



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:51 PM EDT

PDB ID : 5S55 / pdb_00005s55
Title : Tubulin-Z106307058-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.30 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

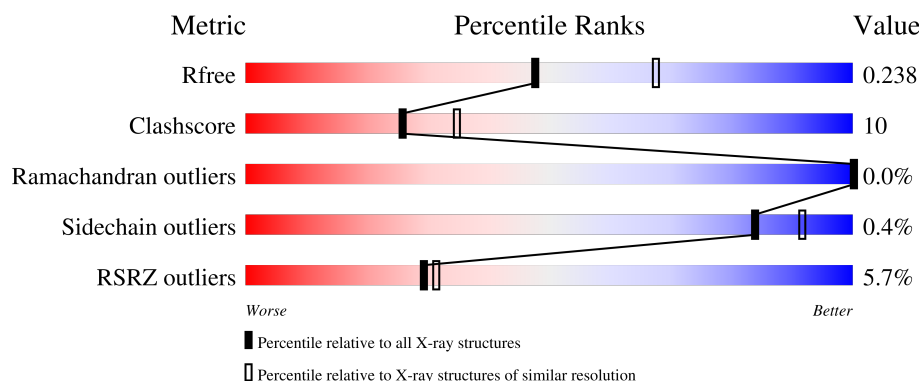
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	8% 71% 20% 9%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 18082 atoms, of which 44 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	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	1	0	0
			3348	2103	573	645	27			
2	D	426	Total	C	N	O	S	5	0	0
			3343	2098	570	648	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	349	Total	C	N	O	S	0	0	0
			2863	1835	492	522	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

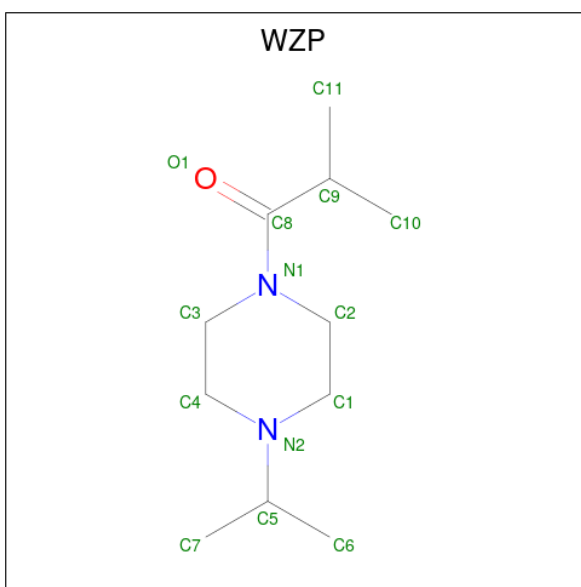
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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



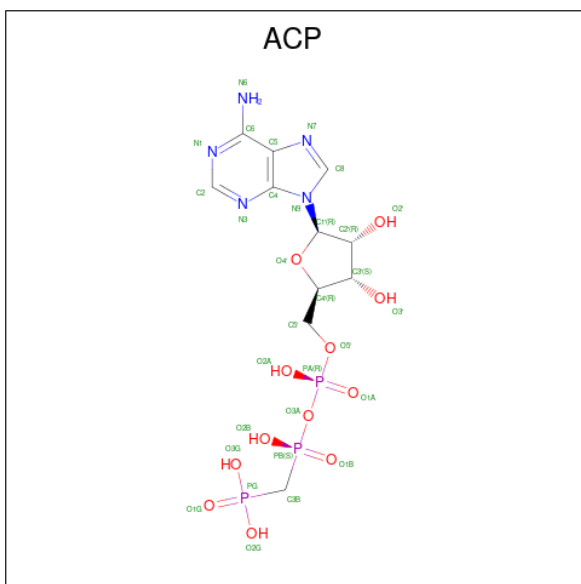
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-methyl-1-[4-(propan-2-yl)piperazin-1-yl]propan-1-one (CCD ID: WZP) (formula: C₁₁H₂₂N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			36	11	22	2	1		
9	D	1	Total	C	H	N	O	0	0
			36	11	22	2	1		

- 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	N	O	P	0	0
			31	11	5	12	3		

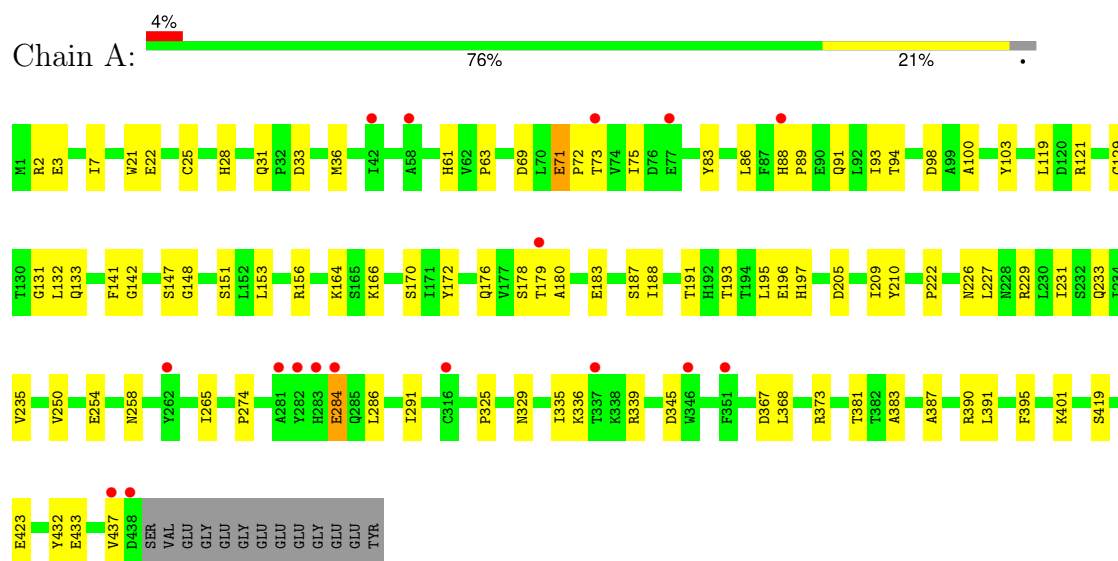
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	73	Total 73	O 73	0	0
11	B	88	Total 88	O 88	0	0
11	C	198	Total 198	O 198	0	0
11	D	32	Total 32	O 32	0	0
11	E	12	Total 12	O 12	0	0
11	F	12	Total 12	O 12	0	0

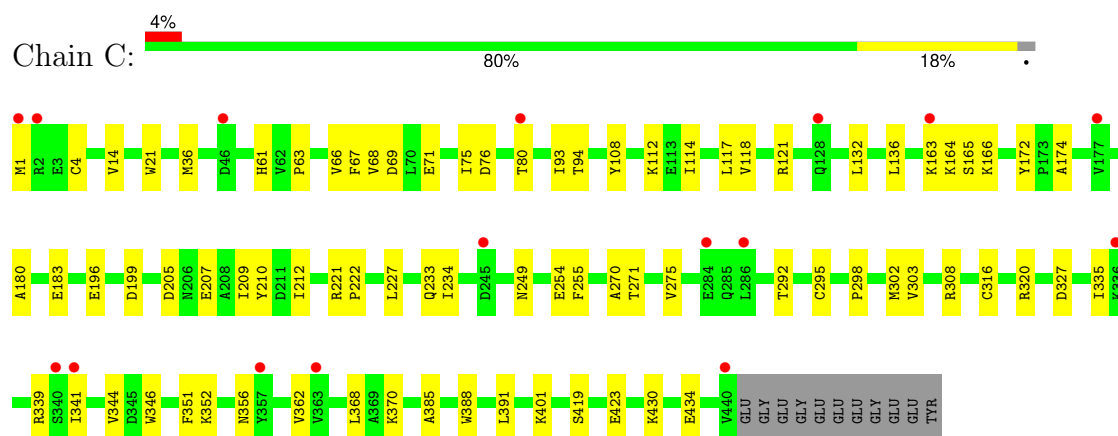
3 Residue-property plots [i](#)

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

- Molecule 1: Tubulin alpha-1B chain

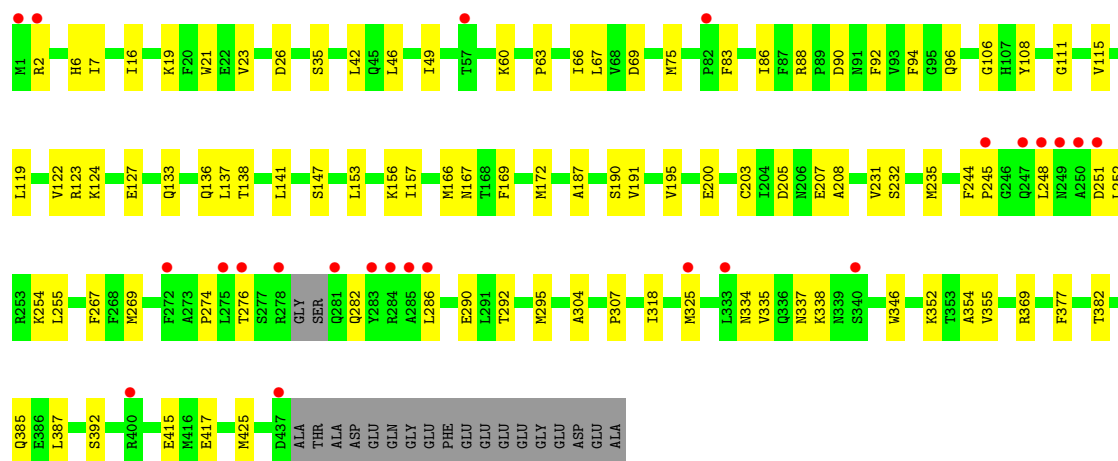


- Molecule 1: Tubulin alpha-1B chain

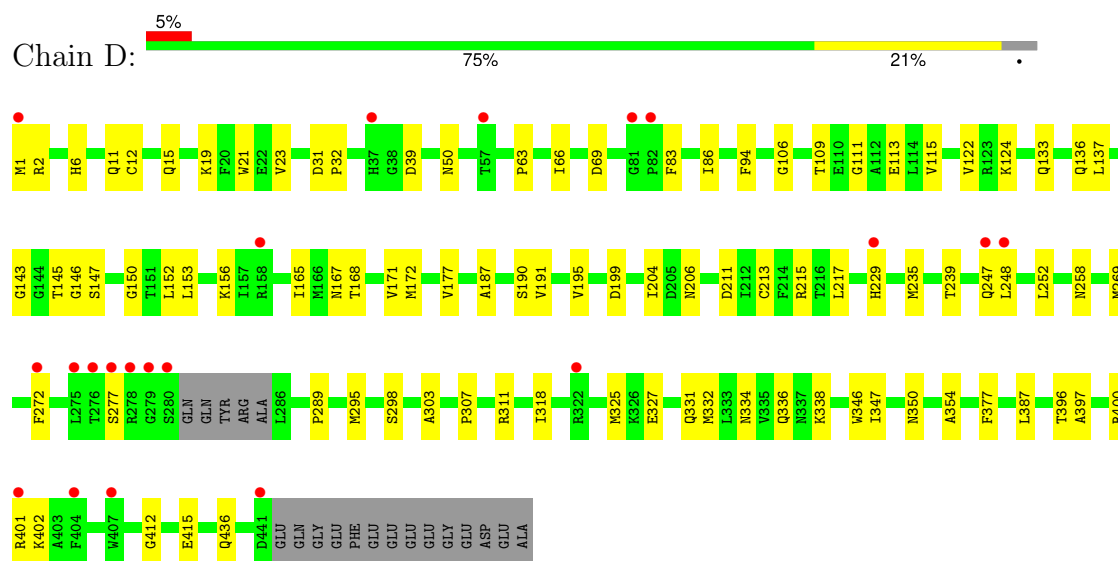


- Molecule 2: Tubulin beta-2B chain

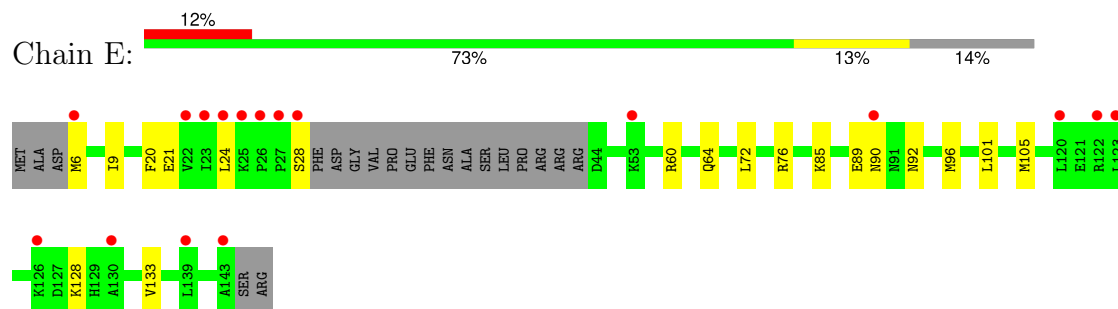




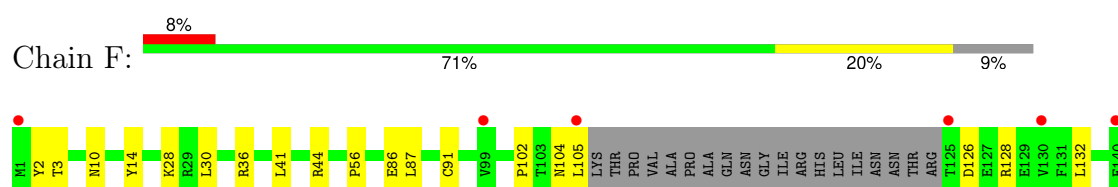
• Molecule 2: Tubulin beta-2B chain

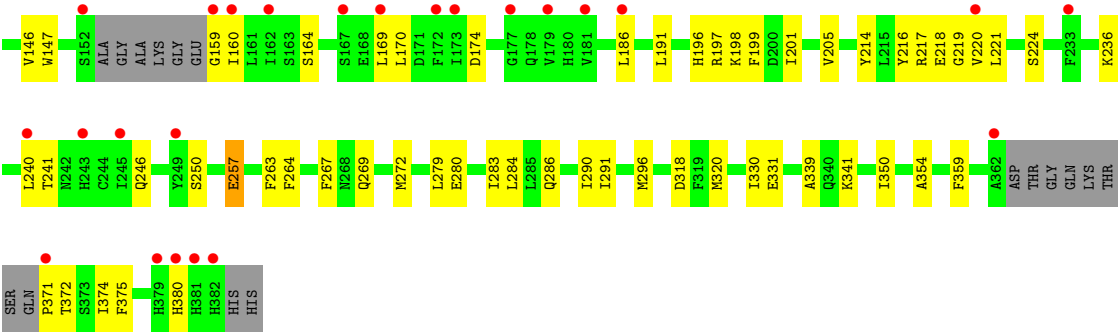


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.64Å 158.15Å 180.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.68 – 2.30 62.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.68-2.30) 99.9 (62.68-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.236 0.211 , 0.238	Depositor DCC
R_{free} test set	6697 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18082	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, WZP, CA, 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	0.12	0/3502	0.28	0/4754
1	C	0.13	0/3521	0.31	0/4780
2	B	0.12	0/3422	0.28	0/4633
2	D	0.11	0/3416	0.27	0/4626
3	E	0.12	0/1022	0.24	0/1356
4	F	0.09	0/2930	0.26	0/3959
All	All	0.12	0/17813	0.28	0/24108

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	71	0
1	C	3443	0	3352	64	0
2	B	3348	0	3223	75	0
2	D	3343	0	3222	66	0
3	E	1014	0	1029	14	0
4	F	2863	0	2826	58	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	B	14	22	0	0	0
9	D	14	22	0	1	0
10	F	31	0	14	4	0
11	A	73	0	0	2	1
11	B	88	0	0	2	0
11	C	198	0	0	3	1
11	D	32	0	0	2	0
11	E	12	0	0	0	0
11	F	12	0	0	0	0
All	All	18038	44	17048	330	1

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 10.

All (330) 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:102:PRO:HG2	4:F:105:LEU:HD13	1.47	0.97
1:A:381:THR:HG22	1:A:383:ALA:H	1.37	0.89
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.55	0.87
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.55	0.86
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.56	0.86
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.59	0.85
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.93	0.84
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.41	0.84
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.58	0.83
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.61	0.82
2:D:217:LEU:HA	2:D:277:SER:HB3	1.63	0.81
1:C:76:ASP:O	1:C:80:THR:HG22	1.84	0.76
4:F:241:THR:HG1	10:F:401:ACP:HO3'	1.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:331:GLU:OE2	10:F:401:ACP:O3G	2.06	0.73
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.71	0.73
4:F:241:THR:OG1	10:F:401:ACP:O3'	2.04	0.73
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.71
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.73	0.71
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.74	0.69
2:B:115:VAL:HG23	2:B:153:LEU:HD23	1.75	0.69
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.28	0.69
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.57	0.68
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.73	0.68
1:A:329:ASN:HB3	3:E:6:MET:HE3	1.76	0.68
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.09	0.67
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.74	0.67
1:C:270:ALA:O	1:C:302:MET:HG2	1.94	0.67
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.61	0.66
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.78	0.66
2:D:83:PHE:O	2:D:86:ILE:HG22	1.96	0.65
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.79	0.65
2:D:397:ALA:O	2:D:401:ARG:NH1	2.30	0.65
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.11	0.64
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.38	0.64
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.79	0.64
2:D:171:VAL:HA	2:D:204:ILE:O	1.98	0.63
4:F:371:PRO:HA	4:F:372:THR:C	2.23	0.63
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.32	0.62
1:A:179:THR:HA	2:B:352:LYS:HD2	1.82	0.62
2:D:152:LEU:O	2:D:156:LYS:HG2	1.99	0.61
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.14	0.61
2:B:147:SER:HG	2:B:190:SER:HG	1.46	0.61
1:A:178:SER:OG	1:A:183:GLU:OE1	2.12	0.61
2:B:69:ASP:O	2:B:94:PHE:HA	2.00	0.61
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.24	0.61
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.82	0.61
4:F:318:ASP:OD2	10:F:401:ACP:O2G	2.19	0.61
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.83	0.61
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.28	0.61
2:D:147:SER:HB2	2:D:190:SER:OG	2.01	0.61
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.82	0.61
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.16	0.60
2:D:191:VAL:O	2:D:195:VAL:HG23	2.02	0.60
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLU:CD	1:A:284:GLU:H	2.10	0.60
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.84	0.59
1:C:419:SER:O	1:C:423:GLU:HG3	2.02	0.59
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.85	0.59
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.84	0.59
2:B:200:GLU:OE2	2:B:255:LEU:HG	2.03	0.58
4:F:159:GLY:C	4:F:160:ILE:HD12	2.28	0.58
1:A:28:HIS:O	1:A:36:MET:HE3	2.03	0.58
2:B:136:GLN:HA	2:B:167:ASN:O	2.02	0.58
2:B:108:TYR:OH	2:B:417:GLU:OE2	2.19	0.58
3:E:72:LEU:O	3:E:76:ARG:HG2	2.03	0.58
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.38	0.58
4:F:246:GLN:O	4:F:250:SER:HB3	2.02	0.58
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.19	0.58
1:C:271:THR:HG21	1:C:295:CYS:O	2.04	0.58
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.86	0.58
1:C:320:ARG:HA	1:C:356:ASN:O	2.03	0.58
2:B:115:VAL:HG23	2:B:153:LEU:CD2	2.33	0.58
1:C:209:ILE:HD11	1:C:302:MET:CE	2.33	0.58
2:B:231:VAL:O	2:B:235:MET:HG3	2.03	0.57
4:F:296:MET:SD	4:F:380:HIS:HB2	2.44	0.57
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.87	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.57
1:C:327:ASP:OD2	11:C:601:HOH:O	2.18	0.57
4:F:371:PRO:HA	4:F:372:THR:O	2.05	0.57
2:D:1:MET:CE	2:D:50:ASN:HB2	2.30	0.57
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.87	0.57
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.87	0.56
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.39	0.56
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.87	0.56
1:C:166:LYS:NZ	11:C:608:HOH:O	2.37	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.88	0.56
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.41	0.55
2:D:1:MET:HG3	2:D:50:ASN:CB	2.36	0.55
2:B:124:LYS:HD3	2:B:124:LYS:C	2.31	0.55
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.89	0.55
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.36	0.55
2:B:295:MET:CG	2:B:377:PHE:HB2	2.37	0.55
2:D:124:LYS:C	2:D:124:LYS:HD3	2.32	0.55
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.89	0.55
1:C:165:SER:HA	1:C:199:ASP:OD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.42	0.54
1:A:69:ASP:O	1:A:94:THR:HA	2.07	0.54
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.89	0.54
2:D:69:ASP:O	2:D:94:PHE:HA	2.07	0.54
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.54
3:E:92:ASN:O	3:E:96:MET:HG2	2.07	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.54
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.39	0.54
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.89	0.54
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.90	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.89	0.54
2:D:1:MET:HE2	2:D:50:ASN:CB	2.35	0.53
2:B:191:VAL:O	2:B:195:VAL:HG23	2.08	0.53
2:D:106:GLY:O	2:D:111:GLY:HA3	2.08	0.53
2:D:412:GLY:C	3:E:133:VAL:HG13	2.34	0.53
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.89	0.53
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.44	0.53
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.40	0.53
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.90	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.53
2:D:187:ALA:O	2:D:191:VAL:HG23	2.08	0.53
1:A:229:ARG:HD2	11:A:601:HOH:O	2.09	0.53
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.44	0.53
4:F:198:LYS:HG2	4:F:199:PHE:H	1.73	0.53
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.24	0.53
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.09	0.53
2:B:46:LEU:HA	2:B:49:ILE:HB	1.90	0.53
2:B:157:ILE:CG2	2:B:166:MET:HE1	2.39	0.52
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.44	0.52
1:A:193:THR:HG23	11:A:627:HOH:O	2.09	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
4:F:3:THR:HB	4:F:30:LEU:HD11	1.92	0.52
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.09	0.52
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.45	0.52
1:A:132:LEU:O	1:A:164:LYS:NZ	2.43	0.51
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.91	0.51
2:D:11:GLN:O	2:D:15:GLN:HG2	2.10	0.51
1:A:329:ASN:HB3	3:E:6:MET:CE	2.39	0.51
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.93	0.51
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.51
2:D:332:MET:O	2:D:336:GLN:HG3	2.11	0.51
2:B:83:PHE:O	2:B:86:ILE:HG22	2.11	0.51
2:D:146:GLY:O	2:D:150:GLY:HA3	2.11	0.51
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.94	0.50
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.35	0.50
4:F:269:GLN:HA	4:F:272:MET:HE2	1.93	0.50
2:B:42:LEU:H	2:B:42:LEU:HD12	1.77	0.50
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.50	0.50
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.92	0.50
2:B:138:THR:HG21	2:B:235:MET:HE1	1.94	0.50
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.93	0.50
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.76	0.50
4:F:350:ILE:O	4:F:354:ALA:HB3	2.12	0.50
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.46	0.50
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.11	0.50
1:C:75:ILE:HB	1:C:94:THR:CG2	2.42	0.50
1:A:141:PHE:HB3	1:A:187:SER:OG	2.11	0.50
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.94	0.49
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.94	0.49
1:A:180:ALA:HB3	1:A:183:GLU:HG3	1.94	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.11	0.49
2:B:387:LEU:C	2:B:387:LEU:HD23	2.37	0.49
4:F:371:PRO:HA	4:F:372:THR:HB	1.93	0.49
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.47	0.49
1:A:179:THR:HG21	2:B:248:LEU:HA	1.94	0.49
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.47	0.49
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.12	0.49
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.12	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.49
1:A:419:SER:O	1:A:423:GLU:HG3	2.13	0.49
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.47	0.49
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.43	0.49
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.95	0.49
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.12	0.49
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.43	0.48
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.48	0.48
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.43	0.48
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.29	0.48
4:F:286:GLN:O	4:F:290:ILE:HG13	2.14	0.48
1:A:231:ILE:O	1:A:235:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:320:MET:CG	4:F:330:ILE:HD11	2.44	0.48
1:C:163:LYS:HG3	3:E:90:ASN:OD1	2.13	0.48
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.96	0.48
2:B:382:THR:O	2:B:385:GLN:HG2	2.14	0.47
1:C:174:ALA:HB2	1:C:207:GLU:N	2.29	0.47
4:F:87:LEU:O	4:F:91:CYS:HB2	2.12	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.95	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.47
2:D:298:SER:HB3	2:D:307:PRO:HD2	1.97	0.47
2:B:415:GLU:HG3	11:B:658:HOH:O	2.14	0.47
1:C:75:ILE:HB	1:C:94:THR:HG21	1.97	0.47
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.95	0.47
2:B:141:LEU:HD12	2:B:172:MET:SD	2.55	0.47
2:B:187:ALA:O	2:B:191:VAL:HG23	2.15	0.47
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.97	0.46
2:D:211:ASP:O	2:D:215:ARG:HB2	2.15	0.46
1:A:75:ILE:HB	1:A:94:THR:HG21	1.97	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.46
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.81	0.46
1:C:362:VAL:HG22	1:C:370:LYS:HD3	1.98	0.46
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.50	0.46
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.30	0.46
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.80	0.46
1:C:132:LEU:HG	1:C:164:LYS:HD3	1.97	0.46
2:D:1:MET:CG	2:D:50:ASN:HB2	2.44	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.46
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.16	0.46
1:A:166:LYS:HE2	1:A:197:HIS:O	2.15	0.46
3:E:9:ILE:HG13	3:E:21:GLU:HB3	1.98	0.46
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.56	0.46
1:C:234:ILE:HG12	1:C:302:MET:CE	2.45	0.46
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.51	0.46
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.15	0.46
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.51	0.46
4:F:3:THR:HA	4:F:28:LYS:O	2.15	0.46
2:B:7:ILE:O	2:B:137:LEU:HA	2.16	0.45
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.97	0.45
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.97	0.45
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.98	0.45
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.51	0.45
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.82	0.45
2:D:19:LYS:HE3	11:D:632:HOH:O	2.15	0.45
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.47	0.45
4:F:197:ARG:HB2	4:F:224:SER:O	2.16	0.45
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.39	0.45
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.45
1:C:117:LEU:HD11	1:C:121:ARG:CZ	2.46	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.45
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.97	0.45
1:C:298:PRO:HG2	1:C:308:ARG:CZ	2.46	0.45
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.51	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.52	0.45
4:F:371:PRO:N	4:F:372:THR:HB	2.31	0.45
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.47	0.45
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.38	0.45
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.99	0.45
2:D:311:ARG:NH1	2:D:436:GLN:O	2.49	0.45
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.51	0.44
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.52	0.44
2:D:289:PRO:HD3	2:D:327:GLU:OE2	2.16	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.44
2:B:248:LEU:CB	2:B:354:ALA:HB2	2.48	0.44
4:F:198:LYS:O	4:F:199:PHE:HB3	2.16	0.44
1:C:234:ILE:HD12	1:C:234:ILE:N	2.33	0.44
2:D:272:PHE:HE2	11:D:631:HOH:O	2.00	0.44
2:D:19:LYS:O	2:D:23:VAL:HG23	2.18	0.44
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.98	0.44
1:A:151:SER:HB2	1:A:193:THR:OG1	2.18	0.44
1:C:270:ALA:C	1:C:302:MET:HG2	2.43	0.44
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.47	0.44
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.00	0.44
1:A:433:GLU:HG3	1:A:437:VAL:HG21	2.00	0.43
2:B:115:VAL:HG21	2:B:156:LYS:HD2	2.00	0.43
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.18	0.43
1:A:227:LEU:O	1:A:231:ILE:HG13	2.18	0.43
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.99	0.43
2:B:205:ASP:OD1	2:B:207:GLU:N	2.50	0.43
2:D:327:GLU:O	2:D:331:GLN:HG2	2.17	0.43
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.53	0.43
3:E:101:LEU:O	3:E:105:MET:HG2	2.18	0.43
1:C:180:ALA:O	1:C:183:GLU:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:160:ILE:HD12	4:F:160:ILE:N	2.33	0.43
1:A:7:ILE:HG21	1:A:153:LEU:HD21	2.00	0.43
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.54	0.43
2:B:318:ILE:N	2:B:318:ILE:HD12	2.33	0.43
2:B:169:PHE:CD1	2:B:235:MET:HE3	2.54	0.43
2:B:295:MET:HE2	2:B:295:MET:HB3	1.91	0.43
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.49	0.43
4:F:240:LEU:HD12	4:F:240:LEU:N	2.34	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.34	0.43
1:A:2:ARG:HB3	1:A:131:GLY:O	2.19	0.43
1:A:75:ILE:HB	1:A:94:THR:CG2	2.48	0.43
2:B:276:THR:HG21	2:B:282:GLN:HA	2.01	0.43
2:B:392:SER:HB2	2:B:425:MET:HE3	2.01	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.54	0.43
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.55	0.42
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.00	0.42
4:F:86:GLU:CD	4:F:86:GLU:H	2.27	0.42
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.19	0.42
2:B:96:GLN:CB	1:C:1:MET:HE2	2.48	0.42
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.83	0.42
4:F:220:VAL:HG11	4:F:339:ALA:HB2	2.00	0.42
1:A:176:GLN:HG3	4:F:56:PRO:CG	2.49	0.42
1:A:387:ALA:HA	1:A:390:ARG:HD3	2.01	0.42
2:B:115:VAL:HG12	11:B:601:HOH:O	2.20	0.42
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.20	0.42
1:C:66:VAL:HG12	1:C:68:VAL:HG23	2.02	0.42
1:C:212:ILE:CG2	1:C:275:VAL:HG11	2.49	0.42
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.50	0.42
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.02	0.42
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.50	0.42
2:D:109:THR:O	2:D:113:GLU:HG2	2.20	0.42
3:E:60:ARG:O	3:E:64:GLN:HG3	2.20	0.42
1:C:196:GLU:HG2	11:C:656:HOH:O	2.20	0.42
2:B:251:ASP:OD1	2:B:252:LEU:N	2.52	0.41
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.55	0.41
2:D:199:ASP:OD1	9:D:503:WZP:N2	2.53	0.41
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.20	0.41
4:F:341:LYS:HG2	4:F:341:LYS:O	2.20	0.41
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.02	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.41
2:B:208:ALA:HB2	2:B:304:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.54	0.41
1:C:108:TYR:O	1:C:112:LYS:HG2	2.21	0.41
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.03	0.41
2:B:325:MET:HE2	2:B:355:VAL:HG21	2.02	0.41
2:D:295:MET:HE3	2:D:295:MET:HB2	1.92	0.41
1:A:119:LEU:HD12	1:A:156:ARG:NH2	2.36	0.41
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.50	0.41
1:C:205:ASP:CB	1:C:303:VAL:HA	2.51	0.41
2:D:145:THR:HB	8:D:501:GDP:O2B	2.21	0.41
2:D:396:THR:O	2:D:400:ARG:HG2	2.21	0.41
1:C:69:ASP:O	1:C:94:THR:HA	2.20	0.41
1:C:234:ILE:HD12	1:C:234:ILE:H	1.85	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.03	0.41
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.21	0.41
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.21	0.41
2:D:235:MET:O	2:D:239:THR:HG23	2.21	0.40
1:A:191:THR:O	1:A:195:LEU:HB2	2.22	0.40
1:C:68:VAL:HG11	1:C:118:VAL:HG21	2.03	0.40
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.56	0.40
4:F:269:GLN:HA	4:F:272:MET:CE	2.51	0.40
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.56	0.40
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.51	0.40
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.57	0.40
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.03	0.40
2:B:35:SER:HG	2:B:60:LYS:HZ3	1.58	0.40
2:D:115:VAL:CG2	2:D:153:LEU:HD23	2.51	0.40
1:A:71:GLU:HG2	1:A:72:PRO:N	2.34	0.40
2:B:19:LYS:HB3	2:B:232:SER:OG	2.20	0.40
2:D:66:ILE:CD1	2:D:122:VAL:HG22	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:668:HOH:O	11:C:718:HOH:O[3_555]	1.96	0.24

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	436/451 (97%)	425 (98%)	11 (2%)	0	100	100
1	C	439/451 (97%)	428 (98%)	11 (2%)	0	100	100
2	B	421/445 (95%)	408 (97%)	13 (3%)	0	100	100
2	D	422/445 (95%)	413 (98%)	9 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	341/384 (89%)	330 (97%)	10 (3%)	1 (0%)	36	46
All	All	2178/2319 (94%)	2122 (97%)	55 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	186	LEU

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	369/379 (97%)	367 (100%)	2 (0%)	81	90
1	C	372/379 (98%)	371 (100%)	1 (0%)	86	93
2	B	367/383 (96%)	367 (100%)	0	100	100
2	D	368/383 (96%)	365 (99%)	3 (1%)	73	86
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	84
4	F	315/342 (92%)	314 (100%)	1 (0%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1901/1993 (95%)	1893 (100%)	8 (0%)	84 92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	284	GLU
1	C	71	GLU
2	D	39	ASP
2	D	229	HIS
2	D	247	GLN
3	E	128	LYS
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
2	B	8	GLN
2	B	133	GLN
2	B	136	GLN
2	B	193	GLN
2	B	349	ASN
2	B	434	GLN
1	C	283	HIS
1	C	300	ASN
1	C	393	HIS
2	D	336	GLN
2	D	349	ASN
3	E	136	ASN
4	F	229	ASN
4	F	333	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 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
10	ACP	F	401	6	31,33,33	1.71	9 (29%)	47,52,52	1.89	10 (21%)
9	WZP	B	504	-	14,14,14	0.27	0	18,19,19	0.88	1 (5%)
8	GDP	B	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.69	6 (13%)
8	GDP	D	501	6	29,30,30	1.16	3 (10%)	45,47,47	1.71	6 (13%)
9	WZP	D	503	-	14,14,14	0.26	0	18,19,19	0.96	1 (5%)
5	GTP	C	501	6	33,34,34	0.98	3 (9%)	50,54,54	1.53	8 (16%)
5	GTP	A	501	6	33,34,34	1.04	3 (9%)	50,54,54	1.51	8 (16%)

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
10	ACP	F	401	6	-	11/19/38/38	0/3/3/3
9	WZP	B	504	-	-	0/12/22/22	0/1/1/1
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
8	GDP	D	501	6	-	4/16/32/32	0/3/3/3
9	WZP	D	503	-	-	4/12/22/22	0/1/1/1
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	ACP	C5-C4	4.78	1.47	1.39
8	B	501	GDP	C5-C4	3.11	1.47	1.38
8	D	501	GDP	C5-C4	3.10	1.47	1.38
10	F	401	ACP	PG-O2G	3.08	1.61	1.55
10	F	401	ACP	PG-O3G	3.04	1.61	1.55
10	F	401	ACP	PB-O3A	2.93	1.61	1.58
10	F	401	ACP	C5-C6	2.75	1.48	1.41
5	A	501	GTP	PA-O3A	2.57	1.62	1.59
8	B	501	GDP	C6-N1	-2.43	1.34	1.38
5	A	501	GTP	PB-O3B	2.39	1.62	1.59
8	D	501	GDP	C6-N1	-2.39	1.34	1.38
10	F	401	ACP	C8-N7	2.34	1.36	1.31
5	C	501	GTP	PB-O3B	2.28	1.62	1.59
10	F	401	ACP	PA-O3A	2.24	1.61	1.59
10	F	401	ACP	PB-O2B	2.20	1.61	1.56
10	F	401	ACP	C5-N7	-2.19	1.35	1.39
5	C	501	GTP	PA-O3A	2.14	1.61	1.59
5	C	501	GTP	C2-N3	2.11	1.38	1.33
8	D	501	GDP	C5-N7	-2.07	1.34	1.39
8	B	501	GDP	C5-N7	-2.06	1.34	1.39
5	A	501	GTP	C2-N3	2.05	1.38	1.33

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-5.92	118.96	128.39
10	F	401	ACP	C5-C4-N3	-5.87	118.64	126.72
8	B	501	GDP	C5-C4-N3	-5.80	119.16	128.39
8	B	501	GDP	C2-N3-C4	5.02	120.94	112.30
8	D	501	GDP	C2-N3-C4	4.97	120.86	112.30
5	C	501	GTP	C5-C4-N3	-4.89	120.61	128.39
5	A	501	GTP	C5-C4-N3	-4.70	120.91	128.39
10	F	401	ACP	N3-C4-N9	4.65	135.07	127.17
5	A	501	GTP	C2-N3-C4	4.50	120.04	112.30
5	C	501	GTP	C2-N3-C4	4.38	119.84	112.30
8	D	501	GDP	N9-C4-N3	4.33	134.61	125.95
8	B	501	GDP	N9-C4-N3	4.20	134.35	125.95
10	F	401	ACP	PB-O3A-PA	-3.92	119.57	132.37
10	F	401	ACP	C2-N3-C4	3.68	120.81	111.83
10	F	401	ACP	C4-C5-N7	-3.48	106.60	110.58
8	B	501	GDP	C6-C5-N7	3.46	136.58	130.29
8	D	501	GDP	C6-C5-N7	3.32	136.32	130.29
10	F	401	ACP	N3-C2-N1	-3.17	123.78	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N9-C4-N3	2.99	131.94	125.95
5	A	501	GTP	N9-C4-N3	2.96	131.87	125.95
9	D	503	WZP	C1-N2-C5	-2.95	108.30	113.01
5	C	501	GTP	C2-N1-C6	-2.83	119.98	125.11
5	A	501	GTP	C2-N1-C6	-2.79	120.05	125.11
9	B	504	WZP	C1-N2-C5	-2.74	108.63	113.01
5	C	501	GTP	N9-C8-N7	-2.69	108.41	113.40
5	C	501	GTP	C8-N7-C5	2.67	109.01	104.26
5	A	501	GTP	N9-C8-N7	-2.64	108.51	113.40
10	F	401	ACP	C4-N9-C8	2.59	108.46	105.74
10	F	401	ACP	C3'-C2'-C1'	2.57	106.32	101.46
8	D	501	GDP	C4-C5-N7	-2.56	106.62	110.67
8	B	501	GDP	C4-C5-N7	-2.52	106.68	110.67
10	F	401	ACP	C5-N7-C8	2.51	107.40	103.45
5	A	501	GTP	O6-C6-C5	-2.46	120.03	126.53
5	A	501	GTP	C5-C6-N1	2.42	119.41	113.25
5	A	501	GTP	C8-N7-C5	2.41	108.55	104.26
5	C	501	GTP	C5-C6-N1	2.28	119.05	113.25
8	B	501	GDP	O6-C6-C5	-2.10	120.99	126.53
5	C	501	GTP	O6-C6-C5	-2.09	121.00	126.53
8	D	501	GDP	O6-C6-C5	-2.09	121.02	126.53
10	F	401	ACP	C6-C5-N7	2.01	135.96	132.09

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
10	F	401	ACP	PG-C3B-PB-O1B
10	F	401	ACP	PG-C3B-PB-O2B
10	F	401	ACP	PG-C3B-PB-O3A

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Mol	Chain	Res	Type	Atoms
10	F	401	ACP	C5'-O5'-PA-O1A
10	F	401	ACP	C5'-O5'-PA-O2A
10	F	401	ACP	C5'-O5'-PA-O3A
10	F	401	ACP	C3'-C4'-C5'-O5'
10	F	401	ACP	O4'-C4'-C5'-O5'
10	F	401	ACP	PB-C3B-PG-O2G
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
9	D	503	WZP	O1-C8-C9-C11
9	D	503	WZP	O1-C8-C9-C10
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
5	C	501	GTP	C4'-C5'-O5'-PA
10	F	401	ACP	PB-C3B-PG-O1G
10	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
9	D	503	WZP	N1-C8-C9-C11
9	D	503	WZP	N1-C8-C9-C10
5	C	501	GTP	PB-O3A-PA-O1A

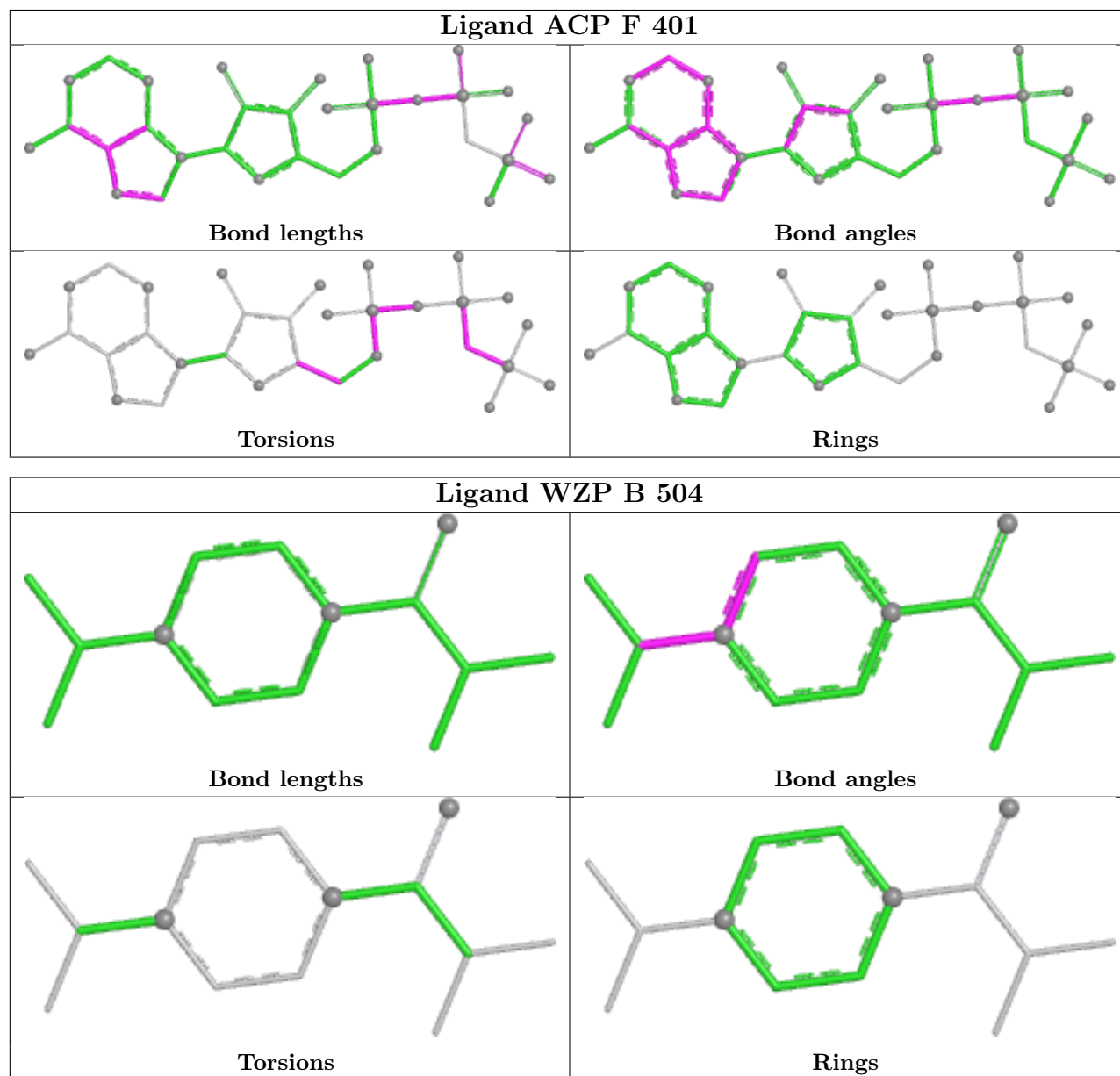
There are no ring outliers.

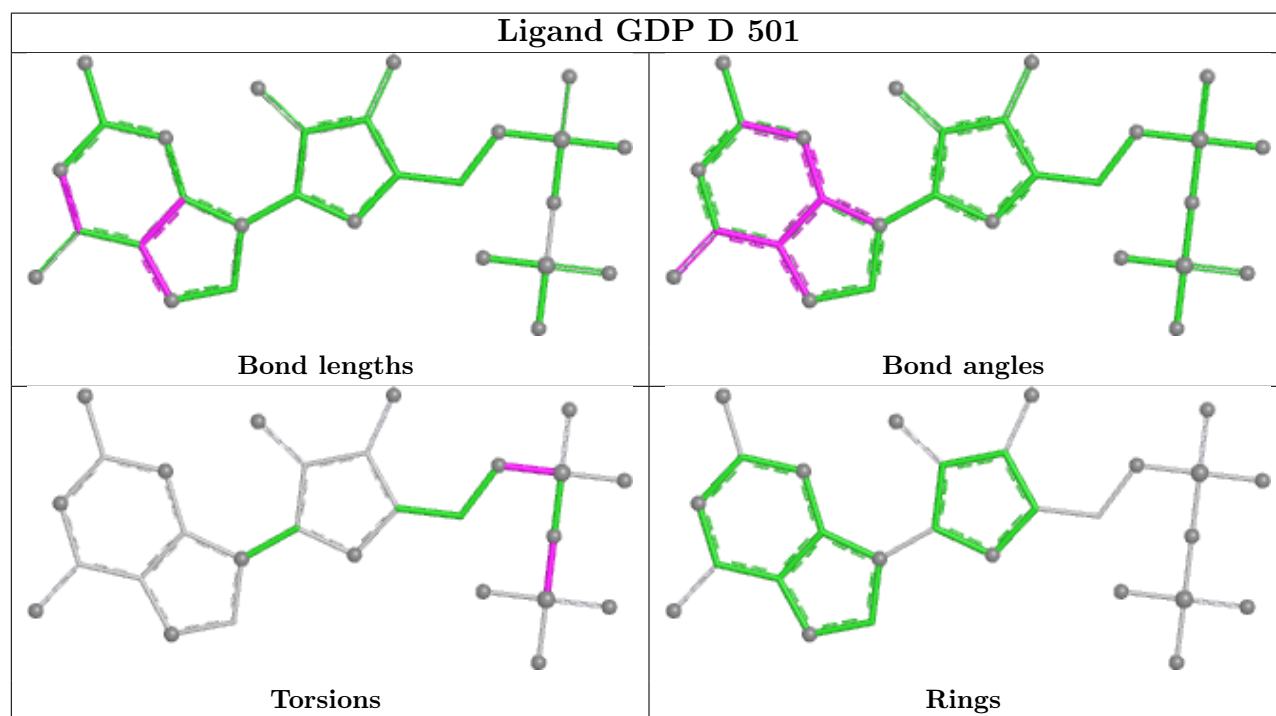
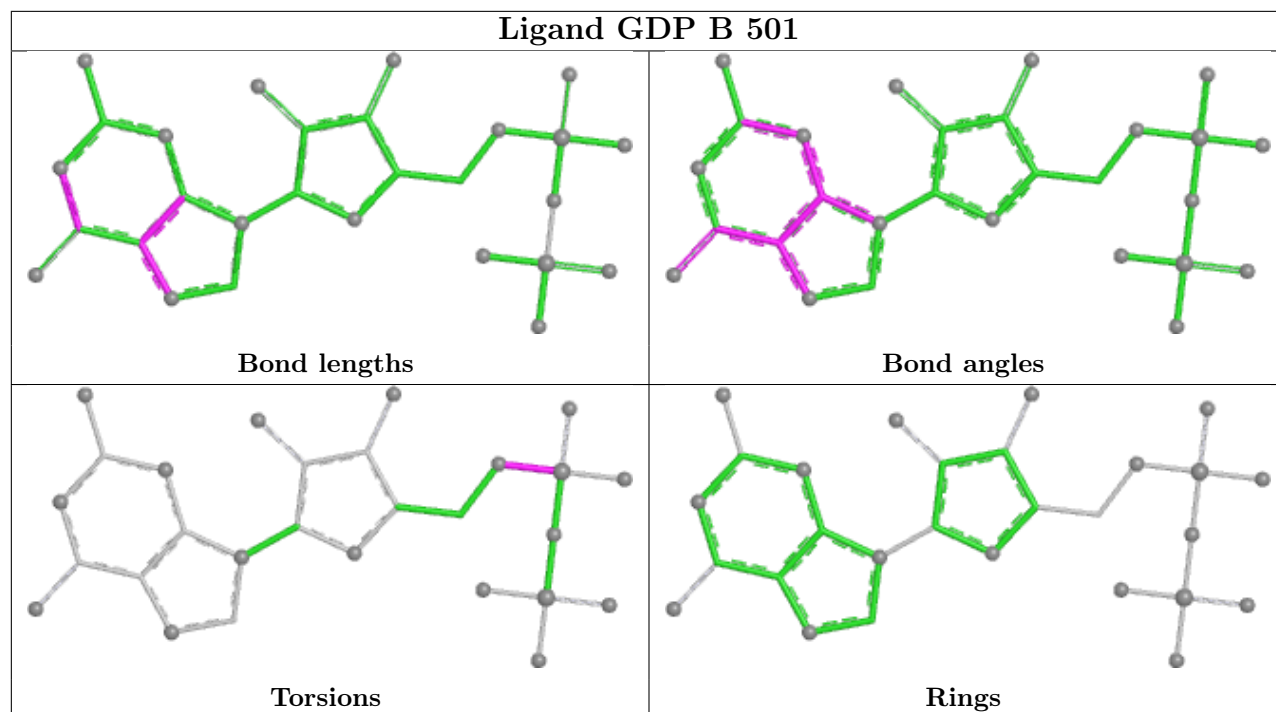
4 monomers are involved in 9 short contacts:

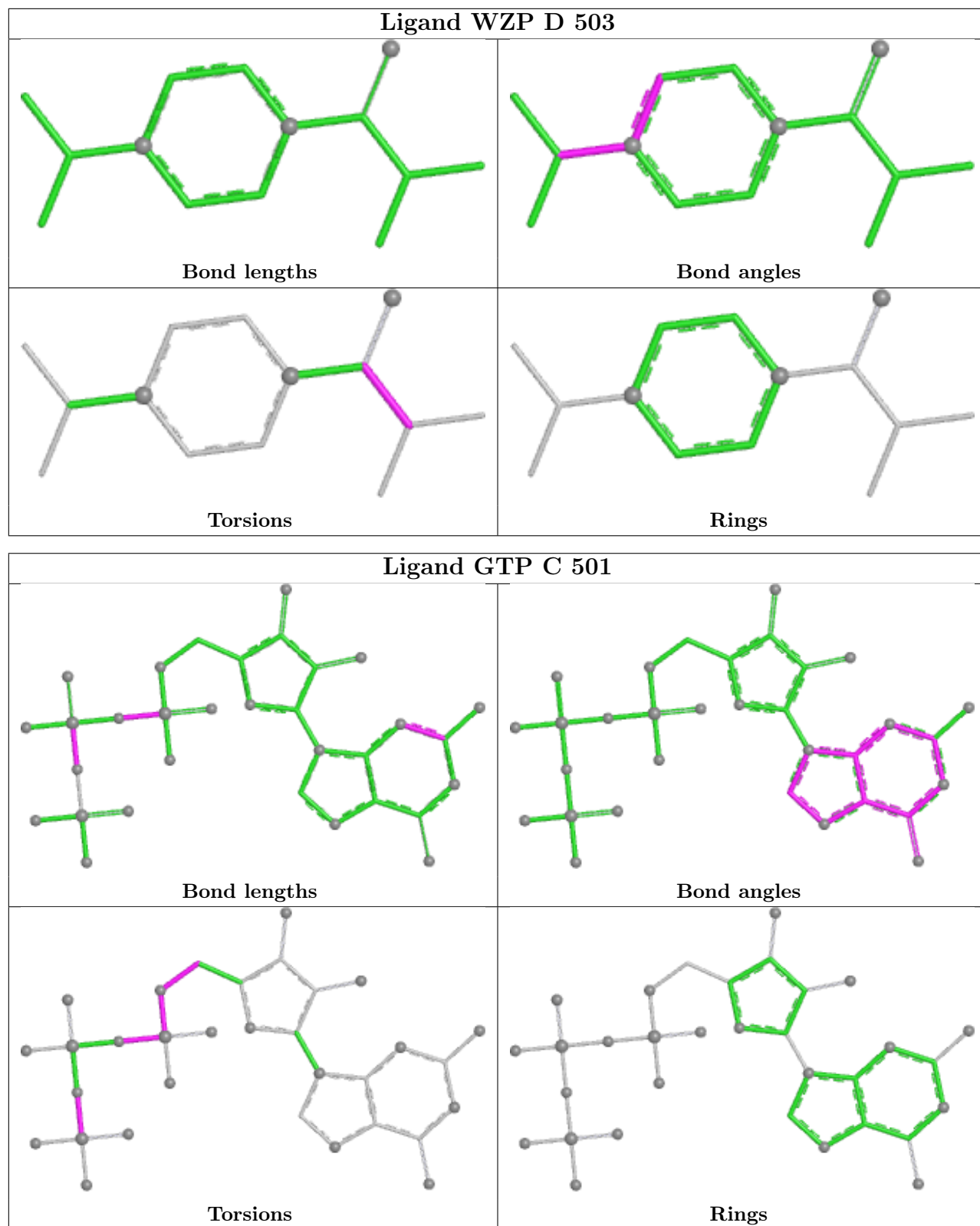
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	401	ACP	4	0
8	D	501	GDP	3	0
9	D	503	WZP	1	0
5	A	501	GTP	1	0

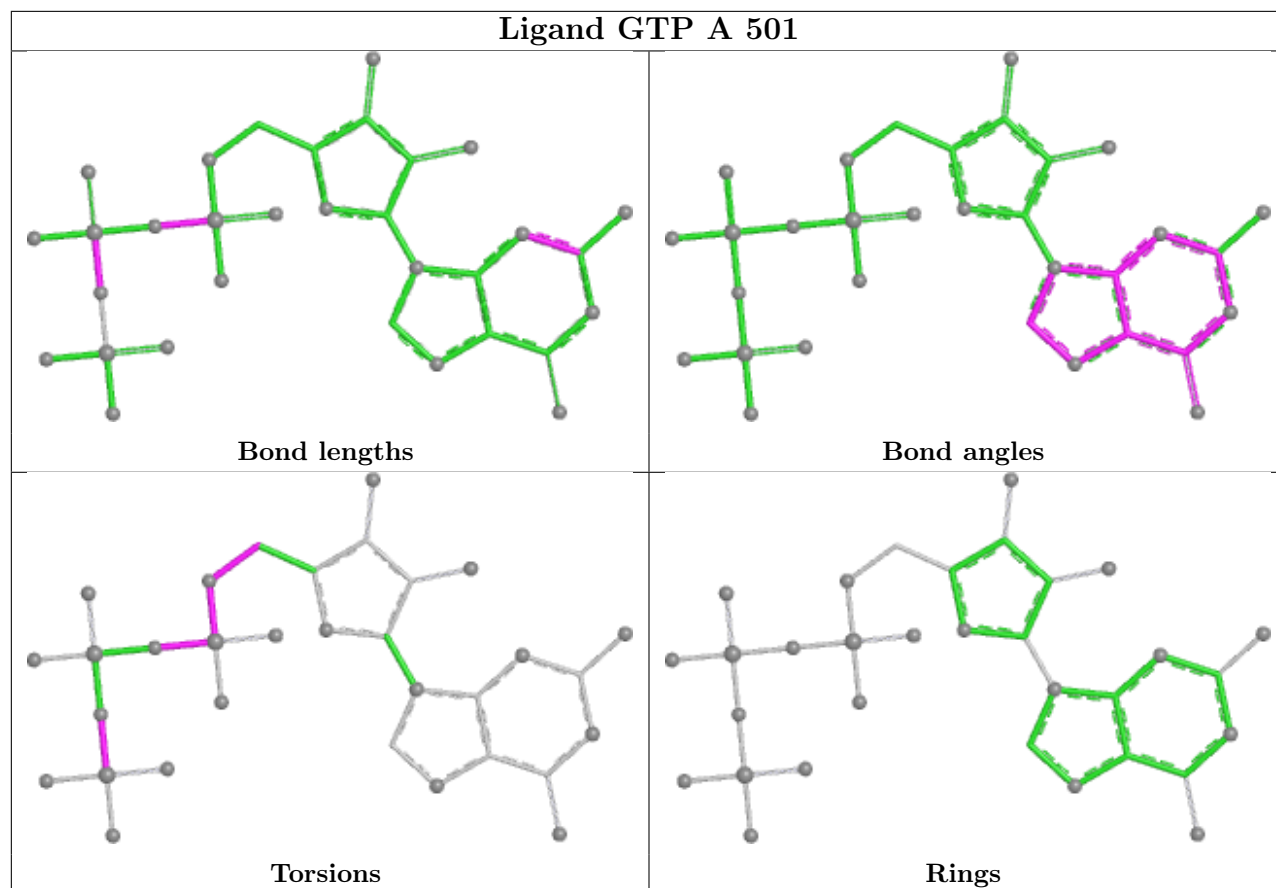
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.36	17 (3%)	43	45	44, 62, 100, 155	0
1	C	440/451 (97%)	0.10	16 (3%)	46	48	25, 50, 75, 118	1 (0%)
2	B	425/445 (95%)	0.39	24 (5%)	30	32	39, 59, 98, 157	1 (0%)
2	D	426/445 (95%)	0.51	21 (4%)	35	36	46, 68, 101, 142	4 (0%)
3	E	123/143 (86%)	0.96	17 (13%)	6	7	51, 69, 114, 147	0
4	F	349/384 (90%)	0.85	30 (8%)	16	17	57, 90, 155, 190	0
All	All	2201/2319 (94%)	0.45	125 (5%)	29	31	25, 64, 118, 190	6 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	248	LEU	6.8
2	B	249	ASN	6.5
3	E	24	LEU	5.1
3	E	143	ALA	5.0
4	F	159	GLY	4.7
1	A	179	THR	4.6
3	E	123	LEU	4.6
4	F	125	THR	4.4
1	C	440	VAL	4.4
4	F	381	HIS	4.4
4	F	371	PRO	4.2
4	F	152	SER	4.1
2	B	285	ALA	4.0
2	D	279	GLY	4.0
3	E	120	LEU	3.9
3	E	6	MET	3.5
2	B	275	LEU	3.5
2	B	1	MET	3.4
2	D	82	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	3.3
2	D	272	PHE	3.3
4	F	240	LEU	3.3
1	A	351	PHE	3.2
3	E	28	SER	3.1
4	F	362	ALA	3.1
2	D	404	PHE	3.1
2	B	250	ALA	3.1
1	A	282	TYR	3.1
4	F	160	ILE	3.0
4	F	105	LEU	3.0
1	A	88	HIS	3.0
3	E	139	LEU	3.0
3	E	122	ARG	3.0
3	E	26	PRO	3.0
2	B	276	THR	2.9
2	D	247	GLN	2.9
4	F	179	VAL	2.9
1	C	340	SER	2.8
4	F	382	HIS	2.8
1	A	438	ASP	2.8
1	C	286	LEU	2.8
1	A	437	VAL	2.8
2	D	276	THR	2.8
1	C	128	GLN	2.8
1	A	77	GLU	2.8
4	F	243	HIS	2.7
4	F	186	LEU	2.7
2	B	57	THR	2.7
3	E	126	LYS	2.7
4	F	167	SER	2.7
2	D	280	SER	2.7
2	D	407	TRP	2.7
4	F	379	HIS	2.6
2	B	82	PRO	2.6
4	F	245	ILE	2.6
2	D	229	HIS	2.6
2	B	251	ASP	2.6
2	B	284	ARG	2.6
2	B	333	LEU	2.6
1	C	163	LYS	2.6
1	C	341	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	247	GLN	2.6
1	A	262	TYR	2.5
2	B	278	ARG	2.5
1	A	284	GLU	2.4
1	C	80	THR	2.4
2	D	278	ARG	2.4
2	D	248	LEU	2.4
1	C	357	TYR	2.4
2	B	281	GLN	2.4
2	B	283	TYR	2.4
1	C	46	ASP	2.4
4	F	181	VAL	2.4
1	C	245	ASP	2.3
2	B	272	PHE	2.3
4	F	173	ILE	2.3
2	B	286	LEU	2.3
1	A	346	TRP	2.3
4	F	177	GLY	2.3
2	D	277	SER	2.3
4	F	162	ILE	2.3
2	B	2	ARG	2.3
1	A	281	ALA	2.3
3	E	23	ILE	2.3
3	E	53	LYS	2.3
1	C	177	VAL	2.3
4	F	99	VAL	2.3
4	F	172	PHE	2.2
2	D	275	LEU	2.2
2	D	441	ASP	2.2
1	A	316	CYS	2.2
4	F	380	HIS	2.2
1	A	42	ILE	2.2
4	F	233	PHE	2.2
1	C	2	ARG	2.2
1	C	363	VAL	2.2
3	E	22	VAL	2.2
2	D	1	MET	2.2
1	C	284	GLU	2.2
3	E	25	LYS	2.2
2	D	81	GLY	2.2
4	F	169	LEU	2.1
2	B	325	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	336	LYS	2.1
1	A	283	HIS	2.1
2	B	400	ARG	2.1
2	D	158	ARG	2.1
2	D	401	ARG	2.1
3	E	90	ASN	2.1
4	F	140	GLU	2.1
3	E	27	PRO	2.1
4	F	130	VAL	2.1
4	F	220	VAL	2.1
2	D	57	THR	2.1
1	C	1	MET	2.1
1	A	58	ALA	2.1
1	A	73	THR	2.0
4	F	1	MET	2.0
2	D	37	HIS	2.0
2	B	437	ASP	2.0
2	D	322	ARG	2.0
1	A	337	THR	2.0
2	B	340	SER	2.0
3	E	130	ALA	2.0
2	B	245	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.71	0.18	100,100,100,100	0

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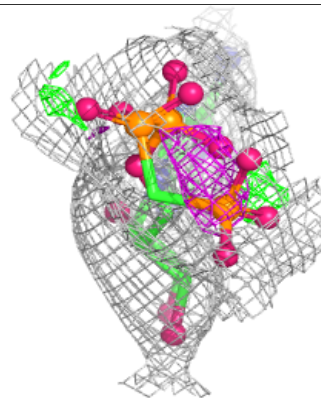
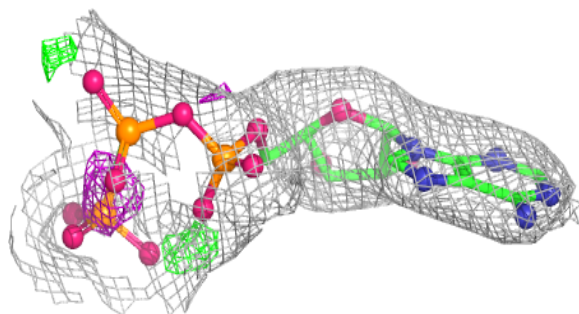
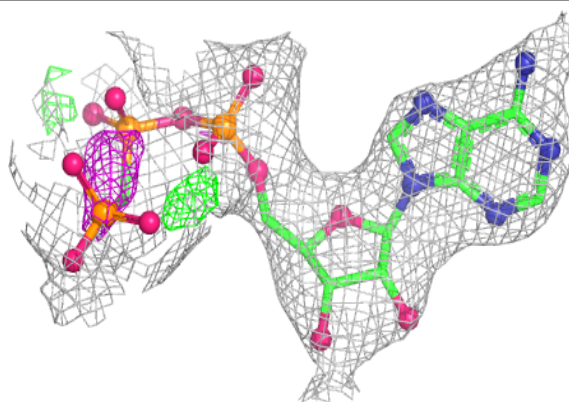
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	ACP	F	401	31/31	0.85	0.12	89,97,105,113	0
9	WZP	D	503	14/14	0.89	0.12	55,70,85,85	0
6	MG	D	502	1/1	0.89	0.09	61,61,61,61	0
8	GDP	D	501	28/28	0.91	0.11	59,65,77,81	0
6	MG	F	402	1/1	0.92	0.11	80,80,80,80	0
7	CA	A	504	1/1	0.93	0.07	90,90,90,90	0
7	CA	A	503	1/1	0.95	0.07	86,86,86,86	0
9	WZP	B	504	14/14	0.96	0.07	52,65,72,75	0
5	GTP	A	501	32/32	0.97	0.06	40,48,52,55	0
5	GTP	C	501	32/32	0.98	0.06	36,42,46,48	0
8	GDP	B	501	28/28	0.98	0.05	39,44,51,56	0
6	MG	B	502	1/1	0.98	0.06	36,36,36,36	0
7	CA	C	503	1/1	0.99	0.02	68,68,68,68	0
6	MG	C	502	1/1	0.99	0.06	43,43,43,43	0
6	MG	A	502	1/1	0.99	0.02	45,45,45,45	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.

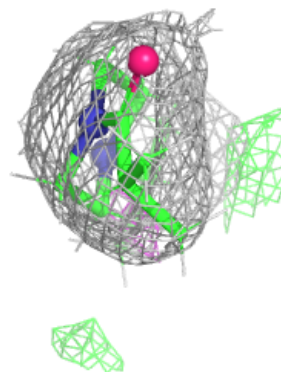
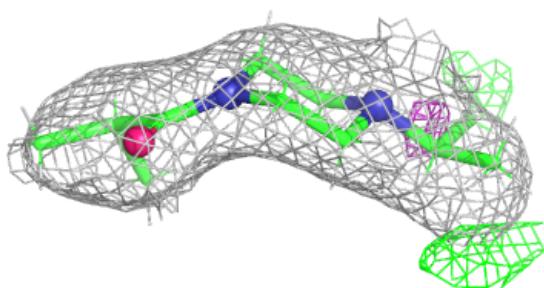
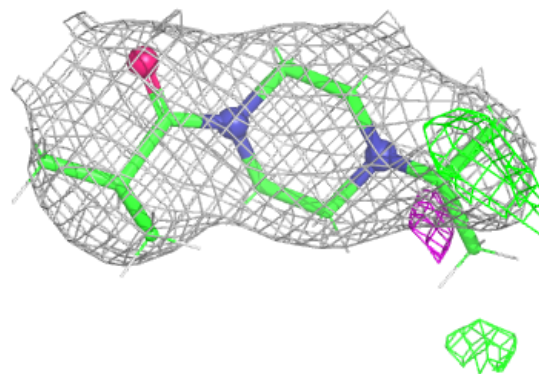
Electron density around ACP F 401:

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



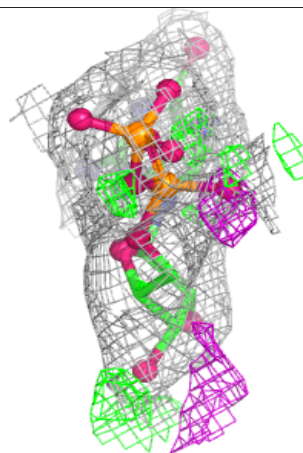
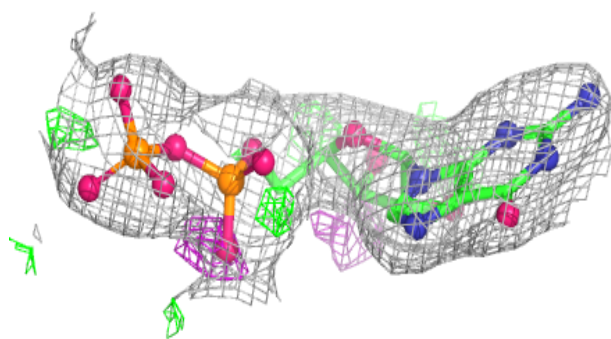
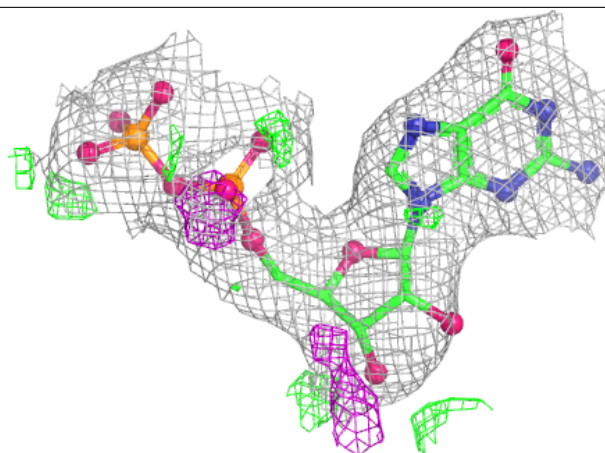
Electron density around WZP D 503:

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



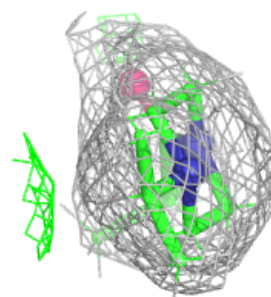
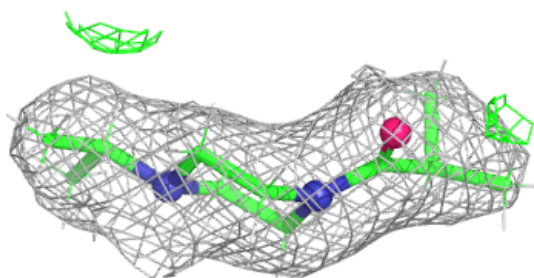
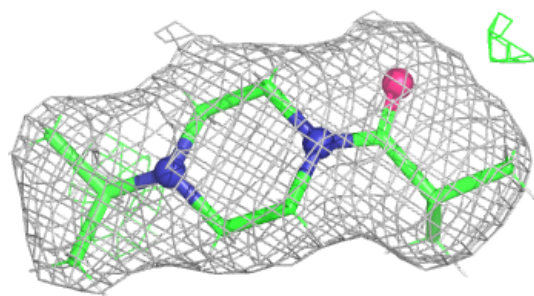
Electron density around GDP D 501:

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

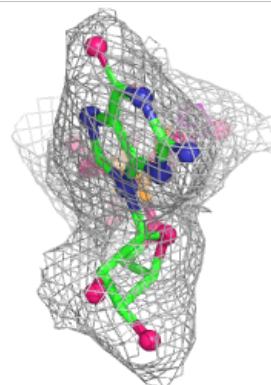
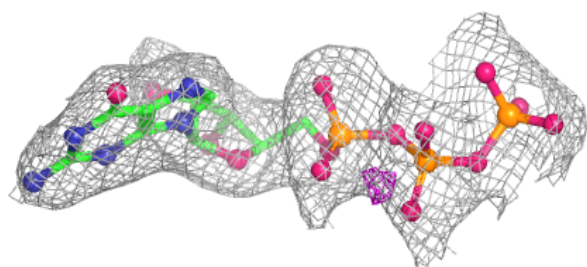
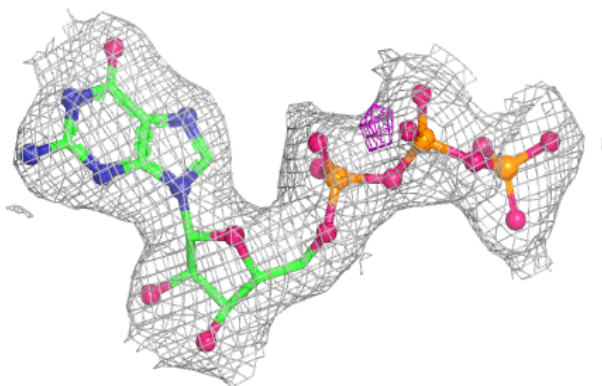


Electron density around WZP B 504:

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

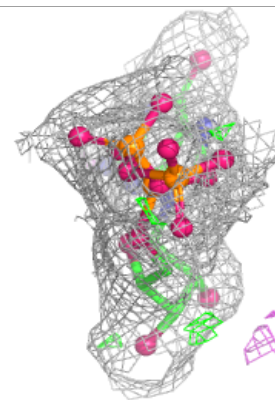
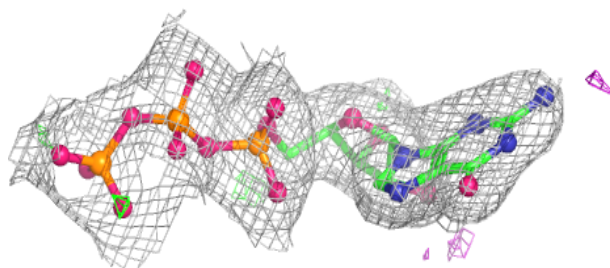
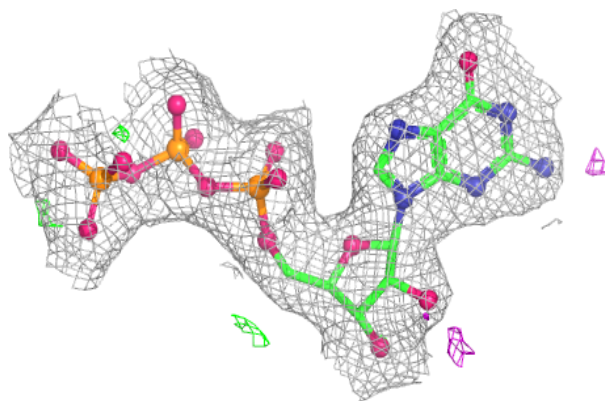
**Electron density around GTP A 501:**

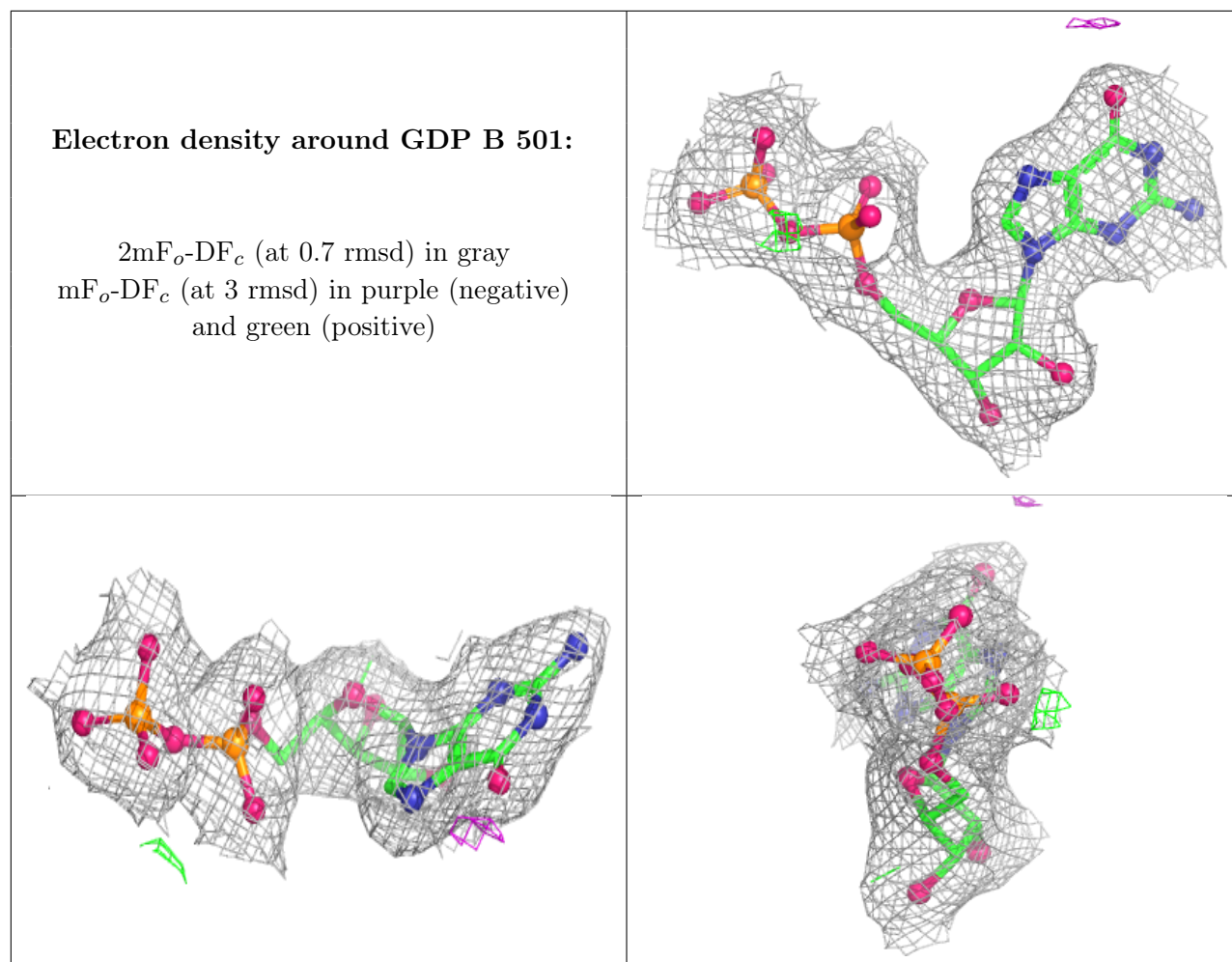
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.