



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:38 PM UTC

PDB ID : 4X1K / pdb_00004x1k
Title : Discovery of cytotoxic Dolastatin 10 analogs with N-terminal modifications
Authors : Parris, K.D.
Deposited on : 2014-11-24
Resolution : 3.50 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

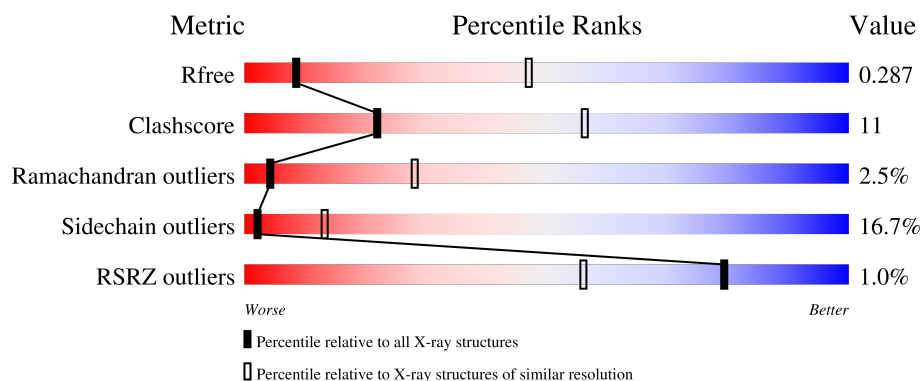
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	% 55% 33% 7% • 5%
1	C	451	% 58% 31% 6% • 5%
2	B	445	2% 54% 33% 7% • •
2	D	445	58% 32% 7% • •
3	E	142	54% 25% 8% 13%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14713 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	2	0
			3351	2124	569	635	23			

- 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).

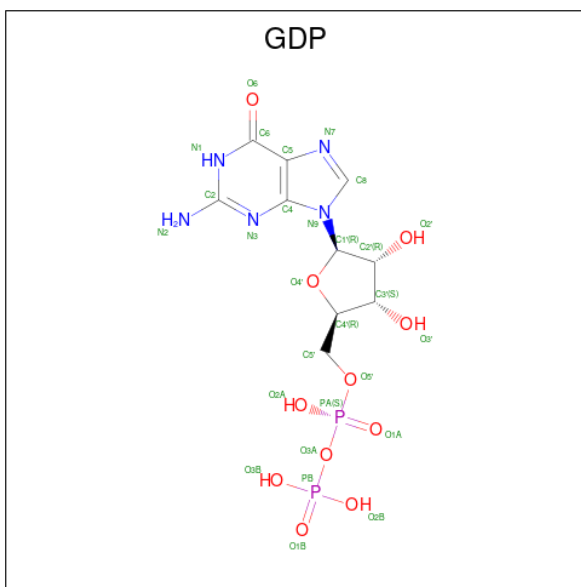


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

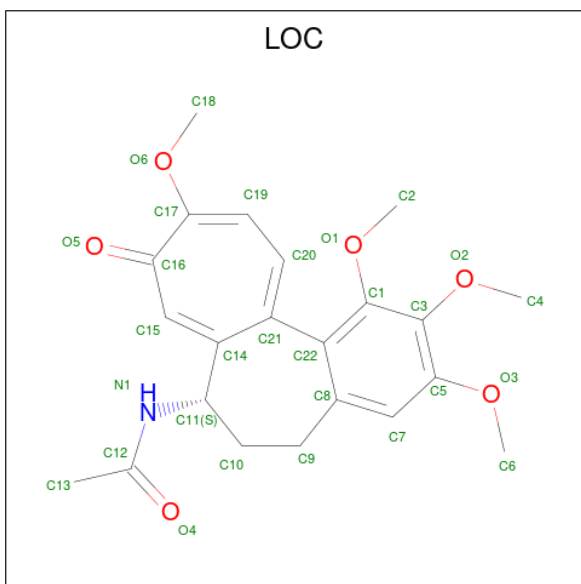
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 7 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (CCD ID: LOC) (formula: C₂₂H₂₅NO₆).



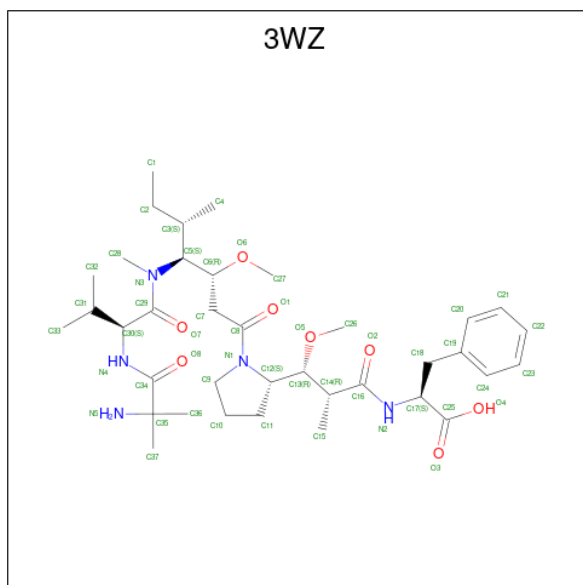
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			29	22	1	6		

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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)-1-{(2S)-2-[(1R,2R)-3-[(1S)-1-carboxy-2-phenylethyl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-oxoheptan-4-yl]-N-methyl-L-valinamide (CCD ID: 3WZ) (formula: $C_{37}H_{61}N_5O_8$).

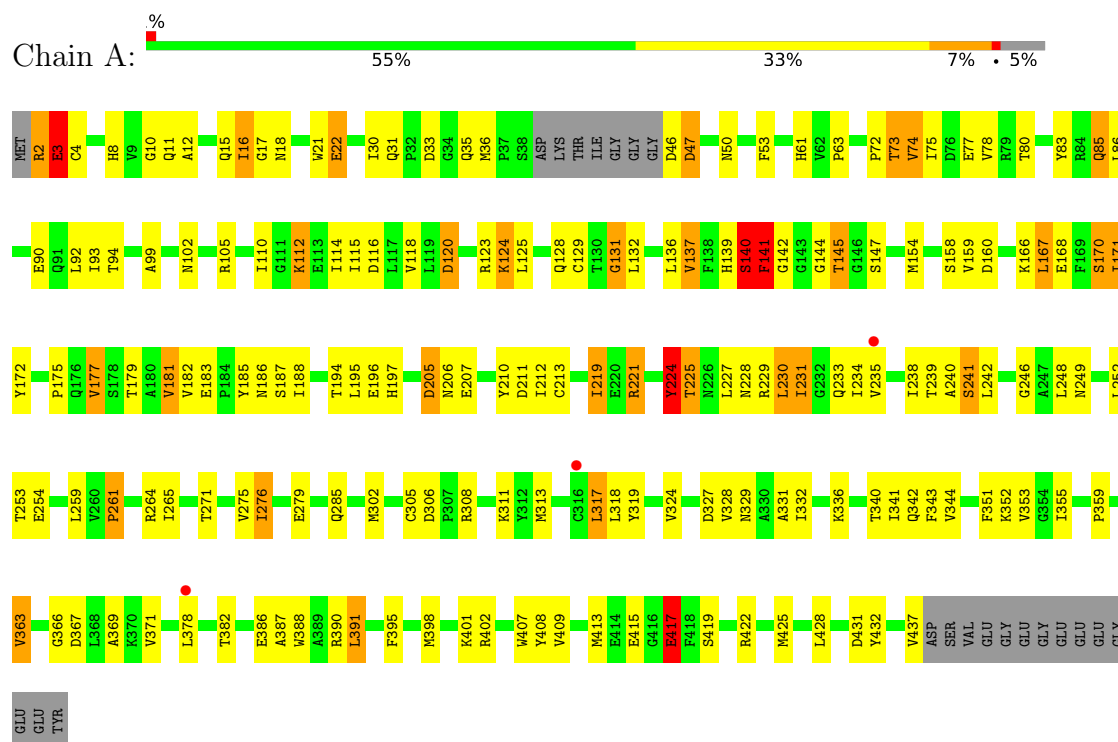


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total 50	C 37	N 5	O 8	0	0
8	D	1	Total 50	C 37	N 5	O 8	0	0

3 Residue-property plots

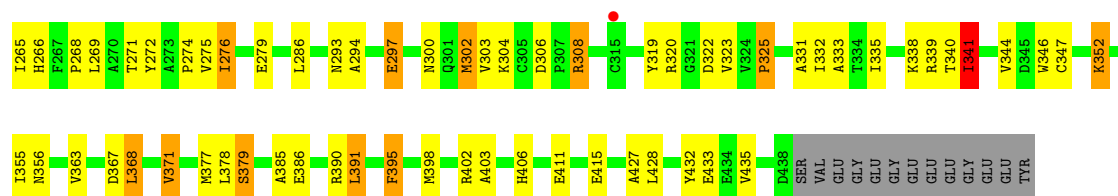
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain

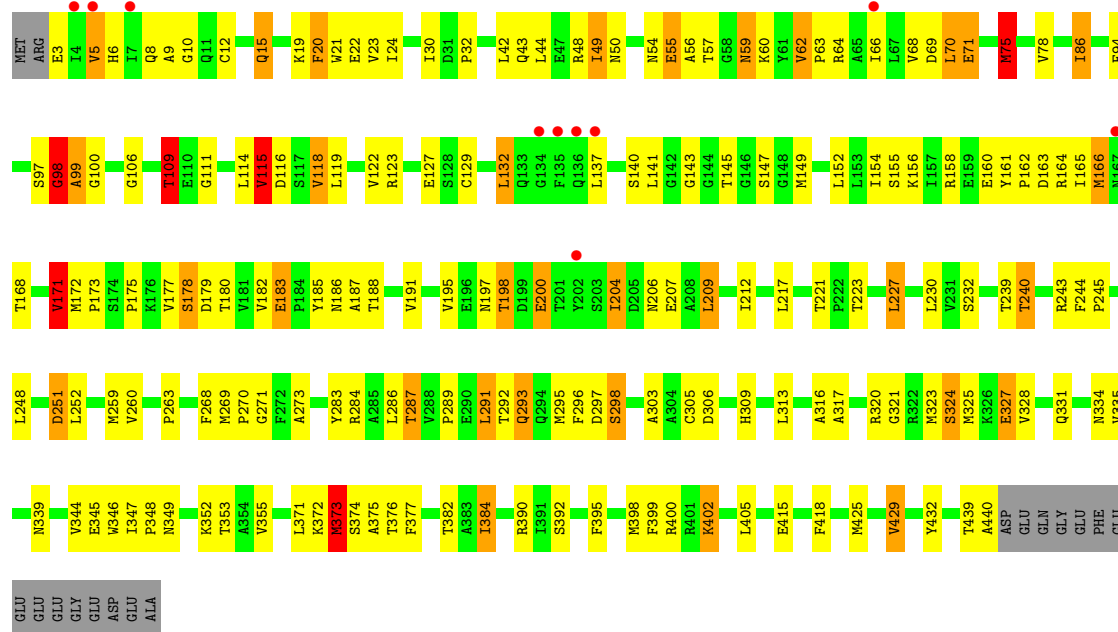


• Molecule 1: Tubulin alpha chain

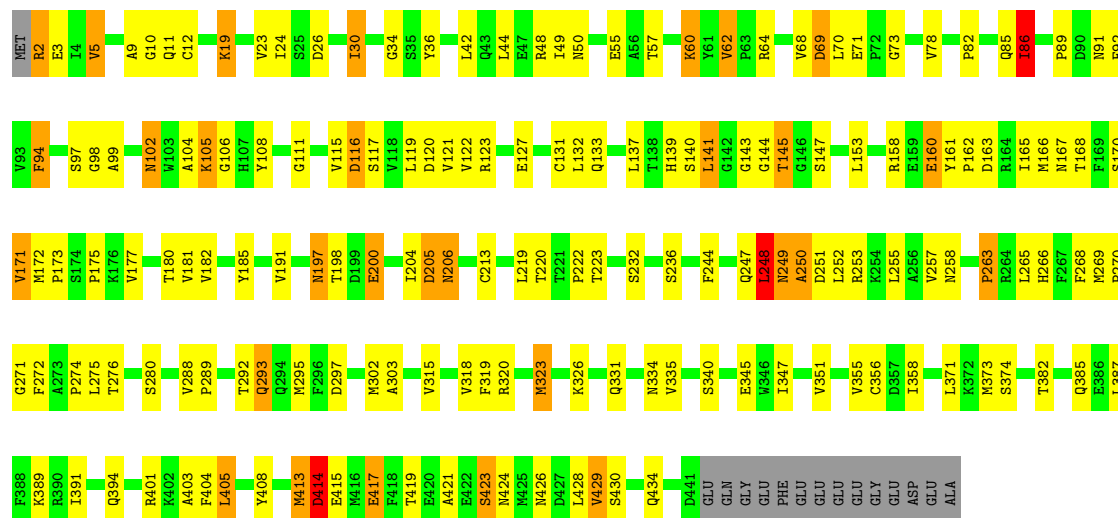




• Molecule 2: Tubulin beta chain

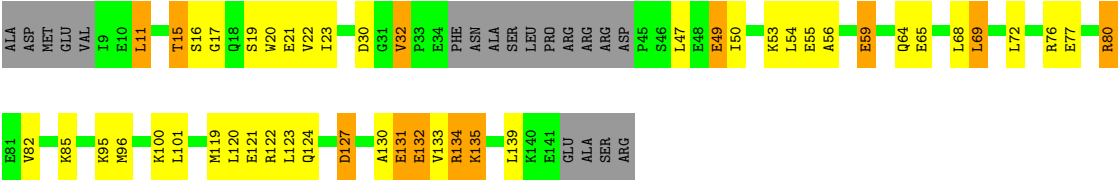


• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4

Chain E: 54% 25% 8% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.73Å 128.30Å 254.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 3.50 45.45 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.1 (45.45-3.50) 97.0 (45.45-3.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.200 , 0.263 0.207 , 0.287	Depositor DCC
R_{free} test set	1816 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	115.6	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 100.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14713	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: MG, GTP, LOC, 3WZ, 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	0.90	1/3440 (0.0%)	1.53	39/4671 (0.8%)
1	C	0.91	0/3432	1.56	37/4662 (0.8%)
2	B	0.92	1/3417 (0.0%)	1.63	62/4634 (1.3%)
2	D	0.91	0/3446	1.56	52/4670 (1.1%)
3	E	0.88	1/1019 (0.1%)	1.61	18/1355 (1.3%)
All	All	0.91	3/14754 (0.0%)	1.57	208/19992 (1.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	75	MET	SD-CE	-5.71	1.65	1.79
3	E	32	VAL	CA-C	5.30	1.58	1.52
1	A	145	THR	CA-C	5.01	1.59	1.52

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	248	LEU	CA-C-N	9.06	138.01	121.70
2	D	248	LEU	C-N-CA	9.06	138.01	121.70
2	D	249	ASN	CA-C-N	8.78	137.51	121.70
2	D	249	ASN	C-N-CA	8.78	137.51	121.70
2	B	399	PHE	N-CA-C	7.59	119.55	111.28
2	B	115	VAL	CA-C-N	7.19	130.23	120.38
2	B	115	VAL	C-N-CA	7.19	130.23	120.38
2	D	69	ASP	CA-CB-CG	7.13	119.73	112.60
1	A	276	ILE	N-CA-C	7.05	118.97	108.46
1	C	308	ARG	N-CA-C	-6.97	104.25	112.89
2	D	191	VAL	CA-C-N	6.91	129.84	120.38
2	D	191	VAL	C-N-CA	6.91	129.84	120.38
2	D	68	VAL	N-CA-C	6.87	117.78	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	207	GLU	N-CA-C	-6.81	103.55	110.97
2	B	327	GLU	CA-C-N	6.70	129.07	120.70
2	B	327	GLU	C-N-CA	6.70	129.07	120.70
1	A	116	ASP	CA-C-N	6.57	129.38	120.38
1	A	116	ASP	C-N-CA	6.57	129.38	120.38
2	B	109	THR	CA-C-N	6.51	129.83	120.79
2	B	109	THR	C-N-CA	6.51	129.83	120.79
3	E	122	ARG	CA-C-N	6.40	129.15	120.44
3	E	122	ARG	C-N-CA	6.40	129.15	120.44
2	D	85	GLN	CA-C-N	6.40	129.55	120.53
2	D	85	GLN	C-N-CA	6.40	129.55	120.53
2	B	334	ASN	CA-C-N	6.37	128.72	120.56
2	B	334	ASN	C-N-CA	6.37	128.72	120.56
2	D	120	ASP	CA-CB-CG	6.36	118.96	112.60
2	B	251	ASP	CA-C-N	6.35	129.07	120.38
2	B	251	ASP	C-N-CA	6.35	129.07	120.38
2	B	10	GLY	CA-C-N	6.33	129.59	120.79
2	B	10	GLY	C-N-CA	6.33	129.59	120.79
1	C	94	THR	N-CA-C	6.33	118.76	108.26
1	A	47	ASP	CA-CB-CG	6.30	118.90	112.60
2	D	78	VAL	CA-C-N	6.29	129.00	120.38
2	D	78	VAL	C-N-CA	6.29	129.00	120.38
1	A	112	LYS	CA-C-N	6.24	128.97	120.54
1	A	112	LYS	C-N-CA	6.24	128.97	120.54
1	C	433	GLU	CA-C-N	6.24	128.55	120.44
1	C	433	GLU	C-N-CA	6.24	128.55	120.44
2	D	334	ASN	N-CA-C	-6.12	104.24	111.03
2	B	15	GLN	CA-C-N	6.11	128.48	120.60
2	B	15	GLN	C-N-CA	6.11	128.48	120.60
2	D	86	ILE	N-CA-C	6.07	117.54	110.62
2	D	405	LEU	N-CA-C	6.06	118.66	111.33
2	D	9	ALA	N-CA-C	6.05	118.77	108.90
1	C	159	VAL	CA-C-N	6.04	128.66	120.38
1	C	159	VAL	C-N-CA	6.04	128.66	120.38
2	D	251	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	73	THR	CA-C-N	5.97	128.08	120.56
1	A	73	THR	C-N-CA	5.97	128.08	120.56
2	D	263	PRO	N-CA-C	5.95	121.69	113.65
2	B	50	ASN	CA-C-N	5.94	128.05	120.56
2	B	50	ASN	C-N-CA	5.94	128.05	120.56
1	C	322	ASP	CA-CB-CG	5.91	118.51	112.60
1	C	81	GLY	CA-C-N	5.90	128.46	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	81	GLY	C-N-CA	5.90	128.46	120.38
2	B	248	LEU	CA-C-N	5.89	132.31	121.70
2	B	248	LEU	C-N-CA	5.89	132.31	121.70
2	B	171	VAL	N-CA-CB	5.89	116.95	110.53
1	C	294	ALA	CA-C-N	5.89	130.02	120.60
1	C	294	ALA	C-N-CA	5.89	130.02	120.60
1	C	179	THR	CB-CA-C	5.83	122.03	110.42
3	E	68	LEU	CA-C-N	5.82	128.36	120.38
3	E	68	LEU	C-N-CA	5.82	128.36	120.38
2	B	56	ALA	CA-C-N	5.78	132.57	121.54
2	B	56	ALA	C-N-CA	5.78	132.57	121.54
1	A	366	GLY	CA-C-N	5.77	128.29	120.44
1	A	366	GLY	C-N-CA	5.77	128.29	120.44
1	A	224	TYR	CA-C-N	5.76	127.93	120.44
1	A	224	TYR	C-N-CA	5.76	127.93	120.44
1	C	98	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	183	GLU	CB-CG-CD	5.75	122.38	112.60
2	B	415	GLU	CA-C-N	5.74	128.25	120.38
2	B	415	GLU	C-N-CA	5.74	128.25	120.38
1	C	3	GLU	N-CA-C	5.74	117.94	110.43
3	E	50	ILE	N-CA-C	-5.74	105.26	110.82
1	A	359	PRO	N-CA-C	5.72	117.68	110.70
2	B	221	THR	CB-CA-C	5.72	120.58	111.15
1	A	3	GLU	N-CA-C	5.71	117.70	110.33
2	B	263	PRO	CA-C-N	5.70	128.49	120.28
2	B	263	PRO	C-N-CA	5.70	128.49	120.28
1	C	247	ALA	CA-C-N	5.70	128.23	120.54
1	C	247	ALA	C-N-CA	5.70	128.23	120.54
2	D	94	PHE	N-CA-C	5.70	118.07	107.99
1	A	318	LEU	N-CA-C	5.69	118.42	108.52
1	C	255	PHE	N-CA-C	-5.68	105.00	111.14
2	B	9	ALA	N-CA-C	5.68	118.50	109.24
2	B	98	GLY	N-CA-C	5.67	126.63	113.18
1	C	16	ILE	CA-C-N	5.67	126.27	119.98
1	C	16	ILE	C-N-CA	5.67	126.27	119.98
2	D	162	PRO	CA-C-N	5.67	130.18	120.72
2	D	162	PRO	C-N-CA	5.67	130.18	120.72
2	D	197	ASN	N-CA-C	5.66	119.76	112.41
2	B	372	LYS	CA-C-N	5.64	132.31	121.54
2	B	372	LYS	C-N-CA	5.64	132.31	121.54
2	B	418	PHE	CA-C-N	5.64	128.15	120.54
2	B	418	PHE	C-N-CA	5.64	128.15	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	175	PRO	CA-C-N	5.63	128.28	120.29
2	D	175	PRO	C-N-CA	5.63	128.28	120.29
1	C	102	ASN	CA-CB-CG	5.62	118.22	112.60
2	B	22	GLU	N-CA-C	-5.61	107.09	114.04
1	C	254	GLU	N-CA-C	-5.60	105.17	112.23
1	A	74	VAL	N-CA-C	5.58	115.78	110.42
1	C	12	ALA	CA-C-N	5.58	126.13	119.94
1	C	12	ALA	C-N-CA	5.58	126.13	119.94
2	D	417	GLU	CA-C-N	5.54	127.98	120.44
2	D	417	GLU	C-N-CA	5.54	127.98	120.44
1	A	132	LEU	CA-C-N	5.54	128.48	120.79
1	A	132	LEU	C-N-CA	5.54	128.48	120.79
2	B	123	ARG	CA-C-N	5.54	127.64	120.44
2	B	123	ARG	C-N-CA	5.54	127.64	120.44
1	C	205	ASP	CA-CB-CG	5.51	118.11	112.60
2	D	139	HIS	CA-C-N	5.51	129.71	121.72
2	D	139	HIS	C-N-CA	5.51	129.71	121.72
1	C	325	PRO	N-CA-C	5.50	123.80	112.47
1	A	419	SER	CA-C-N	5.46	129.01	120.82
1	A	419	SER	C-N-CA	5.46	129.01	120.82
3	E	59	GLU	CA-C-N	5.45	127.89	120.54
3	E	59	GLU	C-N-CA	5.45	127.89	120.54
1	C	21	TRP	N-CA-C	5.43	117.96	111.71
3	E	69	LEU	CA-C-N	5.42	127.48	120.44
3	E	69	LEU	C-N-CA	5.42	127.48	120.44
1	A	415	GLU	CA-C-N	5.41	126.10	119.99
1	A	415	GLU	C-N-CA	5.41	126.10	119.99
1	A	22	GLU	N-CA-C	-5.41	104.25	112.04
2	B	162	PRO	N-CA-C	5.40	120.94	113.65
2	B	251	ASP	CA-CB-CG	5.39	117.99	112.60
2	D	147	SER	N-CA-C	5.38	116.83	111.07
2	B	175	PRO	CA-C-N	5.37	127.93	120.63
2	B	175	PRO	C-N-CA	5.37	127.93	120.63
2	B	239	THR	CB-CA-C	5.37	118.61	111.14
2	B	43	GLN	CA-C-N	5.37	128.22	120.38
2	B	43	GLN	C-N-CA	5.37	128.22	120.38
1	A	102	ASN	CA-CB-CG	5.35	117.95	112.60
2	B	20	PHE	CA-CB-CG	5.33	119.13	113.80
1	C	395	PHE	CA-C-N	5.32	127.67	120.38
1	C	395	PHE	C-N-CA	5.32	127.67	120.38
2	B	317	ALA	N-CA-C	5.32	116.10	107.32
2	D	394	GLN	CA-C-N	5.30	127.34	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	394	GLN	C-N-CA	5.30	127.34	120.44
2	B	22	GLU	CA-C-N	5.30	127.24	120.56
2	B	22	GLU	C-N-CA	5.30	127.24	120.56
2	B	244	PHE	N-CA-C	5.30	118.00	109.15
1	C	215	ARG	N-CA-C	5.29	116.85	111.14
2	D	288	VAL	N-CA-CB	5.29	114.58	110.45
2	D	318	VAL	N-CA-C	5.29	115.20	107.37
1	A	144	GLY	CA-C-N	5.29	129.54	120.71
1	A	144	GLY	C-N-CA	5.29	129.54	120.71
1	A	181	VAL	N-CA-C	5.29	116.01	110.62
2	B	324	SER	CA-C-N	5.28	128.09	120.38
2	B	324	SER	C-N-CA	5.28	128.09	120.38
1	A	228	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	196	GLU	CB-CG-CD	5.26	121.54	112.60
3	E	59	GLU	N-CA-C	-5.24	105.26	110.97
1	C	432	TYR	CA-C-N	5.24	127.56	120.65
1	C	432	TYR	C-N-CA	5.24	127.56	120.65
3	E	127	ASP	N-CA-C	-5.23	107.27	113.97
1	C	385	ALA	CA-C-N	5.23	127.29	120.28
1	C	385	ALA	C-N-CA	5.23	127.29	120.28
2	B	395	PHE	CA-C-N	5.23	129.05	120.63
2	B	395	PHE	C-N-CA	5.23	129.05	120.63
2	D	414	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	339	ASN	CA-CB-CG	5.22	117.82	112.60
2	B	78	VAL	CA-C-N	5.21	127.51	120.38
2	B	78	VAL	C-N-CA	5.21	127.51	120.38
2	D	347	ILE	N-CA-CB	5.20	118.50	111.21
1	A	231	ILE	CA-C-N	5.20	125.75	119.98
1	A	231	ILE	C-N-CA	5.20	125.75	119.98
3	E	85	LYS	CA-C-N	5.20	127.50	120.38
3	E	85	LYS	C-N-CA	5.20	127.50	120.38
2	B	240	THR	N-CA-C	-5.19	106.10	112.90
2	D	163	ASP	CA-CB-CG	5.18	117.78	112.60
2	D	421	ALA	CA-C-N	5.18	127.53	120.54
2	D	421	ALA	C-N-CA	5.18	127.53	120.54
1	A	4	CYS	N-CA-C	5.17	116.61	107.61
3	E	133	VAL	N-CA-C	-5.16	105.81	110.82
2	D	205	ASP	CA-CB-CG	5.16	117.76	112.60
2	D	158	ARG	CA-C-N	5.15	127.63	120.63
2	D	158	ARG	C-N-CA	5.15	127.63	120.63
1	C	333	ALA	CA-C-N	5.13	127.16	120.28
1	C	333	ALA	C-N-CA	5.13	127.16	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	102	ASN	CA-C-N	5.11	127.09	120.44
2	D	102	ASN	C-N-CA	5.11	127.09	120.44
1	A	240	ALA	CA-C-N	5.10	128.76	120.60
1	A	240	ALA	C-N-CA	5.10	128.76	120.60
2	D	244	PHE	N-CA-C	5.08	116.99	109.62
1	A	205	ASP	CA-CB-CG	5.08	117.68	112.60
2	D	236	SER	N-CA-C	-5.07	105.83	111.36
2	D	413	MET	N-CA-C	5.07	117.45	110.35
2	B	390	ARG	CA-C-N	5.07	126.95	120.56
2	B	390	ARG	C-N-CA	5.07	126.95	120.56
1	A	417	GLU	CB-CG-CD	5.06	121.21	112.60
3	E	121	GLU	CA-C-N	5.06	127.37	120.54
3	E	121	GLU	C-N-CA	5.06	127.37	120.54
2	B	429	VAL	CA-C-N	5.06	127.06	120.28
2	B	429	VAL	C-N-CA	5.06	127.06	120.28
2	D	120	ASP	CA-C-N	5.06	127.61	120.42
2	D	120	ASP	C-N-CA	5.06	127.61	120.42
2	B	122	VAL	N-CA-CB	5.05	117.40	110.54
2	D	424	ASN	N-CA-C	-5.04	105.67	111.07
1	C	222	PRO	N-CA-C	5.04	118.80	111.03
3	E	139	LEU	CA-C-N	5.04	127.28	120.38
3	E	139	LEU	C-N-CA	5.04	127.28	120.38
1	C	211	ASP	CA-CB-CG	5.03	117.63	112.60
2	D	297	ASP	CA-CB-CG	5.02	117.62	112.60
2	D	62	VAL	CB-CA-C	5.01	115.22	110.16
1	A	331	ALA	CA-C-N	5.00	126.86	120.56
1	A	331	ALA	C-N-CA	5.00	126.86	120.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3363	0	3274	78	0
1	C	3351	0	3258	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3342	0	3198	84	0
2	D	3369	0	3237	74	0
3	E	1008	0	1022	18	0
4	A	32	0	12	1	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	3	0
7	B	29	0	25	1	0
7	D	29	0	25	2	0
8	B	50	0	60	0	0
8	D	50	0	60	0	0
All	All	14713	0	14207	310	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 11.

All (310) 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:338:LYS:HD3	1:C:340:THR:HG22	1.26	1.16
1:C:338:LYS:HD3	1:C:340:THR:CG2	1.92	0.99
1:C:338:LYS:CD	1:C:340:THR:HG22	1.95	0.97
1:A:33:ASP:HA	1:A:85:GLN:HB3	1.56	0.86
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.59	0.83
2:D:247:GLN:HE22	2:D:355:VAL:H	1.28	0.80
1:C:155:GLU:HB3	3:E:101:LEU:HD21	1.66	0.76
2:B:30:ILE:HG22	2:B:86:ILE:HD11	1.66	0.76
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.69	0.73
1:A:248:LEU:HB2	3:E:19:SER:HB3	1.70	0.73
1:A:246:GLY:HA2	3:E:17:GLY:HA3	1.70	0.71
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.57	0.70
1:A:158:SER:HB2	1:A:197:HIS:HD2	1.56	0.70
2:B:69:ASP:HA	2:B:145:THR:HG21	1.74	0.69
2:B:166:MET:HB3	2:B:198:THR:HG22	1.75	0.69
2:B:259:MET:HE2	2:B:316:ALA:HB2	1.74	0.68
1:A:175:PRO:HA	1:A:179:THR:HG21	1.75	0.67
2:D:12:CYS:SG	2:D:171:VAL:HG11	2.35	0.67
1:C:241:SER:HA	1:C:250:VAL:HB	1.77	0.66
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LYS:HB3	2:B:405:LEU:HD22	1.75	0.66
2:D:401:ARG:HE	2:D:403:ALA:HB2	1.61	0.66
1:A:329:ASN:HD21	3:E:22:VAL:HG11	1.61	0.65
1:A:259:LEU:O	1:A:261:PRO:HD3	1.96	0.65
3:E:11:LEU:HB2	3:E:20:TRP:HA	1.76	0.65
1:A:387:ALA:HA	1:A:390:ARG:HE	1.60	0.65
2:D:270:PRO:HG2	2:D:302:MET:HB2	1.79	0.65
2:B:382:THR:HA	2:B:432:TYR:HD2	1.63	0.64
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.80	0.64
1:C:5:ILE:HD12	1:C:135:PHE:CE2	2.33	0.64
2:D:106:GLY:O	2:D:111:GLY:HA3	1.97	0.64
2:B:331:GLN:O	2:B:335:VAL:HG23	1.97	0.64
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.80	0.64
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.79	0.64
2:D:253:ARG:O	2:D:257:VAL:HG23	1.97	0.64
2:D:272:PHE:CE1	2:D:374:SER:HB2	2.33	0.63
2:B:48:ARG:HH11	2:B:245:PRO:HA	1.63	0.63
2:D:19:LYS:O	2:D:23:VAL:HG23	1.99	0.63
2:D:293:GLN:HE22	2:D:331:GLN:HE21	1.47	0.63
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.79	0.62
2:B:320:ARG:HB2	2:B:374:SER:HB3	1.81	0.62
2:B:179:ASP:HB2	1:C:352:LYS:HG2	1.83	0.61
2:D:250:ALA:HA	7:D:502:LOC:H6B	1.82	0.61
2:B:382:THR:HA	2:B:432:TYR:CD2	2.35	0.60
1:C:276:ILE:HD11	1:C:371:VAL:HG22	1.83	0.60
1:C:308:ARG:NH1	1:C:340:THR:HG21	2.16	0.60
1:A:225:THR:O	1:A:229:ARG:HG2	2.01	0.60
1:C:195:LEU:HD21	1:C:428:LEU:HD13	1.85	0.59
2:B:204:ILE:HD13	2:B:270:PRO:HG2	1.84	0.59
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.84	0.59
2:B:273:ALA:HB3	2:B:375:ALA:HB3	1.84	0.59
2:D:50:ASN:O	2:D:64:ARG:NH2	2.35	0.58
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.38	0.58
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.39	0.58
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.86	0.57
1:C:141:PHE:CE1	1:C:170:SER:HB2	2.40	0.57
2:B:352:LYS:HE3	7:B:502:LOC:O5	2.04	0.57
2:D:36:TYR:CZ	2:D:44:LEU:HD11	2.39	0.57
1:A:317:LEU:HD12	1:A:353:VAL:HG22	1.87	0.57
2:D:133:GLN:HE21	2:D:252:LEU:H	1.52	0.57
1:A:311:LYS:HD3	1:A:344:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:GLN:HE22	2:B:331:GLN:HE21	1.52	0.56
2:B:313:LEU:HA	2:B:344:VAL:HG22	1.88	0.56
2:D:389:LYS:HG3	2:D:429:VAL:HG11	1.87	0.56
1:C:346:TRP:HZ2	1:C:435:VAL:HG22	1.69	0.56
2:D:323:MET:HE3	2:D:373:MET:HE3	1.88	0.55
3:E:130:ALA:HB1	3:E:134:ARG:HH12	1.72	0.55
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.71	0.55
1:A:136:LEU:HD11	1:A:252:LEU:HD21	1.88	0.55
1:A:53:PHE:HB3	1:A:61:HIS:HB3	1.89	0.54
1:A:158:SER:CB	1:A:197:HIS:HD2	2.20	0.54
2:B:191:VAL:O	2:B:195:VAL:HG23	2.08	0.54
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.37	0.54
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.42	0.54
2:B:140:SER:HA	2:B:171:VAL:HG22	1.90	0.54
1:A:154:MET:HG3	1:A:194:THR:HG23	1.89	0.54
1:C:297:GLU:HB3	1:C:300:ASN:HD22	1.73	0.54
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.90	0.53
1:C:259:LEU:O	1:C:261:PRO:HD3	2.08	0.53
1:A:140:SER:HA	1:A:171:ILE:HG22	1.91	0.53
2:D:102:ASN:HB3	2:D:105:LYS:HB2	1.89	0.53
1:A:112:LYS:HE3	3:E:54:LEU:HB3	1.91	0.53
1:A:276:ILE:HG23	1:A:369:ALA:HB3	1.89	0.53
2:D:200:GLU:HB2	2:D:268:PHE:CE1	2.43	0.53
2:B:71:GLU:HB3	2:B:98:GLY:HA2	1.91	0.53
1:C:260:VAL:HG12	1:C:262:TYR:O	2.09	0.53
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.91	0.53
1:C:252:LEU:C	1:C:254:GLU:H	2.16	0.53
2:D:319:PHE:HB2	2:D:355:VAL:HG22	1.91	0.53
1:A:249:ASN:HD22	1:A:254:GLU:HB3	1.74	0.53
2:B:3:GLU:HB2	2:B:132:LEU:HA	1.90	0.52
1:A:207:GLU:O	1:A:210:TYR:HB3	2.09	0.52
2:B:305:CYS:SG	2:B:384:ILE:HA	2.49	0.52
1:C:119:LEU:HD13	1:C:156:ARG:HE	1.73	0.52
1:A:235:VAL:HA	1:A:238:ILE:HD12	1.92	0.52
1:C:266:HIS:O	1:C:268:PRO:HD3	2.09	0.52
2:D:71:GLU:HG2	2:D:98:GLY:HA2	1.92	0.52
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.45	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
2:D:62:VAL:HG23	2:D:86:ILE:O	2.10	0.52
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:274:PRO:HD3	2:D:374:SER:HA	1.92	0.52
1:A:182:VAL:O	1:A:185:TYR:HB2	2.10	0.52
2:B:206:ASN:HA	2:B:209:LEU:HB2	1.91	0.51
1:C:213:CYS:HA	1:C:217:LEU:HB2	1.93	0.51
1:C:188:ILE:HD13	1:C:395:PHE:HB2	1.93	0.51
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.51
1:A:12:ALA:O	1:A:16:ILE:HB	2.11	0.51
3:E:11:LEU:HD23	3:E:21:GLU:HB2	1.92	0.51
1:A:123:ARG:HH12	1:A:160:ASP:HB3	1.75	0.51
2:B:425:MET:O	2:B:429:VAL:HG23	2.09	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.10	0.51
2:B:344:VAL:HG21	2:B:347:ILE:HD12	1.92	0.51
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.93	0.51
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.93	0.50
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.76	0.50
2:B:143:GLY:O	2:B:147:SER:HB3	2.12	0.50
2:B:371:LEU:H	2:B:371:LEU:HD23	1.77	0.50
1:A:3:GLU:HG3	1:A:129:CYS:SG	2.51	0.50
1:A:230:LEU:HD23	1:A:234:ILE:HD11	1.94	0.50
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.94	0.50
2:D:133:GLN:NE2	2:D:252:LEU:H	2.10	0.50
2:B:154:ILE:HA	2:B:166:MET:HE3	1.93	0.50
1:C:249:ASN:HB2	1:C:355:ILE:H	1.77	0.50
2:D:166:MET:HG3	2:D:198:THR:HG22	1.92	0.49
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.93	0.49
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.49
1:C:320:ARG:HB3	1:C:356:ASN:HB3	1.95	0.49
2:D:34:GLY:HA3	2:D:60:LYS:HE3	1.94	0.49
2:D:116:ASP:HA	2:D:119:LEU:HD12	1.95	0.49
1:A:142:GLY:HA2	1:A:186:ASN:HB2	1.94	0.49
1:C:302:MET:HE3	1:C:302:MET:HA	1.95	0.49
2:D:141:LEU:HG	2:D:170:SER:HB3	1.95	0.49
1:A:340:THR:O	1:A:340:THR:HG22	2.13	0.49
3:E:132:GLU:HA	3:E:135:LYS:HB3	1.95	0.49
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.94	0.48
3:E:49:GLU:HG3	3:E:53:LYS:HE2	1.95	0.48
1:A:16:ILE:HD11	1:A:231:ILE:HD13	1.94	0.48
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.48	0.48
1:A:213:CYS:HB3	1:A:219:ILE:HD12	1.95	0.48
2:B:286:LEU:HD23	2:B:291:LEU:HD12	1.95	0.48
2:B:271:GLY:HA3	2:B:377:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:HG22	1:C:180:ALA:H	1.78	0.48
2:D:5:VAL:HG23	2:D:132:LEU:CD1	2.43	0.48
1:A:388:TRP:CE3	1:A:425:MET:HE1	2.48	0.48
1:C:202:PHE:HE2	1:C:378:LEU:HD22	1.78	0.48
2:B:119:LEU:HD21	2:B:156:LYS:HB3	1.95	0.48
2:B:217:LEU:HD11	2:B:230:LEU:HD21	1.96	0.48
2:B:346:TRP:HB3	2:B:440:ALA:HB2	1.96	0.48
1:A:407:TRP:HZ2	2:B:260:VAL:HB	1.78	0.47
1:C:66:VAL:HG12	1:C:68:VAL:HG23	1.95	0.47
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.95	0.47
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.95	0.47
2:D:213:CYS:HB3	2:D:219:LEU:HD12	1.96	0.47
2:D:423:SER:HA	2:D:426:ASN:HB2	1.94	0.47
2:B:21:TRP:CE3	2:B:24:ILE:HD11	2.50	0.47
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.96	0.47
2:B:12:CYS:CB	2:B:140:SER:HB3	2.45	0.47
2:B:179:ASP:HB2	1:C:352:LYS:HE3	1.96	0.47
1:C:224:TYR:HA	1:C:227:LEU:HD12	1.96	0.47
1:A:305:CYS:HB2	1:A:386:GLU:HB2	1.95	0.47
2:B:259:MET:CE	2:B:316:ALA:HB2	2.43	0.47
2:B:71:GLU:HB3	2:B:98:GLY:CA	2.45	0.47
2:D:220:THR:O	2:D:222:PRO:HD3	2.15	0.46
2:B:182:VAL:HA	2:B:398:MET:HE1	1.97	0.46
2:B:98:GLY:C	2:B:100:GLY:H	2.23	0.46
1:C:160:ASP:HB3	1:C:161:TYR:CD1	2.51	0.46
1:A:398:MET:HE2	2:B:348:PRO:HD2	1.96	0.46
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.98	0.46
1:A:229:ARG:HD2	1:A:363:VAL:HG21	1.98	0.46
1:C:119:LEU:CD1	1:C:156:ARG:HE	2.29	0.46
1:A:2:ARG:N	1:A:131:GLY:O	2.48	0.46
1:A:224:TYR:HA	1:A:227:LEU:HD12	1.98	0.46
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.34	0.46
2:B:155:SER:HB2	3:E:76:ARG:HH22	1.80	0.46
2:B:75:MET:HE2	2:B:94:PHE:HB3	1.98	0.45
2:B:119:LEU:HD23	2:B:160:GLU:OE1	2.16	0.45
2:D:185:TYR:HD1	2:D:408:TYR:CE1	2.34	0.45
2:D:272:PHE:HE1	2:D:374:SER:HB2	1.81	0.45
1:A:238:ILE:HG12	1:A:378:LEU:HD21	1.99	0.45
2:B:70:LEU:HD11	2:B:111:GLY:HA2	1.96	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD11	1.98	0.45
1:C:241:SER:OG	1:C:252:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:414:ASP:OD1	2:D:417:GLU:HB2	2.17	0.45
2:B:295:MET:HE3	2:B:377:PHE:HD1	1.82	0.45
2:D:320:ARG:HA	2:D:356:CYS:O	2.16	0.45
1:A:137:VAL:HG23	1:A:168:GLU:HA	1.99	0.45
2:B:19:LYS:HB3	2:B:232:SER:HB3	1.99	0.44
1:C:202:PHE:CE2	1:C:268:PRO:HG2	2.52	0.44
2:D:248:LEU:HB2	2:D:249:ASN:C	2.42	0.44
3:E:130:ALA:HB1	3:E:134:ARG:NH1	2.31	0.44
3:E:56:ALA:HA	3:E:59:GLU:CD	2.42	0.44
1:A:15:GLN:O	1:A:18:ASN:HB2	2.17	0.44
1:A:30:ILE:HA	1:A:36:MET:HB3	1.98	0.44
2:D:5:VAL:HG23	2:D:132:LEU:HD13	2.00	0.44
2:D:387:LEU:O	2:D:391:ILE:HG12	2.16	0.44
1:A:158:SER:HB2	1:A:197:HIS:CD2	2.45	0.44
2:B:44:LEU:HD23	2:B:49:ILE:HD13	1.98	0.44
1:C:377:MET:HE3	1:C:379:SER:OG	2.18	0.44
2:D:89:PRO:HA	2:D:92:PHE:CD1	2.52	0.44
1:A:12:ALA:HA	4:A:600:GTP:C5	2.52	0.44
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.51	0.44
2:D:69:ASP:HA	2:D:145:THR:HG21	1.99	0.44
2:D:104:ALA:HB2	2:D:413:MET:SD	2.58	0.44
1:A:239:THR:HA	1:A:242:LEU:HD12	1.99	0.44
2:B:115:VAL:HG22	2:B:119:LEU:HD13	1.99	0.44
2:D:108:TYR:CE2	3:E:130:ALA:HA	2.52	0.44
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.00	0.44
1:C:23:LEU:HA	1:C:26:LEU:HD12	2.00	0.43
1:C:25:CYS:O	1:C:30:ILE:N	2.51	0.43
1:C:69:ASP:CB	1:C:75:ILE:HD12	2.48	0.43
1:C:231:ILE:HA	1:C:234:ILE:HD12	2.00	0.43
2:D:2:ARG:HB3	2:D:131:CYS:O	2.17	0.43
2:B:173:PRO:HG3	2:B:187:ALA:HB2	1.99	0.43
1:C:331:ALA:O	1:C:335:ILE:HG12	2.19	0.43
2:D:315:VAL:HB	2:D:351:VAL:HG13	2.01	0.43
1:A:395:PHE:CE2	1:A:422:ARG:HB2	2.54	0.43
2:B:54:ASN:HB2	2:B:62:VAL:HG13	2.01	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HG13	2.01	0.43
2:D:10:GLY:HA3	6:D:501:GDP:O1B	2.19	0.43
2:D:91:ASN:HA	2:D:121:VAL:HG11	1.99	0.43
2:D:206:ASN:HD21	6:D:501:GDP:HN22	1.65	0.43
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.82	0.43
2:B:70:LEU:HD11	2:B:111:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:VAL:O	2:B:185:TYR:HB2	2.18	0.43
2:D:181:VAL:HG21	2:D:404:PHE:CZ	2.53	0.43
2:B:209:LEU:HB3	2:B:227:LEU:HG	2.01	0.43
2:B:384:ILE:HG22	2:B:432:TYR:CE2	2.54	0.43
1:C:346:TRP:CZ2	1:C:435:VAL:HG22	2.52	0.43
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.99	0.43
2:B:289:PRO:O	2:B:293:GLN:HG2	2.18	0.43
1:C:93:ILE:HG21	1:C:118:VAL:HG22	2.00	0.43
1:C:182:VAL:O	1:C:185:TYR:HB2	2.18	0.43
2:D:70:LEU:HD21	2:D:111:GLY:HA2	2.00	0.43
2:D:123:ARG:O	2:D:127:GLU:HG2	2.18	0.43
2:D:173:PRO:HB3	6:D:501:GDP:O3'	2.19	0.43
2:D:382:THR:O	2:D:385:GLN:HG2	2.18	0.43
1:A:313:MET:HE1	1:A:382:THR:HG23	1.99	0.43
2:B:306:ASP:O	2:B:309:HIS:HB2	2.19	0.43
1:C:411:GLU:OE2	1:C:411:GLU:HA	2.19	0.43
1:A:31:GLN:C	1:A:33:ASP:H	2.27	0.43
1:A:195:LEU:HD21	1:A:264:ARG:NH1	2.33	0.42
2:D:263:PRO:O	2:D:266:HIS:HD2	2.01	0.42
1:A:319:TYR:HB2	1:A:355:ILE:HG12	2.00	0.42
1:C:11:GLN:HE21	1:C:11:GLN:HB2	1.72	0.42
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.83	0.42
2:B:55:GLU:HG2	2:B:59:ASN:O	2.19	0.42
1:C:154:MET:HE1	1:C:166:LYS:HB3	2.01	0.42
1:A:93:ILE:HG21	1:A:118:VAL:HG22	2.01	0.42
1:A:188:ILE:HG13	1:A:425:MET:HE2	2.00	0.42
1:A:329:ASN:HA	1:A:332:ILE:HB	2.02	0.42
1:C:107:HIS:O	1:C:152:LEU:HD22	2.19	0.42
1:C:132:LEU:HD23	1:C:164:LYS:HE3	2.01	0.42
1:C:340:THR:CG2	1:C:341:ILE:N	2.83	0.42
1:C:386:GLU:O	1:C:390:ARG:HB2	2.19	0.42
2:B:206:ASN:HD21	6:B:501:GDP:HN22	1.67	0.42
1:C:214:ARG:O	1:C:218:ASP:HA	2.20	0.42
1:A:78:VAL:C	1:A:80:THR:H	2.27	0.42
1:A:413:MET:HE3	1:A:417:GLU:HB3	2.01	0.42
2:B:149:MET:O	2:B:152:LEU:HB3	2.20	0.42
2:B:154:ILE:HG22	2:B:197:ASN:HB3	2.02	0.42
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.54	0.42
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.01	0.42
1:A:17:GLY:O	1:A:21:TRP:HD1	2.03	0.41
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.01	0.41
2:D:160:GLU:HB3	2:D:161:TYR:CE1	2.55	0.41
3:E:77:GLU:HA	3:E:80:ARG:HB2	2.03	0.41
2:B:165:ILE:HG22	2:B:252:LEU:HD23	2.01	0.41
2:B:323:MET:HE2	2:B:328:VAL:HG22	2.01	0.41
1:C:99:ALA:HB3	1:C:144:GLY:HA3	2.01	0.41
2:D:289:PRO:O	2:D:293:GLN:HB2	2.20	0.41
1:A:120:ASP:O	1:A:124:LYS:HD2	2.20	0.41
2:B:321:GLY:HA3	2:B:373:MET:HA	2.01	0.41
1:C:69:ASP:HB2	1:C:75:ILE:HD12	2.02	0.41
1:C:195:LEU:HD12	1:C:266:HIS:HE1	1.84	0.41
2:D:295:MET:HE2	2:D:295:MET:HB3	1.58	0.41
1:A:241:SER:HB3	1:A:248:LEU:O	2.21	0.41
1:C:93:ILE:HD13	1:C:118:VAL:HA	2.02	0.41
1:C:180:ALA:HA	7:D:502:LOC:O5	2.21	0.41
1:C:340:THR:HG23	1:C:341:ILE:N	2.34	0.41
2:D:70:LEU:O	2:D:98:GLY:N	2.53	0.41
1:C:201:ALA:H	1:C:266:HIS:HD2	1.69	0.41
2:D:5:VAL:HG13	2:D:64:ARG:HG2	2.02	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.03	0.41
1:A:428:LEU:O	1:A:432:TYR:HD1	2.04	0.41
2:B:183:GLU:HA	2:B:186:ASN:HD22	1.86	0.41
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.56	0.41
1:A:324:VAL:O	1:A:328:VAL:HG23	2.21	0.41
1:A:329:ASN:ND2	3:E:22:VAL:HG11	2.34	0.41
2:B:5:VAL:HG13	2:B:66:ILE:HD13	2.02	0.41
2:B:97:SER:O	2:B:99:ALA:N	2.51	0.41
2:B:114:LEU:O	2:B:118:VAL:HG23	2.21	0.41
2:B:243:ARG:HH22	2:B:320:ARG:HH12	1.69	0.41
1:C:16:ILE:HD11	1:C:231:ILE:HD13	2.03	0.41
2:D:180:THR:HG22	2:D:182:VAL:HG22	2.03	0.41
2:B:114:LEU:HD23	2:B:149:MET:HE1	2.03	0.41
1:C:264:ARG:HH22	1:C:427:ALA:HB3	1.86	0.40
2:D:331:GLN:O	2:D:335:VAL:HG23	2.21	0.40
2:B:160:GLU:HB3	2:B:161:TYR:CD1	2.56	0.40
2:D:140:SER:HA	2:D:171:VAL:HG13	2.03	0.40
1:A:99:ALA:HA	1:A:105:ARG:HG2	2.03	0.40
1:A:140:SER:HB2	1:A:141:PHE:H	1.70	0.40
1:C:101:ASN:HD22	2:D:258:ASN:HD21	1.68	0.40
1:C:398:MET:HB3	1:C:403:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:HD1	1:A:408:TYR:CE1	2.39	0.40
1:C:234:ILE:HG12	1:C:272:TYR:HB2	2.04	0.40
2:D:69:ASP:HB3	2:D:94:PHE:CD1	2.56	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%)	364 (86%)	51 (12%)	10 (2%)	4	29
1	C	428/451 (95%)	363 (85%)	53 (12%)	12 (3%)	4	26
2	B	426/445 (96%)	366 (86%)	47 (11%)	13 (3%)	3	25
2	D	429/445 (96%)	381 (89%)	40 (9%)	8 (2%)	6	33
3	E	119/142 (84%)	108 (91%)	9 (8%)	2 (2%)	7	35
All	All	1827/1934 (94%)	1582 (87%)	200 (11%)	45 (2%)	4	28

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	73	THR
1	A	341	ILE
2	B	60	LYS
2	B	98	GLY
2	B	109	THR
1	C	10	GLY
1	C	109	THR
1	C	249	ASN
2	D	82	PRO
2	D	115	VAL

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Mol	Chain	Res	Type
2	D	250	ALA
3	E	32	VAL
1	A	10	GLY
1	A	72	PRO
1	A	115	ILE
1	A	131	GLY
2	B	57	THR
2	B	99	ALA
2	B	298	SER
2	B	373	MET
1	C	11	GLN
1	C	29	GLY
1	C	250	VAL
2	D	73	GLY
1	A	140	SER
1	A	261	PRO
1	C	115	ILE
2	D	144	GLY
3	E	15	THR
1	A	141	PHE
2	B	178	SER
2	B	283	TYR
2	B	284	ARG
2	D	97	SER
2	B	32	PRO
1	C	265	ILE
1	C	279	GLU
1	C	325	PRO
1	C	32	PRO
1	C	341	ILE
2	D	143	GLY
2	B	183	GLU
2	D	271	GLY
2	B	115	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/378 (96%)	297 (82%)	65 (18%)	2	10
1	C	359/378 (95%)	297 (83%)	62 (17%)	2	11
2	B	364/383 (95%)	306 (84%)	58 (16%)	2	14
2	D	369/383 (96%)	318 (86%)	51 (14%)	3	19
3	E	107/125 (86%)	82 (77%)	25 (23%)	1	4
All	All	1561/1647 (95%)	1300 (83%)	261 (17%)	2	13

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	GLU
1	A	16	ILE
1	A	22	GLU
1	A	35	GLN
1	A	46	ASP
1	A	47	ASP
1	A	50	ASN
1	A	74	VAL
1	A	75	ILE
1	A	77	GLU
1	A	85	GLN
1	A	90	GLU
1	A	92	LEU
1	A	94	THR
1	A	110	ILE
1	A	114	ILE
1	A	120	ASP
1	A	124	LYS
1	A	125	LEU
1	A	128	GLN
1	A	137	VAL
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	166	LYS
1	A	167	LEU
1	A	170	SER
1	A	171	ILE
1	A	177	VAL
1	A	181	VAL

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Mol	Chain	Res	Type
1	A	187	SER
1	A	211	ASP
1	A	212	ILE
1	A	219	ILE
1	A	221	ARG
1	A	224	TYR
1	A	225	THR
1	A	230	LEU
1	A	233	GLN
1	A	241	SER
1	A	253	THR
1	A	271	THR
1	A	275	VAL
1	A	279	GLU
1	A	285	GLN
1	A	302	MET
1	A	306	ASP
1	A	308	ARG
1	A	317	LEU
1	A	327	ASP
1	A	336	LYS
1	A	342	GLN
1	A	343	PHE
1	A	351	PHE
1	A	352	LYS
1	A	363	VAL
1	A	367	ASP
1	A	371	VAL
1	A	391	LEU
1	A	401	LYS
1	A	402	ARG
1	A	409	VAL
1	A	417	GLU
1	A	437	VAL
2	B	5	VAL
2	B	15	GLN
2	B	20	PHE
2	B	23	VAL
2	B	42	LEU
2	B	49	ILE
2	B	55	GLU
2	B	59	ASN

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Mol	Chain	Res	Type
2	B	62	VAL
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	75	MET
2	B	86	ILE
2	B	109	THR
2	B	116	ASP
2	B	118	VAL
2	B	127	GLU
2	B	129	CYS
2	B	132	LEU
2	B	158	ARG
2	B	163	ASP
2	B	164	ARG
2	B	166	MET
2	B	171	VAL
2	B	177	VAL
2	B	178	SER
2	B	180	THR
2	B	188	THR
2	B	198	THR
2	B	200	GLU
2	B	204	ILE
2	B	209	LEU
2	B	212	ILE
2	B	223	THR
2	B	227	LEU
2	B	240	THR
2	B	251	ASP
2	B	287	THR
2	B	291	LEU
2	B	292	THR
2	B	293	GLN
2	B	296	PHE
2	B	297	ASP
2	B	298	SER
2	B	324	SER
2	B	327	GLU
2	B	345	GLU
2	B	349	ASN
2	B	353	THR

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Mol	Chain	Res	Type
2	B	355	VAL
2	B	373	MET
2	B	376	THR
2	B	384	ILE
2	B	392	SER
2	B	400	ARG
2	B	402	LYS
2	B	439	THR
1	C	2	ARG
1	C	4[A]	CYS
1	C	4[B]	CYS
1	C	5	ILE
1	C	11	GLN
1	C	16	ILE
1	C	23	LEU
1	C	33	ASP
1	C	71	GLU
1	C	74	VAL
1	C	77	GLU
1	C	80	THR
1	C	82	THR
1	C	86	LEU
1	C	94	THR
1	C	109	THR
1	C	114	ILE
1	C	120	ASP
1	C	121	ARG
1	C	123	ARG
1	C	125	LEU
1	C	137	VAL
1	C	160	ASP
1	C	165	SER
1	C	170	SER
1	C	177	VAL
1	C	193	THR
1	C	196	GLU
1	C	199	ASP
1	C	219	ILE
1	C	220	GLU
1	C	223	THR
1	C	227	LEU
1	C	245	ASP

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Mol	Chain	Res	Type
1	C	249	ASN
1	C	251	ASP
1	C	252	LEU
1	C	257	THR
1	C	260	VAL
1	C	269	LEU
1	C	271	THR
1	C	276	ILE
1	C	286	LEU
1	C	293	ASN
1	C	297	GLU
1	C	302	MET
1	C	304	LYS
1	C	306	ASP
1	C	332	ILE
1	C	339	ARG
1	C	341	ILE
1	C	344	VAL
1	C	347	CYS
1	C	352	LYS
1	C	363	VAL
1	C	367	ASP
1	C	368	LEU
1	C	371	VAL
1	C	379	SER
1	C	391	LEU
1	C	402	ARG
1	C	415	GLU
2	D	2	ARG
2	D	3	GLU
2	D	5	VAL
2	D	11	GLN
2	D	19	LYS
2	D	24	ILE
2	D	26	ASP
2	D	30	ILE
2	D	42	LEU
2	D	48	ARG
2	D	55	GLU
2	D	57	THR
2	D	60	LYS
2	D	86	ILE

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Mol	Chain	Res	Type
2	D	105	LYS
2	D	116	ASP
2	D	117	SER
2	D	122	VAL
2	D	141	LEU
2	D	145	THR
2	D	153	LEU
2	D	160	GLU
2	D	167	ASN
2	D	171	VAL
2	D	177	VAL
2	D	197	ASN
2	D	200	GLU
2	D	206	ASN
2	D	223	THR
2	D	248	LEU
2	D	255	LEU
2	D	265	LEU
2	D	275	LEU
2	D	276	THR
2	D	280	SER
2	D	293	GLN
2	D	323	MET
2	D	326	LYS
2	D	340	SER
2	D	345	GLU
2	D	358	ILE
2	D	371	LEU
2	D	405	LEU
2	D	414	ASP
2	D	415	GLU
2	D	419	THR
2	D	423	SER
2	D	428	LEU
2	D	429	VAL
2	D	430	SER
2	D	434	GLN
3	E	11	LEU
3	E	15	THR
3	E	16	SER
3	E	23	ILE
3	E	30	ASP

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Mol	Chain	Res	Type
3	E	49	GLU
3	E	55	GLU
3	E	64	GLN
3	E	65	GLU
3	E	69	LEU
3	E	72	LEU
3	E	80	ARG
3	E	82	VAL
3	E	95	LYS
3	E	96	MET
3	E	100	LYS
3	E	119	MET
3	E	120	LEU
3	E	123	LEU
3	E	124	GLN
3	E	127	ASP
3	E	131	GLU
3	E	132	GLU
3	E	134	ARG
3	E	135	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	28	HIS
1	A	50	ASN
1	A	61	HIS
1	A	85	GLN
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS
1	A	249	ASN
2	B	8	GLN
2	B	14	ASN
2	B	91	ASN
2	B	101	ASN
2	B	139	HIS
2	B	193	GLN
2	B	206	ASN
2	B	229	HIS
2	B	293	GLN

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Mol	Chain	Res	Type
2	B	309	HIS
2	B	337	ASN
2	B	385	GLN
2	B	424	ASN
2	B	433	GLN
2	B	434	GLN
2	B	436	GLN
1	C	8	HIS
1	C	11	GLN
1	C	35	GLN
1	C	266	HIS
1	C	293	ASN
1	C	300	ASN
1	C	380	ASN
1	C	393	HIS
2	D	6	HIS
2	D	14	ASN
2	D	43	GLN
2	D	101	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	193	GLN
2	D	206	ASN
2	D	247	GLN
2	D	249	ASN
2	D	258	ASN
2	D	266	HIS
2	D	293	GLN
2	D	300	ASN
2	D	394	GLN
2	D	424	ASN
2	D	426	ASN
3	E	12	ASN
3	E	18	GLN
3	E	51	GLN
3	E	64	GLN
3	E	91	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$
4	GTP	A	600	5	33,34,34	2.23	2 (6%)	50,54,54	0.54	0
8	3WZ	D	503	-	47,51,51	1.14	5 (10%)	54,72,72	1.60	11 (20%)
4	GTP	C	600	5	33,34,34	2.11	2 (6%)	50,54,54	0.54	0
7	LOC	D	502	-	31,31,31	0.47	0	44,44,44	0.87	2 (4%)
6	GDP	B	501	-	29,30,30	0.46	0	45,47,47	0.71	0
6	GDP	D	501	-	29,30,30	0.40	0	45,47,47	0.51	0
7	LOC	B	502	-	31,31,31	0.50	1 (3%)	44,44,44	0.75	1 (2%)
8	3WZ	B	503	-	47,51,51	1.21	6 (12%)	54,72,72	1.54	7 (12%)

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
4	GTP	A	600	5	-	9/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	3WZ	D	503	-	-	15/72/82/82	0/2/2/2
4	GTP	C	600	5	-	10/22/38/38	0/3/3/3
7	LOC	D	502	-	-	0/12/25/25	0/3/3/3
6	GDP	B	501	-	-	6/16/32/32	0/3/3/3
6	GDP	D	501	-	-	3/16/32/32	0/3/3/3
7	LOC	B	502	-	-	0/12/25/25	0/3/3/3
8	3WZ	B	503	-	-	19/72/82/82	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	PA-O3A	-9.04	1.49	1.59
4	C	600	GTP	PB-O3B	-8.67	1.50	1.59
4	A	600	GTP	PB-O3B	-8.62	1.50	1.59
4	C	600	GTP	PA-O3A	-7.91	1.51	1.59
8	D	503	3WZ	C5-N3	5.03	1.58	1.47
8	B	503	3WZ	C5-N3	4.60	1.57	1.47
8	B	503	3WZ	C6-C5	3.87	1.61	1.52
8	B	503	3WZ	O3-C25	3.29	1.31	1.22
8	D	503	3WZ	C6-C5	3.01	1.59	1.52
8	D	503	3WZ	O3-C25	2.99	1.30	1.22
8	B	503	3WZ	C3-C5	2.74	1.60	1.54
8	D	503	3WZ	O4-C25	-2.60	1.22	1.30
8	D	503	3WZ	C3-C5	2.59	1.59	1.54
8	B	503	3WZ	O4-C25	-2.41	1.23	1.30
8	B	503	3WZ	C14-C16	2.31	1.56	1.52
7	B	502	LOC	C11-C14	2.17	1.57	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WZ	C28-N3-C5	-5.43	108.75	119.48
8	B	503	3WZ	C28-N3-C5	-4.98	109.64	119.48
8	B	503	3WZ	C5-N3-C29	4.62	133.58	120.34
8	B	503	3WZ	C4-C3-C5	4.04	122.16	111.38
7	D	502	LOC	C14-C11-N1	3.93	117.41	114.31
8	D	503	3WZ	C30-C29-N3	3.33	125.39	118.80
7	B	502	LOC	C14-C11-N1	3.27	116.89	114.31
8	B	503	3WZ	O5-C13-C14	3.26	113.54	105.83
8	D	503	3WZ	C31-C30-C29	3.12	116.82	110.71
8	D	503	3WZ	O3-C25-C17	-3.02	112.52	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WZ	O7-C29-C30	-2.96	114.38	119.96
8	D	503	3WZ	O4-C25-C17	2.84	123.13	113.51
8	D	503	3WZ	C15-C14-C16	-2.82	103.19	108.77
8	D	503	3WZ	C28-N3-C29	2.73	131.04	122.24
8	B	503	3WZ	O3-C25-C17	-2.61	113.83	122.26
8	B	503	3WZ	O4-C25-C17	2.60	122.32	113.51
8	D	503	3WZ	O8-C34-C35	-2.54	115.78	120.58
8	D	503	3WZ	C14-C16-N2	-2.47	112.70	116.35
8	B	503	3WZ	C30-C29-N3	2.44	123.61	118.80
8	D	503	3WZ	C29-C30-N4	2.38	113.82	108.06
7	D	502	LOC	C10-C11-N1	2.22	113.82	109.76

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600	GTP	PB-O3B-PG-O2G
4	A	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	PB-O3B-PG-O2G
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-O1A
6	D	501	GDP	C5'-O5'-PA-O2A
8	B	503	3WZ	O8-C34-C35-N5
8	B	503	3WZ	N4-C34-C35-N5
8	B	503	3WZ	C3-C5-C6-C7
8	B	503	3WZ	N3-C5-C6-O6
8	B	503	3WZ	C3-C5-C6-O6
8	B	503	3WZ	C2-C3-C5-C6
8	B	503	3WZ	C4-C3-C5-C6
8	B	503	3WZ	C14-C13-O5-C26
8	D	503	3WZ	O8-C34-C35-N5
8	D	503	3WZ	C35-C34-N4-C30
8	D	503	3WZ	O8-C34-N4-C30
8	D	503	3WZ	N3-C5-C6-C7
8	D	503	3WZ	C7-C6-O6-C27
8	B	503	3WZ	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
8	D	503	3WZ	O8-C34-C35-C37
8	D	503	3WZ	N4-C34-C35-C37
8	D	503	3WZ	C29-C30-C31-C33
8	B	503	3WZ	N4-C34-C35-C37
8	B	503	3WZ	O8-C34-C35-C37
8	D	503	3WZ	C29-C30-C31-C32
8	B	503	3WZ	N4-C34-C35-C36
8	B	503	3WZ	C1-C2-C3-C5
8	D	503	3WZ	N4-C30-C31-C33
4	C	600	GTP	PB-O3B-PG-O1G
8	B	503	3WZ	O8-C34-C35-C36
8	B	503	3WZ	C4-C3-C5-N3
8	B	503	3WZ	C2-C3-C5-N3
8	D	503	3WZ	C2-C3-C5-N3
4	A	600	GTP	PB-O3A-PA-O1A
4	C	600	GTP	PB-O3A-PA-O1A
6	B	501	GDP	PB-O3A-PA-O1A
8	D	503	3WZ	C3-C5-C6-C7
8	D	503	3WZ	N3-C5-C6-O6
8	D	503	3WZ	O7-C29-C30-C31
4	A	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O1A
8	B	503	3WZ	N3-C5-C6-C7
4	A	600	GTP	PG-O3B-PB-O2B
6	B	501	GDP	C4'-C5'-O5'-PA
8	D	503	3WZ	N3-C29-C30-C31
4	C	600	GTP	PG-O3B-PB-O1B
4	A	600	GTP	C4'-C5'-O5'-PA
4	C	600	GTP	C4'-C5'-O5'-PA
8	B	503	3WZ	C12-C13-C14-C16
4	A	600	GTP	PG-O3B-PB-O1B
8	B	503	3WZ	C5-C6-C7-C8
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PA-O3A-PB-O2B
4	C	600	GTP	PB-O3A-PA-O2A
6	B	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

5 monomers are involved in 8 short contacts:

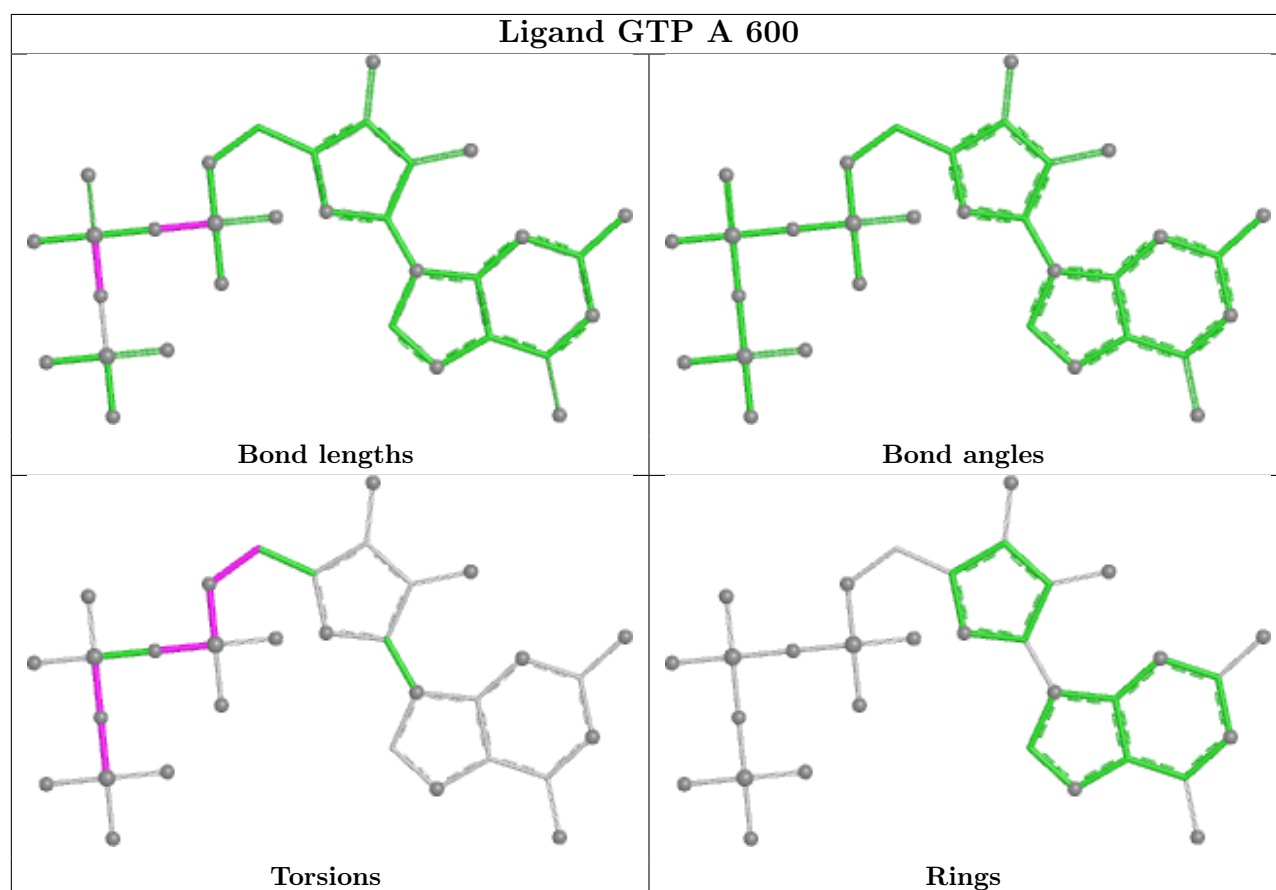
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	1	0

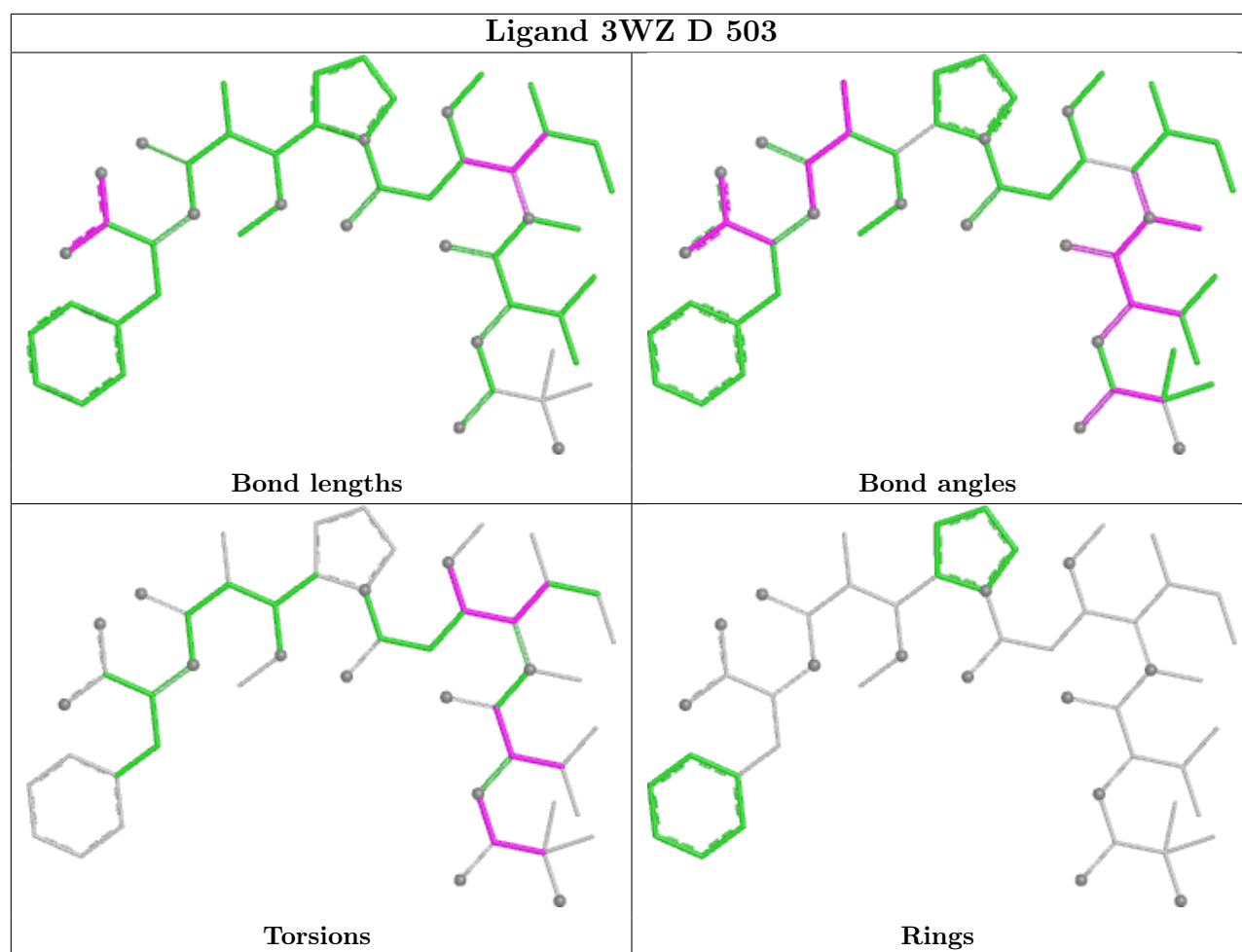
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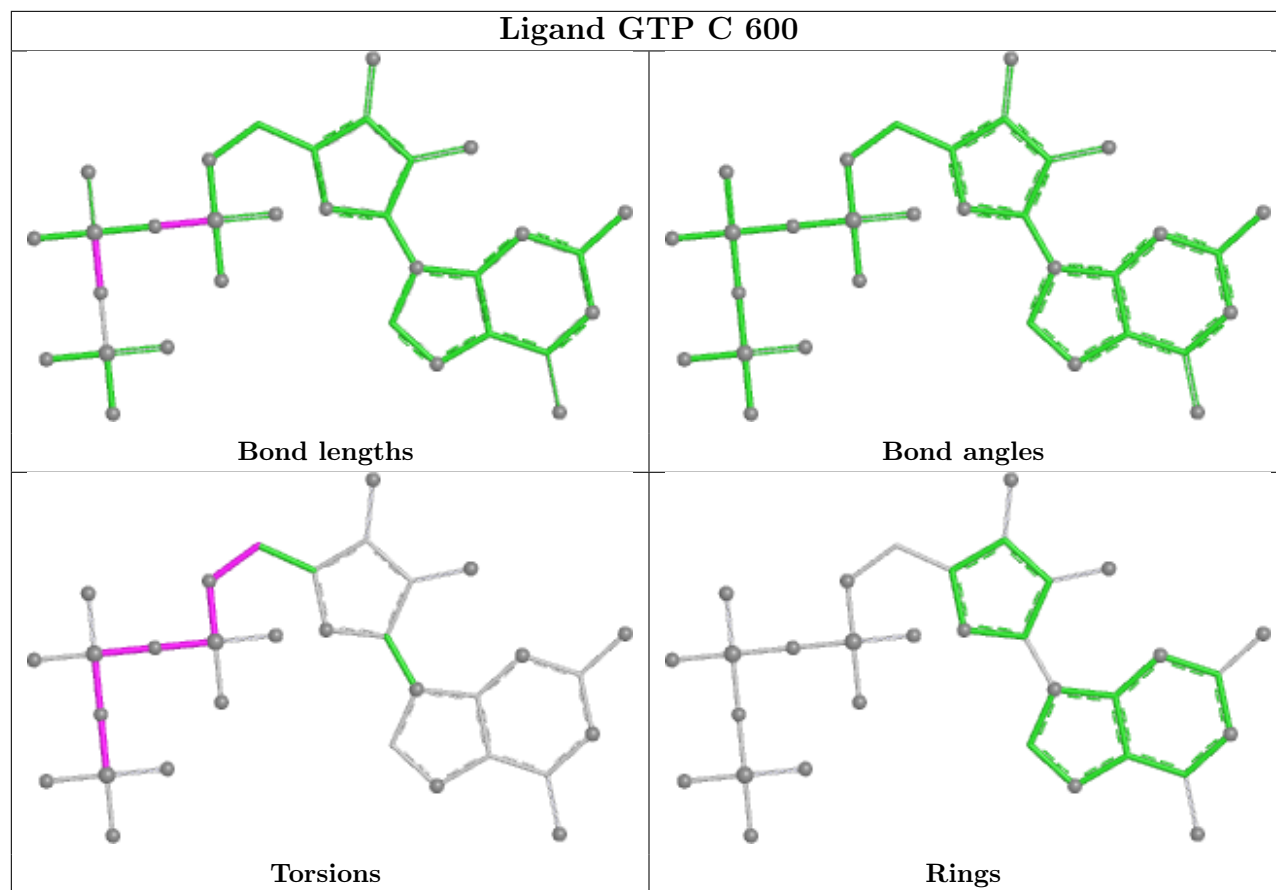
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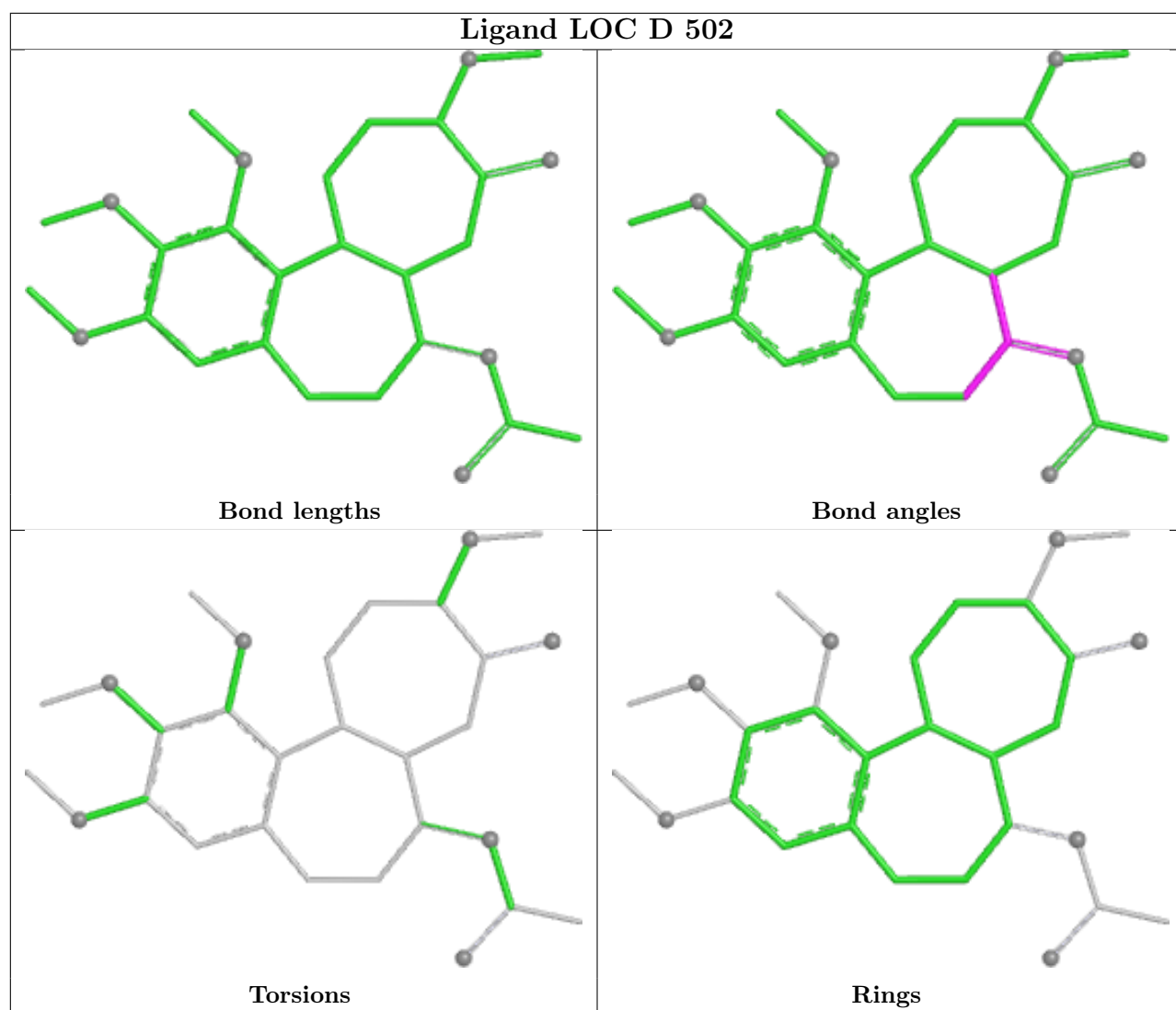
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	502	LOC	2	0
6	B	501	GDP	1	0
6	D	501	GDP	3	0
7	B	502	LOC	1	0

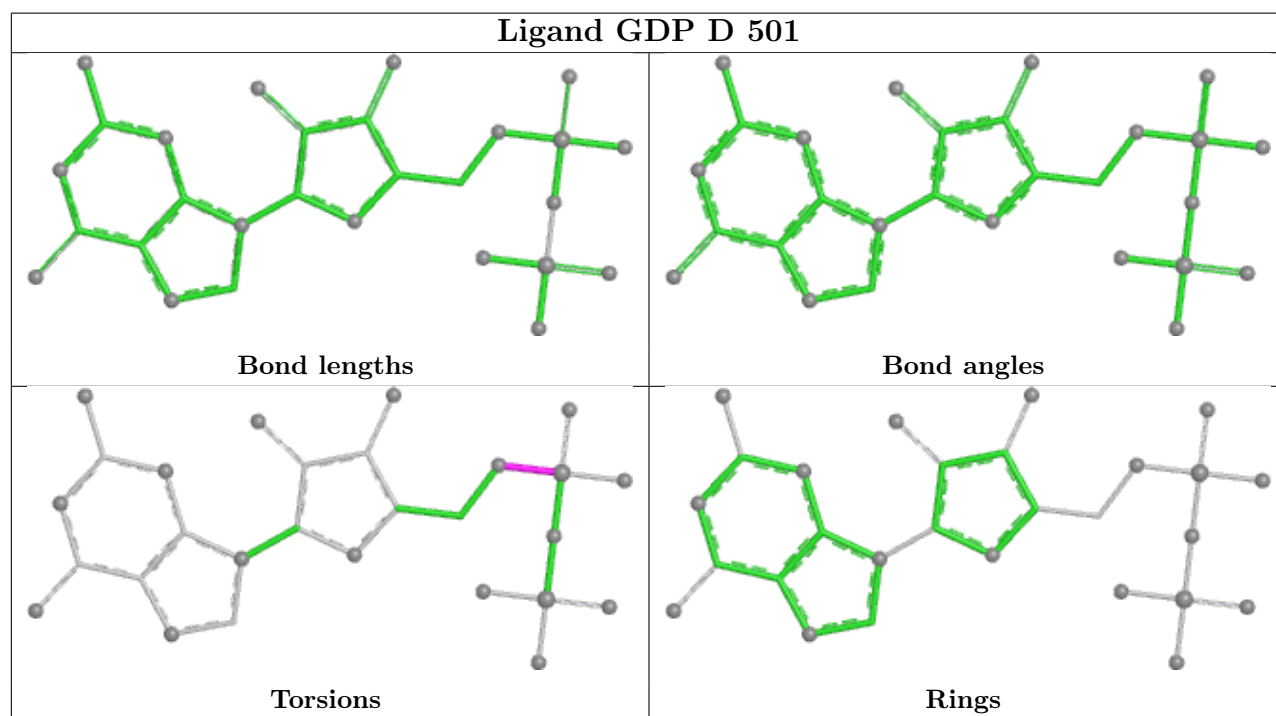
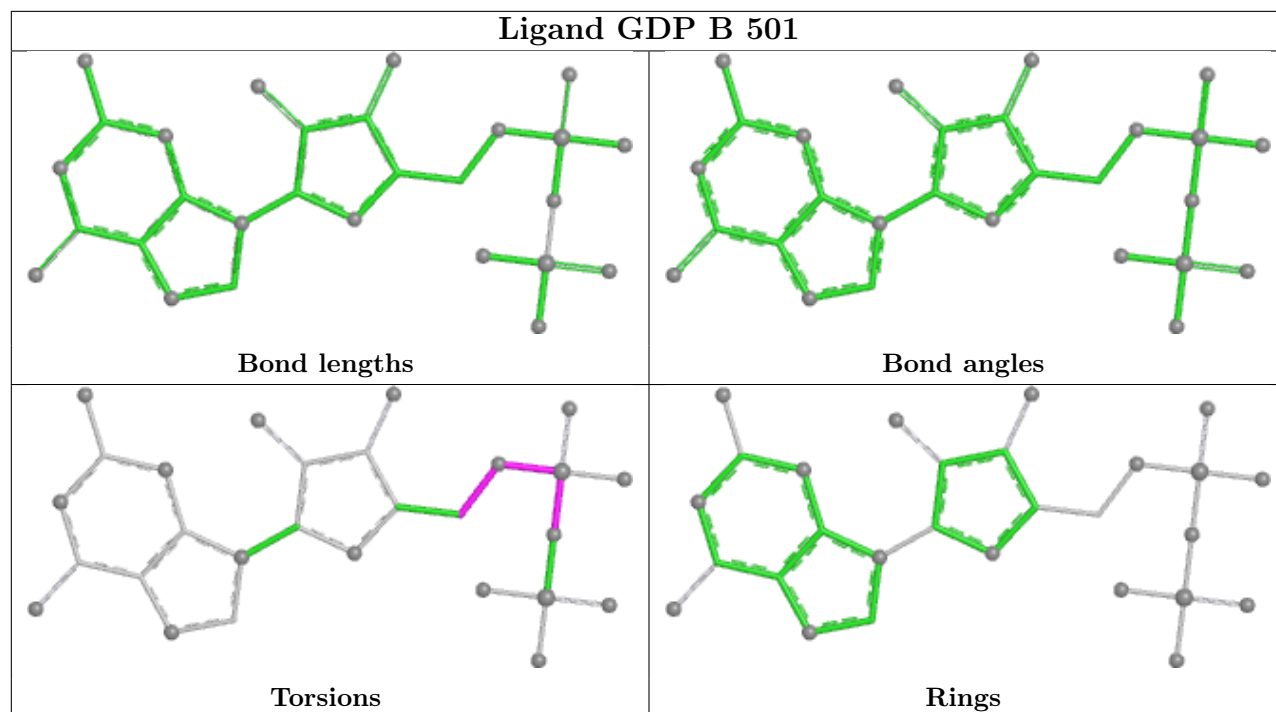
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



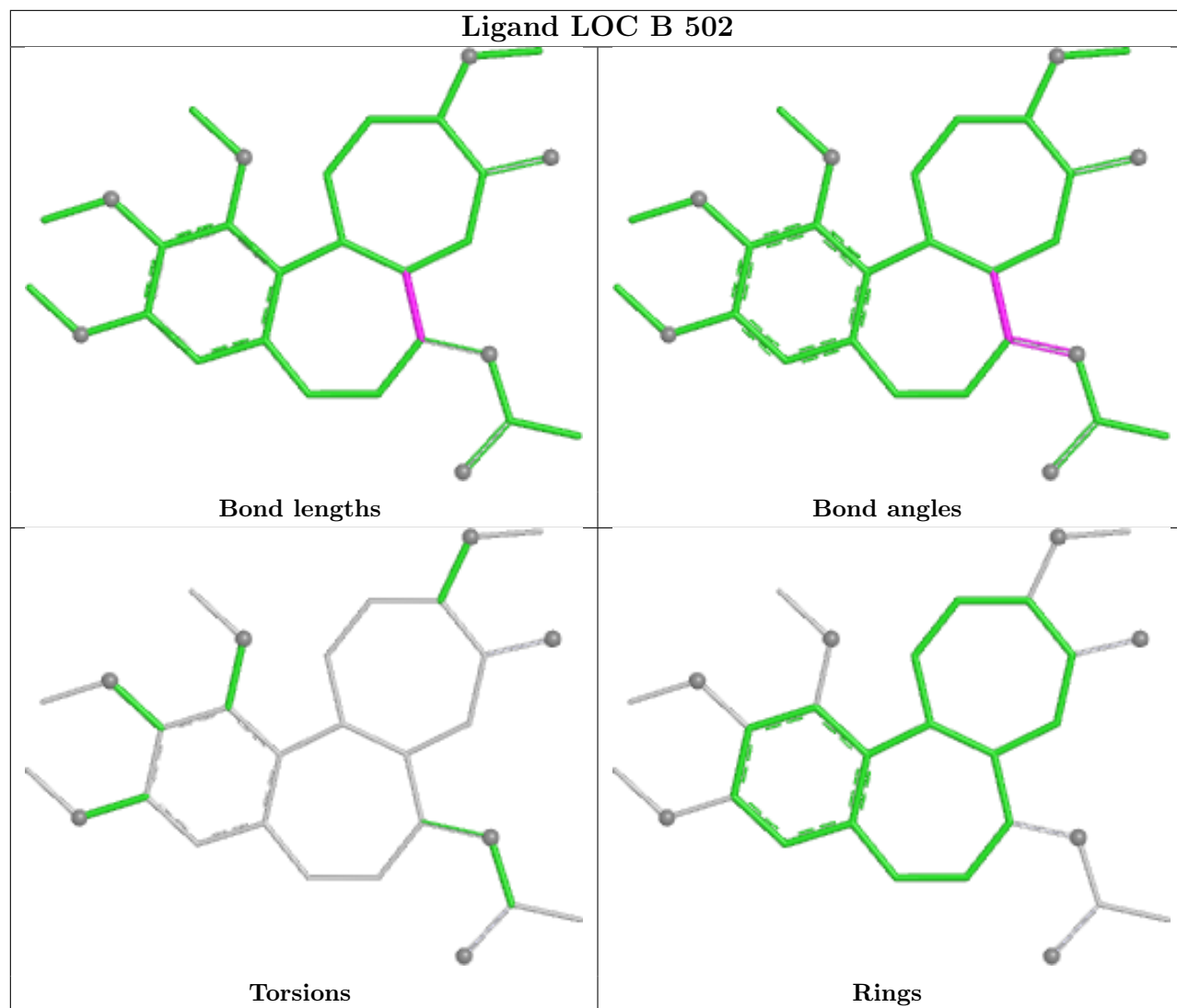


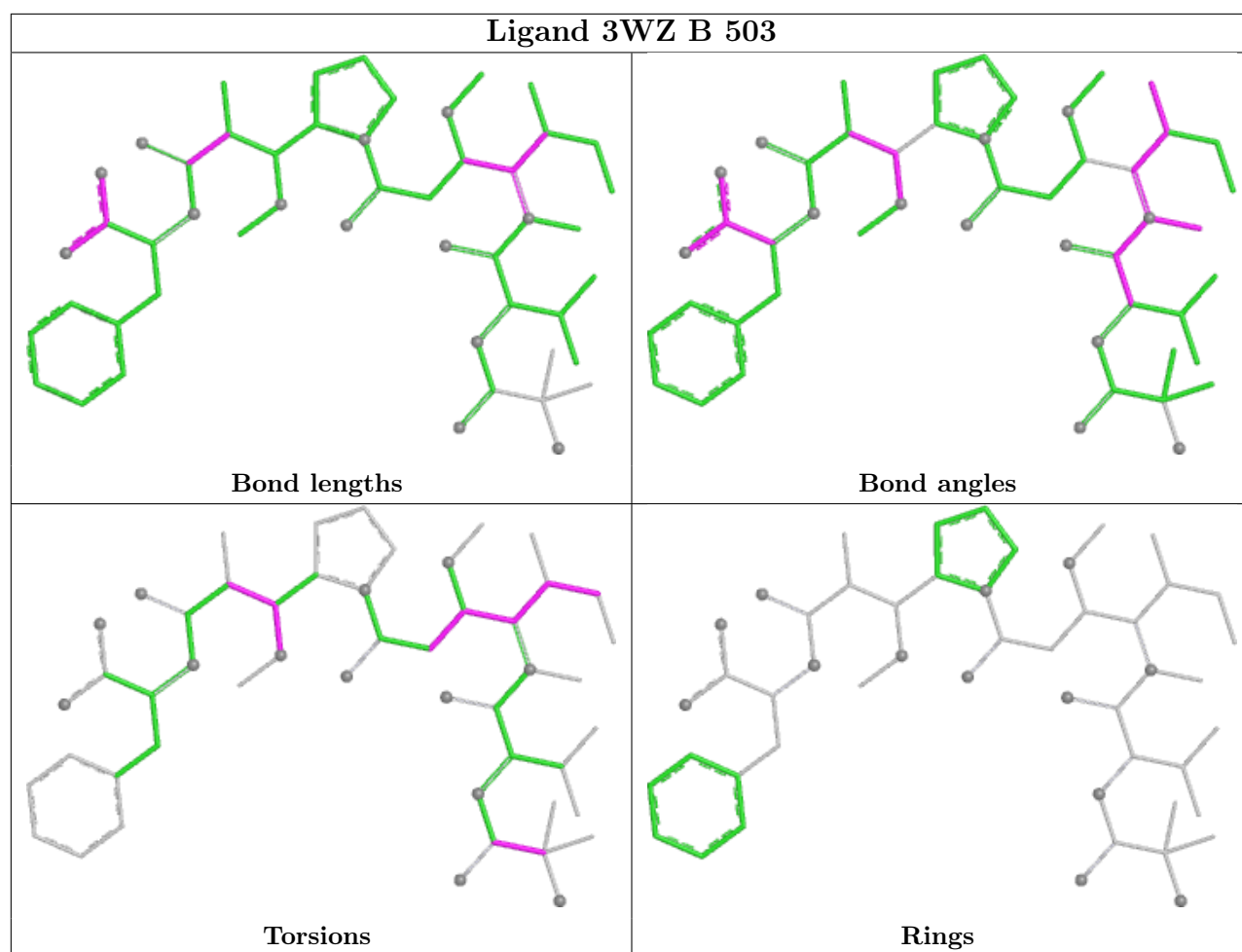






Ligand LOC B 502





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

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	429/451 (95%)	-0.55	3 (0%) 84 63	118, 157, 210, 234	0
1	C	430/451 (95%)	-0.58	5 (1%) 76 52	73, 132, 174, 197	3 (0%)
2	B	428/445 (96%)	-0.48	10 (2%) 61 37	108, 143, 181, 202	2 (0%)
2	D	430/445 (96%)	-0.62	0 100 100	74, 124, 158, 185	3 (0%)
3	E	123/142 (86%)	-0.64	0 100 100	127, 160, 208, 215	0
All	All	1840/1934 (95%)	-0.56	18 (0%) 79 56	73, 142, 190, 234	8 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	5	VAL	5.0
2	B	136	GLN	4.9
2	B	135	PHE	4.7
2	B	202	TYR	4.5
2	B	7	ILE	4.1
1	C	169	PHE	3.9
1	A	378	LEU	3.3
2	B	167	ASN	3.2
2	B	66	ILE	3.2
1	C	315	CYS	2.7
2	B	134	GLY	2.7
1	A	316	CYS	2.3
2	B	4	ILE	2.2
1	C	37	PRO	2.2
1	A	235	VAL	2.2
1	C	122	ILE	2.1
1	C	202	PHE	2.1
2	B	137	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

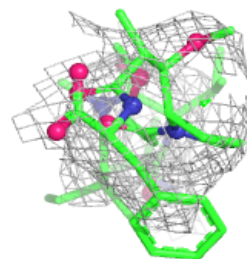
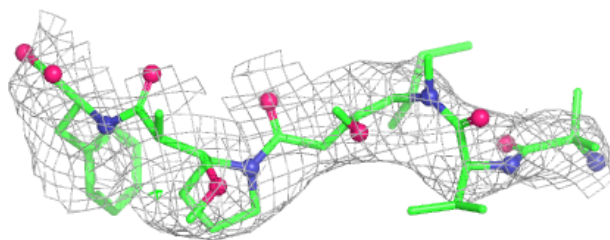
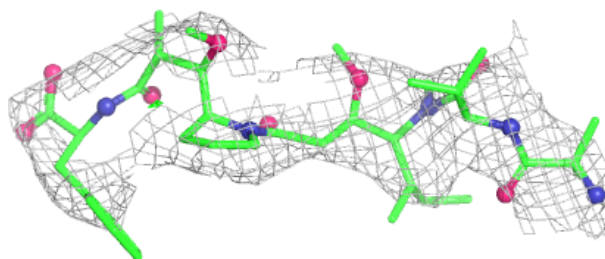
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	C	601	1/1	0.84	0.20	92,92,92,92	0
8	3WZ	B	503	50/50	0.91	0.10	147,163,172,175	0
8	3WZ	D	503	50/50	0.91	0.09	109,139,162,172	0
6	GDP	D	501	28/28	0.92	0.08	110,117,129,130	0
7	LOC	D	502	29/29	0.93	0.10	123,139,142,144	0
4	GTP	A	600	32/32	0.93	0.09	141,151,161,161	0
5	MG	A	601	1/1	0.93	0.11	78,78,78,78	0
4	GTP	C	600	32/32	0.94	0.09	112,116,120,122	0
7	LOC	B	502	29/29	0.95	0.08	153,162,166,167	0
6	GDP	B	501	28/28	0.97	0.05	122,136,140,143	0

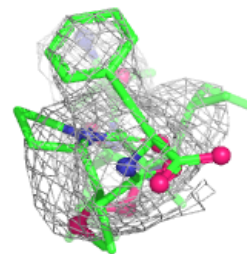
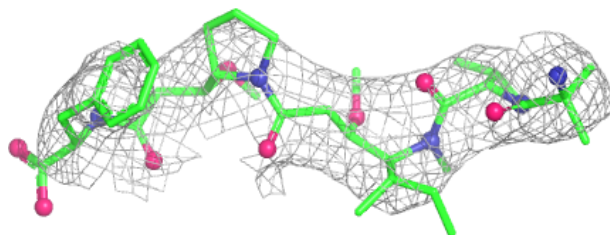
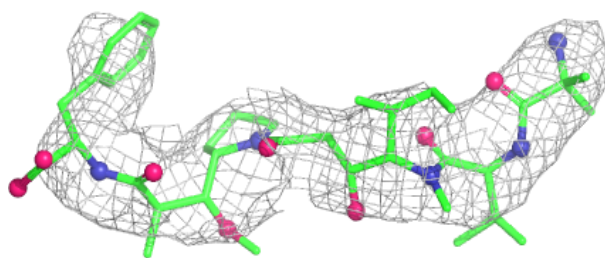
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3WZ 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)

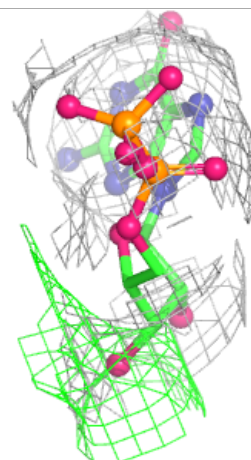
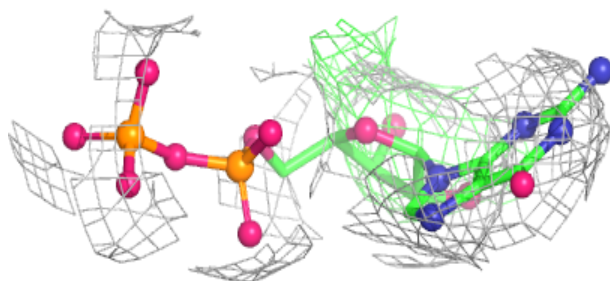
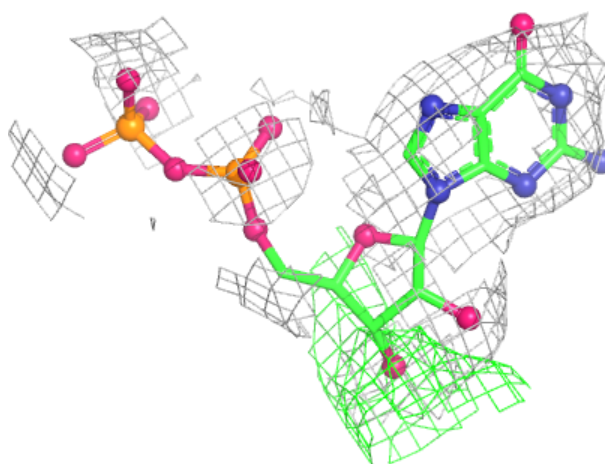
**Electron density around 3WZ D 503:**

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



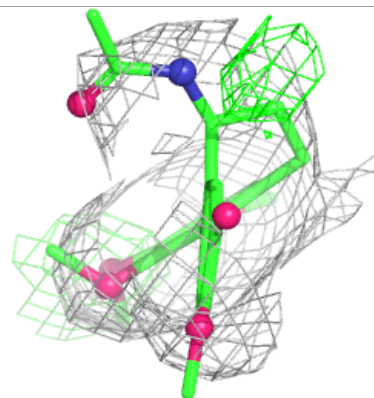
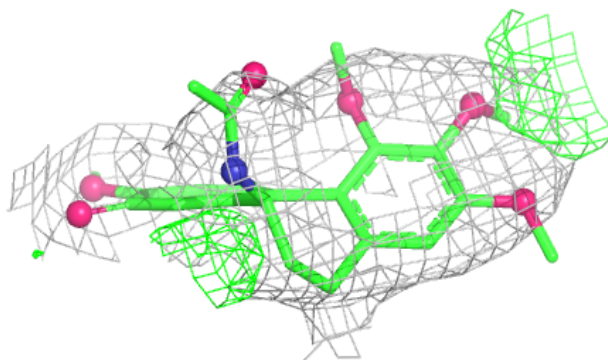
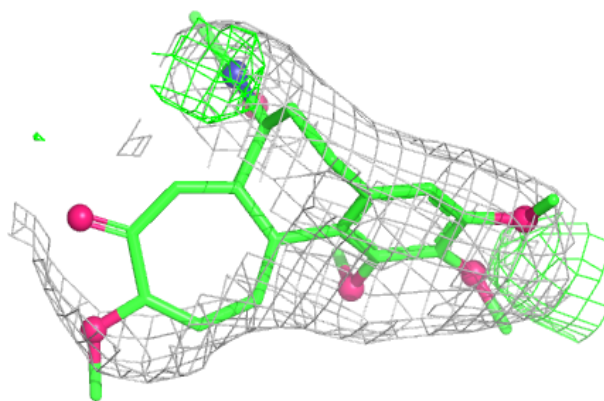
Electron density around GDP D 501:

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

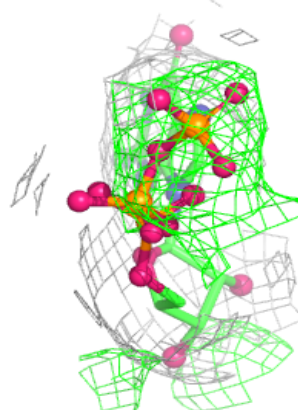
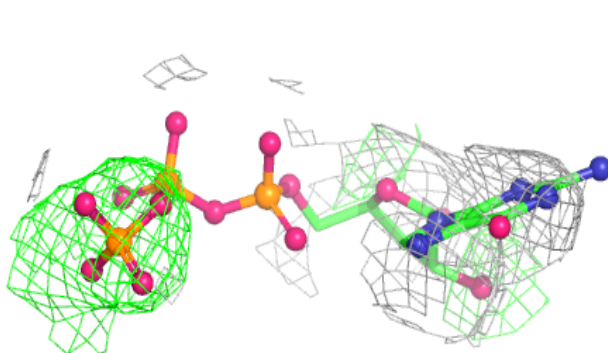
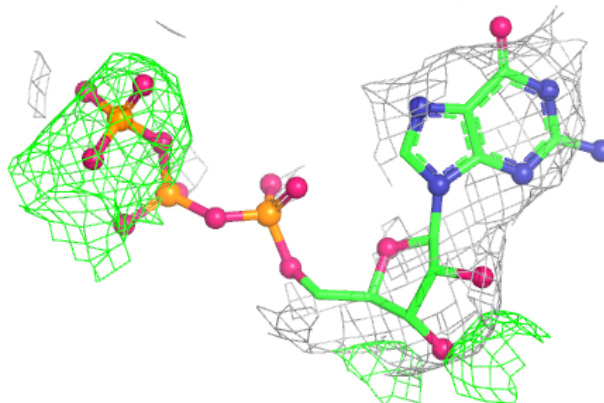


Electron density around LOC D 502:

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

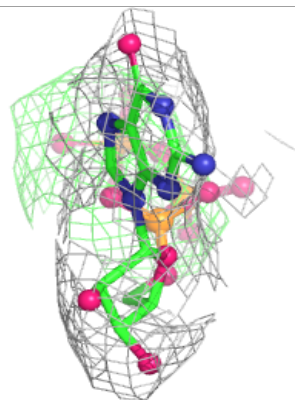
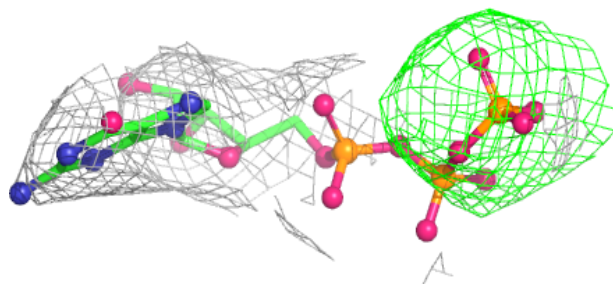
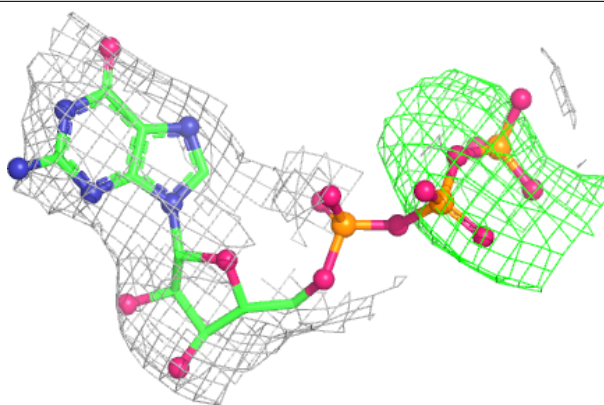
**Electron density around GTP A 600:**

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

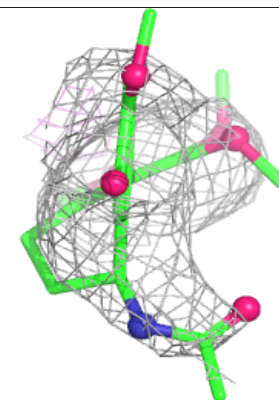
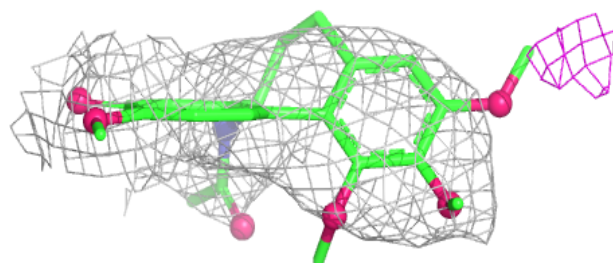
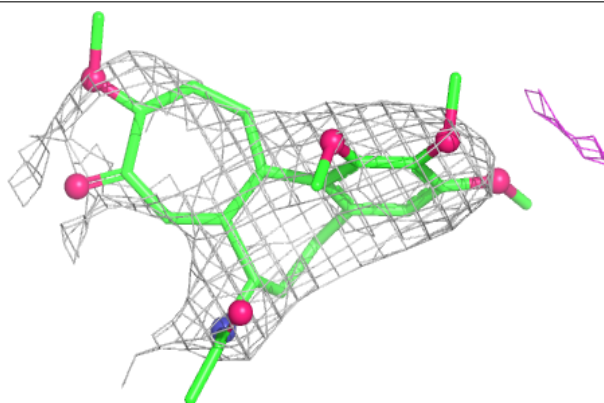


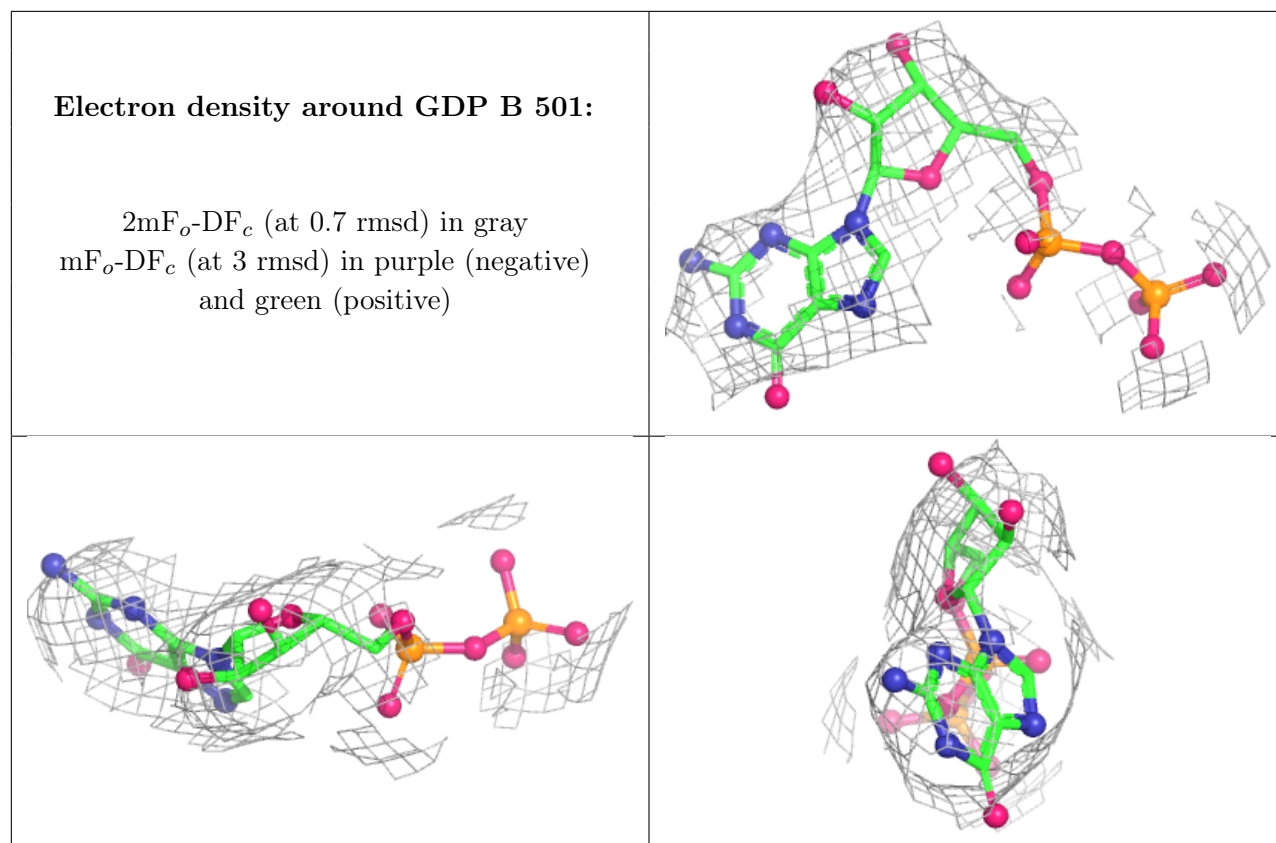
Electron density around GTP C 600:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.