

Full wwPDB X-ray Structure Validation Report (i)

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:	6Y4N
:	Structure of Tubulin Tyrosine Ligase in Complex with Tb116
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:	2020-02-21
:	2.85 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.85 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	А	451	93%	•	·
1	С	451	88%	9%	••
2	В	445	89%	8%	·
2	D	445	^{2%} 90%	6%	·
3	Е	143	80% 6%	14%	_



Mol	Chain	Length	Quality of chain		
			9%		
4	F	384	83%	7%	10%



2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 18400 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	439	Total 3430	C 2170	N 583	O 655	S 22	0	0	0
1	С	440	Total 3484	C 2202	N 594	O 665	S 23	0	5	0

• Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	431	Total 3401	C 2134	N 582	O 658	S 27	0	2	0
2	D	428	Total 3367	C 2112	N 578	O 651	S 26	0	1	0

• Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Е	123	Total 1014	$\begin{array}{c} \mathrm{C} \\ 625 \end{array}$	N 183	O 201	${ m S}{ m 5}$	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	47	MET	-	expression tag	UNP P63043
Е	48	ALA	-	expression tag	UNP P63043

• Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total 2851	C 1826	N 488	O 522	${ m S}$ 15	0	1	0

There are 6 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
Б	Λ	1	Total	С	Ν	Ο	Р	0	0
5	Л	1	32	10	5	14	3	0	0
5	C	1	Total	С	Ν	0	Р	0	0
0	U	1	32	10	5	14	3	0	0
5	Л	1	Total	С	Ν	Ο	Р	0	0
0	D	1	32	10	5	14	3	0	0

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Mg 1 1	0	0
6	В	1	Total Mg 1 1	0	0
6	С	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

• Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Ca 1 1	0	0
7	С	1	Total Ca 1 1	0	0

• Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
8	В	1	Total 28	C 10	N 5	0 11	Р 2	0	0

• Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
9	В	1	Total 12	C 6	N 1	0 4	S 1	0	0

• Molecule 10 is $(2 \{R\})$ -1-methylpiperidine-2-carboxylic acid (three-letter code: O9B) (formula: $C_7H_{13}NO_2$).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
10	В	1	Total 9	С 7	N 1	0 1	0	0

• Molecule 11 is [(1 {R},3 {R})-1-(4-methanoyl-1,3-thiazol-2-yl)-4-methyl-3-(methylamino)pe ntyl] ethanoate (three-letter code: O9K) (formula: $C_{13}H_{20}N_2O_3S$).





Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf
11	В	1	Total 19	C 13	N 2	0 3	S 1	0	0

• Molecule 12 is methyl (2 {S},4 {S})-2,4-bis(azanyl)-5-phenyl-pentanoate (three-letter code: O9N) (formula: $C_{12}H_{18}N_2O_2$).



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
12	В	1	Total 16	C 12	N 2	O 2	0	0

• Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).





Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
13	С	1	Total 10	C 6	0 4	0	0

• Molecule 14 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
14	С	1	Total 7	С 5	N 1	0 1	0	0

• Molecule 15 is benzyl hydrogen carbonate (three-letter code: P6S) (formula: $C_8H_8O_3$).





Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
15	С	1	Total 10	C 8	O 2	0	0

• Molecule 16 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	1	Total C 7 4	CO 43	0	0

• Molecule 17 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
17	F	1	Total 31	C 11	N 5	O 12	Р 3	0	0

• Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	А	116	Total O 116 116	0	0
18	В	143	Total O 143 143	0	0
18	С	174	Total O 174 174	0	0
18	D	67	$\begin{array}{cc} \text{Total} & \text{O} \\ 67 & 67 \end{array}$	0	1
18	Ε	31	Total O 31 31	0	0
18	F	70	Total O 70 70	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: Tubulin alpha-1B chain

• Molecule 3: Stathmin-4





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	104.28Å 154.97Å 183.43Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	78.93 - 2.85	Depositor
Itesolution (A)	78.93 - 2.85	EDS
% Data completeness	$100.0\ (78.93-2.85)$	Depositor
(in resolution range)	$100.0\ (78.93-2.85)$	EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) > 1$	$2.27 (at 2.86 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.7 (6-FEB-2020)	Depositor
B B.	0.183 , 0.220	Depositor
Π, Π_{free}	0.183 , 0.223	DCC
R_{free} test set	3527 reflections $(5.04%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	57.8	Xtriage
Anisotropy	0.328	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 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18400	wwPDB-VP
Average B, all atoms $(Å^2)$	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: GTP, P6S, PEG, O9N, O9B, O9K, MES, PGE, CA, ACP, GDP, MG

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).

Mal	Chain	Bond	lengths	Bond angles	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/3508	0.61	0/4762
1	С	0.45	0/3563	0.61	0/4837
2	В	0.43	0/3476	0.59	0/4709
2	D	0.40	0/3440	0.58	0/4659
3	Е	0.44	0/1022	0.53	0/1356
4	F	0.42	0/2916	0.58	0/3939
All	All	0.43	0/17925	0.59	0/24262

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 (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	А	3430	0	3339	15	0
1	С	3484	0	3386	31	0
2	В	3401	0	3275	24	0
2	D	3367	0	3246	15	0
3	Е	1014	0	1029	9	0
4	F	2851	0	2808	13	0
5	А	32	0	12	0	0



6Y4N	
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	С	32	0	12	0	0
5	D	32	0	12	0	0
6	А	1	0	0	0	0
6	В	1	0	0	0	0
6	С	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	А	1	0	0	0	0
7	С	1	0	0	0	0
8	В	28	0	12	0	0
9	В	12	0	13	2	0
10	В	9	0	0	0	0
11	В	19	0	0	0	0
12	В	16	0	0	0	0
13	С	10	0	14	4	0
14	С	7	0	8	0	0
15	С	10	0	0	0	0
16	D	7	0	10	0	0
17	F	31	0	14	0	0
18	А	116	0	0	8	0
18	В	143	0	0	11	0
18	С	174	0	0	11	0
18	D	67	0	0	6	0
18	Е	31	0	0	7	0
18	F	70	0	0	4	0
All	All	18400	0	17190	106	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 3.

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:E:149:MET:HB3	18:E:223:HOH:O	1.42	1.14
1:C:215:ARG:HB2	18:C:1208:HOH:O	1.68	0.91
3:E:149:MET:CB	18:E:223:HOH:O	2.06	0.88
1:C:113:GLU:HG3	18:C:1197:HOH:O	1.72	0.88
1:A:261:PRO:HD2	18:A:1147:HOH:O	1.74	0.86
1:C:120:ASP:HB2	18:C:1230:HOH:O	1.76	0.86
2:D:262:ARG:NH1	18:D:1101:HOH:O	2.12	0.83
1:A:262:TYR:CE1	18:A:1214:HOH:O	2.33	0.81



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:262:TYR:CD1	18:A:1214:HOH:O	2.39	0.75	
4:F:246:GLN:O	4:F:250:SER:HB3	1.87	0.74	
2:D:306:ARG:NH1	18:D:1103:HOH:O	2.19	0.74	
2:D:72:THR:HG23	18:D:1162:HOH:O	1.88	0.73	
1:C:381:THR:CG2	18:C:1131:HOH:O	2.39	0.71	
1:C:381:THR:HG23	18:C:1131:HOH:O	1.91	0.71	
18:B:1161:HOH:O	3:E:129:LYS:HE2	1.92	0.70	
2:D:2:ARG:NH1	18:D:1104:HOH:O	2.23	0.69	
2:B:197:ASP:OD2	9:B:1003:MES:H52	1.93	0.69	
1:A:85:GLN:HB2	18:A:1105:HOH:O	1.94	0.67	
1:C:262:TYR:HB3	13:C:1004:PGE:H42	1.78	0.65	
2:B:57:ASN:HA	18:B:1102:HOH:O	1.97	0.63	
3:E:88:ASP:N	18:E:201:HOH:O	2.30	0.63	
1:C:296:PHE:CE2	1:C:341:ILE:HD11	2.33	0.63	
2:D:81:PHE:O	2:D:84:ILE:HG22	1.99	0.62	
2:B:323:MET:HB2	18:B:1177:HOH:O	2.02	0.60	
2:B:104:GLY:O	2:B:109:GLY:HA3	2.01	0.60	
2:B:197:ASP:OD1	9:B:1003:MES:H32	2.01	0.60	
2:D:421:GLU:HB2	18:D:1101:HOH:O	2.02	0.59	
1:A:116:ASP:HB2	18:A:1138:HOH:O	2.03	0.58	
3:E:124:ARG:NH2	18:E:202:HOH:O	2.36	0.57	
4:F:19:ARG:HG3	18:F:1147:HOH:O	2.05	0.57	
4:F:292:ARG:HD2	18:F:1151:HOH:O	2.06	0.56	
1:A:262:TYR:HE1	18:A:1214:HOH:O	1.80	0.55	
2:D:115:SER:OG	18:D:1102:HOH:O	2.18	0.55	
2:B:306:ARG:HD3	18:B:1200:HOH:O	2.06	0.55	
1:C:88[B]:HIS:HD2	1:C:90[B]:GLU:H	1.56	0.54	
4:F:379:HIS:HD2	18:F:1149:HOH:O	1.92	0.53	
3:E:99:GLU:HB3	18:E:217:HOH:O	2.08	0.53	
2:B:392:LYS:HG3	18:B:1140:HOH:O	2.09	0.53	
4:F:296[B]:MET:SD	4:F:380:HIS:ND1	2.81	0.53	
2:B:137:HIS:HE1	2:B:168:SER:OG	1.92	0.53	
1:C:1:MET:HG3	1:C:2:ARG:N	2.25	0.52	
4:F:77:LEU:O	4:F:81:ILE:HG12	2.10	0.52	
2:D:134:GLN:HA	2:D:165:ASN:O	2.10	0.52	
1:C:417:GLU:HG2	18:C:1107:HOH:O	2.11	0.51	
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.51	
1:C:320:ARG:HG3	18:C:1176:HOH:O	2.11	0.50	
2:B:81:PHE:O	2:B:84:ILE:HG22	2.12	0.50	
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.94	0.50	
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.49	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:216:LYS:HE2	18:B:1205:HOH:O	2.14	0.48
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.94	0.48
4:F:307:LEU:HD22	4:F:308:HIS:CE1	2.49	0.48
4:F:172:PHE:O	4:F:176:GLN:HG2	2.14	0.48
2:B:261:PRO:O	2:B:264:HIS:HD2	1.97	0.47
2:D:261:PRO:O	2:D:264:HIS:HD2	1.96	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.47
1:C:139:HIS:HE1	1:C:168:GLU:OE1	1.98	0.47
4:F:292:ARG:NH2	18:F:1103:HOH:O	2.47	0.46
2:B:412[B]:GLU:OE2	2:B:412[B]:GLU:HA	2.16	0.46
1:C:434:GLU:O	1:C:437:VAL:HG22	2.16	0.46
1:A:139:HIS:HE1	1:A:168:GLU:OE1	1.98	0.46
2:D:387:ALA:O	2:D:391:ARG:NH1	2.49	0.45
2:B:138:SER:HB2	18:B:1144:HOH:O	2.15	0.45
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.97	0.45
1:C:90[B]:GLU:O	1:C:121:ARG:HD2	2.16	0.45
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.52	0.44
3:E:149:MET:HB2	18:E:223:HOH:O	1.95	0.44
1:A:333:ALA:O	1:A:336:LYS:HG2	2.18	0.44
1:C:69:ASP:O	1:C:94:THR:HA	2.18	0.44
1:C:406:HIS:HD2	18:C:1256:HOH:O	2.00	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
1:A:90:GLU:O	1:A:121:ARG:HD2	2.18	0.43
1:A:357:TYR:CE2	3:E:61:GLY:HA2	2.53	0.43
2:B:262:ARG:HD2	18:B:1228:HOH:O	2.18	0.43
2:D:104:GLY:O	2:D:109:GLY:HA3	2.19	0.43
2:B:30:ILE:CD1	2:B:47:ILE:HD11	2.48	0.43
2:B:262:ARG:CD	18:B:1228:HOH:O	2.67	0.43
4:F:85:PRO:O	4:F:88:SER:OG	2.31	0.43
4:F:296[B]:MET:CE	4:F:380:HIS:ND1	2.82	0.43
2:B:379:LYS:O	2:B:383:GLU:HG3	2.18	0.43
1:C:158:SER:OG	1:C:197:HIS:HD2	2.01	0.43
1:C:204:VAL:HG22	1:C:302[B]:MET:SD	2.59	0.43
1:A:205:ASP:OD2	18:A:1101:HOH:O	2.22	0.42
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.52	0.42
2:B:145:SER:HG	2:B:188:SER:HG	1.65	0.42
1:C:264:ARG:CD	13:C:1004:PGE:H62	2.49	0.42
1:C:264:ARG:HD3	13:C:1004:PGE:H62	2.00	0.42
1:C:100:ALA:HB2	18:C:1155:HOH:O	2.19	0.42
1:C:141:PHE:HE1	18:C:1268:HOH:O	2.03	0.42
2:D:137:HIS:HD2	2:D:144:GLY:O	2.03	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:158:SER:OG	1:A:197:HIS:HD2	2.02	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.19	0.42
2:B:243:PRO:HA	18:B:1107:HOH:O	2.18	0.42
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.50	0.41
4:F:268:ASN:O	4:F:272:MET:HG3	2.20	0.41
1:A:42:ILE:HA	18:A:1107:HOH:O	2.20	0.41
1:C:32:PRO:O	18:C:1101:HOH:O	2.22	0.41
1:C:244:PHE:CZ	1:C:358:GLN:HG2	2.55	0.41
2:B:65:LEU:N	2:B:65:LEU:HD12	2.36	0.41
1:C:270:ALA:HB3	1:C:302[B]:MET:HE2	2.03	0.41
2:D:72:THR:HA	2:D:75:SER:OG	2.20	0.41
1:C:262:TYR:CB	13:C:1004:PGE:H42	2.45	0.41
2:B:195:ASN:ND2	18:B:1108:HOH:O	2.43	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.40
3:E:50:MET:N	18:E:204:HOH:O	2.53	0.40
1:A:3:GLU:O	1:A:133:GLN:HB2	2.22	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	Perce	ntiles
1	А	437/451 (97%)	422 (97%)	15 (3%)	0	100	100
1	С	443/451~(98%)	430 (97%)	13 (3%)	0	100	100
2	В	431/445~(97%)	418 (97%)	12 (3%)	1 (0%)	47	75
2	D	425/445~(96%)	412 (97%)	12 (3%)	1 (0%)	47	75
3	Е	119/143~(83%)	119 (100%)	0	0	100	100
4	F	339/384~(88%)	325 (96%)	14 (4%)	0	100	100
All	All	2194/2319~(95%)	2126 (97%)	66 (3%)	2 (0%)	51	79



All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	279	GLN
2	В	71	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	370/379~(98%)	367~(99%)	3 (1%)	81 93
1	С	376/379~(99%)	365~(97%)	11 (3%)	42 72
2	В	372/381~(98%)	366~(98%)	6(2%)	62 84
2	D	369/381~(97%)	367~(100%)	2(0%)	88 96
3	Ε	110/127~(87%)	108~(98%)	2(2%)	59 82
4	F	313/342~(92%)	306~(98%)	7 (2%)	52 79
All	All	1910/1989~(96%)	1879~(98%)	31 (2%)	62 84

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

Mol	Chain	Res	Type
1	А	42	ILE
1	А	283	HIS
1	А	417	GLU
2	В	33	THR
2	В	115	SER
2	В	137	HIS
2	В	323	MET
2	В	333	VAL
2	В	339	SER
1	С	1	MET
1	С	42	ILE
1	С	71	GLU
1	С	265	ILE
1	С	302[A]	MET
1	С	302[B]	MET



Mol	Chain	Res	Type
1	С	339	ARG
1	С	340	SER
1	С	368	LEU
1	С	381	THR
1	С	417	GLU
2	D	26	ASP
2	D	339	SER
3	Ε	121	GLU
3	Е	170	LYS
4	F	12	SER
4	F	200	ASP
4	F	211	TYR
4	F	252	ASN
4	F	257	GLU
4	F	324	GLU
4	F	363	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	8	HIS
1	А	15	GLN
1	А	139	HIS
1	А	197	HIS
2	В	28	HIS
2	В	137	HIS
2	В	190	HIS
2	В	264	HIS
1	С	8	HIS
1	С	15	GLN
1	С	139	HIS
1	С	197	HIS
1	С	329	ASN
2	D	28	HIS
2	D	137	HIS
2	D	190	HIS
2	D	195	ASN
2	D	264	HIS
4	F	180	HIS
4	F	260	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 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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	Ros Link		Bo	Bond lengths			ond ang	les
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
8	GDP	В	1001	6	24,30,30	0.70	1 (4%)	30,47,47	0.58	0
10	O9B	В	1004	14	7,9,10	0.48	0	7,11,13	0.84	0
12	O9N	В	1006	15,11	16,16,16	0.24	0	18,20,20	0.74	1 (5%)
17	ACP	F	1001	6	27,33,33	1.42	5 (18%)	32,52,52	1.26	5 (15%)
5	GTP	А	1001	6	26,34,34	0.89	1 (3%)	32,54,54	0.57	0
5	GTP	С	1001	6	26,34,34	0.89	1 (3%)	32,54,54	0.58	0
11	O9K	В	1005	14,12	16,19,19	0.28	0	12,25,25	0.98	1 (8%)
13	PGE	С	1004	-	9,9,9	0.24	0	8,8,8	0.28	0
5	GTP	D	1001	6	26,34,34	0.80	0	32,54,54	0.70	1 (3%)
14	VAL	С	1005	10,11	4,6,7	0.60	0	6,7,9	0.91	0
15	P6S	С	1006	12	9,10,11	0.23	0	10,11,13	0.24	0
16	PEG	D	1003	-	6,6,6	0.17	0	5,5,5	0.08	0
9	MES	В	1003	-	12,12,12	0.70	0	14,16,16	0.51	0

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



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	В	1001	6	-	4/12/32/32	0/3/3/3
10	O9B	В	1004	14	-	0/1/13/15	0/1/1/1
12	O9N	В	1006	15,11	-	2/14/14/14	0/1/1/1
17	ACP	F	1001	6	-	5/15/38/38	0/3/3/3
5	GTP	А	1001	6	-	7/18/38/38	0/3/3/3
5	GTP	С	1001	6	-	8/18/38/38	0/3/3/3
11	O9K	В	1005	14,12	-	1/14/20/20	0/1/1/1
13	PGE	С	1004	-	-	<mark>5/7/7/7</mark>	-
5	GTP	D	1001	6	-	3/18/38/38	0/3/3/3
14	VAL	С	1005	10,11	-	1/5/6/8	-
15	P6S	С	1006	12	-	1/4/4/5	0/1/1/1
16	PEG	D	1003	-	-	0/4/4/4	-
9	MES	В	1003	-	-	4/6/14/14	0/1/1/1

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
17	F	1001	ACP	PG-O2G	3.28	1.62	1.54
17	F	1001	ACP	PG-O3G	3.10	1.62	1.54
5	С	1001	GTP	C5-C6	-2.66	1.42	1.47
17	F	1001	ACP	PB-O3A	2.60	1.61	1.58
5	А	1001	GTP	C5-C6	-2.60	1.42	1.47
17	F	1001	ACP	C5-C4	2.44	1.47	1.40
17	F	1001	ACP	PB-O2B	2.34	1.61	1.56
8	В	1001	GDP	C8-N7	-2.08	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
17	F	1001	ACP	N3-C2-N1	-3.60	123.05	128.68
5	D	1001	GTP	O5'-PA-O1A	2.38	118.36	109.07
17	F	1001	ACP	PB-O3A-PA	-2.28	125.33	132.56
17	F	1001	ACP	O2G-PG-O1G	-2.21	106.54	112.39
17	F	1001	ACP	C4-C5-N7	-2.20	107.11	109.40
11	В	1005	O9K	O5-C25-C23	-2.17	122.17	124.22
17	F	1001	ACP	C3'-C2'-C1'	2.06	104.08	100.98
12	В	1006	O9N	C34-C35-N6	2.03	114.85	110.32

There are no chirality outliers.



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Mol	Chain	Res	Type	Atoms
5	А	1001	GTP	C5'-O5'-PA-O1A
5	С	1001	GTP	C5'-O5'-PA-O1A
5	D	1001	GTP	C5'-O5'-PA-O1A
8	В	1001	GDP	C5'-O5'-PA-O1A
9	В	1003	MES	C8-C7-N4-C5
9	В	1003	MES	C7-C8-S-O2S
9	В	1003	MES	C7-C8-S-O3S
12	В	1006	O9N	N6-C35-C44-O8
14	С	1005	VAL	O-C-CA-CB
17	F	1001	ACP	PG-C3B-PB-O1B
17	F	1001	ACP	PG-C3B-PB-O2B
17	F	1001	ACP	PG-C3B-PB-O3A
17	F	1001	ACP	C5'-O5'-PA-O1A
13	С	1004	PGE	O2-C3-C4-O3
13	С	1004	PGE	O3-C5-C6-O4
12	В	1006	O9N	N6-C35-C44-O9
5	А	1001	GTP	C5'-O5'-PA-O3A
5	С	1001	GTP	C5'-O5'-PA-O3A
17	F	1001	ACP	C5'-O5'-PA-O3A
5	А	1001	GTP	C5'-O5'-PA-O2A
5	С	1001	GTP	C5'-O5'-PA-O2A
5	D	1001	GTP	C5'-O5'-PA-O2A
8	В	1001	GDP	C5'-O5'-PA-O2A
9	В	1003	MES	C7-C8-S-O1S
5	А	1001	GTP	PB-O3A-PA-O2A
5	С	1001	GTP	PB-O3A-PA-O2A
13	С	1004	PGE	C6-C5-O3-C4
8	В	1001	GDP	PB-O3A-PA-O2A
13	С	1004	PGE	C4-C3-O2-C2
11	В	1005	O9K	C4-C5-C6-C8
5	С	1001	GTP	PB-O3B-PG-O1G
5	А	1001	GTP	PB-O3B-PG-O3G
5	С	1001	GTP	PB-O3B-PG-O2G
5	С	1001	GTP	PB-O3B-PG-O3G
5	D	1001	GTP	C5'-O5'-PA-O3A
8	В	1001	GDP	C5'-O5'-PA-O3A
13	С	1004	PGE	C1-C2-O2-C3
5	A	1001	GTP	PB-O3A-PA-O1A
5	С	1001	GTP	PB-O3A-PA-O1A
5	A	1001	GTP	PB-O3B-PG-O1G
15	С	1006	P6S	C22-C21-O20-C19

All (41) torsion outliers are listed below:



There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	С	1004	PGE	4	0
9	В	1003	MES	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.



















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, 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	А	439/451~(97%)	0.06	2 (0%) 91 90	37, 57, 83, 98	0
1	С	440/451~(97%)	-0.02	0 100 100	32, 48, 65, 87	0
2	В	431/445~(96%)	-0.01	1 (0%) 95 95	33, 49, 79, 99	0
2	D	428/445~(96%)	0.27	10 (2%) 60 57	45, 69, 92, 123	0
3	Ε	123/143~(86%)	0.06	0 100 100	46, 66, 92, 107	0
4	F	346/384~(90%)	0.63	34 (9%) 7 5	45, 76, 143, 179	0
All	All	2207/2319~(95%)	0.16	47 (2%) 63 60	32, 59, 98, 179	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	1	MET	4.9
4	F	182	ILE	4.4
4	F	234	GLN	4.2
4	F	100	ILE	3.8
2	D	279	GLN	3.8
4	F	147	TRP	3.7
4	F	233	PHE	3.6
4	F	178	GLN	3.5
2	D	275	SER	3.4
4	F	166	ALA	3.4
1	А	439	SER	3.4
4	F	245	ILE	3.2
4	F	161	LEU	3.1
4	F	239	HIS	3.1
4	F	162	ILE	3.1
4	F	173	ILE	3.1
4	F	169	LEU	3.0
4	F	232	ASN	3.0
2	D	274	THR	2.9



Mol	Chain	Res	Type	RSRZ
4	F	148	ILE	2.8
4	F	242	ASN	2.8
4	F	249	TYR	2.8
2	D	1	MET	2.7
4	F	251	LYS	2.7
4	F	177	GLY	2.7
1	А	262	TYR	2.6
4	F	158	GLU	2.6
4	F	140	GLU	2.6
2	D	359	ARG	2.5
2	D	293	MET	2.5
4	F	236	LYS	2.4
4	F	225	SER	2.4
2	D	92	PHE	2.4
4	F	248	GLU	2.4
4	F	372	THR	2.3
4	F	149	ALA	2.3
2	D	48	ASN	2.3
4	F	179	VAL	2.2
4	F	320	MET	2.2
4	F	254	GLY	2.2
4	F	184	LYS	2.2
2	D	390	ARG	2.1
4	F	376	ILE	2.1
4	F	250	SER	2.1
2	D	74	ASP	2.1
4	F	238	CYS	2.0
4	F	240	LEU	2.0

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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,



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
16	PEG	D	1003	7/7	0.61	0.24	93,93,94,94	0
13	PGE	С	1004	10/10	0.87	0.29	70,70,71,71	0
12	O9N	В	1006	16/16	0.90	0.21	58, 59, 69, 69	0
15	P6S	С	1006	10/11	0.92	0.38	71,74,74,74	0
6	MG	В	1002	1/1	0.94	0.23	58,58,58,58	0
6	MG	F	1002	1/1	0.94	0.06	68,68,68,68	0
17	ACP	F	1001	31/31	0.94	0.21	91,94,105,105	0
6	MG	А	1002	1/1	0.96	0.12	45,45,45,45	0
11	O9K	В	1005	19/19	0.97	0.20	47,54,57,57	0
6	MG	D	1002	1/1	0.97	0.04	64,64,64,64	0
9	MES	В	1003	12/12	0.97	0.19	65,65,68,68	0
5	GTP	А	1001	32/32	0.98	0.16	44,46,48,48	0
5	GTP	D	1001	32/32	0.98	0.17	$65,\!68,\!75,\!75$	0
7	CA	А	1003	1/1	0.98	0.15	80,80,80,80	0
14	VAL	С	1005	7/8	0.98	0.21	44,45,46,47	0
7	CA	С	1003	1/1	0.98	0.16	64,64,64,64	0
6	MG	С	1002	1/1	0.98	0.08	42,42,42,42	0
10	O9B	В	1004	9/10	0.98	0.19	42,43,46,46	0
8	GDP	В	1001	28/28	0.99	0.19	38,39,40,41	0
5	GTP	С	1001	32/32	0.99	0.18	41,43,45,46	0

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.

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.













6.5 Other polymers (i)

There are no such residues in this entry.

