,7-trimethoxy-1,3-benzothiazol-2-yl)ethyl]phenol (three-letter code: I8R) (formula: $C_{19}H_{21}NO_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	0	0
			45	19	19	1	5	1		

- Molecule 9 is water.

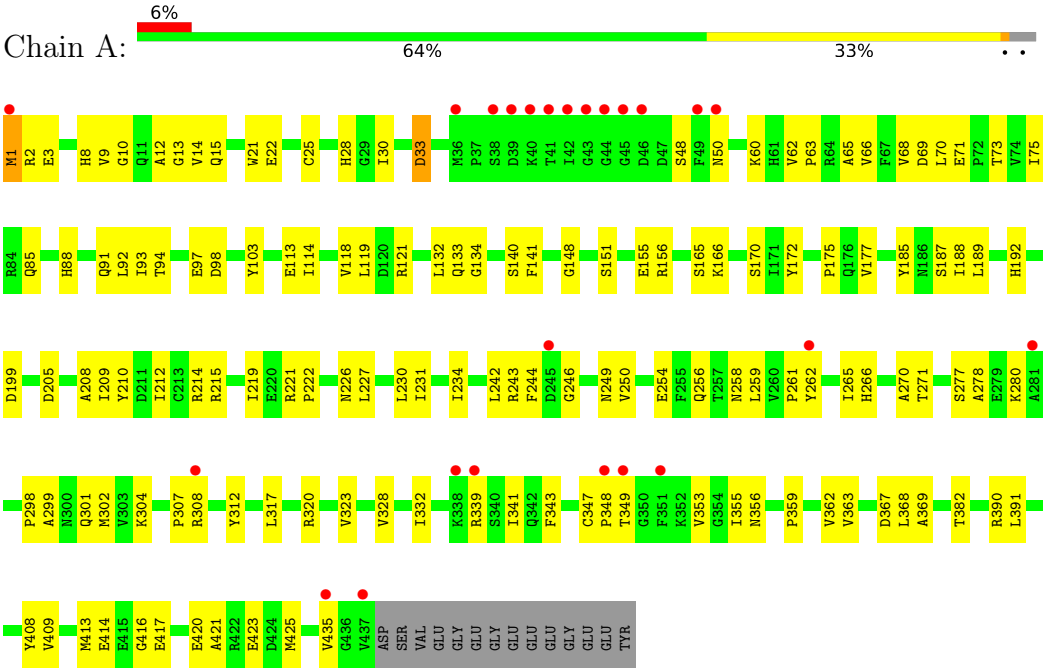
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	93	Total	O	0	0
			93	93		
9	B	61	Total	O	0	0
			61	61		
9	F	46	Total	O	0	0
			46	46		

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.

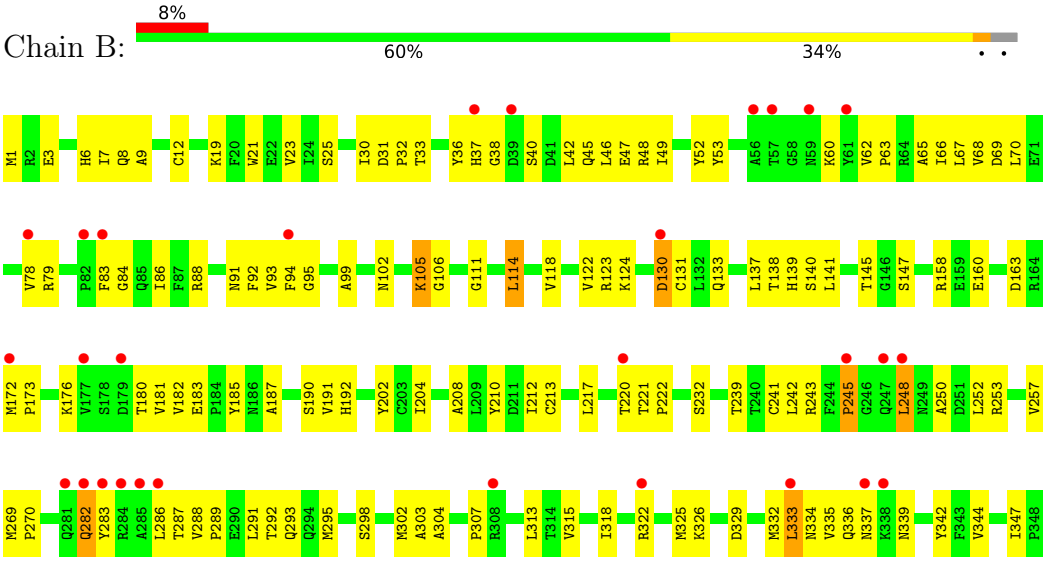
• Molecule 1: Tubulin alpha-1B chain

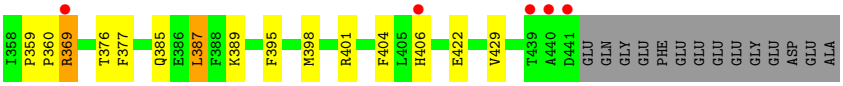
Chain A:



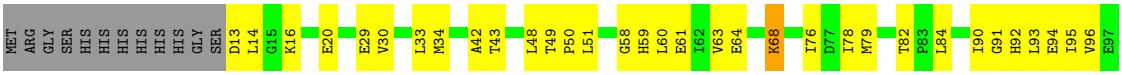
• Molecule 2: Tubulin beta-2B chain

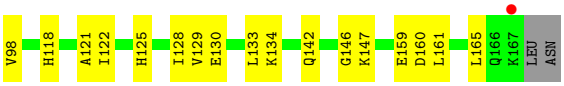
Chain B:





• Molecule 3: Designed Ankyrin Repeat Protein (DARPIN) D1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.47Å 91.89Å 82.43Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	49.19 – 1.82 49.19 – 1.82	Depositor EDS
% Data completeness (in resolution range)	45.5 (49.19-1.82) 43.0 (49.19-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.31 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.205 , 0.255 0.205 , 0.254	Depositor DCC
R_{free} test set	2000 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8287	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, I8R, MG, GDP, GTP

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	0.25	0/3521	0.45	0/4783
2	B	0.24	0/3480	0.45	0/4715
3	F	0.23	0/1178	0.40	0/1601
All	All	0.24	0/8179	0.44	0/11099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3431	0	3343	116	0
2	B	3390	0	3250	137	0
3	F	1159	0	1162	38	0
4	A	32	0	12	1	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	B	28	0	12	1	0
8	B	26	19	0	1	0
9	A	93	0	0	4	0
9	B	61	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	46	0	0	7	0
All	All	8268	19	7779	285	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 18.

All (285) 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)
3:F:121:ALA:HB1	3:F:161:LEU:HD21	1.51	0.90
2:B:295:MET:HE2	2:B:377:PHE:HB2	1.55	0.86
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.59	0.83
2:B:172[B]:MET:HE2	2:B:173:PRO:HD2	1.61	0.83
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.65	0.78
1:A:97:GLU:N	1:A:97:GLU:OE1	2.17	0.77
2:B:180:THR:HG22	2:B:182:VAL:HG22	1.67	0.77
2:B:63:PRO:HD3	2:B:86:ILE:HG13	1.65	0.76
1:A:93:ILE:HG22	1:A:114:ILE:HD11	1.67	0.76
2:B:248:LEU:HD13	2:B:250:ALA:HB2	1.68	0.76
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.68	0.75
1:A:215:ARG:HH22	1:A:299:ALA:HB1	1.51	0.74
2:B:1:MET:N	2:B:131:CYS:SG	2.58	0.74
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.71	0.73
1:A:209:ILE:HD11	1:A:302:MET:HE1	1.71	0.73
1:A:209:ILE:HD11	1:A:302:MET:CE	2.19	0.72
2:B:239:THR:O	2:B:243:ARG:HG3	1.89	0.71
3:F:78:ILE:HG13	3:F:79:MET:HE3	1.74	0.70
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.71	0.70
2:B:172[B]:MET:HG2	2:B:387:LEU:HD21	1.72	0.69
3:F:64:GLU:O	3:F:68:LYS:HE2	1.93	0.69
1:A:1:MET:SD	1:A:50:ASN:ND2	2.66	0.69
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.26	0.69
2:B:1:MET:CE	2:B:133:GLN:HG3	2.23	0.68
1:A:221:ARG:HD3	2:B:326:LYS:HD3	1.76	0.67
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.74	0.67
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.29	0.66
2:B:74:THR:O	2:B:78:VAL:HG23	1.95	0.66
3:F:92:HIS:O	3:F:96:VAL:HG23	1.97	0.65
1:A:413:MET:HE2	1:A:417:GLU:HB3	1.78	0.65
1:A:22:GLU:OE2	1:A:363:VAL:HG11	1.97	0.64
2:B:83:PHE:O	2:B:86:ILE:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:GLN:HG2	2:B:283:TYR:N	2.13	0.63
2:B:333:LEU:HD13	2:B:337:ASN:OD1	1.98	0.62
1:A:362:VAL:HG11	1:A:368:LEU:O	1.99	0.62
1:A:15:GLN:NE2	4:A:501:GTP:O6	2.32	0.62
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.82	0.62
2:B:69:ASP:HB3	2:B:94:PHE:CD2	2.35	0.62
3:F:84:LEU:HD11	3:F:96:VAL:HG13	1.82	0.62
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.82	0.61
2:B:88:ARG:NH1	2:B:91:ASN:OD1	2.33	0.61
1:A:262:TYR:HB2	1:A:265:ILE:HG12	1.81	0.61
2:B:332:MET:O	2:B:336:GLN:HG3	2.00	0.61
1:A:93:ILE:CG2	1:A:114:ILE:HD11	2.31	0.61
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.35	0.61
1:A:156:ARG:NH2	9:A:609:HOH:O	2.33	0.60
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.82	0.60
1:A:271:THR:HG21	1:A:295:CYS:O	2.00	0.60
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.37	0.60
2:B:123:ARG:NH1	2:B:160[A]:GLU:OE2	2.34	0.60
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.17	0.59
3:F:147:LYS:NZ	9:F:202:HOH:O	2.35	0.59
3:F:92:HIS:HB3	9:F:204:HOH:O	2.02	0.59
2:B:69:ASP:HA	2:B:145:THR:HG21	1.85	0.59
1:A:2:ARG:NH1	1:A:133:GLN:HG2	2.18	0.59
2:B:1:MET:HE3	2:B:133:GLN:HG3	1.84	0.59
3:F:43:THR:HG22	3:F:49:THR:HG22	1.85	0.58
2:B:286:LEU:HD11	2:B:291:LEU:HD23	1.85	0.58
1:A:175:PRO:HB3	2:B:349[A]:ASN:OD1	2.04	0.58
2:B:141:LEU:HD12	2:B:172[B]:MET:CE	2.34	0.58
3:F:130:GLU:O	3:F:134:LYS:HD3	2.02	0.58
1:A:246:GLY:O	1:A:250:VAL:HG12	2.03	0.58
2:B:38:GLY:HA3	2:B:45:GLN:NE2	2.19	0.58
2:B:75:MET:HB3	2:B:94:PHE:CD2	2.39	0.58
2:B:75:MET:HB3	2:B:94:PHE:CE2	2.39	0.57
1:A:60:LYS:NZ	1:A:85:GLN:O	2.27	0.57
1:A:317:LEU:HD12	1:A:332:ILE:HD11	1.87	0.57
2:B:3:GLU:OE2	2:B:130:ASP:N	2.26	0.57
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.39	0.57
2:B:63:PRO:CD	2:B:86:ILE:HG13	2.33	0.56
1:A:48:SER:HB2	1:A:244:PHE:HA	1.88	0.56
1:A:308[A]:ARG:HH22	1:A:339:ARG:HH21	1.52	0.56
2:B:12:CYS:HB2	7:B:501:GDP:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:PRO:O	2:B:75:MET:HG2	2.06	0.55
1:A:339:ARG:HB2	1:A:341:ILE:HG12	1.89	0.55
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.88	0.55
1:A:249:ASN:HA	1:A:254:GLU:HG2	1.87	0.55
2:B:23:VAL:HG21	2:B:232:SER:HB2	1.89	0.55
1:A:221:ARG:HB2	2:B:326:LYS:HE3	1.88	0.55
2:B:141:LEU:HD12	2:B:172[A]:MET:SD	2.47	0.55
3:F:94:GLU:CD	3:F:94:GLU:H	2.10	0.55
3:F:125:HIS:O	3:F:129:VAL:HG23	2.07	0.55
2:B:141:LEU:HD12	2:B:172[B]:MET:HE1	1.89	0.54
2:B:181:VAL:HB	2:B:398:MET:SD	2.47	0.54
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.89	0.54
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.38	0.54
2:B:181:VAL:HG11	3:F:90:ILE:HA	1.90	0.54
2:B:318:ILE:CG2	2:B:376:THR:HB	2.37	0.53
2:B:404:PHE:HE2	3:F:90:ILE:HD12	1.74	0.53
2:B:176:LYS:HE3	3:F:160:ASP:OD2	2.09	0.53
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.72	0.53
2:B:1:MET:HE1	2:B:133:GLN:HG3	1.91	0.53
3:F:13:ASP:N	9:F:203:HOH:O	2.40	0.53
2:B:42:LEU:HD22	2:B:245:PRO:HG2	1.90	0.52
2:B:3:GLU:N	2:B:3:GLU:OE1	2.39	0.52
2:B:19:LYS:O	2:B:23:VAL:HG23	2.08	0.52
9:B:642:HOH:O	3:F:79:MET:HG3	2.10	0.52
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.25	0.52
2:B:176:LYS:HD3	2:B:210:TYR:CD1	2.45	0.52
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.92	0.52
1:A:308[A]:ARG:HH22	1:A:339:ARG:NH2	2.07	0.52
2:B:242:LEU:HG	8:B:502:I8R:C9	2.40	0.51
1:A:249:ASN:HA	1:A:254:GLU:CG	2.40	0.51
1:A:409:VAL:HA	1:A:413:MET:O	2.10	0.51
2:B:253:ARG:O	2:B:257:VAL:HG23	2.11	0.51
1:A:151:SER:O	1:A:155:GLU:HG3	2.10	0.51
1:A:166:LYS:HE2	1:A:197:HIS:O	2.11	0.51
1:A:259:LEU:O	1:A:261:PRO:HD3	2.11	0.51
2:B:172[B]:MET:CE	2:B:173:PRO:HD2	2.38	0.51
1:A:301:GLN:HE22	1:A:307:PRO:CD	2.22	0.51
1:A:320:ARG:HA	1:A:356:ASN:O	2.11	0.51
3:F:51:LEU:HD11	3:F:63:VAL:HG13	1.92	0.50
3:F:60:LEU:HD11	3:F:98:VAL:HG21	1.94	0.50
2:B:389:LYS:HE3	2:B:429:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:59:HIS:O	3:F:63:VAL:HG23	2.12	0.50
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.94	0.49
1:A:234:ILE:HG12	1:A:302:MET:SD	2.51	0.49
1:A:270:ALA:O	1:A:302:MET:HG2	2.12	0.49
2:B:208:ALA:O	2:B:212:ILE:HG13	2.13	0.49
3:F:125:HIS:HB3	9:F:236:HOH:O	2.12	0.49
2:B:124:LYS:HD3	2:B:124:LYS:C	2.33	0.49
2:B:130:ASP:N	2:B:130:ASP:OD1	2.45	0.49
2:B:30:ILE:HD12	2:B:30:ILE:N	2.28	0.49
1:A:382:THR:HG21	1:A:435:VAL:HG23	1.95	0.49
2:B:46:LEU:HA	2:B:49:ILE:HB	1.94	0.49
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.41	0.49
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.93	0.49
3:F:16:LYS:NZ	9:F:205:HOH:O	2.45	0.49
2:B:38:GLY:HA3	2:B:45:GLN:HE22	1.77	0.49
2:B:298:SER:HB3	2:B:307:PRO:HD2	1.95	0.49
1:A:416:GLY:O	1:A:420:GLU:HG3	2.11	0.49
2:B:360:PRO:O	2:B:369:ARG:HA	2.13	0.49
2:B:401:ARG:HD2	2:B:401:ARG:N	2.28	0.49
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.95	0.49
2:B:172[B]:MET:HA	2:B:172[B]:MET:HE3	1.95	0.49
2:B:102:ASN:HB3	2:B:105:LYS:HG3	1.94	0.48
1:A:227:LEU:O	1:A:231:ILE:HG13	2.12	0.48
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.95	0.48
2:B:325:MET:HB3	9:B:652:HOH:O	2.13	0.48
1:A:22:GLU:HG3	1:A:83:TYR:OH	2.14	0.48
2:B:62:VAL:HG13	2:B:86:ILE:O	2.13	0.48
2:B:220:THR:O	2:B:222:PRO:HD3	2.14	0.48
2:B:66:ILE:CD1	2:B:122:VAL:HG22	2.43	0.48
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.23	0.48
1:A:3:GLU:O	1:A:133:GLN:HG3	2.14	0.48
2:B:357:ASP:O	2:B:359:PRO:HD3	2.14	0.48
3:F:30:VAL:O	3:F:34:MET:HG3	2.13	0.48
1:A:254:GLU:HG3	1:A:258:ASN:ND2	2.29	0.47
1:A:185:TYR:O	1:A:189:LEU:HG	2.15	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.15	0.47
2:B:313:LEU:HD23	2:B:344:VAL:HG11	1.97	0.47
2:B:72:PRO:HD3	2:B:95:GLY:O	2.15	0.47
1:A:114:ILE:O	1:A:118:VAL:HG23	2.15	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.50	0.47
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:HB2	1:A:91:GLN:CG	2.44	0.47
1:A:280:LYS:HD2	1:A:280:LYS:N	2.30	0.47
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.35	0.47
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.97	0.47
3:F:42:ALA:O	3:F:49:THR:HA	2.15	0.47
1:A:10:GLY:O	1:A:14:VAL:HG23	2.14	0.47
1:A:401:LYS:HE2	9:A:649:HOH:O	2.15	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
2:B:36:TYR:OH	2:B:40:SER:O	2.33	0.47
2:B:147:SER:HB2	2:B:190:SER:OG	2.15	0.46
2:B:180:THR:HB	2:B:183:GLU:HG3	1.96	0.46
3:F:42:ALA:O	3:F:50:PRO:HD3	2.16	0.46
3:F:61:GLU:H	3:F:61:GLU:CD	2.18	0.46
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.97	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.50	0.46
2:B:25:SER:OG	2:B:53:TYR:OH	2.32	0.46
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.50	0.46
2:B:31:ASP:OD2	2:B:33:THR:OG1	2.33	0.46
2:B:47:GLU:HG3	2:B:245:PRO:HG3	1.97	0.46
3:F:58:GLY:HA2	3:F:95:ILE:CD1	2.46	0.46
2:B:187:ALA:O	2:B:191:VAL:HG23	2.15	0.46
1:A:188:ILE:HG22	1:A:421:ALA:HB1	1.97	0.46
2:B:9:ALA:HA	2:B:68:VAL:O	2.16	0.46
2:B:172[B]:MET:HE2	2:B:173:PRO:CD	2.39	0.46
2:B:288:VAL:N	2:B:289:PRO:HD2	2.30	0.46
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.98	0.46
3:F:43:THR:HA	3:F:48:LEU:O	2.16	0.45
1:A:70:LEU:HB2	1:A:98:ASP:HA	1.98	0.45
2:B:182:VAL:O	2:B:185:TYR:HB2	2.16	0.45
1:A:249:ASN:HA	1:A:254:GLU:HB3	1.97	0.45
2:B:360:PRO:C	2:B:369:ARG:HG2	2.36	0.45
3:F:95:ILE:HG13	9:F:204:HOH:O	2.17	0.45
1:A:79:ARG:NH2	1:A:92:LEU:O	2.35	0.45
1:A:199:ASP:HB3	1:A:256:GLN:CG	2.46	0.45
2:B:202:TYR:O	2:B:204:ILE:HD12	2.16	0.45
1:A:3:GLU:OE1	1:A:3:GLU:N	2.49	0.45
1:A:262:TYR:HB2	1:A:265:ILE:CG1	2.45	0.45
1:A:323:VAL:CG1	1:A:355:ILE:HG23	2.46	0.45
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.98	0.45
3:F:16:LYS:O	3:F:20:GLU:HG3	2.17	0.45
1:A:28:HIS:CE1	1:A:243:ARG:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD11	1:A:302:MET:HE3	1.98	0.45
2:B:220:THR:HG23	2:B:221:THR:N	2.32	0.45
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.52	0.45
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.51	0.45
2:B:60:LYS:HE3	2:B:60:LYS:HB3	1.65	0.45
2:B:172[B]:MET:HG3	2:B:173:PRO:HD2	1.97	0.45
2:B:292:THR:CG2	2:B:335:VAL:HG21	2.44	0.45
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.99	0.45
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.53	0.44
1:A:8:HIS:HB3	1:A:13:GLY:O	2.17	0.44
1:A:66:VAL:HG22	1:A:91:GLN:OE1	2.17	0.44
2:B:47:GLU:HG3	2:B:245:PRO:CG	2.47	0.44
1:A:304:LYS:O	1:A:390:ARG:NH1	2.50	0.44
3:F:14:LEU:HD22	3:F:14:LEU:H	1.82	0.44
2:B:8:GLN:OE1	2:B:67:LEU:HD22	2.18	0.44
2:B:172[A]:MET:HG3	2:B:387:LEU:HD11	2.00	0.44
1:A:312:TYR:CE1	1:A:341:ILE:HG23	2.53	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
1:A:343:PHE:HB2	1:A:349:THR:HG22	2.00	0.44
1:A:408:TYR:O	1:A:413:MET:HB3	2.18	0.44
2:B:70:LEU:HD21	2:B:111:GLY:HA2	2.00	0.44
2:B:241:CYS:SG	2:B:318:ILE:HD13	2.57	0.44
2:B:389:LYS:HE3	2:B:429:VAL:HG11	2.00	0.44
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.50	0.44
2:B:36:TYR:O	2:B:37:HIS:ND1	2.50	0.44
1:A:75:ILE:HB	1:A:94:THR:HG21	1.99	0.44
2:B:47:GLU:HB2	2:B:245:PRO:HG3	1.99	0.44
1:A:1:MET:HB2	1:A:2:ARG:H	1.66	0.44
1:A:25:CYS:HB3	1:A:30:ILE:O	2.17	0.44
3:F:91:GLY:HA2	3:F:128:ILE:HD12	1.99	0.44
2:B:52:TYR:HE2	2:B:243:ARG:HG2	1.83	0.43
2:B:75:MET:HB3	2:B:94:PHE:CZ	2.53	0.43
3:F:142:GLN:HB3	3:F:146:GLY:HA2	2.00	0.43
1:A:1:MET:HE2	1:A:1:MET:H3	1.83	0.43
2:B:263:PRO:HG2	2:B:264:ARG:HE	1.83	0.43
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.82	0.43
1:A:33:ASP:N	1:A:33:ASP:OD1	2.51	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.19	0.43
2:B:67:LEU:HD12	2:B:92:PHE:CZ	2.53	0.43
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.54	0.43
2:B:75:MET:HB3	2:B:94:PHE:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:29:GLU:O	3:F:33:LEU:HG	2.18	0.43
1:A:403:ALA:O	1:A:404:PHE:HB2	2.19	0.43
3:F:133:LEU:HD11	3:F:165:LEU:HD13	2.00	0.43
1:A:234:ILE:HD12	1:A:234:ILE:N	2.33	0.42
2:B:204:ILE:HD12	2:B:204:ILE:N	2.33	0.42
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.01	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42
1:A:208:ALA:O	1:A:212:ILE:HG13	2.20	0.42
2:B:12:CYS:SG	2:B:140:SER:HB3	2.59	0.42
2:B:322:ARG:HE	2:B:357:ASP:HB3	1.84	0.42
2:B:289:PRO:O	2:B:293:GLN:HG2	2.19	0.42
2:B:329:ASP:O	2:B:333:LEU:HB2	2.19	0.42
2:B:118:VAL:O	2:B:122:VAL:HG23	2.20	0.42
1:A:88:HIS:HB2	1:A:91:GLN:HG2	2.01	0.42
1:A:214:ARG:HG2	1:A:219:ILE:O	2.20	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.42
3:F:118:HIS:O	3:F:122:ILE:HG13	2.19	0.42
1:A:214:ARG:NH2	9:A:628:HOH:O	2.52	0.42
2:B:69:ASP:HB3	2:B:94:PHE:CE2	2.55	0.42
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.32	0.41
1:A:1:MET:HE2	1:A:1:MET:N	2.35	0.41
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.41
2:B:141:LEU:HD12	2:B:172[B]:MET:HE3	2.02	0.41
1:A:177:VAL:O	1:A:177:VAL:HG13	2.19	0.41
2:B:93:VAL:HG12	2:B:114:LEU:CD2	2.50	0.41
1:A:75:ILE:HB	1:A:94:THR:CG2	2.50	0.41
1:A:323:VAL:HG13	1:A:355:ILE:HG23	2.03	0.41
2:B:287:THR:HB	2:B:289:PRO:HD2	2.02	0.41
2:B:79:ARG:HA	2:B:84:GLY:HA3	2.01	0.41
1:A:62:VAL:HG11	1:A:88:HIS:CD2	2.56	0.41
1:A:277:SER:HB3	1:A:280:LYS:HD3	2.03	0.41
1:A:320:ARG:HG2	1:A:356:ASN:HB3	2.02	0.41
1:A:359:PRO:HG3	9:A:669:HOH:O	2.21	0.41
2:B:6:HIS:HE1	2:B:138:THR:HG23	1.86	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.41
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.79	0.41
2:B:158:ARG:NH1	2:B:166:MET:HB2	2.35	0.41
3:F:79:MET:CE	3:F:79:MET:HA	2.51	0.41
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.40
1:A:93:ILE:HG22	1:A:114:ILE:CD1	2.46	0.40
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:TYR:CD2	2:B:46:LEU:HD21	2.56	0.40
2:B:422:GLU:OE1	2:B:422:GLU:HA	2.21	0.40
1:A:347:CYS:SG	1:A:348:PRO:HD2	2.61	0.40
2:B:68:VAL:O	2:B:69:ASP:HB2	2.20	0.40
3:F:76:ILE:HG22	3:F:82:THR:HG22	2.04	0.40
3:F:128:ILE:HG13	9:F:236:HOH: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	440/451 (98%)	418 (95%)	22 (5%)	0	100	100
2	B	433/445 (97%)	407 (94%)	24 (6%)	2 (0%)	29	15
3	F	154/169 (91%)	149 (97%)	5 (3%)	0	100	100
All	All	1027/1065 (96%)	974 (95%)	51 (5%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	245	PRO
2	B	304	ALA

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	370/379 (98%)	359 (97%)	11 (3%)	41	26
2	B	370/383 (97%)	353 (95%)	17 (5%)	27	12
3	F	121/132 (92%)	118 (98%)	3 (2%)	47	33
All	All	861/894 (96%)	830 (96%)	31 (4%)	37	19

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	33	ASP
1	A	113	GLU
1	A	132	LEU
1	A	195	LEU
1	A	242	LEU
1	A	266	HIS
1	A	283	HIS
1	A	402	ARG
1	A	414	GLU
1	A	423	GLU
2	B	48	ARG
2	B	105	LYS
2	B	114	LEU
2	B	130	ASP
2	B	139[A]	HIS
2	B	139[B]	HIS
2	B	163	ASP
2	B	192	HIS
2	B	248	LEU
2	B	264	ARG
2	B	282	GLN
2	B	333	LEU
2	B	334	ASN
2	B	369	ARG
2	B	387	LEU
2	B	406[A]	HIS
2	B	406[B]	HIS
3	F	68	LYS
3	F	93	LEU
3	F	159	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
8	I8R	B	502	-	25,28,28	1.62	2 (8%)	31,39,39	1.61	3 (9%)
7	GDP	B	501	-	24,30,30	1.21	2 (8%)	31,47,47	1.94	8 (25%)
4	GTP	A	501	5	26,34,34	1.00	1 (3%)	33,54,54	1.83	7 (21%)

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
8	I8R	B	502	-	-	3/12/13/13	0/3/3/3
7	GDP	B	501	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	501	5	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	I8R	C4-C5	-6.29	1.45	1.49
7	B	501	GDP	C5-C6	4.21	1.48	1.41
4	A	501	GTP	C6-N1	3.14	1.38	1.33
8	B	502	I8R	C3-C4	-2.93	1.33	1.53
7	B	501	GDP	C5-C4	2.51	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	502	I8R	C3-C4-C5	7.12	124.61	112.67
4	A	501	GTP	N3-C2-N1	-5.25	120.22	127.22
7	B	501	GDP	C2-N3-C4	4.72	120.75	115.36
4	A	501	GTP	C2-N3-C4	4.31	120.27	115.36
7	B	501	GDP	C2-N1-C6	4.02	122.31	115.93
7	B	501	GDP	C5-C6-N1	-4.00	117.96	123.43
7	B	501	GDP	C4-C5-C6	-3.77	117.20	120.80
4	A	501	GTP	PB-O3B-PG	-3.59	120.51	132.83
4	A	501	GTP	PA-O3A-PB	-3.49	120.85	132.83
7	B	501	GDP	PA-O3A-PB	-3.40	121.17	132.83
8	B	502	I8R	C4-C3-C2	3.25	124.71	113.28
7	B	501	GDP	N3-C2-N1	-3.17	122.99	127.22
4	A	501	GTP	C5-C6-N1	-2.74	119.68	123.43
7	B	501	GDP	C4-C5-N7	-2.65	106.64	109.40
4	A	501	GTP	C2-N1-C6	2.46	119.83	115.93
8	B	502	I8R	C14-C6-N	2.44	113.48	108.19
7	B	501	GDP	C3'-C2'-C1'	2.38	104.56	100.98
4	A	501	GTP	C3'-C2'-C1'	2.31	104.46	100.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O2A
7	B	501	GDP	C5'-O5'-PA-O1A
7	B	501	GDP	C5'-O5'-PA-O2A

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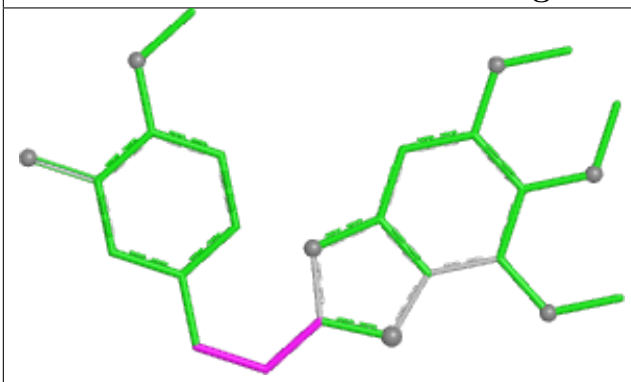
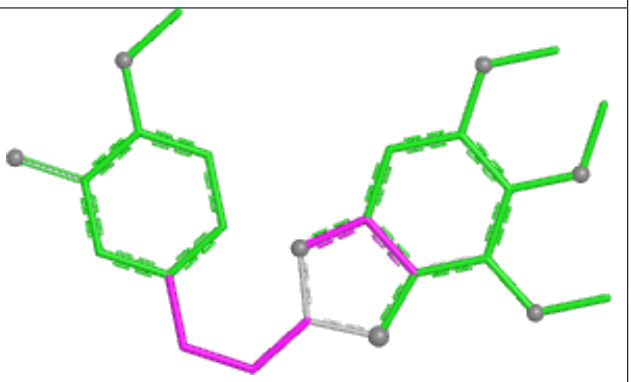
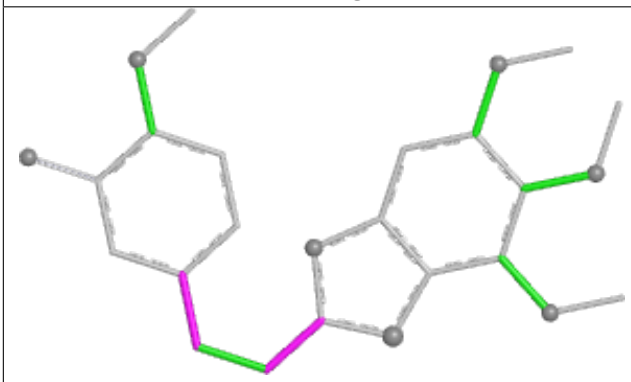
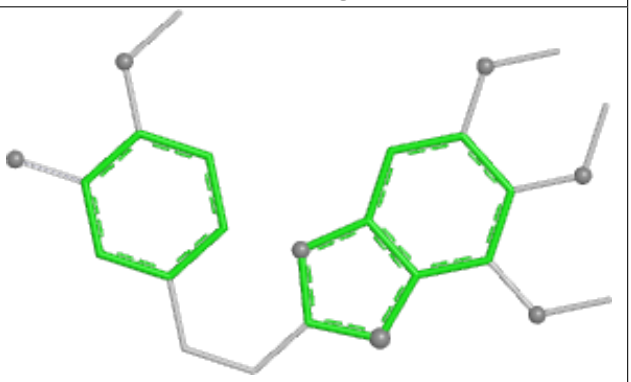
Mol	Chain	Res	Type	Atoms
8	B	502	I8R	C3-C4-C5-N
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C4'-C5'-O5'-PA
8	B	502	I8R	C1-C2-C3-C4
7	B	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	PB-O3A-PA-O2A
4	A	501	GTP	C3'-C4'-C5'-O5'
8	B	502	I8R	C15-C2-C3-C4

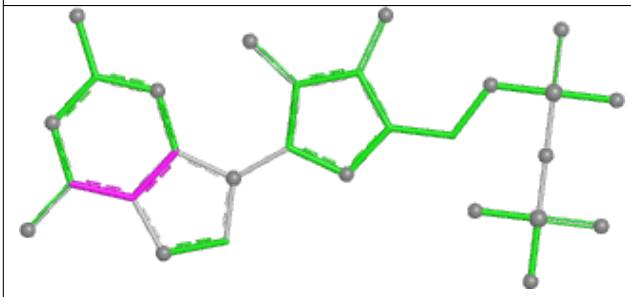
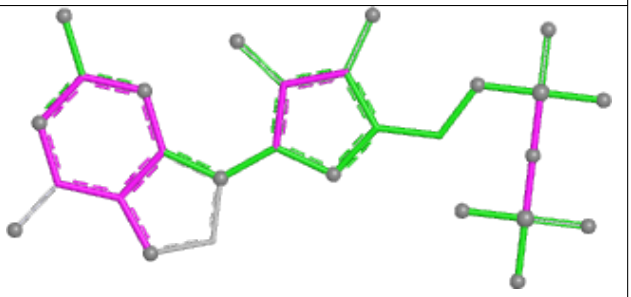
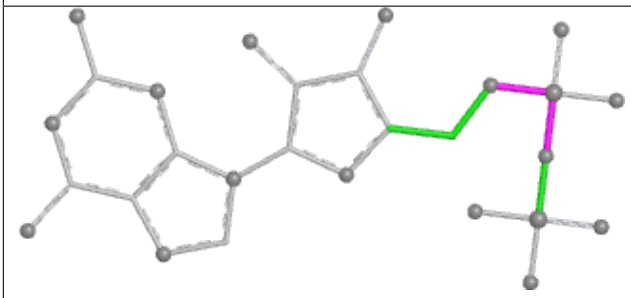
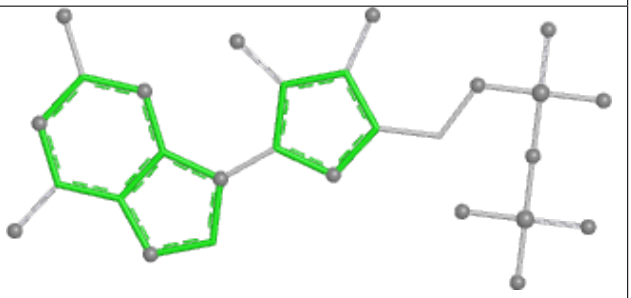
There are no ring outliers.

3 monomers are involved in 3 short contacts:

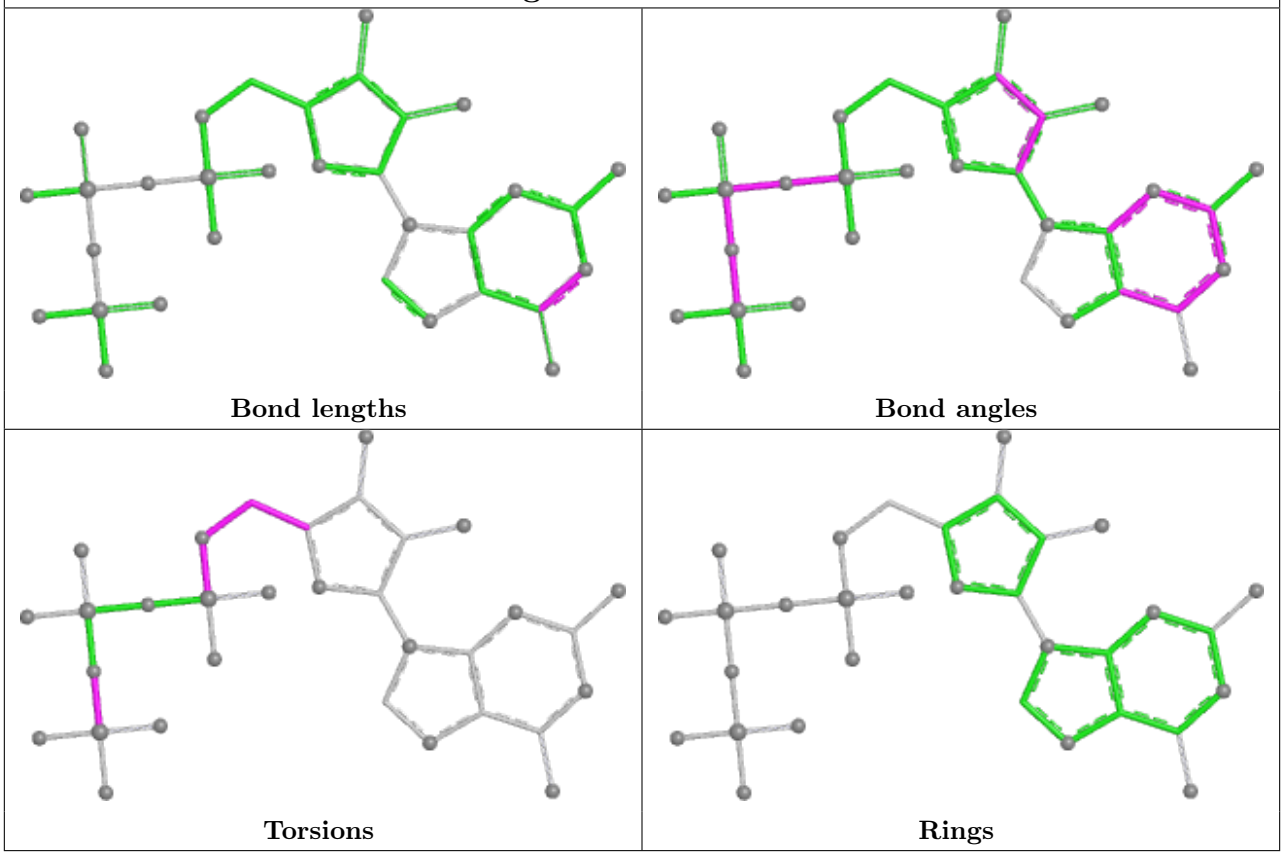
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	502	I8R	1	0
7	B	501	GDP	1	0
4	A	501	GTP	1	0

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 I8R B 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GDP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GTP A 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	360:PRO	C	369:ARG	N	5.08

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	437/451 (96%)	0.57	25 (5%) 23 19	16, 32, 71, 149	0
2	B	431/445 (96%)	0.56	35 (8%) 12 9	17, 37, 73, 110	0
3	F	155/169 (91%)	0.10	1 (0%) 89 88	16, 26, 47, 61	0
All	All	1023/1065 (96%)	0.50	61 (5%) 21 17	16, 33, 70, 149	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	42	ILE	14.5
1	A	281	ALA	11.2
1	A	44	GLY	10.4
1	A	40	LYS	7.7
1	A	41	THR	7.6
1	A	437	VAL	6.8
2	B	179	ASP	6.6
2	B	247	GLN	5.9
2	B	440	ALA	5.8
1	A	43	GLY	5.7
2	B	130	ASP	5.3
2	B	57	THR	5.1
2	B	369	ARG	4.7
2	B	284	ARG	4.6
1	A	45	GLY	4.5
2	B	283	TYR	4.4
2	B	285	ALA	4.2
2	B	281	GLN	4.2
1	A	46	ASP	3.9
2	B	248	LEU	3.5
1	A	282	TYR	3.4
1	A	38	SER	3.4
2	B	59	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
3	F	167	LYS	3.3
1	A	308[A]	ARG	3.3
2	B	61	TYR	3.2
1	A	435	VAL	3.2
2	B	282	GLN	3.2
1	A	349	THR	3.1
1	A	39	ASP	3.1
1	A	1	MET	2.9
1	A	348	PRO	2.9
1	A	339	ARG	2.7
2	B	441	ASP	2.7
2	B	82	PRO	2.7
2	B	337	ASN	2.7
2	B	333	LEU	2.6
2	B	406[A]	HIS	2.6
2	B	220	THR	2.6
2	B	439	THR	2.6
2	B	286	LEU	2.5
2	B	83	PHE	2.5
1	A	36	MET	2.4
1	A	50	ASN	2.4
2	B	308	ARG	2.4
2	B	78	VAL	2.4
2	B	338	LYS	2.3
2	B	39	ASP	2.3
1	A	245	ASP	2.2
1	A	338	LYS	2.2
2	B	37	HIS	2.2
2	B	245	PRO	2.2
1	A	262	TYR	2.2
1	A	351	PHE	2.2
2	B	94	PHE	2.2
2	B	172[A]	MET	2.1
2	B	75	MET	2.1
2	B	322	ARG	2.1
2	B	56	ALA	2.1
2	B	177	VAL	2.0
1	A	49	PHE	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)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.