



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:06 AM UTC

PDB ID : 4X1I / pdb_00004x1i
Title : Discovery of cytotoxic Dolastatin 10 analogs with N-terminal modifications
Authors : Parris, K.D.
Deposited on : 2014-11-24
Resolution : 3.11 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

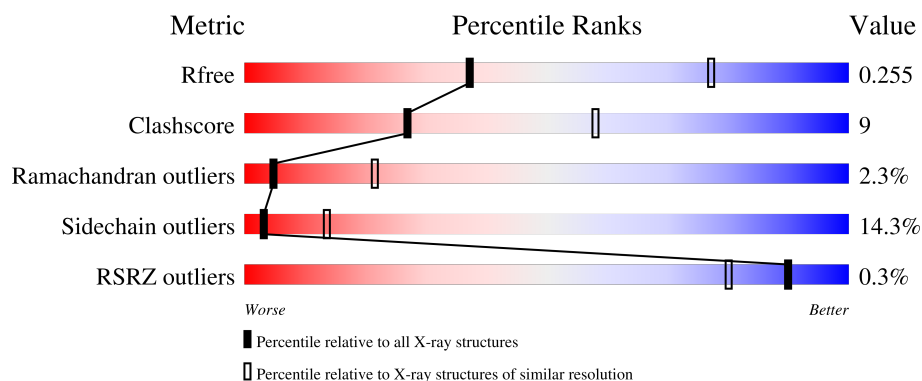
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	63% 26% 6% 5%
1	C	451	64% 24% 7% 5%
2	B	445	61% 28% 6% • •
2	D	445	60% 32% • • • •
3	E	142	59% 20% 7% 13%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14720 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3363	2132	572	638	21			
1	C	430	Total	C	N	O	S	0	3	0
			3354	2126	569	635	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3342	2100	568	649	25			
2	D	430	Total	C	N	O	S	0	1	0
			3369	2112	578	655	24			

- 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
			1008	626	184	195	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

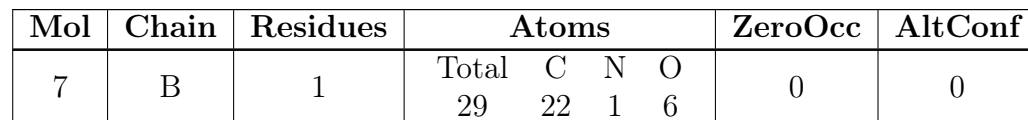
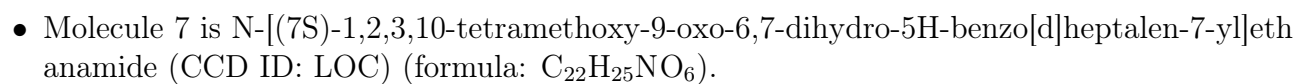


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

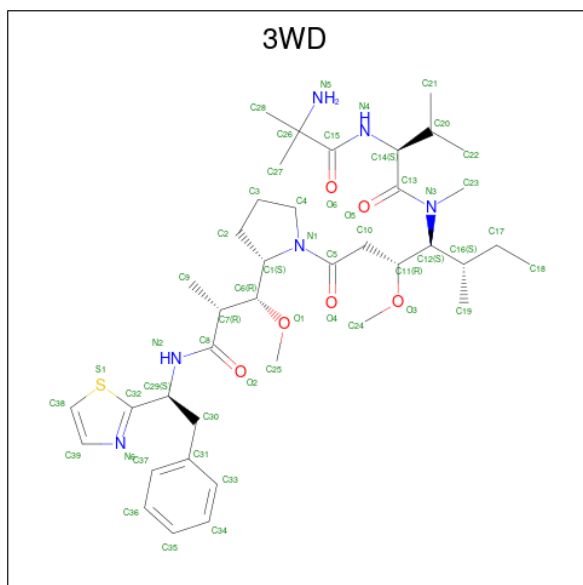


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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			29	22	1	6		

- Molecule 8 is 2-methyl-L-alanyl-N-[(3R,4S,5S)-3-methoxy-1-{(2S)-2-[(1R,2R)-1-methoxy-2-methyl-3-oxo-3-{[(1S)-2-phenyl-1-(1,3-thiazol-2-yl)ethyl]amino}propyl]pyrrolidin-1-yl}-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (CCD ID: 3WD) (formula: C₃₉H₆₂N₆O₆S).

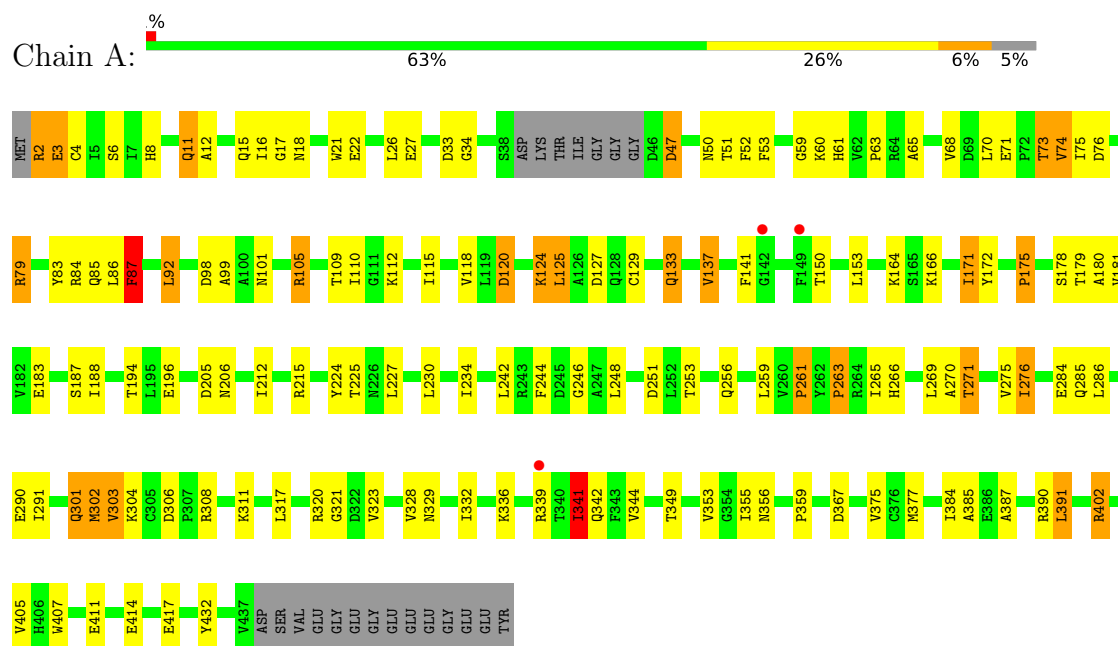


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			52	39	6	6	1		
8	D	1	Total	C	N	O	S	0	0
			52	39	6	6	1		

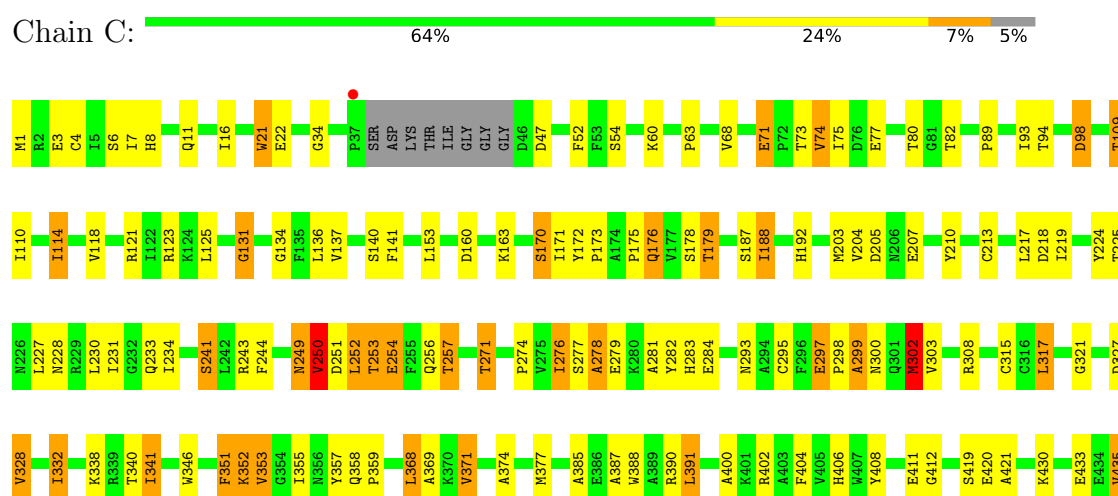
3 Residue-property plots [i](#)

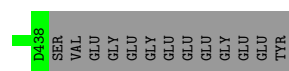
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 chain



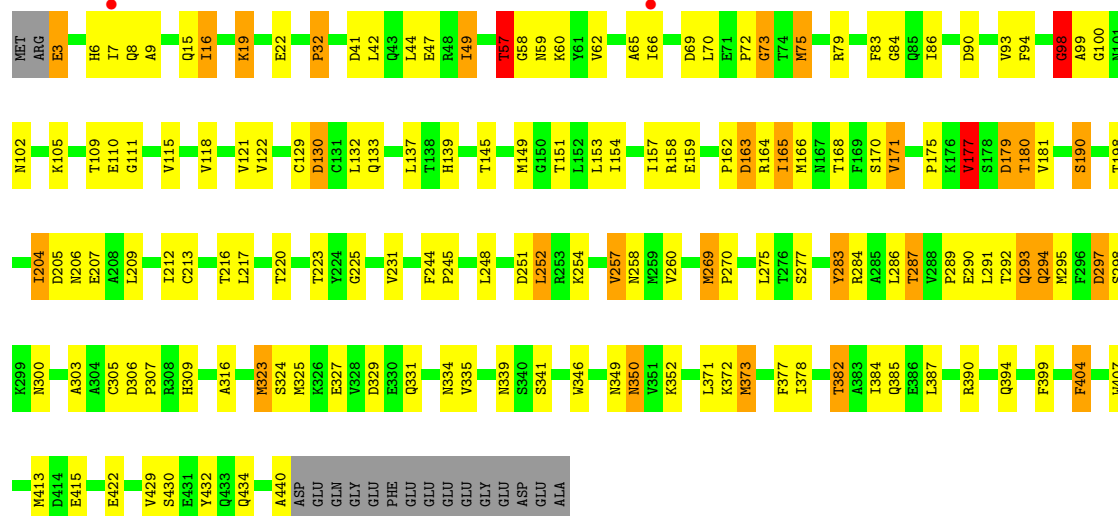
• Molecule 1: Tubulin alpha chain





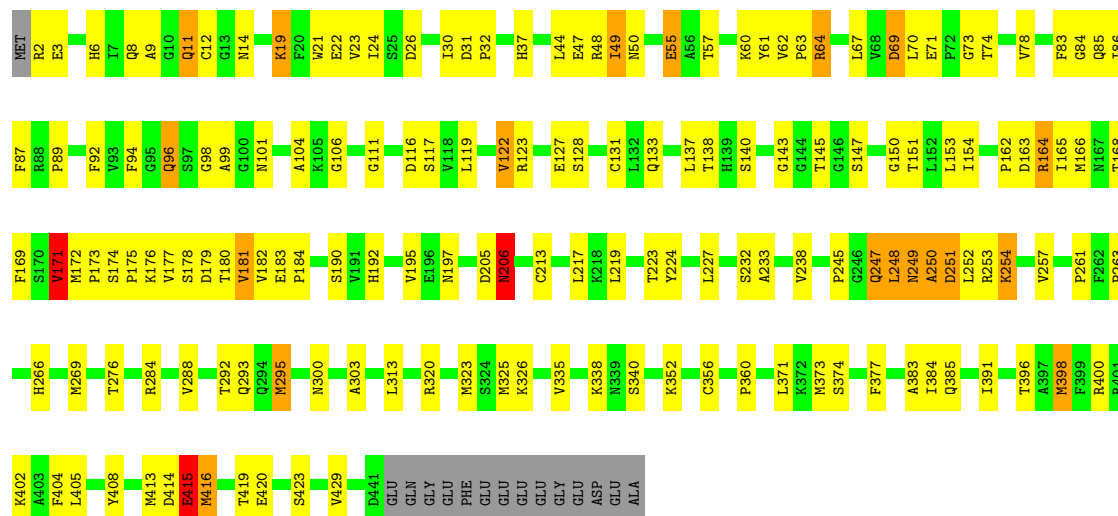
• Molecule 2: Tubulin beta chain

Chain B: 61% 28% 6% . .



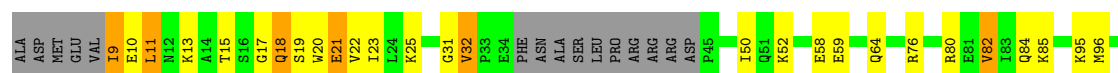
• Molecule 2: Tubulin beta chain

Chain D: 60% 32% . . .



• Molecule 3: Stathmin-4

Chain E: 59% 20% 7% 13%



K100	L101	M105	M108	H115	E121	Q124	E132	K135	N136	K137	E138	L139	K140	E141	GLU	ALA	SER	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.14Å 128.21Å 255.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.30 – 3.11 45.30 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.30-3.11) 99.9 (45.30-3.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.191 , 0.253 (Not available) , 0.255	Depositor DCC
R_{free} test set	1998 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	90.9	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 107.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14720	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, LOC, 3WD, 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	0.84	0/3440	1.49	29/4671 (0.6%)
1	C	0.86	1/3438 (0.0%)	1.48	32/4670 (0.7%)
2	B	0.90	1/3417 (0.0%)	1.57	57/4634 (1.2%)
2	D	0.95	2/3446 (0.1%)	1.54	38/4670 (0.8%)
3	E	0.93	1/1019 (0.1%)	1.65	14/1355 (1.0%)
All	All	0.89	5/14760 (0.0%)	1.53	170/20000 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	32	VAL	CA-C	5.65	1.58	1.52
1	C	302	MET	SD-CE	5.59	1.93	1.79
2	D	398	MET	SD-CE	5.33	1.92	1.79
2	B	260	VAL	CA-C	5.14	1.57	1.53
2	D	206	ASN	C-N	5.03	1.40	1.33

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	ASP	CA-CB-CG	9.06	121.67	112.60
2	D	249	ASN	CA-C-N	8.89	137.70	121.70
2	D	249	ASN	C-N-CA	8.89	137.70	121.70
2	D	177	VAL	N-CA-C	7.72	118.15	111.90
2	B	110	GLU	N-CA-C	7.52	119.17	110.97
2	D	248	LEU	CA-C-N	7.44	135.09	121.70
2	D	248	LEU	C-N-CA	7.44	135.09	121.70
2	D	247	GLN	CA-C-N	7.35	135.57	121.54
2	D	247	GLN	C-N-CA	7.35	135.57	121.54
1	A	359	PRO	N-CA-C	7.28	117.45	110.47
2	B	434	GLN	N-CA-C	-7.22	103.48	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	9	ALA	N-CA-C	7.03	120.35	108.90
2	D	96	GLN	CA-C-N	7.00	129.97	120.38
2	D	96	GLN	C-N-CA	7.00	129.97	120.38
2	B	171	VAL	N-CA-CB	6.89	119.78	111.31
3	E	50	ILE	N-CA-C	-6.87	104.16	110.82
2	B	399	PHE	N-CA-C	6.74	118.63	111.28
2	D	171	VAL	CA-C-N	6.71	129.66	120.67
2	D	171	VAL	C-N-CA	6.71	129.66	120.67
2	B	98	GLY	N-CA-C	6.60	128.83	113.18
1	A	112	LYS	CA-C-N	6.59	129.00	120.44
1	A	112	LYS	C-N-CA	6.59	129.00	120.44
2	D	69	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	306	ASP	CA-CB-CG	6.39	119.00	112.60
2	B	175	PRO	CA-C-N	6.35	129.26	120.63
2	B	175	PRO	C-N-CA	6.35	129.26	120.63
1	C	351	PHE	CA-CB-CG	6.30	120.10	113.80
1	C	250	VAL	N-CA-CB	6.30	121.62	111.23
1	C	328	VAL	N-CA-C	-6.29	104.62	110.53
2	D	162	PRO	CA-C-N	6.14	129.13	120.28
2	D	162	PRO	C-N-CA	6.14	129.13	120.28
1	C	93	ILE	N-CA-C	6.14	116.66	107.51
1	C	254	GLU	N-CA-C	-6.12	104.69	111.36
1	C	175	PRO	CA-C-N	6.12	129.10	120.28
1	C	175	PRO	C-N-CA	6.12	129.10	120.28
1	A	125	LEU	N-CA-C	-6.06	104.60	111.14
2	D	87	PHE	CA-CB-CG	6.05	119.85	113.80
2	B	248	LEU	CA-C-N	5.99	132.49	121.70
2	B	248	LEU	C-N-CA	5.99	132.49	121.70
2	D	163	ASP	CA-CB-CG	5.93	118.53	112.60
2	D	415	GLU	N-CA-C	-5.93	104.90	111.36
2	D	78	VAL	CA-C-N	5.90	128.19	120.28
2	D	78	VAL	C-N-CA	5.90	128.19	120.28
1	A	12	ALA	CA-C-N	5.87	126.60	120.03
1	A	12	ALA	C-N-CA	5.87	126.60	120.03
2	B	115	VAL	N-CA-CB	5.84	116.75	110.62
2	B	415	GLU	CA-C-N	5.79	128.35	120.54
2	B	415	GLU	C-N-CA	5.79	128.35	120.54
2	D	179	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	408	TYR	CA-C-N	5.77	128.04	120.60
1	C	408	TYR	C-N-CA	5.77	128.04	120.60
2	B	157	ILE	CA-C-N	5.76	128.32	120.54
2	B	157	ILE	C-N-CA	5.76	128.32	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	TRP	N-CA-C	5.73	118.30	111.71
2	D	22	GLU	CA-C-N	5.70	127.82	120.70
2	D	22	GLU	C-N-CA	5.70	127.82	120.70
1	A	321	GLY	N-CA-C	5.69	119.72	111.24
2	B	15	GLN	CA-C-N	5.68	127.81	120.70
2	B	15	GLN	C-N-CA	5.68	127.81	120.70
1	A	2	ARG	CA-C-N	5.65	129.13	120.82
1	A	2	ARG	C-N-CA	5.65	129.13	120.82
1	A	71	GLU	CB-CG-CD	5.62	122.15	112.60
2	D	175	PRO	CA-C-N	5.62	128.58	120.38
2	D	175	PRO	C-N-CA	5.62	128.58	120.38
1	C	391	LEU	CA-C-N	5.61	127.80	120.28
1	C	391	LEU	C-N-CA	5.61	127.80	120.28
2	B	413	MET	N-CA-C	5.59	117.74	110.53
3	E	82	VAL	N-CA-CB	5.59	117.72	110.57
2	B	162	PRO	CA-C-N	5.58	128.31	120.28
2	B	162	PRO	C-N-CA	5.58	128.31	120.28
2	B	334	ASN	CA-C-N	5.57	127.58	120.56
2	B	334	ASN	C-N-CA	5.57	127.58	120.56
1	C	433	GLU	CA-C-N	5.57	127.68	120.44
1	C	433	GLU	C-N-CA	5.57	127.68	120.44
1	A	87	PHE	CA-CB-CG	5.56	119.36	113.80
2	B	149	MET	CA-C-N	5.55	126.27	119.99
2	B	149	MET	C-N-CA	5.55	126.27	119.99
2	B	73	GLY	CA-C-N	5.52	127.68	120.28
2	B	73	GLY	C-N-CA	5.52	127.68	120.28
1	C	134	GLY	N-CA-C	5.51	118.02	110.58
2	B	9	ALA	N-CA-C	5.50	117.38	108.41
2	D	313	LEU	N-CA-C	-5.49	104.70	111.40
1	A	342	GLN	N-CA-C	5.47	117.35	110.24
1	C	332	ILE	CA-C-N	5.47	127.55	120.44
1	C	332	ILE	C-N-CA	5.47	127.55	120.44
3	E	138	GLU	CA-C-N	5.41	127.53	120.28
3	E	138	GLU	C-N-CA	5.41	127.53	120.28
1	A	84	ARG	CA-C-N	5.41	128.06	120.28
1	A	84	ARG	C-N-CA	5.41	128.06	120.28
1	A	137	VAL	N-CA-C	5.39	115.86	107.99
2	B	294	GLN	CA-C-N	5.39	127.50	120.28
2	B	294	GLN	C-N-CA	5.39	127.50	120.28
1	C	3	GLU	N-CA-C	5.38	117.66	110.35
1	A	276	ILE	N-CA-C	5.37	116.31	108.53
1	A	385	ALA	CA-C-N	5.37	128.01	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	ALA	C-N-CA	5.37	128.01	120.28
2	B	329	ASP	CA-C-N	5.36	127.47	120.28
2	B	329	ASP	C-N-CA	5.36	127.47	120.28
2	B	372	LYS	CA-C-N	5.36	131.78	121.54
2	B	372	LYS	C-N-CA	5.36	131.78	121.54
1	A	263	PRO	N-CA-C	5.35	120.87	113.65
2	B	41	ASP	CA-C-N	5.34	128.43	120.31
2	B	41	ASP	C-N-CA	5.34	128.43	120.31
2	B	16	ILE	CA-C-N	5.33	125.85	119.94
2	B	16	ILE	C-N-CA	5.33	125.85	119.94
1	A	175	PRO	CA-C-N	5.32	129.11	120.60
1	A	175	PRO	C-N-CA	5.32	129.11	120.60
1	C	188	ILE	N-CA-C	5.31	116.03	110.62
2	B	205	ASP	CA-C-N	5.30	127.91	120.28
2	B	205	ASP	C-N-CA	5.30	127.91	120.28
1	C	74	VAL	N-CA-CB	5.25	116.34	110.51
2	B	171	VAL	CB-CA-C	5.23	117.90	111.25
2	B	292	THR	N-CA-C	5.23	116.84	111.03
1	A	127	ASP	CA-CB-CG	5.22	117.82	112.60
2	B	225	GLY	CA-C-N	5.21	127.53	120.44
2	B	225	GLY	C-N-CA	5.21	127.53	120.44
1	C	341	ILE	N-CA-CB	5.20	117.48	112.28
2	B	180	THR	CA-C-N	5.20	127.86	120.53
2	B	180	THR	C-N-CA	5.20	127.86	120.53
1	A	304	LYS	N-CA-C	5.19	117.74	107.98
1	C	89	PRO	CA-C-N	5.18	127.22	120.28
1	C	89	PRO	C-N-CA	5.18	127.22	120.28
2	D	338	LYS	N-CA-C	-5.16	105.82	112.68
2	D	251	ASP	CA-CB-CG	5.16	117.76	112.60
2	D	233	ALA	CA-C-N	5.15	127.14	120.44
2	D	233	ALA	C-N-CA	5.15	127.14	120.44
2	B	404	PHE	CA-C-N	5.15	127.90	120.38
2	B	404	PHE	C-N-CA	5.15	127.90	120.38
1	C	353	VAL	N-CA-C	5.15	115.37	108.17
1	A	411	GLU	CB-CG-CD	5.14	121.34	112.60
2	D	64	ARG	N-CA-C	-5.14	99.61	108.56
1	A	73	THR	CA-C-N	5.14	127.04	120.56
1	A	73	THR	C-N-CA	5.14	127.04	120.56
3	E	59	GLU	CA-C-N	5.14	127.17	120.28
3	E	59	GLU	C-N-CA	5.14	127.17	120.28
2	D	3	GLU	N-CA-C	5.14	118.09	110.48
1	A	196	GLU	CB-CG-CD	5.12	121.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	171	VAL	CA-C-N	5.11	127.52	120.67
2	B	171	VAL	C-N-CA	5.11	127.52	120.67
1	C	110	ILE	N-CA-C	5.11	116.52	111.67
1	A	4	CYS	N-CA-C	5.10	116.73	108.26
2	B	158	ARG	CA-C-N	5.10	127.62	120.28
2	B	158	ARG	C-N-CA	5.10	127.62	120.28
3	E	115	HIS	N-CA-C	-5.10	105.61	111.07
1	C	390	ARG	CA-C-N	5.09	127.06	120.44
1	C	390	ARG	C-N-CA	5.09	127.06	120.44
3	E	100	LYS	CA-C-N	5.09	127.05	120.44
3	E	100	LYS	C-N-CA	5.09	127.05	120.44
1	C	400	ALA	CA-C-N	5.08	130.34	122.26
1	C	400	ALA	C-N-CA	5.08	130.34	122.26
2	D	94	PHE	N-CA-C	5.08	117.84	109.72
3	E	100	LYS	N-CA-C	-5.08	105.64	111.07
2	D	224	TYR	CA-C-N	5.06	125.60	119.98
2	D	224	TYR	C-N-CA	5.06	125.60	119.98
2	D	300	ASN	CA-C-N	5.05	128.03	120.95
2	D	300	ASN	C-N-CA	5.05	128.03	120.95
2	B	382	THR	CA-C-N	5.05	127.56	120.28
2	B	382	THR	C-N-CA	5.05	127.56	120.28
2	B	251	ASP	CA-C-N	5.04	127.34	120.54
2	B	251	ASP	C-N-CA	5.04	127.34	120.54
2	B	177	VAL	CB-CA-C	5.04	117.06	110.96
3	E	137	LYS	CA-C-N	5.04	127.44	120.29
3	E	137	LYS	C-N-CA	5.04	127.44	120.29
2	B	177	VAL	N-CA-CB	5.02	116.73	111.00
2	B	297	ASP	CA-CB-CG	5.02	117.62	112.60
3	E	85	LYS	CA-C-N	5.01	127.25	120.38
3	E	85	LYS	C-N-CA	5.01	127.25	120.38
1	C	131	GLY	CA-C-N	5.01	128.43	121.02
1	C	131	GLY	C-N-CA	5.01	128.43	121.02
2	D	178	SER	N-CA-C	5.01	116.94	108.02

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	3363	0	3274	60	0
1	C	3354	0	3263	64	0
2	B	3342	0	3198	64	0
2	D	3369	0	3237	70	0
3	E	1008	0	1022	17	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	2	0
7	B	29	0	25	1	0
7	D	29	0	25	0	0
8	B	52	0	62	5	0
8	D	52	0	62	2	0
All	All	14720	0	14216	266	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 9.

All (266) 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)
1:C:252:LEU:HD23	1:C:253:THR:H	1.20	1.06
1:C:241:SER:HA	1:C:250:VAL:HB	1.50	0.91
2:D:133:GLN:HE21	2:D:252:LEU:H	1.16	0.88
1:C:249:ASN:HB2	1:C:355:ILE:H	1.37	0.88
2:D:19:LYS:O	2:D:23:VAL:HG23	1.74	0.88
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.58	0.85
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.27	0.83
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.63	0.81
2:B:206:ASN:HD21	6:B:501:GDP:HN22	1.27	0.80
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.00	0.79
2:D:206:ASN:HD21	6:D:501:GDP:HN22	1.32	0.78
1:C:249:ASN:CB	1:C:355:ILE:H	1.97	0.77
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.65	0.77
2:D:106:GLY:O	2:D:111:GLY:HA3	1.85	0.76
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.69	0.75
1:C:252:LEU:HD23	1:C:253:THR:N	1.98	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:NE	1:C:340:THR:HG21	2.03	0.74
2:D:415:GLU:H	2:D:415:GLU:CD	1.96	0.73
1:C:308:ARG:CZ	1:C:340:THR:HG21	2.21	0.70
3:E:11:LEU:HB2	3:E:20:TRP:HA	1.72	0.70
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.27	0.69
2:B:163:ASP:HB2	2:B:164:ARG:HH21	1.58	0.68
2:D:249:ASN:N	2:D:250:ALA:HB2	2.08	0.68
2:D:71:GLU:HG2	2:D:98:GLY:HA2	1.75	0.68
1:A:171:ILE:HG23	1:A:206:ASN:HD21	1.59	0.68
2:D:184:PRO:HG2	2:D:398:MET:HE1	1.76	0.67
8:D:503:3WD:H38	8:D:503:3WD:H34	1.75	0.67
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.76	0.66
2:B:331:GLN:O	2:B:335:VAL:HG23	1.96	0.66
2:D:249:ASN:H	2:D:250:ALA:HB2	1.62	0.65
2:D:69:ASP:HA	2:D:145:THR:HG21	1.78	0.65
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.80	0.64
2:D:154:ILE:HG22	2:D:197:ASN:HB3	1.79	0.64
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.80	0.63
2:B:22:GLU:HB2	2:B:83:PHE:CD2	2.33	0.62
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.80	0.62
2:B:177:VAL:HA	8:B:503:3WD:H23	1.80	0.62
2:D:192:HIS:O	2:D:195:VAL:HG12	1.99	0.61
1:A:172:TYR:OH	1:A:387:ALA:O	2.12	0.60
1:C:271:THR:HG21	1:C:295:CYS:O	2.01	0.60
2:B:407:TRP:CZ2	1:C:257:THR:HA	2.36	0.60
1:C:141:PHE:CE1	1:C:170:SER:HB2	2.36	0.60
2:B:269:MET:HG2	2:B:303:ALA:HB3	1.84	0.60
2:D:147:SER:HB2	2:D:190:SER:OG	2.02	0.59
2:D:6:HIS:HE1	2:D:8:GLN:NE2	1.97	0.59
2:B:206:ASN:HD22	2:B:209:LEU:HD12	1.67	0.59
1:A:286:LEU:HD23	1:A:290:GLU:HB3	1.85	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.85	0.58
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.49	0.58
1:A:175:PRO:HA	1:A:179:THR:CG2	2.32	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.83	0.58
2:D:396:THR:O	2:D:400:ARG:HB2	2.03	0.58
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.86	0.58
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.22	0.57
2:D:89:PRO:HA	2:D:92:PHE:CD1	2.38	0.57
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.87	0.57
8:B:503:3WD:H20	8:B:503:3WD:H18	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ARG:CD	1:C:340:THR:HG21	2.35	0.57
1:C:338:LYS:HD3	1:C:340:THR:HB	1.87	0.57
2:D:320:ARG:HG2	2:D:356:CYS:HB3	1.87	0.57
1:C:176:GLN:H	1:C:176:GLN:HE21	1.52	0.57
2:B:179:ASP:HB2	1:C:352:LYS:HG2	1.87	0.56
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.88	0.56
1:C:178:SER:O	1:C:179:THR:HG22	2.06	0.56
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.88	0.56
1:C:176:GLN:H	1:C:176:GLN:NE2	2.04	0.56
2:D:44:LEU:HA	2:D:49:ILE:HB	1.88	0.56
1:C:317:LEU:HB2	1:C:353:VAL:HG22	1.88	0.55
1:A:355:ILE:O	3:E:17:GLY:HA2	2.07	0.55
2:D:323:MET:HE3	2:D:373:MET:HG2	1.88	0.55
2:B:79:ARG:HH22	2:B:94:PHE:HE2	1.54	0.55
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.88	0.55
2:B:98:GLY:C	2:B:100:GLY:H	2.15	0.54
2:B:350:ASN:H	2:B:350:ASN:HD22	1.54	0.54
2:D:253:ARG:O	2:D:257:VAL:HG23	2.07	0.54
2:B:16:ILE:HD12	2:B:231:VAL:HG11	1.89	0.54
2:D:12:CYS:SG	2:D:171:VAL:HG11	2.47	0.54
1:C:308:ARG:HD2	1:C:340:THR:HG21	1.89	0.54
2:B:118:VAL:O	2:B:121:VAL:HB	2.08	0.54
2:B:69:ASP:HA	2:B:145:THR:HG21	1.90	0.54
2:D:133:GLN:HE21	2:D:252:LEU:N	1.95	0.54
1:C:34:GLY:HA3	1:C:60:LYS:HG2	1.89	0.53
3:E:11:LEU:HD23	3:E:21:GLU:HB2	1.88	0.53
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.91	0.53
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.90	0.53
2:D:123:ARG:O	2:D:127:GLU:HG2	2.09	0.53
1:C:228:ASN:HA	1:C:231:ILE:HD12	1.89	0.53
1:C:75:ILE:HB	1:C:94:THR:CG2	2.39	0.52
1:A:175:PRO:HA	1:A:179:THR:HG22	1.91	0.52
2:D:104:ALA:HB2	2:D:413:MET:SD	2.50	0.52
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.92	0.52
2:D:269:MET:HE1	2:D:383:ALA:HB3	1.91	0.52
1:A:269:LEU:HD11	1:A:301:GLN:HG2	1.90	0.52
2:D:11:GLN:HA	2:D:74:THR:HG21	1.91	0.52
2:B:290:GLU:O	2:B:294:GLN:HB2	2.10	0.52
1:A:3:GLU:HG3	1:A:129:CYS:HB3	1.92	0.51
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.91	0.51
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:HA	1:A:79:ARG:HG3	1.92	0.51
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.92	0.51
3:E:13:LYS:HA	3:E:18:GLN:HG2	1.93	0.51
2:D:83:PHE:O	2:D:85:GLN:N	2.44	0.51
2:D:181:VAL:HG21	2:D:404:PHE:CZ	2.46	0.51
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.91	0.51
8:B:503:3WD:H1	8:B:503:3WD:O4	2.10	0.51
2:B:382:THR:HA	2:B:432:TYR:CD2	2.46	0.50
1:A:98:ASP:OD2	2:B:254:LYS:HE2	2.11	0.50
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.92	0.50
1:C:321:GLY:HA2	1:C:359:PRO:HA	1.93	0.50
2:B:3:GLU:O	2:B:133:GLN:HG3	2.11	0.50
1:C:241:SER:HB2	1:C:252:LEU:H	1.76	0.50
1:A:402:ARG:HG3	1:A:405:VAL:HG21	1.94	0.50
1:C:406:HIS:CD2	2:D:263:PRO:HG3	2.46	0.50
1:A:328:VAL:HG21	1:A:355:ILE:HD11	1.93	0.50
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.93	0.50
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.92	0.50
1:A:50:ASN:C	1:A:52:PHE:H	2.20	0.50
1:A:68:VAL:HG21	1:A:118:VAL:HG13	1.94	0.50
3:E:101:LEU:HD12	3:E:105:MET:HG2	1.94	0.49
1:A:246:GLY:HA2	3:E:17:GLY:HA3	1.94	0.49
2:B:32:PRO:HB3	2:B:83:PHE:HA	1.93	0.49
2:B:390:ARG:O	2:B:394:GLN:HG3	2.12	0.49
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.94	0.49
2:D:360:PRO:HG2	2:D:371:LEU:HB2	1.95	0.49
1:A:259:LEU:O	1:A:261:PRO:HD3	2.12	0.49
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.47	0.49
1:C:204:VAL:HG22	1:C:302:MET:HG2	1.94	0.49
2:D:50:ASN:O	2:D:64:ARG:NH2	2.46	0.49
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.61	0.48
2:D:150:GLY:O	2:D:154:ILE:HG13	2.13	0.48
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.49	0.48
1:C:192:HIS:CG	1:C:421:ALA:HA	2.48	0.48
1:C:217:LEU:HD21	1:C:368:LEU:HG	1.96	0.48
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.95	0.48
1:C:297:GLU:OE2	1:C:299:ALA:HB3	2.14	0.48
1:C:234:ILE:HG21	1:C:302:MET:SD	2.54	0.47
2:D:55:GLU:HG2	2:D:61:TYR:CE2	2.49	0.47
2:D:44:LEU:HD23	2:D:49:ILE:HD13	1.95	0.47
2:D:151:THR:HA	2:D:154:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:GLU:OE1	3:E:76:ARG:HD2	2.14	0.47
2:B:289:PRO:O	2:B:293:GLN:HG2	2.15	0.47
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.49	0.47
1:C:224:TYR:HA	1:C:227:LEU:HD12	1.96	0.47
2:B:295:MET:HE2	2:B:295:MET:HB3	1.80	0.47
2:B:306:ASP:HB3	2:B:309:HIS:HD2	1.80	0.47
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.47
1:C:274:PRO:HD3	1:C:374:ALA:HA	1.97	0.47
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.96	0.47
2:D:143:GLY:HA3	6:D:501:GDP:O3A	2.15	0.47
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.96	0.47
1:A:11:GLN:HG2	1:A:74:VAL:HG21	1.97	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.50	0.47
1:A:70:LEU:HB2	1:A:98:ASP:HA	1.97	0.46
1:A:244:PHE:HB2	1:A:356:ASN:HD21	1.80	0.46
1:C:252:LEU:CD2	1:C:253:THR:H	2.09	0.46
1:A:15:GLN:O	1:A:18:ASN:HB2	2.14	0.46
2:B:305:CYS:SG	2:B:384:ILE:HA	2.54	0.46
1:C:404:PHE:CD2	2:D:261:PRO:HA	2.51	0.46
2:D:251:ASP:HB3	2:D:254:LYS:HB2	1.97	0.46
2:B:204:ILE:HG22	2:B:209:LEU:HD11	1.98	0.46
1:A:212:ILE:HG22	1:A:275:VAL:HG11	1.98	0.46
2:B:58:GLY:HA3	2:B:59:ASN:C	2.41	0.46
2:B:44:LEU:HD23	2:B:49:ILE:HD13	1.97	0.46
2:B:323:MET:HE3	2:B:373:MET:HE3	1.98	0.46
1:A:212:ILE:HG12	1:A:215:ARG:HH12	1.79	0.46
2:B:6:HIS:O	2:B:65:ALA:HA	2.15	0.46
2:B:324:SER:HB3	2:B:327:GLU:HB2	1.98	0.46
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.98	0.45
2:B:350:ASN:H	2:B:350:ASN:ND2	2.14	0.45
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.51	0.45
1:A:175:PRO:HA	1:A:179:THR:HG21	1.97	0.45
2:B:298:SER:OG	2:B:307:PRO:HD2	2.17	0.45
1:A:286:LEU:HD12	1:A:286:LEU:H	1.82	0.45
2:D:119:LEU:HA	2:D:122:VAL:HG22	1.98	0.45
2:D:263:PRO:O	2:D:266:HIS:HD2	1.99	0.45
2:D:2:ARG:HB3	2:D:131:CYS:O	2.17	0.45
2:B:7:ILE:HG13	2:B:66:ILE:HD13	1.99	0.45
2:B:154:ILE:HA	2:B:166:MET:HE3	1.97	0.45
1:C:141:PHE:HB2	1:C:173:PRO:HD3	1.99	0.45
1:A:205:ASP:HB2	1:A:303:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ALA:H	1:A:183:GLU:CD	2.25	0.45
1:A:263:PRO:O	1:A:266:HIS:HD2	2.00	0.45
1:C:213:CYS:HB3	1:C:219:ILE:HD12	1.99	0.45
1:C:276:ILE:HD13	1:C:369:ALA:HB3	1.99	0.45
3:E:132:GLU:HA	3:E:135:LYS:HB3	1.98	0.45
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.52	0.44
1:A:271:THR:O	1:A:377:MET:N	2.50	0.44
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.99	0.44
1:C:207:GLU:O	1:C:210:TYR:HB3	2.18	0.44
3:E:9:ILE:HD13	3:E:23:ILE:H	1.83	0.44
3:E:80:ARG:O	3:E:84:GLN:HB2	2.16	0.44
1:A:329:ASN:HA	1:A:332:ILE:HD12	1.98	0.44
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.44
2:D:101:ASN:HD22	2:D:180:THR:HG21	1.82	0.44
2:D:416:MET:HE2	2:D:420:GLU:HG3	1.99	0.44
2:B:151:THR:HG21	2:B:190:SER:HA	1.99	0.44
2:D:62:VAL:HG23	2:D:86:ILE:O	2.17	0.44
2:B:346:TRP:CD1	2:B:346:TRP:H	2.34	0.43
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.52	0.43
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.17	0.43
1:C:412:GLY:HA3	3:E:108:ASN:HD22	1.82	0.43
1:A:387:ALA:HA	1:A:390:ARG:HE	1.84	0.43
2:B:346:TRP:HB3	2:B:440:ALA:HB2	2.01	0.43
1:C:298:PRO:C	1:C:300:ASN:H	2.27	0.43
1:C:308:ARG:HD2	1:C:340:THR:CG2	2.48	0.43
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.01	0.43
1:A:311:LYS:HE2	1:A:344:VAL:HA	2.01	0.43
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.53	0.43
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.54	0.43
8:D:503:3WD:C34	8:D:503:3WD:H3	2.49	0.43
1:A:224:TYR:HA	1:A:227:LEU:HD12	2.00	0.42
1:A:349:THR:HB	3:E:25:LYS:HB3	2.01	0.42
2:B:181:VAL:HG11	2:B:404:PHE:CE2	2.54	0.42
1:C:52:PHE:CD1	1:C:243:ARG:HG2	2.54	0.42
2:D:154:ILE:HA	2:D:166:MET:HE3	2.00	0.42
1:C:317:LEU:HG	1:C:377:MET:HG3	2.00	0.42
1:A:83:TYR:HB3	1:A:86:LEU:HD22	2.00	0.42
1:A:99:ALA:HA	1:A:105:ARG:HG2	2.01	0.42
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.55	0.42
2:B:352:LYS:HE3	7:B:502:LOC:O5	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ILE:O	1:C:118:VAL:HG23	2.20	0.42
1:A:33:ASP:HA	1:A:85:GLN:HB2	2.02	0.42
1:A:329:ASN:HD21	3:E:22:VAL:HG11	1.85	0.42
2:D:174:SER:OG	2:D:176:LYS:HB2	2.19	0.42
1:A:34:GLY:HA3	1:A:60:LYS:HB2	2.01	0.42
1:A:133:GLN:HE22	1:A:251:ASP:HA	1.85	0.42
2:B:244:PHE:HA	2:B:245:PRO:HD3	1.86	0.42
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.01	0.42
1:C:346:TRP:HZ2	1:C:435:VAL:HG22	1.85	0.42
2:D:172:MET:HA	2:D:173:PRO:HD3	1.92	0.42
2:B:139:HIS:CE1	2:B:170:SER:OG	2.73	0.42
1:C:249:ASN:HB3	1:C:250:VAL:H	1.59	0.42
1:C:277:SER:C	1:C:279:GLU:H	2.28	0.41
3:E:11:LEU:HB2	3:E:20:TRP:CA	2.45	0.41
1:A:339:ARG:HH21	1:A:341:ILE:HG23	1.85	0.41
2:D:133:GLN:NE2	2:D:252:LEU:H	1.98	0.41
2:B:57:THR:HA	2:B:58:GLY:HA3	1.73	0.41
2:B:204:ILE:HD13	2:B:270:PRO:HG2	2.01	0.41
2:D:14:ASN:HD22	2:D:67:LEU:HD23	1.85	0.41
2:D:32:PRO:HB3	2:D:83:PHE:HA	2.02	0.41
2:D:181:VAL:HG23	2:D:182:VAL:N	2.35	0.41
1:A:3:GLU:HG3	1:A:129:CYS:CB	2.50	0.41
2:D:47:GLU:HB3	2:D:245:PRO:HG3	2.02	0.41
3:E:10:GLU:HA	3:E:20:TRP:HB2	2.02	0.41
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.86	0.41
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.61	0.41
8:B:503:3WD:H2	8:B:503:3WD:H43	2.03	0.41
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.41
2:B:70:LEU:HD21	2:B:111:GLY:HA2	2.03	0.41
1:A:120:ASP:O	1:A:124:LYS:HD2	2.21	0.41
1:A:248:LEU:HB2	3:E:19:SER:HB3	2.03	0.41
2:B:3:GLU:OE2	2:B:130:ASP:N	2.54	0.41
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.83	0.41
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.03	0.41
2:B:19:LYS:HA	2:B:22:GLU:HG2	2.02	0.41
2:D:164:ARG:HH12	2:D:253:ARG:HH11	1.68	0.40
2:D:408:TYR:O	2:D:413:MET:HB2	2.20	0.40
1:A:87:PHE:HB2	1:A:92:LEU:HD11	2.03	0.40
1:A:291:ILE:HD12	1:A:375:VAL:HG12	2.03	0.40
8:B:503:3WD:H9	8:B:503:3WD:H44	1.67	0.40
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:MET:HB3	2:B:198:THR:HA	2.03	0.40
1:C:172:TYR:OH	1:C:387:ALA:O	2.37	0.40
1:C:244:PHE:CE2	1:C:358:GLN:HG3	2.57	0.40
2:D:12:CYS:SG	2:D:171:VAL:CG1	3.08	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	425/451 (94%)	371 (87%)	45 (11%)	9 (2%)	5	23
1	C	429/451 (95%)	383 (89%)	35 (8%)	11 (3%)	4	19
2	B	426/445 (96%)	379 (89%)	35 (8%)	12 (3%)	4	19
2	D	429/445 (96%)	401 (94%)	21 (5%)	7 (2%)	7	29
3	E	119/142 (84%)	109 (92%)	7 (6%)	3 (2%)	4	20
All	All	1828/1934 (94%)	1643 (90%)	143 (8%)	42 (2%)	5	21

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	THR
2	B	57	THR
2	B	60	LYS
2	B	73	GLY
2	B	373	MET
1	C	249	ASN
1	C	283	HIS
2	D	84	GLY
2	D	181	VAL
2	D	248	LEU

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Mol	Chain	Res	Type
2	D	250	ALA
3	E	32	VAL
1	A	59	GLY
1	A	341	ILE
2	B	109	THR
2	B	283	TYR
2	B	284	ARG
1	C	73	THR
1	C	282	TYR
1	C	284	GLU
1	C	299	ALA
2	D	73	GLY
2	D	128	SER
3	E	15	THR
1	A	47	ASP
2	B	84	GLY
1	C	109	THR
1	C	281	ALA
1	A	51	THR
1	A	109	THR
1	A	178	SER
2	B	32	PRO
2	D	340	SER
1	A	261	PRO
2	B	99	ALA
1	C	250	VAL
1	C	278	ALA
1	A	115	ILE
3	E	31	GLY
1	C	131	GLY
2	B	72	PRO
2	B	98	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	362/378 (96%)	307 (85%)	55 (15%)	3	12
1	C	360/378 (95%)	302 (84%)	58 (16%)	2	10
2	B	364/383 (95%)	314 (86%)	50 (14%)	3	15
2	D	369/383 (96%)	325 (88%)	44 (12%)	5	20
3	E	107/125 (86%)	90 (84%)	17 (16%)	2	11
All	All	1562/1647 (95%)	1338 (86%)	224 (14%)	3	13

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	GLU
1	A	6	SER
1	A	11	GLN
1	A	16	ILE
1	A	22	GLU
1	A	26	LEU
1	A	27	GLU
1	A	47	ASP
1	A	74	VAL
1	A	75	ILE
1	A	79	ARG
1	A	87	PHE
1	A	92	LEU
1	A	105	ARG
1	A	120	ASP
1	A	124	LYS
1	A	125	LEU
1	A	133	GLN
1	A	137	VAL
1	A	141	PHE
1	A	150	THR
1	A	153	LEU
1	A	164	LYS
1	A	166	LYS
1	A	171	ILE
1	A	181	VAL
1	A	187	SER
1	A	188	ILE
1	A	194	THR
1	A	225	THR

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	234	ILE
1	A	242	LEU
1	A	253	THR
1	A	256	GLN
1	A	271	THR
1	A	276	ILE
1	A	284	GLU
1	A	285	GLN
1	A	301	GLN
1	A	302	MET
1	A	303	VAL
1	A	308	ARG
1	A	317	LEU
1	A	320	ARG
1	A	323	VAL
1	A	336	LYS
1	A	341	ILE
1	A	367	ASP
1	A	384	ILE
1	A	391	LEU
1	A	402	ARG
1	A	414	GLU
1	A	417	GLU
2	B	3	GLU
2	B	19	LYS
2	B	42	LEU
2	B	47	GLU
2	B	49	ILE
2	B	57	THR
2	B	62	VAL
2	B	75	MET
2	B	86	ILE
2	B	90	ASP
2	B	93	VAL
2	B	122	VAL
2	B	129	CYS
2	B	130	ASP
2	B	132	LEU
2	B	153	LEU
2	B	163	ASP
2	B	165	ILE

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Mol	Chain	Res	Type
2	B	171	VAL
2	B	177	VAL
2	B	179	ASP
2	B	180	THR
2	B	190	SER
2	B	204	ILE
2	B	207	GLU
2	B	212	ILE
2	B	216	THR
2	B	220	THR
2	B	223	THR
2	B	252	LEU
2	B	257	VAL
2	B	269	MET
2	B	277	SER
2	B	283	TYR
2	B	286	LEU
2	B	287	THR
2	B	291	LEU
2	B	293	GLN
2	B	297	ASP
2	B	323	MET
2	B	325	MET
2	B	339	ASN
2	B	341	SER
2	B	349	ASN
2	B	350	ASN
2	B	371	LEU
2	B	377	PHE
2	B	387	LEU
2	B	422	GLU
2	B	430	SER
1	C	1	MET
1	C	11	GLN
1	C	16	ILE
1	C	22	GLU
1	C	47	ASP
1	C	54	SER
1	C	68	VAL
1	C	71	GLU
1	C	74	VAL
1	C	77	GLU

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Mol	Chain	Res	Type
1	C	80	THR
1	C	82	THR
1	C	109	THR
1	C	114	ILE
1	C	121	ARG
1	C	123	ARG
1	C	125	LEU
1	C	137	VAL
1	C	140	SER
1	C	160	ASP
1	C	163	LYS
1	C	170	SER
1	C	171	ILE
1	C	176	GLN
1	C	179	THR
1	C	188	ILE
1	C	203	MET
1	C	218	ASP
1	C	225	THR
1	C	233	GLN
1	C	241	SER
1	C	251	ASP
1	C	252	LEU
1	C	253	THR
1	C	254	GLU
1	C	256	GLN
1	C	257	THR
1	C	271	THR
1	C	276	ILE
1	C	293	ASN
1	C	297	GLU
1	C	302	MET
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	317	LEU
1	C	327	ASP
1	C	332	ILE
1	C	341	ILE
1	C	351	PHE
1	C	352	LYS
1	C	357	TYR
1	C	368	LEU

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Mol	Chain	Res	Type
1	C	371	VAL
1	C	402	ARG
1	C	419	SER
1	C	420	GLU
1	C	430	LYS
1	C	435	VAL
2	D	11	GLN
2	D	19	LYS
2	D	24	ILE
2	D	26	ASP
2	D	30	ILE
2	D	31	ASP
2	D	37	HIS
2	D	48	ARG
2	D	49	ILE
2	D	55	GLU
2	D	57	THR
2	D	60	LYS
2	D	96	GLN
2	D	116	ASP
2	D	117	SER
2	D	122	VAL
2	D	153	LEU
2	D	164	ARG
2	D	171	VAL
2	D	183	GLU
2	D	206	ASN
2	D	223	THR
2	D	227	LEU
2	D	238	VAL
2	D	247	GLN
2	D	254	LYS
2	D	276	THR
2	D	284	ARG
2	D	288	VAL
2	D	293	GLN
2	D	295	MET
2	D	325	MET
2	D	326	LYS
2	D	352	LYS
2	D	374	SER
2	D	384	ILE

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Mol	Chain	Res	Type
2	D	391	ILE
2	D	402	LYS
2	D	405	LEU
2	D	414	ASP
2	D	415	GLU
2	D	416	MET
2	D	419	THR
2	D	423	SER
3	E	9	ILE
3	E	11	LEU
3	E	18	GLN
3	E	21	GLU
3	E	52	LYS
3	E	58	GLU
3	E	64	GLN
3	E	82	VAL
3	E	95	LYS
3	E	96	MET
3	E	101	LEU
3	E	108	ASN
3	E	121	GLU
3	E	124	GLN
3	E	132	GLU
3	E	135	LYS
3	E	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	91	GLN
1	A	139	HIS
1	A	206	ASN
1	A	233	GLN
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	301	GLN
1	A	329	ASN
1	A	356	ASN
1	A	372	GLN

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Mol	Chain	Res	Type
2	B	8	GLN
2	B	14	ASN
2	B	96	GLN
2	B	139	HIS
2	B	197	ASN
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	293	GLN
2	B	309	HIS
2	B	334	ASN
2	B	337	ASN
2	B	349	ASN
2	B	350	ASN
2	B	406	HIS
2	B	426	ASN
2	B	433	GLN
2	B	434	GLN
2	B	436	GLN
1	C	8	HIS
1	C	15	GLN
1	C	35	GLN
1	C	128	GLN
1	C	133	GLN
1	C	176	GLN
1	C	249	ASN
1	C	301	GLN
1	C	406	HIS
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	101	ASN
2	D	133	GLN
2	D	139	HIS
2	D	167	ASN
2	D	193	GLN
2	D	206	ASN
2	D	249	ASN
2	D	266	HIS
2	D	331	GLN
2	D	339	ASN
2	D	426	ASN

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Mol	Chain	Res	Type
2	D	433	GLN
3	E	71	HIS
3	E	84	GLN
3	E	91	ASN
3	E	108	ASN
3	E	111	ASN
3	E	129	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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	3WD	D	503	-	50,54,54	1.05	4 (8%)	58,76,76	1.24	9 (15%)
7	LOC	B	502	-	31,31,31	0.85	1 (3%)	44,44,44	0.61	1 (2%)
6	GDP	B	501	-	29,30,30	0.50	0	45,47,47	0.58	0
6	GDP	D	501	-	29,30,30	0.51	0	45,47,47	0.63	0
8	3WD	B	503	-	50,54,54	1.03	4 (8%)	58,76,76	1.80	11 (18%)
7	LOC	D	502	-	31,31,31	0.44	0	44,44,44	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GTP	C	600	5	33,34,34	2.18	2 (6%)	50,54,54	0.57	0
4	GTP	A	600	5	33,34,34	2.30	2 (6%)	50,54,54	0.52	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
8	3WD	D	503	-	-	13/72/82/82	0/3/3/3
7	LOC	B	502	-	-	0/12/25/25	0/3/3/3
6	GDP	B	501	-	-	4/16/32/32	0/3/3/3
6	GDP	D	501	-	-	3/16/32/32	0/3/3/3
8	3WD	B	503	-	-	25/72/82/82	0/3/3/3
7	LOC	D	502	-	-	0/12/25/25	0/3/3/3
4	GTP	C	600	5	-	3/22/38/38	0/3/3/3
4	GTP	A	600	5	-	4/22/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	PB-O3B	-9.23	1.49	1.59
4	A	600	GTP	PA-O3A	-9.06	1.49	1.59
4	C	600	GTP	PB-O3B	-8.78	1.50	1.59
4	C	600	GTP	PA-O3A	-8.46	1.50	1.59
8	D	503	3WD	C12-N3	4.77	1.57	1.47
8	B	503	3WD	C12-N3	4.40	1.56	1.47
7	B	502	LOC	C11-C14	4.34	1.60	1.53
8	B	503	3WD	C11-C12	4.03	1.61	1.52
8	D	503	3WD	C11-C12	3.20	1.59	1.52
8	D	503	3WD	C7-C8	3.18	1.57	1.52
8	B	503	3WD	C16-C12	2.72	1.60	1.54
8	D	503	3WD	C16-C12	2.56	1.59	1.54
8	B	503	3WD	C29-C32	2.25	1.56	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WD	C23-N3-C12	-5.58	108.46	119.48
8	B	503	3WD	C32-C29-N2	5.07	117.60	109.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	3WD	C23-N3-C12	-5.05	109.50	119.48
8	B	503	3WD	C12-N3-C13	4.67	133.71	120.34
8	B	503	3WD	C29-N2-C8	3.88	129.98	121.65
8	B	503	3WD	C19-C16-C12	3.70	121.26	111.38
8	B	503	3WD	C7-C8-N2	-3.69	110.89	116.35
8	B	503	3WD	C29-C32-S1	3.62	126.60	121.79
8	B	503	3WD	C30-C29-C32	3.21	115.68	111.03
8	D	503	3WD	C20-C14-C13	2.90	116.38	110.71
8	B	503	3WD	C29-C32-N6	-2.84	119.20	123.71
8	D	503	3WD	C14-C13-N3	2.36	123.46	118.80
8	D	503	3WD	O5-C13-C14	-2.31	115.61	119.96
8	D	503	3WD	C11-C10-C5	2.24	115.68	112.38
8	B	503	3WD	C14-C13-N3	2.20	123.14	118.80
8	D	503	3WD	C23-N3-C13	2.14	129.14	122.24
8	D	503	3WD	C20-C14-N4	2.08	116.46	111.44
8	D	503	3WD	C7-C8-N2	-2.08	113.28	116.35
8	B	503	3WD	O1-C6-C7	2.05	110.68	105.83
7	B	502	LOC	C14-C11-N1	2.03	115.91	114.31
8	D	503	3WD	C19-C16-C12	2.01	116.74	111.38

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O2A
8	B	503	3WD	O6-C15-C26-N5
8	B	503	3WD	N4-C15-C26-N5
8	B	503	3WD	O5-C13-N3-C23
8	B	503	3WD	C10-C11-C12-C16
8	B	503	3WD	O3-C11-C12-N3
8	B	503	3WD	O3-C11-C12-C16
8	B	503	3WD	N3-C12-C16-C17
8	B	503	3WD	C11-C12-C16-C17
8	B	503	3WD	N3-C12-C16-C19
8	B	503	3WD	C11-C12-C16-C19

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Mol	Chain	Res	Type	Atoms
8	B	503	3WD	C1-C6-C7-C8
8	B	503	3WD	C7-C6-O1-C25
8	B	503	3WD	C30-C29-N2-C8
8	B	503	3WD	N2-C29-C32-S1
8	D	503	3WD	C10-C11-C12-N3
8	D	503	3WD	C10-C5-N1-C1
8	D	503	3WD	C10-C5-N1-C4
8	D	503	3WD	O6-C15-C26-C27
8	D	503	3WD	N4-C15-C26-C27
8	D	503	3WD	C13-C14-C20-C22
8	B	503	3WD	C16-C12-N3-C13
8	B	503	3WD	N4-C15-C26-C28
8	B	503	3WD	O1-C6-C7-C9
8	B	503	3WD	O6-C15-C26-C28
8	D	503	3WD	N4-C14-C20-C22
8	B	503	3WD	C14-C13-N3-C23
8	B	503	3WD	C19-C16-C17-C18
8	D	503	3WD	C13-C14-C20-C21
8	D	503	3WD	O4-C5-N1-C4
8	B	503	3WD	C29-C30-C31-C37
8	B	503	3WD	C29-C30-C31-C33
4	A	600	GTP	PB-O3A-PA-O1A
4	A	600	GTP	C3'-C4'-C5'-O5'
8	B	503	3WD	N2-C29-C32-N6
8	B	503	3WD	N4-C15-C26-C27
6	D	501	GDP	C5'-O5'-PA-O1A
8	B	503	3WD	N1-C1-C6-C7
6	B	501	GDP	C4'-C5'-O5'-PA
8	D	503	3WD	O5-C13-C14-C20
4	A	600	GTP	O4'-C4'-C5'-O5'
8	D	503	3WD	C5-C10-C11-O3
8	D	503	3WD	N3-C12-C16-C17
8	D	503	3WD	N3-C13-C14-N4
4	A	600	GTP	PB-O3A-PA-O2A

There are no ring outliers.

5 monomers are involved in 11 short contacts:

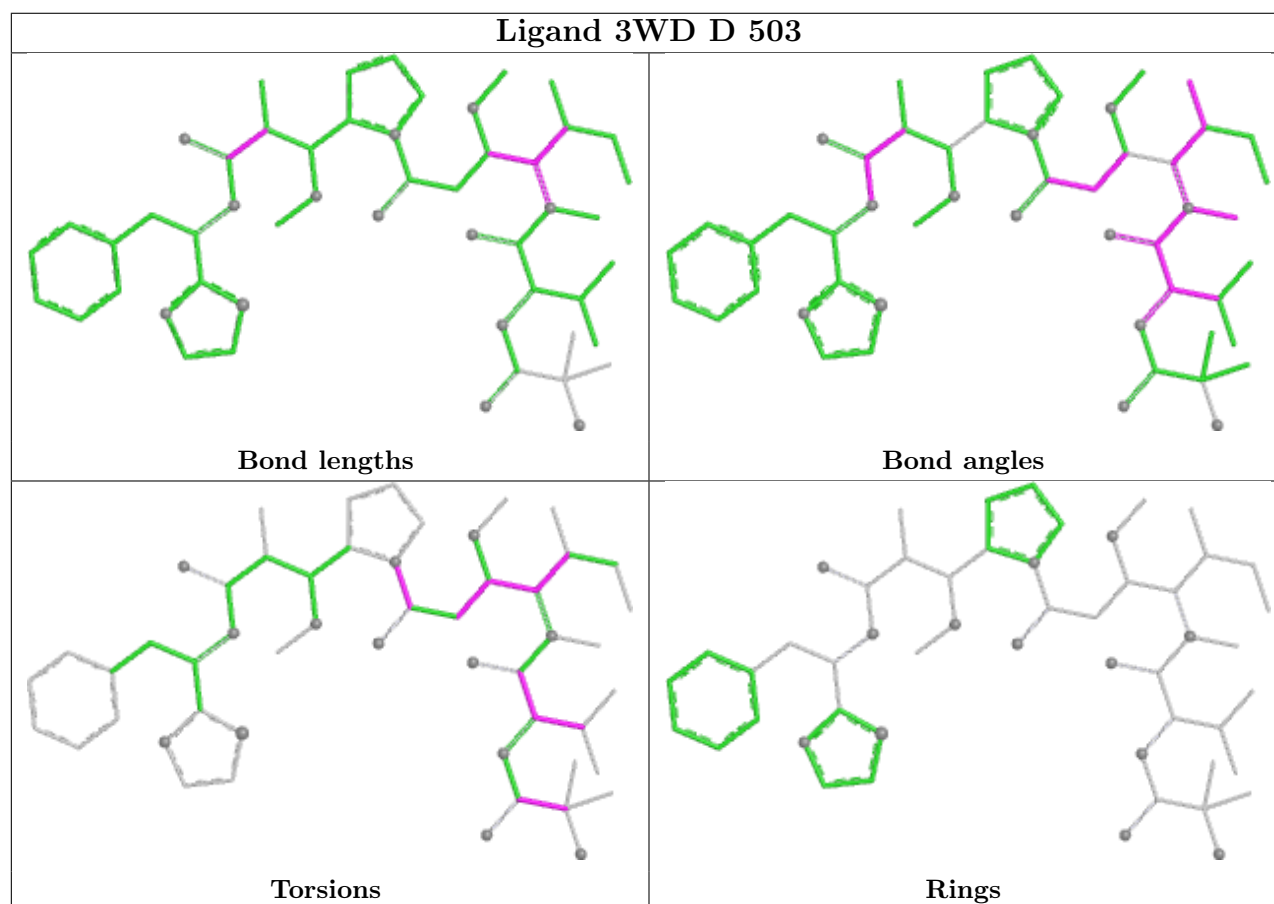
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	503	3WD	2	0
7	B	502	LOC	1	0
6	B	501	GDP	1	0

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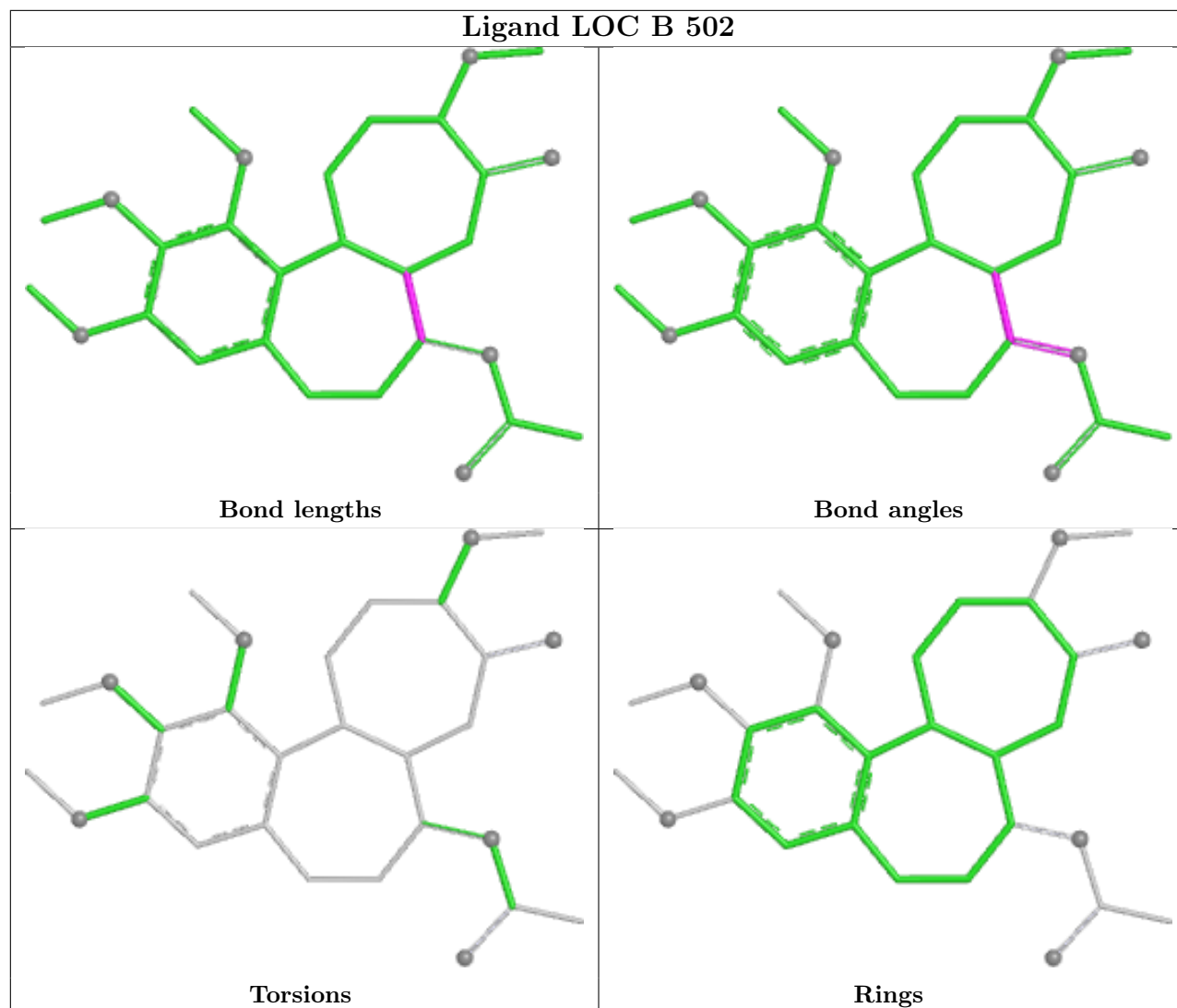
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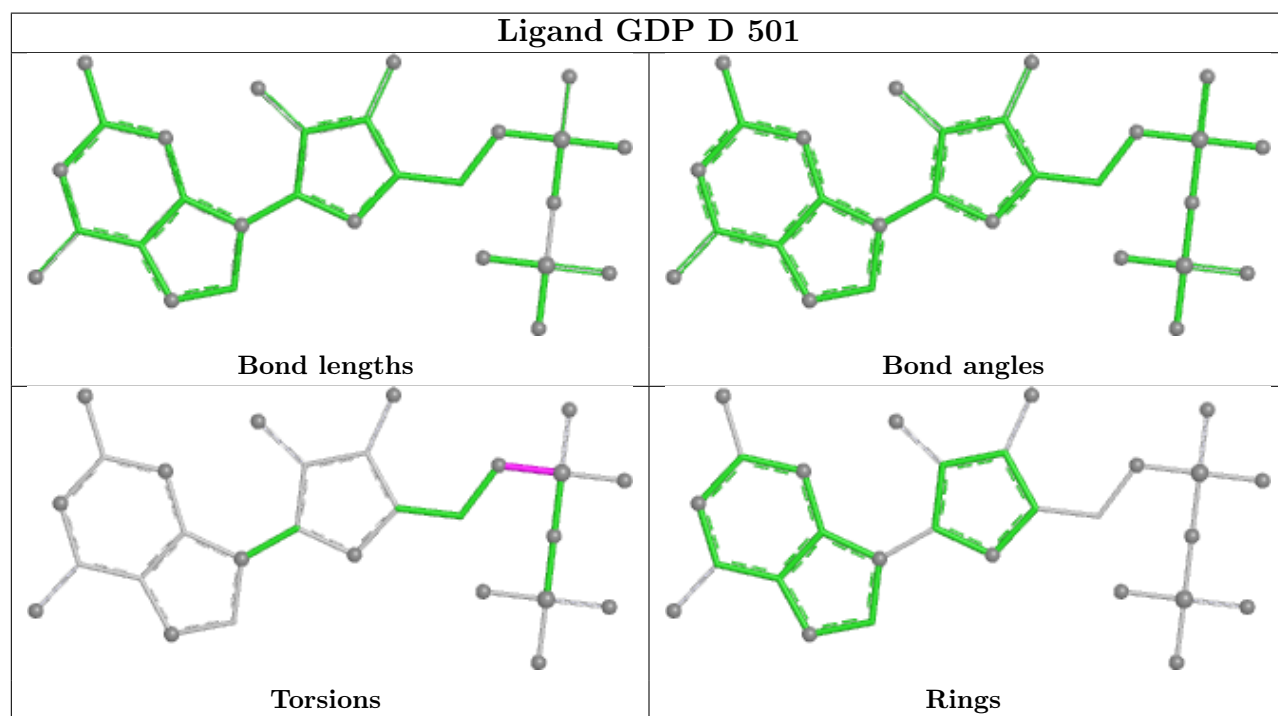
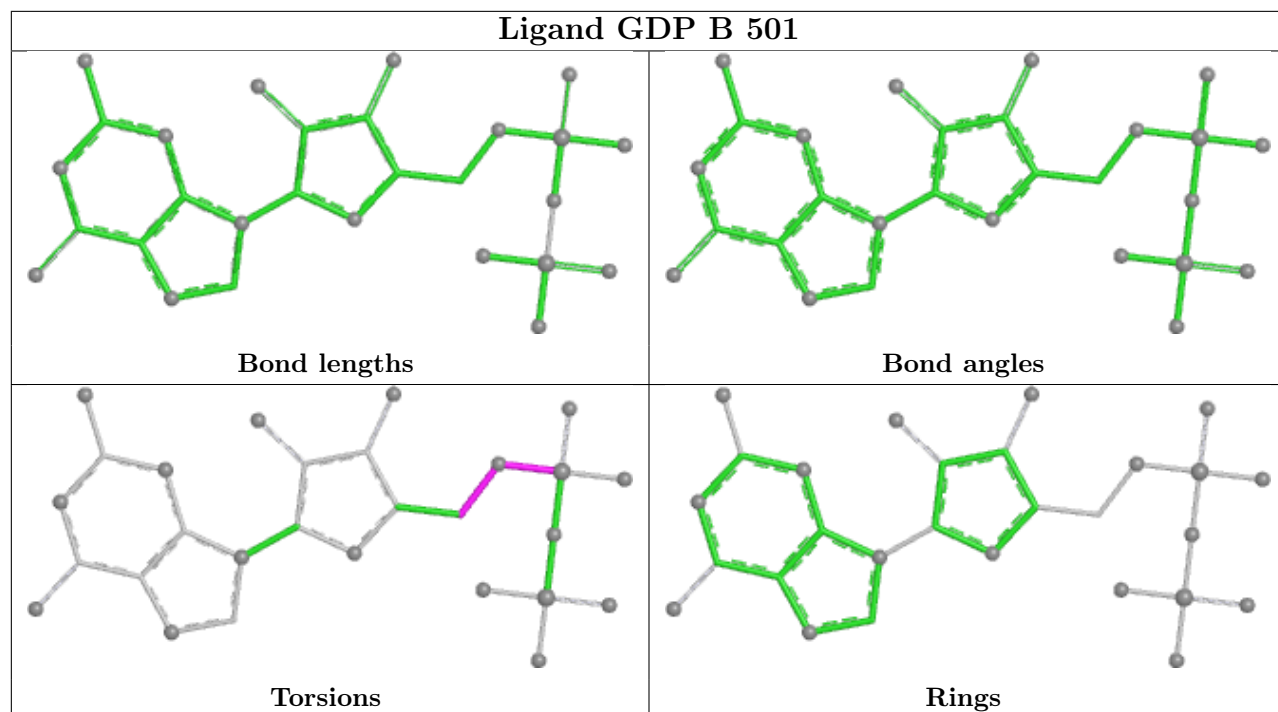
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	GDP	2	0
8	B	503	3WD	5	0

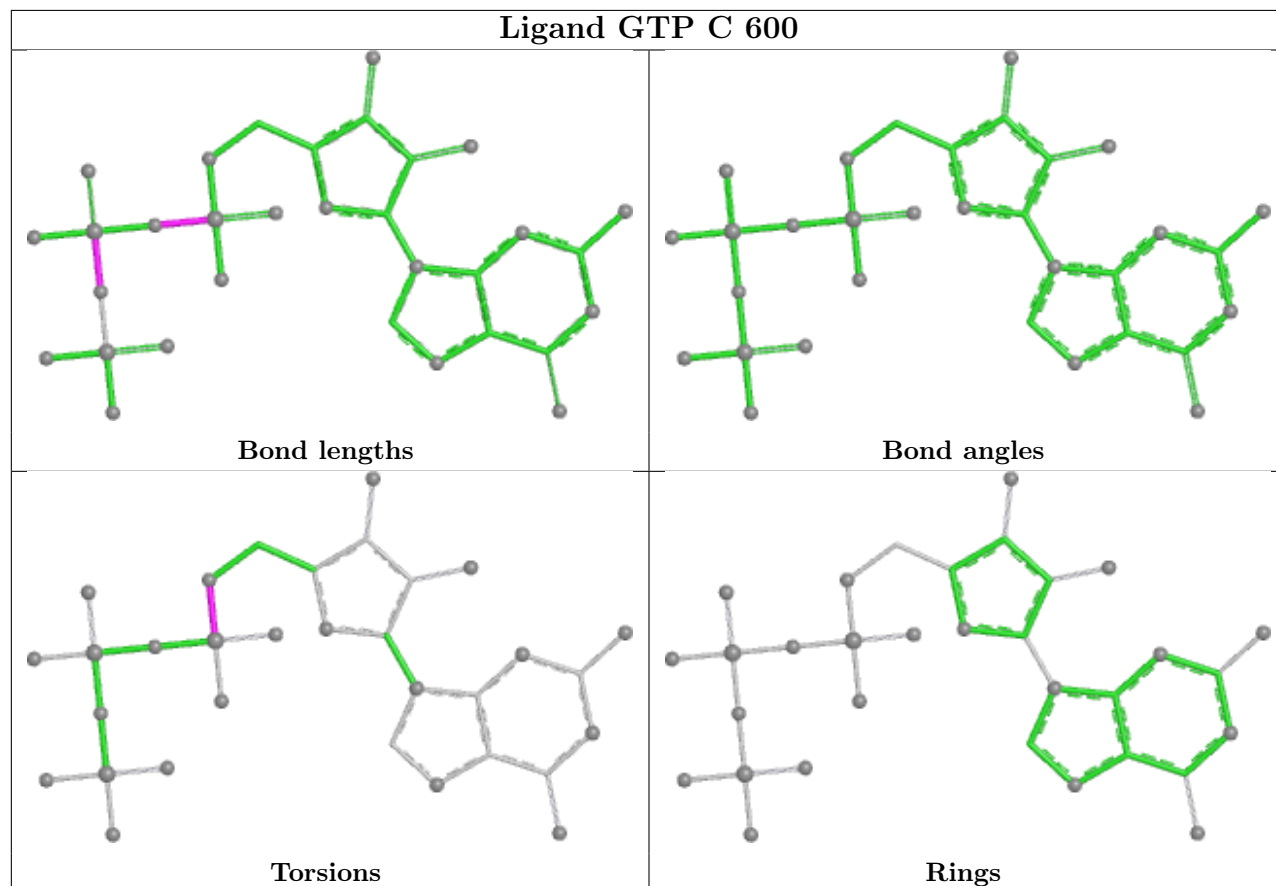
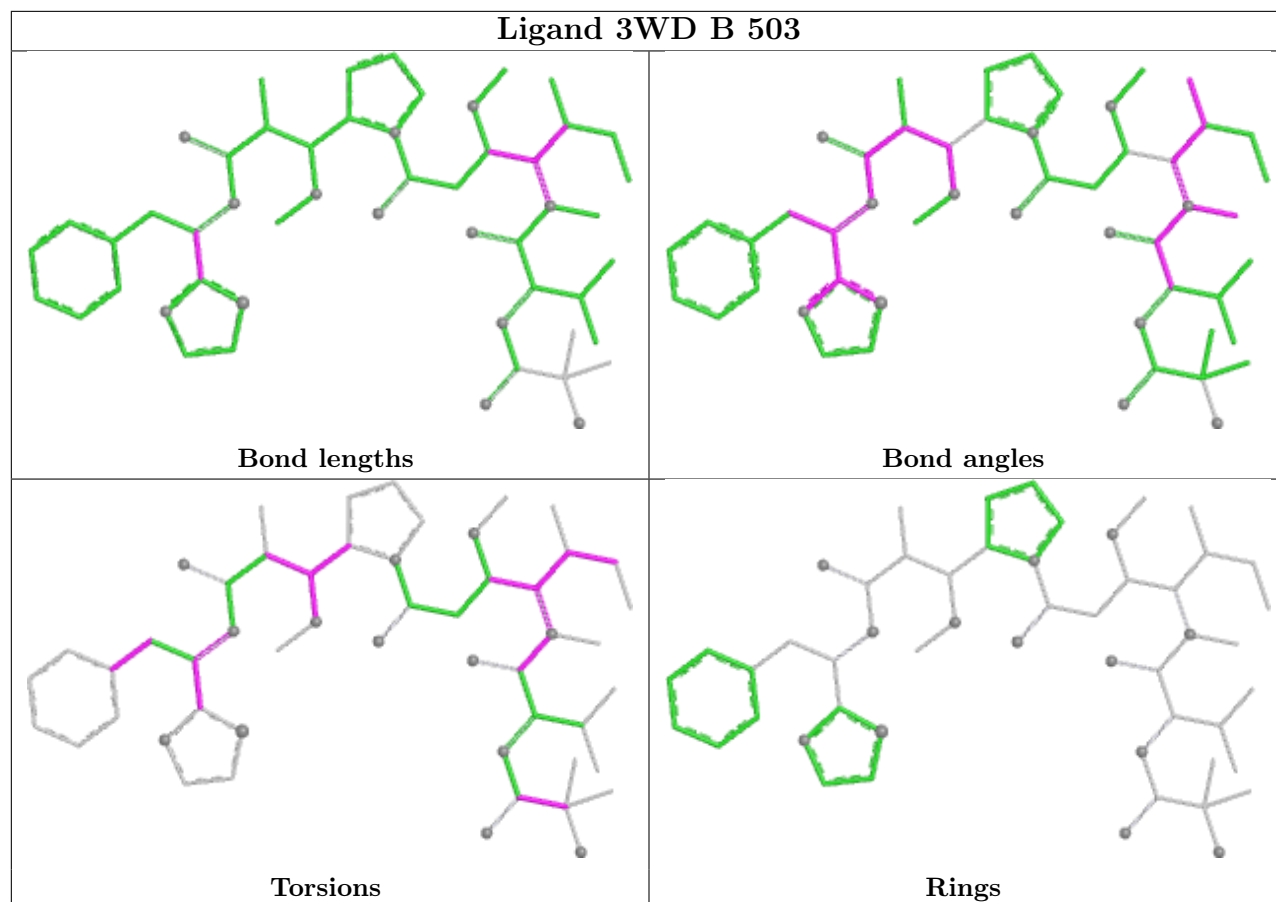
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

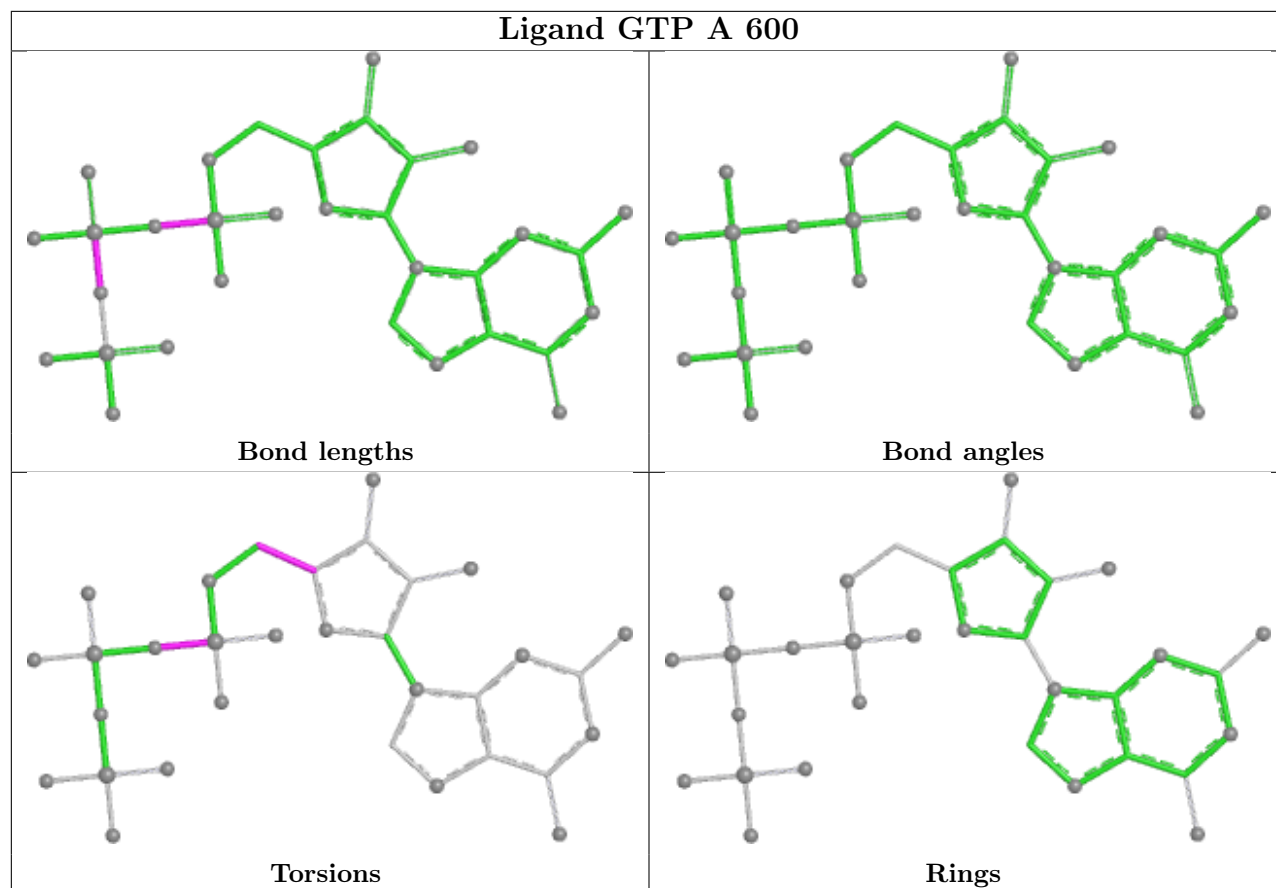


Ligand LOC B 502









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	429/451 (95%)	-0.46	3 (0%) 84 68	92, 139, 188, 216	0
1	C	430/451 (95%)	-0.51	1 (0%) 91 83	49, 99, 145, 171	3 (0%)
2	B	428/445 (96%)	-0.51	2 (0%) 87 73	83, 113, 160, 187	2 (0%)
2	D	430/445 (96%)	-0.66	0 100 100	55, 90, 130, 166	3 (0%)
3	E	123/142 (86%)	-0.53	0 100 100	93, 127, 204, 219	0
All	All	1840/1934 (95%)	-0.53	6 (0%) 90 80	49, 113, 172, 219	8 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	PRO	2.9
2	B	7	ILE	2.8
1	A	142	GLY	2.8
2	B	66	ILE	2.5
1	A	149	PHE	2.1
1	A	339	ARG	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 ⓘ

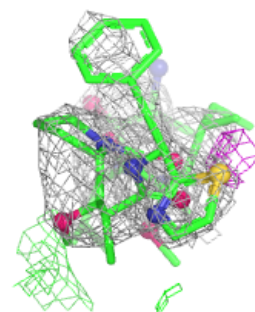
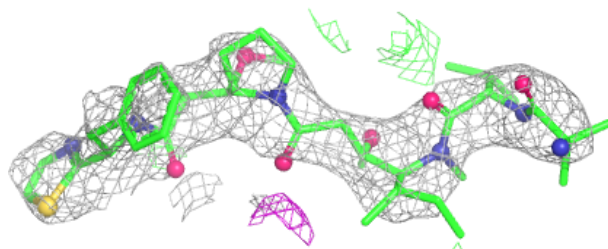
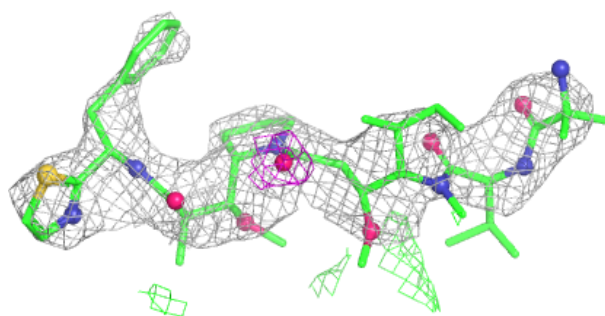
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	3WD	D	503	52/52	0.84	0.12	118,135,146,148	0
8	3WD	B	503	52/52	0.90	0.12	95,112,130,131	0
4	GTP	C	600	32/32	0.95	0.09	73,83,107,109	0
7	LOC	D	502	29/29	0.95	0.10	73,81,88,92	0
7	LOC	B	502	29/29	0.96	0.08	92,106,114,115	0
6	GDP	D	501	28/28	0.96	0.05	68,76,85,89	0
6	GDP	B	501	28/28	0.97	0.05	89,96,101,103	0
4	GTP	A	600	32/32	0.97	0.06	108,122,126,127	0
5	MG	A	601	1/1	0.98	0.09	67,67,67,67	0
5	MG	C	601	1/1	0.98	0.13	37,37,37,37	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.

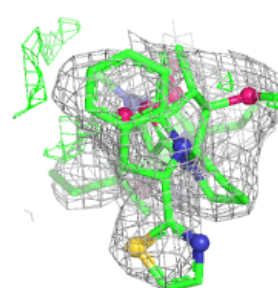
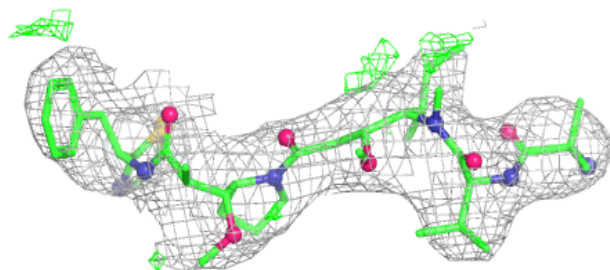
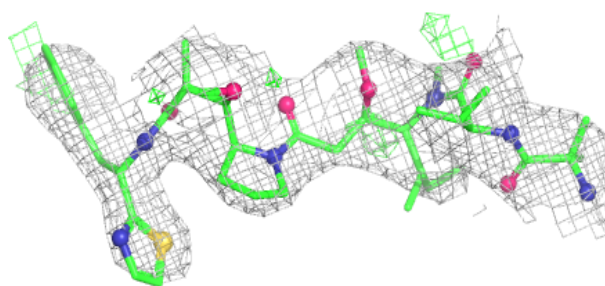
Electron density around 3WD D 503:

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

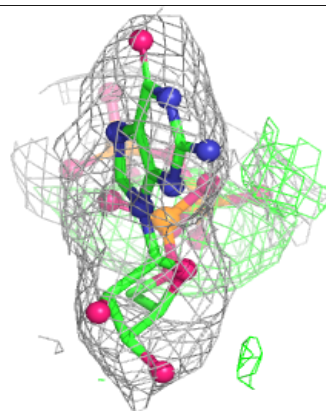
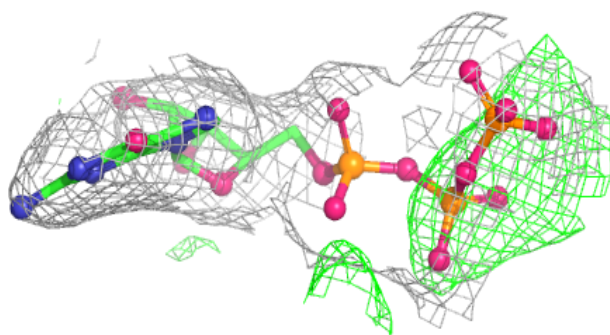
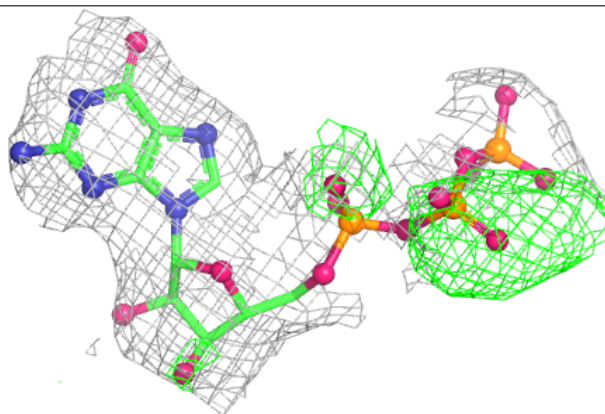


Electron density around 3WD B 503:

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

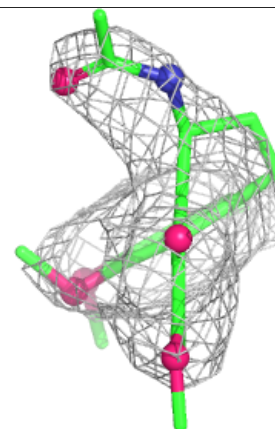
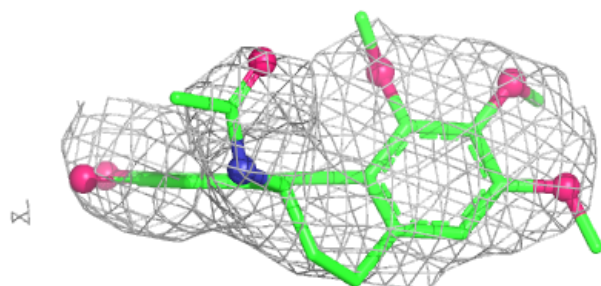
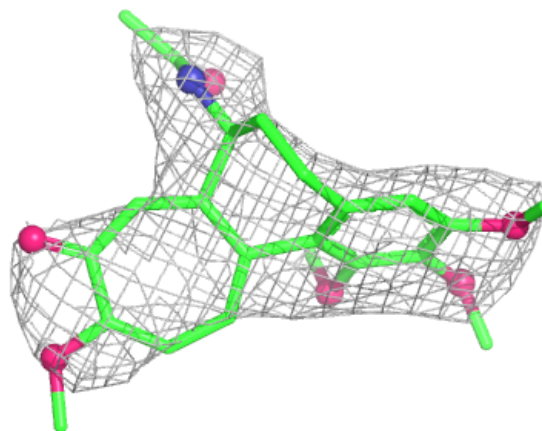
**Electron density around GTP C 600:**

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



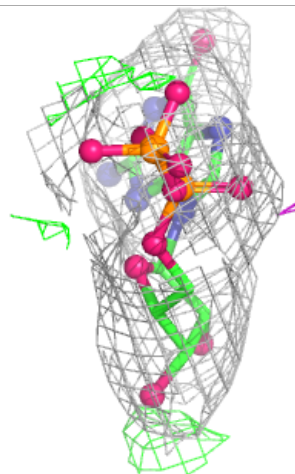
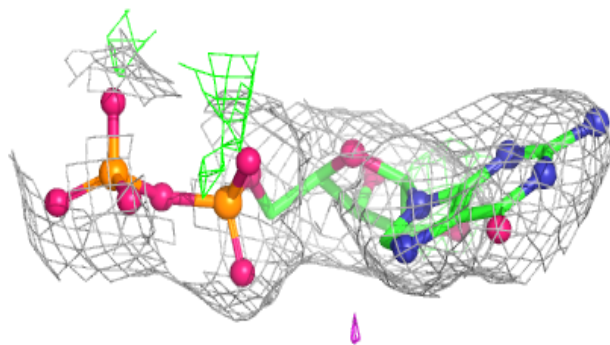
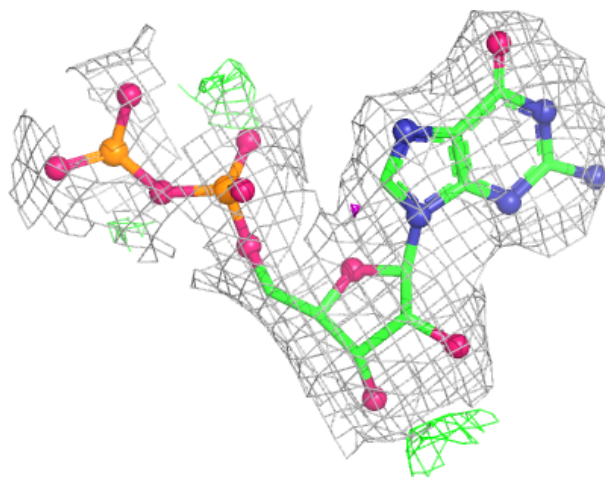
Electron density around LOC B 502:

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



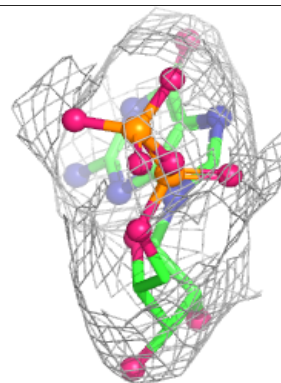
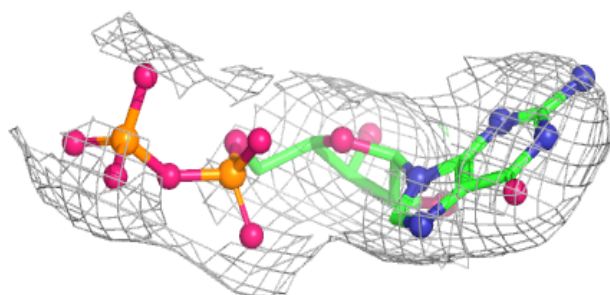
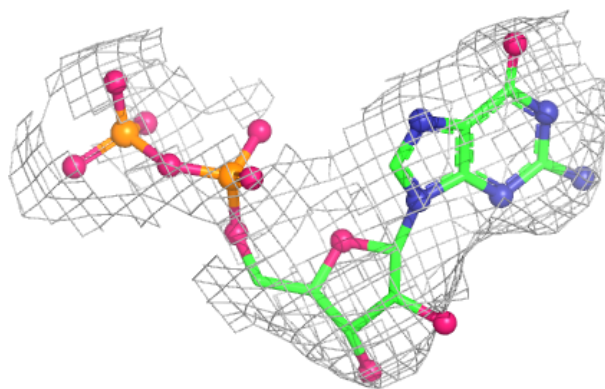
Electron density around GDP D 501:

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

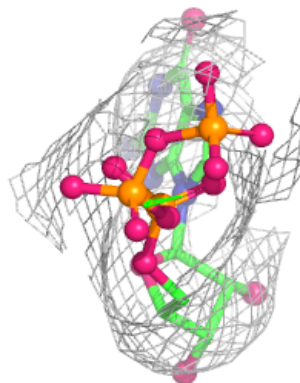
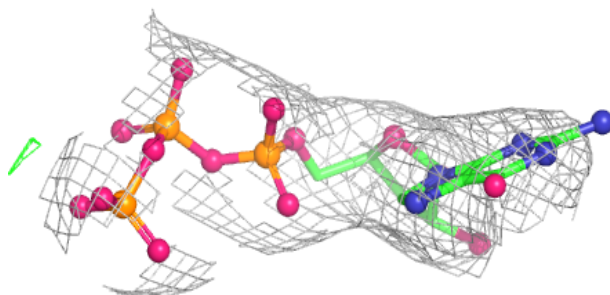
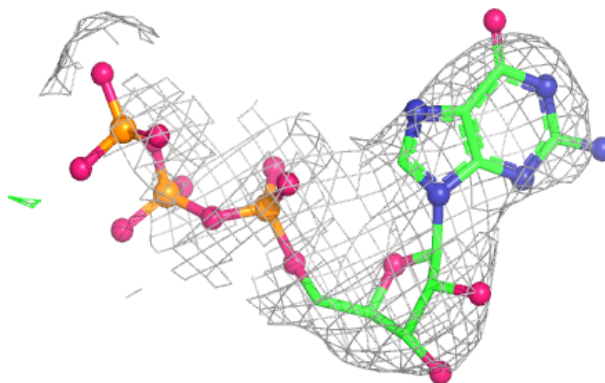


Electron density around GDP B 501:

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

**Electron density around GTP A 600:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.