



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:02 AM UTC

PDB ID : 6GX7 / pdb_00006gx7
Title : Tubulin-CopN-alphaRep complex
Authors : Gigant, B.; Campanacci, V.
Deposited on : 2018-06-26
Resolution : 3.19 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

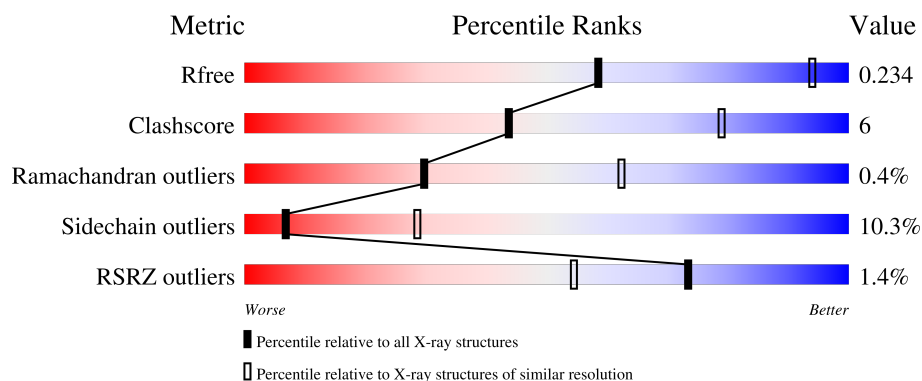
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 $\leq 5\%$. 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	% 70% 21% • 5%
1	C	451	% 74% 18% •• 5%
2	B	445	% 68% 23% • 5%
2	D	445	% 67% 26% • 5%
3	E	201	% 74% 15% • 8%

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Mol	Chain	Length	Quality of chain
3	F	201	% 77% 12% • 8%
4	G	336	2% 70% 14% • 15%
4	H	336	3% 67% 17% • 14%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20365 atoms, of which 24 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3291	2079	561	630	21			
1	C	428	Total	C	N	O	S	0	0	0
			3288	2077	561	630	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	conflict	UNP D0VWZ0
A	340	SER	THR	conflict	UNP D0VWZ0
C	232	SER	GLY	conflict	UNP D0VWZ0
C	340	SER	THR	conflict	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3296	2075	559	636	26			
2	D	423	Total	C	N	O	S	0	0	0
			3298	2076	559	637	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	CYS	SER	conflict	UNP D0VWY9
B	318	ILE	VAL	conflict	UNP D0VWY9
D	203	CYS	SER	conflict	UNP D0VWY9
D	318	ILE	VAL	conflict	UNP D0VWY9

- Molecule 3 is a protein called iiiA5 ALPHAREP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	184	Total	C	N	O	S	0	0	0
			1334	835	239	258	2			
3	F	184	Total	C	N	O	S	0	0	0
			1338	837	239	260	2			

- Molecule 4 is a protein called Low calcium response E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	285	Total	C	N	O	S	0	0	0
			2132	1326	358	441	7			
4	H	290	Total	C	N	O	S	0	0	0
			2146	1335	362	442	7			

There are 42 discrepancies between the modelled and reference sequences:

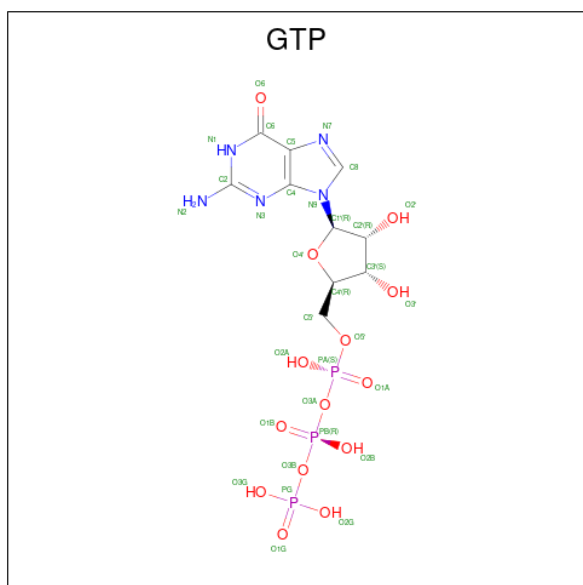
Chain	Residue	Modelled	Actual	Comment	Reference
G	64	MET	-	initiating methionine	UNP Q9Z8L4
G	65	GLY	-	expression tag	UNP Q9Z8L4
G	66	SER	-	expression tag	UNP Q9Z8L4
G	67	SER	-	expression tag	UNP Q9Z8L4
G	68	HIS	-	expression tag	UNP Q9Z8L4
G	69	HIS	-	expression tag	UNP Q9Z8L4
G	70	HIS	-	expression tag	UNP Q9Z8L4
G	71	HIS	-	expression tag	UNP Q9Z8L4
G	72	HIS	-	expression tag	UNP Q9Z8L4
G	73	HIS	-	expression tag	UNP Q9Z8L4
G	74	SER	-	expression tag	UNP Q9Z8L4
G	75	SER	-	expression tag	UNP Q9Z8L4
G	76	GLY	-	expression tag	UNP Q9Z8L4
G	77	LEU	-	expression tag	UNP Q9Z8L4
G	78	VAL	-	expression tag	UNP Q9Z8L4
G	79	PRO	-	expression tag	UNP Q9Z8L4
G	80	ARG	-	expression tag	UNP Q9Z8L4
G	81	GLY	-	expression tag	UNP Q9Z8L4
G	82	SER	-	expression tag	UNP Q9Z8L4
G	83	HIS	-	expression tag	UNP Q9Z8L4
G	84	MET	-	expression tag	UNP Q9Z8L4
H	64	MET	-	initiating methionine	UNP Q9Z8L4
H	65	GLY	-	expression tag	UNP Q9Z8L4
H	66	SER	-	expression tag	UNP Q9Z8L4
H	67	SER	-	expression tag	UNP Q9Z8L4
H	68	HIS	-	expression tag	UNP Q9Z8L4
H	69	HIS	-	expression tag	UNP Q9Z8L4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	70	HIS	-	expression tag	UNP Q9Z8L4
H	71	HIS	-	expression tag	UNP Q9Z8L4
H	72	HIS	-	expression tag	UNP Q9Z8L4
H	73	HIS	-	expression tag	UNP Q9Z8L4
H	74	SER	-	expression tag	UNP Q9Z8L4
H	75	SER	-	expression tag	UNP Q9Z8L4
H	76	GLY	-	expression tag	UNP Q9Z8L4
H	77	LEU	-	expression tag	UNP Q9Z8L4
H	78	VAL	-	expression tag	UNP Q9Z8L4
H	79	PRO	-	expression tag	UNP Q9Z8L4
H	80	ARG	-	expression tag	UNP Q9Z8L4
H	81	GLY	-	expression tag	UNP Q9Z8L4
H	82	SER	-	expression tag	UNP Q9Z8L4
H	83	HIS	-	expression tag	UNP Q9Z8L4
H	84	MET	-	expression tag	UNP Q9Z8L4

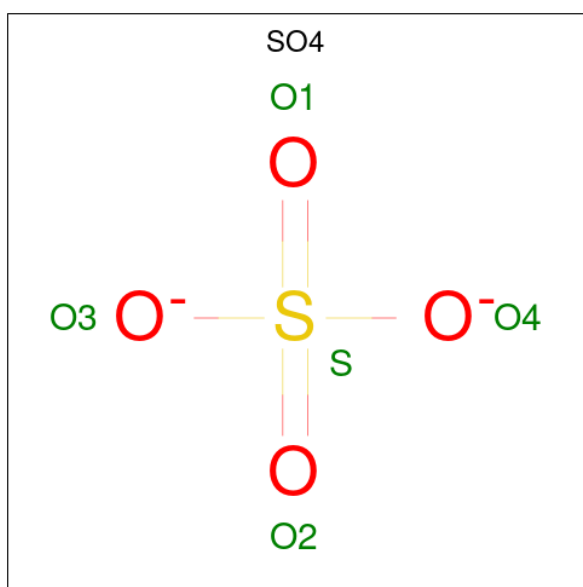
- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

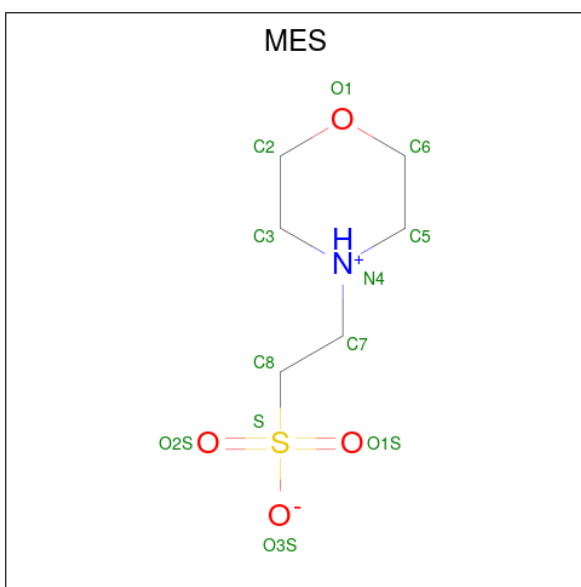
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



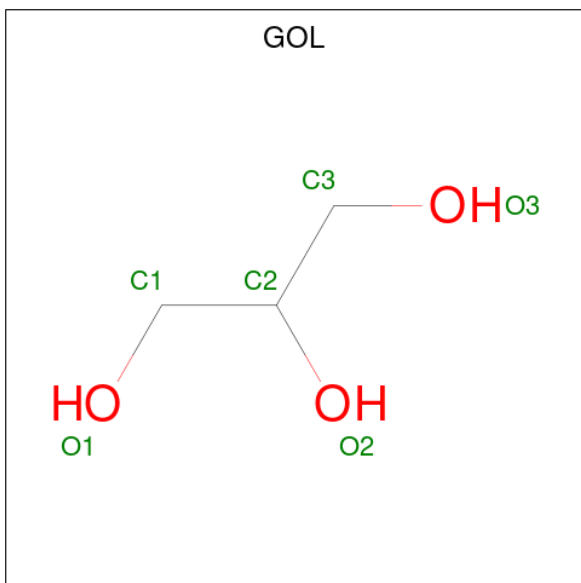
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



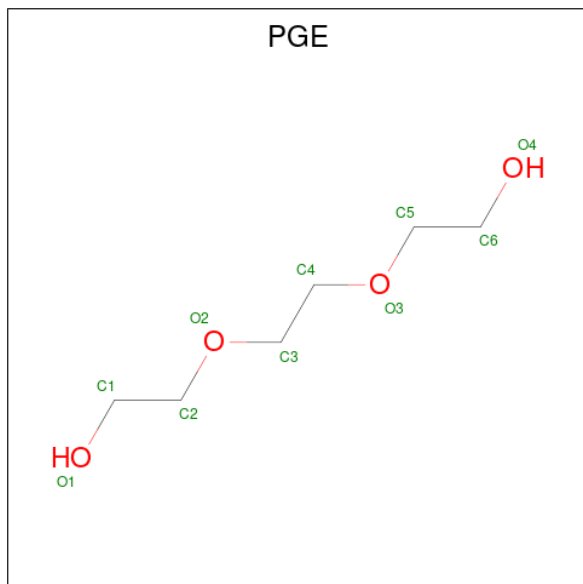
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			14	3	8	3		
9	D	1	Total	C	H	O	0	0
			14	3	8	3		
9	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).

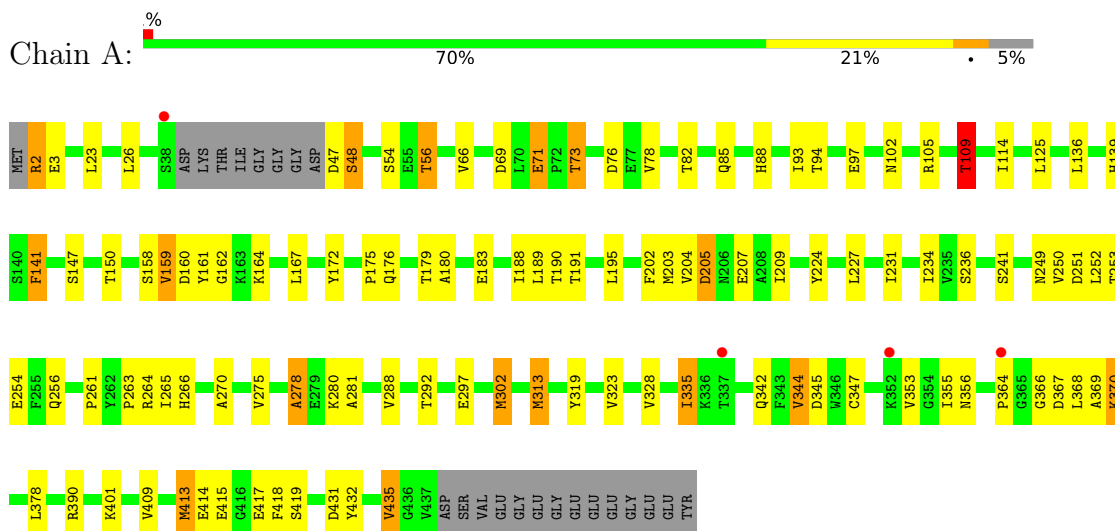


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			10	6	4		

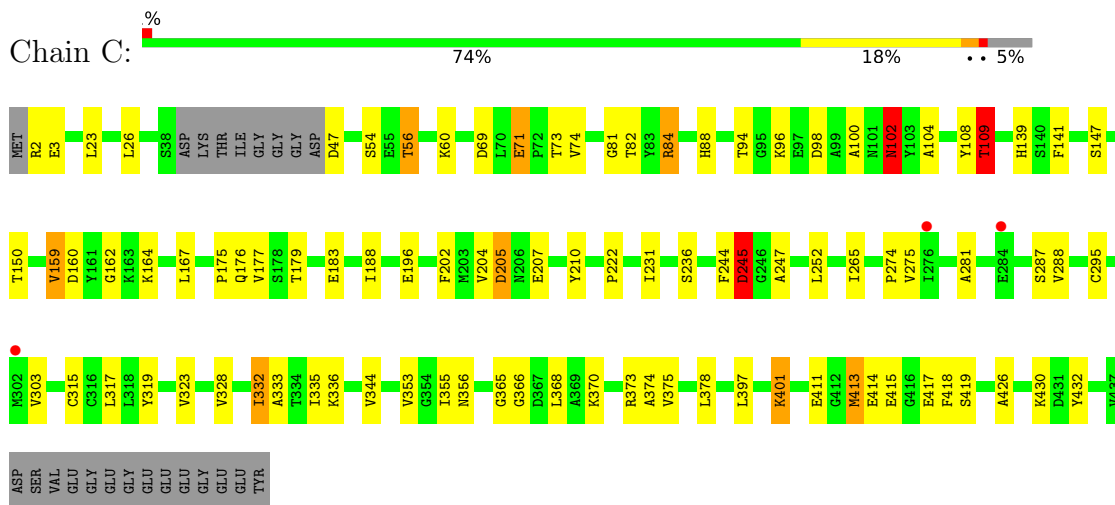
3 Residue-property plots

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 chain

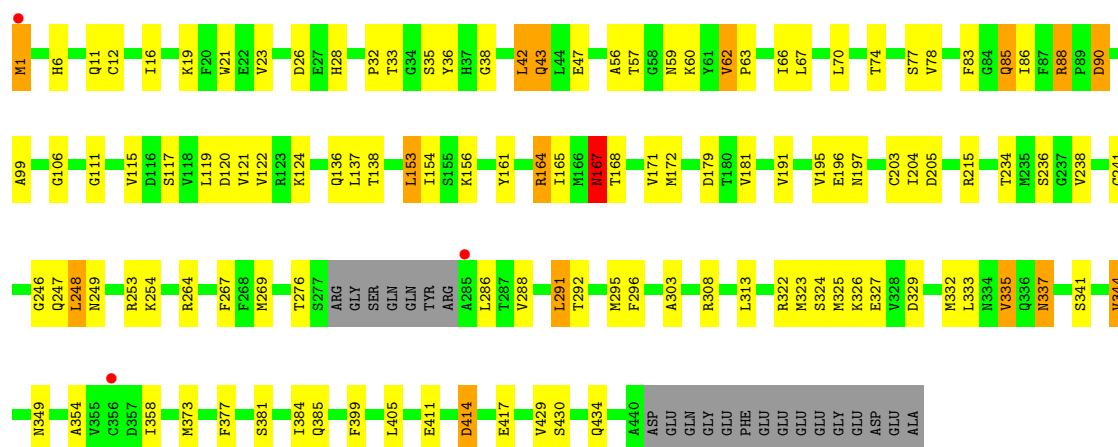


• Molecule 1: Tubulin alpha chain

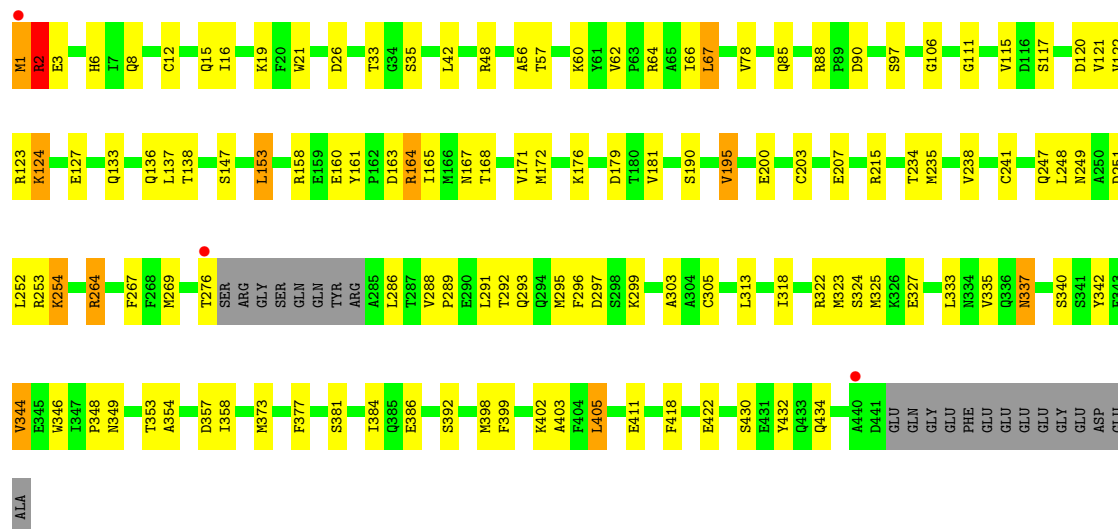


• Molecule 2: Tubulin beta chain

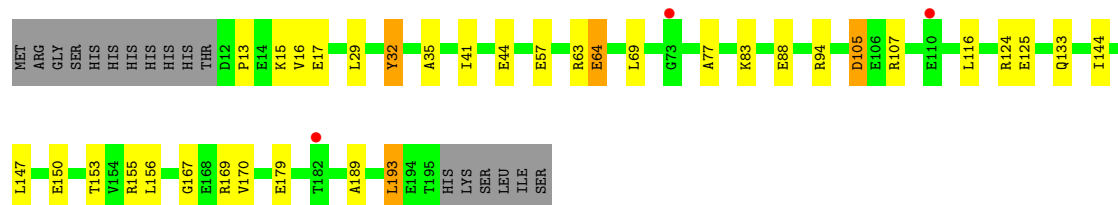
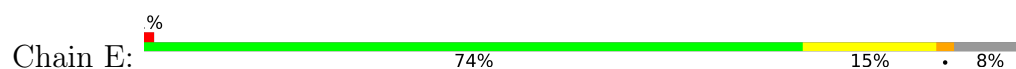




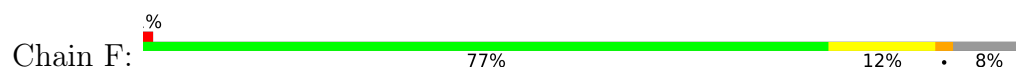
• Molecule 2: Tubulin beta chain

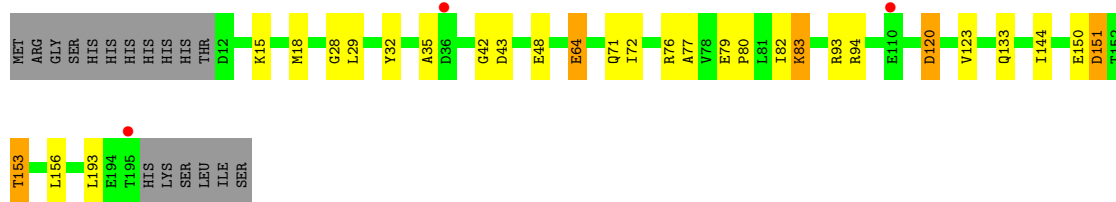


• Molecule 3: iiiA5 ALPHAREP

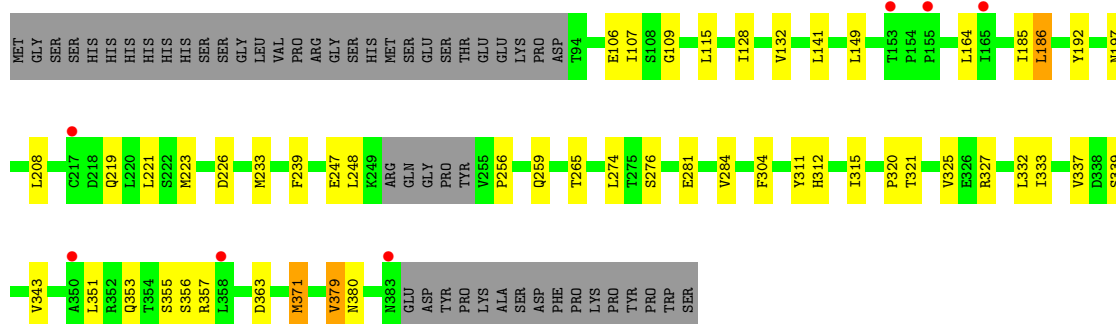


• Molecule 3: iiiA5 ALPHAREP

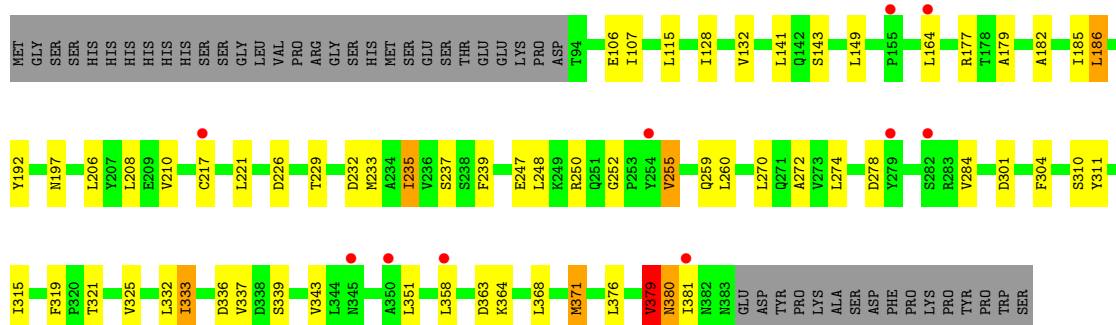




● Molecule 4: Low calcium response E



● Molecule 4: Low calcium response E



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	148.06Å 95.85Å 158.06Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	49.03 – 3.19 49.03 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.03-3.19) 99.2 (49.03-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.173 , 0.210 0.196 , 0.234	Depositor DCC
R_{free} test set	3606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 115.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20365	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MES, PGE, GOL, SO4, MG, 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	0.89	2/3364 (0.1%)	1.46	27/4575 (0.6%)
1	C	0.89	2/3361 (0.1%)	1.47	27/4572 (0.6%)
2	B	0.93	1/3369 (0.0%)	1.41	21/4567 (0.5%)
2	D	0.95	2/3371 (0.1%)	1.44	19/4570 (0.4%)
3	E	0.95	0/1348	1.47	8/1830 (0.4%)
3	F	0.93	1/1352 (0.1%)	1.45	8/1835 (0.4%)
4	G	0.70	0/2158	1.41	6/2937 (0.2%)
4	H	0.71	0/2174	1.41	3/2962 (0.1%)
All	All	0.88	8/20497 (0.0%)	1.44	119/27848 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	MET	C-N	5.60	1.41	1.33
2	B	288	VAL	CA-C	5.53	1.57	1.52
1	A	109	THR	CA-C	5.24	1.59	1.52
3	F	79	GLU	CA-C	5.23	1.59	1.52
1	C	413	MET	SD-CE	-5.19	1.66	1.79
2	D	97	SER	CA-C	5.15	1.55	1.52
1	C	109	THR	CA-C	5.09	1.59	1.52
1	A	413	MET	SD-CE	-5.09	1.66	1.79

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ASP	CA-CB-CG	7.85	120.45	112.60
2	D	249	ASN	CA-C-N	7.49	131.07	120.28
2	D	249	ASN	C-N-CA	7.49	131.07	120.28
1	C	205	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	102	ASN	CA-CB-CG	6.93	119.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	337	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	160	ASP	CA-CB-CG	6.88	119.48	112.60
2	D	163	ASP	CA-CB-CG	6.82	119.42	112.60
2	B	57	THR	CB-CA-C	6.75	120.85	109.84
4	H	278	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	175	PRO	CA-C-N	6.54	129.37	120.54
1	A	175	PRO	C-N-CA	6.54	129.37	120.54
1	C	88	HIS	N-CA-C	-6.50	101.88	109.93
1	C	159	VAL	CA-C-N	6.50	128.98	120.28
1	C	159	VAL	C-N-CA	6.50	128.98	120.28
1	C	175	PRO	CA-C-N	6.40	128.85	120.28
1	C	175	PRO	C-N-CA	6.40	128.85	120.28
1	A	88	HIS	N-CA-C	-6.36	102.05	109.93
1	C	245	ASP	CA-C-N	6.28	125.94	119.92
1	C	245	ASP	C-N-CA	6.28	125.94	119.92
2	B	399	PHE	CA-C-N	6.20	128.50	120.44
2	B	399	PHE	C-N-CA	6.20	128.50	120.44
2	D	432	TYR	CA-C-N	6.19	128.58	120.28
2	D	432	TYR	C-N-CA	6.19	128.58	120.28
1	C	419	SER	CA-C-N	6.18	128.56	120.28
1	C	419	SER	C-N-CA	6.18	128.56	120.28
3	E	105	ASP	CA-C-N	6.18	129.40	120.38
3	E	105	ASP	C-N-CA	6.18	129.40	120.38
2	D	288	VAL	N-CA-CB	6.14	115.24	110.45
1	A	159	VAL	CA-C-N	6.02	128.34	120.28
1	A	159	VAL	C-N-CA	6.02	128.34	120.28
2	B	179	ASP	CA-CB-CG	5.97	118.57	112.60
2	B	248	LEU	CA-C-N	5.96	130.84	122.08
2	B	248	LEU	C-N-CA	5.96	130.84	122.08
2	B	85	GLN	CA-C-N	5.96	128.93	120.53
2	B	85	GLN	C-N-CA	5.96	128.93	120.53
4	H	379	VAL	CA-C-N	5.95	130.12	120.60
4	H	379	VAL	C-N-CA	5.95	130.12	120.60
2	D	1	MET	CA-C-N	5.91	132.84	121.54
2	D	1	MET	C-N-CA	5.91	132.84	121.54
4	G	380	ASN	CA-CB-CG	5.86	118.46	112.60
1	C	247	ALA	N-CA-C	-5.83	104.92	112.68
1	A	390	ARG	CA-C-N	5.80	127.99	120.44
1	A	390	ARG	C-N-CA	5.80	127.99	120.44
2	B	246	GLY	N-CA-C	5.78	118.94	110.38
3	E	13	PRO	CA-C-N	5.78	128.30	120.44
3	E	13	PRO	C-N-CA	5.78	128.30	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ASP	CA-C-N	5.76	132.55	121.54
1	A	47	ASP	C-N-CA	5.76	132.55	121.54
3	F	120	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	281	ALA	CA-C-N	5.74	132.03	121.70
1	A	281	ALA	C-N-CA	5.74	132.03	121.70
1	A	141	PHE	CA-CB-CG	5.71	119.51	113.80
4	G	247	GLU	CA-C-N	5.70	131.91	122.62
4	G	247	GLU	C-N-CA	5.70	131.91	122.62
4	G	109	GLY	CA-C-N	5.67	128.14	120.65
4	G	109	GLY	C-N-CA	5.67	128.14	120.65
2	D	90	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	3	GLU	N-CA-C	5.63	118.00	110.35
1	C	281	ALA	CA-C-N	5.62	131.82	121.70
1	C	281	ALA	C-N-CA	5.62	131.82	121.70
1	C	160	ASP	CA-CB-CG	5.59	118.19	112.60
3	F	93	ARG	CA-C-N	5.59	128.04	120.38
3	F	93	ARG	C-N-CA	5.59	128.04	120.38
1	C	108	TYR	CA-C-N	5.56	132.16	121.54
1	C	108	TYR	C-N-CA	5.56	132.16	121.54
1	A	78	VAL	CA-C-N	5.54	128.26	120.28
1	A	78	VAL	C-N-CA	5.54	128.26	120.28
1	C	47	ASP	CA-CB-CG	5.54	118.14	112.60
2	B	70	LEU	N-CA-C	-5.54	106.02	112.89
1	C	102	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	344	VAL	CA-C-N	5.52	128.44	120.38
1	C	344	VAL	C-N-CA	5.52	128.44	120.38
2	B	414	ASP	CA-C-N	5.47	127.87	120.38
2	B	414	ASP	C-N-CA	5.47	127.87	120.38
4	G	226	ASP	CA-CB-CG	5.41	118.01	112.60
3	F	43	ASP	CA-CB-CG	5.41	118.00	112.60
1	A	344	VAL	CA-C-N	5.39	128.26	120.38
1	A	344	VAL	C-N-CA	5.39	128.26	120.38
1	A	76	ASP	CA-CB-CG	5.31	117.91	112.60
2	B	288	VAL	N-CA-CB	5.27	114.56	110.45
1	C	183	GLU	CB-CG-CD	5.27	121.56	112.60
2	D	418	PHE	CA-C-N	5.26	127.32	120.28
2	D	418	PHE	C-N-CA	5.26	127.32	120.28
1	C	333	ALA	CA-C-N	5.25	127.26	120.44
1	C	333	ALA	C-N-CA	5.25	127.26	120.44
1	C	365	GLY	N-CA-C	-5.24	100.76	113.18
2	D	57	THR	CB-CA-C	5.24	118.61	109.65
2	B	167	ASN	CA-CB-CG	5.23	117.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	191	VAL	CA-C-N	5.23	127.29	120.28
2	B	191	VAL	C-N-CA	5.23	127.29	120.28
2	D	127	GLU	CB-CG-CD	5.22	121.48	112.60
1	A	280	LYS	N-CA-C	5.21	116.64	111.07
1	A	313	MET	N-CA-C	-5.18	107.61	114.04
2	B	337	ASN	CA-CB-CG	5.17	117.77	112.60
2	B	249	ASN	CA-C-N	5.15	127.43	120.38
2	B	249	ASN	C-N-CA	5.15	127.43	120.38
1	A	345	ASP	CA-CB-CG	5.14	117.74	112.60
2	B	90	ASP	CA-CB-CG	5.13	117.73	112.60
2	D	386	GLU	CA-C-N	5.13	127.10	120.44
2	D	386	GLU	C-N-CA	5.13	127.10	120.44
3	F	151	ASP	CA-C-N	5.11	127.08	120.44
3	F	151	ASP	C-N-CA	5.11	127.08	120.44
2	D	357	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	264	ARG	CA-C-N	5.09	131.13	121.97
1	A	264	ARG	C-N-CA	5.09	131.13	121.97
2	B	196	GLU	CB-CG-CD	5.08	121.24	112.60
1	C	177	VAL	CA-C-N	5.07	129.31	121.26
1	C	177	VAL	C-N-CA	5.07	129.31	121.26
3	F	28	GLY	CA-C-N	5.06	127.06	120.28
3	F	28	GLY	C-N-CA	5.06	127.06	120.28
2	D	251	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	278	ALA	CA-C-N	5.05	127.05	120.28
1	A	278	ALA	C-N-CA	5.05	127.05	120.28
2	D	249	ASN	CA-CB-CG	5.04	117.64	112.60
3	E	167	GLY	CA-C-N	5.01	126.99	120.28
3	E	167	GLY	C-N-CA	5.01	126.99	120.28
3	E	169	ARG	CA-C-N	5.00	126.87	120.56
3	E	169	ARG	C-N-CA	5.00	126.87	120.56

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	3291	0	3149	49	0
1	C	3288	0	3142	37	0
2	B	3296	0	3168	48	0
2	D	3298	0	3167	52	0
3	E	1334	0	1294	9	0
3	F	1338	0	1298	6	0
4	G	2132	0	2055	20	0
4	H	2146	0	2053	28	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	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	5	0	0	0	0
7	C	5	0	0	0	0
8	B	24	0	26	2	0
8	D	24	0	26	4	0
9	B	6	8	8	0	0
9	D	12	16	16	0	0
10	D	10	0	14	0	0
All	All	20341	24	19464	242	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 6.

All (242) 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:66:ILE:HD13	2:D:122:VAL:HG22	1.65	0.78
2:D:195:VAL:HG22	2:D:264:ARG:HG2	1.64	0.77
1:A:288:VAL:HG22	1:A:323:VAL:HG12	1.67	0.76
2:D:267:PHE:O	2:D:384:ILE:HD13	1.88	0.73
2:B:195:VAL:HG22	2:B:264:ARG:HG2	1.70	0.73
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.56	0.70
2:D:67:LEU:HD22	2:D:78:VAL:HG11	1.70	0.70
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.74	0.70
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.75	0.69
3:E:189:ALA:O	3:E:193:LEU:HB2	1.96	0.66
2:B:248:LEU:HD23	2:B:354:ALA:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ILE:HG23	1:C:432:TYR:CE2	2.31	0.65
2:B:267:PHE:O	2:B:384:ILE:HD13	1.96	0.65
2:B:67:LEU:HD22	2:B:78:VAL:HG11	1.78	0.65
2:B:161:TYR:HB3	2:B:164:ARG:HG3	1.79	0.63
1:A:319:TYR:HB3	1:A:323:VAL:HG21	1.81	0.62
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.80	0.62
1:A:344:VAL:HG11	1:A:435:VAL:HG12	1.82	0.61
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.36	0.61
4:G:276:SER:OG	4:G:312:HIS:HE1	1.84	0.60
3:E:16:VAL:HG22	3:E:41:ILE:HG21	1.82	0.60
4:H:337:VAL:HG23	4:H:379:VAL:HG12	1.83	0.60
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.82	0.59
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.85	0.59
3:F:42:GLY:HA2	3:F:72:ILE:HG12	1.84	0.59
2:B:313:LEU:HD23	2:B:344:VAL:HG21	1.84	0.59
2:D:8:GLN:NE2	2:D:67:LEU:HD23	2.17	0.58
2:D:296:PHE:HB3	8:D:504:MES:H51	1.86	0.58
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.84	0.58
1:A:431:ASP:O	1:A:435:VAL:HG23	2.04	0.58
1:C:167:LEU:HD21	1:C:202:PHE:HE1	1.68	0.58
1:C:413:MET:HE3	1:C:417:GLU:HB3	1.84	0.58
1:C:288:VAL:HG22	1:C:323:VAL:HG12	1.87	0.57
1:A:203:MET:O	1:A:302:MET:HE1	2.06	0.56
1:A:167:LEU:HD21	1:A:202:PHE:CE1	2.41	0.56
4:H:333:ILE:HG12	4:H:339:SER:HB3	1.88	0.55
1:A:323:VAL:HG23	1:A:355:ILE:HG23	1.88	0.55
4:G:256:PRO:HB2	4:G:259:GLN:HB3	1.88	0.55
2:B:106:GLY:O	2:B:111:GLY:HA3	2.07	0.55
1:A:26:LEU:HD21	1:A:364:PRO:HD2	1.88	0.54
1:A:167:LEU:HD21	1:A:202:PHE:HE1	1.72	0.54
4:G:284:VAL:HG21	4:G:304:PHE:HA	1.89	0.54
2:D:165:ILE:HD11	2:D:253:ARG:HG3	1.90	0.54
1:C:167:LEU:HD21	1:C:202:PHE:CE1	2.44	0.53
2:D:234:THR:O	2:D:238:VAL:HG13	2.07	0.53
4:H:128:ILE:HG21	4:H:164:LEU:HD23	1.90	0.53
1:A:204:VAL:HG11	1:A:231:ILE:HG12	1.90	0.53
2:D:158:ARG:HG3	8:D:503:MES:H62	1.90	0.53
2:D:323:MET:HE2	2:D:373:MET:HG2	1.90	0.53
2:D:115:VAL:HG23	2:D:153:LEU:HG	1.91	0.52
1:C:109:THR:HG21	1:C:411:GLU:OE2	2.08	0.52
1:C:176:GLN:NE2	1:C:207:GLU:HG3	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.91	0.52
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.91	0.52
4:H:221:LEU:HB2	4:H:270:LEU:HD13	1.90	0.52
4:H:252:GLY:H	4:H:255:VAL:HG12	1.73	0.52
2:B:28:HIS:HA	2:B:43:GLN:HG2	1.90	0.52
1:C:287:SER:HA	1:C:373:ARG:HE	1.73	0.52
2:B:234:THR:O	2:B:238:VAL:HG13	2.10	0.52
4:H:311:TYR:OH	4:H:351:LEU:HA	2.09	0.52
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.91	0.52
2:D:292:THR:HA	2:D:295:MET:HE2	1.93	0.51
1:C:81:GLY:O	1:C:84:ARG:HG2	2.10	0.51
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.91	0.51
2:B:42:LEU:HD13	2:B:358:ILE:HD11	1.92	0.51
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.91	0.51
2:B:324:SER:HB3	2:B:327:GLU:HB2	1.92	0.51
4:G:128:ILE:HG21	4:G:164:LEU:HD23	1.92	0.51
2:D:324:SER:HB3	2:D:327:GLU:HB2	1.93	0.51
4:G:192:TYR:CG	4:G:239:PHE:HB2	2.46	0.51
4:G:221:LEU:HD12	4:G:233:MET:HE1	1.92	0.51
2:B:292:THR:HA	2:B:295:MET:HE2	1.93	0.51
1:A:270:ALA:H	1:A:302:MET:HE2	1.75	0.51
1:C:204:VAL:HG11	1:C:231:ILE:HG12	1.92	0.51
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.92	0.50
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.93	0.50
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.76	0.50
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.93	0.50
3:E:29:LEU:HD23	3:E:32:TYR:HE2	1.77	0.50
1:C:100:ALA:HA	2:D:254:LYS:HE2	1.93	0.50
2:B:165:ILE:HD11	2:B:253:ARG:HG3	1.92	0.50
3:E:105:ASP:OD1	3:E:107:ARG:HD3	2.12	0.50
1:C:179:THR:HG21	2:D:247:GLN:HE21	1.77	0.50
4:G:337:VAL:HG23	4:G:379:VAL:HG12	1.94	0.49
2:B:66:ILE:HG12	2:B:121:VAL:HG12	1.94	0.49
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.93	0.49
4:G:311:TYR:OH	4:G:351:LEU:HA	2.13	0.49
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.52	0.49
2:B:62:VAL:HG11	2:B:88:ARG:HG3	1.95	0.49
2:D:381:SER:O	2:D:384:ILE:HD12	2.13	0.49
1:A:209:ILE:HD11	1:A:302:MET:HB3	1.95	0.48
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.48
2:D:136:GLN:HA	2:D:167:ASN:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LEU:HD12	2:D:348:PRO:HG3	1.95	0.48
2:D:167:ASN:OD1	2:D:200:GLU:HG3	2.12	0.48
4:G:141:LEU:HD23	4:G:186:LEU:HD21	1.95	0.48
1:A:409:VAL:HA	1:A:413:MET:O	2.12	0.48
4:H:107:ILE:HG23	4:H:141:LEU:HD22	1.95	0.48
4:G:321:THR:O	4:G:325:VAL:HG23	2.13	0.48
4:H:182:ALA:HB2	4:H:208:LEU:HD11	1.96	0.48
2:B:323:MET:HE2	2:B:373:MET:HG2	1.94	0.48
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.95	0.48
3:F:35:ALA:HB3	3:F:64:GLU:HB3	1.95	0.48
1:A:203:MET:O	1:A:302:MET:CE	2.62	0.48
1:A:224:TYR:HA	1:A:227:LEU:HD12	1.95	0.48
1:C:274:PRO:HD3	1:C:374:ALA:HA	1.96	0.47
2:D:297:ASP:OD1	2:D:299:LYS:HD2	2.14	0.47
4:H:232:ASP:HA	4:H:235:ILE:HD12	1.96	0.47
1:A:189:LEU:CD2	1:A:413:MET:HE1	2.45	0.47
2:B:154:ILE:HG22	2:B:197:ASN:HB3	1.96	0.47
2:D:176:LYS:HD2	2:D:207:GLU:HG3	1.97	0.47
2:D:297:ASP:HA	8:D:504:MES:O2S	2.15	0.47
4:H:368:LEU:HD23	4:H:371:MET:HE3	1.97	0.47
2:D:172:MET:HE3	2:D:203:CYS:SG	2.55	0.47
1:C:210:TYR:CE2	1:C:222:PRO:HD2	2.49	0.47
4:G:219:GLN:O	4:G:223:MET:HB2	2.14	0.47
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.47
1:C:275:VAL:HG23	1:C:368:LEU:HD21	1.96	0.47
1:A:249:ASN:HA	1:A:254:GLU:HB3	1.97	0.47
1:A:93:ILE:HG22	1:A:114:ILE:HD11	1.97	0.47
1:A:261:PRO:HG2	1:A:313:MET:HB3	1.97	0.47
1:C:323:VAL:HG23	1:C:355:ILE:HG23	1.96	0.47
4:H:376:LEU:O	4:H:380:ASN:HB2	2.15	0.47
3:E:35:ALA:HB3	3:E:64:GLU:HB3	1.97	0.46
2:B:308:ARG:HD2	8:B:504:MES:H82	1.98	0.46
2:D:106:GLY:O	2:D:111:GLY:HA3	2.15	0.46
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.97	0.46
1:A:71:GLU:CG	1:A:73:THR:HG23	2.45	0.46
1:A:66:VAL:HG23	1:A:125:LEU:HD22	1.98	0.46
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.97	0.46
4:G:107:ILE:HG23	4:G:141:LEU:HD22	1.96	0.46
1:A:56:THR:HG21	3:E:63:ARG:HH12	1.79	0.46
2:D:318:ILE:HG13	2:D:354:ALA:HB3	1.96	0.46
1:C:69:ASP:O	1:C:94:THR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD13	1:A:302:MET:HG2	1.98	0.46
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.98	0.45
2:D:399:PHE:HE1	2:D:405:LEU:HD21	1.82	0.45
3:F:82:ILE:HG22	3:F:83:LYS:HE2	1.96	0.45
2:B:16:ILE:HD11	2:B:138:THR:HB	1.99	0.45
2:B:66:ILE:HD13	2:B:122:VAL:HG22	1.99	0.45
1:C:202:PHE:CE2	1:C:378:LEU:HD22	2.51	0.45
2:D:313:LEU:HD23	2:D:344:VAL:HG21	1.98	0.45
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.52	0.45
4:G:333:ILE:HG12	4:G:339:SER:HB3	1.98	0.45
4:H:284:VAL:HG21	4:H:304:PHE:HA	1.97	0.45
1:A:105:ARG:HA	1:A:109:THR:HB	1.99	0.45
1:C:317:LEU:HD13	1:C:332:ILE:HD11	1.98	0.45
2:D:42:LEU:HB2	2:D:358:ILE:HD11	1.99	0.45
4:G:149:LEU:HB3	4:G:164:LEU:HD22	1.98	0.45
4:G:320:PRO:HG2	4:G:371:MET:HE3	1.99	0.45
2:D:2:ARG:H	2:D:133:GLN:HG3	1.82	0.45
2:D:138:THR:HG21	2:D:235:MET:HE1	1.99	0.44
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.52	0.44
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.32	0.44
4:G:115:LEU:HD21	4:G:132:VAL:HG22	1.98	0.44
2:D:289:PRO:C	2:D:293:GLN:HE21	2.26	0.44
2:B:172:MET:HB2	2:B:205:ASP:HA	1.99	0.44
2:B:269:MET:HE3	2:B:381:SER:HB3	1.98	0.44
2:D:295:MET:CG	2:D:377:PHE:HB2	2.48	0.44
4:H:336:ASP:HB3	4:H:339:SER:HB2	2.00	0.44
2:B:269:MET:CE	2:B:381:SER:HB3	2.48	0.44
2:D:2:ARG:HB3	2:D:3:GLU:H	1.65	0.44
4:H:143:SER:HB2	4:H:179:ALA:HB1	2.00	0.44
4:H:332:LEU:HD23	4:H:343:VAL:HG11	1.99	0.44
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.36	0.44
3:E:147:LEU:O	3:E:155:ARG:HD3	2.18	0.44
4:G:355:SER:OG	4:G:357:ARG:HG2	2.18	0.44
4:H:221:LEU:HD12	4:H:233:MET:HE1	2.00	0.44
2:B:332:MET:O	2:B:335:VAL:HG12	2.18	0.44
2:D:16:ILE:HD11	2:D:138:THR:HB	2.00	0.44
4:H:149:LEU:HB3	4:H:164:LEU:HD22	2.00	0.44
4:H:192:TYR:CG	4:H:239:PHE:HB2	2.53	0.43
1:C:167:LEU:HD13	1:C:252:LEU:HD22	1.99	0.43
2:D:305:CYS:SG	2:D:384:ILE:HA	2.58	0.43
2:B:67:LEU:CD2	2:B:78:VAL:HG11	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG22	1:C:159:VAL:HG22	2.00	0.43
4:H:106:GLU:HB3	4:H:141:LEU:HD11	1.99	0.43
1:A:179:THR:HG21	2:B:247:GLN:HG3	2.00	0.43
4:H:141:LEU:HD23	4:H:186:LEU:HD21	2.01	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.43
1:A:370:LYS:H	1:A:370:LYS:HG3	1.71	0.43
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.00	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.43
3:F:120:ASP:OD1	3:F:123:VAL:HG23	2.18	0.43
1:A:263:PRO:O	1:A:266:HIS:HD2	2.02	0.43
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.99	0.43
2:D:120:ASP:O	2:D:124:LYS:HD2	2.19	0.43
4:G:281:GLU:HA	4:G:304:PHE:CG	2.54	0.43
1:A:147:SER:HB2	1:A:190:THR:HB	2.01	0.42
1:A:370:LYS:HE2	1:A:370:LYS:O	2.19	0.42
1:A:180:ALA:O	1:A:183:GLU:HG3	2.19	0.42
1:C:401:LYS:HD2	2:D:346:TRP:CG	2.53	0.42
1:A:176:GLN:NE2	1:A:207:GLU:HG3	2.34	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.19	0.42
1:C:56:THR:HG23	1:C:60:LYS:HB2	2.00	0.42
2:D:1:MET:HA	2:D:133:GLN:HG2	2.01	0.42
3:F:151:ASP:OD2	3:F:153:THR:HG23	2.19	0.42
2:B:23:VAL:HG11	2:B:236:SER:HB2	2.01	0.42
1:A:69:ASP:O	1:A:94:THR:HA	2.20	0.42
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.54	0.42
4:G:332:LEU:HD23	4:G:343:VAL:HG11	2.00	0.42
2:D:398:MET:HG2	2:D:403:ALA:HB3	2.01	0.42
4:H:206:LEU:O	4:H:210:VAL:HG23	2.20	0.42
1:A:415:GLU:O	1:A:418:PHE:HB2	2.20	0.42
4:H:177:ARG:HH12	4:H:255:VAL:HG23	1.84	0.42
1:C:415:GLU:O	1:C:418:PHE:HB2	2.20	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.01	0.42
4:H:247:GLU:CB	4:H:255:VAL:HG21	2.50	0.42
1:A:85:GLN:NE2	1:A:85:GLN:HA	2.35	0.41
2:B:1:MET:HE1	2:B:253:ARG:HE	1.84	0.41
2:B:32:PRO:HB3	2:B:83:PHE:HA	2.02	0.41
2:B:381:SER:O	2:B:384:ILE:HD12	2.21	0.41
1:C:244:PHE:HB2	1:C:356:ASN:HD21	1.85	0.41
2:B:115:VAL:HG23	2:B:153:LEU:HG	2.02	0.41
2:B:172:MET:HE3	2:B:203:CYS:SG	2.61	0.41
1:C:319:TYR:CB	1:C:323:VAL:HG21	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD23	1:A:167:LEU:HB3	2.01	0.41
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.56	0.41
4:G:106:GLU:HB3	4:G:141:LEU:HD11	2.01	0.41
4:H:233:MET:HB3	4:H:233:MET:HE2	1.79	0.41
4:H:255:VAL:HG22	4:H:260:LEU:HD11	2.02	0.41
3:E:116:LEU:O	3:E:124:ARG:HD2	2.20	0.41
4:H:115:LEU:HD21	4:H:132:VAL:HG22	2.03	0.41
2:B:373:MET:HE2	2:B:373:MET:HB3	1.98	0.41
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.96	0.41
1:C:426:ALA:O	1:C:430:LYS:HG3	2.21	0.41
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.60	0.41
2:B:296:PHE:HB3	8:B:504:MES:H52	2.02	0.41
1:C:102:ASN:HD21	1:C:104:ALA:HB3	1.86	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.21	0.41
3:E:69:LEU:HD22	3:E:77:ALA:HB2	2.03	0.41
4:H:321:THR:O	4:H:325:VAL:HG23	2.21	0.41
1:A:292:THR:HG22	1:A:335:ILE:HD13	2.02	0.40
2:D:342:TYR:CD2	8:D:504:MES:H22	2.56	0.40
4:H:272:ALA:HB3	4:H:358:LEU:HD21	2.02	0.40
1:C:141:PHE:O	1:C:147:SER:HB3	2.20	0.40
1:C:295:CYS:SG	1:C:375:VAL:HG13	2.61	0.40
2:B:63:PRO:HD3	2:B:86:ILE:HG12	2.03	0.40
3:F:77:ALA:C	3:F:80:PRO:HD2	2.47	0.40
1:A:2:ARG:HG2	1:A:3:GLU:N	2.37	0.40
2:D:248:LEU:HD23	2:D:354:ALA:HB2	2.04	0.40
2:D:398:MET:HE3	2:D:398:MET:HB2	1.95	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	424/451 (94%)	402 (95%)	18 (4%)	4 (1%)	14	47
1	C	424/451 (94%)	403 (95%)	17 (4%)	4 (1%)	14	47
2	B	419/445 (94%)	403 (96%)	15 (4%)	1 (0%)	43	73
2	D	419/445 (94%)	402 (96%)	16 (4%)	1 (0%)	43	73
3	E	182/201 (90%)	180 (99%)	2 (1%)	0	100	100
3	F	182/201 (90%)	180 (99%)	2 (1%)	0	100	100
4	G	281/336 (84%)	276 (98%)	4 (1%)	1 (0%)	30	62
4	H	288/336 (86%)	282 (98%)	6 (2%)	0	100	100
All	All	2619/2866 (91%)	2528 (96%)	80 (3%)	11 (0%)	30	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	GLY
2	D	2	ARG
1	A	48	SER
1	A	109	THR
2	B	99	ALA
1	C	245	ASP
1	C	366	GLY
1	C	109	THR
1	A	162	GLY
1	C	162	GLY
4	G	379	VAL

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	348/379 (92%)	314 (90%)	34 (10%)	7	31
1	C	347/379 (92%)	323 (93%)	24 (7%)	14	45
2	B	359/383 (94%)	315 (88%)	44 (12%)	4	22
2	D	359/383 (94%)	315 (88%)	44 (12%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	120/157 (76%)	102 (85%)	18 (15%)	3	15
3	F	121/157 (77%)	105 (87%)	16 (13%)	4	19
4	G	230/291 (79%)	217 (94%)	13 (6%)	18	51
4	H	228/291 (78%)	204 (90%)	24 (10%)	6	28
All	All	2112/2420 (87%)	1895 (90%)	217 (10%)	7	28

All (217) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	23	LEU
1	A	48	SER
1	A	54	SER
1	A	56	THR
1	A	71	GLU
1	A	73	THR
1	A	82	THR
1	A	97	GLU
1	A	158	SER
1	A	188	ILE
1	A	191	THR
1	A	195	LEU
1	A	236	SER
1	A	241	SER
1	A	250	VAL
1	A	251	ASP
1	A	252	LEU
1	A	253	THR
1	A	256	GLN
1	A	275	VAL
1	A	297	GLU
1	A	302	MET
1	A	335	ILE
1	A	342	GLN
1	A	347	CYS
1	A	356	ASN
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	401	LYS
1	A	414	GLU

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Mol	Chain	Res	Type
1	A	419	SER
1	A	435	VAL
2	B	1	MET
2	B	11	GLN
2	B	19	LYS
2	B	26	ASP
2	B	33	THR
2	B	35	SER
2	B	42	LEU
2	B	43	GLN
2	B	47	GLU
2	B	59	ASN
2	B	62	VAL
2	B	74	THR
2	B	77	SER
2	B	85	GLN
2	B	88	ARG
2	B	117	SER
2	B	120	ASP
2	B	124	LYS
2	B	153	LEU
2	B	164	ARG
2	B	167	ASN
2	B	181	VAL
2	B	215	ARG
2	B	241	CYS
2	B	254	LYS
2	B	276	THR
2	B	286	LEU
2	B	291	LEU
2	B	322	ARG
2	B	325	MET
2	B	326	LYS
2	B	329	ASP
2	B	333	LEU
2	B	335	VAL
2	B	337	ASN
2	B	341	SER
2	B	344	VAL
2	B	349	ASN
2	B	405	LEU
2	B	411	GLU

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Mol	Chain	Res	Type
2	B	414	ASP
2	B	417	GLU
2	B	430	SER
2	B	434	GLN
1	C	2	ARG
1	C	23	LEU
1	C	26	LEU
1	C	54	SER
1	C	56	THR
1	C	71	GLU
1	C	73	THR
1	C	74	VAL
1	C	82	THR
1	C	84	ARG
1	C	96	LYS
1	C	102	ASN
1	C	164	LYS
1	C	188	ILE
1	C	196	GLU
1	C	236	SER
1	C	245	ASP
1	C	315	CYS
1	C	332	ILE
1	C	335	ILE
1	C	336	LYS
1	C	370	LYS
1	C	401	LYS
1	C	414	GLU
2	D	2	ARG
2	D	15	GLN
2	D	19	LYS
2	D	26	ASP
2	D	33	THR
2	D	35	SER
2	D	48	ARG
2	D	62	VAL
2	D	64	ARG
2	D	67	LEU
2	D	85	GLN
2	D	88	ARG
2	D	117	SER
2	D	123	ARG

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Mol	Chain	Res	Type
2	D	124	LYS
2	D	153	LEU
2	D	160	GLU
2	D	164	ARG
2	D	179	ASP
2	D	181	VAL
2	D	195	VAL
2	D	215	ARG
2	D	241	CYS
2	D	254	LYS
2	D	264	ARG
2	D	276	THR
2	D	286	LEU
2	D	291	LEU
2	D	322	ARG
2	D	325	MET
2	D	333	LEU
2	D	335	VAL
2	D	337	ASN
2	D	340	SER
2	D	344	VAL
2	D	349	ASN
2	D	353	THR
2	D	392	SER
2	D	402	LYS
2	D	405	LEU
2	D	411	GLU
2	D	422	GLU
2	D	430	SER
2	D	434	GLN
3	E	15	LYS
3	E	17	GLU
3	E	32	TYR
3	E	44	GLU
3	E	57	GLU
3	E	64	GLU
3	E	83	LYS
3	E	88	GLU
3	E	94	ARG
3	E	125	GLU
3	E	133	GLN
3	E	144	ILE

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Mol	Chain	Res	Type
3	E	150	GLU
3	E	153	THR
3	E	156	LEU
3	E	170	VAL
3	E	179	GLU
3	E	193	LEU
3	F	15	LYS
3	F	18	MET
3	F	29	LEU
3	F	32	TYR
3	F	48	GLU
3	F	64	GLU
3	F	71	GLN
3	F	76	ARG
3	F	83	LYS
3	F	94	ARG
3	F	133	GLN
3	F	144	ILE
3	F	150	GLU
3	F	153	THR
3	F	156	LEU
3	F	193	LEU
4	G	185	ILE
4	G	186	LEU
4	G	197	ASN
4	G	208	LEU
4	G	248	LEU
4	G	265	THR
4	G	274	LEU
4	G	315	ILE
4	G	327	ARG
4	G	353	GLN
4	G	356	SER
4	G	363	ASP
4	G	371	MET
4	H	185	ILE
4	H	186	LEU
4	H	197	ASN
4	H	217	CYS
4	H	226	ASP
4	H	229	THR
4	H	235	ILE

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Mol	Chain	Res	Type
4	H	237	SER
4	H	248	LEU
4	H	250	ARG
4	H	255	VAL
4	H	259	GLN
4	H	274	LEU
4	H	301	ASP
4	H	310	SER
4	H	315	ILE
4	H	319	PHE
4	H	333	ILE
4	H	363	ASP
4	H	364	LYS
4	H	371	MET
4	H	379	VAL
4	H	380	ASN
4	H	381	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	31	GLN
1	A	85	GLN
1	A	102	ASN
1	A	107	HIS
1	A	197	HIS
1	A	216	ASN
1	A	256	GLN
1	A	258	ASN
1	A	309	HIS
1	A	393	HIS
2	B	8	GLN
2	B	101	ASN
2	B	136	GLN
2	B	293	GLN
2	B	334	ASN
2	B	337	ASN
2	B	385	GLN
2	B	394	GLN
2	B	436	GLN
1	C	15	GLN

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Mol	Chain	Res	Type
1	C	31	GLN
1	C	50	ASN
1	C	61	HIS
1	C	102	ASN
1	C	107	HIS
1	C	197	HIS
1	C	216	ASN
1	C	300	ASN
1	C	301	GLN
1	C	329	ASN
1	C	356	ASN
2	D	8	GLN
2	D	15	GLN
2	D	136	GLN
2	D	247	GLN
2	D	249	ASN
2	D	293	GLN
2	D	385	GLN
2	D	436	GLN
4	G	166	GLN
4	G	197	ASN
4	G	215	HIS
4	G	219	GLN
4	G	271	GLN
4	G	312	HIS
4	G	316	ASN
4	G	331	ASN
4	H	215	HIS
4	H	271	GLN
4	H	345	ASN
4	H	380	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z > 2$
9	GOL	B	505	-	5,5,5	0.76	0	5,5,5	0.48	0
9	GOL	D	506	-	5,5,5	0.58	0	5,5,5	0.35	0
7	SO4	C	503	-	4,4,4	0.25	0	6,6,6	0.29	0
8	MES	B	503	-	12,12,12	0.69	0	15,16,16	0.32	0
9	GOL	D	507	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GTP	A	501	6	33,34,34	0.57	1 (3%)	50,54,54	0.60	0
7	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.28	0
5	GTP	B	501	6	33,34,34	0.36	0	50,54,54	0.63	1 (2%)
5	GTP	D	501	6	33,34,34	0.43	0	50,54,54	0.72	1 (2%)
8	MES	D	504	-	12,12,12	0.57	0	15,16,16	0.84	1 (6%)
8	MES	B	504	-	12,12,12	0.64	0	15,16,16	0.31	0
8	MES	D	503	-	12,12,12	0.70	0	15,16,16	0.34	0
5	GTP	C	501	6	33,34,34	0.36	0	50,54,54	0.57	0
10	PGE	D	505	-	9,9,9	0.24	0	8,8,8	0.19	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 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
9	GOL	B	505	-	-	1/4/4/4	-
9	GOL	D	506	-	-	2/4/4/4	-
9	GOL	D	507	-	-	0/4/4/4	-
8	MES	B	503	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
5	GTP	B	501	6	-	4/22/38/38	0/3/3/3
5	GTP	D	501	6	-	7/22/38/38	0/3/3/3
8	MES	D	504	-	-	2/6/14/14	0/1/1/1
8	MES	B	504	-	-	5/6/14/14	0/1/1/1
8	MES	D	503	-	-	2/6/14/14	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
10	PGE	D	505	-	-	1/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	PG-O2G	2.35	1.63	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	O5'-PA-O1A	2.32	118.13	108.94
8	D	504	MES	C8-C7-N4	-2.30	103.67	112.36
5	B	501	GTP	O5'-PA-O1A	2.10	117.26	108.94

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	B	501	GTP	C5'-O5'-PA-O3A
5	B	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
8	B	504	MES	C7-C8-S-O1S
8	D	503	MES	C8-C7-N4-C5
9	D	506	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	B	503	MES	C8-C7-N4-C3
8	B	503	MES	C8-C7-N4-C5
8	D	503	MES	C8-C7-N4-C3
8	B	504	MES	C7-C8-S-O3S
9	B	505	GOL	O1-C1-C2-O2
8	B	504	MES	C7-C8-S-O2S
5	D	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	B	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	504	MES	C8-C7-N4-C3
8	B	504	MES	C8-C7-N4-C5
8	D	504	MES	C8-C7-N4-C3
8	D	504	MES	C8-C7-N4-C5
5	D	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
9	D	506	GOL	O1-C1-C2-O2
5	A	501	GTP	PB-O3A-PA-O1A
5	B	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
10	D	505	PGE	O2-C3-C4-O3

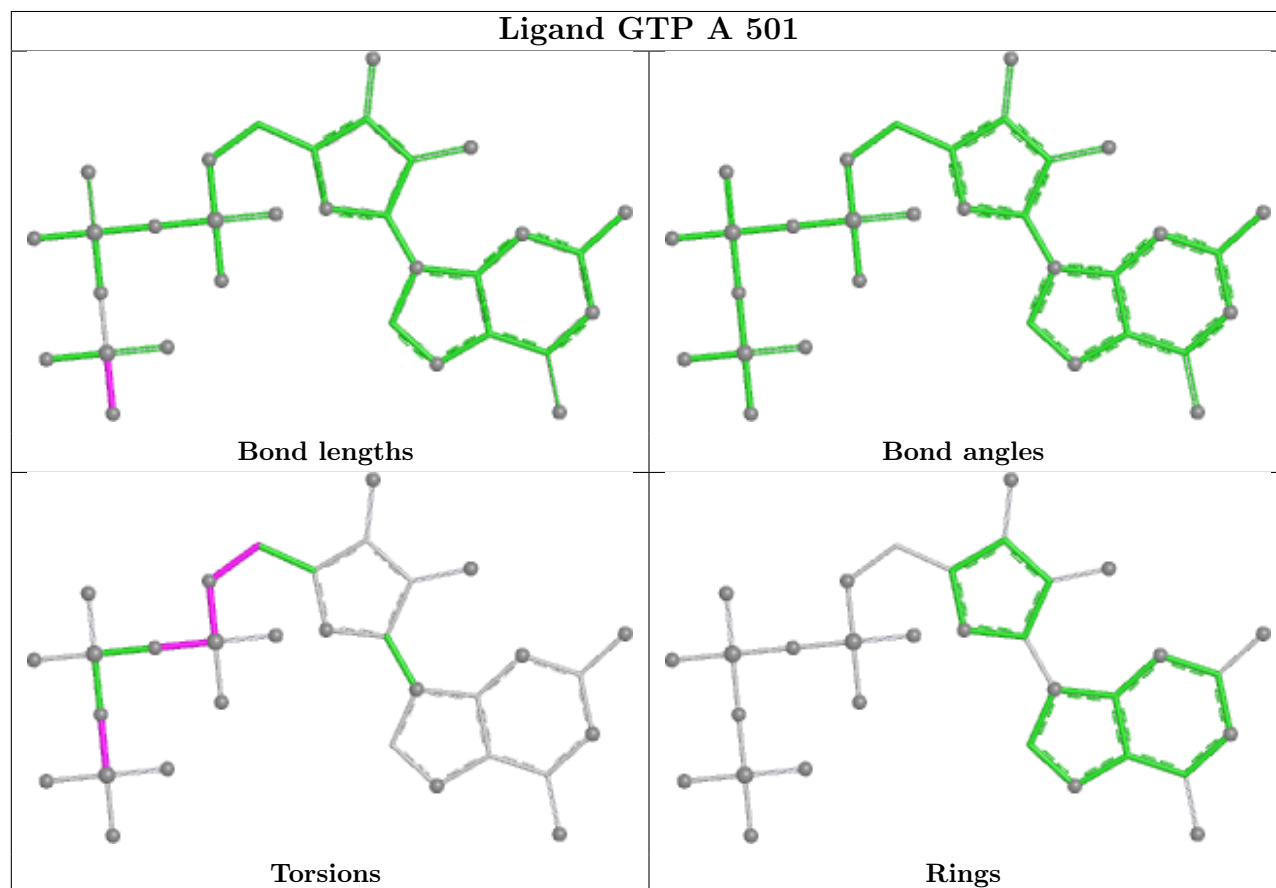
There are no ring outliers.

3 monomers are involved in 6 short contacts:

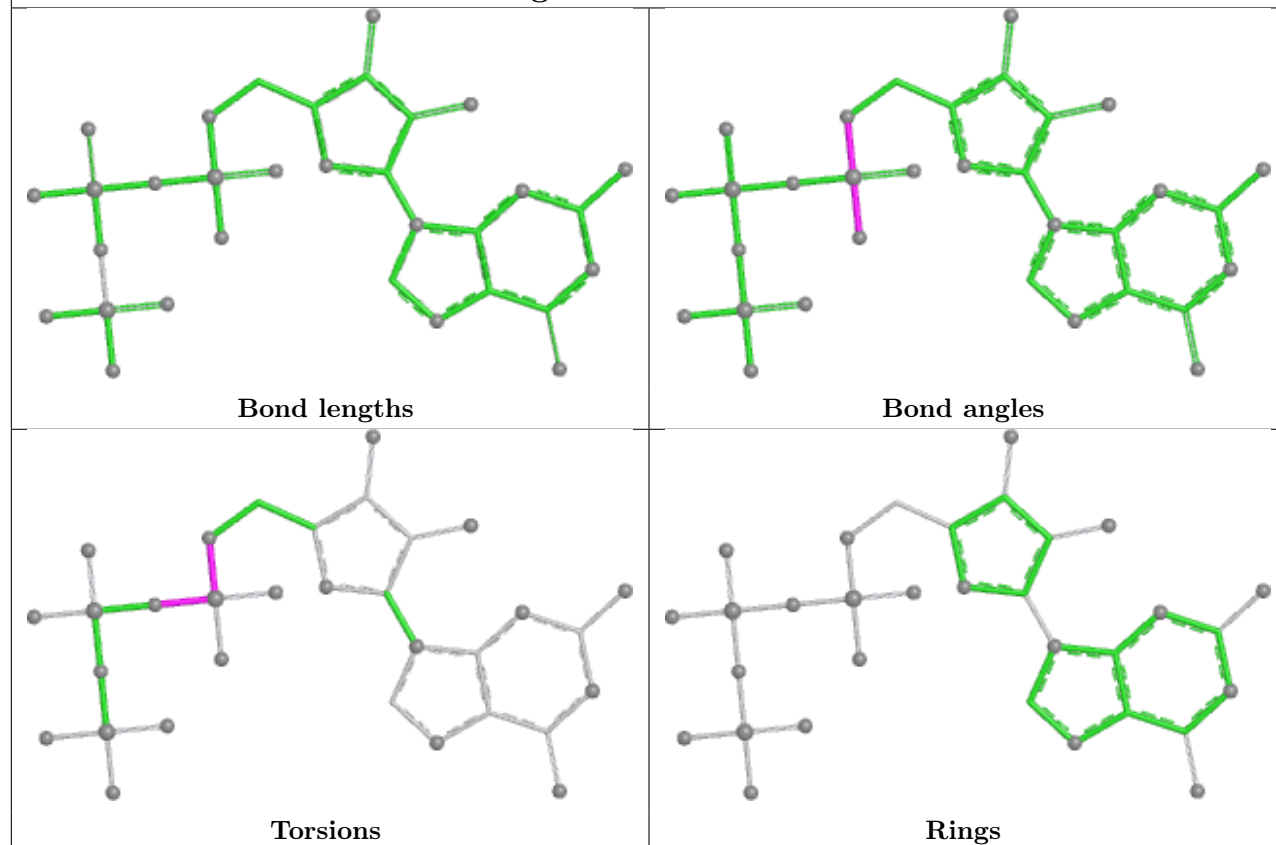
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	504	MES	3	0
8	B	504	MES	2	0
8	D	503	MES	1	0

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 than 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.

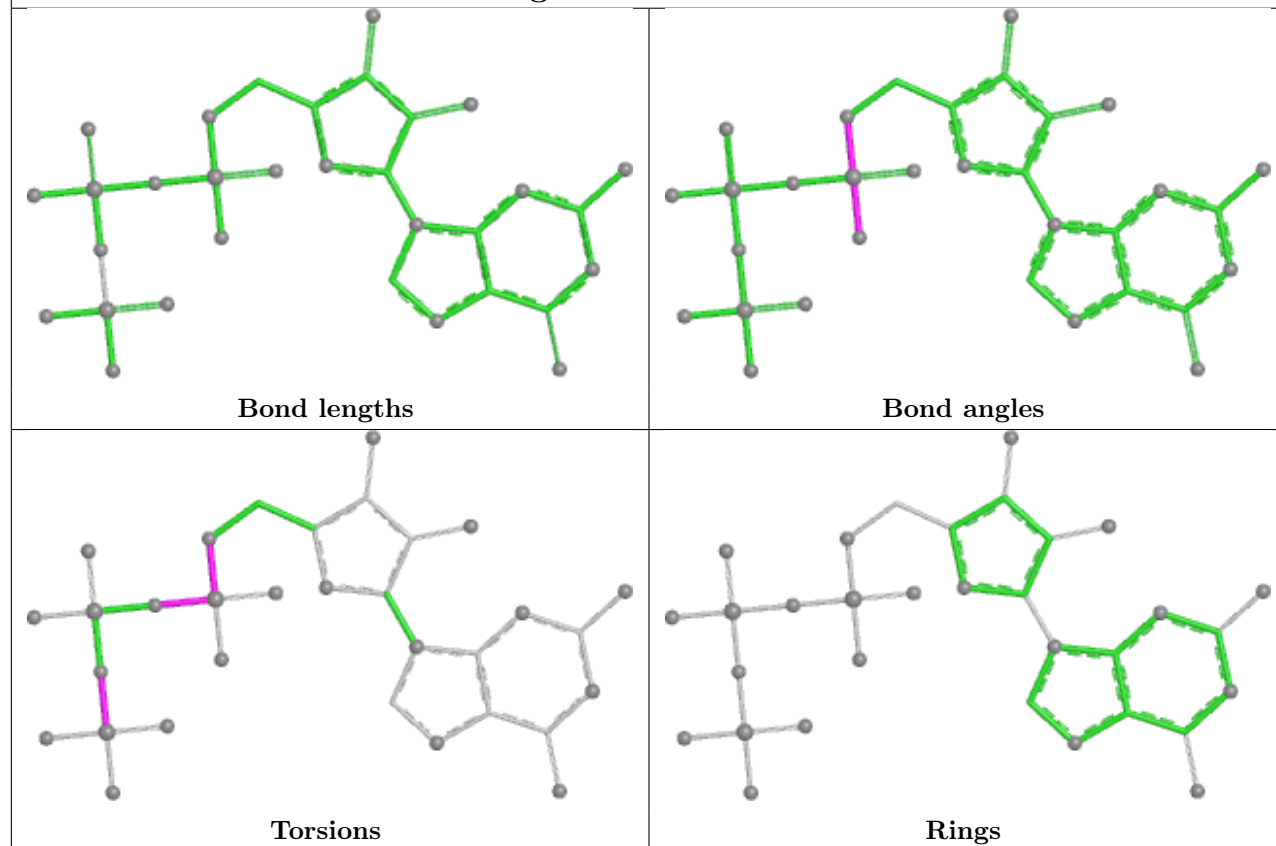
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

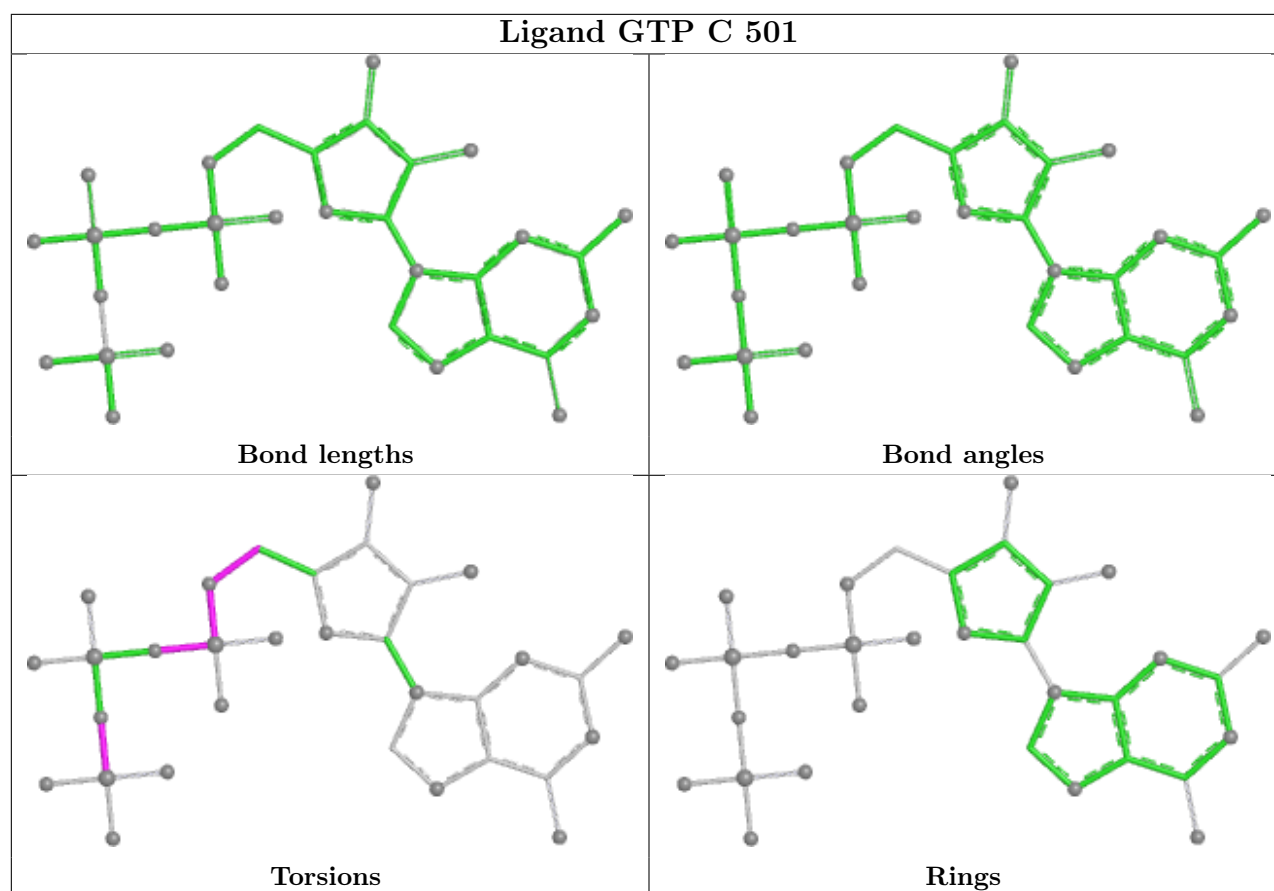


Ligand GTP B 501



Ligand GTP D 501





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

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	428/451 (94%)	-0.19	4 (0%)	81 64	55, 95, 156, 183	2 (0%)
1	C	428/451 (94%)	-0.21	3 (0%)	84 69	58, 94, 152, 176	2 (0%)
2	B	423/445 (95%)	-0.15	3 (0%)	84 69	64, 92, 124, 153	0
2	D	423/445 (95%)	-0.15	3 (0%)	84 69	62, 86, 121, 165	0
3	E	184/201 (91%)	-0.11	3 (1%)	70 51	77, 109, 182, 191	0
3	F	184/201 (91%)	-0.06	3 (1%)	70 51	77, 110, 187, 200	0
4	G	285/336 (84%)	0.27	7 (2%)	58 39	104, 164, 269, 279	0
4	H	290/336 (86%)	0.28	10 (3%)	48 30	92, 166, 250, 270	0
All	All	2645/2866 (92%)	-0.06	36 (1%)	73 54	55, 103, 218, 279	4 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	282	SER	3.9
4	G	155	PRO	3.3
2	D	440	ALA	3.0
4	H	279	TYR	3.0
4	G	350	ALA	2.9
2	B	356	CYS	2.8
3	F	110	GLU	2.8
2	D	1	MET	2.8
1	A	364	PRO	2.8
4	H	155	PRO	2.7
4	H	217	CYS	2.6
3	F	195	THR	2.6
4	H	350	ALA	2.6
2	B	1	MET	2.5
3	E	182	THR	2.5
4	G	217	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	345	ASN	2.4
4	G	165	ILE	2.4
4	H	358	LEU	2.4
4	G	383	ASN	2.3
1	C	302	MET	2.3
1	C	284	GLU	2.3
2	B	285	ALA	2.3
4	H	381	ILE	2.2
3	E	110	GLU	2.2
2	D	276	THR	2.2
3	E	73	GLY	2.2
4	G	153	THR	2.2
1	A	38	SER	2.2
3	F	36	ASP	2.2
4	H	164	LEU	2.1
1	A	352	LYS	2.1
4	G	358	LEU	2.1
1	A	337	THR	2.1
4	H	254	TYR	2.1
1	C	276	ILE	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 oligosaccharides 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.

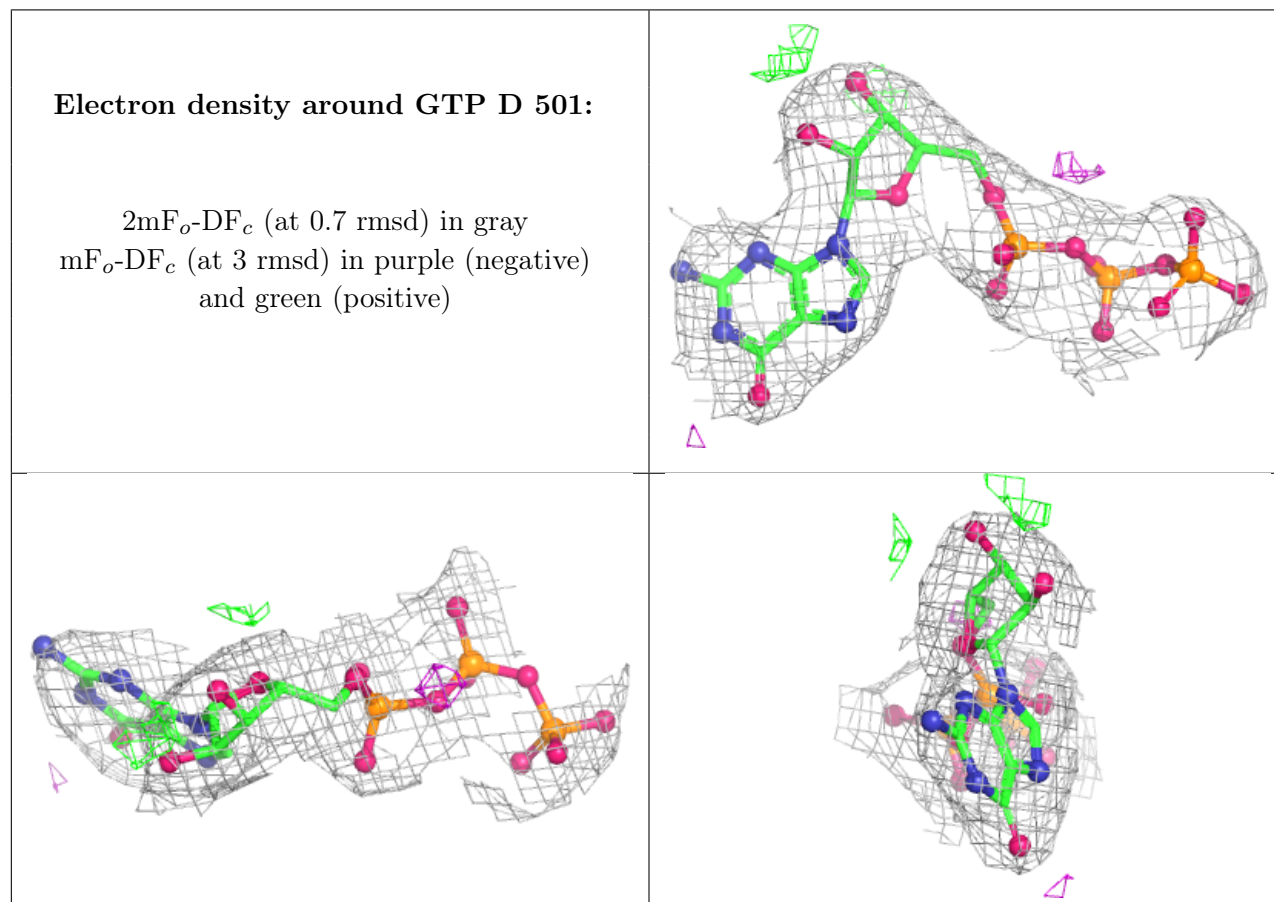
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	SO4	A	503	5/5	0.79	0.10	172,174,174,175	0
7	SO4	C	503	5/5	0.85	0.12	168,169,170,171	0
10	PGE	D	505	10/10	0.88	0.14	129,136,140,140	0

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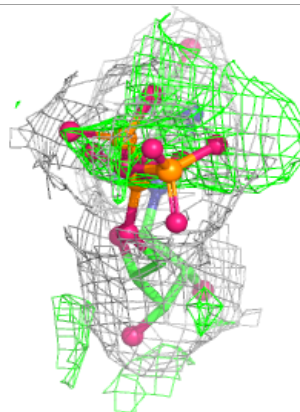
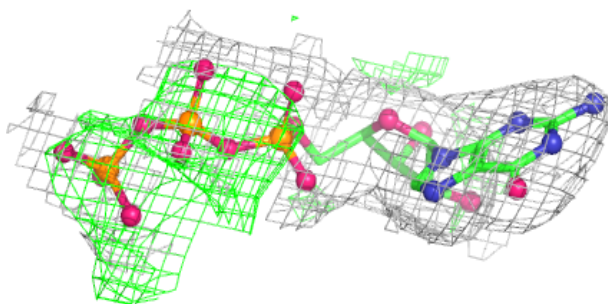
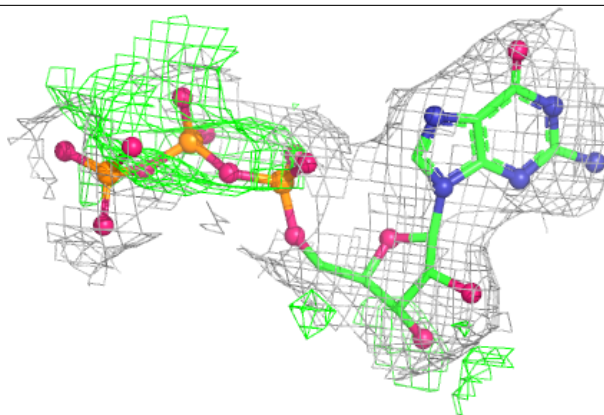
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	D	507	6/6	0.89	0.23	63,69,77,78	0
6	MG	B	502	1/1	0.91	0.10	85,85,85,85	0
6	MG	C	502	1/1	0.91	0.14	61,61,61,61	0
6	MG	A	502	1/1	0.91	0.21	60,60,60,60	0
9	GOL	D	506	6/6	0.92	0.15	58,65,72,75	0
9	GOL	B	505	6/6	0.93	0.19	49,55,63,69	0
8	MES	B	503	12/12	0.95	0.10	104,107,118,118	0
8	MES	D	503	12/12	0.95	0.09	92,99,121,122	0
6	MG	D	502	1/1	0.95	0.07	76,76,76,76	0
5	GTP	D	501	32/32	0.96	0.07	78,88,117,121	0
8	MES	D	504	12/12	0.96	0.10	88,91,111,112	0
8	MES	B	504	12/12	0.96	0.11	104,107,111,112	0
5	GTP	A	501	32/32	0.97	0.08	71,81,93,95	0
5	GTP	B	501	32/32	0.97	0.07	73,88,123,126	0
5	GTP	C	501	32/32	0.97	0.07	77,81,85,87	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.

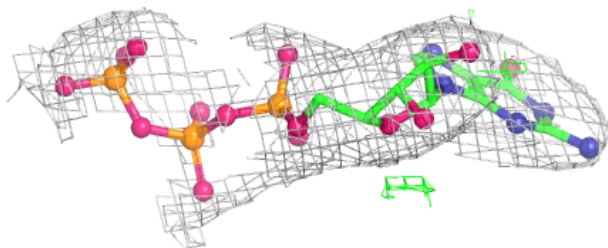
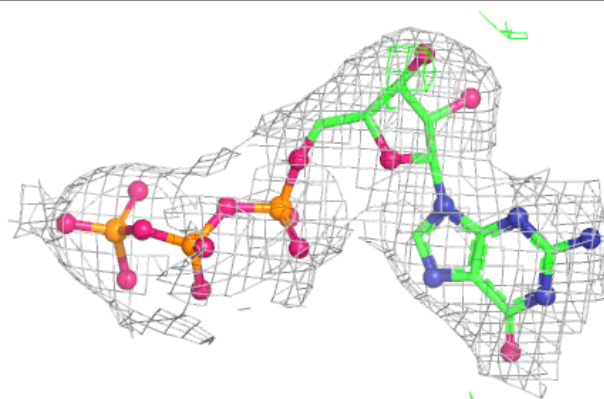


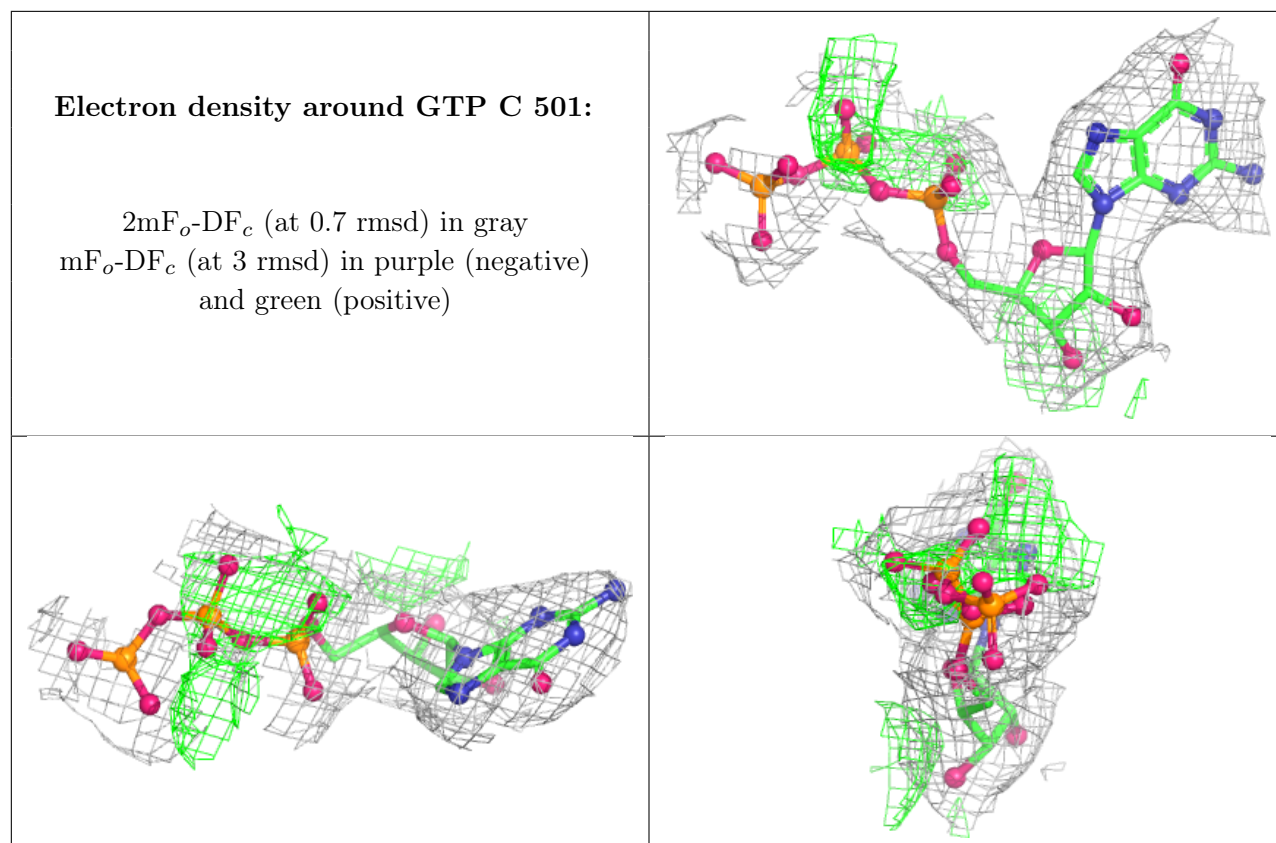
Electron density around GTP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GTP B 501:**

$2mF_o-DF_c$ (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.