



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:43 AM UTC

PDB ID : 8HUH / pdb_00008huh
Title : Crystal structure of T2R-TTL-3a complex
Authors : Wang, Y.X.; Chen, J.J.
Deposited on : 2022-12-23
Resolution : 2.80 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

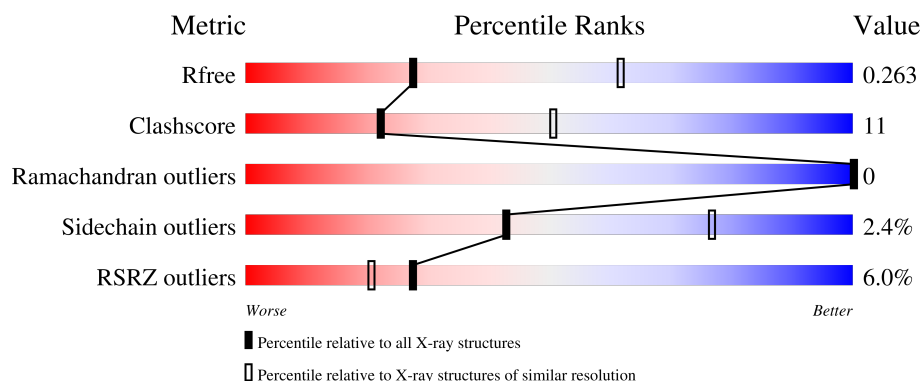
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	450	0% 71% 26% •
1	C	450	0% 81% 17% •
2	B	445	2% 73% 23% •
2	D	445	11% 67% 26% • 5%
3	E	143	3% 67% 15% • 15%

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Mol	Chain	Length	Quality of chain
4	F	384	15% 62% 19% • 18%

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 16899 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3403	2156	579	646	22			
1	C	440	Total	C	N	O	S	0	0	0
			3427	2169	581	655	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3336	2098	570	642	26			
2	D	421	Total	C	N	O	S	0	0	0
			3156	1975	534	622	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	1	0
			983	605	178	195	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	316	Total	C	N	O	S	0	0	0
			2383	1531	404	437	11			

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		

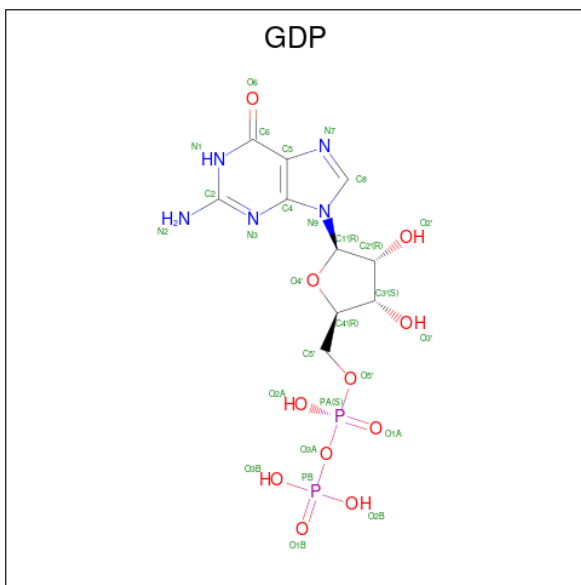
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



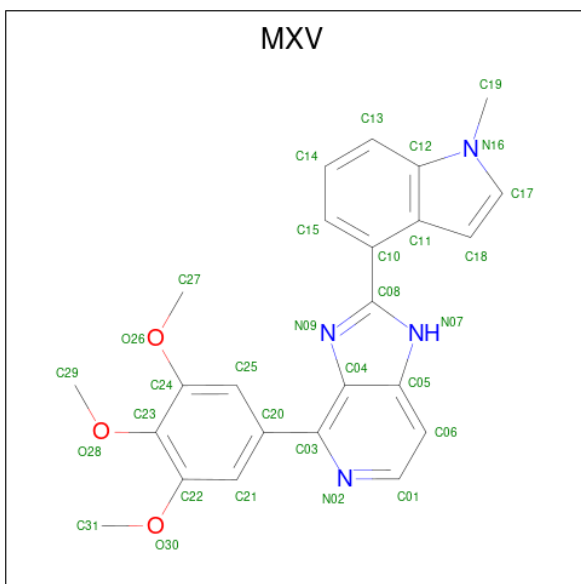
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



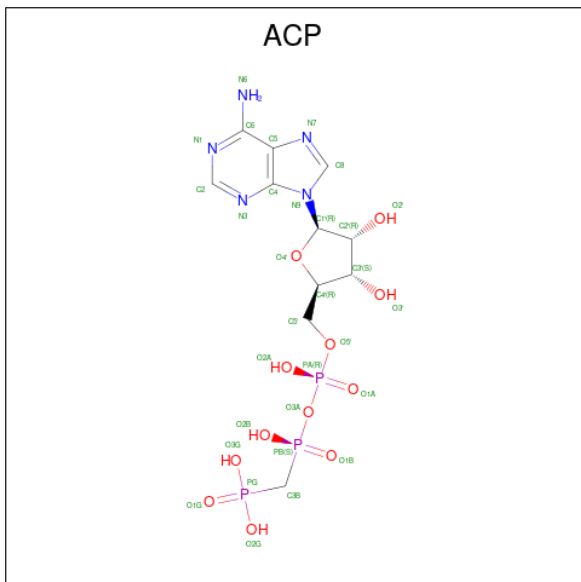
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 2-(1-methylindol-4-yl)-4-(3,4,5-trimethoxyphenyl)-1 {H}-imidazo[4,5-c]pyridine (CCD ID: MXV) (formula: C₂₄H₂₂N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			31	24	4	3		

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

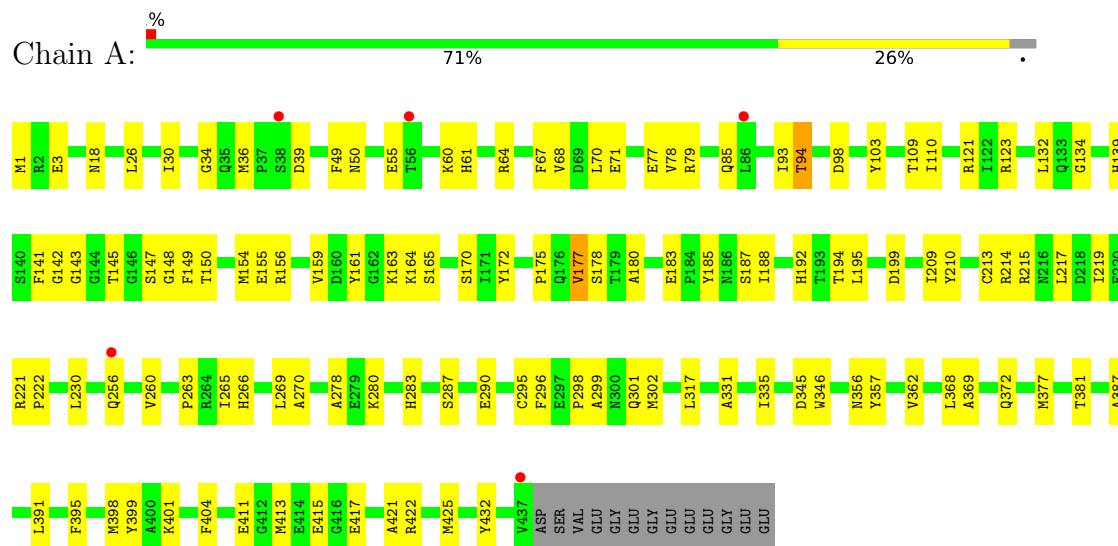


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

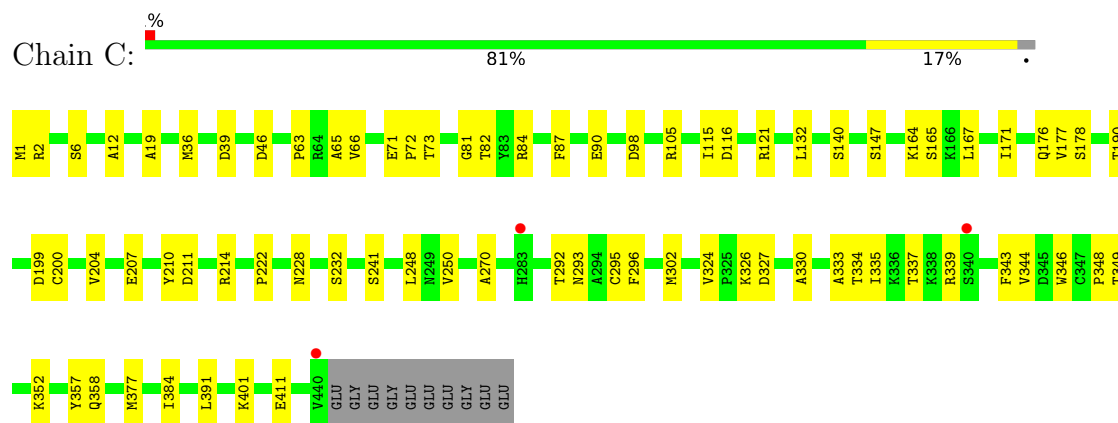
3 Residue-property plots

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

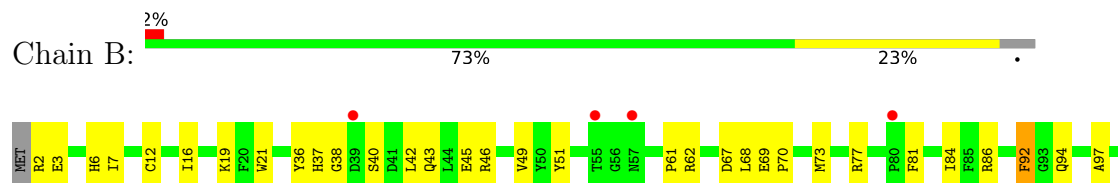
• Molecule 1: Tubulin alpha-1B chain

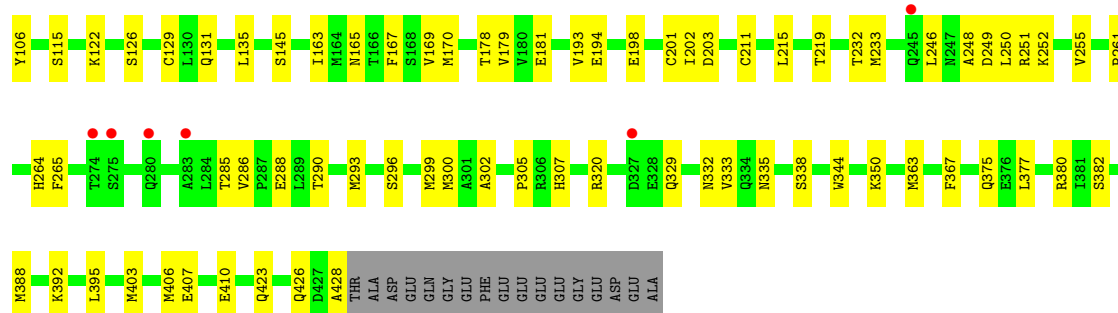


• Molecule 1: Tubulin alpha-1B chain

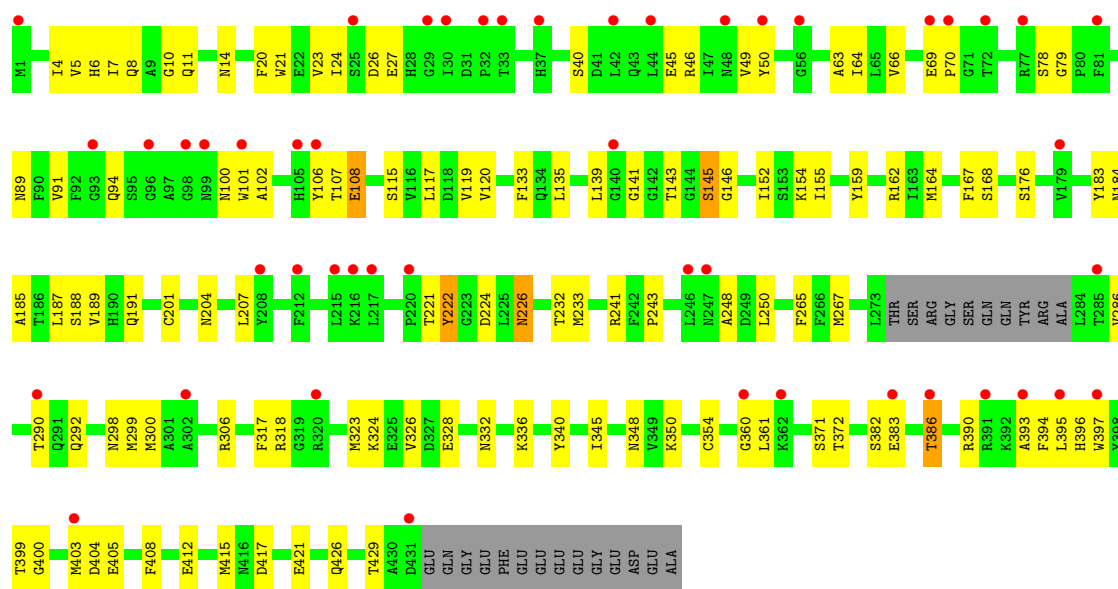


• Molecule 2: Tubulin beta-2B chain

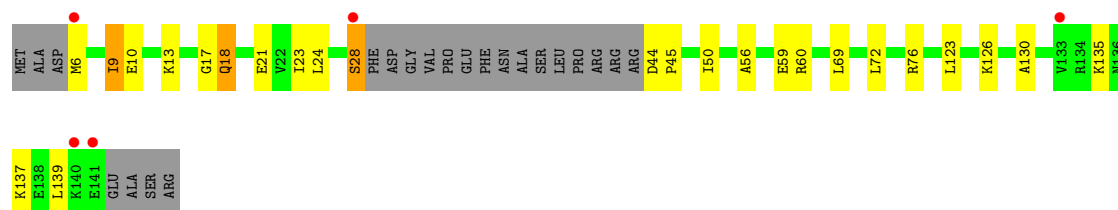




• Molecule 2: Tubulin beta-2B chain

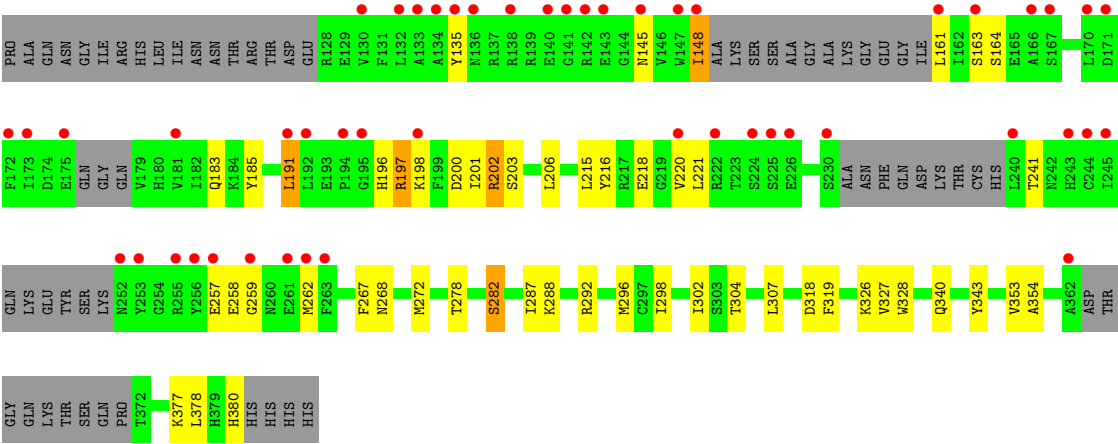


• Molecule 3: Stathmin-4



• Molecule 4: TTL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.19Å 157.88Å 182.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.80 19.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.89-2.80) 99.0 (19.89-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.79Å)	Xtriage
Refinement program	PHENIX v1.2	Depositor
R, R_{free}	0.214 , 0.266 0.214 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (2.65%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16899	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: MG, CA, MES, MXV, ACP, GDP, 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	0.44	0/3480	0.65	0/4725
1	C	0.45	0/3505	0.67	0/4759
2	B	0.49	2/3411 (0.1%)	0.66	0/4622
2	D	0.46	1/3224 (0.0%)	0.73	5/4389 (0.1%)
3	E	0.44	0/995	0.62	0/1327
4	F	0.36	0/2434	0.58	3/3311 (0.1%)
All	All	0.44	3/17049 (0.0%)	0.66	8/23133 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	286	VAL	CA-CB	6.37	1.57	1.54
2	D	226	ASN	CB-CG	5.36	1.65	1.52
2	B	302	ALA	CA-C	-5.25	1.47	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	393	ALA	N-CA-C	16.44	128.66	111.07
2	D	145	SER	N-CA-C	11.81	125.42	111.02
2	D	226	ASN	N-CA-C	-6.91	104.72	113.01
4	F	197	ARG	N-CA-C	6.62	119.72	109.07
4	F	88	SER	N-CA-C	5.59	119.11	111.39
2	D	390	ARG	N-CA-C	-5.48	105.30	111.28
2	D	226	ASN	CA-CB-CG	5.25	117.85	112.60
4	F	89	GLU	CB-CA-C	-5.05	110.77	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3318	88	0
1	C	3427	0	3325	51	0
2	B	3336	0	3197	74	0
2	D	3156	0	2893	78	0
3	E	983	0	966	22	0
4	F	2383	0	2181	51	0
5	A	32	0	12	0	0
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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	5	0
9	B	24	0	24	2	0
10	B	31	0	0	2	0
11	F	31	0	14	2	0
All	All	16899	0	15966	348	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (348) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.62	0.79
1:A:175:PRO:HA	1:A:178:SER:HB2	1.64	0.79
4:F:79:LYS:O	4:F:83:THR:HG22	1.83	0.77
2:D:292:GLN:HE21	2:D:298:ASN:HD21	1.31	0.77
2:D:324:LYS:O	2:D:328:GLU:HG3	1.89	0.72
2:D:226:ASN:OD1	8:D:501:GDP:N1	2.19	0.72
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.70	0.72
1:A:79:ARG:HH22	1:A:94:THR:HG22	1.56	0.71
2:D:204:ASN:HA	2:D:207:LEU:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HE1	1:A:49:PHE:CZ	2.27	0.70
4:F:197:ARG:NH2	4:F:257:GLU:OE1	2.23	0.70
2:D:143:THR:N	8:D:501:GDP:O1B	2.26	0.69
4:F:135:TYR:O	4:F:145:ASN:ND2	2.25	0.69
1:A:163:LYS:H	1:A:163:LYS:HD3	1.57	0.69
1:C:167:LEU:HD22	1:C:200:CYS:HB3	1.73	0.68
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.75	0.68
4:F:197:ARG:HH22	4:F:257:GLU:CD	2.01	0.68
2:D:100:ASN:HD22	2:D:397:TRP:HE3	1.40	0.66
11:F:401:ACP:H5'2	11:F:401:ACP:O1B	1.97	0.65
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.26	0.65
2:B:81:PHE:O	2:B:84:ILE:HG22	1.97	0.64
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.64
2:B:375:GLN:HE22	2:B:423:GLN:NE2	1.95	0.64
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.80	0.63
2:B:211:CYS:HA	2:B:215:LEU:HD12	1.79	0.63
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.80	0.63
2:D:107:THR:OG1	2:D:108:GLU:N	2.31	0.63
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.80	0.62
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.35	0.62
1:C:178:SER:OG	2:D:350:LYS:NZ	2.31	0.62
1:A:36:MET:HE3	1:A:39:ASP:HB2	1.82	0.61
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.66	0.61
1:A:331:ALA:O	1:A:335:ILE:HG13	2.01	0.60
2:B:299:MET:HE3	2:B:305:PRO:HG3	1.82	0.60
2:B:3:GLU:HB3	2:B:62:ARG:NH1	2.16	0.60
2:B:307:HIS:O	2:B:426:GLN:NE2	2.35	0.60
2:B:406:MET:HE3	2:B:410:GLU:HG3	1.84	0.60
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.37	0.59
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.83	0.59
4:F:200:ASP:OD1	4:F:241:THR:OG1	2.21	0.59
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.84	0.59
1:C:211:ASP:OD1	1:C:214:ARG:NH2	2.36	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.59
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.84	0.59
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.85	0.59
2:B:2:ARG:HB3	2:B:131:GLN:HG2	1.85	0.59
2:D:70:PRO:HG3	2:D:94:GLN:HA	1.85	0.58
1:A:79:ARG:HH12	1:A:94:THR:HG21	1.68	0.58
1:C:132:LEU:O	1:C:164:LYS:NZ	2.37	0.58
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:HH11	2:B:46:ARG:HG2	1.68	0.58
1:A:143:GLY:O	1:A:147:SER:HB3	2.03	0.58
2:D:221:THR:HG23	2:D:224:ASP:H	1.68	0.58
4:F:148:ILE:N	4:F:183:GLN:O	2.30	0.57
2:D:152:ILE:HD12	2:D:164:MET:SD	2.45	0.57
4:F:4:PHE:CZ	4:F:18:SER:HB2	2.40	0.57
4:F:3:THR:OG1	4:F:37:PHE:HA	2.05	0.57
4:F:10:ASN:C	4:F:10:ASN:HD22	2.12	0.57
2:D:11:GLN:N	8:D:501:GDP:O2B	2.33	0.56
1:A:109:THR:HG21	1:A:411:GLU:OE1	2.06	0.56
2:B:165:ASN:OD1	2:B:198:GLU:HB2	2.05	0.56
4:F:191:LEU:H	4:F:191:LEU:HD12	1.71	0.56
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.87	0.56
2:B:203:ASP:OD2	2:B:380:ARG:NH1	2.35	0.56
2:D:183:TYR:CD1	2:D:408:PHE:HE2	2.23	0.56
4:F:202:ARG:HH21	4:F:318:ASP:CG	2.13	0.56
2:B:40:SER:OG	2:B:42:LEU:HB2	2.06	0.56
3:E:44:ASP:OD1	3:E:44:ASP:N	2.37	0.56
1:A:401:LYS:HE2	2:B:428:ALA:HB1	1.88	0.56
2:D:404:ASP:OD1	2:D:405:GLU:N	2.39	0.56
1:A:103:TYR:HD1	1:A:147:SER:OG	1.88	0.56
1:C:81:GLY:O	1:C:84:ARG:HG2	2.05	0.56
4:F:292:ARG:HG2	4:F:296:MET:HE1	1.86	0.56
4:F:262:MET:HE2	4:F:267:PHE:HA	1.88	0.55
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.41	0.55
2:B:350:LYS:HB2	10:B:505:MXV:C12	2.36	0.55
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.89	0.55
4:F:81:ILE:HA	4:F:87:LEU:HD23	1.87	0.55
2:B:296:SER:N	9:B:504:MES:O3S	2.35	0.55
3:E:135:LYS:O	3:E:139:LEU:HB2	2.07	0.55
4:F:268:ASN:O	4:F:272:MET:HG3	2.07	0.55
1:A:163:LYS:HE2	1:A:164:LYS:HZ2	1.71	0.55
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.42	0.55
1:A:34:GLY:O	1:A:61:HIS:N	2.32	0.54
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.71	0.54
2:B:86:ARG:HE	2:B:122:LYS:HZ3	1.56	0.54
1:A:177:VAL:O	1:A:177:VAL:HG22	2.07	0.54
2:D:23:VAL:O	2:D:27:GLU:HG3	2.07	0.54
2:B:2:ARG:HB3	2:B:131:GLN:CG	2.37	0.54
2:B:38:GLY:HA3	2:B:43:GLN:HE22	1.72	0.54
2:B:392:LYS:HB3	2:B:395:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:50:TYR:CE2	2:D:241:ARG:HG2	2.43	0.54
2:B:178:THR:O	2:B:181:GLU:HG3	2.07	0.54
1:A:180:ALA:O	1:A:183:GLU:HG3	2.08	0.54
2:D:101:TRP:HD1	2:D:145:SER:OG	1.91	0.54
4:F:278:THR:O	4:F:282:SER:OG	2.25	0.54
1:A:296:PHE:CZ	1:A:377:MET:HE1	2.42	0.53
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.90	0.53
2:D:78:SER:OG	2:D:79:GLY:N	2.40	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HD11	1.90	0.53
1:A:213:CYS:O	1:A:217:LEU:HB2	2.09	0.53
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.40	0.53
1:A:185:TYR:OH	1:A:398:MET:HB3	2.08	0.53
2:B:12:CYS:O	2:B:16:ILE:HG12	2.09	0.53
2:D:394:PHE:O	2:D:397:TRP:HB2	2.09	0.53
1:A:134:GLY:HA2	1:A:164:LYS:HB3	1.89	0.52
2:D:189:VAL:HG21	2:D:415:MET:HE3	1.91	0.52
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.44	0.52
1:A:132:LEU:HD23	1:A:164:LYS:HG3	1.92	0.52
2:D:139:LEU:HG	2:D:188:SER:CB	2.40	0.52
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.45	0.51
2:D:139:LEU:HG	2:D:188:SER:HB3	1.93	0.51
2:B:232:THR:OG1	2:B:300:MET:HE3	2.10	0.51
2:B:338:SER:OG	4:F:34:ASN:ND2	2.37	0.51
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.46	0.51
2:D:141:GLY:O	2:D:184:ASN:ND2	2.43	0.51
4:F:326:LYS:HD3	4:F:328:TRP:CE2	2.46	0.51
2:B:249:ASP:OD1	2:B:252:LYS:HB2	2.10	0.51
4:F:40:MET:HE1	4:F:48:PRO:HD2	1.92	0.51
3:E:6:MET:HE2	3:E:6:MET:HA	1.92	0.51
4:F:340:GLN:HA	4:F:343:TYR:HD1	1.76	0.50
4:F:203:SER:HB3	4:F:215:LEU:HD11	1.92	0.50
2:B:329:GLN:O	2:B:332:ASN:HB3	2.12	0.50
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.94	0.50
2:B:86:ARG:HE	2:B:122:LYS:NZ	2.09	0.50
2:B:68:LEU:CD1	2:B:97:ALA:HB2	2.42	0.50
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.94	0.50
4:F:21:LEU:O	4:F:24:THR:OG1	2.29	0.50
1:A:39:ASP:OD2	1:A:61:HIS:HE1	1.95	0.50
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.38	0.50
2:D:141:GLY:HA3	8:D:501:GDP:O5'	2.12	0.50
2:B:7:ILE:O	2:B:135:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:MET:HE3	2:D:371:SER:HB3	1.94	0.49
4:F:4:PHE:HZ	4:F:18:SER:HB2	1.75	0.49
2:D:417:ASP:O	2:D:421:GLU:HG3	2.12	0.49
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.95	0.48
1:A:60:LYS:NZ	1:A:85:GLN:O	2.46	0.48
1:A:134:GLY:HA3	1:A:165:SER:O	2.13	0.48
2:B:2:ARG:O	2:B:49:VAL:HG13	2.13	0.48
2:D:159:TYR:HB3	2:D:162:ARG:HG3	1.95	0.48
2:B:169:VAL:HA	2:B:202:ILE:O	2.14	0.48
1:C:19:ALA:HB1	1:C:232:SER:OG	2.13	0.48
4:F:258:GLU:OE1	4:F:259:GLY:N	2.47	0.48
2:D:46:ARG:NH2	2:D:248:ALA:O	2.46	0.48
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
2:D:383:GLU:HA	2:D:386:THR:HG22	1.96	0.48
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.96	0.48
4:F:288:LYS:HG2	4:F:378:LEU:HD22	1.95	0.48
1:A:154:MET:HG3	1:A:194:THR:HG23	1.94	0.47
1:C:330:ALA:O	1:C:334:THR:HG23	2.14	0.47
2:D:290:THR:HG22	2:D:317:PHE:CZ	2.49	0.47
1:A:295:CYS:HB3	1:A:377:MET:HE3	1.94	0.47
1:A:163:LYS:HG2	1:A:164:LYS:HD3	1.96	0.47
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.96	0.47
1:A:362:VAL:HG21	1:A:368:LEU:O	2.13	0.47
2:D:117:LEU:HA	2:D:120:VAL:HG22	1.95	0.47
2:B:170:MET:HE3	2:B:377:LEU:HD21	1.96	0.47
2:D:286:VAL:O	2:D:290:THR:HG23	2.14	0.47
1:A:30:ILE:HG12	1:A:36:MET:HB2	1.95	0.47
1:A:296:PHE:CE2	1:A:377:MET:HE1	2.50	0.47
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.32	0.47
1:A:155:GLU:HB3	3:E:50:ILE:HD11	1.97	0.47
2:B:293:MET:CG	2:B:367:PHE:HB2	2.44	0.47
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.49	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.47
2:B:36:TYR:C	2:B:37:HIS:HD1	2.21	0.47
2:B:122:LYS:HE3	2:B:122:LYS:HB3	1.75	0.47
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.49	0.47
2:D:63:ALA:C	2:D:64:ILE:HD13	2.40	0.47
1:C:147:SER:HB2	1:C:190:THR:OG1	2.15	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.50	0.47
2:B:335:ASN:OD1	4:F:36:ARG:NH1	2.47	0.47
2:D:191:GLN:OE1	3:E:126:LYS:NZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HG	1:A:145:THR:HG23	1.96	0.46
1:A:132:LEU:O	1:A:164:LYS:HE2	2.15	0.46
2:D:183:TYR:O	2:D:187:LEU:HD12	2.15	0.46
1:A:317:LEU:HD21	1:A:377:MET:HE2	1.97	0.46
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.97	0.46
2:D:50:TYR:HE2	2:D:241:ARG:HG2	1.80	0.46
1:A:163:LYS:H	1:A:163:LYS:CD	2.27	0.46
2:D:6:HIS:CE1	2:D:8:GLN:HG2	2.50	0.46
2:D:400:GLY:O	3:E:137:LYS:HG3	2.15	0.46
1:A:49:PHE:CD1	1:A:49:PHE:C	2.93	0.46
1:A:123:ARG:HG3	1:A:123:ARG:NH1	2.31	0.46
1:A:345:ASP:O	3:E:28:SER:N	2.47	0.46
1:C:204:VAL:HG22	1:C:302:MET:HE1	1.97	0.46
2:D:332:ASN:HD21	2:D:336:LYS:HE3	1.81	0.46
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.98	0.46
1:A:399:TYR:OH	1:A:415:GLU:HG2	2.17	0.45
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.51	0.45
1:C:12:ALA:HB3	1:C:140:SER:HB3	1.98	0.45
1:A:192:HIS:CG	1:A:421:ALA:HA	2.52	0.45
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.45
2:D:45:GLU:OE1	2:D:243:PRO:HB3	2.15	0.45
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.50	0.45
2:B:2:ARG:HA	2:B:129:CYS:O	2.16	0.45
2:B:70:PRO:HG3	2:B:94:GLN:HE22	1.81	0.45
2:D:139:LEU:HB3	2:D:185:ALA:HA	1.96	0.45
2:D:267:MET:SD	2:D:299:MET:HG3	2.56	0.45
2:D:290:THR:HG22	2:D:317:PHE:HZ	1.81	0.45
4:F:87:LEU:HD13	4:F:87:LEU:N	2.30	0.45
1:A:55:GLU:HG2	1:A:61:HIS:CE1	2.52	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.45
1:C:171:ILE:HD12	1:C:171:ILE:N	2.31	0.45
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.98	0.45
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.52	0.45
2:B:193:VAL:HG12	2:B:194:GLU:HG3	1.99	0.45
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.56	0.45
1:C:292:THR:O	1:C:295:CYS:HB2	2.17	0.45
3:E:72:LEU:O	3:E:76:ARG:HG2	2.17	0.45
4:F:3:THR:O	4:F:38:ASN:HB2	2.17	0.45
1:C:140:SER:HA	1:C:171:ILE:HB	1.99	0.45
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.67	0.45
2:D:323:MET:HA	2:D:326:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:394:PHE:O	2:D:395:LEU:C	2.59	0.45
1:A:109:THR:OG1	1:A:110:ILE:N	2.50	0.45
1:A:156:ARG:O	1:A:159:VAL:HG22	2.17	0.45
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.99	0.45
3:E:23:ILE:C	3:E:24:LEU:HD12	2.42	0.45
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.52	0.44
1:A:287:SER:OG	1:A:290:GLU:HG3	2.17	0.44
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.44
1:C:204:VAL:HG22	1:C:302:MET:CE	2.47	0.44
1:C:296:PHE:CE2	1:C:377:MET:HE1	2.52	0.44
4:F:87:LEU:N	4:F:87:LEU:CD1	2.80	0.44
2:B:329:GLN:O	2:B:333:VAL:HG23	2.16	0.44
2:D:10:GLY:O	2:D:14:ASN:ND2	2.27	0.44
2:D:306:ARG:HG3	2:D:340:TYR:CZ	2.52	0.44
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.53	0.44
2:D:7:ILE:HG12	2:D:64:ILE:HB	2.00	0.44
4:F:287:ILE:HG12	4:F:319:PHE:CE2	2.51	0.44
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.32	0.44
1:C:293:ASN:OD1	1:C:339:ARG:NH1	2.51	0.44
2:D:318:ARG:HG2	2:D:354:CYS:HB3	1.99	0.44
1:A:398:MET:HE3	1:A:404:PHE:CD2	2.52	0.44
1:C:176:GLN:NE2	1:C:207:GLU:HG3	2.33	0.44
2:D:7:ILE:O	2:D:135:LEU:HD12	2.17	0.44
2:D:232:THR:OG1	2:D:300:MET:HE3	2.18	0.44
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.99	0.44
1:A:280:LYS:HD3	1:A:283:HIS:HB2	2.00	0.44
2:B:94:GLN:OE1	1:C:1:MET:HE2	2.17	0.44
2:B:261:PRO:O	2:B:264:HIS:ND1	2.50	0.44
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.18	0.44
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.44
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.53	0.43
2:B:67:ASP:O	2:B:92:PHE:HA	2.17	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.53	0.43
2:B:296:SER:HA	2:B:299:MET:HG2	1.99	0.43
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.43
9:B:504:MES:H81	9:B:504:MES:H51	1.64	0.43
1:C:46:ASP:OD1	1:C:46:ASP:N	2.49	0.43
2:D:66:VAL:HA	2:D:91:VAL:O	2.18	0.43
3:E:10:GLU:O	3:E:10:GLU:HG2	2.17	0.43
4:F:3:THR:HB	4:F:30:LEU:HD11	2.00	0.43
2:B:94:GLN:HB3	1:C:1:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:TYR:OH	2:B:407:GLU:OE2	2.24	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.54	0.43
2:D:89:ASN:HA	2:D:119:VAL:HG11	2.01	0.43
2:D:221:THR:OG1	2:D:222:TYR:N	2.51	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.00	0.43
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.53	0.43
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.00	0.43
2:D:106:TYR:HE2	3:E:130:ALA:HA	1.83	0.43
4:F:163:SER:OG	4:F:164:SER:N	2.50	0.43
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.82	0.43
2:B:320:ARG:HH11	2:B:320:ARG:HG2	1.84	0.43
2:D:164:MET:HE2	2:D:164:MET:HB2	1.90	0.43
4:F:298:ILE:HD12	4:F:302:ILE:HD13	2.00	0.43
1:A:221:ARG:HA	1:A:221:ARG:HD2	1.63	0.43
1:A:401:LYS:HD3	2:B:344:TRP:CD2	2.54	0.43
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.01	0.43
2:D:395:LEU:O	2:D:399:THR:HG22	2.19	0.43
1:A:269:LEU:HD11	1:A:301:GLN:HB3	2.01	0.43
2:B:246:LEU:HD12	2:B:246:LEU:HA	1.81	0.43
2:B:251:ARG:O	2:B:255:VAL:HG23	2.18	0.43
2:B:363:MET:HE3	2:B:363:MET:HB3	1.82	0.43
3:E:69:LEU:HD23	3:E:69:LEU:HA	1.82	0.43
2:B:388:MET:HE3	2:B:388:MET:HB2	1.76	0.42
3:E:13:LYS:HZ2	3:E:13:LYS:HB3	1.83	0.42
4:F:288:LYS:HG2	4:F:378:LEU:CD2	2.49	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.19	0.42
2:D:395:LEU:O	2:D:396:HIS:C	2.60	0.42
4:F:221:LEU:HD12	4:F:221:LEU:HA	1.45	0.42
1:A:68:VAL:HG22	1:A:93:ILE:HB	2.01	0.42
2:D:372:THR:OG1	2:D:426:GLN:HG3	2.19	0.42
2:B:46:ARG:O	2:B:49:VAL:HG23	2.18	0.42
2:B:285:THR:HG23	2:B:288:GLU:OE1	2.19	0.42
1:A:346:TRP:CD1	1:A:346:TRP:H	2.37	0.42
2:B:219:THR:HG21	1:C:326:LYS:HB2	2.01	0.42
1:A:172:TYR:CE2	1:A:387:ALA:HB1	2.54	0.42
2:B:51:TYR:O	2:B:62:ARG:NH2	2.53	0.42
1:C:1:MET:HB2	1:C:2:ARG:H	1.48	0.42
2:D:4:ILE:HD12	2:D:49:VAL:CG1	2.50	0.42
2:B:403:MET:HE2	2:B:403:MET:HB3	1.91	0.42
3:E:44:ASP:HA	3:E:45:PRO:HD3	1.80	0.42
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:PRO:O	1:A:266:HIS:ND1	2.41	0.42
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.46	0.42
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.35	0.42
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.44	0.42
1:A:195:LEU:HD23	1:A:195:LEU:HA	1.88	0.42
1:A:199:ASP:HB3	1:A:256:GLN:HG2	2.02	0.42
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.20	0.42
4:F:287:ILE:HG12	4:F:319:PHE:CD2	2.55	0.42
1:C:228:ASN:O	1:C:232:SER:OG	2.35	0.41
3:E:56:ALA:O	3:E:59:GLU:HG3	2.20	0.41
4:F:197:ARG:CZ	4:F:257:GLU:OE1	2.68	0.41
1:C:6:SER:O	1:C:65:ALA:HA	2.20	0.41
1:C:105:ARG:NH1	1:C:411:GLU:OE2	2.51	0.41
2:D:106:TYR:CE2	3:E:130:ALA:HA	2.54	0.41
2:D:201:CYS:SG	2:D:265:PHE:HB3	2.60	0.41
1:A:163:LYS:HE2	1:A:164:LYS:NZ	2.35	0.41
2:B:126:SER:O	2:B:126:SER:OG	2.38	0.41
2:B:293:MET:HG3	2:B:367:PHE:HB2	2.02	0.41
1:C:71:GLU:OE2	1:C:73:THR:N	2.49	0.41
1:C:90:GLU:HB3	1:C:121:ARG:HD2	2.01	0.41
3:E:123:LEU:O	3:E:126:LYS:HB3	2.19	0.41
4:F:191:LEU:HD23	4:F:196:HIS:HE1	1.84	0.41
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.85	0.41
1:A:67:PHE:N	1:A:67:PHE:CD2	2.89	0.41
1:C:270:ALA:CB	1:C:302:MET:HE2	2.49	0.41
2:D:139:LEU:HD13	2:D:168:SER:HB3	2.02	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.83	0.41
1:A:142:GLY:HA3	1:A:183:GLU:OE1	2.21	0.41
1:C:36:MET:HG2	1:C:39:ASP:H	1.85	0.41
1:C:204:VAL:HG22	1:C:302:MET:SD	2.61	0.41
1:C:358:GLN:H	1:C:358:GLN:CD	2.28	0.41
4:F:74:LYS:HE2	11:F:401:ACP:O2A	2.21	0.41
2:B:290:THR:HG22	2:B:333:VAL:HG21	2.03	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.41
2:B:203:ASP:CG	2:B:380:ARG:HH22	2.28	0.41
1:C:401:LYS:NZ	2:D:429:THR:O	2.40	0.41
4:F:296:MET:HE1	4:F:380:HIS:HB3	2.02	0.41
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.55	0.41
2:B:167:PHE:CE2	2:B:233:MET:HG2	2.56	0.41
2:D:332:ASN:ND2	2:D:336:LYS:HE3	2.36	0.41
2:B:36:TYR:HE1	2:B:43:GLN:NE2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:GLU:HA	2:D:70:PRO:HD3	1.92	0.40
2:D:360:GLY:C	2:D:361:LEU:HD23	2.45	0.40
4:F:200:ASP:O	4:F:221:LEU:HD12	2.19	0.40
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.02	0.40
1:A:214:ARG:HG2	1:A:219:ILE:O	2.22	0.40
2:B:248:ALA:HA	10:B:505:MXV:N02	2.36	0.40
1:C:115:ILE:HG23	1:C:116:ASP:N	2.36	0.40
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.56	0.40
2:D:102:ALA:HB2	2:D:403:MET:CE	2.52	0.40
2:D:141:GLY:CA	8:D:501:GDP:H5'	2.51	0.40
4:F:287:ILE:HG13	4:F:327:VAL:HG11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	409 (94%)	26 (6%)	0	100	100
1	C	438/450 (97%)	421 (96%)	17 (4%)	0	100	100
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	D	417/445 (94%)	395 (95%)	22 (5%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	302/384 (79%)	290 (96%)	12 (4%)	0	100	100
All	All	2135/2317 (92%)	2045 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	365/378 (97%)	360 (99%)	5 (1%)	59	85
1	C	368/378 (97%)	363 (99%)	5 (1%)	59	85
2	B	362/383 (94%)	354 (98%)	8 (2%)	45	78
2	D	326/383 (85%)	316 (97%)	10 (3%)	35	70
3	E	104/127 (82%)	101 (97%)	3 (3%)	37	73
4	F	233/342 (68%)	221 (95%)	12 (5%)	21	53
All	All	1758/1991 (88%)	1715 (98%)	43 (2%)	43	77

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLU
1	A	94	THR
1	A	177	VAL
1	A	356	ASN
1	A	381	THR
2	B	19	LYS
2	B	45	GLU
2	B	69	GLU
2	B	77	ARG
2	B	92	PHE
2	B	115	SER
2	B	145	SER
2	B	382	SER
1	C	66	VAL
1	C	82	THR
1	C	177	VAL
1	C	241	SER
1	C	384	ILE
2	D	26	ASP
2	D	40	SER
2	D	108	GLU
2	D	115	SER

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Mol	Chain	Res	Type
2	D	155	ILE
2	D	176	SER
2	D	222	TYR
2	D	382	SER
2	D	386	THR
2	D	412	GLU
3	E	9	ILE
3	E	18	GLN
3	E	28	SER
4	F	12	SER
4	F	13	VAL
4	F	26	GLN
4	F	87	LEU
4	F	148	ILE
4	F	161	LEU
4	F	191	LEU
4	F	202	ARG
4	F	220	VAL
4	F	282	SER
4	F	353	VAL
4	F	377	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	61	HIS
1	A	128	GLN
1	A	393	HIS
2	B	43	GLN
2	B	83	GLN
2	B	191	GLN
2	B	423	GLN
1	C	128	GLN
1	C	356	ASN
1	C	406	HIS
2	D	6	HIS
2	D	8	GLN
2	D	134	GLN
2	D	292	GLN
2	D	335	ASN
2	D	337	ASN

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Mol	Chain	Res	Type
2	D	347	ASN
2	D	375	GLN
2	D	396	HIS
3	E	103	GLN
3	E	108	ASN
3	E	124	GLN
4	F	183	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	D	501	-	29,30,30	1.64	6 (20%)	45,47,47	2.10	10 (22%)
11	ACP	F	401	-	31,33,33	1.34	2 (6%)	47,52,52	0.92	2 (4%)
8	GDP	B	501	6	29,30,30	1.47	3 (10%)	45,47,47	1.94	10 (22%)
9	MES	B	504	-	12,12,12	2.53	1 (8%)	15,16,16	1.94	4 (26%)
10	MXV	B	505	-	35,35,35	2.28	8 (22%)	48,51,51	2.10	10 (20%)

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	1.01	3 (9%)	50,54,54	1.80	12 (24%)
9	MES	B	503	-	12,12,12	2.30	1 (8%)	15,16,16	1.94	5 (33%)
5	GTP	C	501	6	33,34,34	0.86	0	50,54,54	1.80	14 (28%)

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
8	GDP	D	501	-	-	4/16/32/32	0/3/3/3
11	ACP	F	401	-	-	4/19/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	MXV	B	505	-	-	0/14/14/14	0/5/5/5
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-8.42	1.65	1.77
10	B	505	MXV	C20-C03	-8.38	1.39	1.49
9	B	503	MES	C8-S	-7.56	1.67	1.77
8	B	501	GDP	PA-O3A	5.48	1.65	1.59
11	F	401	ACP	PB-O3A	5.24	1.64	1.58
11	F	401	ACP	PA-O3A	5.19	1.65	1.59
10	B	505	MXV	C10-C08	-4.87	1.38	1.47
10	B	505	MXV	C11-C12	-4.45	1.37	1.41
8	D	501	GDP	C6-N1	-4.43	1.30	1.38
10	B	505	MXV	C17-N16	-4.25	1.33	1.37
8	D	501	GDP	C5-N7	-3.86	1.31	1.39
10	B	505	MXV	C03-C04	3.25	1.43	1.40
10	B	505	MXV	O30-C22	2.76	1.41	1.37
8	B	501	GDP	C5-C4	2.70	1.46	1.38
8	B	501	GDP	C6-N1	-2.56	1.34	1.38
5	A	501	GTP	C2-N3	2.43	1.39	1.33
10	B	505	MXV	C13-C12	2.42	1.43	1.39
8	D	501	GDP	C5-C4	2.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C8-N9	-2.29	1.32	1.37
8	D	501	GDP	C2-N1	-2.28	1.32	1.37
10	B	505	MXV	C04-N09	-2.17	1.35	1.39
5	A	501	GTP	PA-O3A	2.16	1.61	1.59
5	A	501	GTP	C5-N7	-2.12	1.34	1.39
8	D	501	GDP	O4'-C4'	-2.01	1.40	1.45

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-7.88	115.85	128.39
10	B	505	MXV	C04-C05-N07	6.05	108.57	105.13
8	B	501	GDP	C5-C4-N3	-6.02	118.82	128.39
9	B	504	MES	C5-N4-C3	5.77	121.27	108.84
8	D	501	GDP	C2-N3-C4	5.33	121.48	112.30
5	A	501	GTP	C5-C4-N3	-5.17	120.17	128.39
8	B	501	GDP	C2-N3-C4	5.16	121.19	112.30
8	D	501	GDP	N9-C4-N3	5.16	136.27	125.95
5	C	501	GTP	C2-N3-C4	4.97	120.86	112.30
5	C	501	GTP	C5-C4-N3	-4.85	120.67	128.39
10	B	505	MXV	C05-C04-N09	-4.73	106.21	110.31
8	B	501	GDP	N9-C4-N3	4.55	135.05	125.95
10	B	505	MXV	C06-C05-C04	-4.51	118.33	122.57
11	F	401	ACP	PB-O3A-PA	-4.48	117.74	132.37
5	A	501	GTP	O2B-PB-O3B	4.47	119.34	107.27
10	B	505	MXV	C31-O30-C22	-4.33	111.16	117.51
5	A	501	GTP	C2-N3-C4	4.28	119.68	112.30
9	B	503	MES	C5-N4-C3	4.25	117.99	108.84
10	B	505	MXV	C12-N16-C17	3.96	110.83	108.35
10	B	505	MXV	C13-C12-C11	-3.91	119.17	122.36
8	B	501	GDP	C6-C5-N7	3.71	137.04	130.29
10	B	505	MXV	C18-C17-N16	-3.67	106.92	110.39
9	B	503	MES	C6-C5-N4	-3.66	104.56	110.12
5	C	501	GTP	O2B-PB-O3B	3.52	116.79	107.27
5	A	501	GTP	N9-C4-N3	3.37	132.70	125.95
5	A	501	GTP	C2-N1-C6	-3.36	119.02	125.11
8	D	501	GDP	C4-C5-N7	-3.12	105.73	110.67
5	C	501	GTP	C8-N7-C5	3.06	109.72	104.26
10	B	505	MXV	C04-C03-N02	3.04	119.70	118.02
8	B	501	GDP	C4-C5-N7	-3.03	105.86	110.67
11	F	401	ACP	O2B-PB-O1B	-3.03	100.10	109.95
5	C	501	GTP	N9-C8-N7	-2.98	107.87	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O2A-PA-O3A	2.89	115.09	107.27
5	A	501	GTP	O6-C6-C5	-2.87	118.95	126.53
8	B	501	GDP	O2A-PA-O3A	2.81	114.87	107.27
9	B	503	MES	O3S-S-C8	2.71	111.31	106.00
8	D	501	GDP	C3'-C2'-C1'	2.69	106.55	101.46
5	A	501	GTP	N9-C8-N7	-2.67	108.45	113.40
8	D	501	GDP	C6-C5-N7	2.64	135.09	130.29
5	C	501	GTP	N9-C4-N3	2.63	131.22	125.95
5	C	501	GTP	C2-N1-C6	-2.62	120.36	125.11
5	A	501	GTP	O2G-PG-O3B	2.62	113.41	104.64
5	A	501	GTP	O2A-PA-O3A	2.59	114.27	107.27
9	B	503	MES	C7-N4-C5	2.59	118.14	111.24
8	D	501	GDP	C2-N1-C6	-2.56	120.47	125.11
5	A	501	GTP	O3B-PB-O1B	-2.52	103.12	110.70
5	A	501	GTP	C8-N7-C5	2.50	108.72	104.26
5	C	501	GTP	N2-C2-N1	2.47	121.98	116.76
10	B	505	MXV	O30-C22-C23	2.42	119.28	115.14
5	A	501	GTP	C5-C6-N1	2.40	119.37	113.25
8	B	501	GDP	C8-N7-C5	2.38	108.50	104.26
9	B	504	MES	C6-C5-N4	-2.37	106.52	110.12
5	C	501	GTP	O6-C6-C5	-2.36	120.31	126.53
5	C	501	GTP	C4-C5-N7	-2.35	106.95	110.67
9	B	504	MES	C8-C7-N4	-2.34	103.51	112.36
5	C	501	GTP	C5-C6-N1	2.25	118.97	113.25
8	D	501	GDP	O3B-PB-O2B	2.24	116.21	107.80
8	B	501	GDP	C5-C6-N1	2.18	118.81	113.25
8	D	501	GDP	C5'-C4'-C3'	-2.16	107.44	115.21
9	B	503	MES	O1S-S-C8	2.13	109.95	106.73
5	C	501	GTP	O3'-C3'-C4'	-2.13	104.97	111.08
8	B	501	GDP	O6-C6-C5	-2.12	120.94	126.53
8	B	501	GDP	C2-N1-C6	-2.11	121.28	125.11
10	B	505	MXV	C14-C13-C12	2.11	122.55	118.28
8	D	501	GDP	C8-N7-C5	2.09	107.98	104.26
9	B	504	MES	O2S-S-C8	2.04	109.81	106.73
5	C	501	GTP	N1-C2-N3	-2.02	119.62	123.32

There are no chirality outliers.

All (33) 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

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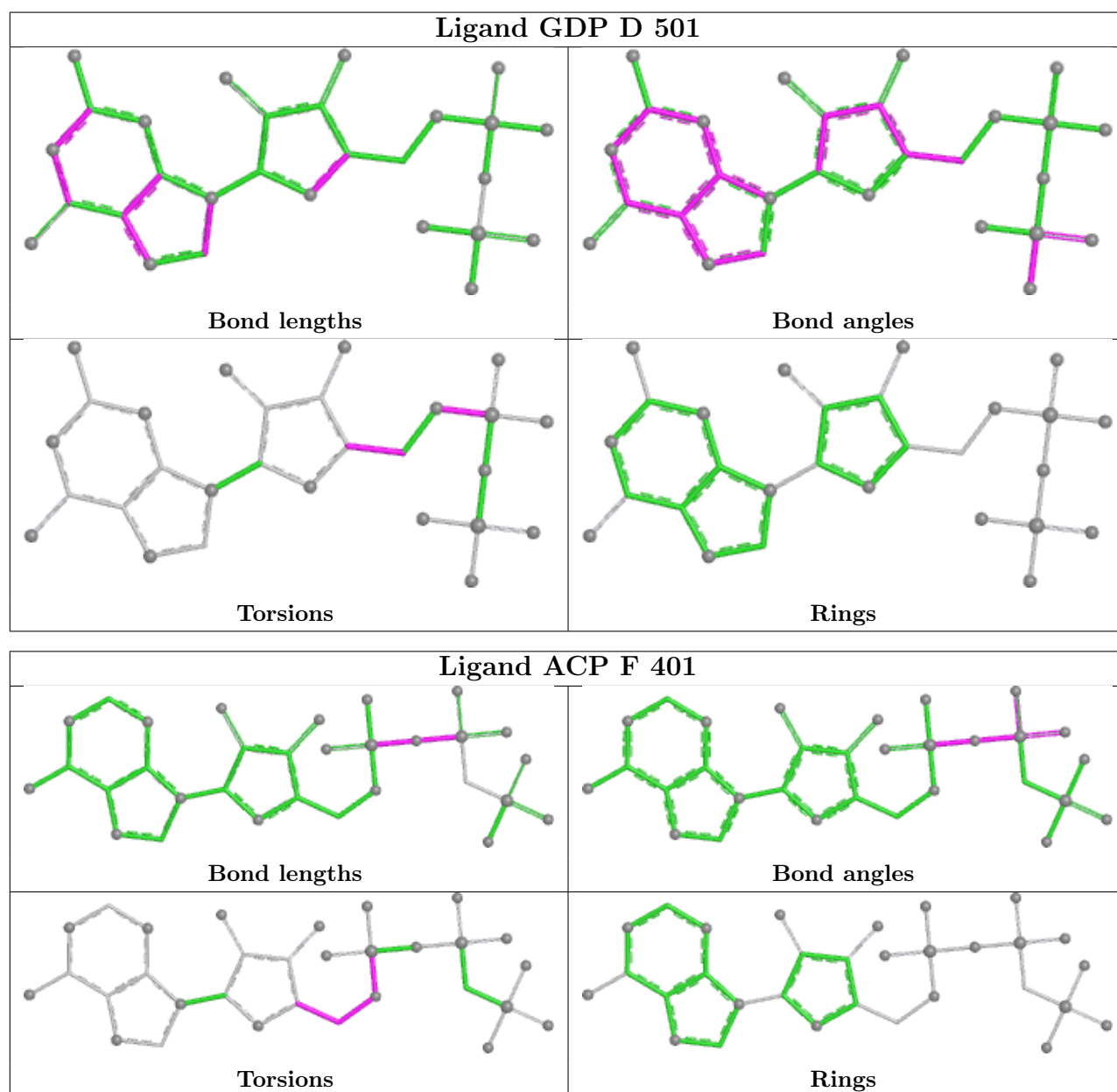
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C5
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O3S
11	F	401	ACP	C5'-O5'-PA-O1A
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	503	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	C4'-C5'-O5'-PA
5	A	501	GTP	PG-O3B-PB-O1B
5	C	501	GTP	PG-O3B-PB-O1B
5	A	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PG-O3B-PB-O2B

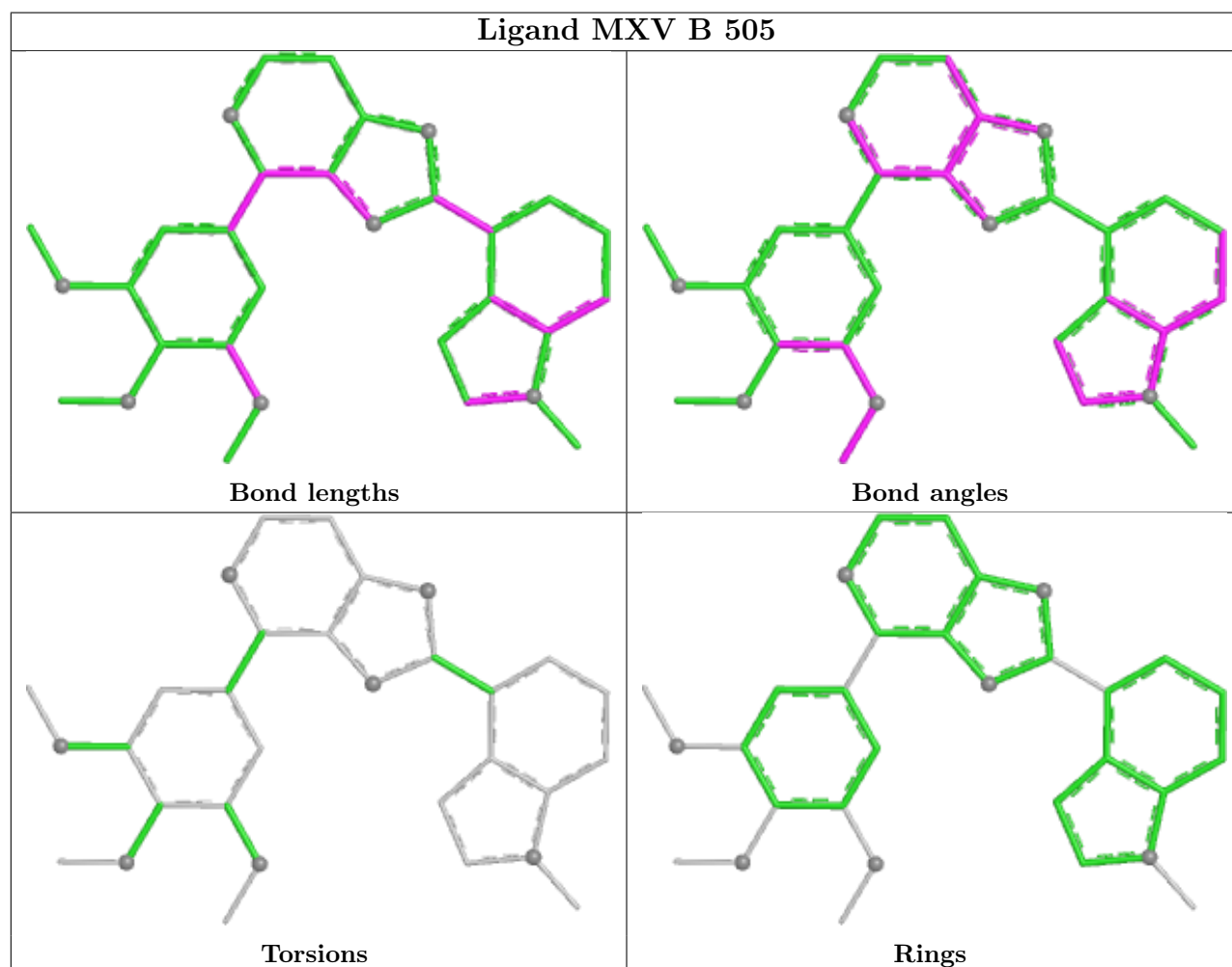
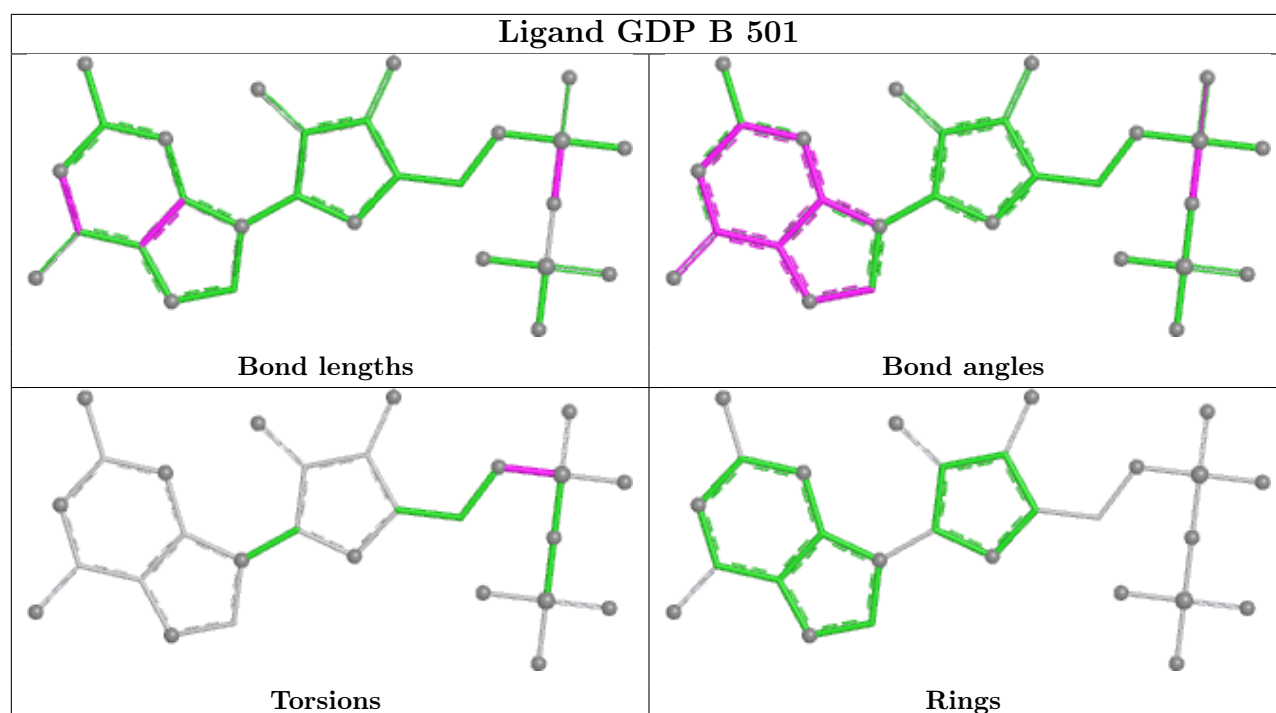
There are no ring outliers.

5 monomers are involved in 12 short contacts:

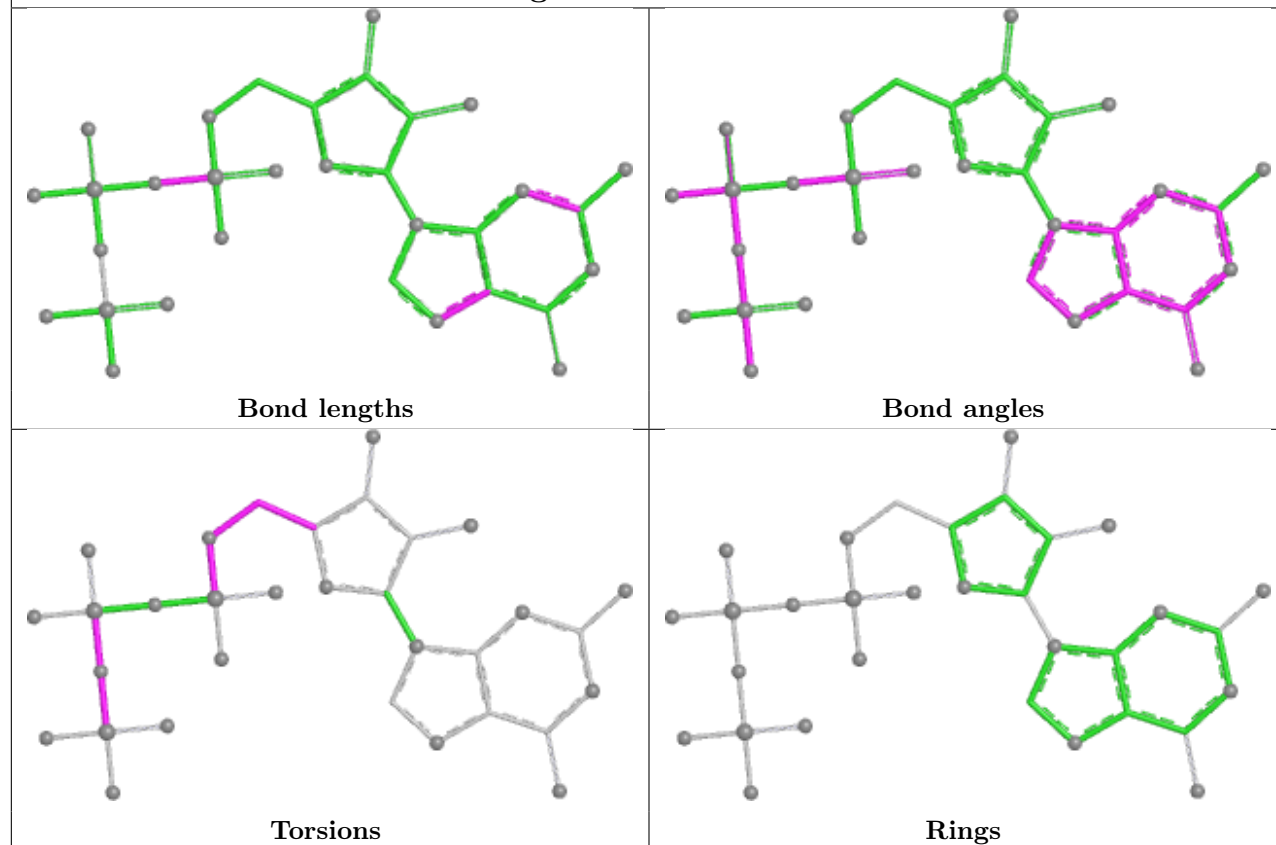
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	5	0
11	F	401	ACP	2	0
8	B	501	GDP	1	0
9	B	504	MES	2	0
10	B	505	MXV	2	0

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.

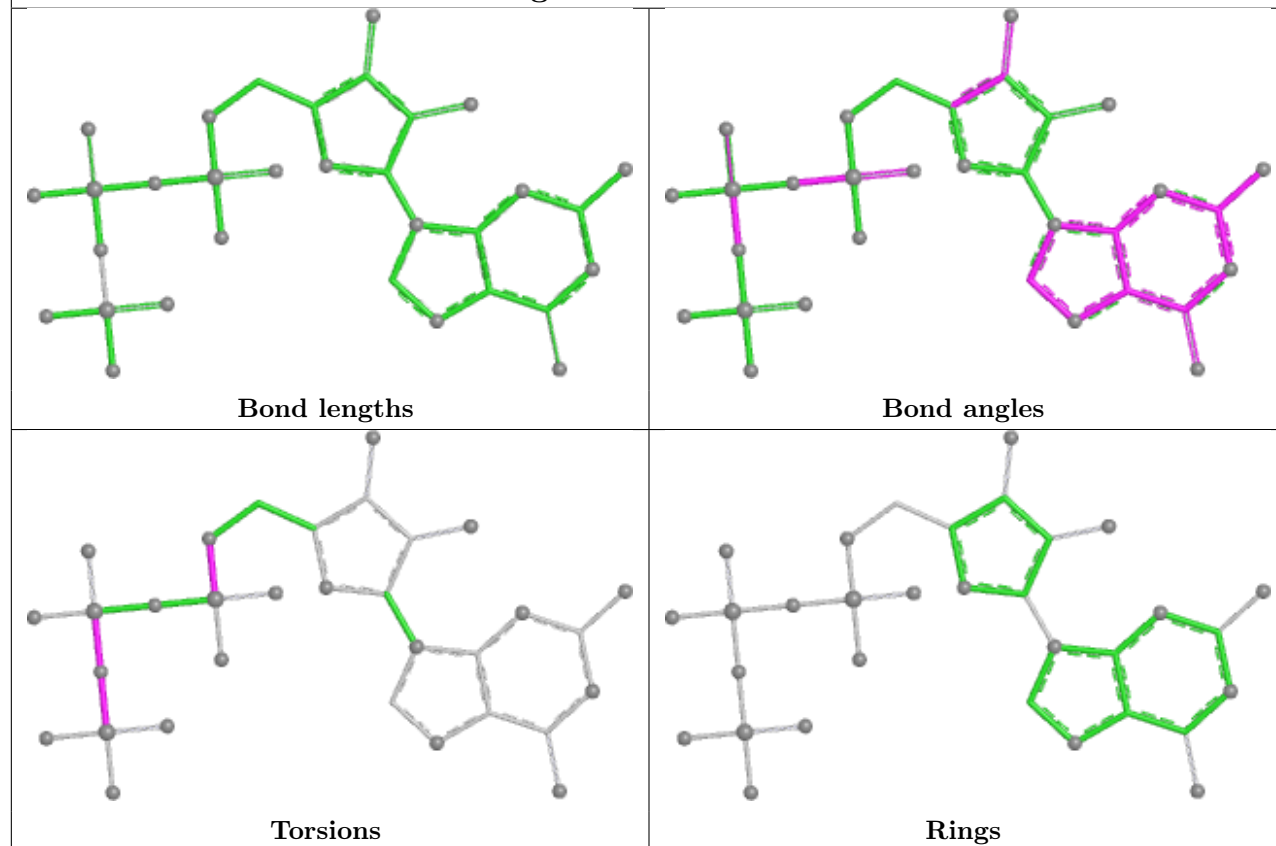




Ligand GTP A 501



Ligand GTP C 501



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	437/450 (97%)	-0.10	5 (1%) 78 70	30, 52, 78, 90	0
1	C	440/450 (97%)	-0.52	3 (0%) 84 77	23, 38, 64, 82	0
2	B	427/445 (95%)	-0.15	10 (2%) 61 51	25, 48, 85, 128	0
2	D	421/445 (94%)	0.72	48 (11%) 10 7	35, 74, 109, 130	0
3	E	121/143 (84%)	0.41	5 (4%) 41 33	36, 67, 108, 122	1 (0%)
4	F	316/384 (82%)	0.88	58 (18%) 3 2	40, 79, 134, 150	0
All	All	2162/2317 (93%)	0.13	129 (5%) 27 21	23, 56, 107, 150	1 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	225	SER	5.8
4	F	167	SER	4.8
4	F	253	TYR	4.6
2	D	216	LYS	4.5
4	F	243	HIS	4.5
4	F	244	CYS	4.2
2	D	1	MET	4.2
4	F	140	GLU	4.2
2	D	99	ASN	4.1
4	F	181	VAL	4.1
4	F	362	ALA	3.9
4	F	143	GLU	3.8
4	F	147	TRP	3.8
2	D	98	GLY	3.8
4	F	99	VAL	3.7
4	F	226	GLU	3.6
4	F	198	LYS	3.6
2	D	37	HIS	3.6
2	B	57	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	171	ASP	3.5
2	D	106	TYR	3.5
4	F	191	LEU	3.4
4	F	256	TYR	3.4
4	F	161	LEU	3.3
2	D	383	GLU	3.3
2	D	247	ASN	3.3
2	D	29	GLY	3.3
4	F	252	ASN	3.2
2	B	55	THR	3.2
2	D	393	ALA	3.1
4	F	224	SER	3.1
2	D	69	GLU	3.1
4	F	88	SER	3.1
4	F	230	SER	3.1
4	F	148	ILE	3.1
3	E	140	LYS	3.1
2	D	302	ALA	3.0
4	F	195	GLY	3.0
4	F	261	GLU	3.0
2	D	215	LEU	2.9
2	B	327	ASP	2.9
4	F	257	GLU	2.9
4	F	222	ARG	2.9
3	E	133	VAL	2.9
4	F	263	PHE	2.9
2	D	360	GLY	2.9
2	D	140	GLY	2.8
4	F	166	ALA	2.8
4	F	255	ARG	2.8
3	E	141	GLU	2.8
1	C	440	VAL	2.8
4	F	194	PRO	2.8
1	A	86	LEU	2.7
2	D	72	THR	2.7
2	D	208	TYR	2.7
4	F	170	LEU	2.7
2	D	105	HIS	2.7
2	D	386	THR	2.7
1	C	340	SER	2.7
4	F	259	GLY	2.6
2	B	245	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	283	HIS	2.6
2	D	101	TRP	2.6
2	B	80	PRO	2.6
2	D	395	LEU	2.6
2	D	220	PRO	2.6
4	F	136	ASN	2.5
2	D	362	LYS	2.5
2	D	42	LEU	2.5
2	D	403	MET	2.5
2	D	56	GLY	2.5
2	D	32	PRO	2.4
1	A	38	SER	2.4
2	D	25	SER	2.4
2	D	391	ARG	2.4
2	D	81	PHE	2.4
2	D	212	PHE	2.4
4	F	163	SER	2.4
4	F	262	MET	2.4
2	D	44	LEU	2.4
4	F	100	ILE	2.4
4	F	10	ASN	2.3
4	F	172	PHE	2.3
2	B	274	THR	2.3
2	D	246	LEU	2.3
4	F	240	LEU	2.3
3	E	6	MET	2.3
2	D	397	TRP	2.3
4	F	98	TYR	2.3
4	F	142	ARG	2.3
4	F	130	VAL	2.3
4	F	25	GLY	2.3
2	D	77	ARG	2.3
2	D	70	PRO	2.2
2	D	290	THR	2.2
4	F	220	VAL	2.2
4	F	135	TYR	2.2
2	D	93	GLY	2.2
2	B	280	GLN	2.2
3	E	28	SER	2.2
4	F	89	GLU	2.2
2	D	30	ILE	2.2
4	F	141	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	217	LEU	2.2
4	F	134	ALA	2.2
1	A	256	GLN	2.2
2	D	33	THR	2.2
2	D	320	ARG	2.1
4	F	173	ILE	2.1
4	F	145	ASN	2.1
2	D	96	GLY	2.1
2	D	285	THR	2.1
4	F	175	GLU	2.1
2	B	39	ASP	2.1
1	A	56	THR	2.1
4	F	133	ALA	2.1
4	F	245	ILE	2.1
2	D	179	VAL	2.1
4	F	102	PRO	2.1
2	D	48	ASN	2.1
4	F	192	LEU	2.1
4	F	138	ARG	2.1
2	D	50	TYR	2.1
2	B	275	SER	2.0
1	A	437	VAL	2.0
4	F	132	LEU	2.0
2	B	283	ALA	2.0
2	D	431	ASP	2.0
4	F	9	GLU	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](#)

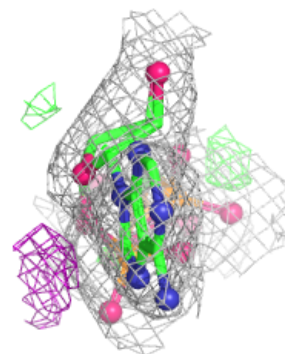
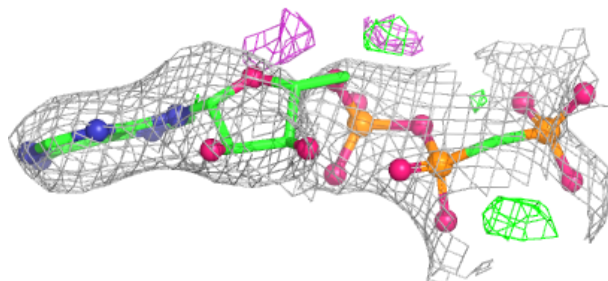
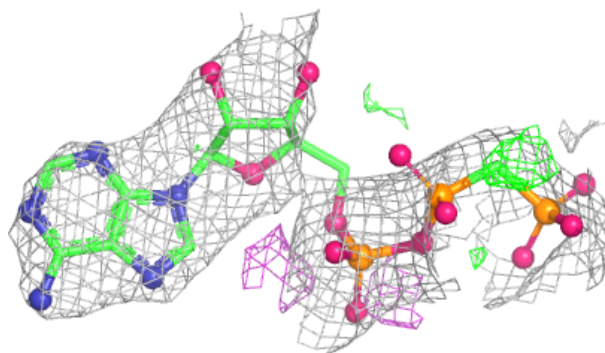
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	ACP	F	401	31/31	0.73	0.17	93,117,154,164	0
8	GDP	D	501	28/28	0.83	0.15	65,77,89,96	0
9	MES	B	503	12/12	0.89	0.13	47,59,80,84	0
10	MXV	B	505	31/31	0.90	0.10	41,51,57,61	0
9	MES	B	504	12/12	0.90	0.11	74,78,87,92	0
6	MG	C	502	1/1	0.95	0.21	37,37,37,37	0
8	GDP	B	501	28/28	0.97	0.07	22,37,46,68	0
6	MG	B	502	1/1	0.97	0.23	40,40,40,40	0
5	GTP	A	501	32/32	0.97	0.06	34,40,45,45	0
7	CA	A	503	1/1	0.98	0.03	82,82,82,82	0
7	CA	C	503	1/1	0.98	0.04	57,57,57,57	0
5	GTP	C	501	32/32	0.98	0.05	29,34,37,39	0
6	MG	A	502	1/1	0.98	0.21	39,39,39,39	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.

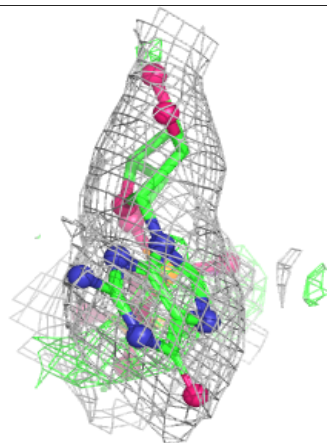
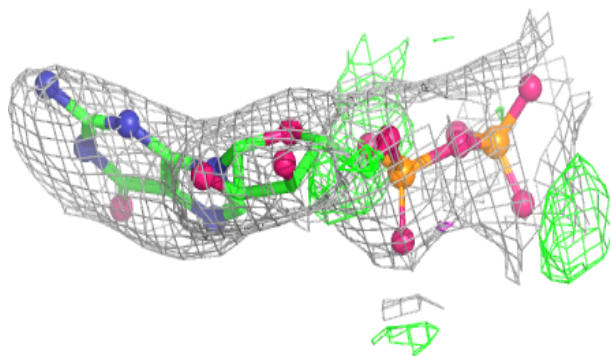
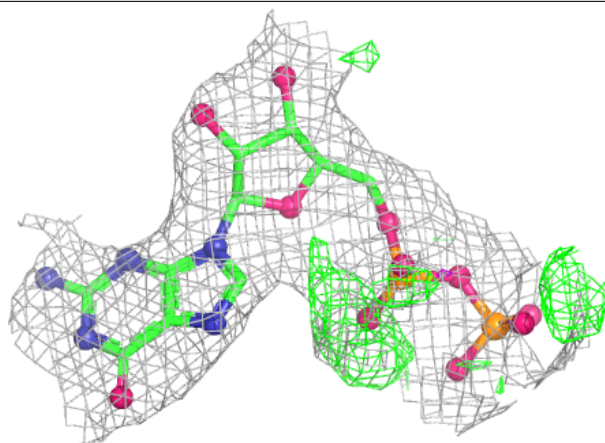
Electron density around ACP F 401:

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



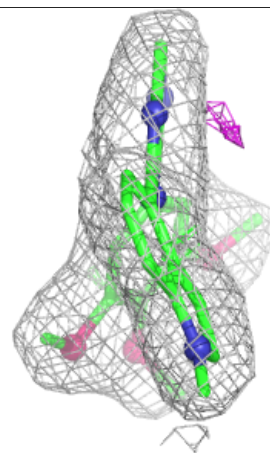
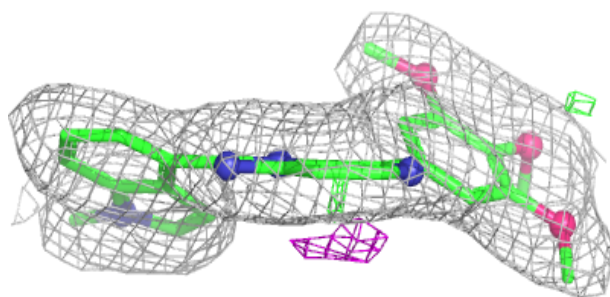
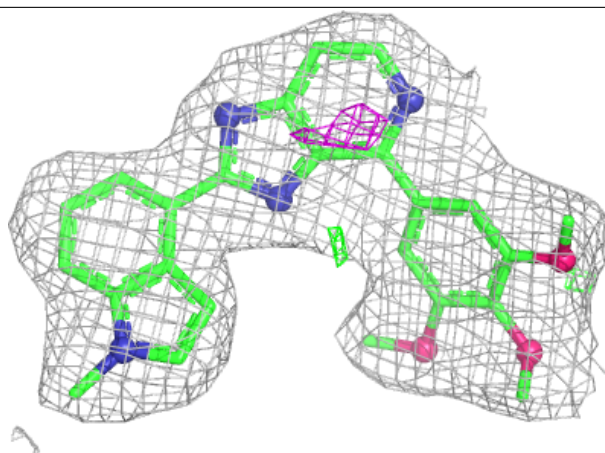
Electron density around GDP D 501:

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



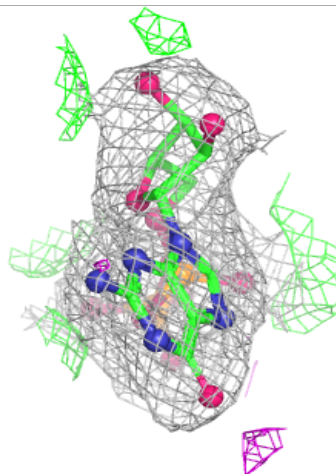
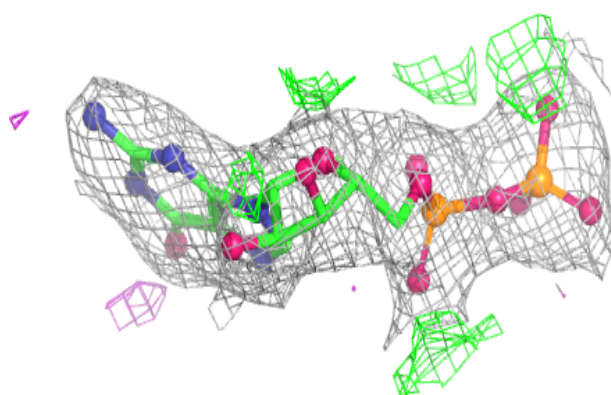
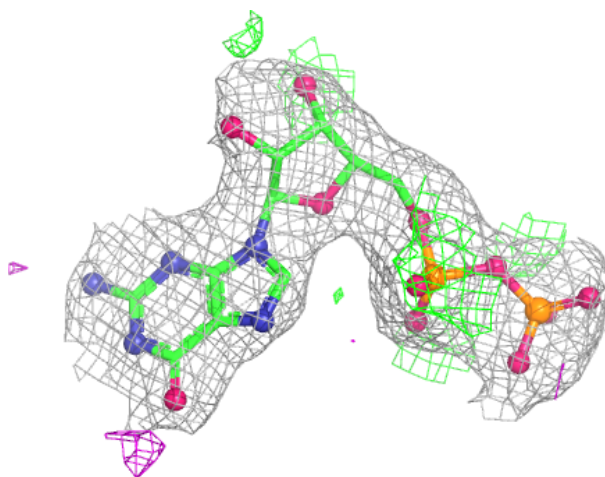
Electron density around MXV B 505:

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



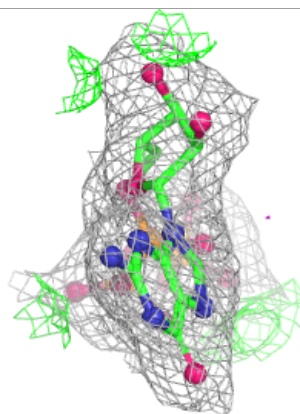
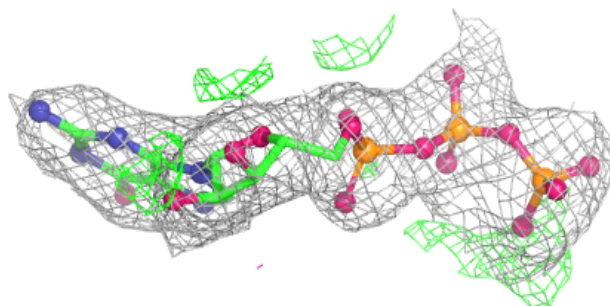
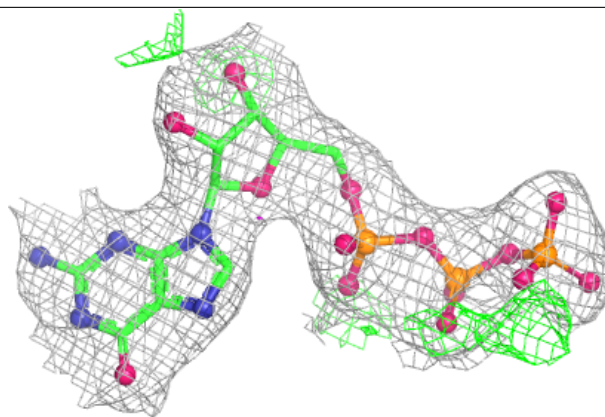
Electron density around GDP B 501:

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

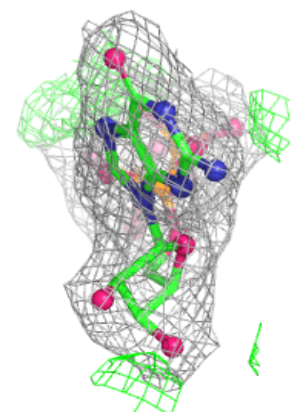
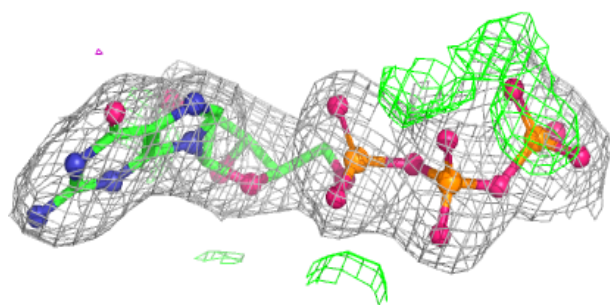
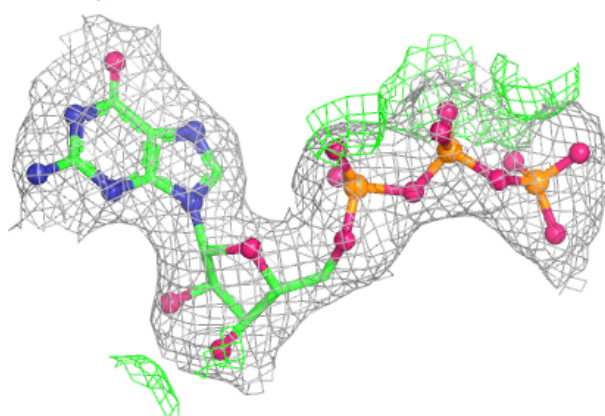


Electron density around GTP A 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.