



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:04 PM UTC

PDB ID : 5S5R / pdb_00005s5r
Title : Tubulin-Z33452106-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

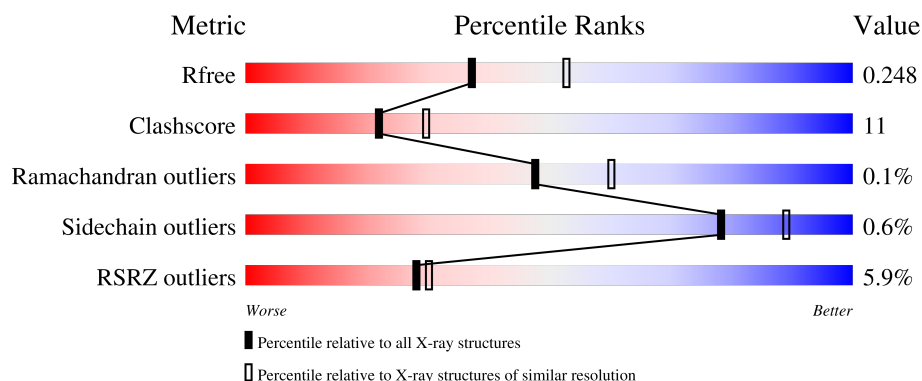
1 Overall quality at a glance

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	4% 78% 19% ••
1	C	451	4% 76% 22% •
2	B	445	4% 70% 25% •
2	D	445	8% 70% 27% •
3	E	143	6% 70% 16% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	8% 71% 21% 8%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18069 atoms, of which 13 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	2	0	0
			3348	2103	573	645	27			
2	D	431	Total	C	N	O	S	5	0	0
			3368	2113	575	653	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	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	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		

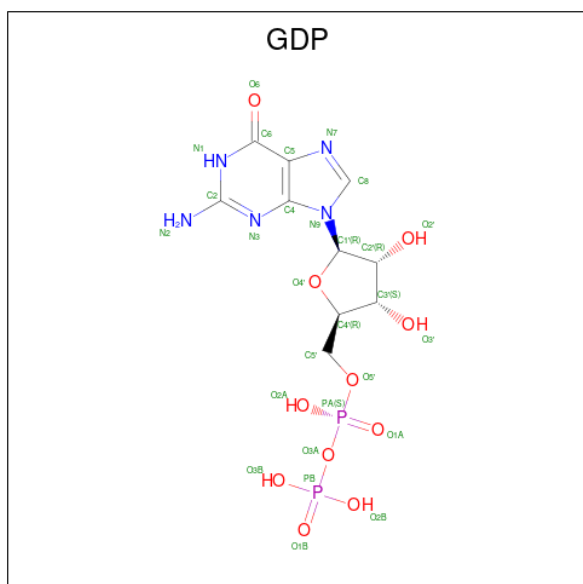
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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	D	2	Total	Mg	0	0
			2	2		
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).



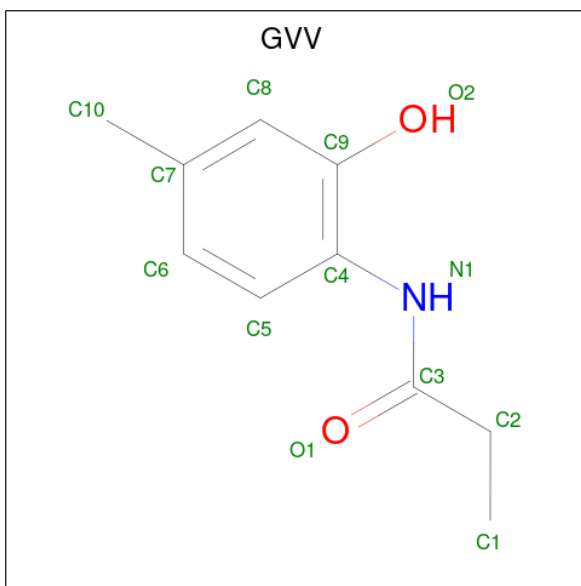
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
8	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



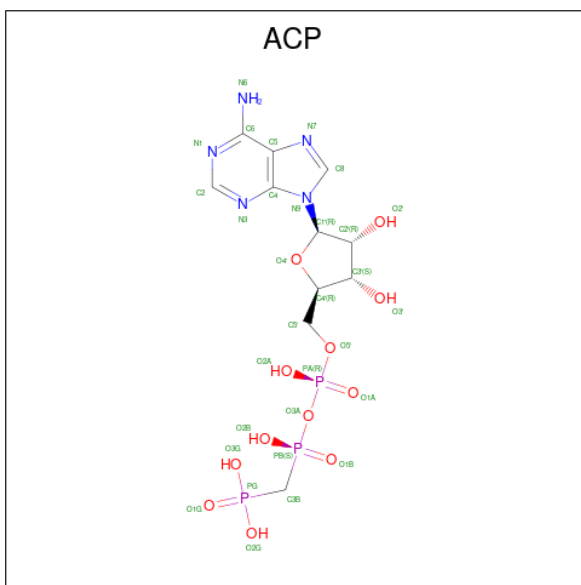
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is {N}-(4-methyl-2-oxidanyl-phenyl)propanamide (CCD ID: GVV) (formula: $C_{10}H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			26	10	13	1	2		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

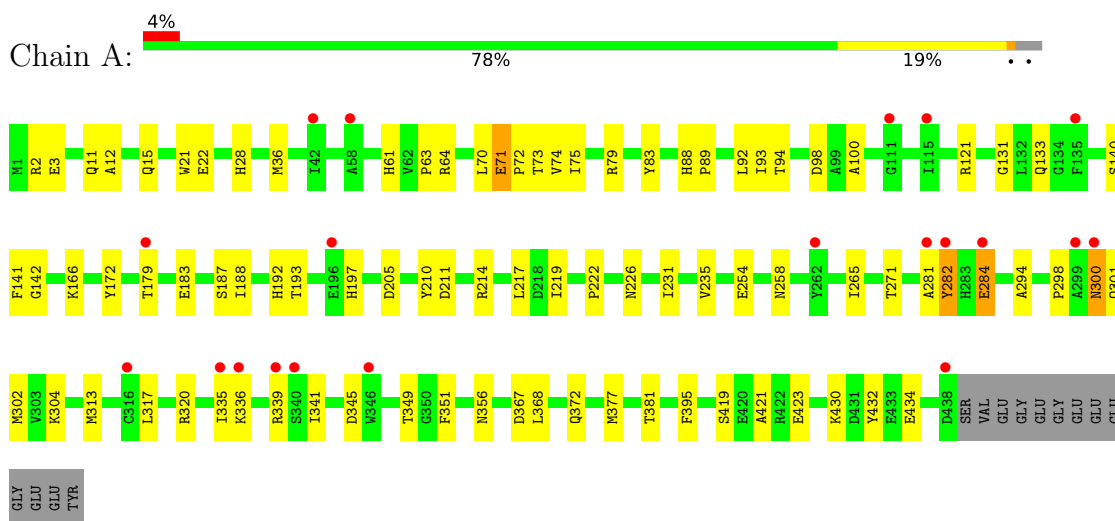
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	71	Total O 71 71	0	0
12	B	86	Total O 86 86	0	0
12	C	180	Total O 180 180	0	0
12	D	32	Total O 32 32	0	0
12	E	15	Total O 15 15	0	0
12	F	13	Total O 13 13	0	0

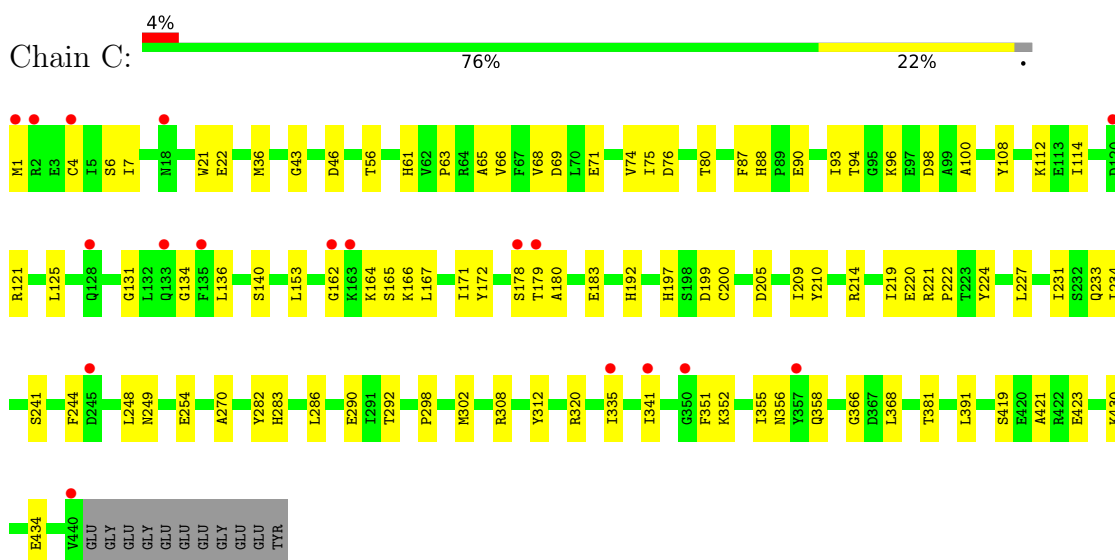
3 Residue-property plots [i](#)

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

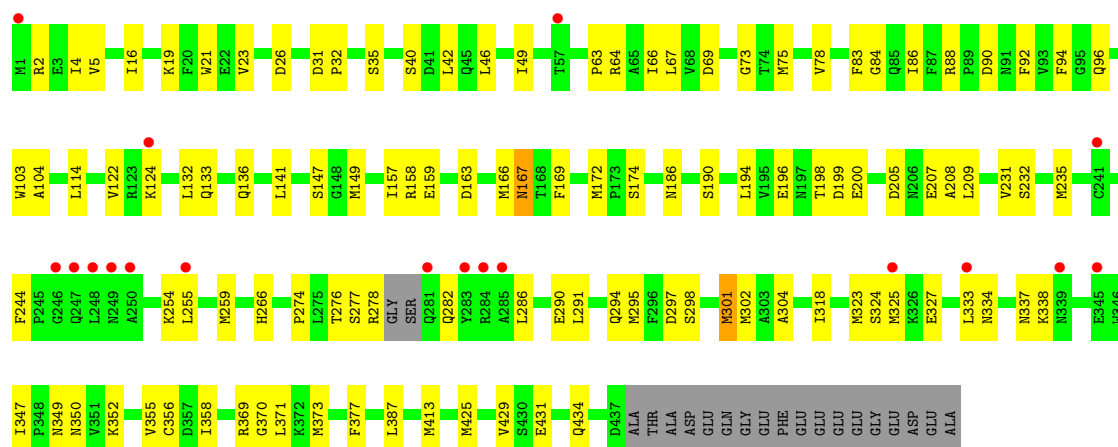


- Molecule 1: Tubulin alpha-1B chain

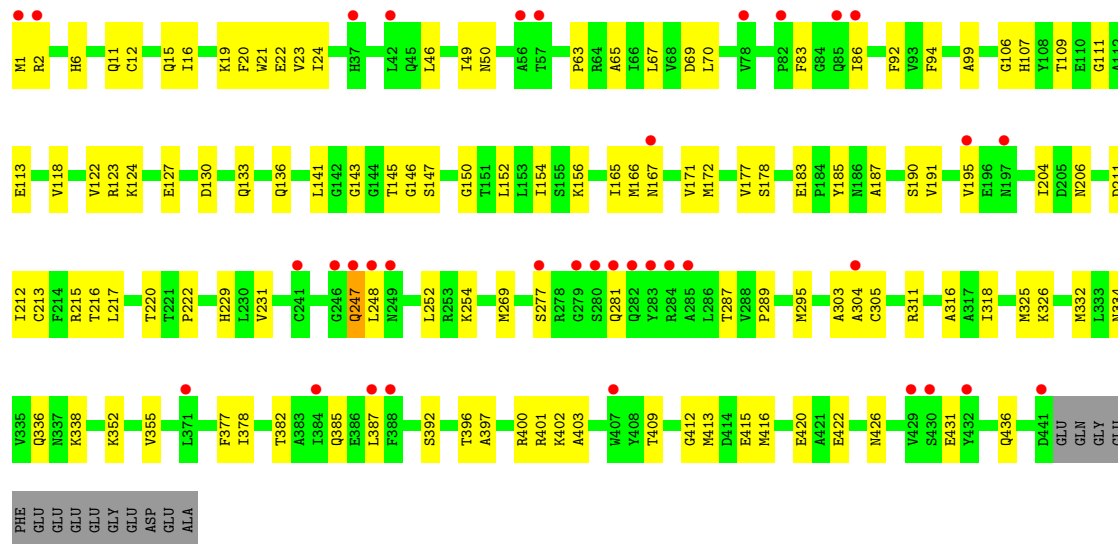


- Molecule 2: Tubulin beta-2B chain

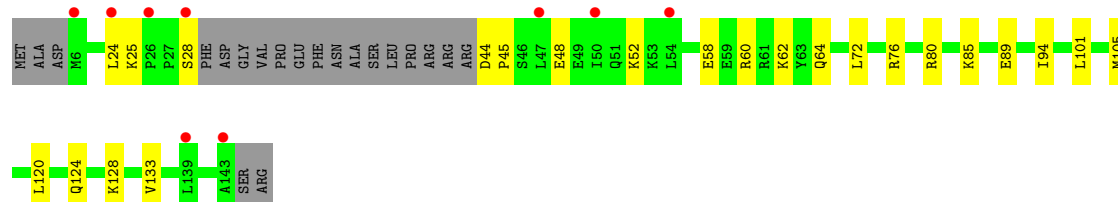




• Molecule 2: Tubulin beta-2B chain

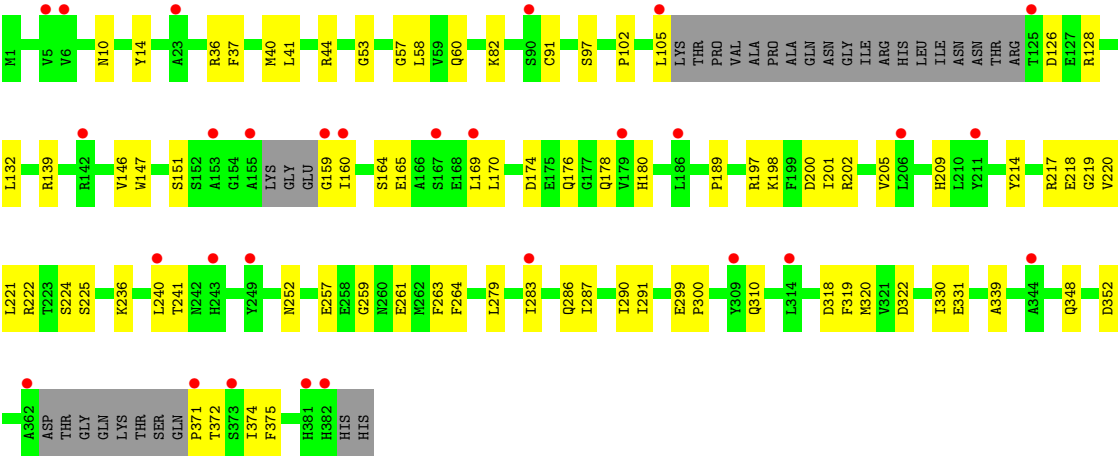


• Molecule 3: Stathmin-4



• 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	105.24Å 159.48Å 178.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.81 – 2.30 72.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (72.81-2.30) 99.4 (72.81-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.244 0.211 , 0.248	Depositor DCC
R_{free} test set	6575 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18069	wwPDB-VP
Average B, all atoms (Å ²)	81.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GVV, MES, CA, ACP, GDP, 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	0.11	0/3502	0.29	0/4754
1	C	0.13	0/3521	0.31	0/4780
2	B	0.12	0/3422	0.30	0/4633
2	D	0.10	0/3442	0.27	0/4664
3	E	0.11	0/1022	0.23	0/1356
4	F	0.09	0/2944	0.27	0/3978
All	All	0.11	0/17853	0.29	0/24165

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	64	0
1	C	3443	0	3352	74	1
2	B	3348	0	3223	84	0
2	D	3368	0	3236	87	0
3	E	1014	0	1029	19	1
4	F	2877	0	2839	60	0
5	A	32	0	12	2	0

Continued on next page...

Continued from previous page...

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	D	2	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	12	0	12	2	0
10	B	13	13	0	2	0
11	F	31	0	14	5	0
12	A	71	0	0	4	0
12	B	86	0	0	1	0
12	C	180	0	0	6	0
12	D	32	0	0	2	0
12	E	15	0	0	2	0
12	F	13	0	0	1	0
All	All	18056	13	17087	371	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 11.

All (371) 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)
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.45	0.98
2:D:217:LEU:HA	2:D:277:SER:HB3	1.50	0.91
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.57	0.84
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.96	0.83
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.00	0.79
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.64	0.79
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.45	0.79
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.65	0.79
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.65	0.78
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.66	0.76
4:F:91:CYS:HA	12:F:512:HOH:O	1.87	0.74
1:C:1:MET:O	12:C:601:HOH:O	2.04	0.74
1:C:76:ASP:O	1:C:80:THR:HG22	1.88	0.74
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:OD2	12:C:602:HOH:O	2.07	0.72
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.72
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.36	0.71
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.70	0.71
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.73	0.70
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.16	0.69
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.74	0.69
1:C:209:ILE:HD11	1:C:302:MET:CE	2.22	0.69
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.75	0.69
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.75	0.68
2:D:397:ALA:O	2:D:401:ARG:NH1	2.26	0.68
2:D:332:MET:O	2:D:336:GLN:HG3	1.94	0.67
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.93	0.67
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.24	0.67
1:A:179:THR:HA	2:B:352:LYS:HD2	1.77	0.67
2:D:83:PHE:O	2:D:86:ILE:HG22	1.93	0.67
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.77	0.66
3:E:44:ASP:OD2	12:E:201:HOH:O	2.13	0.66
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.79	0.65
1:C:178:SER:OG	2:D:352:LYS:NZ	2.29	0.65
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.32	0.65
4:F:371:PRO:HA	4:F:372:THR:C	2.20	0.65
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.79	0.65
3:E:85:LYS:NZ	12:E:202:HOH:O	2.30	0.65
1:C:270:ALA:O	1:C:302:MET:HG2	1.96	0.65
1:A:28:HIS:O	1:A:36:MET:HE3	1.96	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.77	0.65
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.97	0.65
2:B:83:PHE:O	2:B:86:ILE:HG22	1.98	0.64
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.62	0.64
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.80	0.64
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.79	0.64
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.32	0.63
1:C:320:ARG:HA	1:C:356:ASN:O	1.98	0.63
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.34	0.63
2:D:1:MET:CE	2:D:50:ASN:HB2	2.26	0.63
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.80	0.63
4:F:320:MET:CG	4:F:330:ILE:HD11	2.28	0.63
2:B:69:ASP:O	2:B:94:PHE:HA	1.99	0.62
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.81	0.62
2:D:392:SER:O	2:D:396:THR:HG22	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:LEU:HD12	2:B:172:MET:SD	2.40	0.62
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.81	0.61
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.33	0.61
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.17	0.61
4:F:159:GLY:C	4:F:160:ILE:HD12	2.26	0.61
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.14	0.61
2:B:163:ASP:OD1	12:B:601:HOH:O	2.16	0.61
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.82	0.61
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.36	0.60
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.34	0.60
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.81	0.60
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.84	0.60
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.02	0.59
10:B:505:GVV:O2	10:B:505:GVV:O1	2.20	0.59
2:B:167:ASN:OD1	2:B:200:GLU:HB2	2.02	0.59
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.37	0.59
2:B:298:SER:HA	2:B:301:MET:HG3	1.83	0.59
2:D:106:GLY:O	2:D:111:GLY:HA3	2.02	0.59
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.85	0.59
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.16	0.59
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.33	0.59
2:D:318:ILE:HG12	12:D:607:HOH:O	2.02	0.59
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
1:C:179:THR:HG21	12:C:659:HOH:O	2.03	0.58
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.38	0.58
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.84	0.58
2:D:69:ASP:O	2:D:94:PHE:HA	2.03	0.58
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.04	0.58
3:E:72:LEU:O	3:E:76:ARG:HG2	2.04	0.58
4:F:371:PRO:HA	4:F:372:THR:O	2.03	0.57
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.86	0.57
2:D:431:GLU:OE1	12:D:601:HOH:O	2.17	0.57
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.39	0.57
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.38	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.56
4:F:371:PRO:HA	4:F:372:THR:HB	1.86	0.56
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.86	0.56
2:B:136:GLN:HA	2:B:167:ASN:O	2.04	0.56
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.21	0.56
1:C:308:ARG:HD2	12:C:724:HOH:O	2.06	0.56
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.88	0.56
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.21	0.55
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.55
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.88	0.55
2:B:370:GLY:O	2:B:371:LEU:HD23	2.06	0.55
2:D:124:LYS:C	2:D:124:LYS:HD3	2.31	0.55
1:A:141:PHE:HB3	1:A:187:SER:OG	2.07	0.55
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.89	0.55
2:B:96:GLN:CB	1:C:1:MET:HE2	2.37	0.55
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.37	0.55
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.43	0.54
2:B:4:ILE:O	2:B:64:ARG:HD2	2.08	0.54
4:F:198:LYS:HE3	4:F:320:MET:HE1	1.88	0.54
1:A:284:GLU:CD	1:A:284:GLU:H	2.15	0.54
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.38	0.54
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.88	0.54
4:F:371:PRO:CA	4:F:372:THR:HB	2.38	0.54
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.72	0.54
2:D:152:LEU:O	2:D:156:LYS:HG2	2.06	0.54
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.90	0.54
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.43	0.54
2:B:205:ASP:OD1	2:B:207:GLU:N	2.37	0.53
3:E:85:LYS:O	3:E:89:GLU:HG3	2.07	0.53
2:D:109:THR:O	2:D:113:GLU:HG2	2.09	0.53
4:F:82:LYS:NZ	4:F:97:SER:O	2.36	0.53
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.90	0.53
2:B:46:LEU:HA	2:B:49:ILE:HB	1.91	0.53
1:C:43:GLY:HA2	1:C:56:THR:O	2.09	0.53
3:E:60:ARG:O	3:E:64:GLN:HG3	2.09	0.53
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.38	0.52
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.25	0.52
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.91	0.52
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.52
2:B:295:MET:CG	2:B:377:PHE:HB2	2.40	0.52
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.90	0.52
2:D:147:SER:HB2	2:D:190:SER:OG	2.09	0.52
1:C:22:GLU:OE1	12:C:603:HOH:O	2.19	0.52
1:A:71:GLU:HG2	1:A:72:PRO:N	2.24	0.52
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.92	0.52
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.52
2:D:12:CYS:HB2	8:D:502:GDP:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.09	0.52
2:D:107:HIS:O	2:D:152:LEU:HD22	2.09	0.52
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.92	0.51
1:C:166:LYS:HE2	1:C:197:HIS:O	2.11	0.51
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.92	0.51
2:B:169:PHE:CD1	2:B:235:MET:HE3	2.45	0.51
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.93	0.51
1:C:214:ARG:HG2	1:C:219:ILE:O	2.11	0.51
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.45	0.50
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.46	0.50
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.47	0.50
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.77	0.50
2:B:318:ILE:N	2:B:318:ILE:HD12	2.26	0.50
2:D:211:ASP:O	2:D:215:ARG:HB2	2.12	0.50
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.27	0.50
2:B:199:ASP:OD1	9:B:504:MES:H62	2.11	0.50
1:C:224:TYR:HE2	2:D:247:GLN:HE21	1.60	0.50
2:B:114:LEU:O	2:B:114:LEU:HG	2.11	0.50
2:B:104:ALA:HB2	2:B:413:MET:SD	2.51	0.50
4:F:259:GLY:O	4:F:261:GLU:HG3	2.12	0.50
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.42	0.49
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.77	0.49
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.27	0.49
2:D:191:VAL:O	2:D:195:VAL:HG23	2.12	0.49
2:B:124:LYS:HD3	2:B:124:LYS:C	2.38	0.49
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.37	0.49
1:A:302:MET:N	1:A:302:MET:HE2	2.28	0.49
1:C:419:SER:O	1:C:423:GLU:HG3	2.12	0.49
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.47	0.49
1:A:231:ILE:O	1:A:235:VAL:HG23	2.13	0.49
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.48	0.49
2:B:276:THR:HG22	2:B:277:SER:O	2.13	0.49
2:D:146:GLY:O	2:D:150:GLY:HA3	2.13	0.49
1:A:214:ARG:HG2	1:A:219:ILE:O	2.13	0.49
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.28	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.48	0.48
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.43	0.48
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.13	0.48
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.96	0.48
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.94	0.48
1:A:300:ASN:HB3	12:A:602:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:141:LEU:HA	2:D:147:SER:HB3	1.94	0.48
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.46	0.48
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.96	0.48
2:D:412:GLY:C	3:E:133:VAL:HG13	2.39	0.48
1:A:294:ALA:O	1:A:300:ASN:ND2	2.45	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.50	0.47
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.95	0.47
1:C:220:GLU:HB3	2:D:326:LYS:HD2	1.96	0.47
1:C:241:SER:HA	1:C:249:ASN:OD1	2.14	0.47
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.79	0.47
2:B:174:SER:OG	2:B:207:GLU:HB2	2.14	0.47
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.96	0.47
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.96	0.47
2:B:147:SER:HG	2:B:190:SER:HG	1.60	0.47
1:C:75:ILE:HB	1:C:94:THR:CG2	2.44	0.47
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.97	0.47
1:C:234:ILE:HG12	1:C:302:MET:CE	2.42	0.47
1:A:298:PRO:HA	1:A:301:GLN:CD	2.40	0.47
1:C:66:VAL:HG12	1:C:68:VAL:HG23	1.96	0.47
2:B:231:VAL:O	2:B:235:MET:HG3	2.15	0.46
1:C:108:TYR:O	1:C:112:LYS:HG2	2.15	0.46
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.97	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.46
2:D:409:THR:HA	2:D:413:MET:O	2.15	0.46
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.30	0.46
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.96	0.46
2:D:187:ALA:O	2:D:191:VAL:HG23	2.16	0.46
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.46
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.46
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.98	0.46
1:A:74:VAL:HB	12:A:612:HOH:O	2.15	0.46
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.97	0.46
1:C:134:GLY:HA2	1:C:164:LYS:HG2	1.98	0.46
2:D:416:MET:O	2:D:420:GLU:HG3	2.15	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.46
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.43	0.46
1:C:234:ILE:HD12	1:C:234:ILE:N	2.31	0.46
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.51	0.46
1:C:192:HIS:CG	1:C:421:ALA:HA	2.51	0.46
2:D:20:PHE:CE2	2:D:24:ILE:HD13	2.51	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.55	0.45
2:D:12:CYS:O	2:D:16:ILE:HG12	2.16	0.45
3:E:120:LEU:O	3:E:124:GLN:HG3	2.16	0.45
2:B:255:LEU:CD1	2:B:259:MET:HG3	2.46	0.45
2:D:145:THR:HB	8:D:502:GDP:O2B	2.16	0.45
2:D:318:ILE:N	2:D:318:ILE:HD12	2.30	0.45
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.31	0.45
2:D:143:GLY:HA3	8:D:502:GDP:O3A	2.16	0.45
2:D:325:MET:HE2	2:D:355:VAL:HG21	1.97	0.45
4:F:197:ARG:HB2	4:F:224:SER:O	2.17	0.45
2:B:40:SER:OG	2:B:42:LEU:HD13	2.16	0.45
2:D:11:GLN:O	2:D:15:GLN:HG2	2.16	0.45
2:D:150:GLY:O	2:D:154:ILE:HG13	2.16	0.45
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.45
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.99	0.45
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.51	0.45
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.52	0.45
1:A:349:THR:HB	3:E:25:LYS:HB3	1.98	0.45
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.97	0.45
2:B:355:VAL:HG12	2:B:356:CYS:N	2.32	0.45
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.98	0.45
1:C:180:ALA:O	1:C:183:GLU:HG3	2.15	0.45
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.45
2:B:431:GLU:O	2:B:434:GLN:HG2	2.17	0.45
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.45
3:E:48:GLU:O	3:E:52:LYS:HG3	2.17	0.45
4:F:209:HIS:HB2	4:F:310:GLN:OE1	2.17	0.45
4:F:225:SER:HB2	4:F:252:ASN:O	2.17	0.45
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.47	0.45
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.99	0.45
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.99	0.44
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.99	0.44
2:D:382:THR:O	2:D:385:GLN:HG2	2.17	0.44
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.99	0.44
4:F:371:PRO:HA	4:F:372:THR:CB	2.47	0.44
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.46	0.44
2:B:19:LYS:O	2:B:23:VAL:HG23	2.18	0.44
2:B:31:ASP:OD1	2:B:35:SER:N	2.50	0.44
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.98	0.44
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.48	0.44
1:A:265:ILE:CG2	1:A:313:MET:HE1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:O	2:D:23:VAL:HG23	2.18	0.44
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.17	0.44
4:F:202:ARG:HB3	4:F:220:VAL:CG2	2.47	0.44
1:A:419:SER:O	1:A:423:GLU:HG3	2.18	0.44
2:B:323:MET:CE	2:B:373:MET:HB2	2.48	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.99	0.44
2:B:198:THR:OG1	2:B:266:HIS:NE2	2.51	0.44
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.99	0.44
1:A:271:THR:CG2	1:A:300:ASN:HD22	2.31	0.44
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.32	0.44
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.53	0.44
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.52	0.44
2:B:324:SER:HB3	2:B:327:GLU:HB3	2.00	0.44
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.99	0.44
2:D:220:THR:C	2:D:222:PRO:HD3	2.43	0.43
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.52	0.43
1:C:234:ILE:HD12	1:C:234:ILE:H	1.83	0.43
2:D:185:TYR:HE2	2:D:403:ALA:O	2.01	0.43
1:A:193:THR:HG23	12:A:651:HOH:O	2.19	0.43
1:A:320:ARG:HD2	12:A:652:HOH:O	2.18	0.43
2:D:287:THR:HB	2:D:289:PRO:HD2	1.99	0.43
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.54	0.43
2:B:425:MET:O	2:B:429:VAL:HG23	2.19	0.43
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.00	0.43
4:F:222:ARG:O	4:F:241:THR:HB	2.18	0.43
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.49	0.43
2:D:118:VAL:O	2:D:122:VAL:HG23	2.19	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.43
2:D:123:ARG:O	2:D:127:GLU:HG3	2.19	0.43
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.43	0.43
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.36	0.43
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.84	0.43
2:B:209:LEU:HD23	2:B:302:MET:HG2	1.99	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
2:D:15:GLN:O	2:D:19:LYS:HG2	2.19	0.43
4:F:201:ILE:HG12	4:F:221:LEU:HG	2.01	0.43
2:B:255:LEU:HD11	2:B:259:MET:HG3	2.01	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.19	0.42
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.55	0.42
2:B:147:SER:OG	2:B:190:SER:OG	2.30	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:ALA:O	2:D:305:CYS:N	2.47	0.42
4:F:146:VAL:HG22	4:F:164:SER:HB3	2.00	0.42
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.42
2:B:16:ILE:HG21	2:B:231:VAL:HG11	2.01	0.42
2:D:2:ARG:HB3	2:D:133:GLN:HG2	2.01	0.42
2:D:311:ARG:NH1	2:D:436:GLN:O	2.51	0.42
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.18	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.44	0.42
1:A:179:THR:HA	2:B:352:LYS:CD	2.49	0.42
2:B:42:LEU:H	2:B:42:LEU:HD12	1.84	0.42
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.55	0.42
4:F:53:GLY:N	4:F:60:GLN:OE1	2.41	0.42
2:B:158:ARG:NH1	2:B:196:GLU:O	2.52	0.42
2:B:297:ASP:OD1	2:B:298:SER:N	2.53	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.02	0.42
4:F:222:ARG:NH2	4:F:318:ASP:OD1	2.51	0.42
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.51	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.42
1:C:6:SER:O	1:C:65:ALA:HA	2.20	0.42
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.50	0.42
2:D:212:ILE:O	2:D:216:THR:HB	2.19	0.42
4:F:372:THR:O	4:F:372:THR:HG22	2.19	0.42
1:A:70:LEU:HB2	1:A:98:ASP:HA	2.01	0.41
2:B:42:LEU:HD12	2:B:42:LEU:N	2.35	0.41
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.19	0.41
2:B:290:GLU:O	2:B:294:GLN:HG3	2.19	0.41
2:D:204:ILE:HG21	2:D:231:VAL:HG22	2.02	0.41
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.21	0.41
4:F:279:LEU:HD12	4:F:283:ILE:HB	2.03	0.41
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.50	0.41
1:C:71:GLU:HB3	1:C:98:ASP:HB3	2.02	0.41
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.02	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HD13	2.02	0.41
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.50	0.41
1:C:74:VAL:HB	12:C:620:HOH:O	2.21	0.41
1:A:281:ALA:O	1:A:282:TYR:HD2	2.04	0.41
1:C:227:LEU:O	1:C:231:ILE:HG13	2.20	0.41
2:D:325:MET:HE3	2:D:325:MET:HB2	1.99	0.41
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.38	0.41
1:A:75:ILE:HD12	1:A:94:THR:HG22	2.01	0.41
2:B:333:LEU:HD13	4:F:57:GLY:HA3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:ASN:O	2:B:352:LYS:HE2	2.20	0.41
1:C:46:ASP:OD1	1:C:46:ASP:N	2.52	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.41
10:B:505:GVV:O2	10:B:505:GVV:C3	2.69	0.40
2:B:42:LEU:CB	2:B:358:ILE:HD11	2.50	0.40
2:D:46:LEU:HA	2:D:49:ILE:HB	2.03	0.40
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.04	0.40
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.29	0.40
4:F:225:SER:O	4:F:252:ASN:HB2	2.21	0.40
2:B:78:VAL:O	2:B:84:GLY:HA3	2.21	0.40
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.21	0.40
2:D:63:PRO:O	2:D:65:ALA:N	2.54	0.40
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.03	0.40
4:F:189:PRO:HA	4:F:322:ASP:HA	2.03	0.40
1:A:192:HIS:CG	1:A:421:ALA:HA	2.57	0.40
1:A:430:LYS:O	1:A:434:GLU:HG3	2.21	0.40
2:B:194:LEU:HD22	2:B:198:THR:HG21	2.03	0.40
9:B:504:MES:H81	9:B:504:MES:H51	1.79	0.40
1:C:75:ILE:HB	1:C:94:THR:HG21	2.04	0.40
2:D:1:MET:HG3	2:D:50:ASN:HB2	2.03	0.40
2:D:63:PRO:HD3	2:D:86:ILE:HG12	2.03	0.40
2:D:154:ILE:HG23	2:D:166:MET:HG2	2.04	0.40
3:E:58:GLU:O	3:E:62:LYS:HG3	2.21	0.40
1:A:2:ARG:HB3	1:A:131:GLY:O	2.21	0.40
1:A:320:ARG:HA	1:A:356:ASN:O	2.22	0.40
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.21	0.40
2:B:369:ARG:HA	2:B:369:ARG:HD3	1.96	0.40
1:C:282:TYR:O	1:C:283:HIS:HB2	2.21	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)
1:C:366:GLY:O	3:E:80:ARG:NH1[4_455]	2.16	0.04

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%)	427 (98%)	9 (2%)	0	100	100
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	421/445 (95%)	410 (97%)	10 (2%)	1 (0%)	43	55
2	D	429/445 (96%)	417 (97%)	10 (2%)	2 (0%)	24	31
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	344/384 (90%)	325 (94%)	19 (6%)	0	100	100
All	All	2188/2319 (94%)	2127 (97%)	58 (3%)	3 (0%)	48	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	281	GLN
2	D	304	ALA
2	B	73	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	369/379 (97%)	364 (99%)	5 (1%)	59	76
1	C	372/379 (98%)	371 (100%)	1 (0%)	86	93
2	B	367/383 (96%)	364 (99%)	3 (1%)	73	86
2	D	368/383 (96%)	366 (100%)	2 (0%)	81	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	110/127 (87%)	109 (99%)	1 (1%)	70	84
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1901/1993 (95%)	1889 (99%)	12 (1%)	78	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	A	381	THR
2	B	167	ASN
2	B	291	LEU
2	B	301	MET
1	C	381	THR
2	D	229	HIS
2	D	247	GLN
3	E	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	176	GLN
1	A	300	ASN
1	A	301	GLN
1	A	329	ASN
2	B	15	GLN
2	B	193	GLN
2	B	282	GLN
2	B	293	GLN
2	B	294	GLN
2	B	337	ASN
2	B	349	ASN
1	C	11	GLN
1	C	15	GLN
1	C	101	ASN
2	D	8	GLN
2	D	14	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	37	HIS
2	D	136	GLN
3	E	12	ASN
3	E	71	HIS
3	E	92	ASN
3	E	136	ASN
4	F	180	HIS
4	F	196	HIS
4	F	269	GLN
4	F	348	GLN
4	F	379	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
5	GTP	C	501	6	33,34,34	1.06	3 (9%)	50,54,54	1.50	9 (18%)
10	GVV	B	505	-	13,13,13	0.26	0	17,17,17	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	6	33,34,34	0.96	2 (6%)	50,54,54	1.56	9 (18%)
11	ACP	F	401	6	31,33,33	1.68	8 (25%)	47,52,52	1.88	9 (19%)
8	GDP	B	501	6	29,30,30	1.14	3 (10%)	45,47,47	1.73	6 (13%)
8	GDP	D	502	6	29,30,30	1.16	3 (10%)	45,47,47	1.73	6 (13%)
9	MES	B	504	-	12,12,12	2.23	1 (8%)	15,16,16	1.95	4 (26%)

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
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
10	GVV	B	505	-	-	2/6/6/6	0/1/1/1
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
11	ACP	F	401	6	-	11/19/38/38	0/3/3/3
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3
8	GDP	D	502	6	-	3/16/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.45	1.67	1.77
11	F	401	ACP	C5-C4	4.83	1.47	1.39
8	B	501	GDP	C5-C4	3.08	1.47	1.38
8	D	502	GDP	C5-C4	3.06	1.47	1.38
11	F	401	ACP	PG-O3G	2.97	1.61	1.55
11	F	401	ACP	PG-O2G	2.96	1.61	1.55
11	F	401	ACP	C5-C6	2.69	1.48	1.41
11	F	401	ACP	PB-O3A	2.66	1.61	1.58
5	C	501	GTP	PA-O3A	2.60	1.62	1.59
5	C	501	GTP	PB-O3B	2.60	1.62	1.59
8	B	501	GDP	C6-N1	-2.44	1.34	1.38
8	D	502	GDP	C6-N1	-2.43	1.34	1.38
11	F	401	ACP	C8-N7	2.34	1.36	1.31
5	A	501	GTP	PB-O3B	2.27	1.62	1.59
11	F	401	ACP	C5-N7	-2.26	1.35	1.39
5	C	501	GTP	C2-N3	2.22	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O2B	2.16	1.61	1.56
5	A	501	GTP	C2-N3	2.09	1.38	1.33
8	D	502	GDP	C5-N7	-2.07	1.34	1.39
8	B	501	GDP	C5-N7	-2.05	1.35	1.39

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	502	GDP	C5-C4-N3	-6.07	118.73	128.39
8	B	501	GDP	C5-C4-N3	-5.93	118.94	128.39
11	F	401	ACP	C5-C4-N3	-5.72	118.83	126.72
8	B	501	GDP	C2-N3-C4	5.07	121.04	112.30
8	D	502	GDP	C2-N3-C4	5.07	121.02	112.30
5	A	501	GTP	C5-C4-N3	-4.97	120.47	128.39
5	A	501	GTP	C2-N3-C4	4.81	120.58	112.30
5	C	501	GTP	C5-C4-N3	-4.79	120.77	128.39
11	F	401	ACP	N3-C4-N9	4.66	135.09	127.17
8	D	502	GDP	N9-C4-N3	4.45	134.85	125.95
5	C	501	GTP	C2-N3-C4	4.38	119.85	112.30
9	B	504	MES	C5-N4-C3	4.33	118.17	108.84
8	B	501	GDP	N9-C4-N3	4.32	134.59	125.95
11	F	401	ACP	PB-O3A-PA	-3.97	119.42	132.37
11	F	401	ACP	C2-N3-C4	3.61	120.64	111.83
8	B	501	GDP	C6-C5-N7	3.56	136.76	130.29
11	F	401	ACP	C4-C5-N7	-3.31	106.79	110.58
8	D	502	GDP	C6-C5-N7	3.29	136.27	130.29
11	F	401	ACP	N3-C2-N1	-3.16	123.80	128.58
9	B	504	MES	O1S-S-C8	3.08	111.38	106.73
5	C	501	GTP	N9-C4-N3	3.05	132.05	125.95
5	A	501	GTP	N9-C4-N3	2.97	131.90	125.95
5	A	501	GTP	C2-N1-C6	-2.88	119.89	125.11
5	C	501	GTP	C2-N1-C6	-2.83	119.98	125.11
9	B	504	MES	C6-C5-N4	-2.82	105.83	110.12
5	A	501	GTP	N9-C8-N7	-2.76	108.28	113.40
11	F	401	ACP	C4-N9-C8	2.76	108.64	105.74
5	A	501	GTP	C8-N7-C5	2.72	109.11	104.26
8	B	501	GDP	C4-C5-N7	-2.68	106.42	110.67
11	F	401	ACP	C3'-C2'-C1'	2.65	106.48	101.46
5	C	501	GTP	N9-C8-N7	-2.65	108.49	113.40
9	B	504	MES	C7-N4-C5	2.64	118.26	111.24
8	D	502	GDP	C4-C5-N7	-2.61	106.53	110.67
5	C	501	GTP	C5-C6-N1	2.49	119.60	113.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	2.48	119.56	113.25
11	F	401	ACP	C5-N7-C8	2.44	107.29	103.45
5	C	501	GTP	C8-N7-C5	2.37	108.49	104.26
5	C	501	GTP	O6-C6-C5	-2.27	120.54	126.53
5	A	501	GTP	O6-C6-C5	-2.22	120.67	126.53
8	B	501	GDP	O6-C6-C5	-2.17	120.81	126.53
8	D	502	GDP	O6-C6-C5	-2.14	120.88	126.53
5	C	501	GTP	O2A-PA-O3A	2.10	112.95	107.27
5	A	501	GTP	C4-C5-N7	-2.08	107.38	110.67

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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	502	GDP	PA-O3A-PB-O2B
8	D	502	GDP	C5'-O5'-PA-O3A
8	D	502	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O3A
11	F	401	ACP	O4'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	MES	C7-C8-S-O2S
10	B	505	GVV	C5-C4-N1-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	B	505	GVV	C9-C4-N1-C3
11	F	401	ACP	PG-C3B-PB-O2B
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA
8	B	501	GDP	PB-O3A-PA-O2A

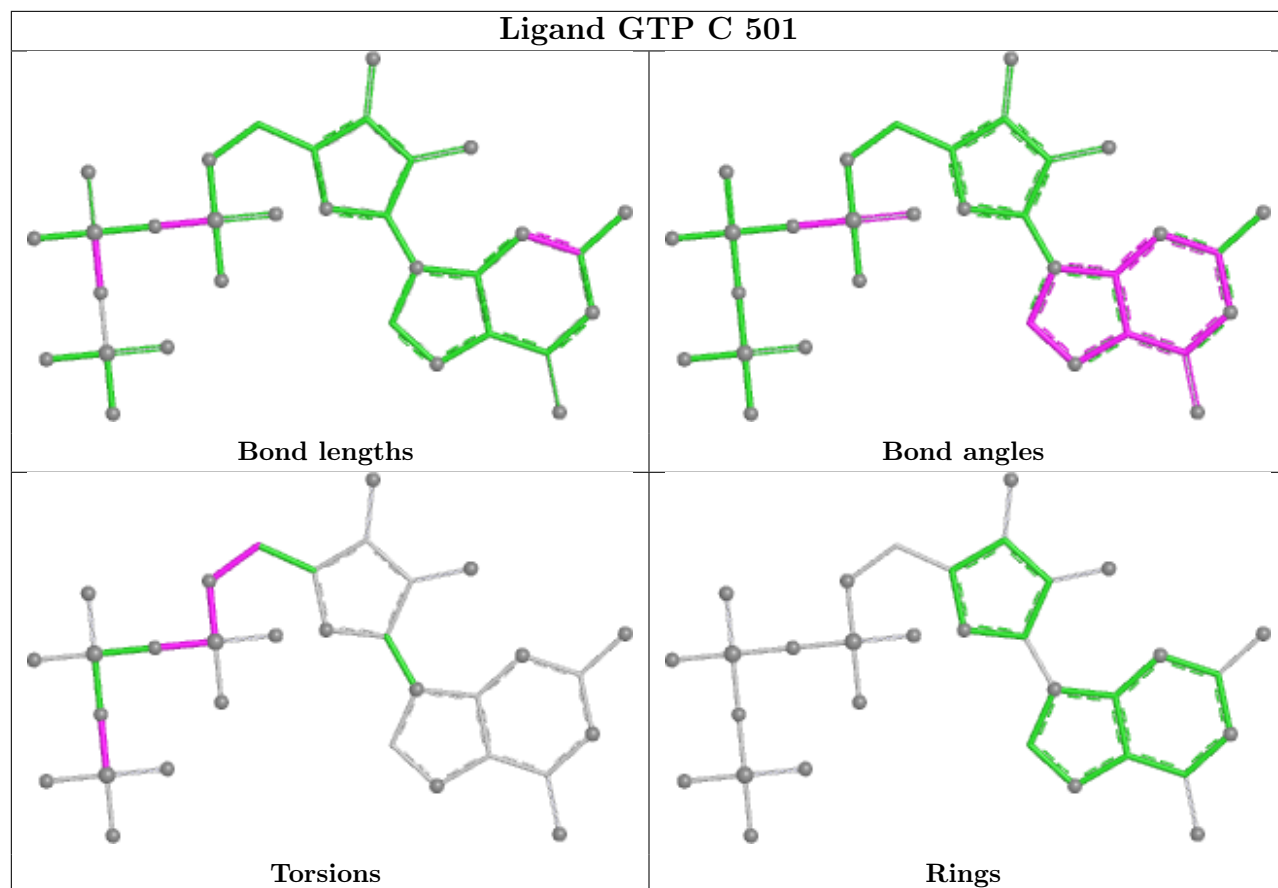
There are no ring outliers.

5 monomers are involved in 14 short contacts:

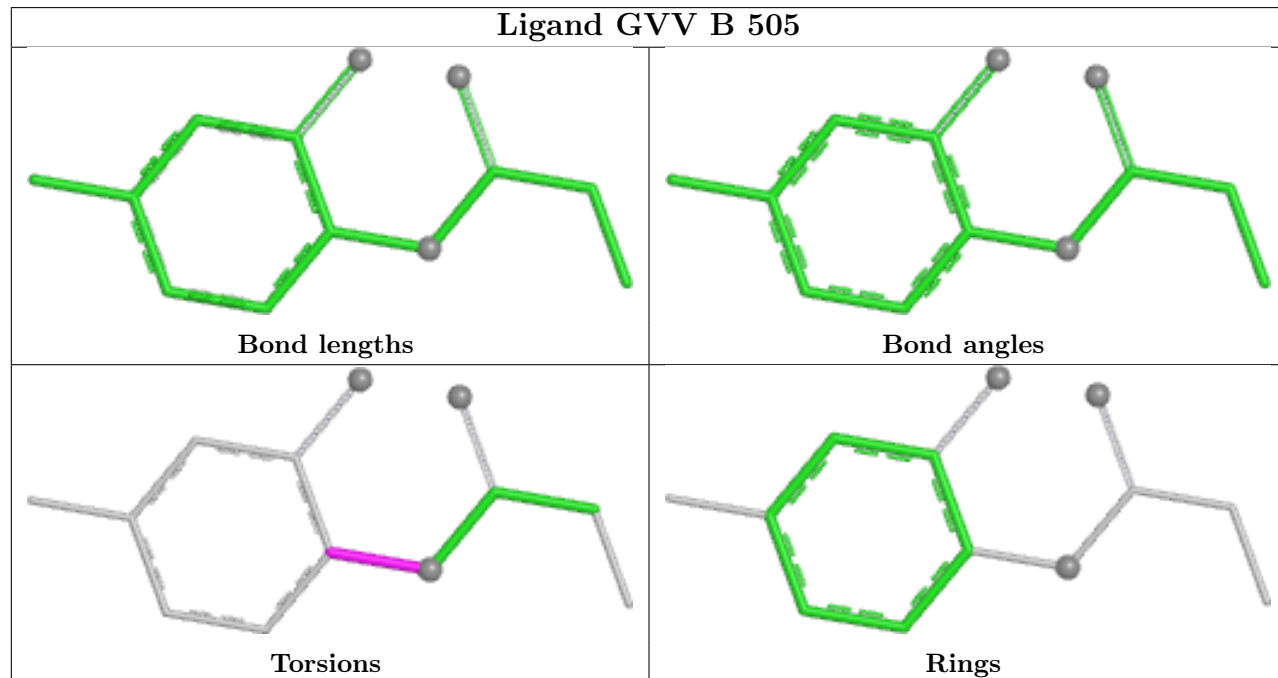
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	GVV	2	0
5	A	501	GTP	2	0
11	F	401	ACP	5	0
8	D	502	GDP	3	0
9	B	504	MES	2	0

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

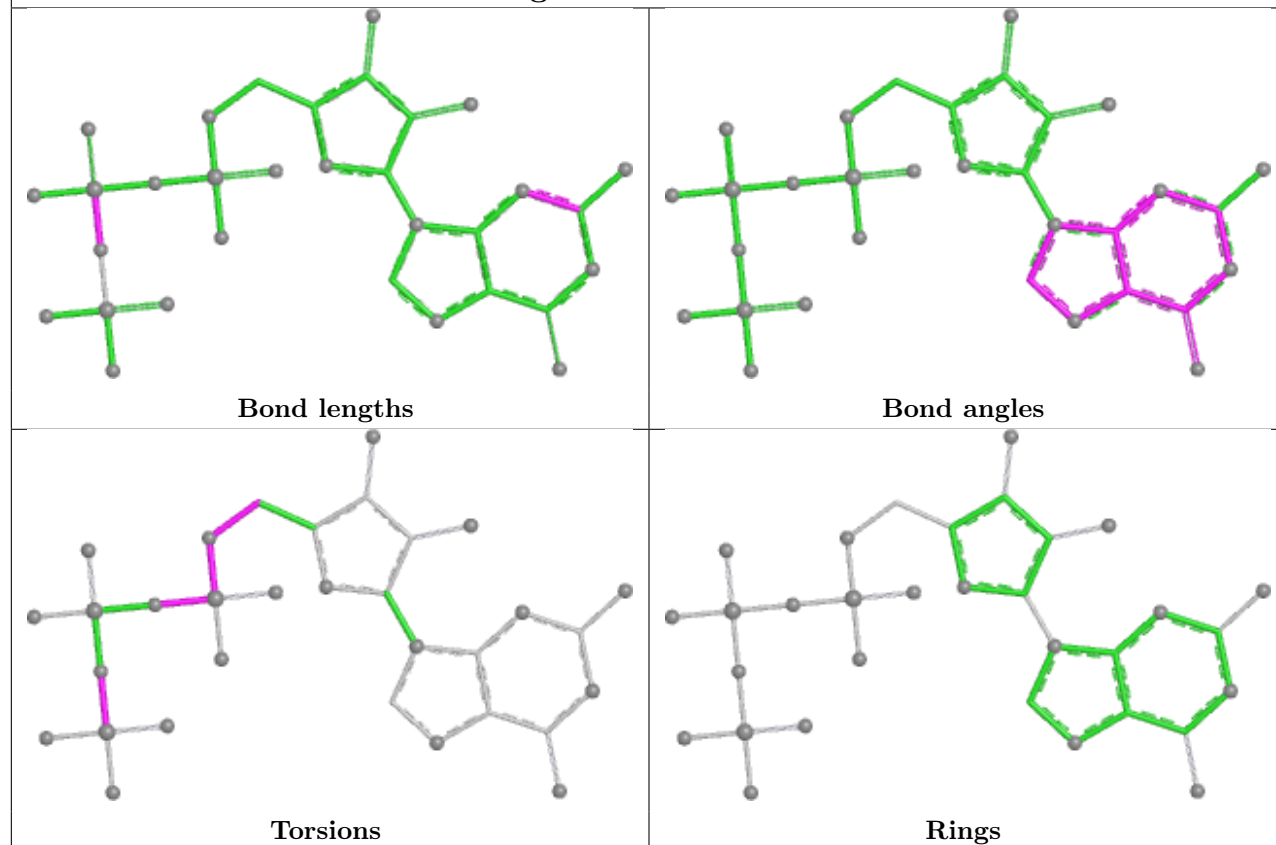
Ligand GTP C 501



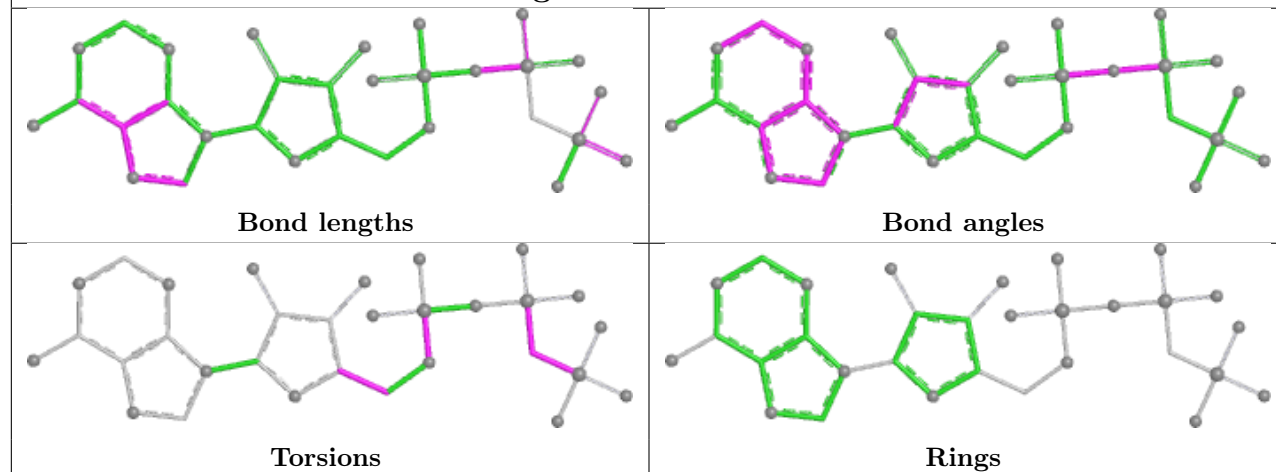
Ligand GVV B 505

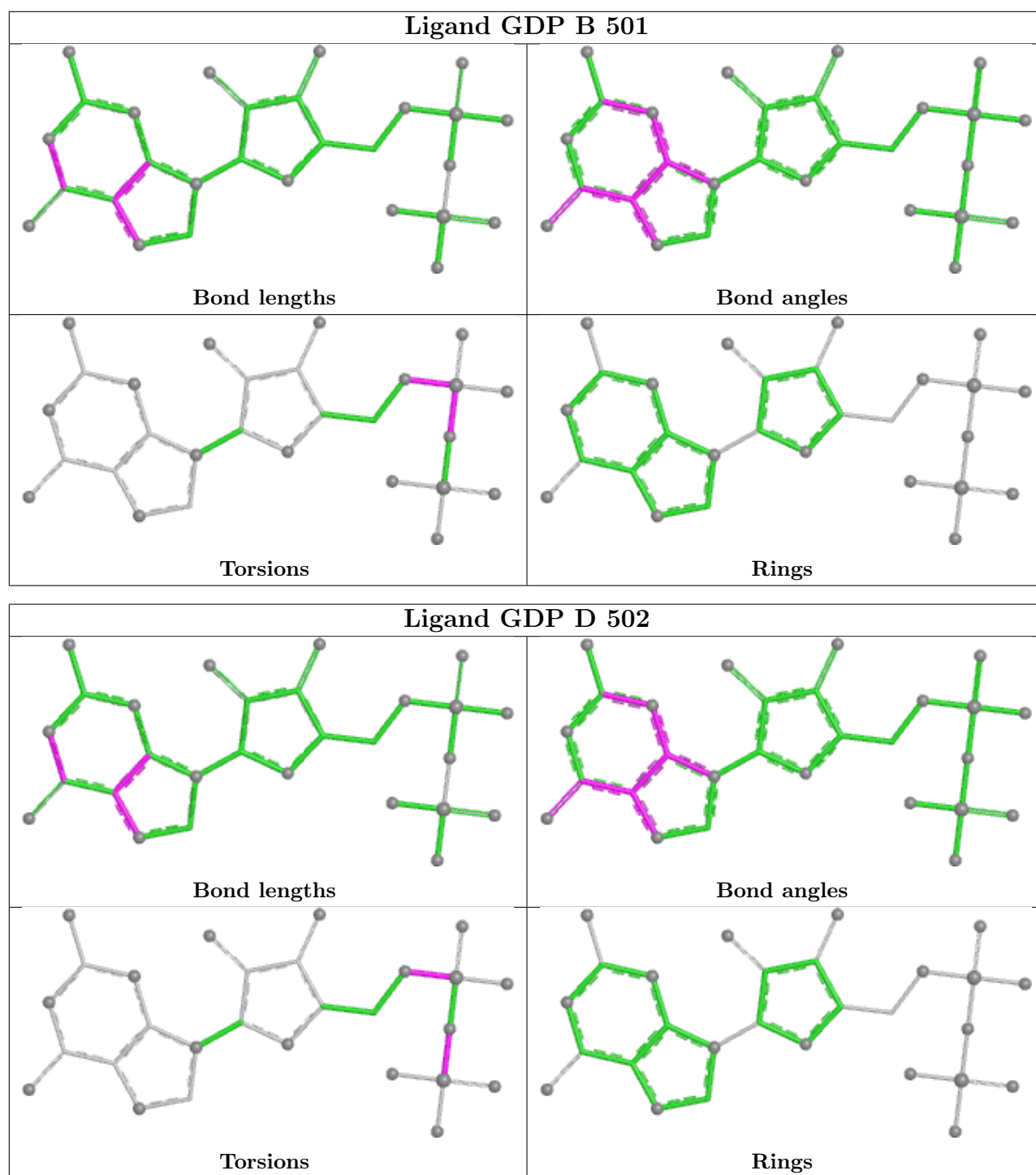


Ligand GTP A 501



Ligand ACP F 401





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%)	0.47	20 (4%)	37	39	52, 71, 109, 170	0
1	C	440/451 (97%)	0.27	18 (4%)	41	43	32, 60, 85, 119	1 (0%)
2	B	425/445 (95%)	0.52	18 (4%)	40	42	43, 70, 119, 160	3 (0%)
2	D	431/445 (96%)	0.73	36 (8%)	17	18	57, 82, 124, 169	4 (0%)
3	E	123/143 (86%)	0.99	9 (7%)	21	23	60, 89, 135, 152	0
4	F	352/384 (91%)	0.85	29 (8%)	17	19	69, 104, 172, 195	0
All	All	2209/2319 (95%)	0.58	130 (5%)	28	30	32, 75, 135, 195	8 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	6.7
2	B	248	LEU	5.4
1	C	440	VAL	5.0
4	F	159	GLY	4.7
2	B	249	ASN	4.5
2	D	248	LEU	4.5
2	D	283	TYR	4.3
4	F	371	PRO	4.2
1	C	357	TYR	4.2
2	D	285	ALA	3.9
2	B	241	CYS	3.7
2	B	250	ALA	3.7
3	E	143	ALA	3.7
2	D	407	TRP	3.7
1	A	282	TYR	3.5
4	F	362	ALA	3.4
2	B	1	MET	3.4
3	E	26	PRO	3.4
2	D	429	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	125	THR	3.4
2	D	284	ARG	3.3
2	D	304	ALA	3.3
2	D	241	CYS	3.3
3	E	50	ILE	3.3
4	F	344	ALA	3.2
4	F	105	LEU	3.2
2	D	82	PRO	3.2
1	C	128	GLN	3.2
2	B	247	GLN	3.2
2	D	56	ALA	3.1
2	B	333	LEU	3.1
2	D	281	GLN	3.1
2	D	441	ASP	3.1
2	D	282	GLN	3.1
3	E	6	MET	3.1
4	F	186	LEU	3.0
4	F	382	HIS	3.0
1	A	438	ASP	2.9
2	D	279	GLY	2.9
1	A	340	SER	2.9
1	A	281	ALA	2.9
4	F	240	LEU	2.9
4	F	167	SER	2.9
1	C	135	PHE	2.8
4	F	160	ILE	2.8
4	F	243	HIS	2.8
2	D	388	PHE	2.8
1	A	335	ILE	2.7
1	C	341	ILE	2.7
3	E	28	SER	2.7
1	C	163	LYS	2.7
2	D	197	ASN	2.7
1	C	245	ASP	2.7
2	D	249	ASN	2.7
1	A	115	ILE	2.7
2	B	255	LEU	2.7
4	F	206	LEU	2.7
4	F	249	TYR	2.6
4	F	373	SER	2.6
1	A	196	GLU	2.6
2	D	246	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	2.6
2	D	247	GLN	2.5
3	E	24	LEU	2.5
3	E	139	LEU	2.5
2	B	285	ALA	2.5
2	B	339	ASN	2.5
2	D	85	GLN	2.5
2	D	2	ARG	2.5
2	D	42	LEU	2.5
2	D	167	ASN	2.5
1	A	316	CYS	2.4
2	B	345	GLU	2.4
1	A	179	THR	2.4
2	D	277	SER	2.4
2	D	57	THR	2.4
1	C	4[A]	CYS	2.4
2	D	430	SER	2.3
1	A	262	TYR	2.3
2	B	283	TYR	2.3
1	C	2	ARG	2.3
1	A	111	GLY	2.3
1	C	162	GLY	2.3
4	F	211	TYR	2.3
4	F	90	SER	2.3
2	B	325	MET	2.3
4	F	283	ILE	2.3
1	C	1	MET	2.2
4	F	309	TYR	2.2
2	D	371	LEU	2.2
4	F	169	LEU	2.2
1	A	135	PHE	2.2
1	C	179	THR	2.2
2	D	280	SER	2.2
4	F	5	VAL	2.2
1	C	133	GLN	2.2
1	A	299	ALA	2.2
2	D	432	TYR	2.2
1	A	346	TRP	2.2
2	D	86	ILE	2.2
2	D	384	ILE	2.2
2	B	57	THR	2.2
3	E	47	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	314	LEU	2.1
2	D	78	VAL	2.1
2	D	195	VAL	2.1
2	B	284	ARG	2.1
1	A	284	GLU	2.1
2	B	281	GLN	2.1
2	D	37	HIS	2.1
4	F	381	HIS	2.1
1	C	178	SER	2.1
2	B	124	LYS	2.1
1	C	18	ASN	2.1
4	F	179	VAL	2.1
1	C	350	GLY	2.1
2	D	387	LEU	2.1
3	E	54	LEU	2.1
1	C	335	ILE	2.1
1	A	58	ALA	2.0
1	A	42	ILE	2.0
1	A	339	ARG	2.0
4	F	6	VAL	2.0
4	F	142	ARG	2.0
2	B	246	GLY	2.0
4	F	23	ALA	2.0
4	F	153	ALA	2.0
1	A	300	ASN	2.0
1	C	120	ASP	2.0
1	A	336	LYS	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,

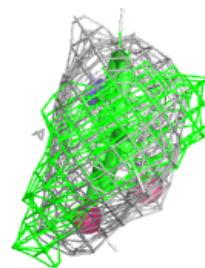
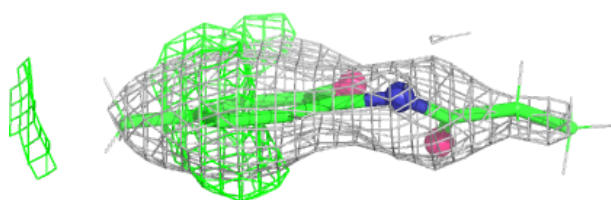
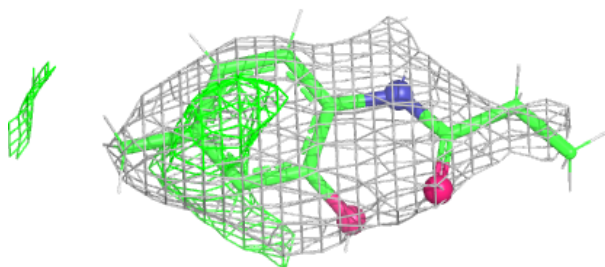
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.74	0.16	121,121,121,121	0
7	CA	A	504	1/1	0.84	0.12	106,106,106,106	0
6	MG	F	402	1/1	0.86	0.12	99,99,99,99	0
9	MES	B	504	12/12	0.87	0.15	89,94,106,114	0
10	GVV	B	505	13/13	0.87	0.27	47,57,69,70	26
11	ACP	F	401	31/31	0.88	0.10	98,110,119,124	0
6	MG	D	503	1/1	0.89	0.08	80,80,80,80	0
8	GDP	D	502	28/28	0.93	0.11	70,77,86,93	0
6	MG	D	501	1/1	0.95	0.07	58,58,58,58	0
6	MG	B	502	1/1	0.97	0.09	43,43,43,43	0
5	GTP	C	501	32/32	0.98	0.06	43,50,53,56	0
8	GDP	B	501	28/28	0.98	0.05	45,51,56,60	0
5	GTP	A	501	32/32	0.98	0.06	47,55,60,61	0
7	CA	A	503	1/1	0.99	0.04	87,87,87,87	0
6	MG	A	502	1/1	0.99	0.03	54,54,54,54	0
7	CA	C	502	1/1	1.00	0.02	77,77,77,77	0

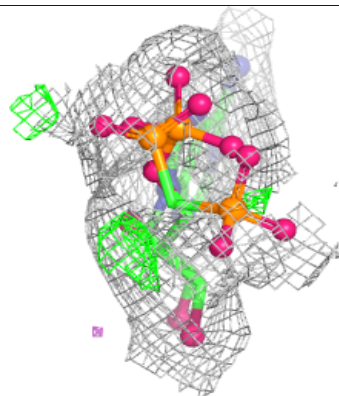
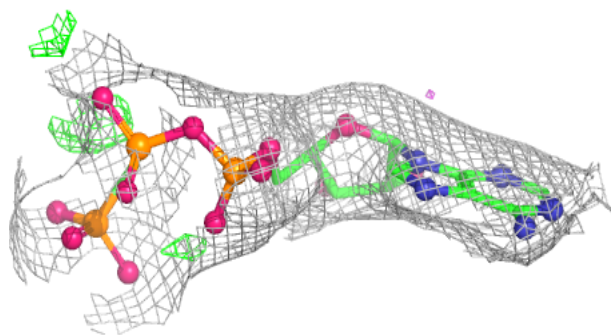
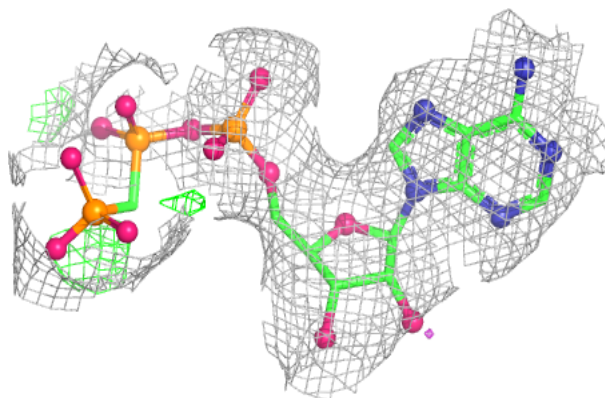
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GVV B 505:

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

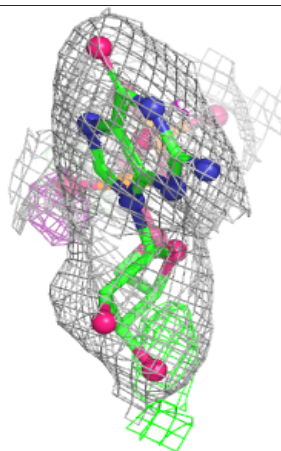
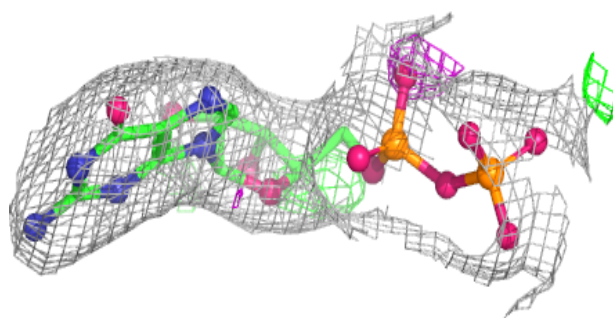
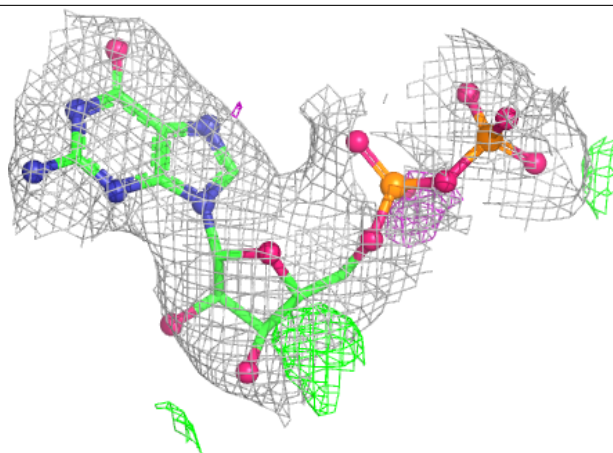
**Electron density around ACP F 401:**

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

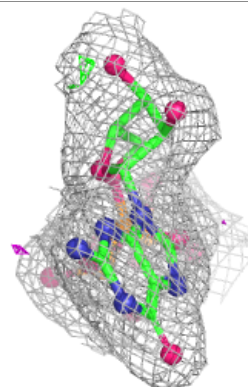
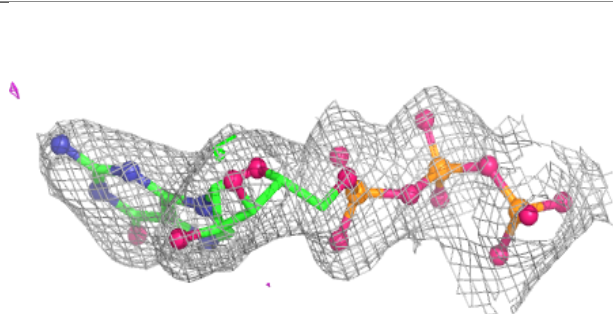
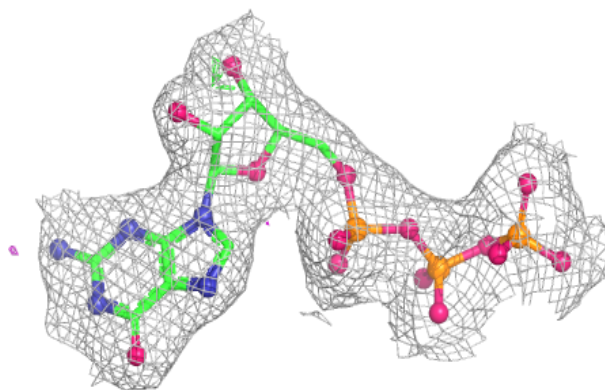


Electron density around GDP D 502:

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

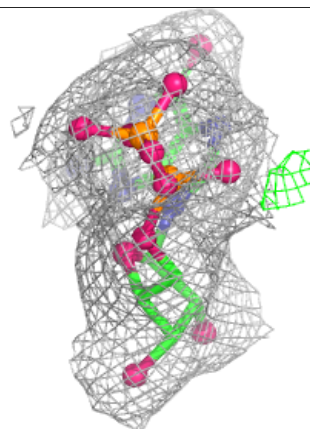
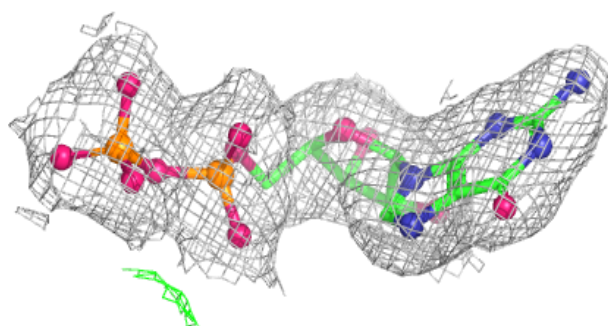
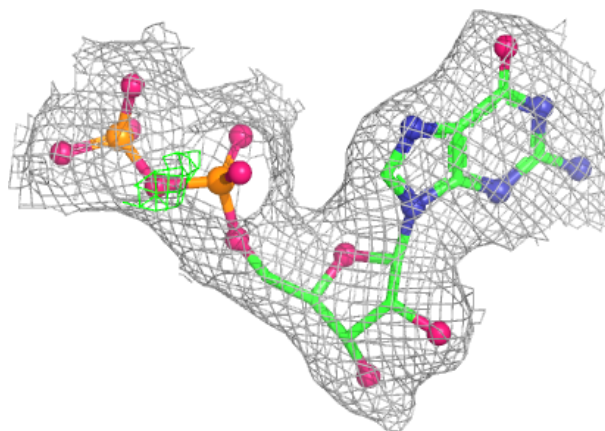
**Electron density around GTP C 501:**

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

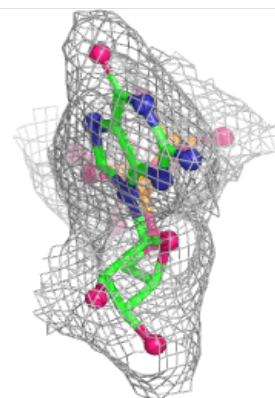
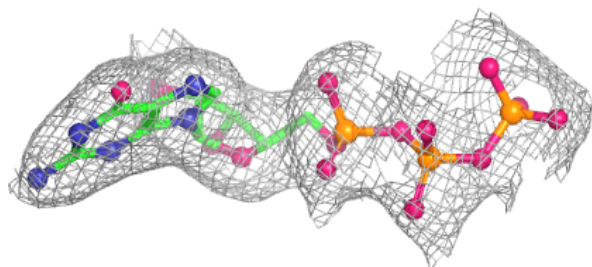
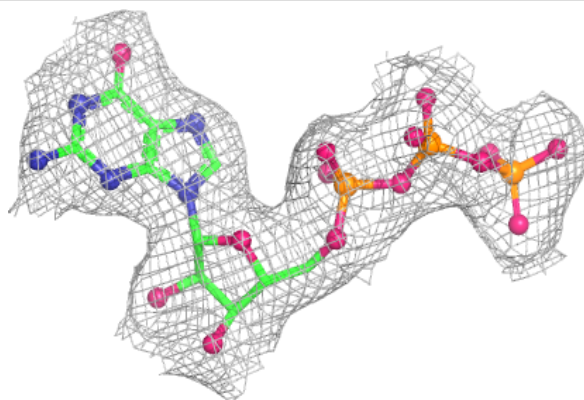


Electron density around GDP B 501:

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

**Electron density around GTP A 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 [i](#)

There are no such residues in this entry.