wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 05:59 AM JST

PDB ID	:	7EXC
Title	:	Crystal structure of T2R-TTL-1129A2 complex
Authors	:	Yang, J.H.; Yan, W.
Deposited on	:	2021-05-26
Resolution	:	2.39 Å(reported)

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

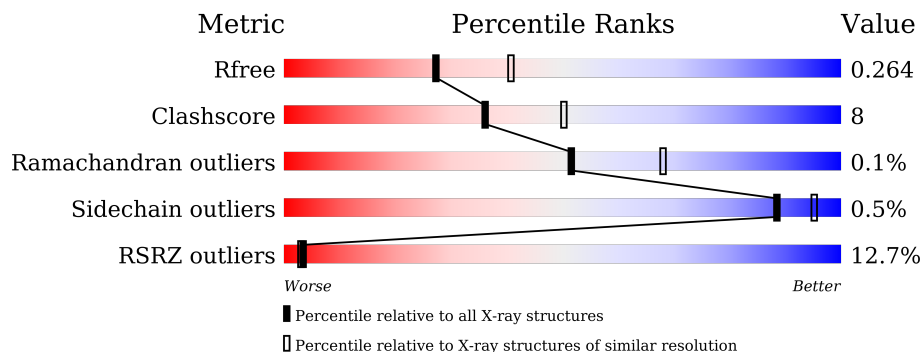|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.39 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.264
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		0.5%
RSRZ outliers		12.7%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	3% / 85% 11% ·
1	C	451	2% / 86% 11% ·
2	B	445	5% / 82% 13% ·
2	D	445	20% / 76% 18% · 5%
3	E	189	6% / 50% 12% ·· 36%
4	F	384	35% / 71% 16% · 12%

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 34877 atoms, of which 16830 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	A	437	Total 6733	C 2163	H 3317	N 581	O 650	S 22	0	0	0
1	C	440	Total 6772	C 2175	H 3335	N 584	O 656	S 22	0	0	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total 6560	C 2108	H 3204	N 576	O 647	S 25	0	0	0
2	D	421	Total 6457	C 2078	H 3153	N 562	O 638	S 26	0	0	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total 2013	C 617	H 1013	N 181	O 197	S 5	0	0	0

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	338	Total 5494	C 1785	H 2709	N 482	O 504	S 14	0	0	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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: $C_{10}H_{16}N_5O_{14}P_3$).
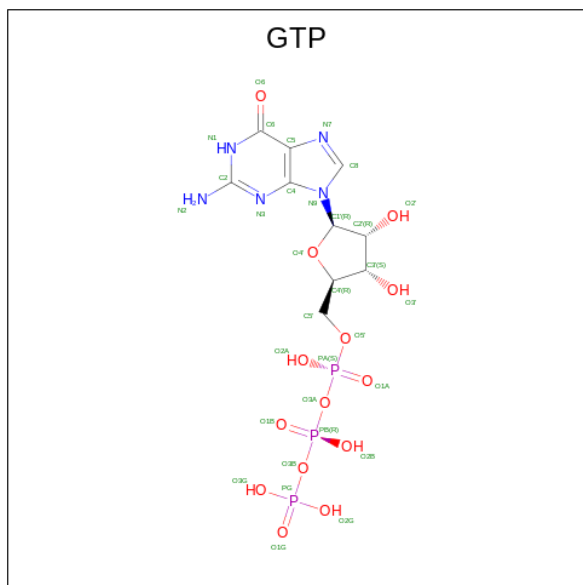
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	42	0
			42	10	10	5	14	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	1	0
			1	1		
6	B	1	Total	Mg	1	0
			1	1		
6	C	1	Total	Mg	1	0
			1	1		
6	D	1	Total	Mg	1	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total Ca 1 1		1	0
7	C	1	Total Ca 1 1		1	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
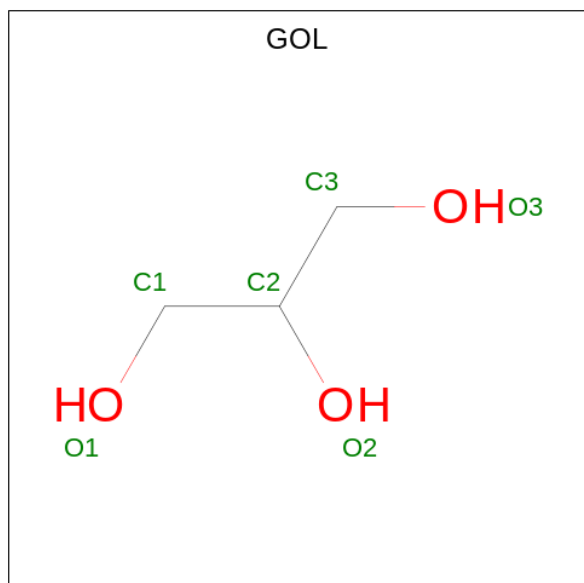
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total C H O 14 3 8 3				14	0

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

MES
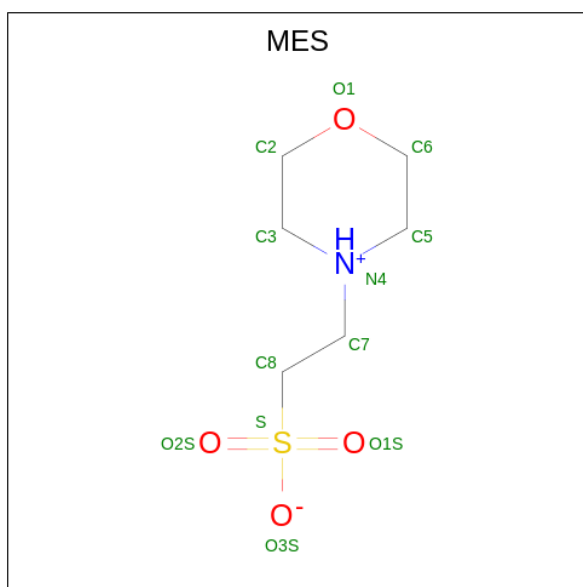
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	25	0
			25	6	13	1	4	1		

- Molecule 10 is N-[[3-(1,3-benzodioxol-5-yloxy)phenyl]methyl]-9H-pyrido[3,4-b]indol-3-amine (three-letter code: JEL) (formula: $C_{25}H_{19}N_3O_3$) (labeled as "Ligand of Interest" by depositor).
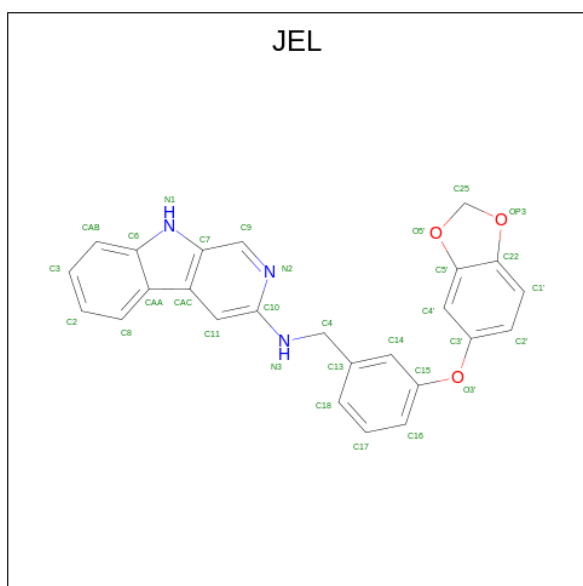
JEL

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			50	25	19	3	3		
10	D	1	Total	C	H	N	O	0	0
			50	25	19	3	3		

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
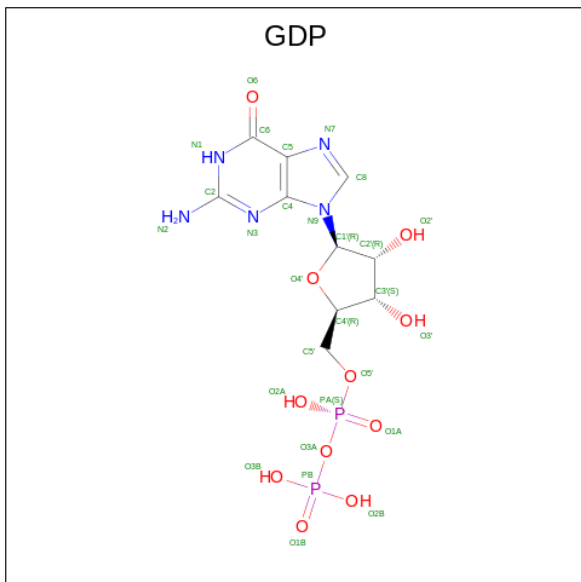
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
11	B	1	38	10	10	5	11	2	38	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
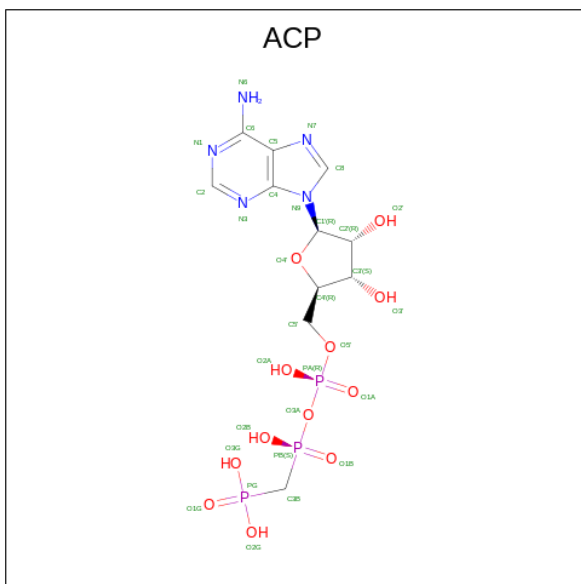
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
12	F	1	31	11	5	12	3	31	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	125	Total O 125 125		0	0
13	B	99	Total O 99 99		0	0
13	C	202	Total O 202 202		0	0
13	D	29	Total O 29 29		0	0
13	E	19	Total O 19 19		0	0
13	F	34	Total O 34 34		0	0

# 3 Residue-property plots ⓘ

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
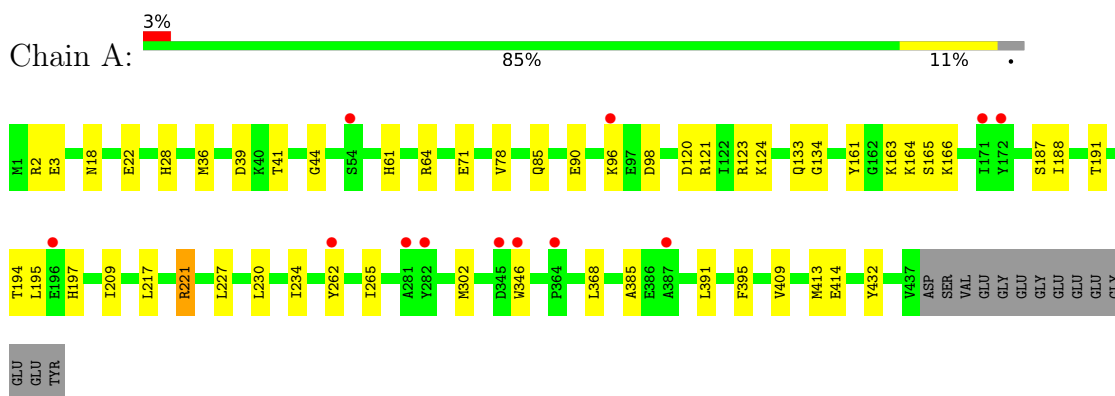
Chain A:

• Molecule 1: Tubulin alpha-1B chain

Chain C:
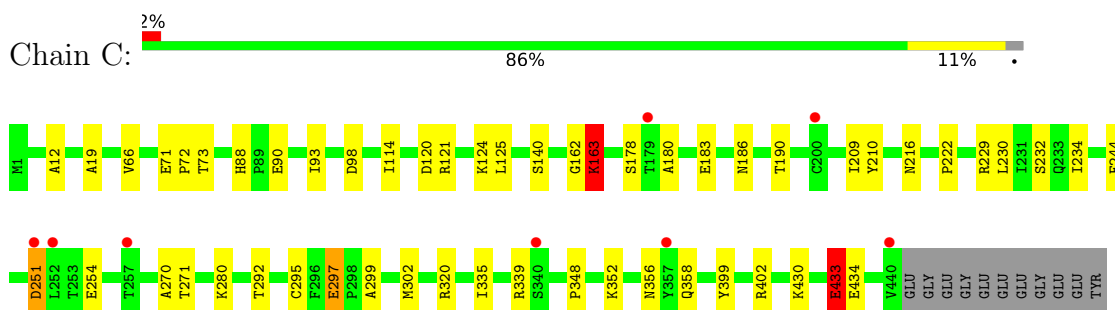
• Molecule 2: Tubulin beta chain
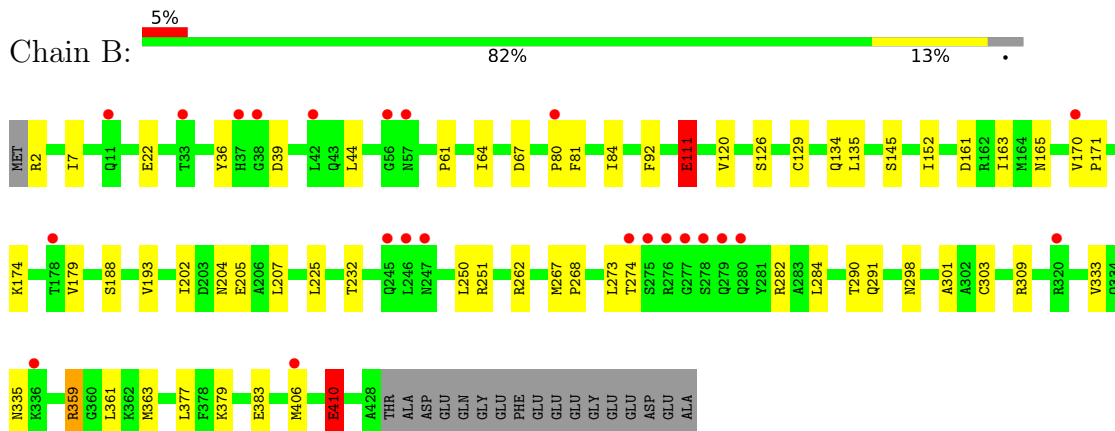
Chain B:

• Molecule 2: Tubulin beta chain

Chain D:
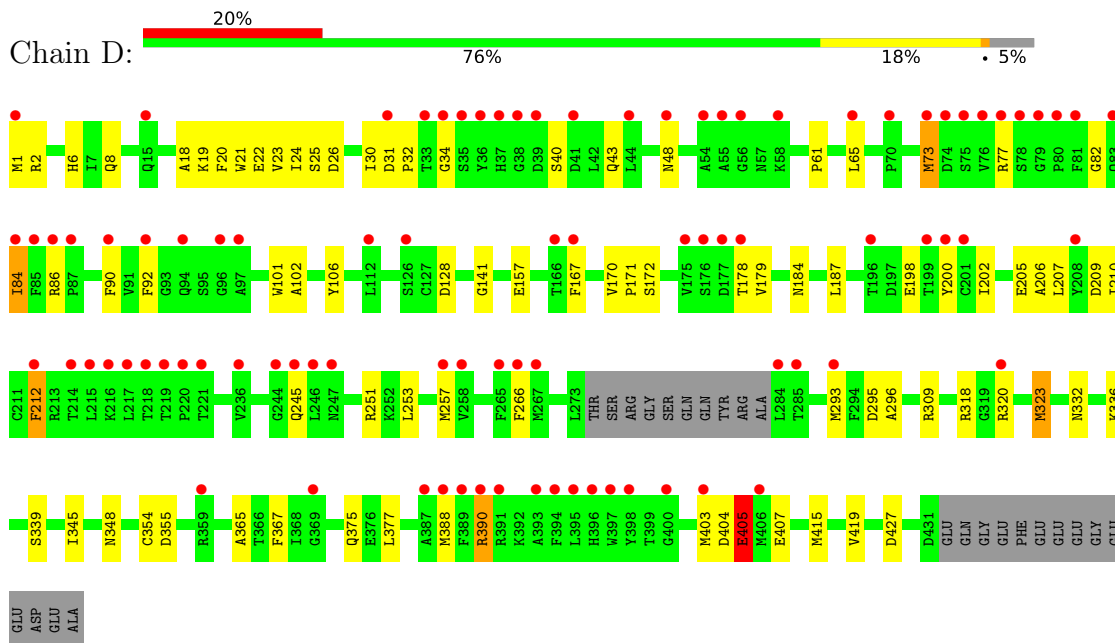
• Molecule 3: Stathmin-4

Chain E:
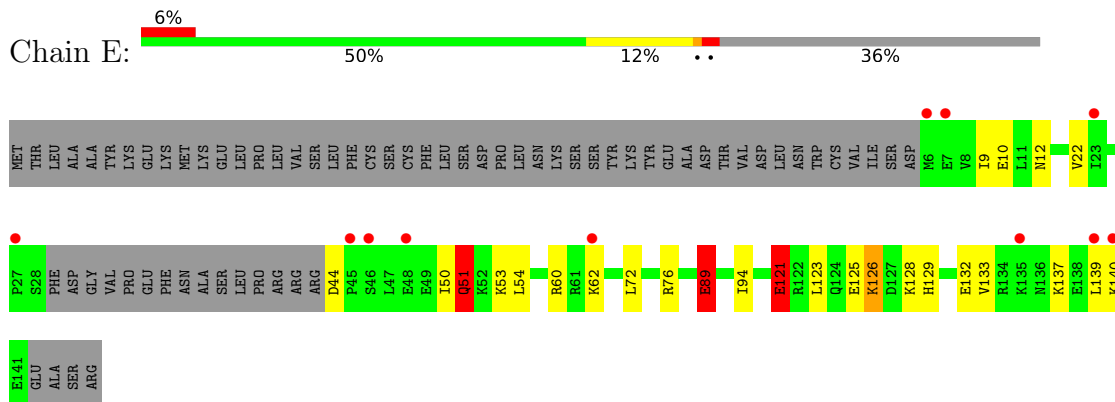
• Molecule 4: Tubulin tyrosine ligase

Chain F:

SER LYS N252 Y253 G254 R255 Y256 E257 E258 E261 M262 F263 F264 L271 A274 L275 I283 M296 E299 K305 M320 Q340 K341 L342 Y343 L346 C347 Q348 D352 L361 A362 ASP THR GLY GLN LYS THR SER GLN PRO T372 S373 H379 H380 H381 H382 H383
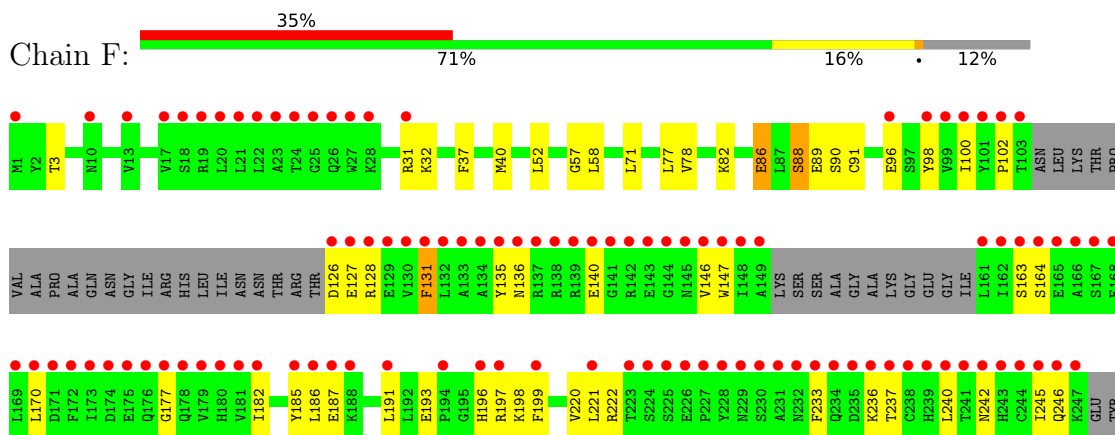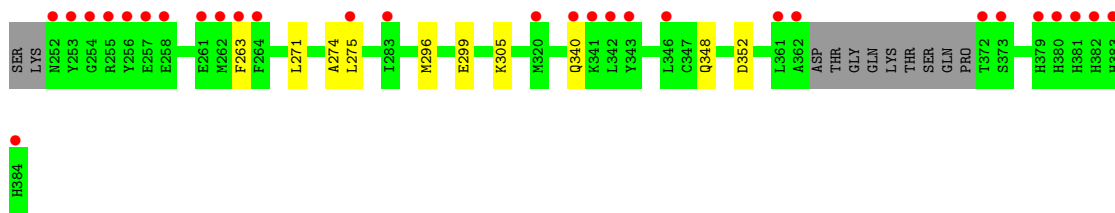
H384

4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.25Å 157.38Å 181.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.39 49.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.39) 96.9 (49.85-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.218 , 0.264 0.218 , 0.264	Depositor DCC
R_{free} test set	2318 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.4	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	0.92	EDS
Total number of atoms	34877	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: GOL, JEL, GTP, CA, MES, GDP, ACP, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.30	0/3494	0.55	3/4743 (0.1%)
1	C	0.66	7/3515 (0.2%)	0.78	14/4772 (0.3%)
2	B	0.36	2/3431 (0.1%)	0.64	9/4649 (0.2%)
2	D	0.43	4/3377 (0.1%)	0.71	11/4576 (0.2%)
3	E	0.66	3/1008 (0.3%)	0.98	12/1337 (0.9%)
4	F	0.39	2/2851 (0.1%)	0.69	7/3851 (0.2%)
All	All	0.47	18/17676 (0.1%)	0.70	56/23928 (0.2%)

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	2
2	B	0	3
2	D	0	3
3	E	0	3
4	F	0	1
All	All	0	12

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	LYS	CE-NZ	20.27	1.99	1.49
1	C	433	GLU	CB-CG	19.05	1.88	1.52
1	C	433	GLU	CG-CD	11.87	1.69	1.51
2	D	323	MET	CG-SD	9.83	2.06	1.81
1	C	163	LYS	CB-CG	9.41	1.77	1.52

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	GLU	OE1-CD-OE2	-18.69	100.87	123.30
1	C	433	GLU	OE1-CD-OE2	-17.29	102.56	123.30
4	F	86	GLU	OE1-CD-OE2	-15.97	104.14	123.30
1	C	433	GLU	CG-CD-OE2	-15.70	86.91	118.30
1	C	251	ASP	CB-CG-OD1	15.40	132.16	118.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	111	GLU	Sidechain
2	B	359	ARG	Sidechain
2	B	410	GLU	Sidechain
1	C	251	ASP	Sidechain
1	C	433	GLU	Sidechain

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	3416	3317	3330	44	0
1	C	3437	3335	3348	48	0
2	B	3356	3204	3234	42	0
2	D	3304	3153	3185	74	0
3	E	1000	1013	1018	25	0
4	F	2785	2709	2737	47	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	12	13	12	0	0
10	B	31	19	0	0	0

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	31	19	0	2	0
11	B	28	10	12	0	0
12	F	31	0	14	0	0
13	A	125	0	0	3	0
13	B	99	0	0	3	0
13	C	202	0	0	6	0
13	D	29	0	0	6	0
13	E	19	0	0	2	0
13	F	34	0	0	0	0
All	All	18047	16830	16934	274	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.

The worst 5 of 274 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)
2:D:323:MET:CG	2:D:323:MET:CB	1.78	1.59
1:C:163:LYS:CG	1:C:163:LYS:CB	1.78	1.57
3:E:126:LYS:CE	3:E:126:LYS:NZ	1.69	1.56
1:C:433:GLU:CB	1:C:433:GLU:CG	1.88	1.50
2:D:323:MET:CE	2:D:323:MET:SD	2.03	1.47

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	427 (98%)	8 (2%)	0	100	100
1	C	438/451 (97%)	425 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	425/445 (96%)	415 (98%)	10 (2%)	0	100	100
2	D	417/445 (94%)	400 (96%)	17 (4%)	0	100	100
3	E	117/189 (62%)	112 (96%)	5 (4%)	0	100	100
4	F	328/384 (85%)	314 (96%)	12 (4%)	2 (1%)	25	36
All	All	2160/2365 (91%)	2093 (97%)	65 (3%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU
4	F	88	SER

5.3.2　Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	367 (100%)	1 (0%)	92	97
1	C	371/379 (98%)	370 (100%)	1 (0%)	92	97
2	B	367/381 (96%)	365 (100%)	2 (0%)	88	95
2	D	362/381 (95%)	360 (99%)	2 (1%)	86	94
3	E	109/171 (64%)	108 (99%)	1 (1%)	78	90
4	F	305/342 (89%)	303 (99%)	2 (1%)	84	92
All	All	1882/2033 (93%)	1873 (100%)	9 (0%)	88	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	131	PHE
4	F	222	ARG
1	C	163	LYS
2	D	86	ARG
2	D	212	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	293	ASN
2	D	6	HIS
2	D	8	GLN
2	D	37	HIS
3	E	51	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 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	#$|Z| > 2$
10	JEL	D	502	-	35,36,36	1.42	2 (5%)	49,51,51	1.38	8 (16%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.61	7 (21%)
11	GDP	B	504	6	24,30,30	0.94	2 (8%)	30,47,47	1.31	4 (13%)
5	GTP	D	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.50	7 (21%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.61	7 (21%)
8	GOL	A	504	-	5,5,5	0.77	0	5,5,5	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
12	ACP	F	401	-	27,33,33	1.35	5 (18%)	32,52,52	1.42	4 (12%)
9	MES	B	502	-	12,12,12	2.22	1 (8%)	14,16,16	1.77	5 (35%)
10	JEL	B	503	-	35,36,36	1.39	2 (5%)	49,51,51	1.30	7 (14%)

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
10	JEL	D	502	-	-	0/9/15/15	0/6/6/6
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
11	GDP	B	504	6	-	2/12/32/32	0/3/3/3
5	GTP	D	501	6	-	4/18/38/38	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
12	ACP	F	401	-	-	4/15/38/38	0/3/3/3
9	MES	B	502	-	-	3/6/14/14	0/1/1/1
10	JEL	B	503	-	-	0/9/15/15	0/6/6/6

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.45	1.66	1.77
10	D	502	JEL	C10-N3	5.69	1.44	1.36
10	B	503	JEL	C10-N3	5.42	1.44	1.36
5	C	501	GTP	C5-C6	-4.06	1.39	1.47
5	D	501	GTP	C5-C6	-3.96	1.39	1.47

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	502	JEL	C9-N2-C10	4.56	122.43	117.81
10	B	503	JEL	C9-N2-C10	4.21	122.07	117.81
12	F	401	ACP	PB-O3A-PA	-3.87	120.28	132.56
5	A	501	GTP	PB-O3B-PG	-3.78	119.85	132.83
5	C	501	GTP	PB-O3B-PG	-3.74	120.00	132.83

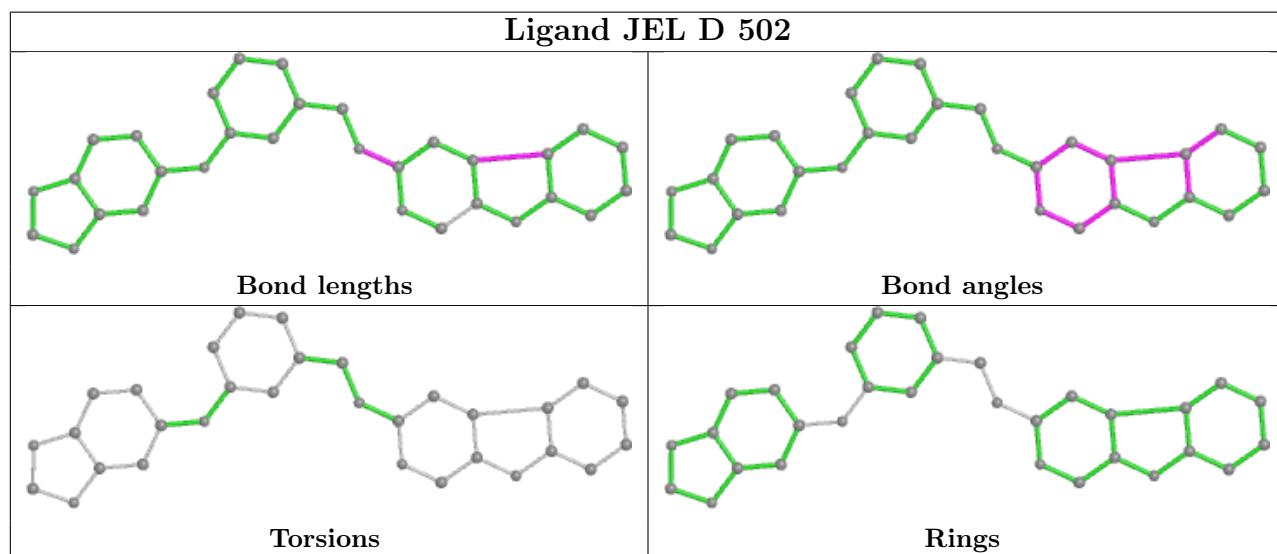There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	504	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	502	JEL	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 JEL D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 504

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ACP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand JEL B 503

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	437/451 (96%)	0.37	12 (2%)	54	52	25, 41, 64, 79	0
1	C	440/451 (97%)	0.27	8 (1%)	68	66	21, 34, 57, 79	0
2	B	427/445 (95%)	0.48	23 (5%)	25	24	20, 40, 71, 118	0
2	D	421/445 (94%)	1.23	90 (21%)	0	0	33, 67, 97, 132	0
3	E	121/189 (64%)	0.79	11 (9%)	9	8	29, 62, 88, 109	0
4	F	338/384 (88%)	1.92	133 (39%)	0	0	36, 72, 125, 141	0
All	All	2184/2365 (92%)	0.80	277 (12%)	3	3	20, 49, 95, 141	0

The worst 5 of 277 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	12.9
4	F	169	LEU	12.3
4	F	233	PHE	12.1
4	F	173	ILE	12.0
4	F	130	VAL	11.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.