Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 08:21 AM EDT

PDB ID	:	4X1I
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)

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

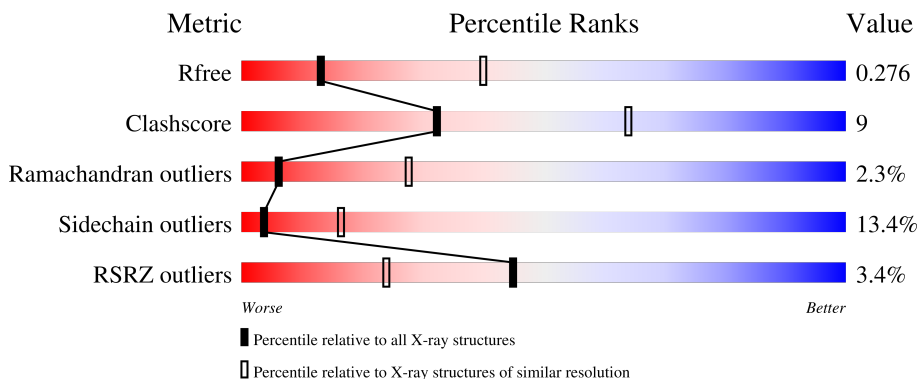|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.276
Clashscore		9
Ramachandran outliers		2.3%
Sidechain outliers		13.4%
RSRZ outliers		3.4%

Worse · · · *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (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 <=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	5% — 67% · 25% · 5%
1	C	451	.% — 67% · 23% · 5% · 5%
2	B	445	3% — 67% · 25% · ·
2	D	445	66% · 27% · ·
3	E	142	14% — 63% · 18% · 5% · 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 3363	C 2132	N 572	O 638	S 21	0	0	0
1	C	430	Total 3354	C 2126	N 569	O 635	S 24	0	3	0

- Molecule 2 is a protein called Tubulin beta chain.

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

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total 1008	C 626	N 184	O 195	S 3	0	0	0

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 (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

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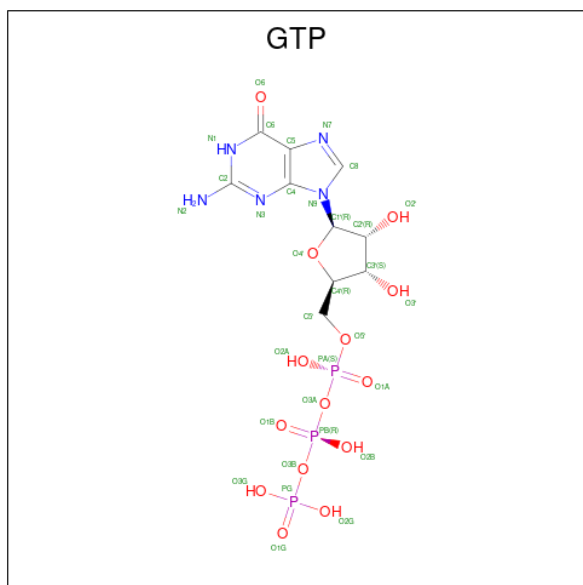
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: 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 (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

GDP

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

- Molecule 7 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]eth anamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).
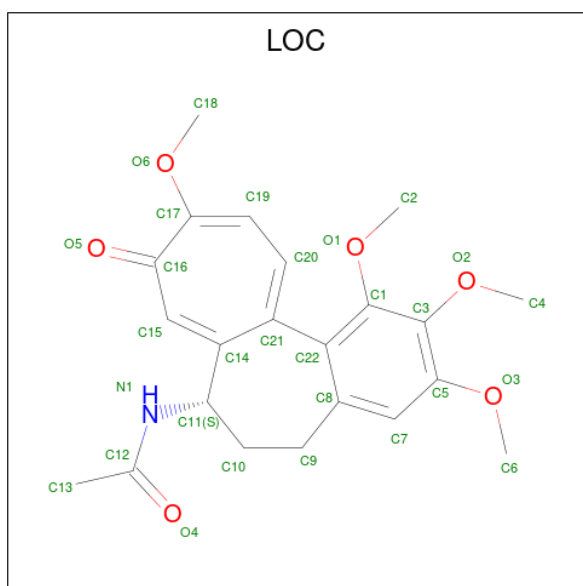

LOC

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)-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 (three-letter code: 3WD) (formula: $C_{39}H_{62}N_6O_6S$).
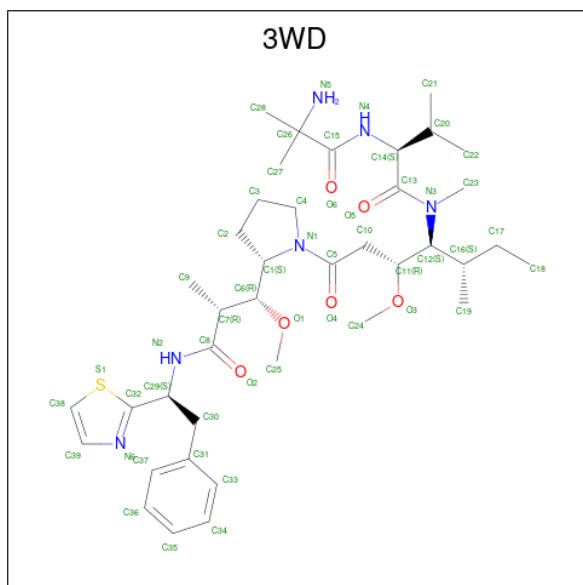
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			52	39	6	6	1		
8	D	1	Total	C	N	O	S	0	0
			52	39	6	6	1		

3 Residue-property plots ⓘ

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.
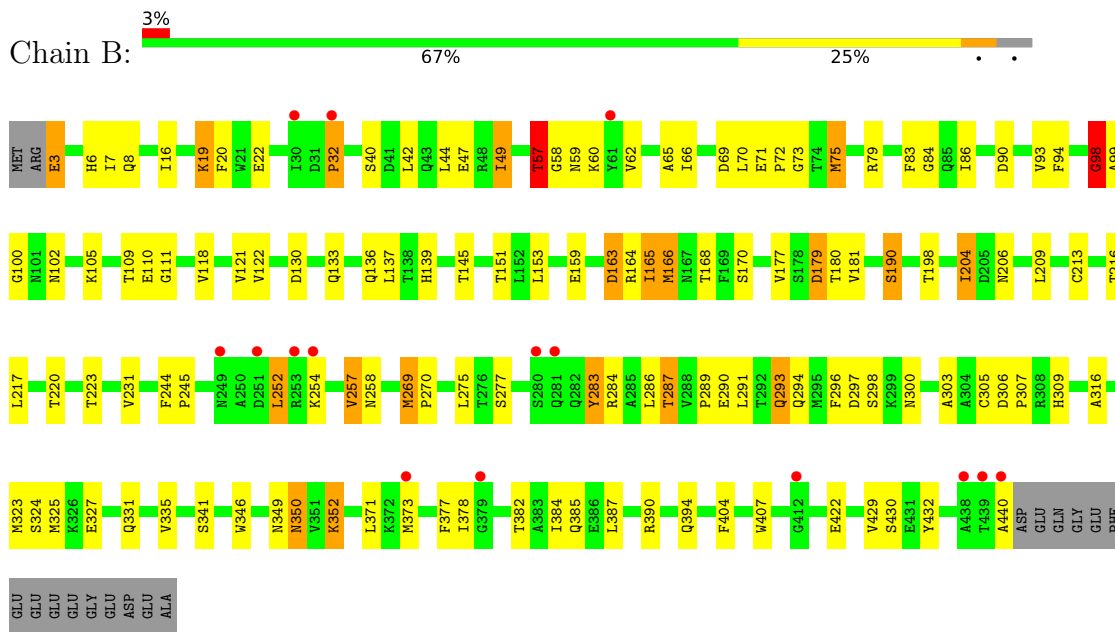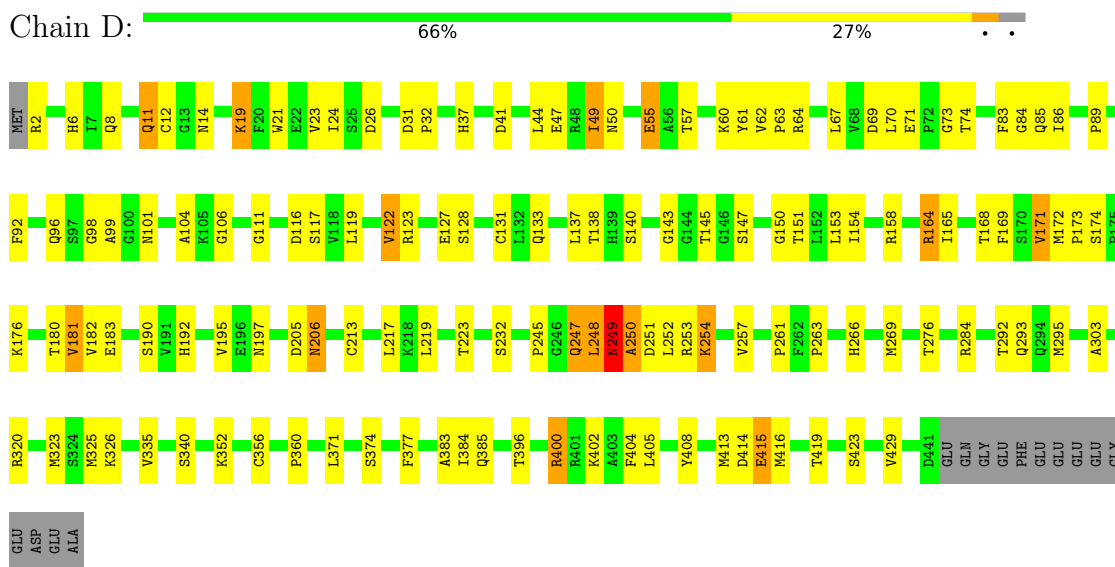
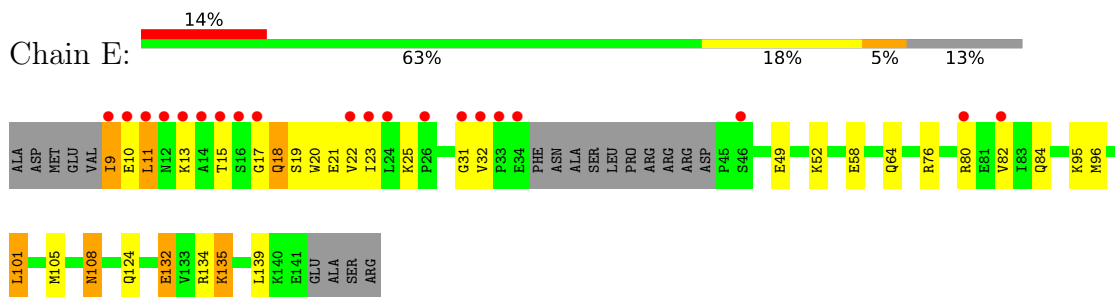• Molecule 1: Tubulin alpha chain
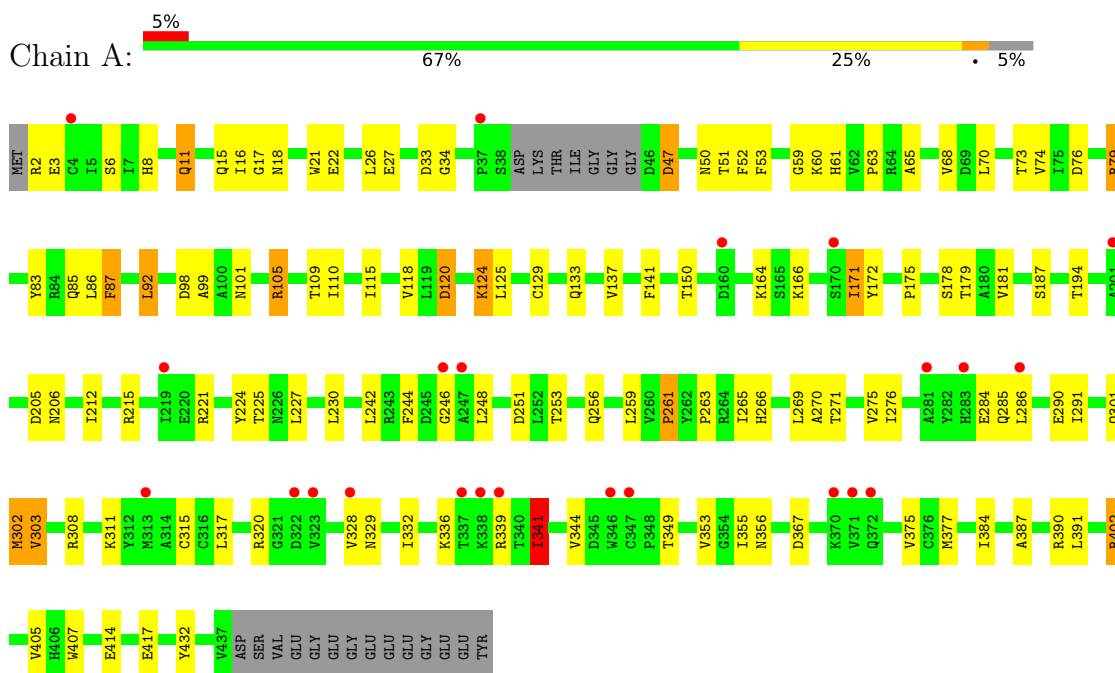
• Molecule 1: Tubulin alpha chain

• Molecule 2: Tubulin beta chain

Chain B:

3%

67% 25%

• Molecule 2: Tubulin beta chain

Chain D:

66% 27%

• Molecule 3: Stathmin-4

Chain E:

14%

63% 18% 5% 13%

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.14Å 128.21Å 255.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.30 – 3.11 40.36 – 3.11	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.30-3.11) 99.9 (40.36-3.11)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.191 , 0.253 0.194 , 0.276	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)	0.28 , 84.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, LOC, 3WD, MG, GTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.48	0/3440	0.74	0/4671
1	C	0.52	0/3438	0.76	0/4670
2	B	0.53	0/3417	0.80	1/4634 (0.0%)
2	D	0.57	0/3446	0.81	3/4670 (0.1%)
3	E	0.53	0/1019	0.76	0/1355
All	All	0.53	0/14760	0.78	4/20000 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	249	ASN	C-N-CA	6.40	137.70	121.70
2	B	98	GLY	N-CA-C	6.29	128.83	113.10
2	D	247	GLN	C-N-CA	5.55	135.57	121.70
2	D	248	LEU	C-N-CA	5.36	135.09	121.70

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	59	0
1	C	3354	0	3263	61	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3342	0	3198	60	0
2	D	3369	0	3237	66	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	254	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 (254) 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: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
1:C:308:ARG:NE	1:C:340:THR:HG21	2.03	0.74
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:D:415:GLU:H	2:D:415:GLU:CD	1.96	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:75:MET:HE1	2:B:94:PHE:HB3	1.89	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:98:GLY:C	2:B:100:GLY:H	2.15	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:LEU:HD23	2:B:49:ILE:HD13	1.97	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
1:A:50:ASN:C	1:A:52:PHE:H	2.20	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:58:GLY:HA3	2:B:59:ASN:C	2.41	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:269:MET:HE1	2:D:383:ALA:HB3	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
2:B:166:MET:HB3	2:B:198:THR:HA	2.03	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/451 (94%)	371 (87%)	45 (11%)	9 (2%)	7	29
1	C	429/451 (95%)	383 (89%)	35 (8%)	11 (3%)	5	25
2	B	426/445 (96%)	379 (89%)	35 (8%)	12 (3%)	5	24
2	D	429/445 (96%)	401 (94%)	21 (5%)	7 (2%)	9	36
3	E	119/142 (84%)	109 (92%)	7 (6%)	3 (2%)	5	26
All	All	1828/1934 (94%)	1643 (90%)	143 (8%)	42 (2%)	6	28

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
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

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Mol	Chain	Res	Type
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%)	316 (87%)	46 (13%)	4	18
1	C	360/378 (95%)	305 (85%)	55 (15%)	2	12
2	B	364/383 (95%)	314 (86%)	50 (14%)	3	16
2	D	369/383 (96%)	327 (89%)	42 (11%)	5	23
3	E	107/125 (86%)	90 (84%)	17 (16%)	2	11
All	All	1562/1647 (95%)	1352 (87%)	210 (13%)	4	16

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
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

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Mol	Chain	Res	Type
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	137	VAL
1	A	141	PHE
1	A	150	THR
1	A	164	LYS
1	A	166	LYS
1	A	171	ILE
1	A	181	VAL
1	A	187	SER
1	A	194	THR
1	A	221	ARG
1	A	225	THR
1	A	230	LEU
1	A	242	LEU
1	A	253	THR
1	A	256	GLN
1	A	276	ILE
1	A	284	GLU
1	A	285	GLN
1	A	302	MET
1	A	303	VAL
1	A	308	ARG
1	A	315	CYS
1	A	317	LEU
1	A	320	ARG
1	A	336	LYS
1	A	341	ILE
1	A	367	ASP
1	A	384	ILE
1	A	402	ARG
1	A	414	GLU
1	A	417	GLU
2	B	3	GLU
2	B	19	LYS
2	B	20	PHE
2	B	40	SER

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Mol	Chain	Res	Type
2	B	42	LEU
2	B	47	GLU
2	B	49	ILE
2	B	57	THR
2	B	62	VAL
2	B	71	GLU
2	B	75	MET
2	B	86	ILE
2	B	90	ASP
2	B	93	VAL
2	B	110	GLU
2	B	122	VAL
2	B	136	GLN
2	B	153	LEU
2	B	163	ASP
2	B	165	ILE
2	B	166	MET
2	B	179	ASP
2	B	180	THR
2	B	190	SER
2	B	204	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	296	PHE
2	B	297	ASP
2	B	323	MET
2	B	325	MET
2	B	341	SER
2	B	349	ASN
2	B	350	ASN
2	B	352	LYS
2	B	371	LEU

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Mol	Chain	Res	Type
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	80	THR
1	C	82	THR
1	C	84	ARG
1	C	109	THR
1	C	112	LYS
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	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	276	ILE
1	C	293	ASN
1	C	297	GLU
1	C	302	MET
1	C	315[A]	CYS

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Mol	Chain	Res	Type
1	C	315[B]	CYS
1	C	317	LEU
1	C	327	ASP
1	C	332	ILE
1	C	338	LYS
1	C	339	ARG
1	C	341	ILE
1	C	352	LYS
1	C	357	TYR
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	401	LYS
1	C	402	ARG
1	C	419	SER
1	C	420	GLU
1	C	435	VAL
2	D	11	GLN
2	D	19	LYS
2	D	24	ILE
2	D	26	ASP
2	D	31	ASP
2	D	37	HIS
2	D	41	ASP
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	158	ARG
2	D	164	ARG
2	D	171	VAL
2	D	183	GLU
2	D	206	ASN
2	D	223	THR
2	D	247	GLN
2	D	249	ASN
2	D	254	LYS

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Mol	Chain	Res	Type
2	D	276	THR
2	D	284	ARG
2	D	293	GLN
2	D	323	MET
2	D	325	MET
2	D	326	LYS
2	D	352	LYS
2	D	374	SER
2	D	384	ILE
2	D	400	ARG
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	49	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	124	GLN
3	E	132	GLU
3	E	134	ARG
3	E	135	LYS
3	E	139	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	91	GLN
1	A	139	HIS
1	A	197	HIS

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	301	GLN
1	A	329	ASN
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
2	B	59	ASN
2	B	139	HIS
2	B	206	ASN
2	B	229	HIS
2	B	266	HIS
2	B	309	HIS
2	B	331	GLN
2	B	349	ASN
2	B	350	ASN
2	B	406	HIS
2	B	426	ASN
1	C	8	HIS
1	C	11	GLN
1	C	139	HIS
1	C	176	GLN
1	C	249	ASN
1	C	301	GLN
1	C	406	HIS
2	D	6	HIS
2	D	14	ASN
2	D	101	ASN
2	D	133	GLN
2	D	139	HIS
2	D	206	ASN
2	D	249	ASN
2	D	266	HIS
2	D	281	GLN
2	D	300	ASN
2	D	331	GLN
2	D	339	ASN
2	D	385	GLN
2	D	433	GLN
3	E	18	GLN
3	E	71	HIS

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Mol	Chain	Res	Type
3	E	108	ASN
3	E	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
6	GDP	D	501	-	24,30,30	0.75	1 (4%)	30,47,47	0.81	0
8	3WD	B	503	-	48,54,54	0.99	3 (6%)	50,76,76	1.72	9 (18%)
6	GDP	B	501	-	24,30,30	0.77	1 (4%)	30,47,47	0.82	0
7	LOC	B	502	-	31,31,31	0.77	1 (3%)	44,44,44	0.60	0
7	LOC	D	502	-	31,31,31	0.44	0	44,44,44	0.56	0
4	GTP	A	600	5	26,34,34	0.76	0	32,54,54	0.72	0
8	3WD	D	503	-	48,54,54	1.03	4 (8%)	50,76,76	1.32	9 (18%)
4	GTP	C	600	5	26,34,34	0.76	1 (3%)	32,54,54	0.78	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
6	GDP	D	501	-	-	3/12/32/32	0/3/3/3
8	3WD	B	503	-	-	22/66/82/82	0/3/3/3
6	GDP	B	501	-	-	4/12/32/32	0/3/3/3
7	LOC	B	502	-	-	0/12/25/25	0/3/3/3
7	LOC	D	502	-	-	0/12/25/25	0/3/3/3
4	GTP	A	600	5	-	5/18/38/38	0/3/3/3
8	3WD	D	503	-	-	15/66/82/82	0/3/3/3
4	GTP	C	600	5	-	3/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	3WD	C12-N3	4.77	1.57	1.47
8	B	503	3WD	C12-N3	4.40	1.56	1.47
8	B	503	3WD	C11-C12	4.01	1.61	1.52
7	B	502	LOC	C11-C14	3.82	1.60	1.53
8	D	503	3WD	C11-C12	3.19	1.59	1.52
8	D	503	3WD	C7-C8	3.03	1.57	1.52
8	B	503	3WD	C16-C12	2.57	1.60	1.54
8	D	503	3WD	C16-C12	2.42	1.59	1.54
4	C	600	GTP	C8-N7	-2.23	1.31	1.35
6	B	501	GDP	C8-N7	-2.06	1.31	1.35
6	D	501	GDP	C8-N7	-2.02	1.31	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WD	C23-N3-C12	-5.59	108.46	119.46
8	B	503	3WD	C23-N3-C12	-5.06	109.50	119.46
8	B	503	3WD	C12-N3-C13	4.67	133.71	120.34
8	B	503	3WD	C29-N2-C8	4.53	129.98	123.19
8	B	503	3WD	C7-C8-N2	-3.66	110.89	116.44
8	B	503	3WD	C19-C16-C12	3.64	121.26	111.20
8	B	503	3WD	C30-C29-C32	3.05	115.68	110.64
8	D	503	3WD	C20-C14-C13	2.79	116.38	110.73
8	B	503	3WD	C30-C29-N2	2.70	113.92	109.01
8	D	503	3WD	C14-C13-N3	2.29	123.46	118.74
8	D	503	3WD	O5-C13-C14	-2.25	115.61	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	3WD	C14-C13-N3	2.13	123.14	118.74
8	D	503	3WD	C23-N3-C13	2.12	129.14	122.26
8	D	503	3WD	C11-C10-C5	2.11	115.68	112.42
8	D	503	3WD	C7-C8-N2	-2.08	113.28	116.44
8	B	503	3WD	O1-C6-C7	2.05	110.68	105.83
8	D	503	3WD	C20-C14-N4	2.03	116.46	111.43
8	D	503	3WD	C19-C16-C12	2.00	116.74	111.20

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O2A
8	B	503	3WD	O5-C13-N3-C23
8	B	503	3WD	C16-C12-N3-C13
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
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	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	C14-C13-N3-C23
8	B	503	3WD	N4-C15-C26-C28
8	B	503	3WD	O1-C6-C7-C9
8	D	503	3WD	N4-C14-C20-C22
8	B	503	3WD	O6-C15-C26-C28
8	B	503	3WD	C19-C16-C17-C18
8	D	503	3WD	C13-C14-C20-C21

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Mol	Chain	Res	Type	Atoms
8	D	503	3WD	O4-C5-N1-C4
8	B	503	3WD	C29-C30-C31-C37
8	B	503	3WD	C29-C30-C31-C33
6	B	501	GDP	C4'-C5'-O5'-PA
8	D	503	3WD	C5-C10-C11-C12
6	D	501	GDP	C5'-O5'-PA-O3A
8	D	503	3WD	C5-C10-C11-O3
4	A	600	GTP	PB-O3A-PA-O1A
6	D	501	GDP	C5'-O5'-PA-O1A
8	B	503	3WD	N4-C15-C26-C27
8	B	503	3WD	N1-C1-C6-C7
4	A	600	GTP	C3'-C4'-C5'-O5'
8	D	503	3WD	O5-C13-C14-C20
8	D	503	3WD	N3-C13-C14-N4
4	A	600	GTP	O4'-C4'-C5'-O5'
4	A	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
6	B	501	GDP	C5'-O5'-PA-O3A
8	D	503	3WD	O5-C13-C14-N4
4	A	600	GTP	C5'-O5'-PA-O1A
8	D	503	3WD	N3-C12-C16-C17
8	B	503	3WD	O5-C13-N3-C12

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	501	GDP	2	0
8	B	503	3WD	5	0
6	B	501	GDP	1	0
7	B	502	LOC	1	0
8	D	503	3WD	2	0

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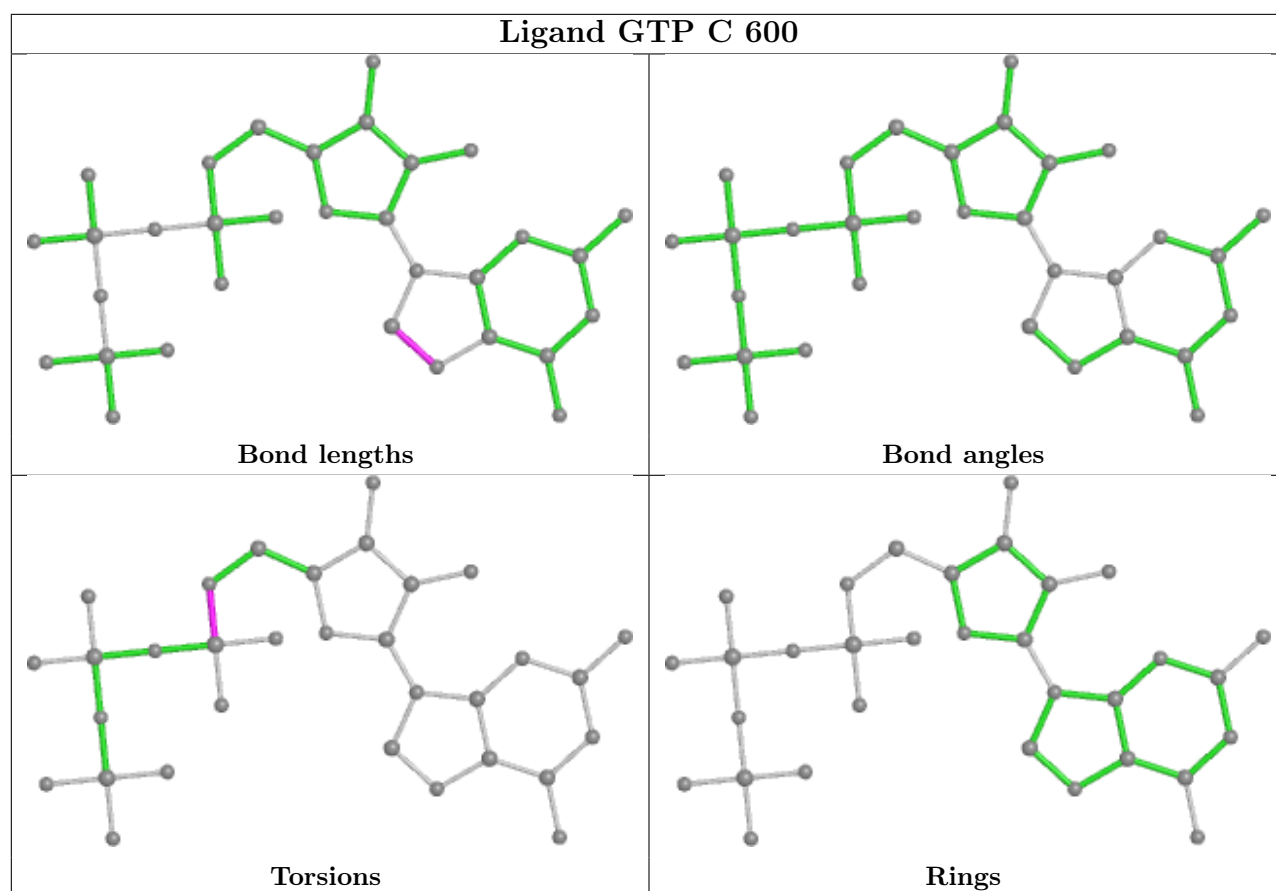
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP D 501

Bond lengths   Bond angles

Torsions   Rings

Ligand 3WD B 503

Bond lengths   Bond angles

Torsions   Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand LOC B 502

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand 3WD D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 600

Bond lengths

Bond angles

Torsions

Rings

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(Å²)	Q<0.9
1	A	429/451 (95%)	0.21	23 (5%)	25	12	92, 139, 188, 216	0
1	C	430/451 (95%)	-0.08	5 (1%)	79	63	66, 99, 145, 171	0
2	B	428/445 (96%)	-0.01	15 (3%)	44	23	83, 114, 160, 187	2 (0%)
2	D	430/445 (96%)	-0.23	0	100	100	62, 90, 130, 166	2 (0%)
3	E	123/142 (86%)	0.54	20 (16%)	1	1	93, 127, 204, 219	0
All	All	1840/1934 (95%)	0.01	63 (3%)	45	24	62, 113, 172, 219	4 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	9	ILE	5.6
3	E	16	SER	5.1
3	E	12	ASN	4.7
3	E	31	GLY	4.2
1	A	346	TRP	4.1
1	A	371	VAL	4.1
3	E	24	LEU	4.0
2	B	439	THR	4.0
1	A	347	CYS	3.8
3	E	22	VAL	3.8
3	E	14	ALA	3.7
1	C	253	THR	3.7
1	A	338	LYS	3.6
2	B	373	MET	3.6
2	B	30	ILE	3.5
1	A	372	GLN	3.4
3	E	26	PRO	3.4
1	A	247	ALA	3.3
1	A	201	ALA	3.2
2	B	251	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	219	ILE	3.0
1	A	323	VAL	3.0
3	E	17	GLY	2.8
3	E	13	LYS	2.8
3	E	10	GLU	2.8
1	A	170	SER	2.8
1	A	322	ASP	2.8
1	A	339	ARG	2.8
2	B	281	GLN	2.8
3	E	11	LEU	2.7
2	B	379	GLY	2.7
1	A	313	MET	2.7
2	B	438	ALA	2.7
3	E	80	ARG	2.6
2	B	440	ALA	2.6
3	E	15	THR	2.6
3	E	32	VAL	2.6
1	A	337	THR	2.6
2	B	249	ASN	2.5
2	B	32	PRO	2.5
1	A	370	LYS	2.5
1	A	4	CYS	2.5
1	C	199	ASP	2.4
3	E	46	SER	2.4
2	B	254	LYS	2.4
2	B	253	ARG	2.4
3	E	82	VAL	2.3
1	A	283	HIS	2.3
1	A	246	GLY	2.3
2	B	412	GLY	2.3
1	A	328	VAL	2.3
1	A	281	ALA	2.2
2	B	280	SER	2.2
1	A	286	LEU	2.2
1	A	37	PRO	2.2
1	C	35	GLN	2.2
3	E	23	ILE	2.1
3	E	33	PRO	2.1
1	A	160	ASP	2.1
1	C	252	LEU	2.1
3	E	34	GLU	2.0
1	C	200	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	61	TYR	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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	0.88	0.30	118,135,146,148	0
8	3WD	B	503	52/52	0.91	0.21	95,112,130,131	0
7	LOC	D	502	29/29	0.94	0.23	73,81,88,92	0
4	GTP	C	600	32/32	0.95	0.28	73,83,107,109	0
4	GTP	A	600	32/32	0.95	0.32	108,122,126,127	0
7	LOC	B	502	29/29	0.96	0.24	92,106,114,115	0
6	GDP	B	501	28/28	0.97	0.23	89,96,101,103	0
5	MG	C	601	1/1	0.98	0.33	37,37,37,37	0
6	GDP	D	501	28/28	0.98	0.22	68,76,85,89	0
5	MG	A	601	1/1	0.99	0.36	67,67,67,67	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.
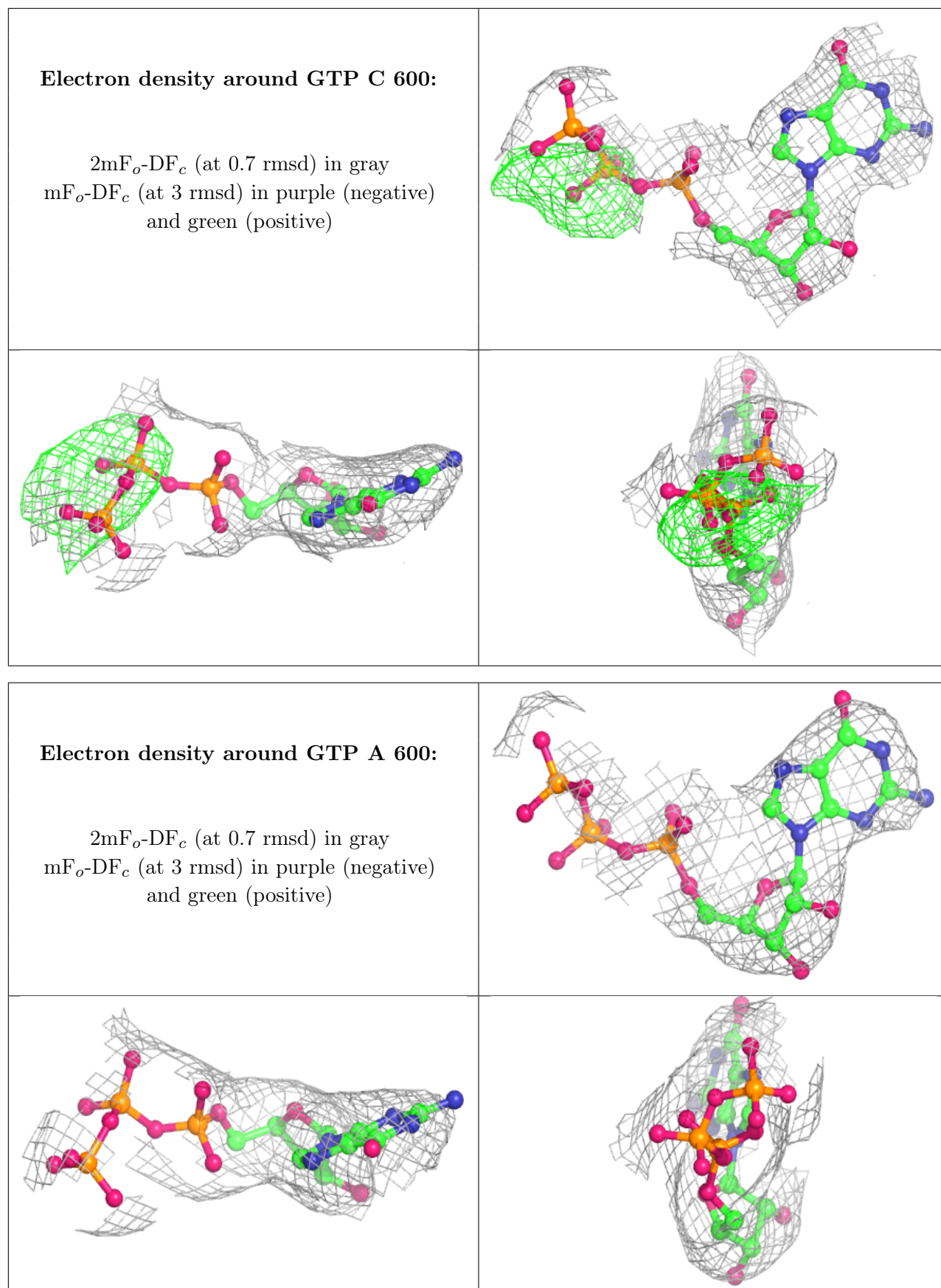
Electron density around 3WD D 503:

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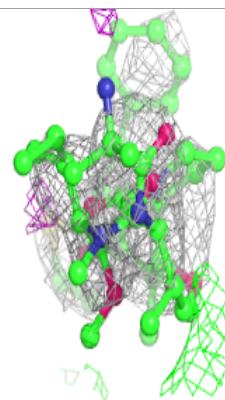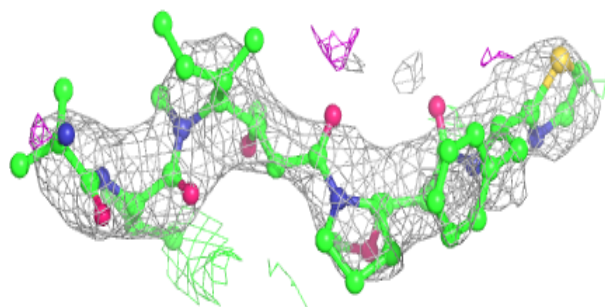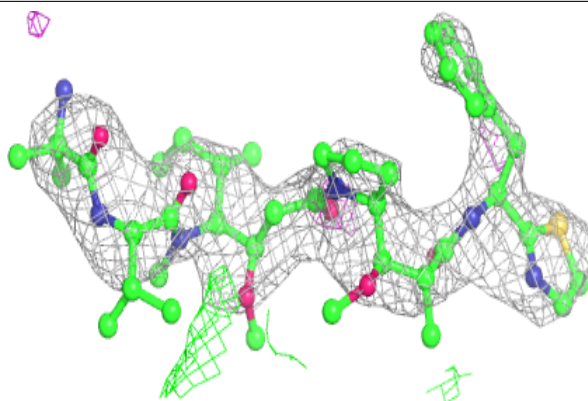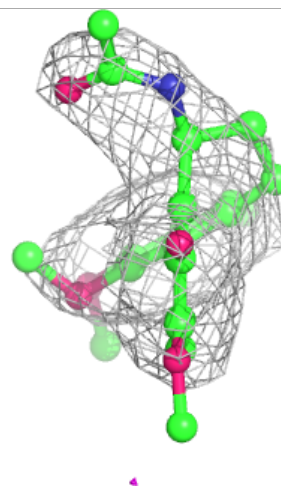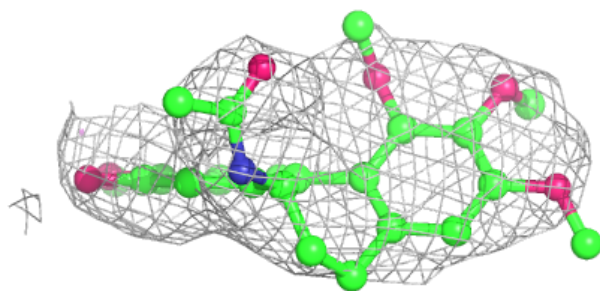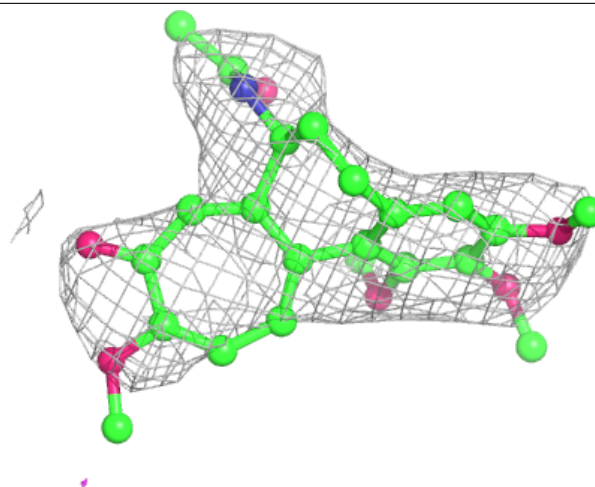

Electron density around 3WD B 503:

$2mF_o$-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 GTP A 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
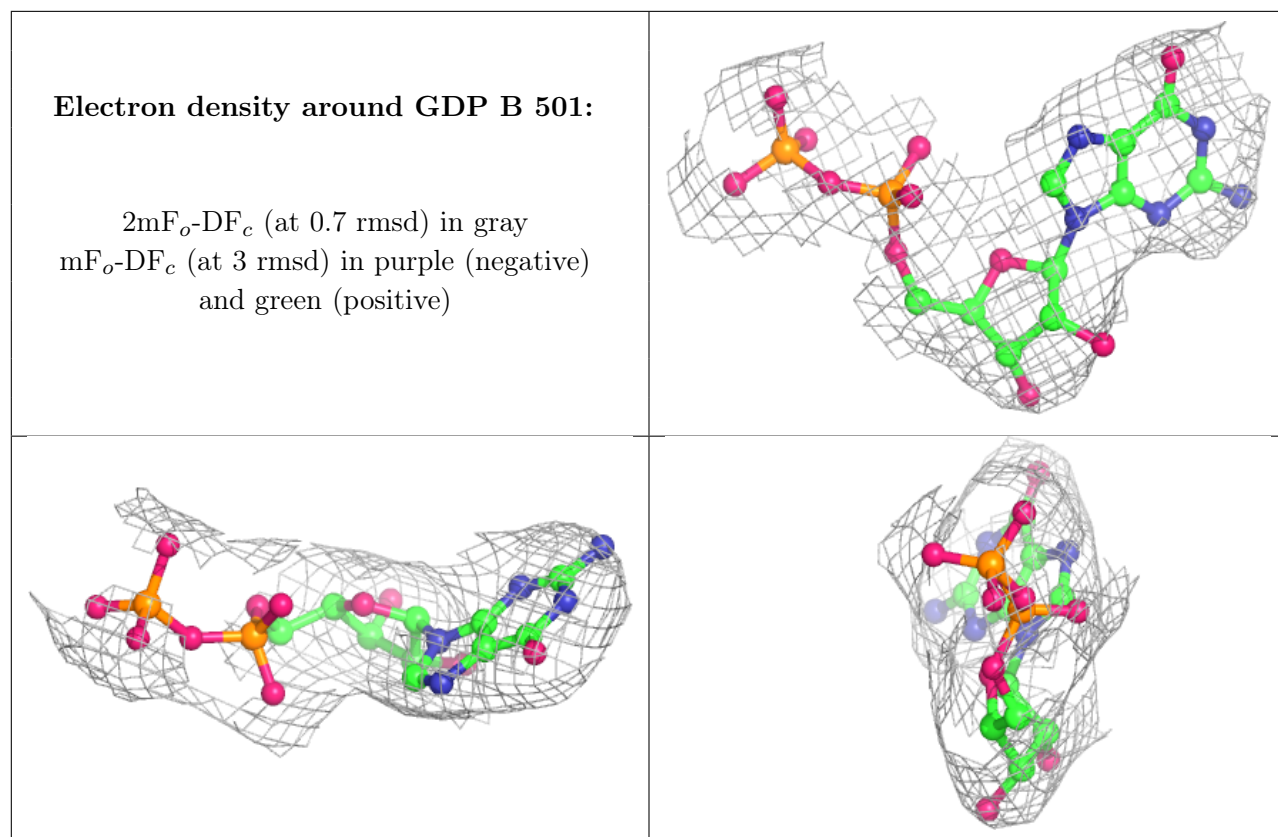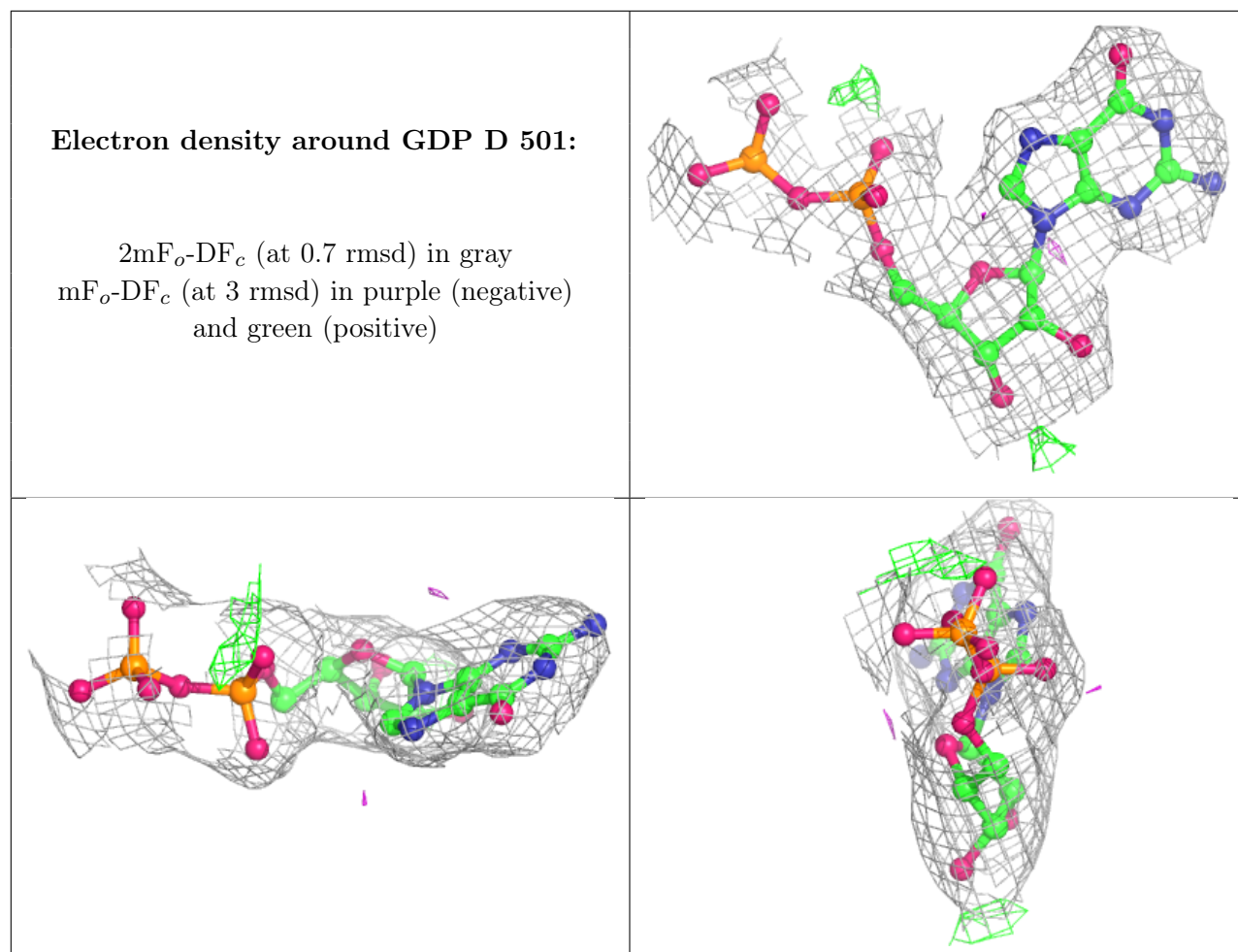and green (positive)
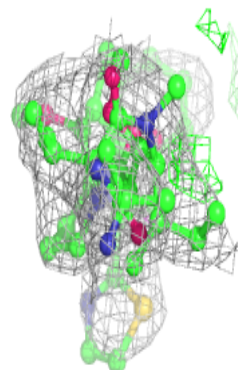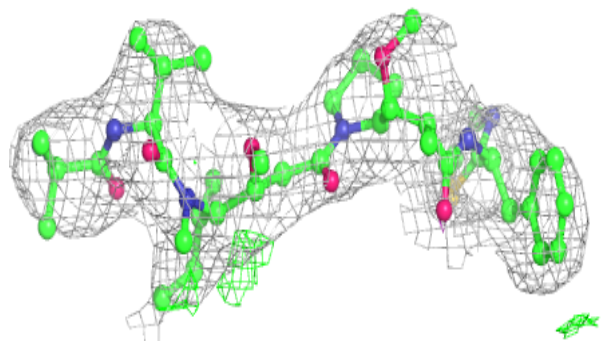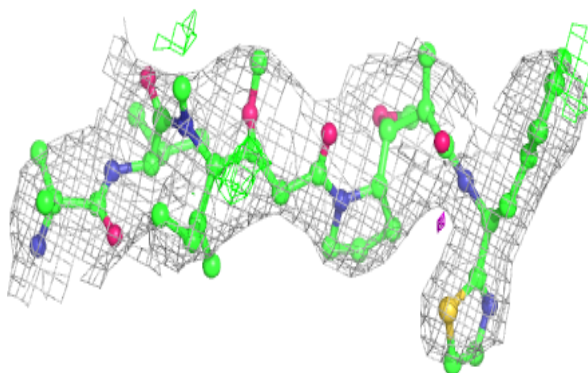
Electron density around LOC B 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.