



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 02:32 PM UTC

PDB ID : 5BMV / pdb_00005bmv
Title : CRYSTAL STRUCTURE OF TUBULIN-STATHMIN-TTL-Vinblastine COMPLEX
Authors : Wang, Y.; Chen, Q.; Zhang, R.
Deposited on : 2015-05-23
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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<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

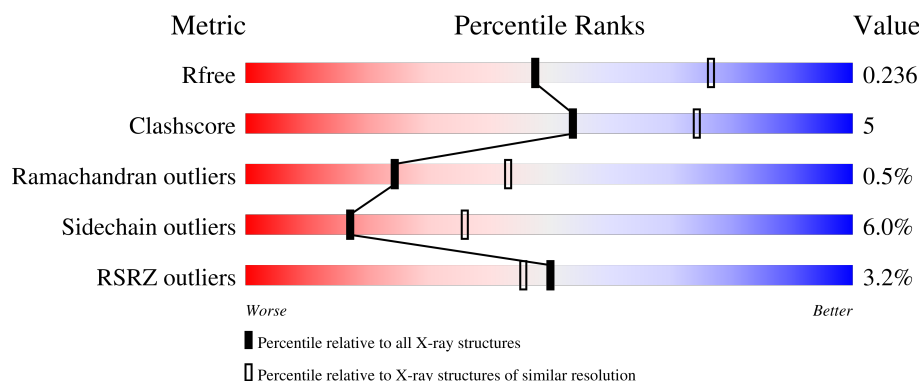
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	88% 9% .
1	C	451	2% 86% 10% ..
2	B	445	2% 79% 15% ..
2	D	445	4% 74% 19% 5%
3	E	143	2% 69% 15% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	C	504	-	-	X	-
8	GOL	C	505	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17912 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	A	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	1	0
			3446	2180	585	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3360	2111	576	647	26			
2	D	422	Total	C	N	O	S	0	0	0
			3311	2082	563	640	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2849	1825	492	518	14			

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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	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 CALCIUM ION (CCD ID: CA) (formula: Ca).

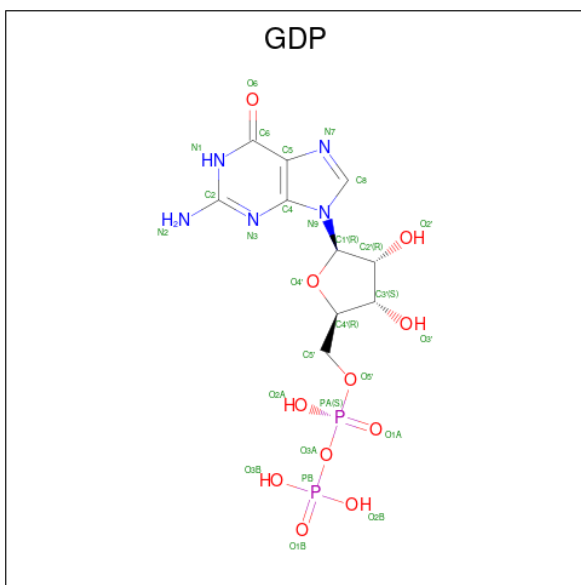
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



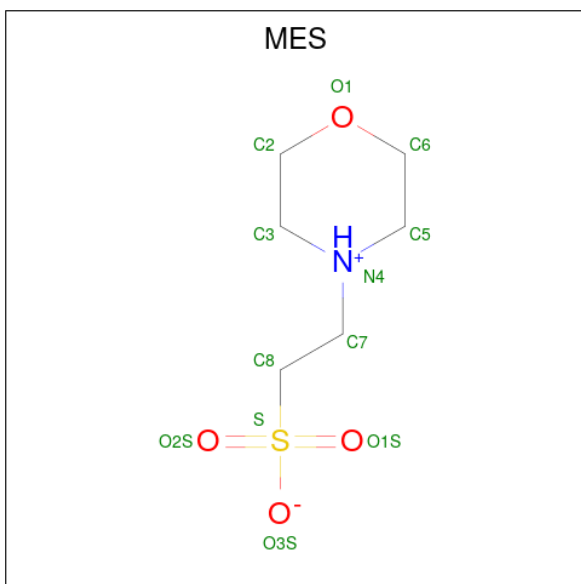
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



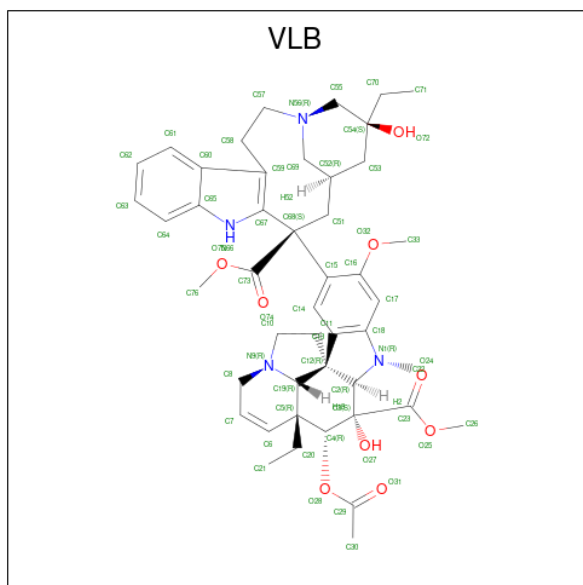
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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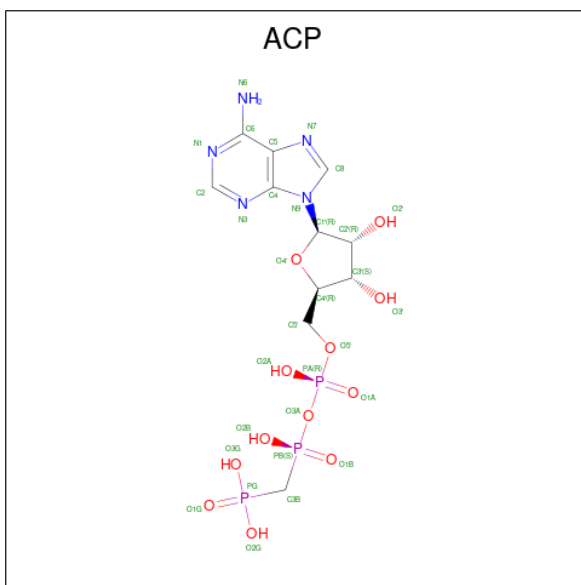
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (CCD ID: VLB) (formula: $C_{46}H_{58}N_4O_9$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O		0	0
			59	46	4	9			

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

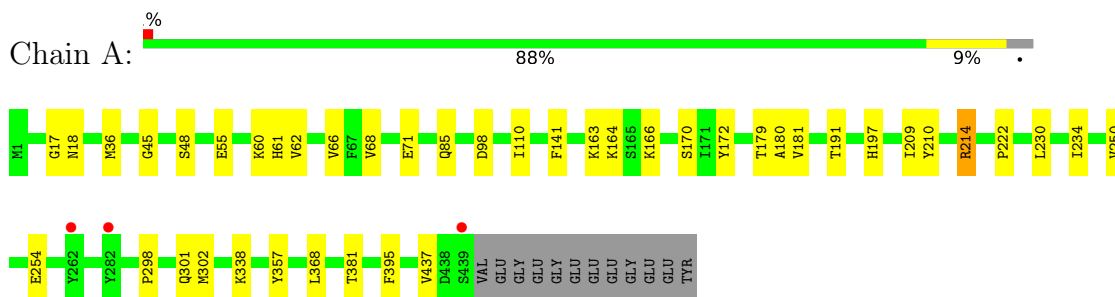
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	47	Total O 47 47	0	0
13	B	56	Total O 56 56	0	0
13	C	83	Total O 83 83	0	0
13	D	8	Total O 8 8	0	0
13	E	1	Total O 1 1	0	0
13	F	24	Total O 24 24	0	0

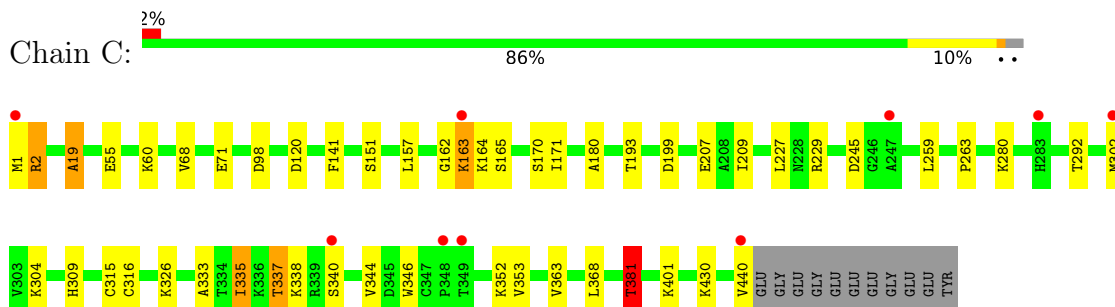
3 Residue-property plots [i](#)

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.

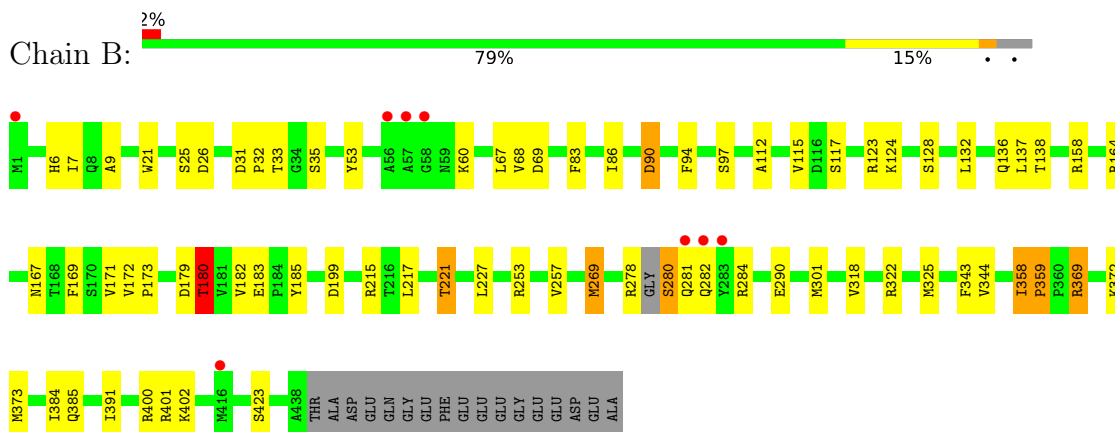
- Molecule 1: Tubulin alpha-1B chain



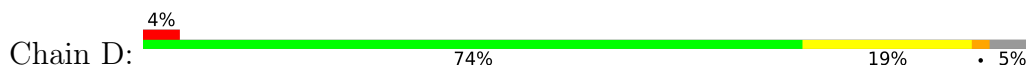
- Molecule 1: Tubulin alpha-1B chain

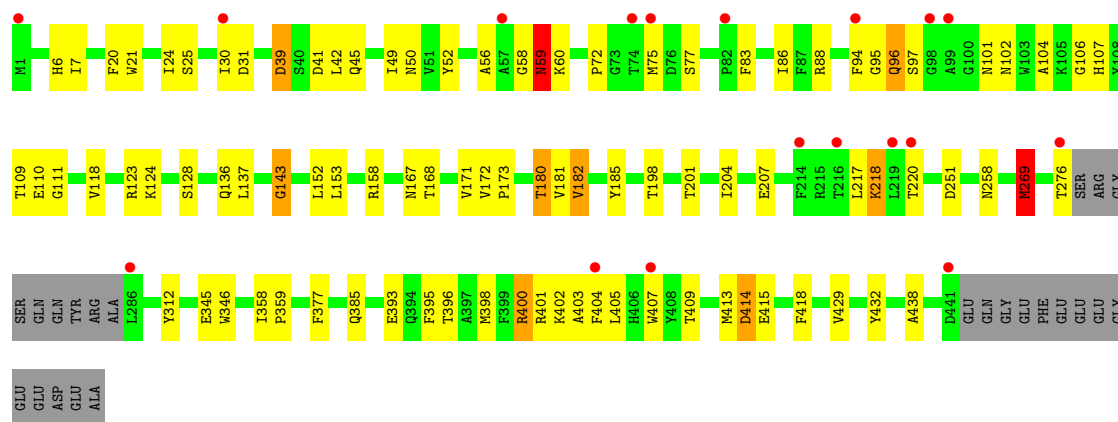


- Molecule 2: Tubulin beta chain

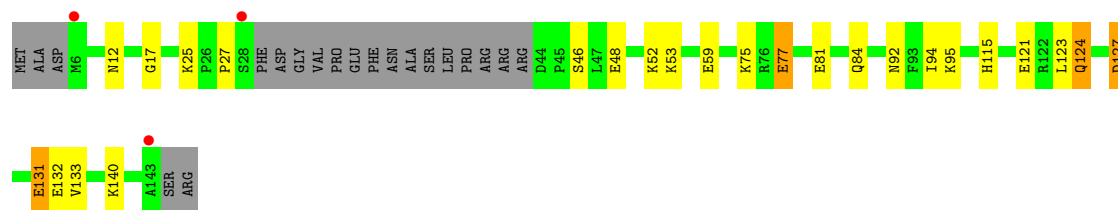


- Molecule 2: Tubulin beta chain

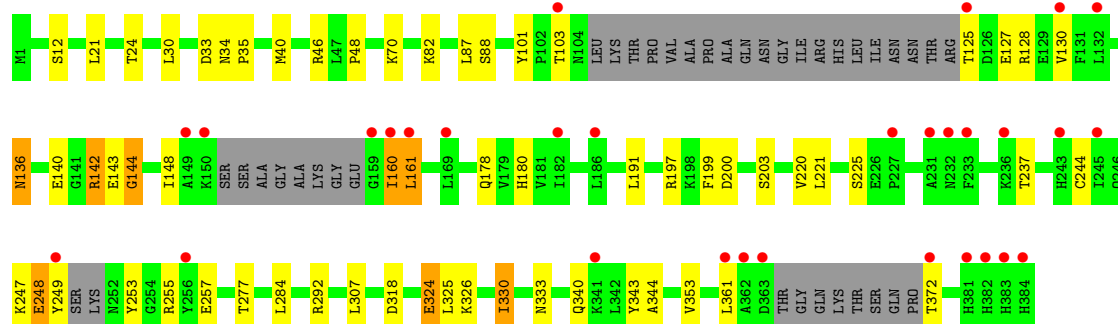
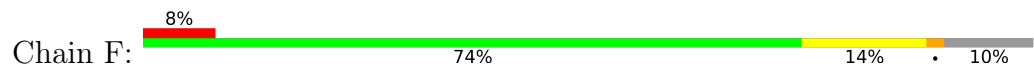




• Molecule 3: Stathmin-4



• Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 157.42Å 183.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.50) 99.5 (50.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.184 , 0.235 0.192 , 0.236	Depositor DCC
R_{free} test set	4906 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17912	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GOL, ACP, MG, GTP, VLB, MES, CA, GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.00	1/3508 (0.0%)	1.05	3/4762 (0.1%)
1	C	1.07	2/3524 (0.1%)	1.06	4/4785 (0.1%)
2	B	1.11	7/3434 (0.2%)	1.09	13/4651 (0.3%)
2	D	0.94	4/3384 (0.1%)	1.08	12/4586 (0.3%)
3	E	1.01	0/1022	1.11	1/1356 (0.1%)
4	F	0.82	0/2916	0.98	2/3940 (0.1%)
All	All	1.00	14/17788 (0.1%)	1.06	35/24080 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
4	F	0	1
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	171	VAL	C-O	-6.99	1.16	1.24
2	B	172	VAL	C-N	6.51	1.41	1.33
2	D	358	ILE	C-N	6.06	1.40	1.33
2	D	172	VAL	C-N	5.94	1.40	1.33
2	B	359	PRO	C-N	5.68	1.40	1.33
2	B	358	ILE	C-N	5.67	1.40	1.33
2	B	318	VAL	C-O	-5.57	1.18	1.24
1	C	353	VAL	C-O	-5.56	1.18	1.24
2	B	179	ASP	CB-CG	-5.46	1.38	1.52
2	B	183	GLU	C-O	-5.42	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	19	ALA	N-CA	-5.34	1.40	1.46
2	D	173	PRO	N-CD	5.30	1.55	1.47
2	D	359	PRO	N-CD	5.27	1.55	1.47
1	A	180	ALA	CA-C	-5.01	1.46	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	269	MET	CA-C-N	-7.62	112.97	120.52
2	D	269	MET	C-N-CA	-7.62	112.97	120.52
1	C	381	THR	CB-CA-C	-7.51	95.63	109.37
2	D	358	ILE	CA-C-N	-7.00	113.17	120.38
2	D	358	ILE	C-N-CA	-7.00	113.17	120.38
2	B	359	PRO	CA-C-N	-6.97	113.47	120.31
2	B	359	PRO	C-N-CA	-6.97	113.47	120.31
2	B	358	ILE	CA-C-N	-6.96	113.22	120.38
2	B	358	ILE	C-N-CA	-6.96	113.22	120.38
2	B	172	VAL	CA-C-N	-6.40	114.03	120.31
2	B	172	VAL	C-N-CA	-6.40	114.03	120.31
2	B	269	MET	CB-CA-C	-5.89	103.31	110.08
2	B	180	THR	CB-CA-C	5.79	119.29	109.80
2	D	56	ALA	N-CA-C	-5.76	100.65	109.41
3	E	84	GLN	N-CA-C	-5.68	105.17	111.36
4	F	161	LEU	N-CA-C	5.67	118.71	109.06
2	B	179	ASP	CB-CA-C	-5.62	99.58	109.02
1	C	338	LYS	N-CA-C	5.61	118.91	112.57
2	B	173	PRO	N-CA-C	5.57	120.03	111.57
2	D	172	VAL	CA-C-N	-5.56	113.51	120.51
2	D	172	VAL	C-N-CA	-5.56	113.51	120.51
1	C	68	VAL	CB-CA-C	-5.55	102.23	110.33
2	D	359	PRO	CA-C-N	-5.47	113.00	119.84
2	D	359	PRO	C-N-CA	-5.47	113.00	119.84
1	A	172	TYR	CA-C-N	5.34	125.10	119.76
1	A	172	TYR	C-N-CA	5.34	125.10	119.76
2	D	393	GLU	N-CA-C	-5.27	105.18	111.03
1	C	259	LEU	N-CA-C	5.26	118.96	112.54
2	B	179	ASP	N-CA-CB	-5.25	103.92	110.90
2	D	118	VAL	N-CA-C	-5.21	105.63	110.53
2	B	215	ARG	CB-CA-C	-5.07	102.90	110.90
2	D	58	GLY	N-CA-C	-5.06	106.45	114.10
2	B	391	ILE	CB-CA-C	-5.06	105.31	112.14
4	F	340	GLN	N-CA-C	5.05	117.17	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	THR	N-CA-C	-5.02	105.51	111.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	163	LYS	Peptide
4	F	136	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3340	18	0
1	C	3446	0	3354	33	0
2	B	3360	0	3242	41	0
2	D	3311	0	3192	47	0
3	E	1014	0	1029	11	0
4	F	2849	0	2796	24	0
5	A	32	0	12	1	0
5	C	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	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	0	0
8	B	6	0	8	1	0
8	C	18	0	24	11	0
9	B	28	0	12	0	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	C	59	0	58	5	0
12	F	31	0	14	2	0
13	A	47	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	56	0	0	1	0
13	C	83	0	0	6	0
13	D	8	0	0	2	0
13	E	1	0	0	0	0
13	F	24	0	0	1	0
All	All	17912	0	17155	172	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 5.

All (172) 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:B:35:SER:OG	2:B:60:LYS:NZ	1.65	1.30
2:D:432:TYR:OH	13:D:601:HOH:O	1.71	1.09
11:C:507:VLB:H582	11:C:507:VLB:H511	1.43	1.01
2:B:33:THR:HG22	2:B:60:LYS:HE3	1.58	0.85
2:B:83:PHE:O	2:B:86:ILE:HG22	1.79	0.82
2:B:33:THR:CG2	2:B:60:LYS:HE3	2.14	0.77
2:D:96:GLN:HG2	2:D:97:SER:N	1.99	0.77
1:C:381:THR:HG23	13:C:667:HOH:O	1.87	0.73
2:B:278:ARG:C	2:B:280:SER:N	2.49	0.71
8:C:506:GOL:O1	8:C:506:GOL:O3	2.11	0.69
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.75	0.68
11:C:507:VLB:H582	11:C:507:VLB:C51	2.23	0.68
2:D:185:TYR:CD1	2:D:418:PHE:HE2	2.12	0.67
13:C:663:HOH:O	3:E:115:HIS:HE1	1.76	0.67
2:B:33:THR:HG22	2:B:60:LYS:CE	2.26	0.64
2:D:7:ILE:O	2:D:137:LEU:HD12	1.96	0.63
3:E:131:GLU:HA	3:E:131:GLU:OE2	1.96	0.63
4:F:148:ILE:HD11	4:F:160:ILE:HD11	1.79	0.63
1:A:60:LYS:NZ	1:A:85:GLN:O	2.18	0.62
2:B:199:ASP:OD1	10:B:504:MES:H32	1.99	0.62
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.36	0.61
11:C:507:VLB:C73	11:C:507:VLB:O32	2.47	0.61
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.35	0.61
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.33	0.61
2:B:35:SER:HG	2:B:60:LYS:NZ	1.95	0.61
2:B:132:LEU:O	2:B:164:ARG:NH1	2.30	0.61
2:D:414:ASP:OD1	2:D:415:GLU:N	2.34	0.60
2:B:401:ARG:HH21	8:B:506:GOL:H11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:217:LEU:C	2:D:218:LYS:HG2	2.27	0.60
2:D:136:GLN:HA	2:D:167:ASN:O	2.01	0.60
1:C:309:HIS:CE1	13:C:612:HOH:O	2.55	0.59
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.38	0.59
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.85	0.58
1:C:229:ARG:HG2	8:C:505:GOL:O2	2.04	0.57
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.12	0.57
2:D:21:TRP:O	2:D:25:SER:OG	2.09	0.57
2:B:221:THR:O	2:B:221:THR:CG2	2.53	0.56
2:D:143:GLY:HA3	9:D:501:GDP:O3A	2.05	0.56
4:F:324:GLU:O	4:F:325:LEU:HB2	2.05	0.55
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.42	0.55
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.26	0.54
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.89	0.54
2:B:31:ASP:OD1	2:B:33:THR:HB	2.07	0.54
3:E:124:GLN:O	3:E:127:ASP:N	2.40	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.53
2:B:269:MET:HE1	2:B:301:MET:HG3	1.90	0.53
2:D:401:ARG:O	2:D:403:ALA:N	2.41	0.53
2:D:59:ASN:N	2:D:59:ASN:OD1	2.40	0.53
2:B:284:ARG:NH2	2:B:290:GLU:OE1	2.43	0.52
1:C:229:ARG:CG	8:C:505:GOL:O2	2.57	0.52
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.44	0.52
3:E:124:GLN:HA	3:E:124:GLN:OE1	2.10	0.52
1:C:207:GLU:OE2	8:C:504:GOL:H11	2.09	0.52
2:B:180:THR:HB	13:C:608:HOH:O	2.09	0.51
2:B:90:ASP:OD1	2:B:90:ASP:N	2.44	0.51
1:C:363:VAL:HG21	8:C:505:GOL:H11	1.93	0.51
2:D:39:ASP:OD1	2:D:39:ASP:N	2.41	0.51
1:C:304:LYS:HG3	8:C:504:GOL:H12	1.93	0.51
4:F:318:ASP:OD2	12:F:401:ACP:O3G	2.29	0.50
2:B:253:ARG:O	2:B:257:VAL:HG23	2.12	0.50
4:F:191:LEU:HA	4:F:197:ARG:O	2.10	0.50
1:C:1:MET:O	1:C:2:ARG:HB2	2.11	0.50
1:C:171:ILE:HD13	1:C:171:ILE:N	2.25	0.50
2:D:182:VAL:HG22	2:D:185:TYR:HD2	1.76	0.50
2:D:181:VAL:O	2:D:398:MET:HE1	2.12	0.50
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.94	0.50
4:F:200:ASP:OD2	12:F:401:ACP:O3'	2.30	0.49
1:C:229:ARG:HG2	8:C:505:GOL:C2	2.41	0.49
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.12	0.49
4:F:343:TYR:O	4:F:344:ALA:C	2.55	0.49
1:C:209:ILE:HD11	1:C:302:MET:HG2	1.93	0.49
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.12	0.48
2:B:343:PHE:O	2:B:344:VAL:C	2.53	0.48
4:F:21:LEU:O	4:F:24:THR:OG1	2.27	0.48
4:F:248:GLU:O	4:F:249:TYR:CD2	2.66	0.48
1:C:19:ALA:HA	8:C:505:GOL:H12	1.95	0.48
3:E:121:GLU:O	3:E:124:GLN:HB2	2.13	0.48
2:D:96:GLN:HG2	2:D:97:SER:H	1.76	0.48
2:B:164:ARG:HD2	13:B:614:HOH:O	2.13	0.48
11:C:507:VLB:H213	11:C:507:VLB:H19	1.72	0.48
1:A:17:GLY:O	1:A:18:ASN:C	2.56	0.48
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.96	0.47
2:D:400:ARG:HG3	2:D:401:ARG:N	2.30	0.47
1:C:304:LYS:HE3	8:C:504:GOL:H31	1.95	0.47
1:A:110:ILE:HG22	1:A:110:ILE:O	2.15	0.47
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.15	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.50	0.47
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.46
1:C:55:GLU:HA	1:C:60:LYS:O	2.14	0.46
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.98	0.46
2:D:102:ASN:ND2	2:D:407:TRP:O	2.47	0.46
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.96	0.46
2:B:227:LEU:HD22	11:C:507:VLB:H711	1.97	0.46
2:B:373:MET:HE2	2:B:373:MET:HA	1.97	0.46
2:D:104:ALA:HB2	2:D:413:MET:SD	2.56	0.46
2:D:102:ASN:OD1	2:D:102:ASN:C	2.59	0.46
2:B:158:ARG:NE	10:B:504:MES:O1	2.49	0.46
2:D:41:ASP:C	2:D:45:GLN:H	2.24	0.46
1:C:381:THR:CG2	13:C:667:HOH:O	2.53	0.46
2:B:199:ASP:OD2	10:B:504:MES:H52	2.16	0.45
2:D:41:ASP:C	2:D:45:GLN:N	2.73	0.45
2:B:278:ARG:O	2:B:280:SER:N	2.50	0.45
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.99	0.45
2:D:83:PHE:O	2:D:86:ILE:HG22	2.16	0.45
4:F:247:LYS:HE3	4:F:253:TYR:CZ	2.52	0.45
4:F:143:GLU:O	4:F:144:GLY:C	2.60	0.45
2:B:25:SER:HA	2:B:53:TYR:OH	2.17	0.44
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.17	0.44
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:B:67:LEU:HD12	2:B:67:LEU:N	2.32	0.44
2:D:107:HIS:O	2:D:152:LEU:HD22	2.18	0.44
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.52	0.44
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.53	0.44
2:D:109:THR:OG1	2:D:110:GLU:N	2.51	0.44
4:F:46:ARG:HB3	4:F:46:ARG:NH2	2.33	0.43
2:B:158:ARG:HG3	10:B:504:MES:H62	2.00	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.18	0.43
1:A:166:LYS:HE2	1:A:197:HIS:O	2.18	0.43
1:A:395:PHE:C	1:A:395:PHE:CD1	2.96	0.43
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.77	0.43
3:E:46:SER:C	3:E:48:GLU:N	2.76	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.43	0.43
4:F:333:ASN:HB3	13:F:518:HOH:O	2.18	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.43
1:C:304:LYS:HB3	8:C:504:GOL:H31	2.01	0.42
2:D:101:ASN:ND2	2:D:180:THR:HG21	2.34	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.59	0.42
2:B:112:ALA:O	2:B:115:VAL:HG12	2.19	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.42
2:D:438:ALA:O	13:D:602:HOH:O	2.21	0.42
2:B:269:MET:CE	2:B:301:MET:HG3	2.49	0.42
3:E:77:GLU:O	3:E:81:GLU:HG3	2.19	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
4:F:101:TYR:O	4:F:128:ARG:NH2	2.52	0.42
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.54	0.42
2:B:9:ALA:HA	2:B:68:VAL:O	2.20	0.42
1:C:304:LYS:CB	8:C:504:GOL:H31	2.50	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.20	0.41
2:D:123:ARG:O	2:D:124:LYS:C	2.63	0.41
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.02	0.41
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.89	0.41
1:C:263:PRO:HD2	13:C:641:HOH:O	2.20	0.41
2:B:97:SER:O	1:C:2:ARG:NH2	2.53	0.41
2:D:395:PHE:CD1	2:D:395:PHE:C	2.97	0.41
1:C:316:CYS:HA	1:C:352:LYS:O	2.20	0.41
2:D:168:THR:HG23	2:D:198:THR:HG21	2.02	0.41
2:D:52:TYR:OH	2:D:136:GLN:OE1	2.32	0.41
2:D:269:MET:HE3	2:D:269:MET:HB3	1.91	0.41
2:D:251:ASP:OD1	2:D:251:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:136:ASN:O	4:F:140:GLU:HG2	2.21	0.41
2:D:31:ASP:OD1	2:D:31:ASP:C	2.63	0.41
4:F:178:GLN:OE1	4:F:178:GLN:N	2.54	0.41
1:A:45:GLY:HA3	13:A:624:HOH:O	2.21	0.41
2:B:384:ILE:O	2:B:385:GLN:C	2.63	0.41
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.41
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.51	0.41
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.41
2:D:168:THR:OG1	2:D:201:THR:HG23	2.21	0.40
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.56	0.40
2:B:182:VAL:O	2:B:185:TYR:HB2	2.20	0.40
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.40
2:D:185:TYR:CD1	2:D:418:PHE:CE2	3.02	0.40
2:B:180:THR:HG22	1:C:352:LYS:NZ	2.37	0.40
2:D:72:PRO:HG3	2:D:95:GLY:O	2.22	0.40
2:B:69:ASP:O	2:B:94:PHE:HA	2.21	0.40
1:C:151:SER:HB2	1:C:193:THR:HG22	2.03	0.40
2:D:403:ALA:C	2:D:405:LEU:H	2.30	0.40
3:E:46:SER:C	3:E:48:GLU:H	2.29	0.40
4:F:244:CYS:O	4:F:247:LYS:N	2.55	0.40
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.97	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	437/451 (97%)	417 (95%)	20 (5%)	0	100	100
1	C	439/451 (97%)	423 (96%)	14 (3%)	2 (0%)	24	43
2	B	423/445 (95%)	417 (99%)	6 (1%)	0	100	100
2	D	418/445 (94%)	390 (93%)	23 (6%)	5 (1%)	10	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	119/143 (83%)	111 (93%)	7 (6%)	1 (1%)	16	31
4	F	336/384 (88%)	306 (91%)	27 (8%)	3 (1%)	14	27
All	All	2172/2319 (94%)	2064 (95%)	97 (4%)	11 (0%)	24	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	402	LYS
3	E	27	PRO
1	C	2	ARG
1	C	164	LYS
2	D	143	GLY
2	D	404	PHE
4	F	142	ARG
2	D	59	ASN
2	D	180	THR
4	F	88	SER
4	F	144	GLY

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	370/379 (98%)	355 (96%)	15 (4%)	27	53
1	C	372/379 (98%)	359 (96%)	13 (4%)	32	58
2	B	368/381 (97%)	348 (95%)	20 (5%)	20	41
2	D	363/381 (95%)	340 (94%)	23 (6%)	16	34
3	E	110/127 (87%)	95 (86%)	15 (14%)	3	8
4	F	312/342 (91%)	285 (91%)	27 (9%)	9	21
All	All	1895/1989 (95%)	1782 (94%)	113 (6%)	17	36

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	62	VAL
1	A	66	VAL
1	A	68	VAL
1	A	71	GLU
1	A	163	LYS
1	A	164	LYS
1	A	179	THR
1	A	181	VAL
1	A	214	ARG
1	A	234	ILE
1	A	338	LYS
1	A	368	LEU
1	A	381	THR
1	A	437	VAL
2	B	90	ASP
2	B	117	SER
2	B	123	ARG
2	B	124	LYS
2	B	128	SER
2	B	180	THR
2	B	217	LEU
2	B	221	THR
2	B	280	SER
2	B	281	GLN
2	B	282	GLN
2	B	322	ARG
2	B	325	MET
2	B	358	ILE
2	B	359	PRO
2	B	369	ARG
2	B	372	LYS
2	B	400	ARG
2	B	402	LYS
2	B	423	SER
1	C	120	ASP
1	C	163	LYS
1	C	245	ASP
1	C	280	LYS
1	C	315	CYS
1	C	326	LYS
1	C	335	ILE
1	C	337	THR

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Mol	Chain	Res	Type
1	C	340	SER
1	C	368	LEU
1	C	381	THR
1	C	430	LYS
1	C	440	VAL
2	D	30	ILE
2	D	39	ASP
2	D	42	LEU
2	D	49	ILE
2	D	50	ASN
2	D	59	ASN
2	D	60	LYS
2	D	77	SER
2	D	88	ARG
2	D	96	GLN
2	D	128	SER
2	D	153	LEU
2	D	182	VAL
2	D	207	GLU
2	D	218	LYS
2	D	220	THR
2	D	269	MET
2	D	276	THR
2	D	345	GLU
2	D	396	THR
2	D	400	ARG
2	D	409	THR
2	D	414	ASP
3	E	12	ASN
3	E	25	LYS
3	E	52	LYS
3	E	53	LYS
3	E	59	GLU
3	E	75	LYS
3	E	77	GLU
3	E	92	ASN
3	E	95	LYS
3	E	124	GLN
3	E	127	ASP
3	E	131	GLU
3	E	132	GLU
3	E	133	VAL

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Mol	Chain	Res	Type
3	E	140	LYS
4	F	12	SER
4	F	30	LEU
4	F	33	ASP
4	F	70	LYS
4	F	87	LEU
4	F	103	THR
4	F	125	THR
4	F	130	VAL
4	F	142	ARG
4	F	160	ILE
4	F	161	LEU
4	F	180	HIS
4	F	203	SER
4	F	220	VAL
4	F	225	SER
4	F	237	THR
4	F	248	GLU
4	F	255	ARG
4	F	277	THR
4	F	292	ARG
4	F	307	LEU
4	F	324	GLU
4	F	326	LYS
4	F	330	ILE
4	F	353	VAL
4	F	361	LEU
4	F	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	18	ASN
1	A	283	HIS
1	A	300	ASN
1	A	309	HIS
2	B	11	GLN
2	B	101	ASN
2	B	193	GLN
2	B	281	GLN
2	B	294	GLN

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Mol	Chain	Res	Type
2	B	331	GLN
2	B	394	GLN
1	C	15	GLN
1	C	309	HIS
1	C	356	ASN
2	D	45	GLN
2	D	96	GLN
2	D	101	ASN
2	D	167	ASN
2	D	294	GLN
2	D	385	GLN
3	E	18	GLN
3	E	136	ASN
4	F	26	GLN
4	F	104	ASN
4	F	136	ASN
4	F	229	ASN
4	F	232	ASN
4	F	306	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	GOL	B	506	-	5,5,5	0.42	0	5,5,5	0.34	0
5	GTP	A	501	6	33,34,34	1.25	4 (12%)	50,54,54	1.93	13 (26%)
9	GDP	B	501	6	29,30,30	1.44	5 (17%)	45,47,47	1.61	6 (13%)
11	VLB	C	507	-	66,67,67	2.77	19 (28%)	82,108,108	2.34	22 (26%)
8	GOL	A	506	-	5,5,5	0.77	0	5,5,5	0.52	0
8	GOL	C	506	-	5,5,5	0.37	0	5,5,5	0.67	0
8	GOL	A	505	-	5,5,5	0.46	0	5,5,5	1.16	0
8	GOL	A	504	-	5,5,5	0.49	0	5,5,5	0.57	0
8	GOL	C	504	-	5,5,5	0.65	0	5,5,5	1.06	0
9	GDP	D	501	6	29,30,30	1.50	5 (17%)	45,47,47	2.02	12 (26%)
8	GOL	C	505	-	5,5,5	0.67	0	5,5,5	0.78	0
10	MES	B	504	-	12,12,12	2.33	3 (25%)	15,16,16	5.72	8 (53%)
10	MES	B	505	-	12,12,12	2.41	1 (8%)	15,16,16	1.33	1 (6%)
12	ACP	F	401	-	31,33,33	2.38	11 (35%)	47,52,52	1.81	10 (21%)
5	GTP	C	501	6	33,34,34	1.28	6 (18%)	50,54,54	1.50	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	506	-	-	2/4/4/4	-
5	GTP	A	501	6	-	3/22/38/38	0/3/3/3
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
11	VLB	C	507	-	-	8/40/131/131	0/7/9/9
8	GOL	A	506	-	-	2/4/4/4	-
8	GOL	C	506	-	-	2/4/4/4	-
8	GOL	A	505	-	-	2/4/4/4	-
8	GOL	A	504	-	-	2/4/4/4	-
8	GOL	C	504	-	-	2/4/4/4	-
9	GDP	D	501	6	-	3/16/32/32	0/3/3/3
8	GOL	C	505	-	-	1/4/4/4	-
10	MES	B	504	-	-	5/6/14/14	0/1/1/1
10	MES	B	505	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	ACP	F	401	-	-	6/19/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	507	VLB	C6-C7	12.38	1.54	1.32
10	B	505	MES	C8-S	-7.94	1.66	1.77
10	B	504	MES	C8-S	-6.73	1.68	1.77
11	C	507	VLB	C12-C13	-6.34	1.41	1.51
11	C	507	VLB	C68-C73	-6.16	1.45	1.53
12	F	401	ACP	PB-O3A	6.01	1.65	1.58
11	C	507	VLB	C60-C65	-6.01	1.33	1.41
12	F	401	ACP	PG-O1G	5.98	1.62	1.50
12	F	401	ACP	PA-O3A	5.01	1.64	1.59
12	F	401	ACP	C5-C4	4.77	1.47	1.39
11	C	507	VLB	C68-C67	-4.62	1.44	1.52
11	C	507	VLB	C58-C59	-4.43	1.44	1.51
11	C	507	VLB	C60-C59	-4.36	1.36	1.44
11	C	507	VLB	C57-C58	4.32	1.61	1.52
11	C	507	VLB	C18-C13	-4.25	1.34	1.39
9	D	501	GDP	PA-O3A	4.04	1.63	1.59
11	C	507	VLB	C19-N9	3.85	1.53	1.47
11	C	507	VLB	C20-C5	-3.40	1.49	1.55
9	B	501	GDP	C6-N1	-3.34	1.32	1.38
5	C	501	GTP	C6-N1	-3.27	1.32	1.38
11	C	507	VLB	C17-C18	-3.23	1.34	1.39
11	C	507	VLB	C14-C13	-3.22	1.34	1.39
12	F	401	ACP	PG-O3G	3.16	1.62	1.55
9	B	501	GDP	C5-N7	-3.13	1.32	1.39
11	C	507	VLB	C68-C15	-3.08	1.45	1.54
12	F	401	ACP	PG-O2G	-3.03	1.48	1.55
11	C	507	VLB	C67-N66	-2.95	1.33	1.38
9	B	501	GDP	C5-C4	2.95	1.46	1.38
9	D	501	GDP	C5-C4	2.92	1.46	1.38
9	D	501	GDP	C5-N7	-2.91	1.33	1.39
11	C	507	VLB	O75-C73	2.85	1.38	1.33
10	B	504	MES	O2S-S	2.84	1.53	1.45
5	A	501	GTP	C5-C4	2.82	1.46	1.38
12	F	401	ACP	C5-C6	2.82	1.48	1.41
5	A	501	GTP	C5-N7	-2.68	1.33	1.39
11	C	507	VLB	C61-C60	-2.63	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	PA-O3A	2.61	1.62	1.59
9	B	501	GDP	PA-O3A	2.54	1.62	1.59
5	C	501	GTP	C4-N9	-2.49	1.31	1.38
11	C	507	VLB	C18-N1	-2.49	1.35	1.39
12	F	401	ACP	C8-N7	2.45	1.36	1.31
9	D	501	GDP	C6-N1	-2.38	1.34	1.38
5	C	501	GTP	C5-C4	2.32	1.45	1.38
11	C	507	VLB	C65-N66	-2.30	1.34	1.38
5	A	501	GTP	PB-O3B	2.27	1.62	1.59
12	F	401	ACP	PB-O2B	2.23	1.61	1.56
12	F	401	ACP	C5-N7	-2.16	1.35	1.39
10	B	504	MES	O1S-S	2.11	1.51	1.45
9	D	501	GDP	C2-N3	2.10	1.38	1.33
5	A	501	GTP	C2-N3	2.08	1.38	1.33
9	B	501	GDP	C4-N9	-2.07	1.32	1.38
5	C	501	GTP	C5-N7	-2.05	1.35	1.39
12	F	401	ACP	C4-N9	-2.04	1.33	1.37
5	C	501	GTP	C8-N7	2.04	1.38	1.32

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O3S-S-O1S	-12.56	79.98	111.40
10	B	504	MES	O3S-S-C8	-9.89	86.66	106.00
10	B	504	MES	O1S-S-C8	9.88	121.66	106.73
11	C	507	VLB	C8-C7-C6	-8.62	109.72	123.13
10	B	504	MES	O3S-S-O2S	-8.17	90.97	111.40
11	C	507	VLB	C19-C5-C6	7.14	115.39	108.27
9	D	501	GDP	C5-C4-N3	-6.90	117.40	128.39
10	B	504	MES	O2S-S-C8	6.16	116.03	106.73
5	A	501	GTP	C5-C4-N3	-5.60	119.48	128.39
12	F	401	ACP	C5-C4-N3	-5.55	119.07	126.72
11	C	507	VLB	C5-C6-C7	-5.43	112.34	123.88
9	B	501	GDP	C5-C4-N3	-5.12	120.25	128.39
9	D	501	GDP	N9-C4-N3	5.10	136.15	125.95
11	C	507	VLB	O28-C29-C30	4.86	119.75	111.09
11	C	507	VLB	C11-C12-C13	-4.85	103.53	112.36
9	D	501	GDP	C2-N3-C4	4.64	120.30	112.30
12	F	401	ACP	N3-C4-N9	4.55	134.91	127.17
5	A	501	GTP	N9-C4-N3	4.53	135.02	125.95
11	C	507	VLB	C12-C19-C5	-4.48	114.88	118.20
11	C	507	VLB	C59-C67-N66	-4.34	105.35	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	507	VLB	C4-O28-C29	4.28	124.13	117.65
11	C	507	VLB	O28-C4-C3	4.25	112.93	106.29
5	C	501	GTP	C2-N3-C4	4.06	119.29	112.30
5	C	501	GTP	C5-C4-N3	-3.88	122.21	128.39
5	A	501	GTP	C2-N3-C4	3.83	118.89	112.30
12	F	401	ACP	C2-N3-C4	3.74	120.96	111.83
9	B	501	GDP	N9-C4-N3	3.72	133.39	125.95
12	F	401	ACP	N3-C2-N1	-3.64	123.07	128.58
11	C	507	VLB	C52-C69-N56	3.61	117.24	111.20
11	C	507	VLB	C5-C19-N9	3.53	119.15	111.72
9	B	501	GDP	C6-C5-N7	3.51	136.68	130.29
5	A	501	GTP	O6-C6-C5	-3.50	117.28	126.53
11	C	507	VLB	C13-C12-C2	3.44	107.46	102.11
12	F	401	ACP	C4-C5-N7	-3.37	106.73	110.58
10	B	504	MES	C5-N4-C3	3.26	115.86	108.84
9	D	501	GDP	O3B-PB-O1B	3.24	123.47	110.83
5	A	501	GTP	C4-C5-N7	-3.23	105.55	110.67
12	F	401	ACP	C4-N9-C8	3.21	109.11	105.74
5	A	501	GTP	C8-N7-C5	3.21	109.98	104.26
10	B	505	MES	O2S-S-C8	3.12	111.45	106.73
5	A	501	GTP	N9-C8-N7	-3.07	107.70	113.40
5	C	501	GTP	C6-C5-N7	3.04	135.83	130.29
5	A	501	GTP	C6-C5-N7	3.03	135.81	130.29
9	B	501	GDP	C4-C5-N7	-2.87	106.13	110.67
9	B	501	GDP	C2-N3-C4	2.87	117.24	112.30
9	D	501	GDP	C2-N1-C6	-2.84	119.95	125.11
10	B	504	MES	C6-C5-N4	2.82	114.41	110.12
11	C	507	VLB	C53-C52-C69	2.80	111.82	108.67
11	C	507	VLB	C63-C62-C61	-2.80	116.79	120.24
5	A	501	GTP	C8-N9-C4	2.77	111.22	106.03
9	D	501	GDP	O3A-PA-O1A	2.74	118.94	110.70
11	C	507	VLB	C13-C18-N1	2.72	113.90	110.93
5	C	501	GTP	O2A-PA-O1A	2.67	124.88	112.44
11	C	507	VLB	C2-C12-C19	2.65	118.55	114.07
11	C	507	VLB	O75-C73-C68	2.65	115.48	111.21
5	A	501	GTP	O3G-PG-O3B	-2.56	96.05	104.64
12	F	401	ACP	C5-N7-C8	2.54	107.45	103.45
5	A	501	GTP	C2-N1-C6	-2.54	120.50	125.11
9	D	501	GDP	O6-C6-C5	-2.50	119.94	126.53
5	A	501	GTP	O6-C6-N1	2.48	124.78	120.11
9	D	501	GDP	C4-C5-N7	-2.48	106.74	110.67
9	D	501	GDP	C6-C5-N7	2.46	134.77	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O2A-PA-O3A	2.46	113.92	107.27
11	C	507	VLB	C17-C18-C13	-2.45	119.18	121.99
9	D	501	GDP	O3A-PB-O1B	-2.39	98.47	111.04
5	C	501	GTP	N2-C2-N1	2.38	121.79	116.76
9	B	501	GDP	C8-N7-C5	2.32	108.40	104.26
5	A	501	GTP	O3G-PG-O1G	2.31	119.85	110.83
12	F	401	ACP	N9-C8-N7	-2.29	110.68	113.94
11	C	507	VLB	C8-N9-C19	2.26	118.20	112.48
9	D	501	GDP	C5-C6-N1	2.24	118.96	113.25
9	D	501	GDP	O2A-PA-O5'	2.22	117.61	107.57
12	F	401	ACP	C6-C5-N7	2.19	136.31	132.09
5	C	501	GTP	C4-C5-N7	-2.15	107.26	110.67
11	C	507	VLB	C70-C54-C55	-2.13	106.84	111.80
10	B	504	MES	O2S-S-O1S	2.11	120.68	113.82
11	C	507	VLB	C65-C60-C59	2.10	108.75	106.84
5	C	501	GTP	N9-C4-N3	2.04	130.03	125.95
12	F	401	ACP	C2-N1-C6	2.01	122.03	118.73
11	C	507	VLB	C11-C12-C2	-2.01	108.28	112.17
5	C	501	GTP	O6-C6-C5	-2.00	121.25	126.53

There are no chirality outliers.

All (47) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
11	C	507	VLB	C58-C57-N56-C69
12	F	401	ACP	PG-C3B-PB-O1B
12	F	401	ACP	PG-C3B-PB-O2B
12	F	401	ACP	PG-C3B-PB-O3A
11	C	507	VLB	C30-C29-O28-C4
11	C	507	VLB	O31-C29-O28-C4
8	A	504	GOL	C1-C2-C3-O3
8	C	504	GOL	O1-C1-C2-C3
8	C	506	GOL	C1-C2-C3-O3
8	A	505	GOL	O1-C1-C2-O2
12	F	401	ACP	O4'-C4'-C5'-O5'
12	F	401	ACP	PB-O3A-PA-O1A
8	B	506	GOL	O2-C2-C3-O3
8	C	505	GOL	O1-C1-C2-O2
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	N4-C7-C8-S
9	D	501	GDP	C5'-O5'-PA-O2A
8	A	504	GOL	O2-C2-C3-O3
10	B	504	MES	C8-C7-N4-C3
8	C	504	GOL	O1-C1-C2-O2
11	C	507	VLB	C67-C68-C73-O75
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	504	MES	C7-C8-S-O2S
11	C	507	VLB	C3-C23-O25-C26
11	C	507	VLB	C67-C68-C73-O74
5	C	501	GTP	PB-O3A-PA-O1A
11	C	507	VLB	C58-C57-N56-C55
12	F	401	ACP	C3'-C4'-C5'-O5'
11	C	507	VLB	N56-C57-C58-C59

There are no ring outliers.

9 monomers are involved in 25 short contacts:

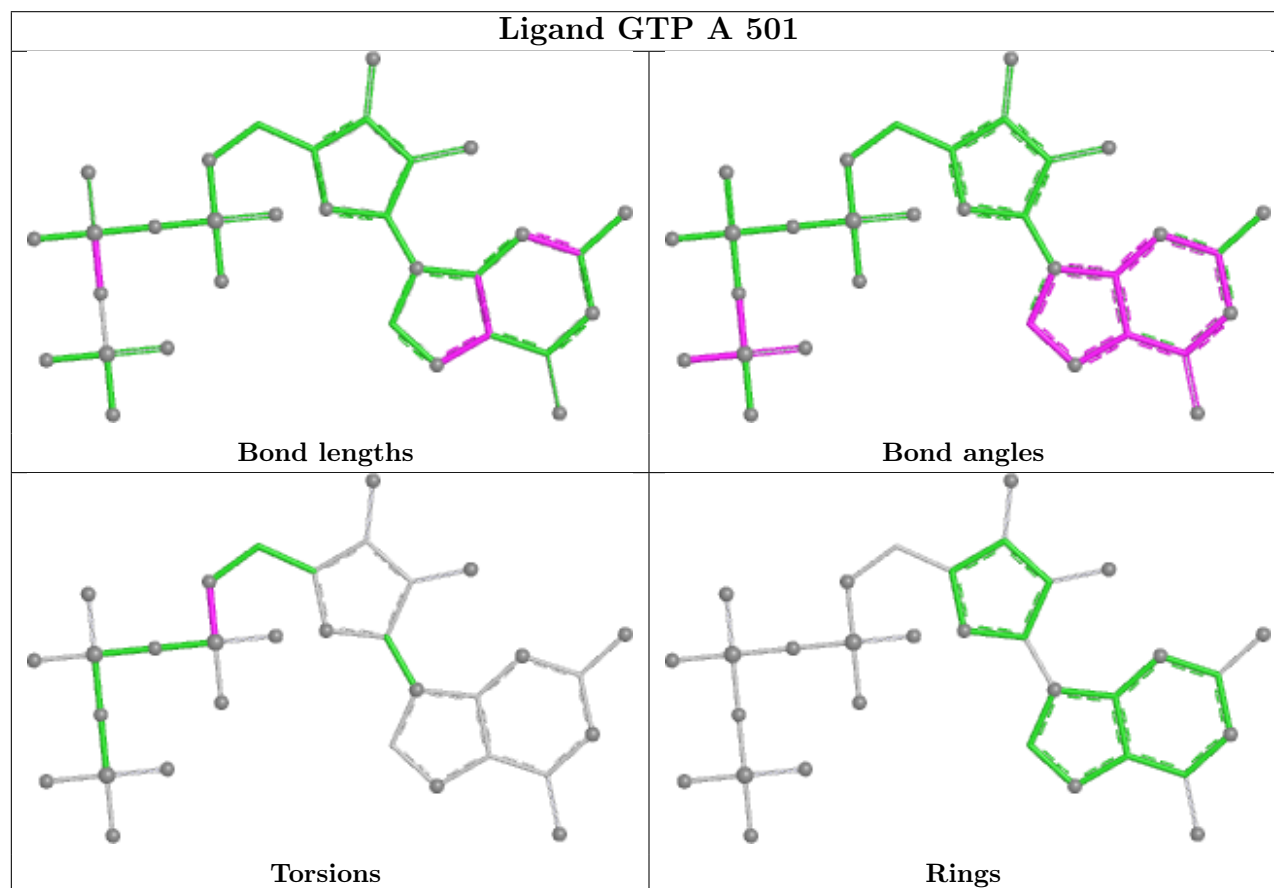
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	506	GOL	1	0
5	A	501	GTP	1	0
11	C	507	VLB	5	0
8	C	506	GOL	1	0
8	C	504	GOL	5	0
9	D	501	GDP	1	0
8	C	505	GOL	5	0
10	B	504	MES	4	0

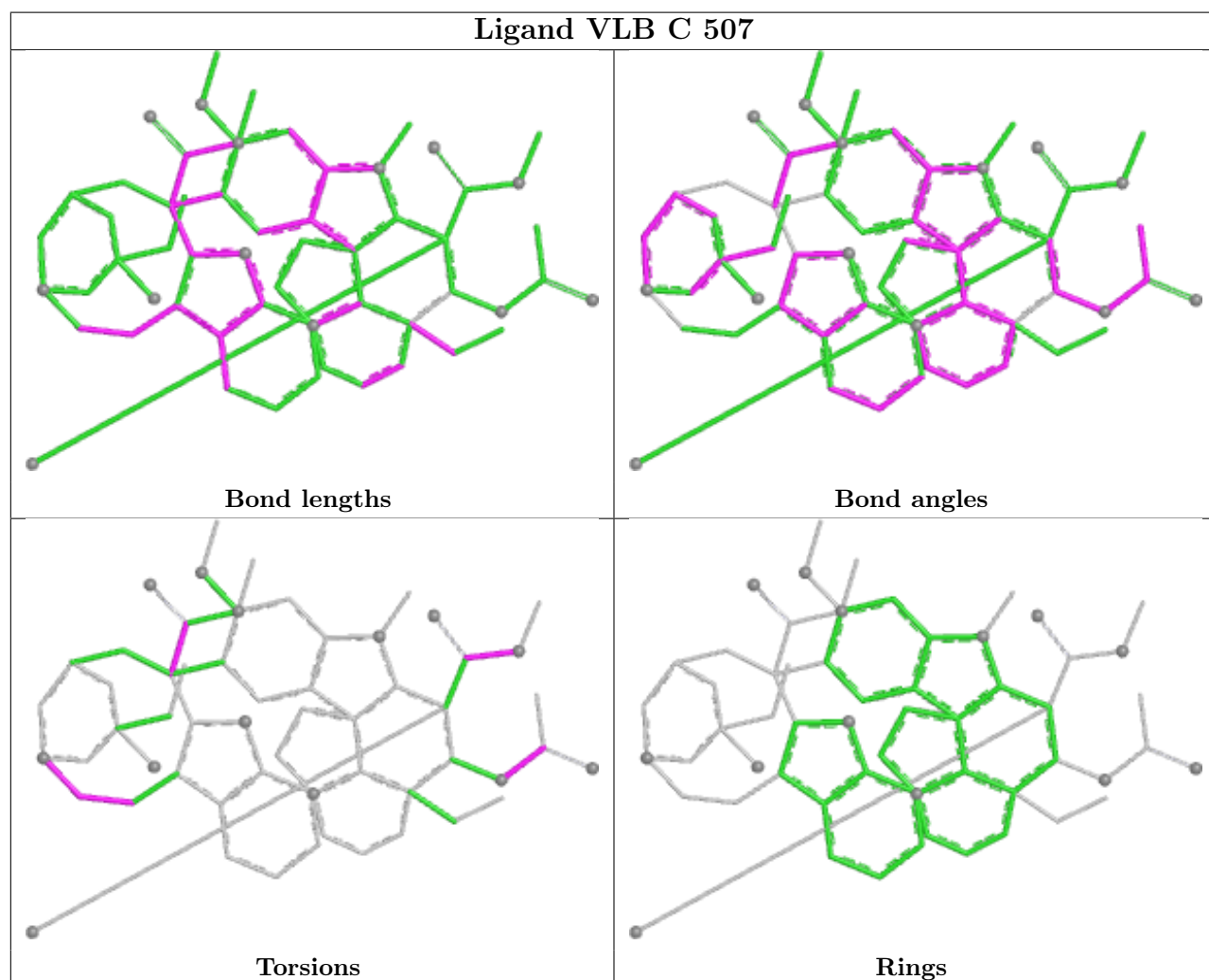
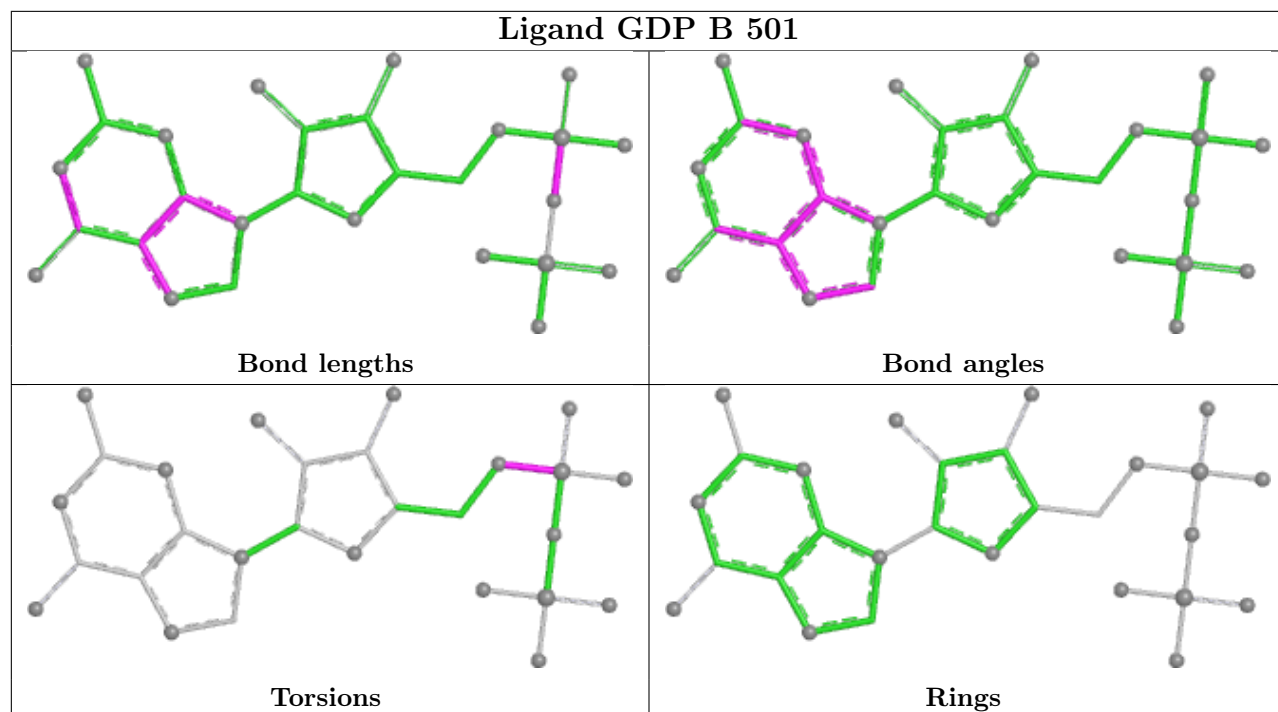
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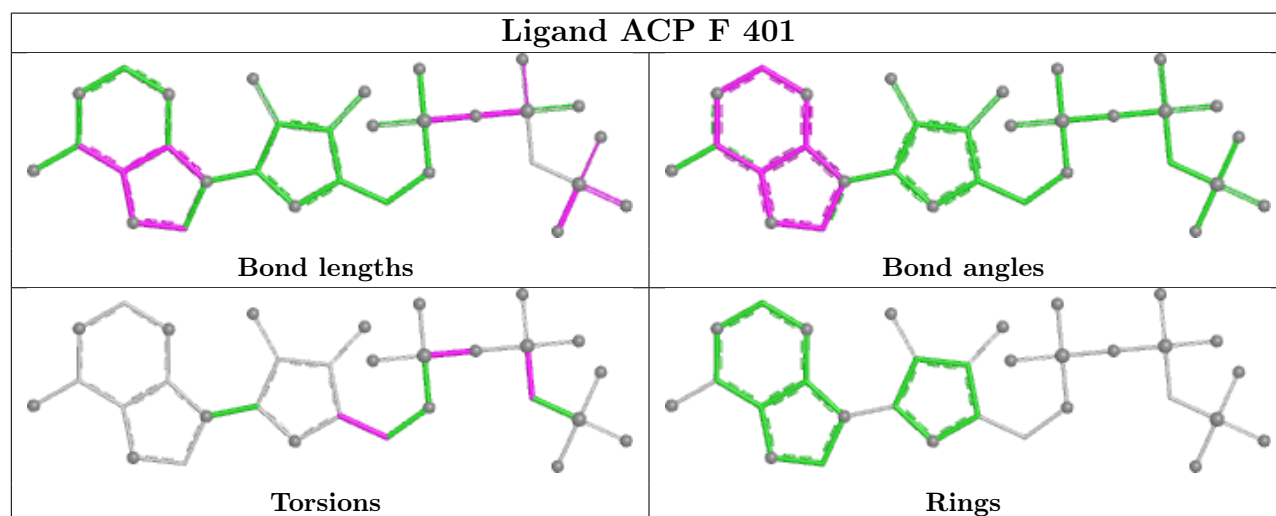
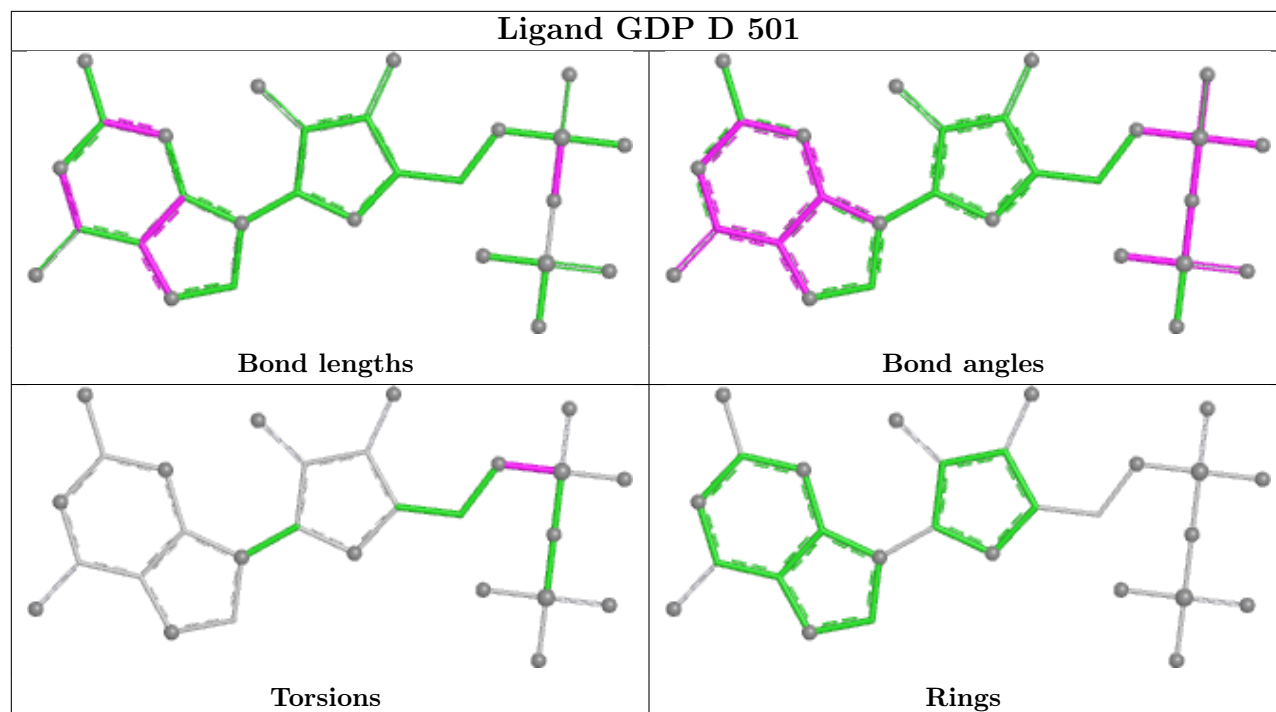
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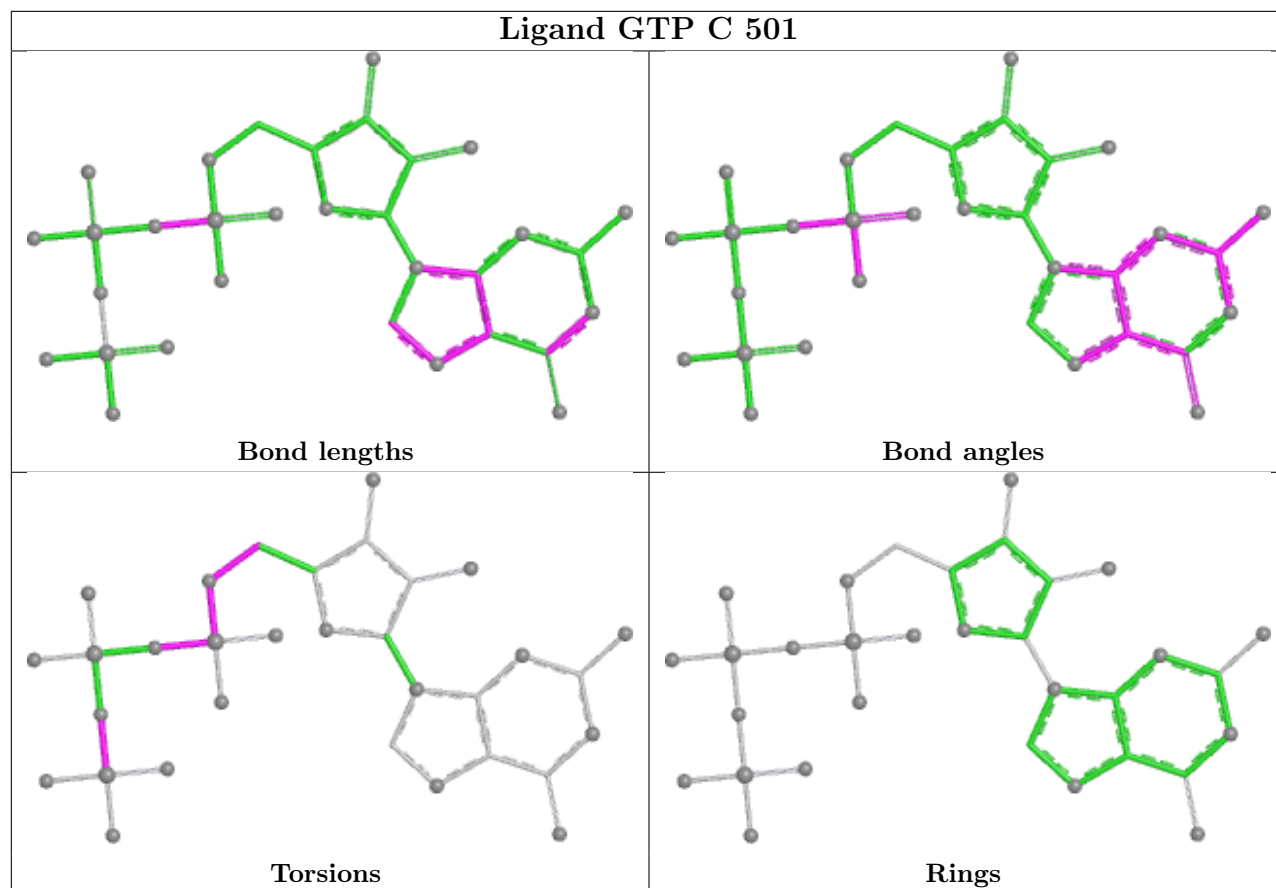
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	2	0

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 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.









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	439/451 (97%)	-0.21	3 (0%) 84 81	26, 45, 74, 106	0
1	C	440/451 (97%)	-0.35	9 (2%) 65 61	22, 38, 66, 97	1 (0%)
2	B	427/445 (95%)	-0.32	8 (1%) 66 62	24, 38, 75, 109	0
2	D	422/445 (94%)	0.31	18 (4%) 40 35	33, 58, 89, 111	0
3	E	123/143 (86%)	0.48	3 (2%) 59 55	35, 62, 101, 125	0
4	F	346/384 (90%)	0.51	30 (8%) 16 14	33, 68, 121, 136	0
All	All	2197/2319 (94%)	-0.01	71 (3%) 50 46	22, 49, 95, 136	1 (0%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	4.1
4	F	125	THR	3.7
4	F	150	LYS	3.7
1	C	440	VAL	3.6
4	F	149	ALA	3.6
2	D	407	TRP	3.4
2	D	1	MET	3.4
3	E	143	ALA	3.4
4	F	159	GLY	3.3
4	F	249	TYR	3.2
4	F	383	HIS	3.2
1	C	163	LYS	3.1
2	B	283	TYR	3.1
3	E	6	MET	3.1
1	A	282	TYR	3.0
2	D	94	PHE	3.0
4	F	161	LEU	3.0
1	A	439	SER	3.0
4	F	245	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	276	THR	2.9
4	F	382	HIS	2.9
4	F	381	HIS	2.8
4	F	362	ALA	2.8
4	F	231	ALA	2.8
3	E	28	SER	2.6
2	B	281	GLN	2.6
4	F	130	VAL	2.6
1	C	283	HIS	2.6
2	D	75	MET	2.6
4	F	103	THR	2.6
4	F	236	LYS	2.6
1	C	340	SER	2.5
2	D	286	LEU	2.5
1	A	262	TYR	2.5
4	F	341	LYS	2.5
4	F	233	PHE	2.4
4	F	363	ASP	2.4
2	D	404	PHE	2.4
1	C	348	PRO	2.4
4	F	132	LEU	2.4
2	B	56	ALA	2.4
4	F	232	ASN	2.3
2	B	57	ALA	2.3
4	F	372	THR	2.3
2	D	98	GLY	2.3
4	F	243	HIS	2.3
1	C	1	MET	2.3
4	F	256	TYR	2.3
2	D	99	ALA	2.2
4	F	182	ILE	2.2
1	C	247	ALA	2.2
1	C	349	THR	2.2
2	B	282	GLN	2.2
2	B	58	GLY	2.2
2	D	74	THR	2.2
2	D	216	THR	2.2
2	D	220	THR	2.2
4	F	186	LEU	2.2
4	F	160	ILE	2.2
2	D	57	ALA	2.1
2	D	441	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	361	LEU	2.1
2	D	82	PRO	2.1
2	B	416	MET	2.1
2	D	219	LEU	2.0
4	F	169	LEU	2.0
1	C	302	MET	2.0
4	F	384	HIS	2.0
2	D	214	PHE	2.0
2	D	30	ILE	2.0
4	F	227	PRO	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
6	MG	B	502	1/1	0.61	0.14	74,74,74,74	0
6	MG	D	502	1/1	0.67	0.27	53,53,53,53	0
8	GOL	A	504	6/6	0.71	0.17	70,74,80,86	0
8	GOL	C	505	6/6	0.77	0.28	81,96,107,130	0
8	GOL	B	506	6/6	0.86	0.14	80,84,88,88	0
8	GOL	A	505	6/6	0.86	0.16	61,65,68,69	0
12	ACP	F	401	31/31	0.86	0.10	72,85,113,115	0
10	MES	B	504	12/12	0.88	0.14	53,63,74,82	0
8	GOL	A	506	6/6	0.88	0.14	56,64,70,71	0
9	GDP	D	501	28/28	0.90	0.10	44,48,60,67	0
8	GOL	C	504	6/6	0.91	0.14	55,69,70,72	0
8	GOL	C	506	6/6	0.92	0.11	49,62,65,74	0
10	MES	B	505	12/12	0.93	0.11	65,71,76,76	0

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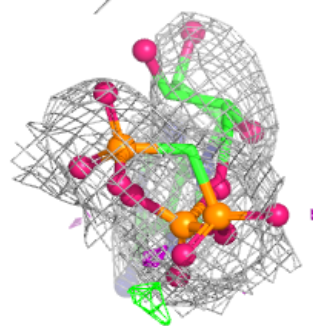
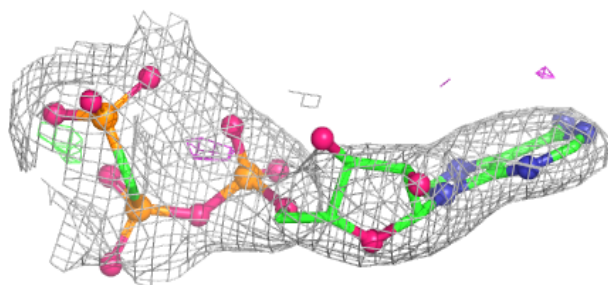
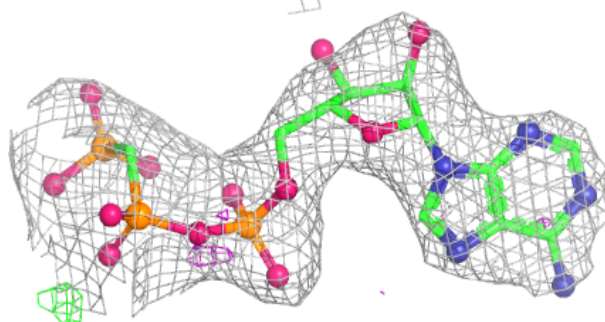
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	VLB	C	507	59/59	0.95	0.07	28,35,44,49	0
7	CA	B	503	1/1	0.98	0.04	76,76,76,76	0
5	GTP	A	501	32/32	0.99	0.04	25,30,34,34	0
5	GTP	C	501	32/32	0.99	0.04	25,28,32,33	0
9	GDP	B	501	28/28	0.99	0.04	23,26,28,29	0
7	CA	A	503	1/1	0.99	0.04	62,62,62,62	0
6	MG	A	502	1/1	1.00	0.02	36,36,36,36	0
7	CA	C	503	1/1	1.00	0.03	49,49,49,49	0
6	MG	C	502	1/1	1.00	0.02	28,28,28,28	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.

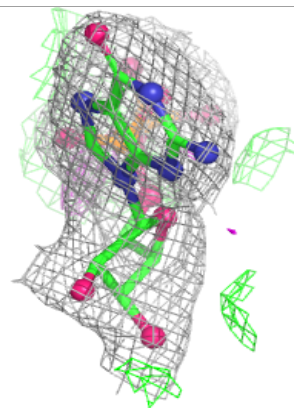
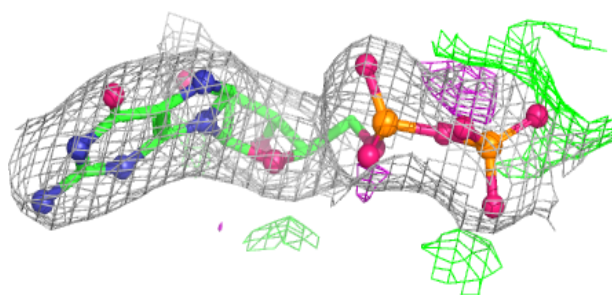
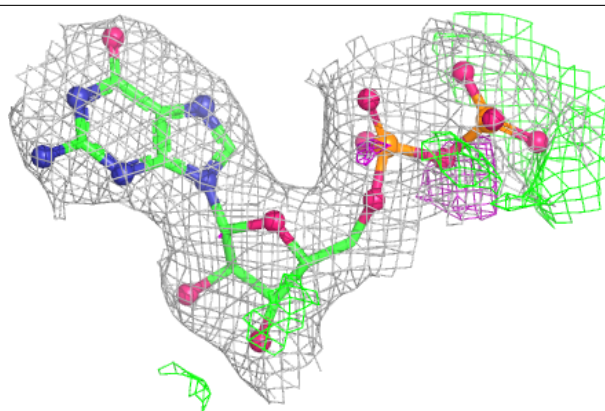
Electron density around ACP F 401:

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



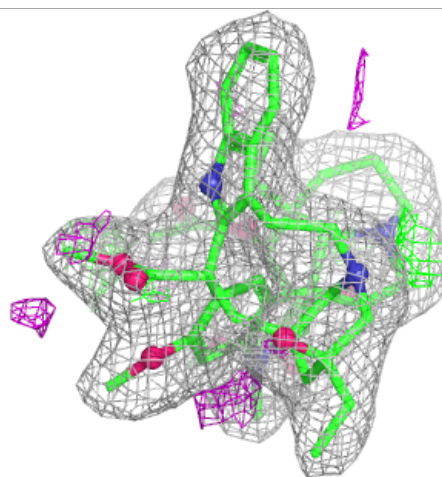
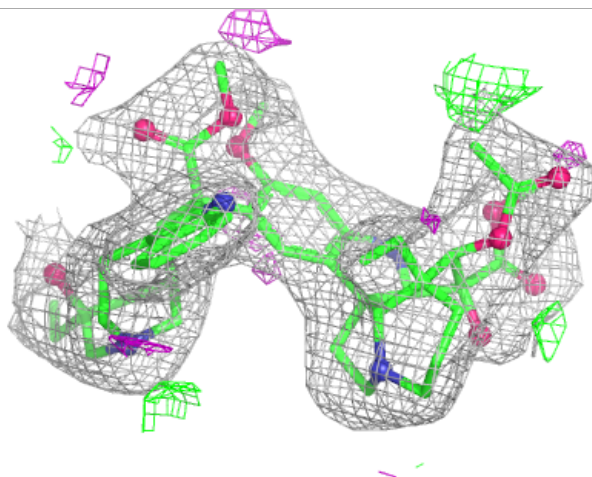
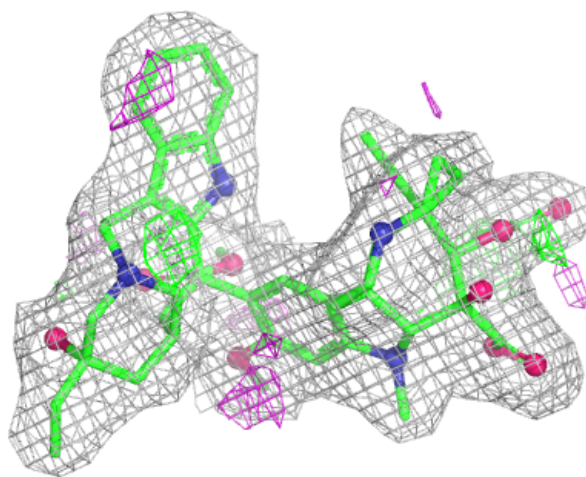
Electron density around GDP D 501:

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



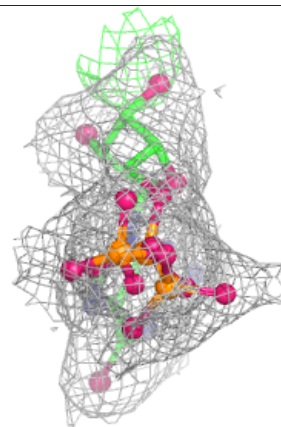
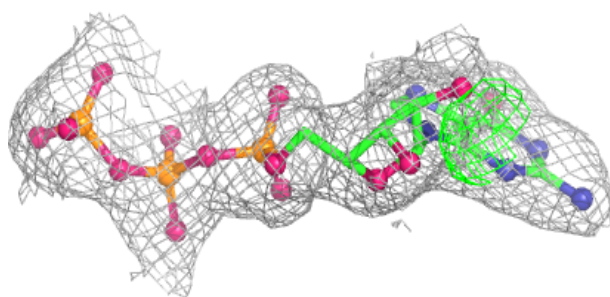
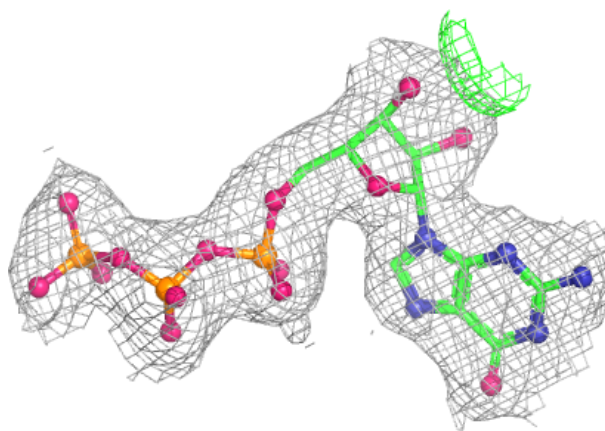
Electron density around VLB C 507:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

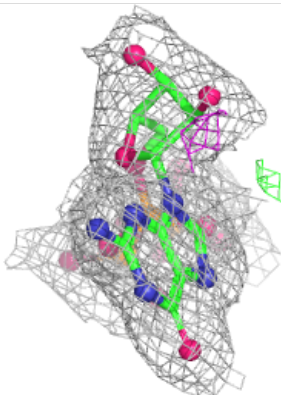
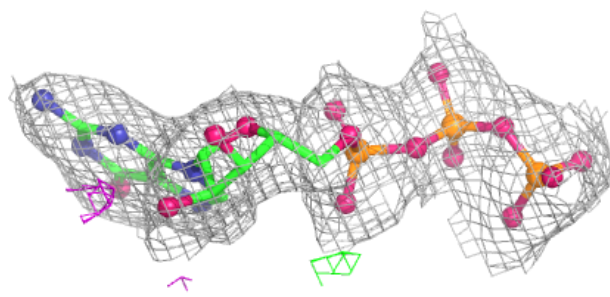
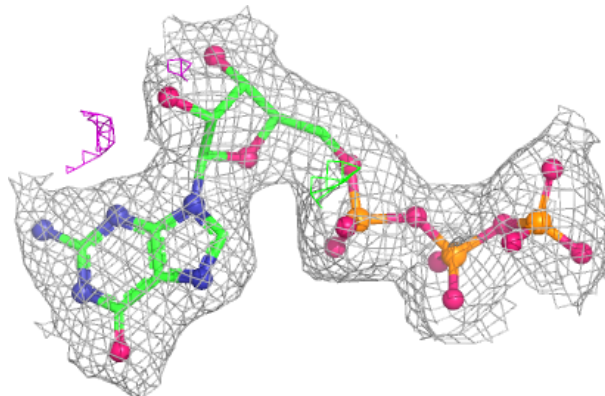


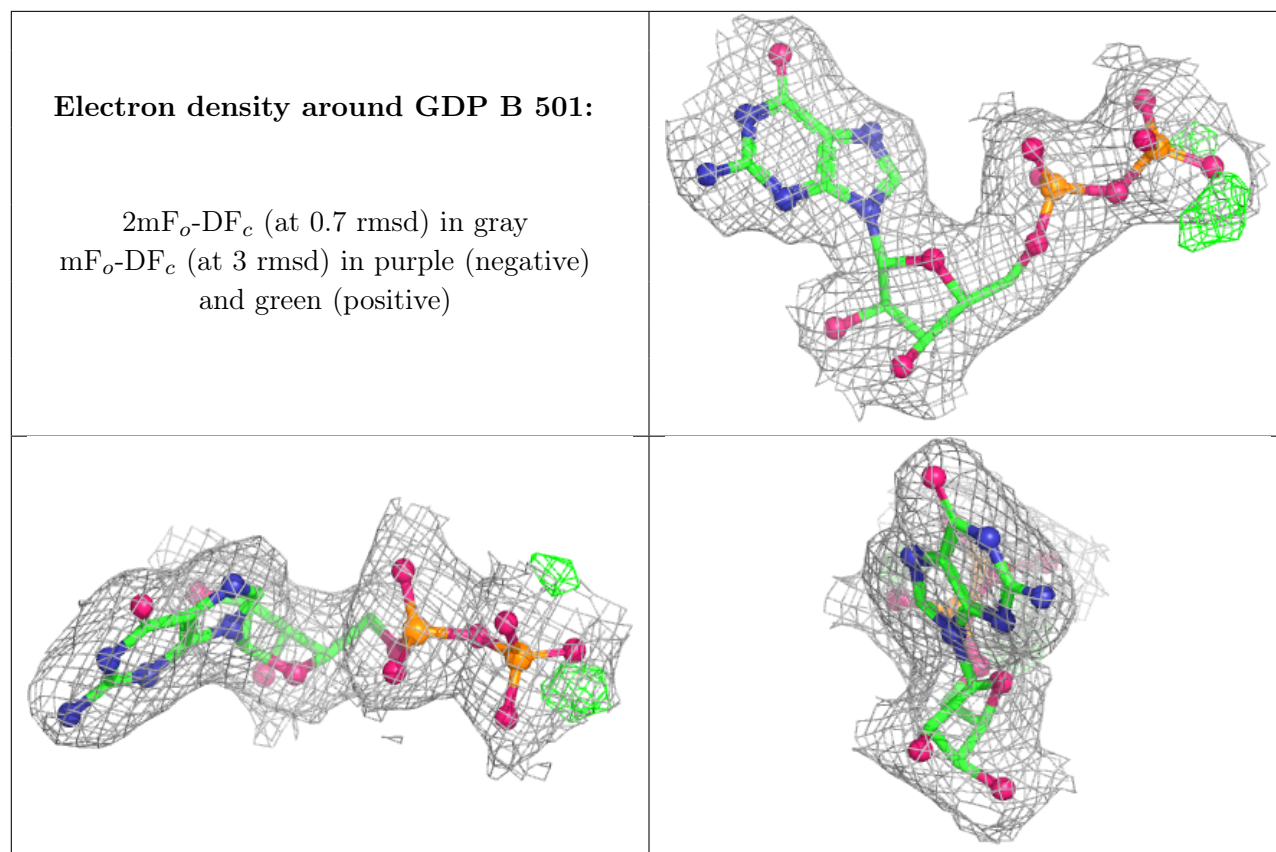
Electron density around GTP A 501:

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

**Electron density around GTP C 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.