



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:32 PM UTC

PDB ID : 8CLB / pdb_00008clb
Title : Colchicine bound to tubulin (T2R-TTL) complex
Authors : Wranik, M.; Kepa, M.W.; Bertrand, Q.; Weinert, T.; Steinmetz, M.; Standfuss, J.
Deposited on : 2023-02-16
Resolution : 3.00 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

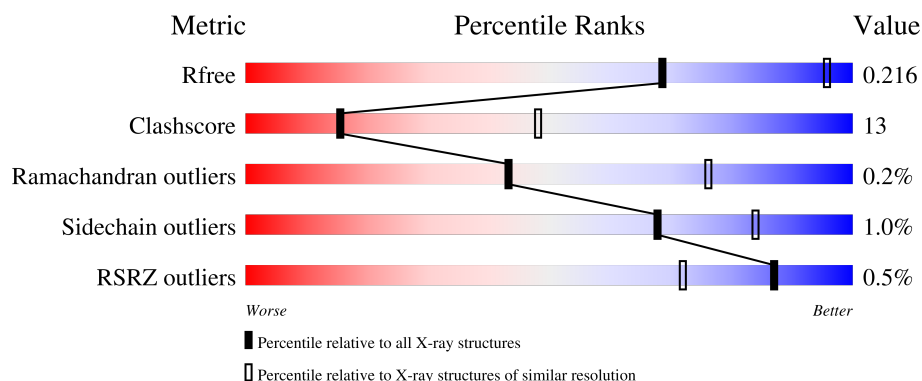
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	440	 71% 28% .
1	C	440	 77% 23% .
2	B	431	 75% 23% .
2	D	431	 65% 32% .
3	E	121	 80% 19% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	320	2% 68% 30%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34597 atoms, of which 17054 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	439	Total	C	H	N	O	S	0	13	0
			6913	2214	3431	582	661	25			
1	C	440	Total	C	H	N	O	S	0	10	0
			6893	2205	3412	587	665	24			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	423	Total	C	H	N	O	S	1	9	0
			6646	2126	3271	569	653	27			
2	D	421	Total	C	H	N	O	S	5	4	0
			6533	2091	3211	561	642	28			

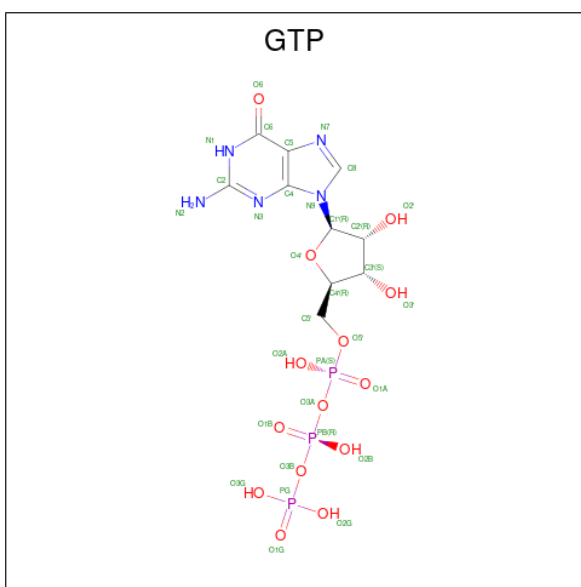
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	1	0
			2032	621	1026	182	198	5			

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	320	Total	C	H	N	O	S	13	5	0
			5281	1711	2641	437	478	14			

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			44	10	12	5	14	3		

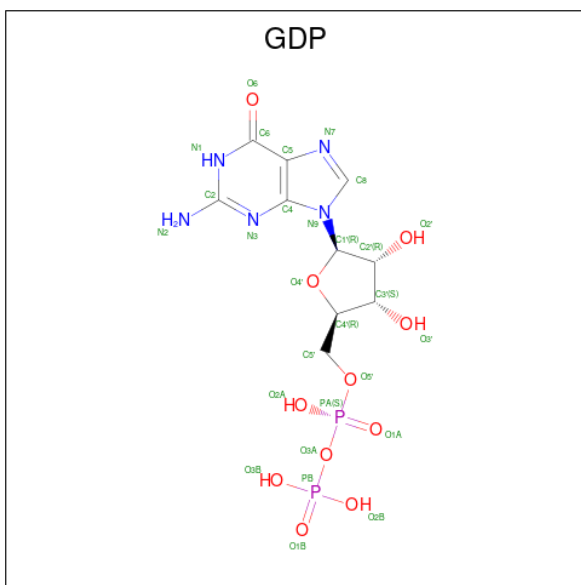
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

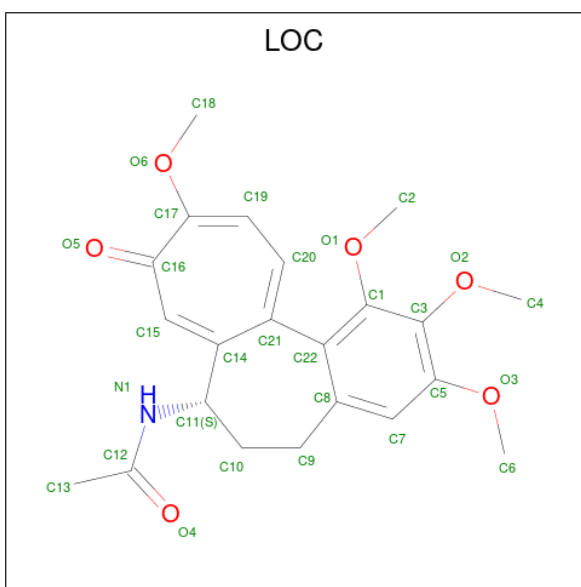
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total 40	C 10	H 12	N 5	O 11	P 2	0	0
8	D	1	Total 40	C 10	H 12	N 5	O 11	P 2	0	0

- Molecule 9 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) (labeled as "Ligand of Interest" by depositor).



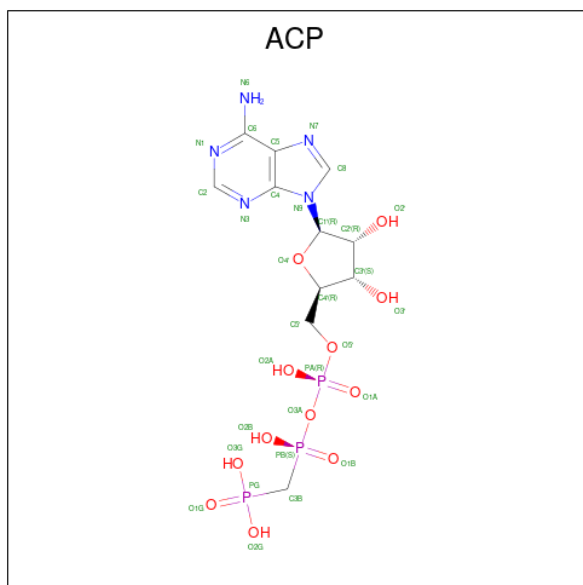
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			29	22	1	6		

Continued on next page...

Continued from previous page...

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

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

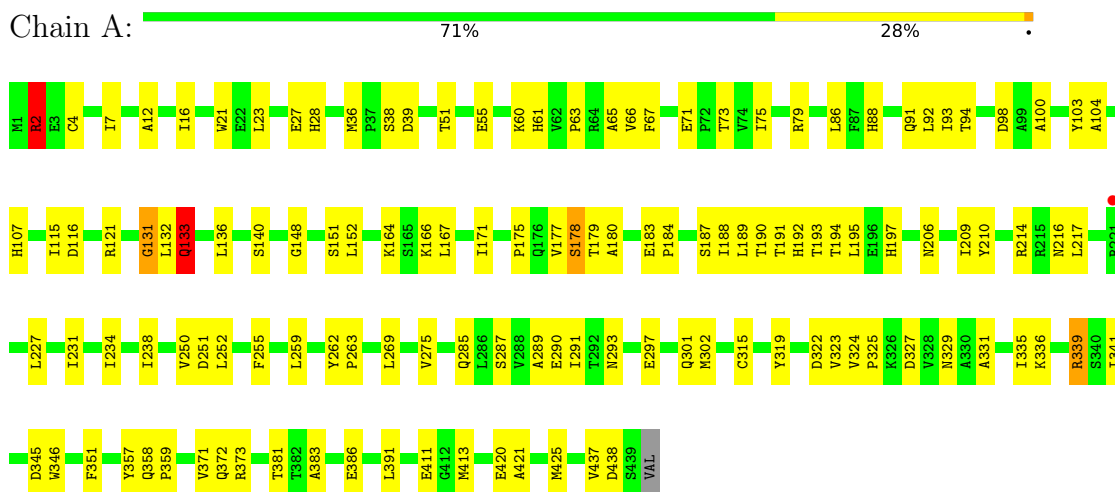
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	7	Total	O	0	0
			7	7		
11	B	5	Total	O	0	0
			5	5		
11	C	6	Total	O	0	0
			6	6		
11	D	1	Total	O	0	0
			1	1		
11	E	1	Total	O	0	0
			1	1		
11	F	2	Total	O	0	0
			2	2		

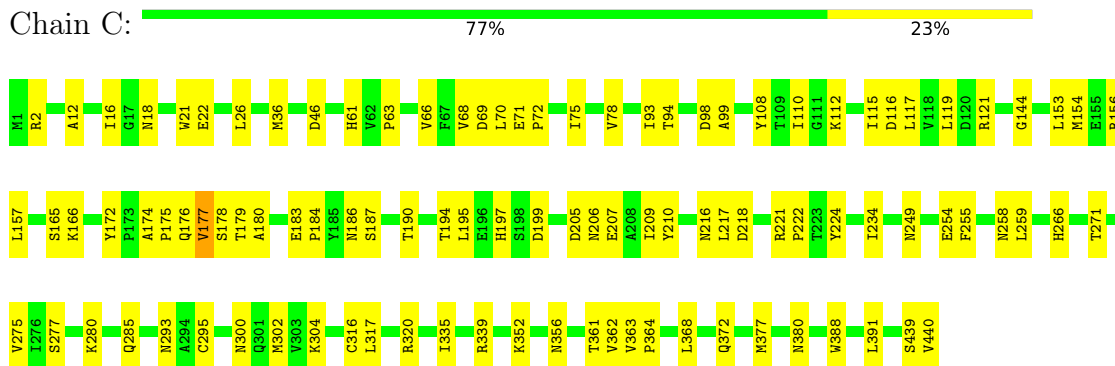
3 Residue-property plots

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.

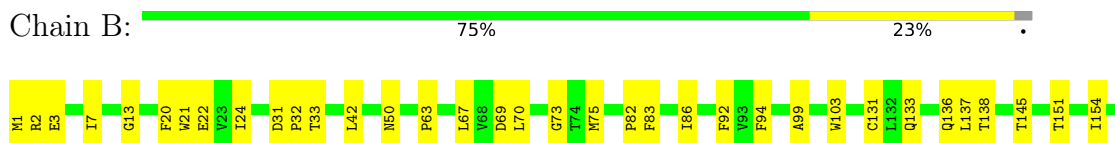
• Molecule 1: Tubulin alpha-1B chain

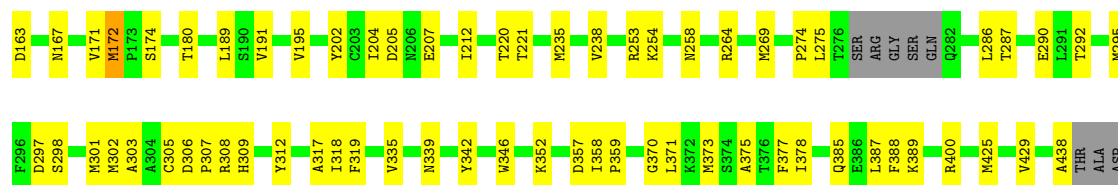


• Molecule 1: Tubulin alpha-1B chain



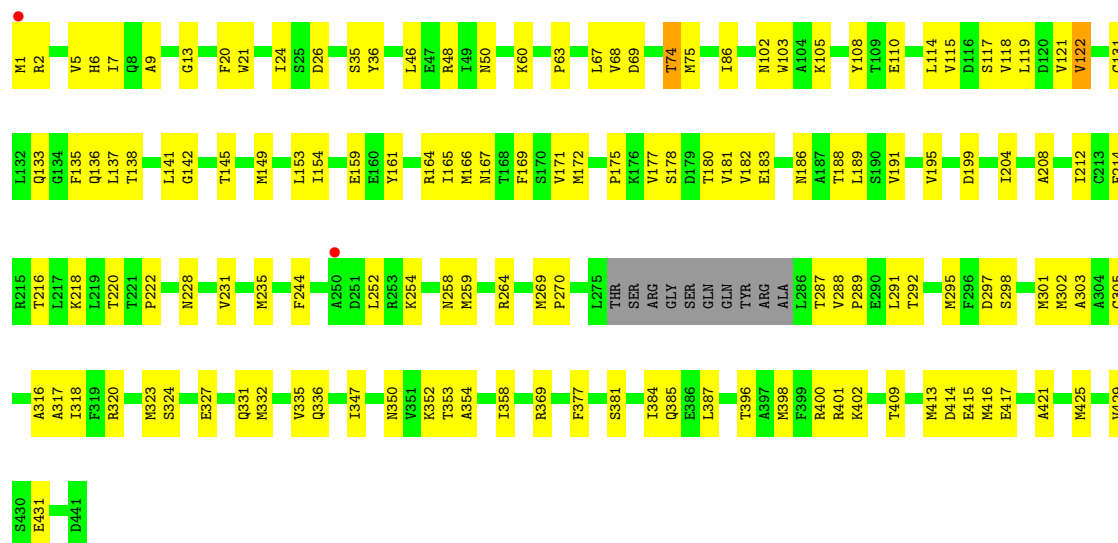
• Molecule 2: Tubulin beta-2B chain





• Molecule 2: Tubulin beta-2B chain

Chain D: 65% 32% .



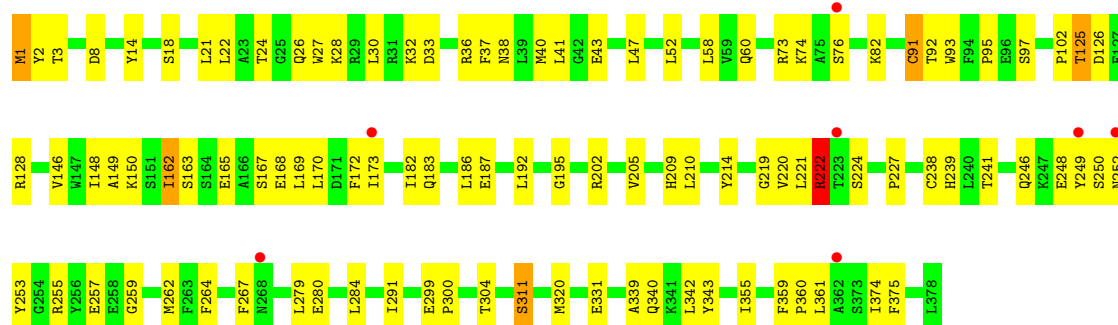
• Molecule 3: Stathmin-4

Chain E: 80% 19% .



• Molecule 4: Tubulin-Tyrosine Ligase

Chain F: 68% 30% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.71Å 160.61Å 180.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.18 – 3.00 15.18 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (15.18-3.00) 98.9 (15.18-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20_4487	Depositor
R, R_{free}	0.163 , 0.214 0.172 , 0.216	Depositor DCC
R_{free} test set	2000 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.50 , 122.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34597	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: GDP, CA, LOC, ACP, 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	0.34	0/3599	0.48	1/4888 (0.0%)
1	C	0.37	0/3589	0.51	0/4874
2	B	0.39	0/3473	0.56	0/4704
2	D	0.32	0/3407	0.49	2/4618 (0.0%)
3	E	0.35	0/1017	0.44	0/1349
4	F	0.35	0/2712	0.53	0/3663
All	All	0.36	0/17797	0.51	3/24096 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	3
2	B	0	1
2	D	0	1
4	F	0	1
All	All	0	8

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	302	MET	N-CA-C	-5.67	106.69	113.21
2	D	75	MET	N-CA-C	-5.52	105.36	111.71
1	A	133	GLN	N-CA-C	-5.07	107.27	113.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ARG	Sidechain
1	A	339	ARG	Sidechain
2	B	264	ARG	Sidechain
1	C	2	ARG	Sidechain
1	C	221	ARG	Sidechain
1	C	339	ARG	Sidechain
2	D	401	ARG	Sidechain
4	F	222	ARG	Sidechain

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	3482	3431	3430	110	0
1	C	3481	3412	3409	72	0
2	B	3375	3271	3268	90	0
2	D	3322	3211	3210	112	0
3	E	1006	1026	1026	19	0
4	F	2640	2641	2641	77	0
5	A	32	12	12	0	0
5	C	32	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	12	12	0	0
8	D	28	12	12	3	0
9	B	29	0	25	2	0
9	D	29	0	25	5	0
10	F	31	14	14	1	0
11	A	7	0	0	0	0
11	B	5	0	0	0	0
11	C	6	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	2	0	0	0	0
All	All	17543	17054	17096	464	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 13.

All (464) 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)
4:F:128:ARG:HE	4:F:170:LEU:HD22	1.37	0.88
2:B:75:MET:HE3	2:B:94:PHE:HB3	1.55	0.86
1:A:381:THR:HG22	1:A:383:ALA:H	1.41	0.86
2:D:118:VAL:HG21	2:D:153:LEU:HD21	1.56	0.84
2:D:175:PRO:HA	2:D:178:SER:HB2	1.56	0.83
4:F:125:THR:HG22	4:F:126:ASP:HA	1.61	0.82
4:F:149:ALA:HB2	4:F:182:ILE:HG12	1.63	0.81
2:B:1:MET:N	2:B:131:CYS:HB3	1.96	0.80
1:A:166:LYS:HE2	1:A:197:HIS:O	1.84	0.78
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.66	0.78
1:A:2:ARG:NH2	1:A:250[A]:VAL:HG13	2.00	0.77
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.21	0.76
2:B:75:MET:CE	2:B:94:PHE:HB3	2.15	0.76
2:B:136:GLN:HA	2:B:167:ASN:O	1.86	0.76
4:F:339:ALA:HB3	4:F:342:LEU:HD13	1.68	0.76
2:B:1:MET:H2	2:B:131:CYS:HB3	1.51	0.76
2:D:191:VAL:HG11	2:D:425:MET:HE2	1.67	0.75
1:C:177:VAL:HG21	1:C:206:ASN:HB3	1.69	0.74
1:A:2:ARG:HH21	1:A:250[A]:VAL:HG13	1.53	0.74
1:A:75:ILE:HG23	1:A:92:LEU:HD12	1.69	0.73
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.71	0.72
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.54	0.72
1:A:67:PHE:HB2	1:A:92:LEU:HD13	1.71	0.72
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.70	0.72
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.71	0.71
1:A:297:GLU:HG2	1:A:339:ARG:HH22	1.55	0.71
2:B:83:PHE:O	2:B:86:ILE:HG22	1.90	0.71
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.71	0.70
2:D:142:GLY:HA3	8:D:501:GDP:H4'	1.74	0.69
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.22	0.69
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.75	0.69
1:A:63:PRO:CG	1:A:86:LEU:HD21	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.74	0.68
2:B:388:PHE:HD1	2:B:425:MET:HE2	1.59	0.67
1:C:175:PRO:HA	1:C:179:THR:CG2	2.25	0.67
2:D:63:PRO:HD3	2:D:86:ILE:HG12	1.75	0.67
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.75	0.67
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.30	0.67
2:B:317:ALA:C	2:B:318:ILE:HD12	2.19	0.67
2:D:105:LYS:HD3	2:D:110:GLU:HG3	1.78	0.66
1:A:4:CYS:SG	1:A:252:LEU:HD21	2.35	0.66
1:A:371:VAL:HG12	1:A:373:ARG:H	1.61	0.66
2:B:1:MET:HE3	2:B:50[B]:ASN:ND2	2.12	0.65
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.31	0.64
2:D:171:VAL:HA	2:D:204:ILE:O	1.98	0.64
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.78	0.64
2:D:2:ARG:HB3	2:D:133:GLN:HE21	1.63	0.63
2:D:214:PHE:O	2:D:218:LYS:HA	1.99	0.63
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.34	0.63
2:D:204:ILE:HD13	2:D:231:VAL:HG13	1.79	0.63
4:F:128:ARG:NE	4:F:170:LEU:HD22	2.12	0.63
1:C:175:PRO:HA	1:C:179:THR:HG21	1.81	0.63
4:F:209:HIS:CD2	4:F:210:LEU:HG	2.35	0.62
1:A:293:ASN:ND2	1:A:339:ARG:HH21	1.98	0.62
4:F:246:GLN:O	4:F:253:TYR:HB2	1.98	0.62
2:B:287:THR:HG22	2:B:290:GLU:CG	2.29	0.62
1:C:216:ASN:HB3	1:C:275:VAL:O	2.00	0.62
4:F:374:ILE:HD11	4:F:375:PHE:CE2	2.34	0.62
1:A:357:TYR:CD2	3:E:17:GLY:HA2	2.34	0.62
2:B:287:THR:HG23	2:B:290:GLU:H	1.63	0.61
2:D:118:VAL:CG2	2:D:153:LEU:HD21	2.29	0.61
1:C:12:ALA:O	1:C:16:ILE:HG12	2.00	0.61
2:D:181:VAL:O	2:D:398:MET:HE1	2.00	0.61
2:B:352:LYS:HG2	9:B:503:LOC:H18B	1.83	0.61
2:B:388:PHE:CD1	2:B:425:MET:HE2	2.35	0.61
1:A:103:TYR:HD2	1:A:413:MET:HE1	1.66	0.61
2:D:269[B]:MET:CE	2:D:305:CYS:HB2	2.30	0.61
9:B:503:LOC:O1	9:B:503:LOC:H20	2.01	0.61
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.36	0.60
1:A:63:PRO:HG2	1:A:86:LEU:HD21	1.83	0.60
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.32	0.60
1:C:165:SER:HA	1:C:199:ASP:OD2	2.02	0.60
1:A:285:GLN:HG3	1:A:372[B]:GLN:OE1	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:PRO:HB3	2:B:286:LEU:HD12	1.84	0.60
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.17	0.60
2:B:191:VAL:O	2:B:195:VAL:HG23	2.02	0.60
4:F:1:MET:HE2	4:F:28:LYS:HB2	1.83	0.59
4:F:91:CYS:SG	4:F:93:TRP:CD2	2.96	0.59
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.38	0.59
4:F:165:GLU:HG2	4:F:167:SER:H	1.68	0.59
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.85	0.59
1:A:190:THR:O	1:A:194:THR:HG22	2.03	0.58
1:C:180:ALA:HB1	2:D:258:ASN:OD1	2.03	0.58
2:B:370:GLY:O	2:B:371:LEU:HD23	2.03	0.58
1:A:324:VAL:HG23	1:A:327:ASP:H	1.68	0.58
2:D:188:THR:HG22	2:D:421:ALA:HB1	1.86	0.58
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.22	0.58
4:F:148:ILE:HB	4:F:162:ILE:HG23	1.85	0.58
1:A:329:ASN:HB3	3:E:6:MET:HE1	1.84	0.58
2:D:396:THR:O	2:D:400:ARG:HB2	2.04	0.57
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.85	0.57
2:B:400:ARG:HD2	1:C:439:SER:HB3	1.87	0.57
1:C:166:LYS:HE2	1:C:197:HIS:O	2.04	0.57
1:C:271:THR:HG23	1:C:300:ASN:O	2.04	0.57
2:B:163:ASP:O	2:B:253:ARG:NH2	2.37	0.57
2:D:172:MET:HE2	2:D:387:LEU:HD21	1.85	0.57
1:A:322:ASP:O	1:A:373:ARG:NH1	2.36	0.57
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.39	0.57
1:C:72:PRO:CG	2:D:1:MET:HE2	2.34	0.57
1:C:440:VAL:HG12	1:C:440:VAL:O	2.05	0.57
2:B:292:THR:HG22	2:B:319:PHE:CZ	2.40	0.56
1:A:227:LEU:O	1:A:231:ILE:HG13	2.06	0.56
2:D:269[A]:MET:HE2	2:D:305:CYS:HB2	1.86	0.56
2:D:318:ILE:HG13	2:D:354:ALA:HB3	1.87	0.56
3:E:96:MET:O	3:E:100:LYS:HB2	2.06	0.56
2:B:13:GLY:HA2	2:B:138[B]:THR:HG22	1.87	0.56
1:A:285:GLN:HG3	1:A:372[B]:GLN:CD	2.30	0.56
2:D:141:LEU:HD12	2:D:172:MET:CE	2.35	0.56
1:C:75:ILE:HD12	1:C:94:THR:CG2	2.35	0.56
1:A:7:ILE:HG23	1:A:66[B]:VAL:HG13	1.87	0.56
2:D:180:THR:HG22	2:D:181:VAL:N	2.20	0.56
2:D:220:THR:O	2:D:222:PRO:HD3	2.06	0.56
4:F:202:ARG:HB3	4:F:220:VAL:CG1	2.36	0.56
1:C:293[B]:ASN:CG	1:C:335:ILE:HD11	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:VAL:O	2:D:122:VAL:HG13	2.05	0.56
4:F:320:MET:HE1	10:F:401:ACP:N3	2.22	0.55
2:B:308:ARG:HG2	2:B:342:TYR:CE2	2.41	0.55
1:C:209:ILE:HD11	1:C:302:MET:SD	2.46	0.55
2:D:244:PHE:CZ	2:D:358:ILE:HD11	2.40	0.55
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.87	0.55
2:D:413:MET:HE3	2:D:417:GLU:CD	2.32	0.55
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.87	0.55
1:C:18:ASN:ND2	1:C:78:VAL:HG22	2.20	0.55
2:D:358:ILE:O	2:D:358:ILE:HG13	2.04	0.55
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.89	0.55
1:A:325:PRO:O	1:A:329:ASN:ND2	2.40	0.55
1:A:206:ASN:OD1	1:A:209[B]:ILE:HD11	2.07	0.55
4:F:149:ALA:CB	4:F:182:ILE:HG12	2.35	0.55
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.71	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.42	0.54
2:D:69:ASP:HA	2:D:145:THR:HG21	1.90	0.54
1:A:88:HIS:N	1:A:91:GLN:OE1	2.36	0.54
1:A:167:LEU:HD22	1:A:252:LEU:HD12	1.89	0.54
3:E:60:ARG:O	3:E:64:GLN:HG3	2.08	0.54
1:A:28:HIS:O	1:A:36:MET:HE3	2.08	0.54
2:B:151:THR:HA	2:B:154:ILE:HD12	1.90	0.54
9:D:503:LOC:O1	9:D:503:LOC:H20	2.08	0.54
3:E:51:GLN:O	3:E:55:GLU:HG3	2.08	0.54
1:C:361:THR:HG22	1:C:362:VAL:N	2.22	0.53
2:D:332:MET:O	2:D:336:GLN:HG3	2.07	0.53
2:B:22[A]:GLU:OE2	2:B:82:PRO:HG2	2.08	0.53
4:F:21:LEU:HD22	4:F:27:TRP:CD2	2.43	0.53
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.90	0.53
1:C:218:ASP:OD2	1:C:280:LYS:HE3	2.09	0.53
1:C:259:LEU:O	1:C:380:ASN:ND2	2.39	0.53
2:D:115:VAL:O	2:D:119:LEU:HG	2.08	0.53
1:A:289:ALA:HA	1:A:331:ALA:HB2	1.91	0.53
2:B:292:THR:HG22	2:B:319:PHE:HZ	1.74	0.53
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.90	0.53
2:D:108:TYR:O	3:E:134:ARG:NH1	2.41	0.53
1:A:151:SER:HB2	1:A:193:THR:CG2	2.37	0.53
1:A:437:VAL:HG12	1:A:438:ASP:N	2.23	0.53
4:F:74:LYS:HE3	4:F:331:GLU:OE1	2.09	0.53
2:D:141:LEU:HD12	2:D:172:MET:SD	2.49	0.53
2:D:9:ALA:O	2:D:13:GLY:HA3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:8:ASP:HB2	4:F:43:GLU:HA	1.91	0.53
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.44	0.53
1:A:315[A]:CYS:HG	1:A:351:PHE:HD2	1.56	0.53
1:C:70:LEU:HD13	1:C:110:ILE:HG22	1.89	0.53
2:B:22[B]:GLU:HG3	2:B:83:PHE:CE1	2.44	0.52
1:C:190:THR:O	1:C:194[B]:THR:HG23	2.09	0.52
2:D:288:VAL:HG12	2:D:331:GLN:HG3	1.91	0.52
2:B:220:THR:HG23	2:B:221:THR:HG22	1.91	0.52
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.09	0.52
4:F:73:ARG:HB2	4:F:76[B]:SER:OG	2.09	0.52
2:B:31:ASP:CG	2:B:33:THR:HG22	2.34	0.52
2:D:2:ARG:HB3	2:D:133:GLN:NE2	2.24	0.52
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.44	0.52
2:B:286:LEU:HD22	2:B:290:GLU:CB	2.39	0.52
2:B:295:MET:SD	2:B:375:ALA:HB1	2.49	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.52
1:C:317:LEU:HD23	1:C:377:MET:HG3	1.92	0.52
2:D:269[B]:MET:HE1	2:D:305:CYS:HB2	1.92	0.52
4:F:250:SER:C	4:F:253:TYR:H	2.17	0.52
2:B:69:ASP:HA	2:B:145:THR:HG21	1.93	0.51
2:D:183:GLU:OE2	8:D:501:GDP:H3'	2.10	0.51
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.10	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.45	0.51
2:D:324:SER:OG	2:D:327:GLU:HB2	2.10	0.51
2:B:286:LEU:HD22	2:B:290:GLU:HB3	1.92	0.51
1:C:69:ASP:O	1:C:94:THR:HA	2.10	0.51
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.10	0.51
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.45	0.51
2:B:346:TRP:HE1	2:B:438:ALA:CB	2.24	0.51
2:B:31:ASP:OD2	2:B:33:THR:HG22	2.10	0.51
2:D:26:ASP:OD2	2:D:369:ARG:HD3	2.11	0.51
2:D:269[A]:MET:CE	2:D:305:CYS:HB2	2.41	0.51
2:D:180:THR:HG22	2:D:182:VAL:H	1.74	0.51
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.93	0.51
4:F:32:LYS:HG3	4:F:33:ASP:N	2.25	0.50
1:C:271:THR:HG21	1:C:295[B]:CYS:HA	1.93	0.50
1:A:91:GLN:C	1:A:92:LEU:HD22	2.36	0.50
2:D:141:LEU:HD12	2:D:172:MET:HE1	1.93	0.50
2:D:352:LYS:HG3	9:D:503:LOC:C16	2.42	0.50
4:F:21:LEU:HD22	4:F:27:TRP:CE2	2.46	0.50
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:HIS:CD2	1:A:152:LEU:HB2	2.46	0.50
1:A:191:THR:O	1:A:195:LEU:HB2	2.12	0.50
2:B:238:VAL:HG22	2:B:378:ILE:HD11	1.94	0.50
2:D:1:MET:O	2:D:131:CYS:HB3	2.11	0.50
1:A:335:ILE:C	1:A:335:ILE:HD12	2.37	0.50
2:B:7:ILE:O	2:B:137:LEU:HA	2.12	0.50
1:C:115:ILE:HG23	1:C:116:ASP:N	2.26	0.50
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.46	0.50
3:E:132:GLU:O	3:E:136:ASN:HB2	2.11	0.50
1:A:79:ARG:NH2	1:A:94:THR:HG21	2.26	0.50
2:B:1:MET:HB2	2:B:3:GLU:OE2	2.12	0.50
1:C:175:PRO:HA	1:C:179:THR:HG22	1.94	0.50
2:B:137:LEU:CD2	2:B:154:ILE:HD11	2.42	0.50
4:F:148:ILE:HG12	4:F:150:LYS:HG2	1.92	0.50
1:C:72:PRO:CD	2:D:1:MET:HE2	2.41	0.49
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.11	0.49
2:B:1:MET:HE3	2:B:50[B]:ASN:HD22	1.76	0.49
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.94	0.49
2:B:180:THR:HA	1:C:258:ASN:HD21	1.75	0.49
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.95	0.49
1:C:46:ASP:OD1	1:C:46:ASP:N	2.43	0.49
2:D:67:LEU:N	2:D:67:LEU:HD12	2.27	0.49
2:D:301:MET:C	2:D:303:ALA:H	2.20	0.49
2:D:20:PHE:O	2:D:24:ILE:HG12	2.13	0.49
2:B:67:LEU:N	2:B:67:LEU:HD12	2.27	0.49
1:A:36:MET:HB3	1:A:61:HIS:NE2	2.27	0.49
1:C:154:MET:HE2	1:C:194[A]:THR:CG2	2.42	0.49
4:F:304:THR:HG21	4:F:311:SER:HB2	1.95	0.49
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.42	0.49
2:B:287:THR:HG22	2:B:290:GLU:HG3	1.92	0.49
2:B:295:MET:CG	2:B:377:PHE:HB2	2.43	0.49
4:F:339:ALA:HB3	4:F:342:LEU:CD1	2.39	0.49
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.95	0.49
2:D:297:ASP:OD1	2:D:298:SER:N	2.46	0.49
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.41	0.49
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.48	0.49
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.48	0.49
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.95	0.49
2:B:346:TRP:HE1	2:B:438:ALA:HB3	1.78	0.49
1:C:186:ASN:O	1:C:190:THR:HG22	2.12	0.49
2:D:5:VAL:HB	2:D:135:PHE:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:O	1:A:259:LEU:HB2	2.13	0.48
2:B:274:PRO:HB3	2:B:286:LEU:CD1	2.42	0.48
1:C:99:ALA:HB3	1:C:144:GLY:HA3	1.95	0.48
2:B:318:ILE:HD12	2:B:318:ILE:N	2.28	0.48
1:C:271:THR:HG21	1:C:295[A]:CYS:HA	1.94	0.48
4:F:102:PRO:HB3	4:F:173:ILE:CG2	2.44	0.48
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.43	0.48
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.49	0.48
1:C:108:TYR:O	1:C:112:LYS:HG2	2.13	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.48	0.48
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.95	0.48
1:A:252:LEU:HD22	1:A:252:LEU:H	1.78	0.48
2:B:171:VAL:HA	2:B:204:ILE:O	2.14	0.48
2:B:286:LEU:O	2:B:373:MET:HE2	2.14	0.48
2:D:258:ASN:HB3	9:D:503:LOC:C16	2.43	0.48
2:D:287:THR:CB	2:D:289:PRO:HD2	2.44	0.48
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.94	0.48
1:A:180:ALA:HB1	2:B:258:ASN:OD1	2.12	0.48
1:A:339:ARG:HB2	1:A:341:ILE:HD11	1.96	0.48
1:C:70:LEU:HD13	1:C:110:ILE:HG21	1.93	0.48
4:F:102:PRO:HA	4:F:173:ILE:HG22	1.96	0.48
4:F:168:GLU:OE1	4:F:168:GLU:N	2.39	0.48
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.96	0.47
1:A:336:LYS:HD3	1:A:336:LYS:O	2.14	0.47
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.49	0.47
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.95	0.47
2:B:357:ASP:O	2:B:359:PRO:HD3	2.14	0.47
1:A:115:ILE:HG23	1:A:116:ASP:N	2.30	0.47
4:F:3:THR:HB	4:F:30:LEU:HD11	1.97	0.47
1:A:2:ARG:O	1:A:51[A]:THR:HG22	2.14	0.47
2:D:191:VAL:HB	2:D:425:MET:CE	2.45	0.47
2:D:191:VAL:O	2:D:195:VAL:HG23	2.14	0.47
1:A:383:ALA:O	1:A:386:GLU:HG3	2.14	0.47
1:A:209[B]:ILE:HG13	1:A:227:LEU:HD22	1.96	0.47
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.96	0.47
4:F:36:ARG:HA	4:F:58:LEU:CD1	2.44	0.47
1:A:71:GLU:OE1	1:A:73:THR:HG22	2.15	0.46
2:D:177:VAL:HG12	2:D:177:VAL:O	2.15	0.46
2:D:381:SER:O	2:D:384[B]:ILE:HG22	2.15	0.46
2:D:402:LYS:HE2	2:D:415:GLU:OE2	2.14	0.46
1:A:175:PRO:HA	1:A:179:THR:OG1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:GLN:HA	2:D:167:ASN:O	2.15	0.46
4:F:148:ILE:HG23	4:F:148:ILE:O	2.16	0.46
1:A:269:LEU:HD11	1:A:301:GLN:HB3	1.97	0.46
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.97	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.97	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
1:C:363:VAL:HG23	1:C:364:PRO:HD2	1.97	0.46
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.50	0.46
1:C:249:ASN:ND2	1:C:356[A]:ASN:OD1	2.49	0.46
2:D:159:GLU:HG3	3:E:123:LEU:HD13	1.98	0.46
2:B:75:MET:HG2	2:B:94:PHE:CD2	2.51	0.46
2:B:287:THR:CG2	2:B:290:GLU:H	2.28	0.46
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.98	0.46
4:F:192:LEU:CD1	4:F:262:MET:HE1	2.46	0.45
1:A:36:MET:HE2	1:A:38:SER:HB2	1.97	0.45
4:F:253:TYR:OH	4:F:259:GLY:HA2	2.17	0.45
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.47	0.45
2:D:7:ILE:O	2:D:137:LEU:HA	2.16	0.45
2:D:414:ASP:OD2	2:D:416:MET:HB2	2.16	0.45
4:F:186:LEU:HD12	4:F:320:MET:HG2	1.99	0.45
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.45
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.98	0.45
4:F:195:GLY:O	4:F:227:PRO:HB3	2.16	0.45
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.98	0.45
1:A:341:ILE:N	1:A:341:ILE:HD12	2.32	0.45
2:B:335:VAL:O	2:B:339:ASN:ND2	2.41	0.45
1:C:217:LEU:HD21	1:C:368:LEU:HD23	1.99	0.45
2:D:409:THR:O	3:E:140:LYS:HE3	2.17	0.45
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.99	0.45
2:B:212:ILE:HG23	2:B:275:LEU:HD13	1.99	0.45
2:D:161:TYR:HB3	2:D:164:ARG:CG	2.47	0.45
1:A:23:LEU:O	1:A:27:GLU:HG3	2.17	0.45
1:A:177:VAL:O	1:A:178:SER:C	2.60	0.45
2:D:191:VAL:CG1	2:D:425:MET:HE2	2.43	0.45
4:F:47:LEU:C	4:F:47:LEU:HD23	2.42	0.45
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.52	0.45
4:F:267:PHE:CD2	4:F:279:LEU:HD13	2.51	0.45
1:C:177:VAL:CG2	1:C:206:ASN:HB3	2.45	0.45
2:D:244:PHE:CZ	2:D:358:ILE:CD1	3.00	0.45
4:F:165:GLU:HB3	4:F:168:GLU:OE2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:NE	1:A:251:ASP:HB3	2.32	0.44
2:B:1:MET:HE2	2:B:3:GLU:OE2	2.17	0.44
1:C:176:GLN:CD	1:C:176:GLN:H	2.26	0.44
4:F:168:GLU:HG2	4:F:169:LEU:N	2.32	0.44
4:F:202:ARG:NH2	4:F:222:ARG:HH12	2.15	0.44
4:F:37:PHE:O	4:F:60:GLN:HG2	2.18	0.44
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.00	0.44
2:D:119:LEU:O	2:D:122:VAL:HG22	2.18	0.44
3:E:53:LYS:HE2	3:E:53:LYS:HB3	1.84	0.44
2:D:259:MET:HE2	2:D:316:ALA:CB	2.47	0.44
1:A:131:GLY:O	1:A:132:LEU:C	2.59	0.44
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.50	0.44
2:D:258:ASN:O	9:D:503:LOC:H18A	2.18	0.44
4:F:2:TYR:OH	4:F:360:PRO:O	2.33	0.44
1:A:75:ILE:CG2	1:A:92:LEU:HD12	2.45	0.44
1:A:287:SER:OG	1:A:290:GLU:HG3	2.17	0.44
2:B:69:ASP:O	2:B:94:PHE:HA	2.18	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.00	0.44
2:D:228:ASN:CG	8:D:501:GDP:HN1	2.26	0.44
2:D:295:MET:CG	2:D:377:PHE:HB2	2.48	0.44
4:F:250:SER:C	4:F:253:TYR:N	2.76	0.44
2:B:42:LEU:HD12	2:B:358:ILE:HD11	1.99	0.44
3:E:6:MET:HG2	3:E:24:LEU:CD2	2.48	0.44
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.00	0.44
4:F:299:GLU:N	4:F:300:PRO:HD2	2.33	0.44
2:D:117:SER:O	2:D:121:VAL:HG23	2.17	0.44
4:F:221:LEU:HD22	4:F:262:MET:HE3	1.99	0.44
1:A:71:GLU:CD	1:A:73:THR:HG22	2.42	0.43
2:D:48:ARG:HD3	2:D:48:ARG:HA	1.77	0.43
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.98	0.43
1:C:183:GLU:N	1:C:184:PRO:CD	2.82	0.43
1:C:234:ILE:HD12	1:C:234:ILE:N	2.33	0.43
3:E:48:GLU:O	3:E:52:LYS:HG3	2.18	0.43
1:A:217:LEU:HD21	1:A:275:VAL:HG12	2.00	0.43
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.53	0.43
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.33	0.43
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.43
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.01	0.43
2:D:35:SER:OG	2:D:60:LYS:HE3	2.17	0.43
4:F:82:LYS:NZ	4:F:97:SER:O	2.48	0.43
1:A:234:ILE:O	1:A:238:ILE:HG13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:O	3:E:61:ARG:HD3	2.18	0.43
2:B:63:PRO:HD3	2:B:86:ILE:HG12	2.00	0.43
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.76	0.43
2:B:287:THR:HG22	2:B:290:GLU:CB	2.48	0.43
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.19	0.43
4:F:37:PHE:HZ	4:F:52:LEU:CD2	2.32	0.43
4:F:238:CYS:HG	4:F:239:HIS:CE1	2.35	0.43
4:F:172:PHE:HD1	4:F:172:PHE:O	2.01	0.43
4:F:284[A]:LEU:HD12	4:F:284[A]:LEU:HA	1.78	0.43
2:B:305:CYS:O	2:B:307:PRO:HD3	2.19	0.43
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.54	0.43
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.53	0.43
1:A:55:GLU:HA	1:A:60:LYS:O	2.18	0.43
2:B:287:THR:HG22	2:B:290:GLU:HB2	2.00	0.43
2:D:220:THR:C	2:D:222:PRO:HD3	2.44	0.42
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.59	0.42
3:E:75:LYS:O	3:E:79:GLU:HG3	2.19	0.42
4:F:91:CYS:C	4:F:92:THR:HG23	2.44	0.42
2:B:286:LEU:HD23	2:B:286:LEU:HA	1.84	0.42
2:D:9:ALA:HA	2:D:68:VAL:O	2.19	0.42
1:A:100:ALA:HA	2:B:254:LYS:CG	2.49	0.42
1:A:285:GLN:OE1	1:A:285:GLN:N	2.51	0.42
1:A:262:TYR:HE2	1:A:346:TRP:CH2	2.37	0.42
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.42
1:C:72:PRO:CG	2:D:1:MET:CE	2.96	0.42
2:D:114:LEU:HG	2:D:114:LEU:O	2.18	0.42
2:D:208:ALA:O	2:D:212:ILE:HG13	2.19	0.42
2:D:320:ARG:O	2:D:323:MET:HE1	2.19	0.42
4:F:18:SER:O	4:F:22:LEU:HG	2.19	0.42
1:A:39:ASP:OD2	1:A:61:HIS:HE1	2.03	0.42
2:D:50:ASN:HD22	2:D:50:ASN:H	1.68	0.42
2:D:212:ILE:O	2:D:216:THR:HB	2.19	0.42
4:F:24:THR:HG22	4:F:26:GLN:HG3	2.02	0.42
2:D:317:ALA:O	2:D:353:THR:HA	2.20	0.42
2:B:20:PHE:CE2	2:B:24:ILE:HD13	2.55	0.42
1:A:93:ILE:HD11	1:A:121:ARG:CG	2.45	0.42
1:A:319:TYR:HB3	1:A:323:VAL:HG21	2.01	0.42
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.01	0.42
1:C:277:SER:OG	1:C:280:LYS:HG3	2.20	0.42
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.46	0.42
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:264:ARG:NE	2:D:431:GLU:OE2	2.52	0.41
2:D:269[B]:MET:HE3	2:D:305:CYS:HB2	2.02	0.41
1:A:104:ALA:CB	1:A:413:MET:HE3	2.47	0.41
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.86	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.41
2:D:102:ASN:HD22	2:D:105:LYS:HG3	1.84	0.41
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.02	0.41
3:E:47:LEU:HD23	3:E:47:LEU:O	2.21	0.41
4:F:21:LEU:HD21	4:F:355:ILE:HG21	2.03	0.41
4:F:38:ASN:O	4:F:60:GLN:HA	2.20	0.41
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.50	0.41
1:A:209[A]:ILE:HG22	1:A:227:LEU:CD2	2.49	0.41
2:B:269:MET:HE3	2:B:301:MET:HB3	2.02	0.41
1:C:22:GLU:O	1:C:26:LEU:HG	2.20	0.41
1:C:117:LEU:HD21	1:C:121:ARG:NH2	2.35	0.41
1:C:178:SER:HB2	1:C:224:TYR:OH	2.20	0.41
1:C:361:THR:CG2	1:C:362:VAL:N	2.84	0.41
2:B:269:MET:HE2	2:B:269:MET:HB3	1.79	0.41
1:C:153:LEU:O	1:C:157:LEU:HG	2.20	0.41
2:D:414:ASP:N	2:D:414:ASP:OD1	2.53	0.41
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.50	0.41
1:A:151:SER:HB2	1:A:193:THR:HG22	2.00	0.41
1:A:209[A]:ILE:HG22	1:A:227:LEU:HD22	2.01	0.41
1:C:72:PRO:HG2	2:D:1:MET:CE	2.51	0.41
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.56	0.41
4:F:168:GLU:O	4:F:172:PHE:HB2	2.21	0.41
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.95	0.41
2:D:115:VAL:HG23	2:D:153:LEU:HD23	2.02	0.41
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.02	0.41
2:D:270:PRO:HA	2:D:377:PHE:O	2.20	0.41
4:F:224:SER:HB2	4:F:241:THR:HG22	2.03	0.41
1:A:132:LEU:O	1:A:164:LYS:NZ	2.51	0.41
1:A:358:GLN:HA	1:A:359:PRO:HD3	1.95	0.41
2:D:291:LEU:HD12	2:D:291:LEU:HA	1.86	0.41
1:A:209[B]:ILE:HD13	1:A:231:ILE:HD11	2.02	0.41
1:A:262:TYR:HA	1:A:263:PRO:HD3	1.92	0.41
1:A:437:VAL:CG1	1:A:438:ASP:N	2.84	0.41
1:C:277:SER:HG	1:C:280:LYS:HG3	1.85	0.41
4:F:24:THR:CG2	4:F:361:LEU:HD13	2.50	0.41
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	2.02	0.41
4:F:252:ASN:ND2	4:F:255:ARG:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:279:LEU:HG	4:F:284[B]:LEU:HG	2.03	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.41
2:B:20:PHE:CD1	2:B:235:MET:HE2	2.56	0.40
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.39	0.40
1:A:133:GLN:HB2	1:A:252:LEU:HD23	2.04	0.40
1:A:183:GLU:N	1:A:184:PRO:CD	2.85	0.40
1:A:192:HIS:NE2	1:A:420[A]:GLU:HG2	2.36	0.40
2:B:295:MET:HE2	2:B:295:MET:HB3	1.86	0.40
4:F:24:THR:HG23	4:F:361:LEU:HD13	2.03	0.40
1:A:302[A]:MET:HE2	1:A:302[A]:MET:HA	2.02	0.40
2:B:387:LEU:HD23	2:B:387:LEU:C	2.46	0.40
1:C:195:LEU:HD12	1:C:266:HIS:CE1	2.57	0.40
4:F:24:THR:HG22	4:F:26:GLN:H	1.86	0.40
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.57	0.40
2:D:145:THR:O	2:D:149:MET:HB3	2.20	0.40
2:D:254:LYS:HG2	9:D:503:LOC:H10	2.04	0.40
4:F:1:MET:HE3	4:F:26:GLN:C	2.46	0.40
2:B:205:ASP:HB3	2:B:303:ALA:HA	2.03	0.40
2:D:287:THR:HB	2:D:289:PRO:HD2	2.03	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	450/440 (102%)	431 (96%)	17 (4%)	2 (0%)	30	65
1	C	448/440 (102%)	432 (96%)	15 (3%)	1 (0%)	43	76
2	B	428/431 (99%)	406 (95%)	21 (5%)	1 (0%)	43	76
2	D	421/431 (98%)	400 (95%)	20 (5%)	1 (0%)	43	76
3	E	118/121 (98%)	116 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	310/320 (97%)	288 (93%)	22 (7%)	0	100	100
All	All	2175/2183 (100%)	2073 (95%)	97 (4%)	5 (0%)	43	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	VAL
1	A	178	SER
2	D	74	THR
2	B	73	GLY
1	A	131	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	382/371 (103%)	380 (100%)	2 (0%)	81	89
1	C	381/371 (103%)	381 (100%)	0	100	100
2	B	374/372 (100%)	372 (100%)	2 (0%)	81	89
2	D	367/372 (99%)	365 (100%)	2 (0%)	81	89
3	E	110/109 (101%)	108 (98%)	2 (2%)	51	77
4	F	294/289 (102%)	284 (97%)	10 (3%)	32	66
All	All	1908/1884 (101%)	1890 (99%)	18 (1%)	68	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	133	GLN
2	B	172	MET
2	B	302	MET
2	D	74	THR
2	D	122	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	6	MET
3	E	8	VAL
4	F	1	MET
4	F	91	CYS
4	F	125	THR
4	F	162	ILE
4	F	163	SER
4	F	222	ARG
4	F	248	GLU
4	F	249	TYR
4	F	257	GLU
4	F	311	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	LOC	B	503	-	31,31,31	0.98	3 (9%)	44,44,44	1.57	6 (13%)
9	LOC	D	503	-	31,31,31	1.01	2 (6%)	44,44,44	1.70	5 (11%)
10	ACP	F	401	-	31,33,33	0.75	2 (6%)	47,52,52	0.68	1 (2%)
5	GTP	C	501	6	33,34,34	0.58	0	50,54,54	0.49	0
5	GTP	A	501	6	33,34,34	0.57	0	50,54,54	0.51	0
8	GDP	B	501	6	29,30,30	0.54	0	45,47,47	0.43	0
8	GDP	D	501	6	29,30,30	0.52	0	45,47,47	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LOC	B	503	-	-	2/12/25/25	0/3/3/3
9	LOC	D	503	-	-	4/12/25/25	0/3/3/3
10	ACP	F	401	-	-	6/19/38/38	0/3/3/3
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3
8	GDP	D	501	6	-	5/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	503	LOC	C22-C21	-3.27	1.46	1.50
9	B	503	LOC	C22-C21	-2.96	1.46	1.50
9	D	503	LOC	C20-C21	2.94	1.42	1.37
9	B	503	LOC	C20-C21	2.75	1.42	1.37
10	F	401	ACP	PB-O2B	-2.35	1.50	1.56
9	B	503	LOC	C21-C14	2.03	1.46	1.43
10	F	401	ACP	PG-O2G	-2.03	1.50	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	503	LOC	O6-C17-C16	7.58	116.57	109.60
9	B	503	LOC	O6-C17-C16	7.02	116.05	109.60
9	D	503	LOC	C14-C11-N1	-4.05	111.11	114.31
9	D	503	LOC	O6-C17-C19	-3.83	116.73	122.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	LOC	O6-C17-C19	-3.61	117.04	122.29
9	B	503	LOC	C14-C11-N1	-3.43	111.60	114.31
9	D	503	LOC	C14-C15-C16	-3.19	128.52	134.20
9	B	503	LOC	C9-C10-C11	-2.84	108.68	112.13
9	D	503	LOC	C9-C10-C11	-2.84	108.69	112.13
9	B	503	LOC	C14-C15-C16	-2.59	129.59	134.20
10	F	401	ACP	O1G-PG-C3B	-2.56	105.80	111.37
9	B	503	LOC	C20-C21-C14	-2.25	122.39	124.67

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	503	LOC	C19-C17-O6-C18
9	B	503	LOC	C16-C17-O6-C18
9	D	503	LOC	C19-C17-O6-C18
9	D	503	LOC	C16-C17-O6-C18
10	F	401	ACP	PG-C3B-PB-O1B
10	F	401	ACP	PG-C3B-PB-O2B
10	F	401	ACP	PG-C3B-PB-O3A
10	F	401	ACP	C5'-O5'-PA-O3A
9	D	503	LOC	C3-C5-O3-C6
10	F	401	ACP	PB-O3A-PA-O5'
9	D	503	LOC	C7-C5-O3-C6
8	D	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
10	F	401	ACP	C5'-O5'-PA-O1A
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A

Continued on next page...

Continued from previous page...

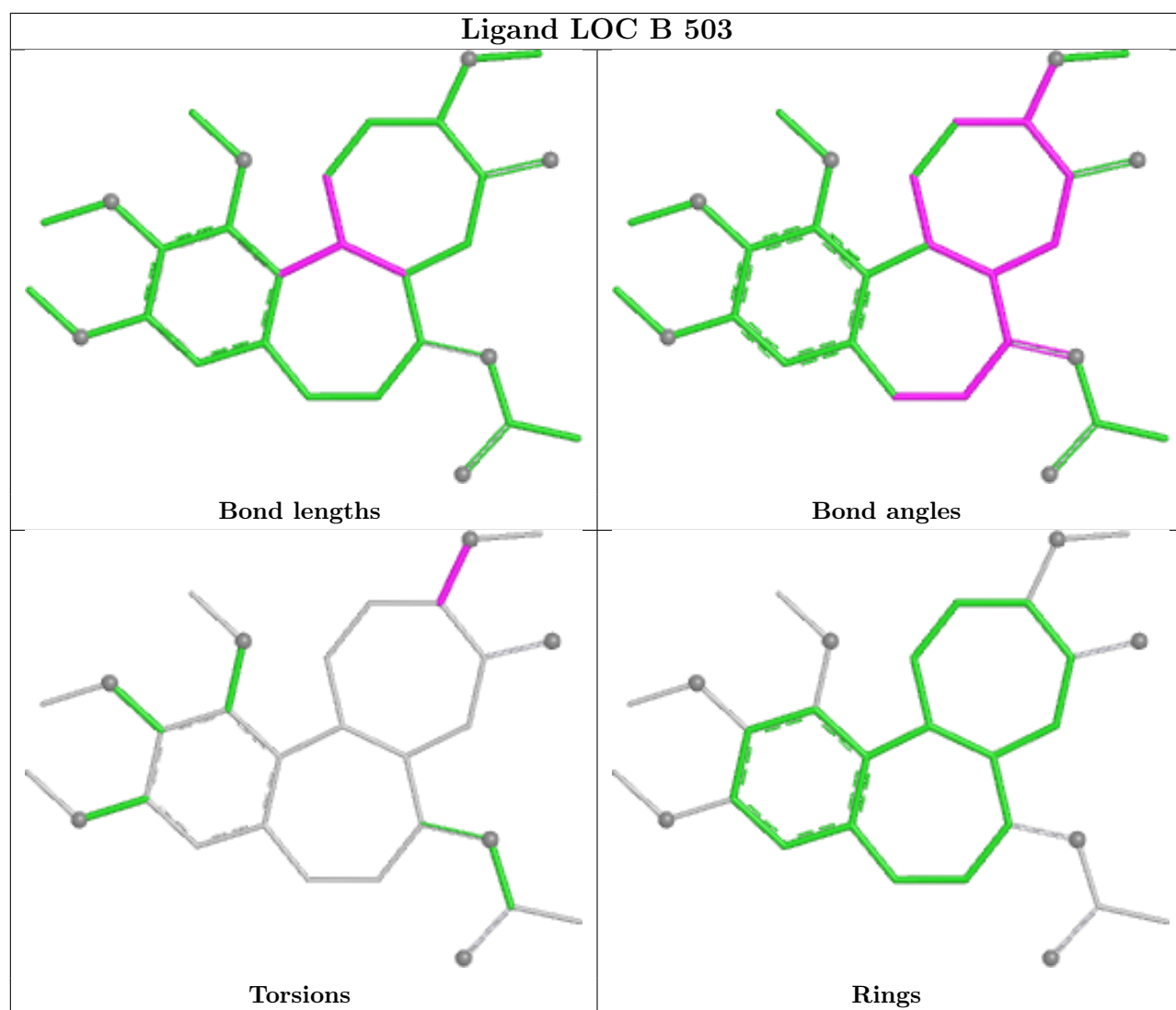
Mol	Chain	Res	Type	Atoms
8	D	501	GDP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

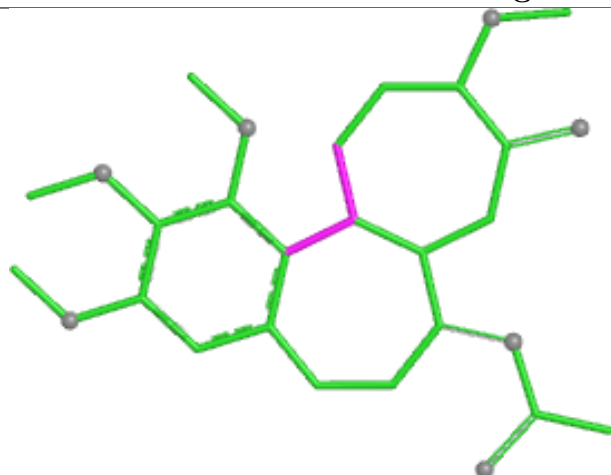
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	503	LOC	2	0
9	D	503	LOC	5	0
10	F	401	ACP	1	0
8	D	501	GDP	3	0

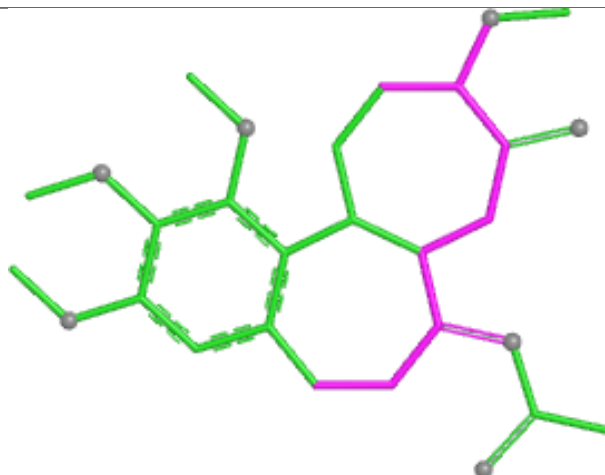
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



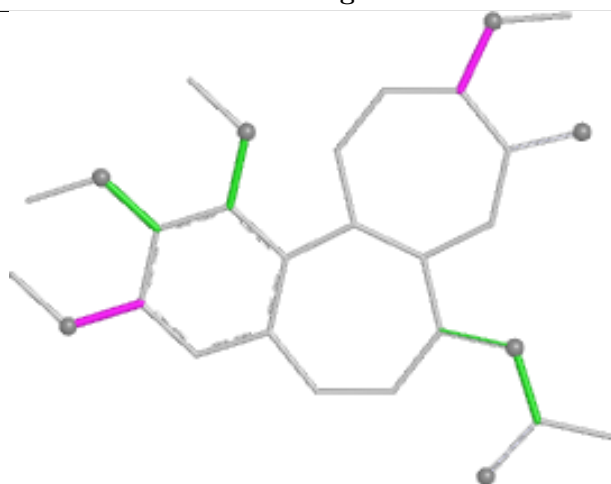
Ligand LOC D 503



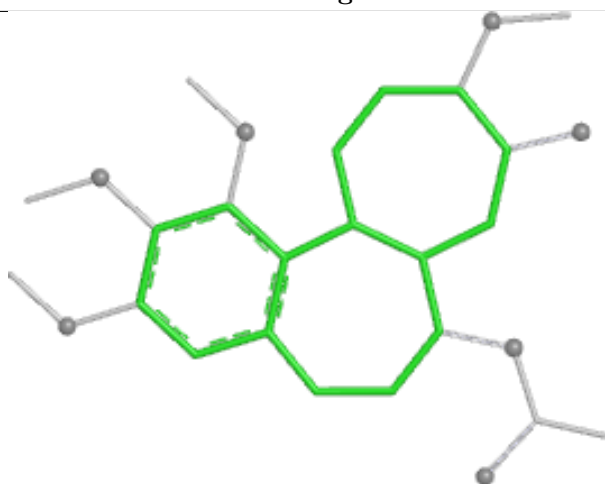
Bond lengths



Bond angles

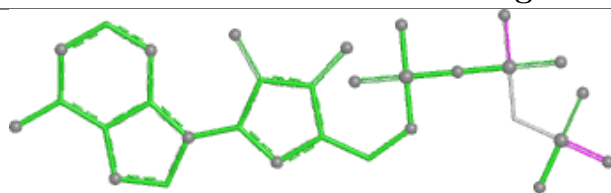


Torsions

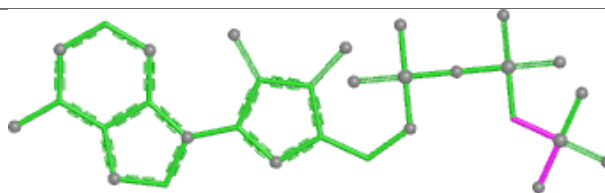


Rings

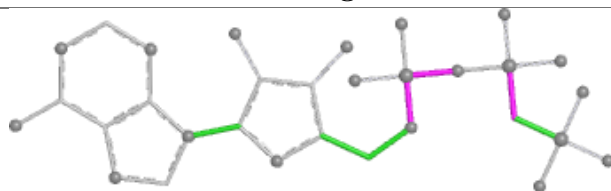
Ligand ACP F 401



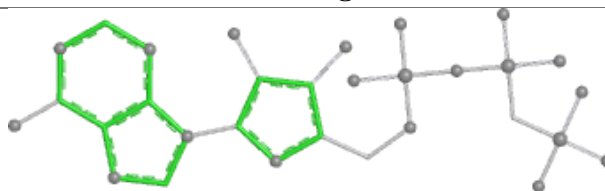
Bond lengths



Bond angles

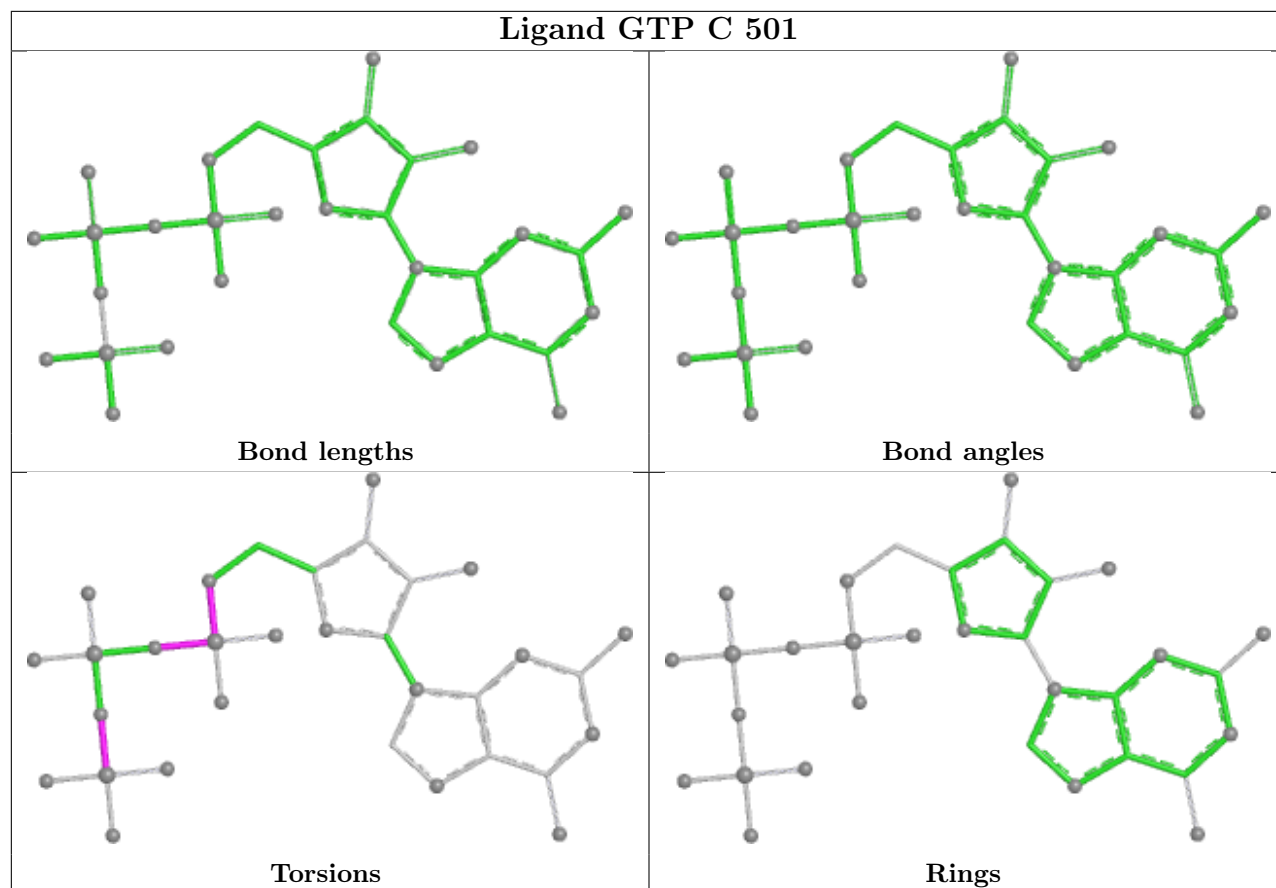


Torsions

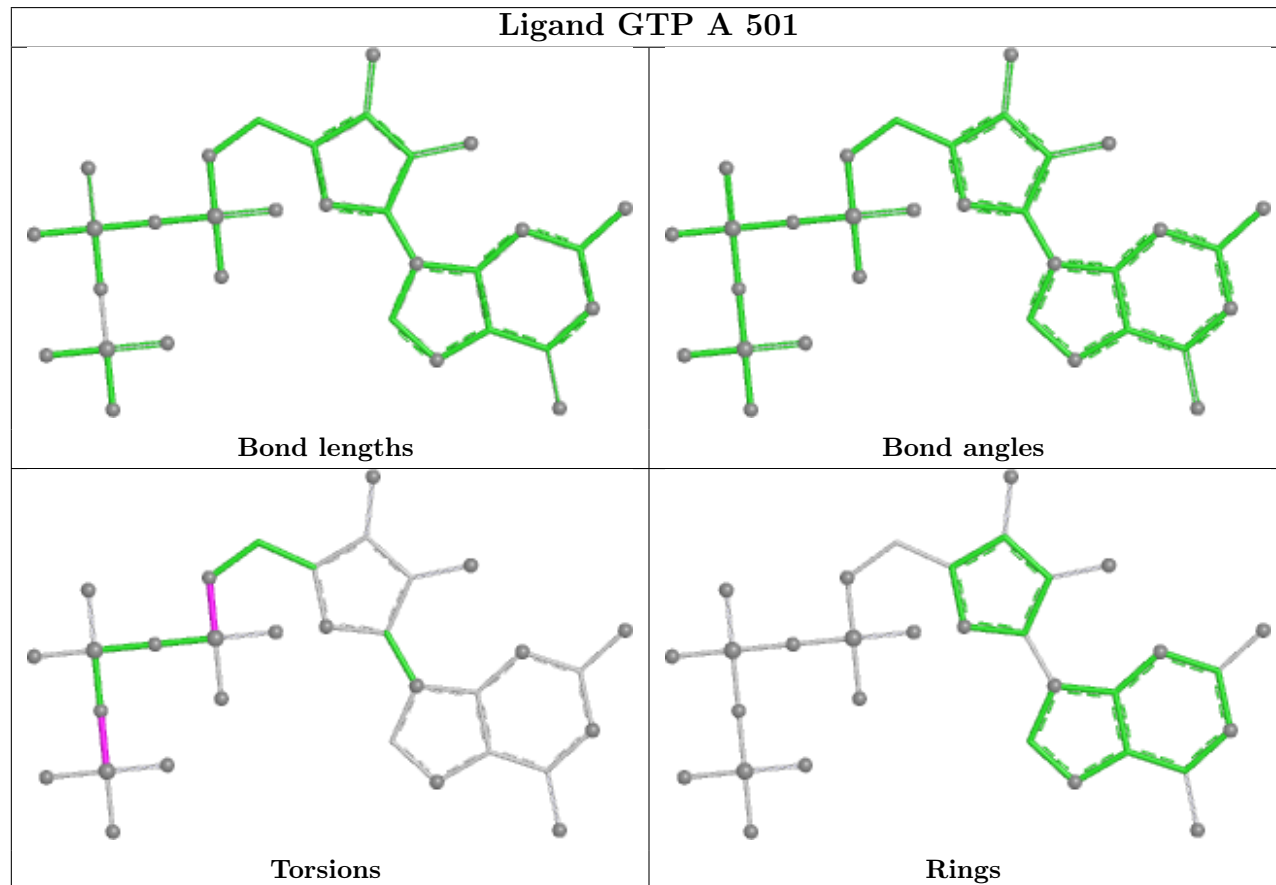


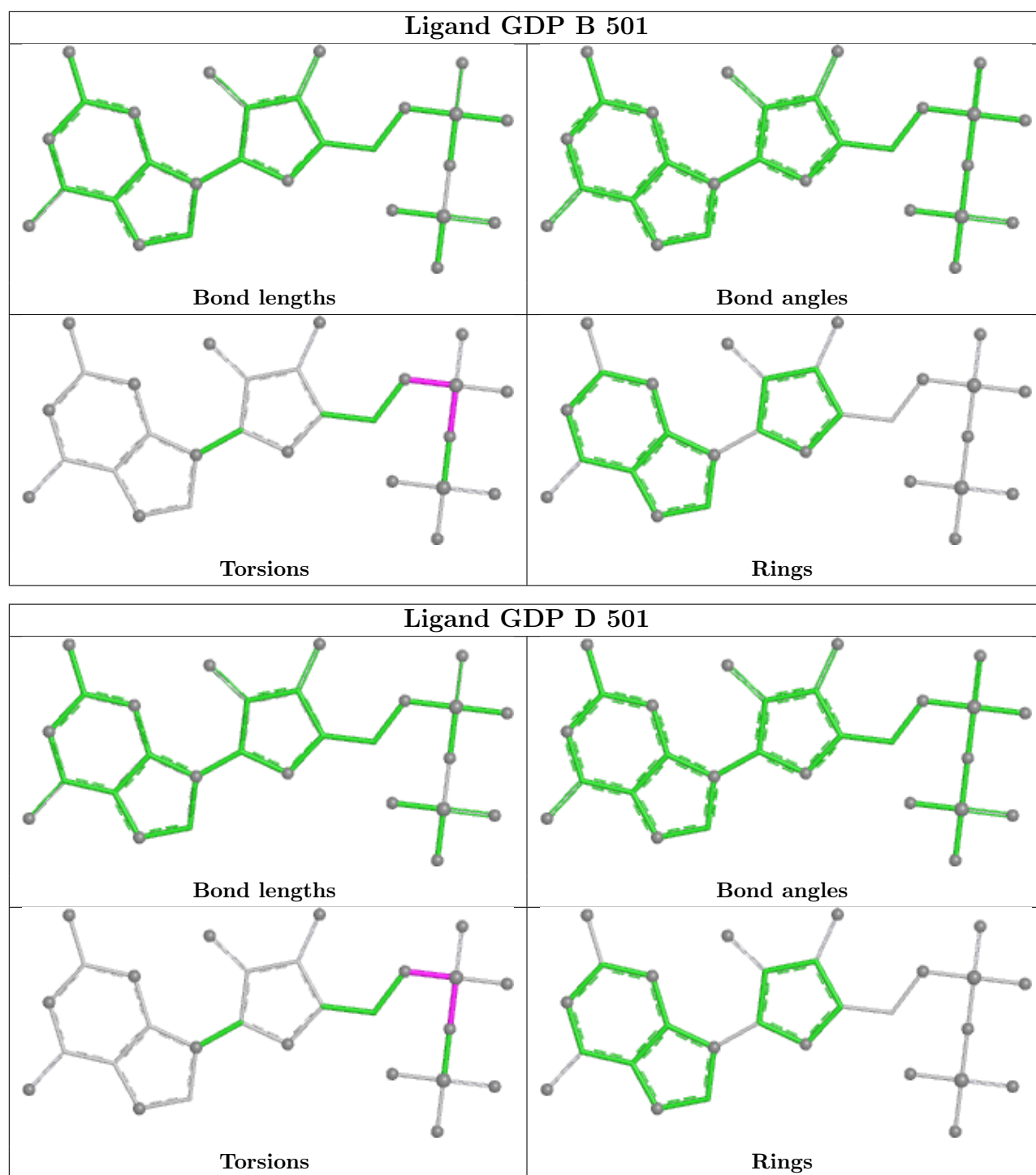
Rings

Ligand GTP C 501



Ligand GTP A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	F	6
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	28:SER	C	44:ASP	N	32.70
1	F	362:ALA	C	373:SER	N	19.68
1	F	102:PRO	C	125:THR	N	12.42
1	F	151:SER	C	162:ILE	N	11.70
1	F	136:ASN	C	144:GLY	N	11.08
1	F	173:ILE	C	179:VAL	N	8.40
1	F	231:ALA	C	235:ASP	N	6.52

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/440 (99%)	-0.44	1 (0%) 91 83	23, 62, 111, 188	13 (2%)
1	C	440/440 (100%)	-0.59	0 100 100	20, 48, 84, 146	10 (2%)
2	B	423/431 (98%)	-0.50	0 100 100	19, 55, 102, 141	12 (2%)
2	D	421/431 (97%)	-0.39	2 (0%) 87 72	27, 74, 114, 151	8 (1%)
3	E	121/121 (100%)	-0.25	1 (0%) 82 64	28, 77, 125, 193	1 (0%)
4	F	320/320 (100%)	-0.09	7 (2%) 62 39	32, 91, 164, 196	5 (1%)
All	All	2164/2183 (99%)	-0.41	11 (0%) 87 72	19, 64, 125, 196	49 (2%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	45	PRO	3.5
4	F	173	ILE	3.3
4	F	76[A]	SER	3.2
1	A	221	ARG	3.0
4	F	268	ASN	2.7
4	F	252	ASN	2.4
2	D	1	MET	2.2
2	D	250	ALA	2.2
4	F	223	THR	2.1
4	F	249	TYR	2.1
4	F	362	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

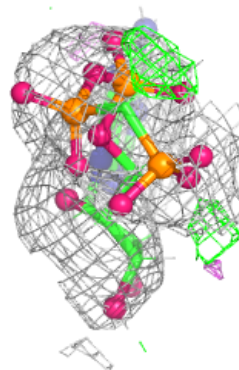
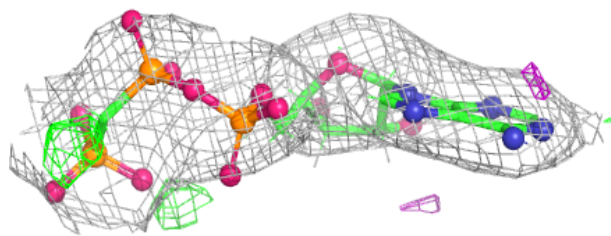
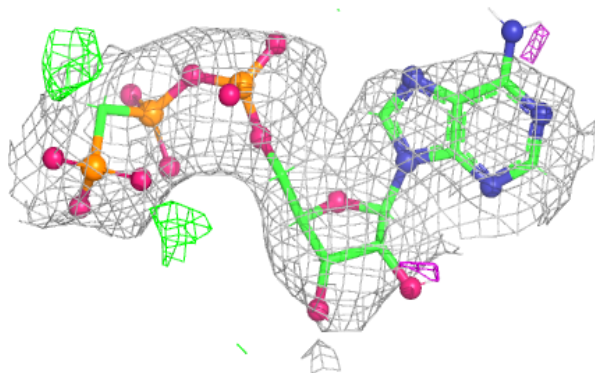
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	502	1/1	0.74	0.12	84,84,84,84	0
10	ACP	F	401	31/31	0.76	0.13	99,114,139,150	0
9	LOC	D	503	29/29	0.89	0.10	29,34,42,45	0
8	GDP	D	501	28/28	0.90	0.12	54,72,94,112	0
6	MG	A	502	1/1	0.95	0.16	43,43,43,43	0
9	LOC	B	503	29/29	0.95	0.07	30,35,40,42	0
6	MG	B	502	1/1	0.95	0.20	43,43,43,43	0
5	GTP	A	501	32/32	0.95	0.08	30,43,54,65	0
6	MG	C	502	1/1	0.96	0.19	37,37,37,37	0
8	GDP	B	501	28/28	0.96	0.07	35,42,56,68	0
7	CA	C	503	1/1	0.97	0.05	91,91,91,91	0
5	GTP	C	501	32/32	0.97	0.07	31,44,50,56	0
7	CA	A	503	1/1	0.99	0.04	98,98,98,98	0

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

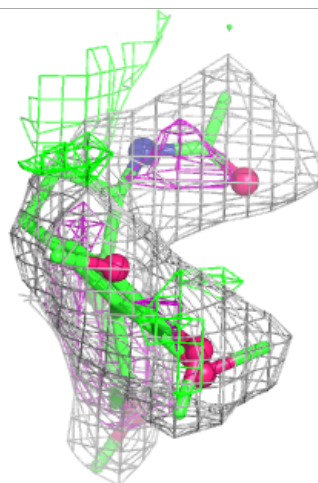
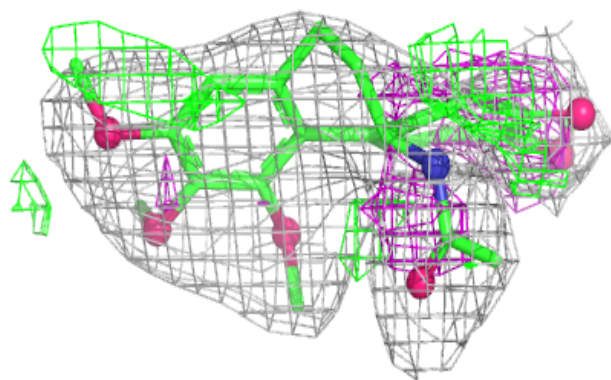
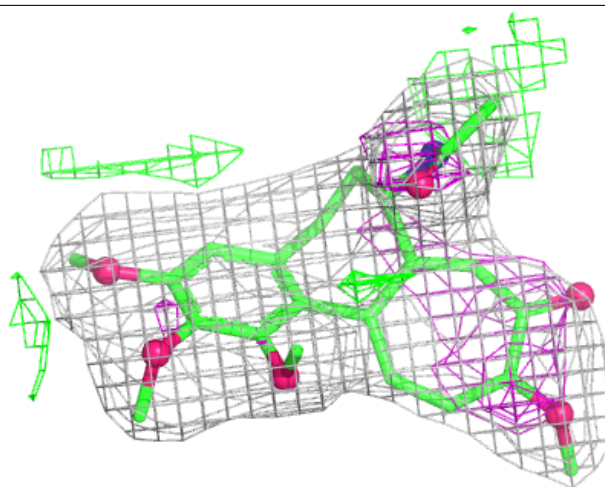
Electron density around ACP F 401:

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



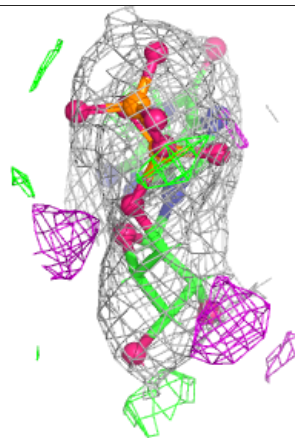
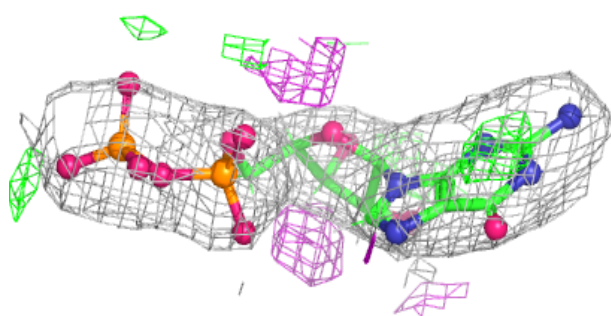
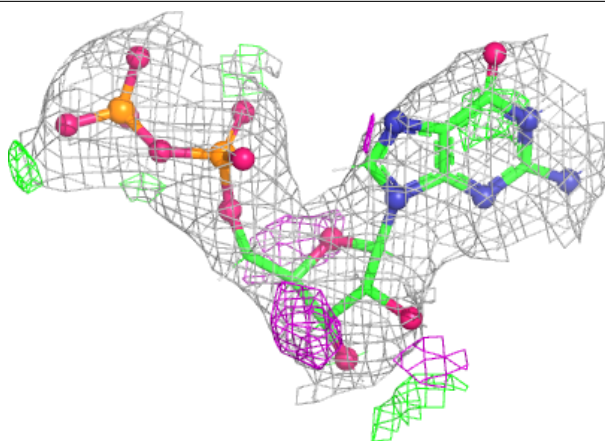
Electron density around LOC D 503:

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

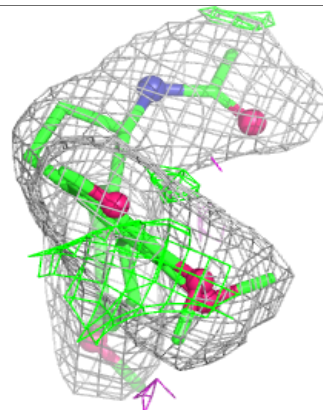
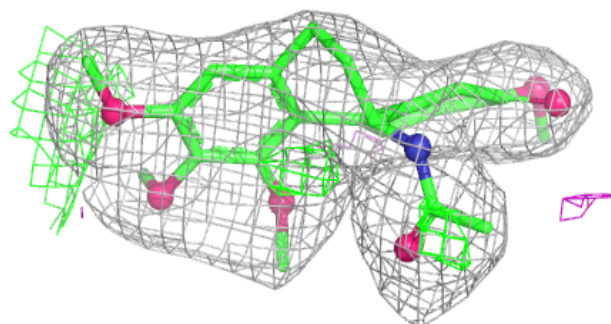
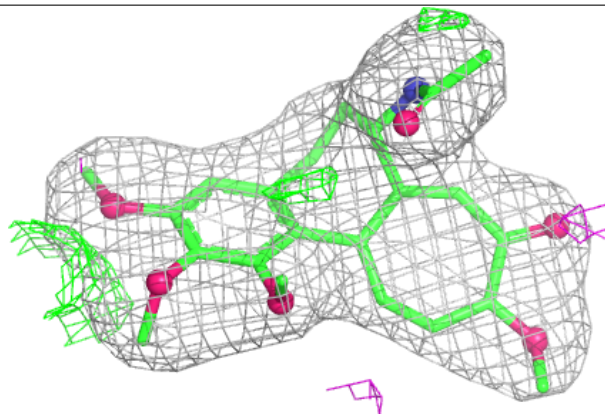


Electron density around GDP D 501:

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

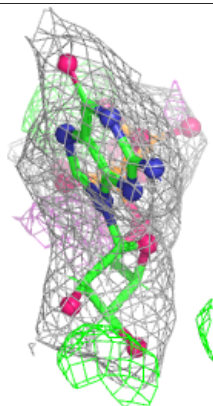
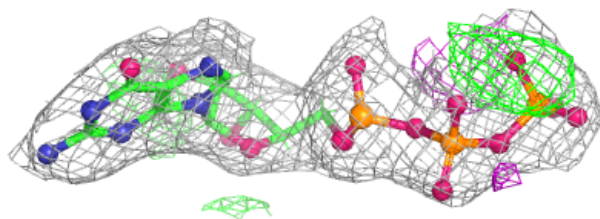
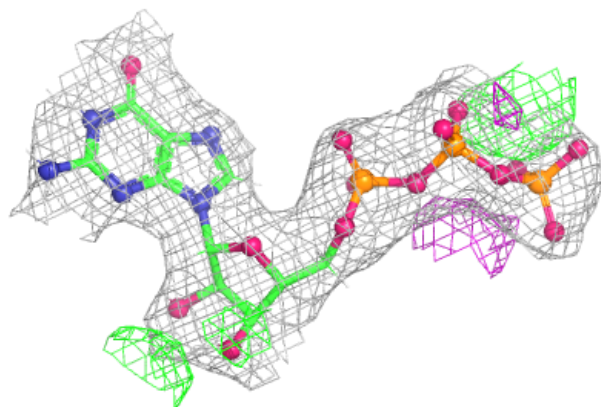
**Electron density around LOC B 503:**

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



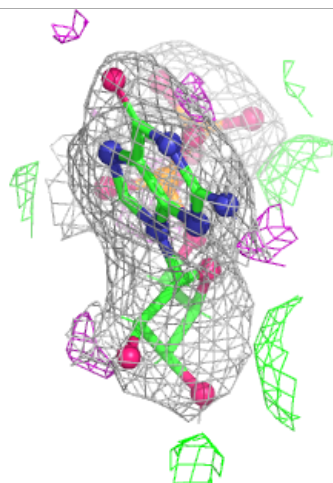
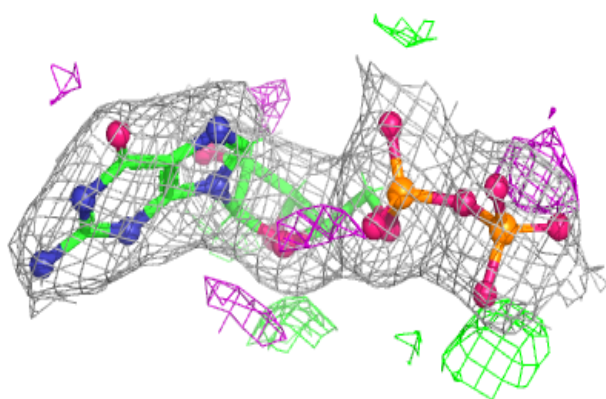
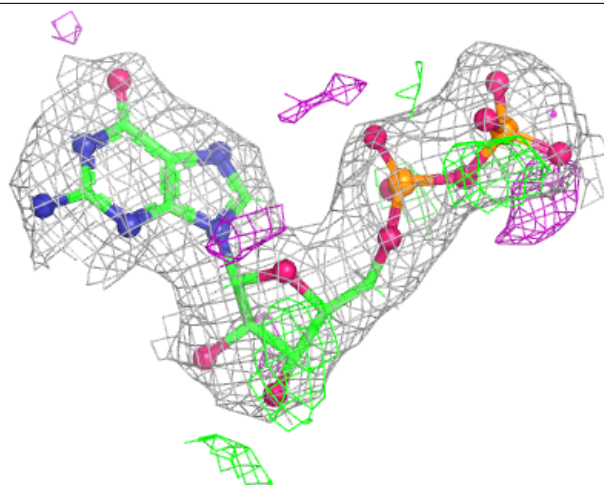
Electron density around GTP A 501:

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



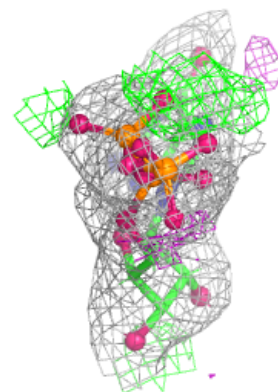
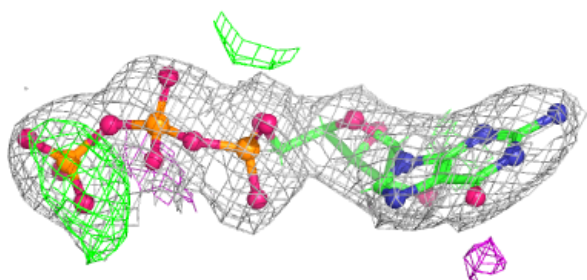
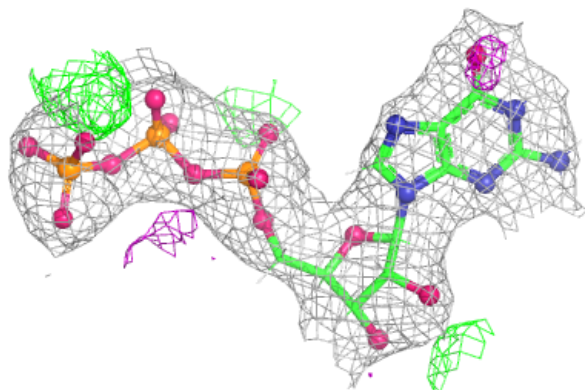
Electron density around GDP B 501:

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



Electron density around GTP C 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.