



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:44 AM EDT

PDB ID : 9H31 / pdb_00009h31
Title : T2R-TTL-PROTAC4 complex
Authors : Maiocchi, A.; Abel, A.-C.; Steinmetz, M.O.; Passarella, D.; Protà, A.E.
Deposited on : 2024-10-15
Resolution : 2.20 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

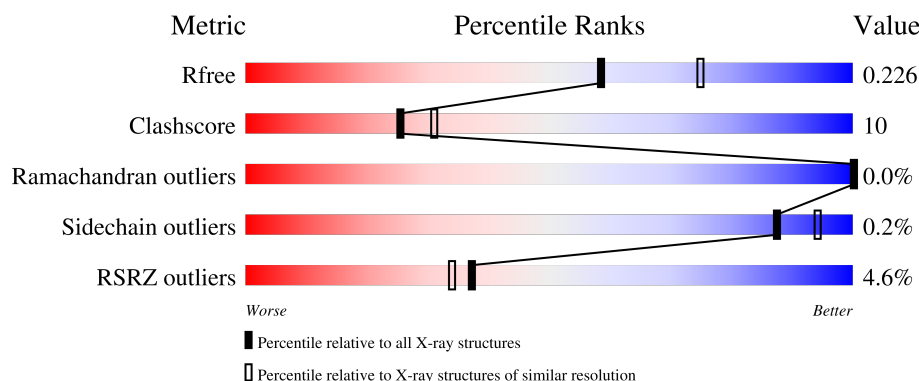
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	<div> <div>4%</div> <div>78%</div> <div>19%</div> <div>.</div> </div>
1	C	451	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	B	445	<div> <div>4%</div> <div>72%</div> <div>23%</div> <div>5%</div> </div>
2	D	445	<div> <div>5%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>
3	E	143	<div> <div>6%</div> <div>70%</div> <div>16%</div> <div>14%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '7%', followed by a large green segment labeled '70%', then a yellow segment labeled '20%', and a small grey segment at the end labeled '10%'.

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18122 atoms, of which 82 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	423	Total	C	N	O	S	0	1	0
			3345	2102	572	644	27			
2	D	426	Total	C	N	O	S	0	0	0
			3342	2098	570	647	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			

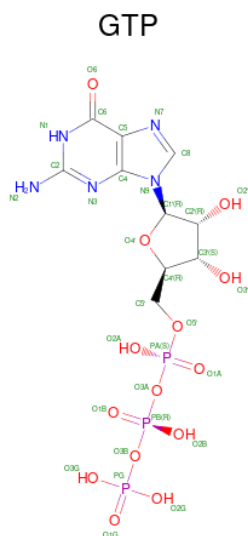
There are 2 discrepancies between the modelled and reference sequences:

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	345	Total	C	N	O	S	0	0	0
			2822	1809	485	514	14			

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



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

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

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

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

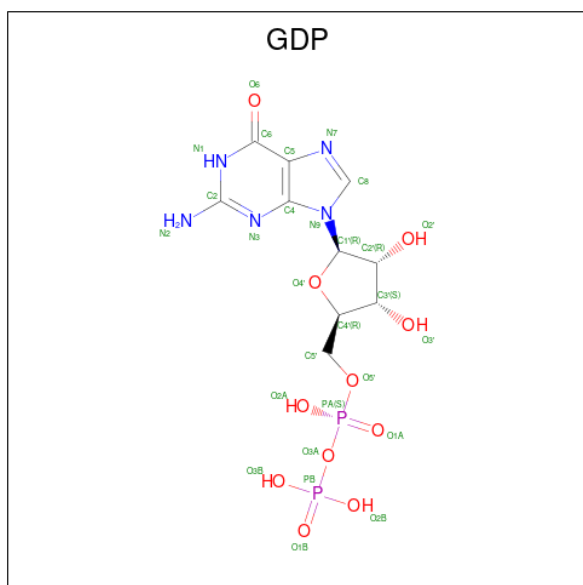
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0

Continued on next page...

Continued from previous page...

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

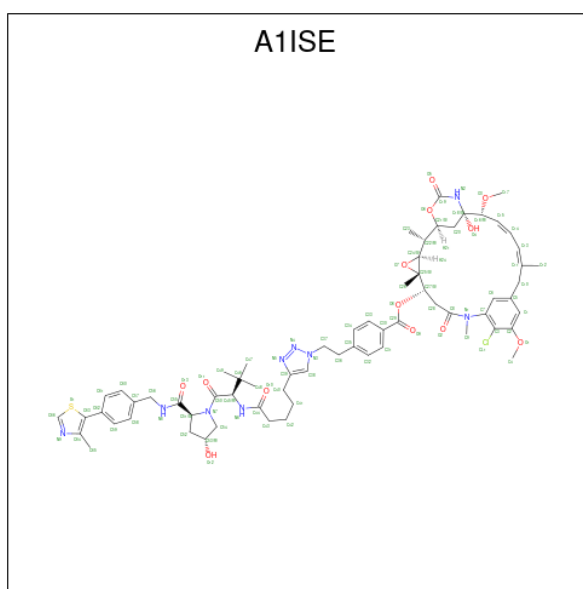
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





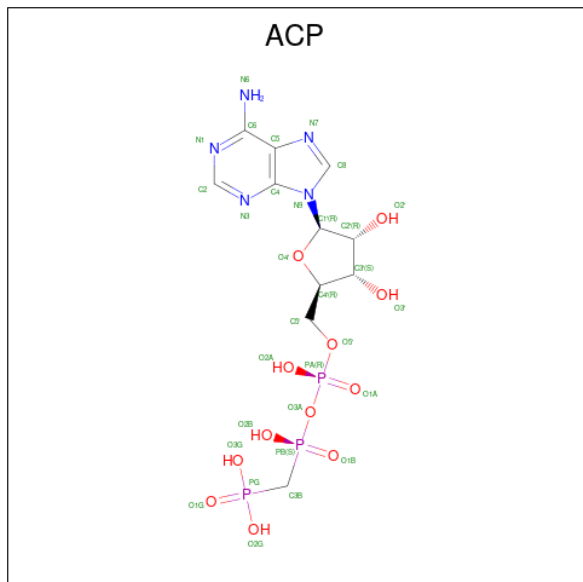
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is N-[5-(1-{2-[4-({[(1S,2R,3S,5S,6S,16E,18E,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1 10,14.0 3,5]hexacosa-10(26),11,13,16,18-pentaen-6-yl]oxy}carbonyl)phenyl]ethyl}-1H-1,2,3-triazol-4-yl)pentanoyl]-3-methyl-D-valyl-(4R)-4-hydroxy-N-{[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl}-L-prolinamide (CCD ID: A1ISE) (formula: C₆₆H₈₂ClN₉O₁₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
10	D	1	Total	C	Cl	H	N	O	S	0	0
			172	66	1	82	9	13	1		

- 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

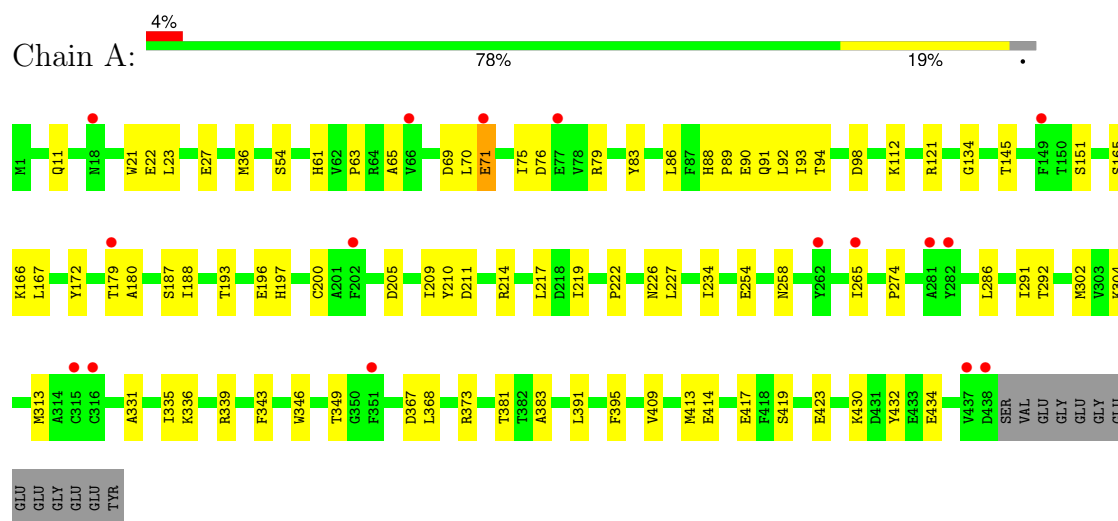
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	63	Total O 63 63	0	0
12	B	99	Total O 99 99	0	0
12	C	166	Total O 166 166	0	0
12	D	31	Total O 31 31	0	0
12	E	11	Total O 11 11	0	0
12	F	18	Total O 18 18	0	0

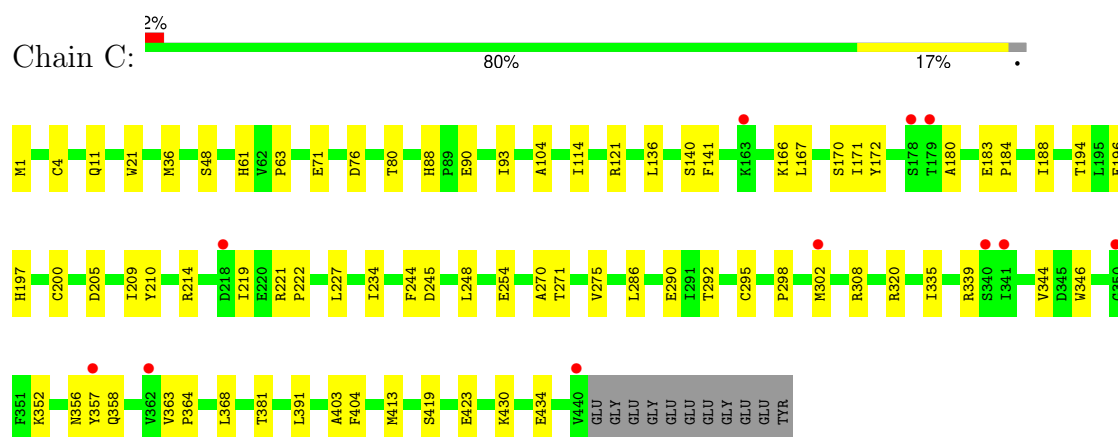
3 Residue-property plots

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.

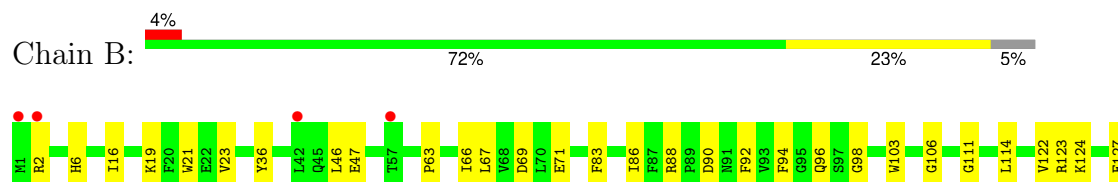
• Molecule 1: Tubulin alpha-1B chain

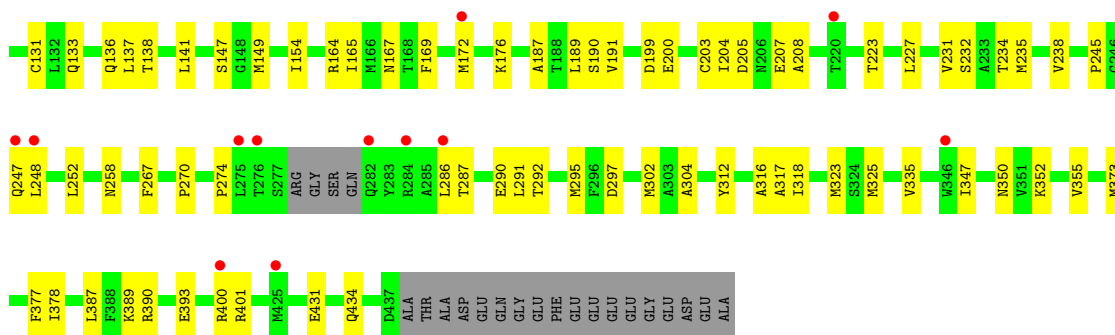


• Molecule 1: Tubulin alpha-1B chain

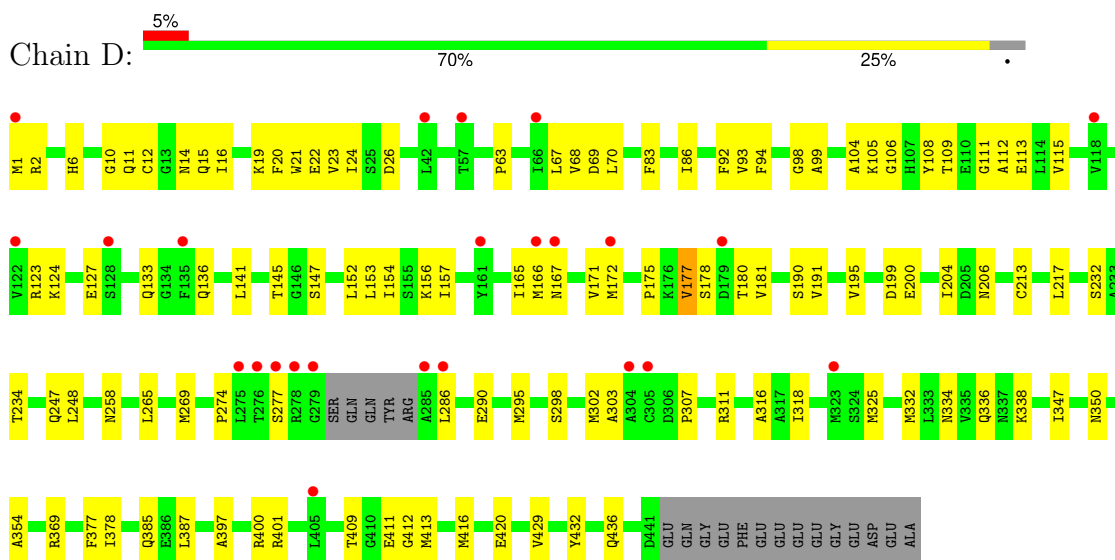


• Molecule 2: Tubulin beta-2B chain

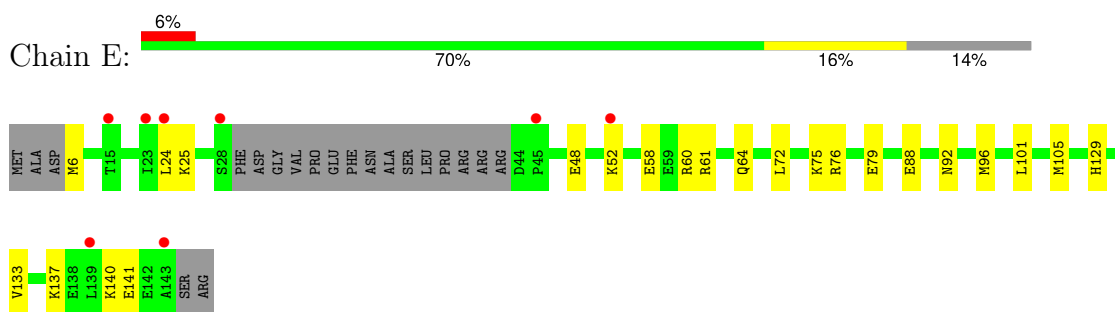




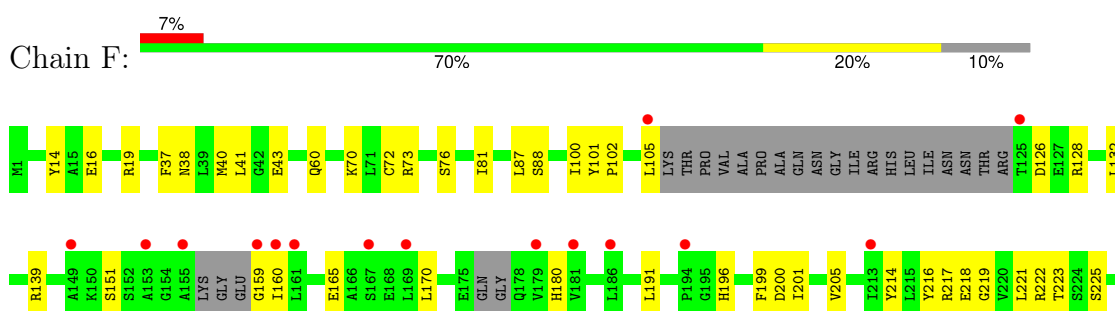
• Molecule 2: Tubulin beta-2B chain

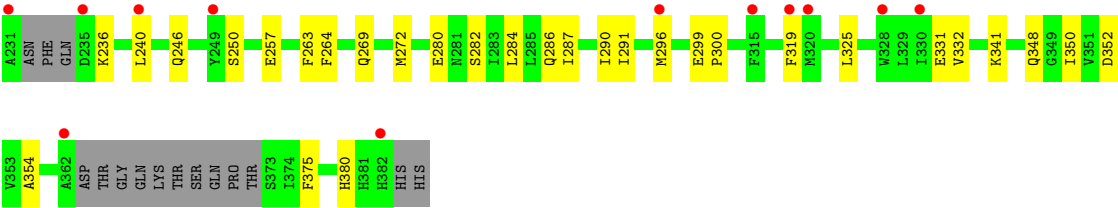


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.50Å 156.57Å 181.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.62 – 2.20 49.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.62-2.20) 100.0 (49.62-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.203 , 0.227 0.203 , 0.226	Depositor DCC
R_{free} test set	7550 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18122	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, MG, ACP, AIISE, CA, GTP, GDP

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	0.07	0/3502	0.21	0/4754
1	C	0.09	0/3521	0.24	0/4780
2	B	0.08	0/3419	0.22	0/4629
2	D	0.07	0/3415	0.19	0/4625
3	E	0.05	0/1022	0.13	0/1356
4	F	0.05	0/2885	0.19	0/3895
All	All	0.07	0/17764	0.21	0/24039

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	65	0
1	C	3443	0	3352	55	0
2	B	3345	0	3227	77	0
2	D	3342	0	3222	82	0
3	E	1014	0	1029	21	0
4	F	2822	0	2788	49	0
5	A	32	0	12	1	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	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	13	1	0
10	D	90	82	0	0	0
11	F	31	0	14	0	0
12	A	63	0	0	1	0
12	B	99	0	0	3	0
12	C	166	0	0	1	0
12	D	31	0	0	0	0
12	E	11	0	0	0	0
12	F	18	0	0	1	0
All	All	18040	82	17027	332	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 10.

All (332) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.40	1.03
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.43	1.01
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.43	0.98
1:A:381:THR:HG22	1:A:383:ALA:H	1.29	0.94
2:D:180:THR:HG22	2:D:181:VAL:H	1.41	0.84
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.64	0.78
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.67	0.77
1:A:71:GLU:OE1	12:A:601:HOH:O	2.03	0.76
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.68	0.75
2:D:1:MET:HA	2:D:1:MET:HE2	1.71	0.73
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.71	0.72
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.70	0.72
2:B:83:PHE:O	2:B:86:ILE:HG22	1.91	0.71
2:D:83:PHE:O	2:D:86:ILE:HG22	1.91	0.71
2:D:217:LEU:HA	2:D:277:SER:HB3	1.73	0.70
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.73	0.70
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.58	0.69
1:C:76:ASP:O	1:C:80:THR:HG22	1.94	0.68
4:F:14:TYR:OH	12:F:501:HOH:O	2.12	0.68
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.09	0.67
2:D:136:GLN:HA	2:D:167:ASN:O	1.94	0.67
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.30	0.67
2:B:323:MET:HE2	2:B:373:MET:HE3	1.77	0.67
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.25	0.67
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.76	0.67
2:B:147:SER:HG	2:B:190:SER:HG	1.43	0.66
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.76	0.66
1:C:209:ILE:HD11	1:C:302:MET:CE	2.26	0.66
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.78	0.65
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.79	0.65
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.77	0.65
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.79	0.65
1:A:187:SER:CB	1:A:391:LEU:HD21	2.27	0.65
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.22	0.65
2:D:409:THR:O	3:E:140:LYS:NZ	2.30	0.64
2:D:10:GLY:O	2:D:14:ASN:ND2	2.26	0.64
4:F:280:GLU:OE1	4:F:284:LEU:HD23	1.98	0.64
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.79	0.64
4:F:246:GLN:O	4:F:250:SER:HB3	1.97	0.63
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.81	0.63
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.63
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.81	0.63
1:C:320:ARG:HA	1:C:356:ASN:O	2.00	0.62
3:E:137:LYS:O	3:E:141:GLU:HG2	2.00	0.62
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.83	0.61
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.01	0.61
2:B:96:GLN:CB	1:C:1:MET:HE2	2.30	0.60
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.19	0.60
3:E:6:MET:HE2	3:E:24:LEU:CD2	2.30	0.60
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.36	0.60
1:C:48:SER:OG	1:C:245:ASP:HB2	2.02	0.60
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	2.01	0.59
1:A:430:LYS:O	1:A:434:GLU:HG3	2.02	0.59
2:D:191:VAL:O	2:D:195:VAL:HG23	2.02	0.59
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.38	0.58
1:C:214:ARG:HG2	1:C:219:ILE:O	2.03	0.58
2:D:104:ALA:HB2	2:D:413:MET:SD	2.43	0.58
2:D:145:THR:HB	8:D:501:GDP:O2B	2.03	0.58
2:D:147:SER:HB2	2:D:190:SER:OG	2.03	0.58
2:B:71:GLU:HG3	2:B:98:GLY:HA2	1.83	0.58
2:D:167:ASN:OD1	2:D:200:GLU:HG3	2.03	0.58
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.34	0.58
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.85	0.58
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.39	0.57
1:C:11:GLN:HE22	2:D:247:GLN:HE22	1.51	0.57
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.36	0.57
2:B:207:GLU:OE1	2:B:390:ARG:NH1	2.37	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.03	0.57
2:B:106:GLY:O	2:B:111:GLY:HA3	2.04	0.57
4:F:43:GLU:OE1	4:F:43:GLU:N	2.27	0.57
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.40	0.57
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.86	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.56
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.21	0.56
2:B:323:MET:CE	2:B:373:MET:HE3	2.36	0.56
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.41	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.06	0.56
2:B:123:ARG:O	2:B:127:GLU:HG3	2.06	0.56
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.88	0.55
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.06	0.55
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.89	0.55
2:D:298:SER:HB3	2:D:307:PRO:HD2	1.87	0.55
1:A:83:TYR:HB3	1:A:86:LEU:HD12	1.89	0.55
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.42	0.54
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.89	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.42	0.54
2:D:109:THR:O	2:D:113:GLU:HG2	2.06	0.54
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.07	0.54
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.89	0.54
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.37	0.54
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.43	0.54
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.90	0.54
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.90	0.54
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.90	0.53
4:F:159:GLY:C	4:F:160:ILE:HD12	2.33	0.53
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.43	0.53
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.08	0.53
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.40	0.53
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.24	0.53
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.90	0.53
4:F:331:GLU:HG2	4:F:332:VAL:N	2.24	0.52
1:C:166:LYS:HE2	1:C:197:HIS:O	2.10	0.52
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.52
2:B:141:LEU:HD12	2:B:172:MET:SD	2.49	0.52
1:C:104:ALA:HB2	1:C:413:MET:SD	2.50	0.52
3:E:92:ASN:O	3:E:96:MET:HG2	2.09	0.52
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.91	0.52
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.25	0.52
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.08	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.52
2:D:175:PRO:HA	2:D:178:SER:HB3	1.90	0.52
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.25	0.51
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.91	0.51
2:B:187:ALA:O	2:B:191:VAL:HG23	2.11	0.51
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.50	0.51
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.93	0.51
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.10	0.51
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.41	0.51
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.92	0.51
3:E:129:HIS:O	3:E:133:VAL:HG23	2.11	0.51
2:D:397:ALA:O	2:D:401:ARG:NH1	2.43	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.46	0.50
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.92	0.50
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.46	0.50
2:D:295:MET:CE	2:D:377:PHE:HB2	2.41	0.50
2:D:123:ARG:O	2:D:127:GLU:HG3	2.11	0.50
2:B:400:ARG:HG3	2:B:401:ARG:HG2	1.93	0.50
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.23	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.11	0.49
2:B:124:LYS:HD3	2:B:124:LYS:C	2.38	0.49
2:D:69:ASP:O	2:D:94:PHE:HA	2.11	0.49
2:D:180:THR:HG22	2:D:181:VAL:N	2.19	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.95	0.49
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.49
2:B:83:PHE:N	12:B:601:HOH:O	2.31	0.49
2:B:248:LEU:CD2	2:B:352:LYS:HB3	2.42	0.49
2:D:1:MET:HE2	2:D:1:MET:CA	2.41	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.49
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.94	0.49
1:A:214:ARG:HG2	1:A:219:ILE:O	2.12	0.49
1:C:180:ALA:O	1:C:183:GLU:HG3	2.12	0.49
2:D:171:VAL:HA	2:D:204:ILE:O	2.13	0.49
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.46	0.49
2:B:317:ALA:C	2:B:318:ILE:HD12	2.38	0.49
2:D:411:GLU:HA	3:E:137:LYS:HZ3	1.77	0.48
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.48	0.48
2:B:47:GLU:HG2	2:B:245:PRO:CG	2.30	0.48
2:B:389:LYS:O	2:B:393:GLU:HG3	2.14	0.48
2:D:416:MET:O	2:D:420:GLU:HG3	2.13	0.48
4:F:296:MET:SD	4:F:380:HIS:HB2	2.53	0.48
1:C:419:SER:O	1:C:423:GLU:HG3	2.13	0.48
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.49	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.31	0.48
4:F:102:PRO:HD2	4:F:105:LEU:HD22	1.95	0.48
4:F:199:PHE:CB	4:F:223:THR:HG22	2.44	0.48
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.38	0.48
2:D:387:LEU:HD23	2:D:387:LEU:C	2.38	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.48
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.95	0.48
1:C:271:THR:HG21	1:C:295:CYS:O	2.13	0.48
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.95	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.13	0.48
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.14	0.47
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.14	0.47
1:A:23:LEU:O	1:A:27:GLU:HG3	2.14	0.47
2:B:205:ASP:CG	2:B:390:ARG:HH22	2.21	0.47
4:F:101:TYR:N	4:F:126:ASP:OD1	2.30	0.47
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.97	0.47
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.55	0.47
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.48	0.47
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.96	0.47
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.50	0.47
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:ILE:HG23	1:C:339:ARG:CG	2.43	0.47
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.97	0.47
4:F:286:GLN:O	4:F:290:ILE:HG13	2.15	0.47
1:A:54:SER:O	1:A:61:HIS:HA	2.15	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.47
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.97	0.47
4:F:160:ILE:HD12	4:F:160:ILE:N	2.30	0.47
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.97	0.46
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.46
2:D:124:LYS:C	2:D:124:LYS:HD3	2.40	0.46
1:A:134:GLY:HA3	1:A:165:SER:O	2.15	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.46
1:A:69:ASP:O	1:A:94:THR:HA	2.15	0.46
2:B:164:ARG:O	9:B:504:MES:H71	2.15	0.46
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.51	0.46
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.96	0.46
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.97	0.46
4:F:269:GLN:HA	4:F:272:MET:HE2	1.97	0.46
1:A:346:TRP:H	1:A:346:TRP:CD1	2.33	0.46
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.81	0.46
2:B:67:LEU:N	2:B:67:LEU:HD12	2.31	0.46
1:C:270:ALA:O	1:C:302:MET:HG2	2.15	0.46
1:A:88:HIS:ND1	1:A:90:GLU:HB2	2.31	0.45
1:A:381:THR:HG22	1:A:383:ALA:N	2.13	0.45
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.45
4:F:70:LYS:HA	4:F:76:SER:HB3	1.98	0.45
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.97	0.45
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.43	0.45
2:D:332:MET:O	2:D:336:GLN:HG3	2.16	0.45
4:F:299:GLU:HB3	4:F:300:PRO:HD3	1.97	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.51	0.45
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.51	0.45
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.99	0.45
2:D:177:VAL:HG11	2:D:206:ASN:HB3	1.99	0.45
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.16	0.45
4:F:225:SER:OG	4:F:250:SER:OG	2.27	0.45
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.95	0.45
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.99	0.45
2:B:318:ILE:HD12	2:B:318:ILE:N	2.31	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.99	0.45
2:D:152:LEU:O	2:D:156:LYS:HG2	2.16	0.45
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.98	0.45
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.99	0.45
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.52	0.45
1:A:331:ALA:O	1:A:335:ILE:HG13	2.17	0.45
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.99	0.45
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.47	0.44
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.98	0.44
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.44
2:D:19:LYS:O	2:D:23:VAL:HG23	2.17	0.44
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.99	0.44
4:F:87:LEU:O	4:F:88:SER:OG	2.26	0.44
4:F:128:ARG:HH12	4:F:170:LEU:HB3	1.81	0.44
1:A:75:ILE:HB	1:A:94:THR:CG2	2.48	0.44
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.98	0.44
2:B:325:MET:HE2	2:B:355:VAL:HB	1.99	0.44
3:E:101:LEU:O	3:E:105:MET:HG2	2.17	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.44
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.17	0.44
2:B:2:ARG:HA	2:B:131:CYS:O	2.18	0.44
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.52	0.44
2:B:431:GLU:O	2:B:434:GLN:HG2	2.17	0.44
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.48	0.44
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.99	0.44
1:A:179:THR:HG21	2:B:247:GLN:HG3	2.00	0.44
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.98	0.44
1:C:234:ILE:HG12	1:C:302:MET:SD	2.57	0.44
2:D:316:ALA:HB3	2:D:378:ILE:HB	2.00	0.44
1:A:419:SER:O	1:A:423:GLU:HG3	2.18	0.43
2:B:147:SER:OG	2:B:190:SER:OG	2.22	0.43
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.53	0.43
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.41	0.43
1:A:414:GLU:OE2	3:E:60:ARG:NH1	2.52	0.43
2:B:387:LEU:C	2:B:387:LEU:HD23	2.44	0.43
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.53	0.43
2:D:67:LEU:N	2:D:67:LEU:HD12	2.33	0.43
2:B:390:ARG:NE	12:B:612:HOH:O	2.50	0.43
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.99	0.43
4:F:72:CYS:O	4:F:73:ARG:HD2	2.18	0.43
1:A:265:ILE:HG21	1:A:313:MET:HE1	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB2	1:A:193:THR:OG1	2.18	0.43
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.54	0.43
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.91	0.43
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.00	0.43
4:F:199:PHE:HB2	4:F:223:THR:HG22	2.01	0.43
1:C:270:ALA:HB3	1:C:302:MET:HG3	2.01	0.43
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.53	0.43
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.54	0.43
1:A:349:THR:HB	3:E:25:LYS:HB3	2.01	0.42
2:B:234:THR:OG1	2:B:302:MET:HE3	2.19	0.42
4:F:38:ASN:O	4:F:60:GLN:HA	2.19	0.42
2:B:223:THR:O	2:B:227:LEU:HD13	2.19	0.42
4:F:151:SER:HB3	4:F:180:HIS:CG	2.54	0.42
2:B:295:MET:CG	2:B:377:PHE:HB2	2.49	0.42
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.18	0.42
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.55	0.42
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.47	0.42
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.44	0.42
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.20	0.42
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.01	0.42
2:B:19:LYS:O	2:B:23:VAL:HG23	2.19	0.42
2:D:141:LEU:HD12	2:D:172:MET:SD	2.59	0.42
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.20	0.42
4:F:280:GLU:HA	4:F:284:LEU:HB3	2.01	0.42
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.30	0.42
1:C:248:LEU:HD23	1:C:357:TYR:OH	2.20	0.42
2:D:70:LEU:HB3	2:D:98:GLY:HA2	2.01	0.42
2:D:108:TYR:CE1	3:E:133:VAL:HG21	2.55	0.42
1:C:136:LEU:HD23	1:C:167:LEU:HB2	2.02	0.42
1:C:194:THR:O	1:C:194:THR:HG22	2.19	0.42
2:D:177:VAL:O	2:D:177:VAL:HG22	2.19	0.42
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.42
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.42	0.42
1:C:180:ALA:HA	2:D:258:ASN:OD1	2.20	0.42
2:D:11:GLN:O	2:D:15:GLN:HG2	2.20	0.42
2:D:265:LEU:HD22	2:D:432:TYR:CZ	2.55	0.42
2:B:199:ASP:C	2:B:200:GLU:HG3	2.44	0.41
2:D:412:GLY:C	3:E:133:VAL:HG13	2.45	0.41
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.55	0.41
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.51	0.41
2:B:297:ASP:HA	12:B:630:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.52	0.41
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.01	0.41
2:D:12:CYS:O	2:D:16:ILE:HG12	2.20	0.41
3:E:6:MET:HG3	3:E:24:LEU:CD2	2.50	0.41
2:D:112:ALA:O	2:D:115:VAL:HG12	2.20	0.41
2:D:234:THR:OG1	2:D:302:MET:HE3	2.19	0.41
3:E:88:GLU:OE1	3:E:88:GLU:HA	2.20	0.41
1:A:234:ILE:HD12	1:A:234:ILE:N	2.35	0.41
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.55	0.41
2:D:311:ARG:NH1	2:D:436:GLN:O	2.54	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.41
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.55	0.41
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.46	0.41
1:C:196:GLU:HG2	12:C:652:HOH:O	2.21	0.41
1:C:234:ILE:HD12	1:C:234:ILE:N	2.36	0.41
2:B:208:ALA:HB2	2:B:304:ALA:HB2	2.02	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.41
2:D:153:LEU:O	2:D:157:ILE:HG13	2.21	0.41
1:A:11:GLN:HE22	2:B:247:GLN:NE2	2.20	0.41
1:A:112:LYS:HE3	3:E:58:GLU:OE1	2.21	0.41
2:B:286:LEU:HD23	2:B:291:LEU:HD23	2.03	0.41
2:D:105:LYS:HE2	2:D:411:GLU:OE2	2.21	0.41
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.86	0.41
2:B:287:THR:OG1	2:B:290:GLU:HG3	2.21	0.40
1:C:403:ALA:O	1:C:404:PHE:HB2	2.21	0.40
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.55	0.40
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.02	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.22	0.40
2:D:68:VAL:HA	2:D:93:VAL:O	2.22	0.40
2:B:138:THR:HG21	2:B:235:MET:HE1	2.03	0.40
1:C:184:PRO:O	1:C:188:ILE:HD13	2.20	0.40
2:B:312:TYR:CE1	2:B:377:PHE:HZ	2.40	0.40
4:F:132:LEU:HD21	4:F:170:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	426 (98%)	10 (2%)	0	100	100
1	C	439/451 (97%)	431 (98%)	8 (2%)	0	100	100
2	B	420/445 (94%)	415 (99%)	5 (1%)	0	100	100
2	D	422/445 (95%)	411 (97%)	10 (2%)	1 (0%)	43	51
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	333/384 (87%)	325 (98%)	8 (2%)	0	100	100
All	All	2169/2319 (94%)	2126 (98%)	42 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	177	VAL

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%)	368 (100%)	1 (0%)	86	93
1	C	372/379 (98%)	370 (100%)	2 (0%)	81	90
2	B	368/383 (96%)	368 (100%)	0	100	100
2	D	367/383 (96%)	367 (100%)	0	100	100
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	309/342 (90%)	309 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1895/1993 (95%)	1892 (100%)	3 (0%)	87 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	C	71	GLU
1	C	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	216	ASN
2	B	193	GLN
2	B	282	GLN
2	B	294	GLN
2	B	349	ASN
2	B	385	GLN
2	B	434	GLN
1	C	11	GLN
1	C	101	ASN
1	C	393	HIS
2	D	50	ASN
2	D	247	GLN
2	D	294	GLN
2	D	300	ASN
2	D	334	ASN
2	D	339	ASN
2	D	349	ASN
2	D	426	ASN
3	E	12	ASN
3	E	92	ASN
3	E	103	GLN
3	E	115	HIS
3	E	136	ASN
4	F	269	GLN
4	F	306	HIS
4	F	348	GLN
4	F	379	HIS
4	F	380	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	0.95	2 (6%)	50,54,54	1.53	9 (18%)
11	ACP	F	401	6	31,33,33	2.15	3 (9%)	47,52,52	1.01	4 (8%)
8	GDP	B	501	6	29,30,30	1.16	2 (6%)	45,47,47	1.72	6 (13%)
10	A1ISE	D	503	-	95,98,98	1.38	9 (9%)	125,144,144	2.37	39 (31%)
5	GTP	A	501	6	33,34,34	0.97	2 (6%)	50,54,54	1.50	8 (16%)
9	MES	B	504	-	12,12,12	1.14	1 (8%)	15,16,16	0.70	0
8	GDP	D	501	6	29,30,30	1.15	3 (10%)	45,47,47	1.72	6 (13%)

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	-	7/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	6	-	3/19/38/38	0/3/3/3
8	GDP	B	501	6	-	3/16/32/32	0/3/3/3
10	A1ISE	D	503	-	-	22/93/131/131	0/7/9/9
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
8	GDP	D	501	6	-	0/16/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	401	ACP	PB-O3A	10.81	1.70	1.58
10	D	503	A1ISE	C14-C15	8.05	1.63	1.33
10	D	503	A1ISE	O7-C25	-4.81	1.40	1.46
10	D	503	A1ISE	O7-C24	-3.54	1.40	1.45
8	D	501	GDP	C5-C4	3.11	1.47	1.38
8	B	501	GDP	C5-C4	3.10	1.47	1.38
9	B	504	MES	C8-S	3.02	1.81	1.77
10	D	503	A1ISE	O6-C21	-2.87	1.42	1.46
10	D	503	A1ISE	C25-C24	2.55	1.50	1.47
10	D	503	A1ISE	C10-C11	-2.49	1.50	1.52
10	D	503	A1ISE	C38-N3	2.43	1.38	1.34
8	D	501	GDP	C6-N1	-2.43	1.34	1.38
11	F	401	ACP	PA-O3A	2.42	1.62	1.59
8	B	501	GDP	C6-N1	-2.38	1.34	1.38
5	A	501	GTP	PA-O3A	2.17	1.61	1.59
11	F	401	ACP	PB-O2B	-2.17	1.51	1.56
5	A	501	GTP	C2-N3	2.14	1.38	1.33
5	C	501	GTP	C2-N3	2.12	1.38	1.33
5	C	501	GTP	PB-O3B	2.10	1.61	1.59
10	D	503	A1ISE	O8-C27	-2.05	1.43	1.46
10	D	503	A1ISE	C64-N9	-2.03	1.35	1.38
8	D	501	GDP	C5-N7	-2.02	1.35	1.39

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	A1ISE	O6-C21-C22	10.04	124.96	105.68
10	D	503	A1ISE	O7-C24-C22	8.14	127.17	117.41
10	D	503	A1ISE	C25-O7-C24	7.29	64.94	60.81
8	D	501	GDP	C5-C4-N3	-5.95	118.92	128.39
8	B	501	GDP	C5-C4-N3	-5.93	118.95	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	A1ISE	C52-C51-N7	5.88	110.17	103.17
10	D	503	A1ISE	C45-C50-N7	5.33	124.82	118.46
8	B	501	GDP	C2-N3-C4	5.05	120.99	112.30
10	D	503	A1ISE	O8-C29-C30	4.98	119.90	111.90
8	D	501	GDP	C2-N3-C4	4.96	120.84	112.30
10	D	503	A1ISE	C26-C25-C24	-4.88	110.48	121.17
5	C	501	GTP	C5-C4-N3	-4.84	120.69	128.39
5	A	501	GTP	C5-C4-N3	-4.76	120.82	128.39
5	C	501	GTP	C2-N3-C4	4.49	120.04	112.30
5	A	501	GTP	C2-N3-C4	4.48	120.02	112.30
10	D	503	A1ISE	C62-C63-C64	-4.48	124.73	130.81
8	B	501	GDP	N9-C4-N3	4.42	134.80	125.95
8	D	501	GDP	N9-C4-N3	4.36	134.67	125.95
10	D	503	A1ISE	O1-C2-C3	4.30	120.15	115.44
10	D	503	A1ISE	C14-C13-C11	-4.08	121.94	127.69
10	D	503	A1ISE	C52-C53-C54	3.83	107.45	103.18
10	D	503	A1ISE	C50-C45-N6	3.81	112.03	107.40
11	F	401	ACP	O1G-PG-C3B	-3.71	103.28	111.37
10	D	503	A1ISE	O7-C25-C26	-3.51	109.18	114.12
10	D	503	A1ISE	O7-C24-C25	-3.51	57.44	59.82
8	D	501	GDP	C6-C5-N7	3.39	136.47	130.29
8	B	501	GDP	C6-C5-N7	3.32	136.34	130.29
10	D	503	A1ISE	C43-C44-N6	3.21	121.52	115.86
10	D	503	A1ISE	O6-C19-O5	-3.17	113.25	118.05
10	D	503	A1ISE	N3-N4-N5	3.15	109.85	107.02
10	D	503	A1ISE	C57-C56-N8	-3.15	106.44	113.07
10	D	503	A1ISE	C63-C64-N9	-3.13	111.98	114.99
5	C	501	GTP	N9-C4-N3	3.10	132.16	125.95
11	F	401	ACP	O2B-PB-O1B	3.01	119.74	109.95
5	A	501	GTP	N9-C4-N3	3.00	131.96	125.95
10	D	503	A1ISE	C54-N7-C51	-2.90	107.99	111.83
10	D	503	A1ISE	C64-C63-S1	2.87	111.39	109.64
10	D	503	A1ISE	C40-C39-C38	-2.81	124.82	130.26
5	C	501	GTP	C2-N1-C6	-2.80	120.04	125.11
10	D	503	A1ISE	O7-C25-C24	-2.78	57.61	59.38
5	A	501	GTP	C2-N1-C6	-2.77	120.09	125.11
10	D	503	A1ISE	C62-C63-S1	2.74	123.87	118.77
5	A	501	GTP	N9-C8-N7	-2.73	108.34	113.40
5	C	501	GTP	N9-C8-N7	-2.70	108.40	113.40
8	D	501	GDP	C4-C5-N7	-2.61	106.54	110.67
10	D	503	A1ISE	C37-N3-N4	2.59	125.98	120.78
5	A	501	GTP	C8-N7-C5	2.51	108.73	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	503	A1ISE	C27-O8-C29	-2.51	113.15	117.52
10	D	503	A1ISE	O1-C2-C1	-2.50	119.76	124.08
5	C	501	GTP	C8-N7-C5	2.49	108.70	104.26
10	D	503	A1ISE	C36-C37-N3	-2.49	109.20	111.90
8	B	501	GDP	C4-C5-N7	-2.48	106.74	110.67
5	C	501	GTP	C5-C6-N1	2.47	119.53	113.25
10	D	503	A1ISE	C38-N3-N4	-2.46	108.36	110.75
5	A	501	GTP	C5-C6-N1	2.44	119.47	113.25
10	D	503	A1ISE	C66-N9-C64	2.36	113.37	110.71
10	D	503	A1ISE	O6-C19-N2	2.32	123.11	118.78
11	F	401	ACP	PB-O3A-PA	-2.28	124.94	132.37
5	C	501	GTP	O6-C6-C5	-2.28	120.53	126.53
5	A	501	GTP	O6-C6-C5	-2.27	120.55	126.53
8	B	501	GDP	O6-C6-C5	-2.25	120.59	126.53
10	D	503	A1ISE	C42-C43-C44	-2.24	106.99	113.19
10	D	503	A1ISE	C53-C54-N7	2.20	105.13	103.00
10	D	503	A1ISE	O8-C27-C28	2.19	109.32	105.09
11	F	401	ACP	O3G-PG-O2G	2.16	114.13	107.96
10	D	503	A1ISE	C4-O1-C2	-2.10	114.43	117.51
10	D	503	A1ISE	O2-C8-C28	-2.10	118.15	122.07
8	D	501	GDP	O6-C6-C5	-2.07	121.06	126.53
5	C	501	GTP	O2A-PA-O3A	2.06	112.85	107.27
10	D	503	A1ISE	O10-C44-N6	-2.06	119.47	122.95
10	D	503	A1ISE	O8-C29-O9	-2.03	120.25	123.55
10	D	503	A1ISE	C13-C14-C15	-2.00	119.79	124.43

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
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
10	D	503	A1ISE	C12-C11-C13-C14
10	D	503	A1ISE	C15-C16-O3-C17
10	D	503	A1ISE	C3-C2-O1-C4
10	D	503	A1ISE	N6-C45-C50-N7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	D	503	A1ISE	N6-C45-C50-O11
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
10	D	503	A1ISE	C30-C29-O8-C27
10	D	503	A1ISE	C1-C2-O1-C4
10	D	503	A1ISE	O9-C29-O8-C27
10	D	503	A1ISE	C25-C27-O8-C29
10	D	503	A1ISE	C52-C51-C55-O13
10	D	503	A1ISE	O8-C29-C30-C31
10	D	503	A1ISE	O8-C29-C30-C33
10	D	503	A1ISE	C52-C51-C55-N8
10	D	503	A1ISE	N7-C51-C55-O13
10	D	503	A1ISE	N7-C51-C55-N8
10	D	503	A1ISE	O9-C29-C30-C31
10	D	503	A1ISE	O9-C29-C30-C33
5	A	501	GTP	PB-O3B-PG-O2G
10	D	503	A1ISE	C28-C27-O8-C29
5	C	501	GTP	PB-O3A-PA-O2A
10	D	503	A1ISE	C27-C28-C8-N1
10	D	503	A1ISE	C27-C28-C8-O2
10	D	503	A1ISE	C24-C25-C27-O8
10	D	503	A1ISE	C20-C21-C22-C23
5	A	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A

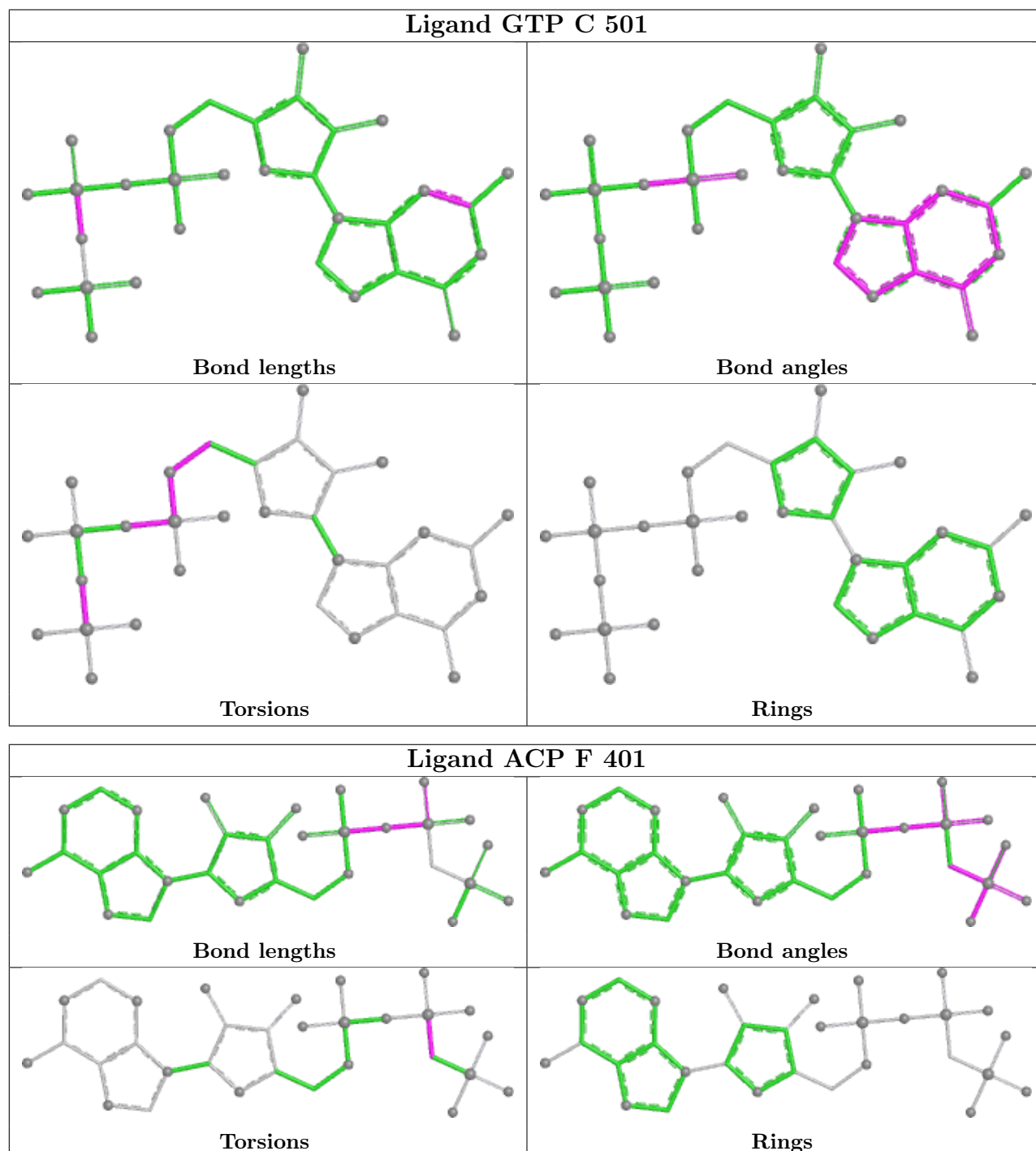
There are no ring outliers.

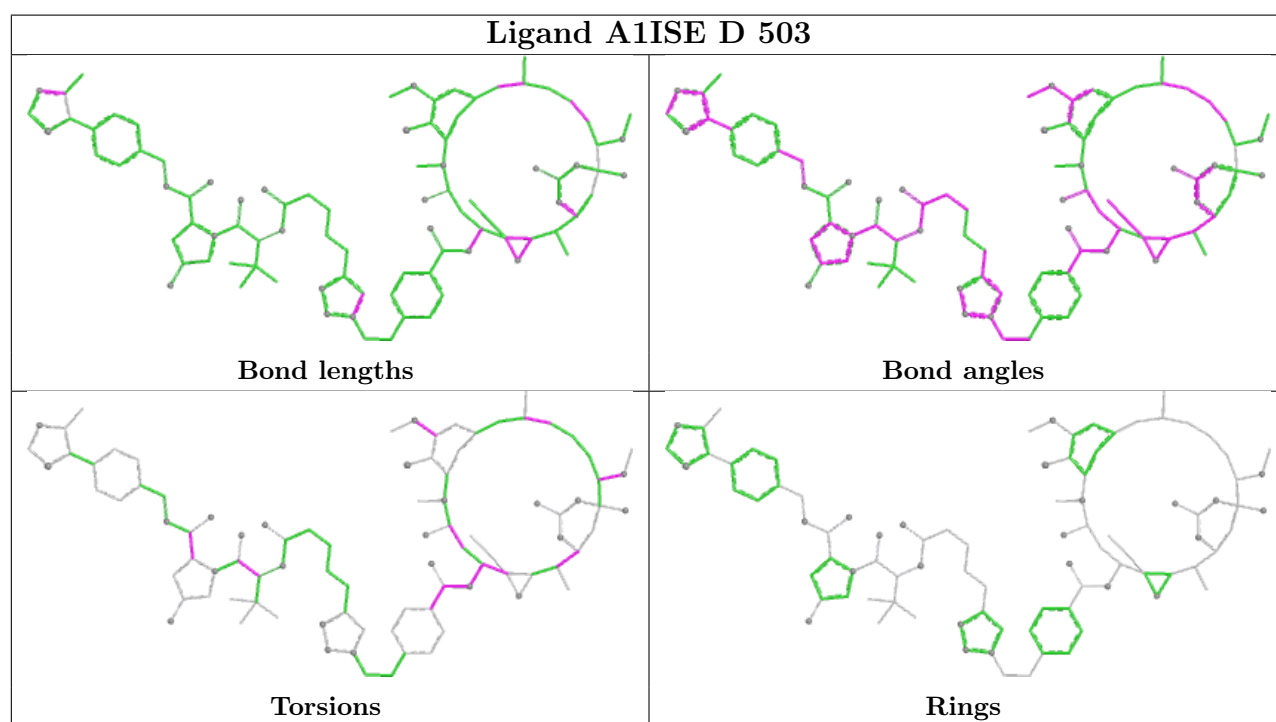
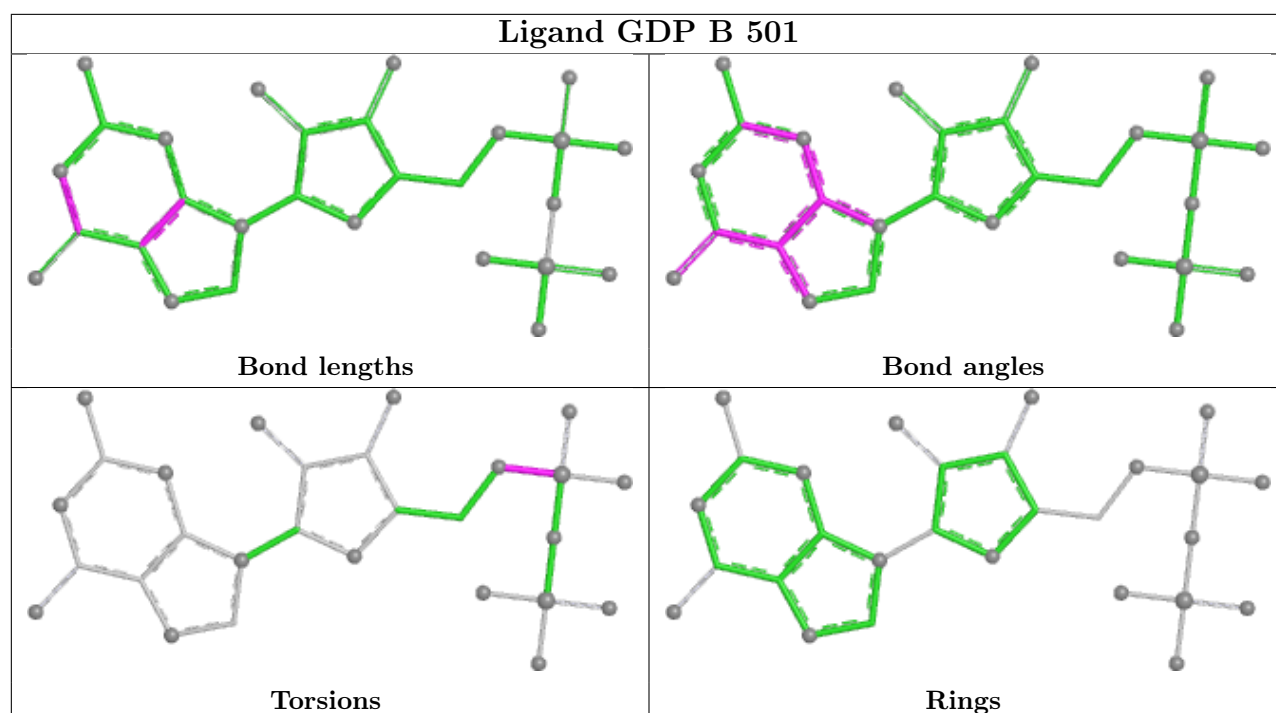
3 monomers are involved in 4 short contacts:

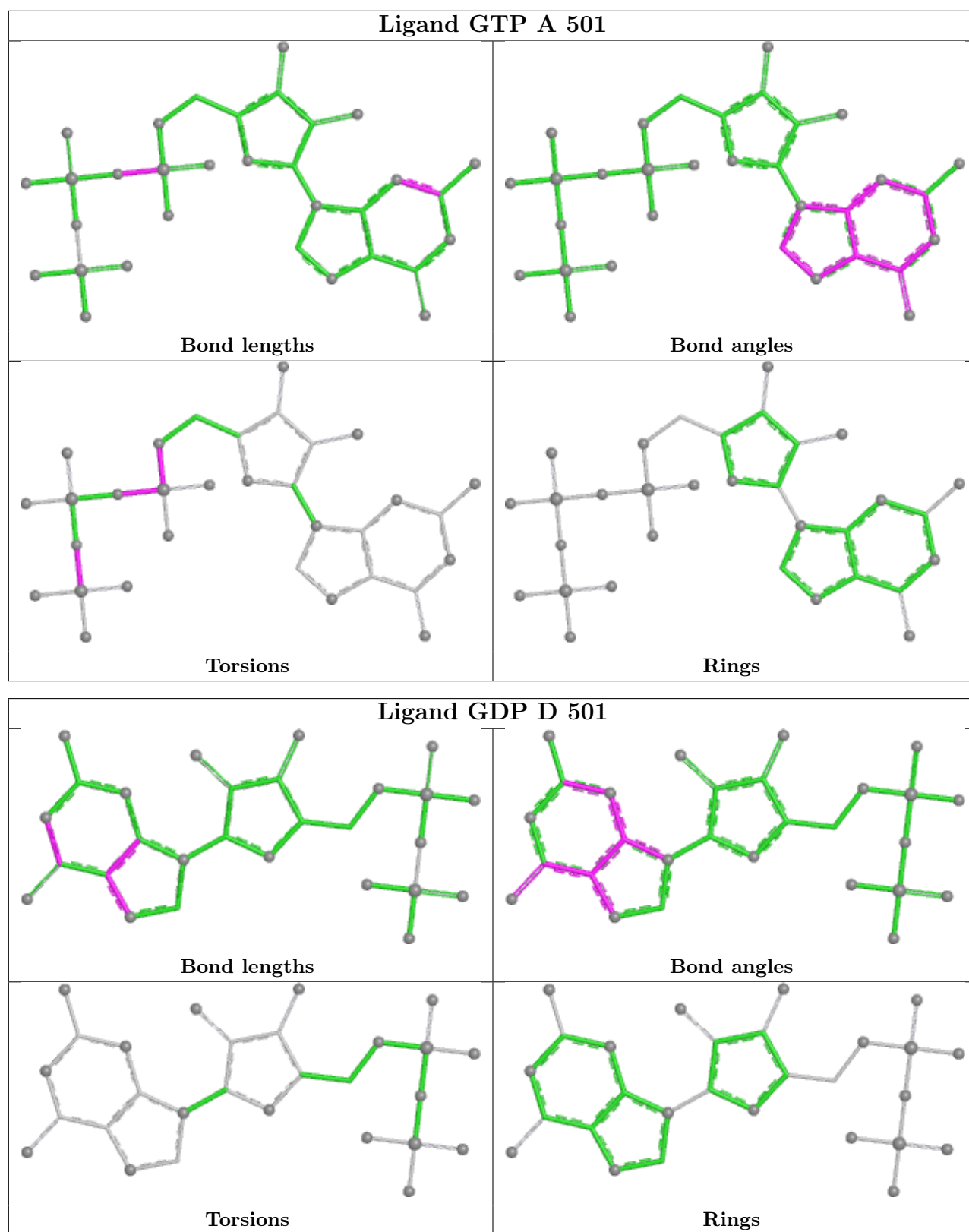
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	504	MES	1	0
8	D	501	GDP	2	0

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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.49	16 (3%)	45	42	60, 81, 107, 158	0
1	C	440/451 (97%)	0.25	11 (2%)	58	55	30, 66, 85, 119	1 (0%)
2	B	423/445 (95%)	0.43	16 (3%)	44	41	36, 73, 104, 132	1 (0%)
2	D	426/445 (95%)	0.67	24 (5%)	30	27	61, 93, 125, 155	0
3	E	123/143 (86%)	0.86	8 (6%)	25	22	69, 96, 140, 163	0
4	F	345/384 (89%)	0.76	27 (7%)	19	16	74, 109, 164, 189	0
All	All	2195/2319 (94%)	0.53	102 (4%)	37	34	30, 83, 135, 189	2 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	5.7
2	D	279	GLY	5.4
2	D	172	MET	5.3
1	C	341	ILE	4.9
2	B	1	MET	4.7
2	D	277	SER	4.4
4	F	231	ALA	4.3
3	E	143	ALA	4.0
2	D	276	THR	4.0
4	F	159	GLY	4.0
2	D	122	VAL	3.5
1	A	281	ALA	3.3
2	B	276	THR	3.3
1	C	440	VAL	3.2
3	E	23	ILE	3.2
4	F	362	ALA	3.1
2	D	161	TYR	3.1
4	F	330	ILE	3.1
2	B	248	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	357	TYR	3.0
4	F	125	THR	3.0
1	C	163	LYS	3.0
2	B	275	LEU	3.0
3	E	24	LEU	2.9
1	A	179	THR	2.9
1	A	282	TYR	2.9
1	C	340	SER	2.9
2	B	57	THR	2.9
3	E	28	SER	2.8
1	A	438	ASP	2.8
4	F	320	MET	2.7
1	A	351	PHE	2.7
2	D	285	ALA	2.7
4	F	153	ALA	2.7
1	C	302	MET	2.7
4	F	194	PRO	2.6
4	F	382	HIS	2.6
2	B	247	GLN	2.6
4	F	105	LEU	2.6
2	D	167	ASN	2.6
4	F	149	ALA	2.6
2	B	346	TRP	2.6
1	A	437	VAL	2.6
3	E	45	PRO	2.6
2	D	166	MET	2.5
2	D	118	VAL	2.5
4	F	181	VAL	2.5
4	F	249	TYR	2.5
4	F	161	LEU	2.5
2	B	286	LEU	2.5
4	F	186	LEU	2.5
1	A	316	CYS	2.5
1	C	350	GLY	2.5
1	C	178	SER	2.4
4	F	319	PHE	2.4
4	F	296	MET	2.4
2	D	304	ALA	2.4
2	D	323	MET	2.4
2	D	286	LEU	2.4
2	B	400	ARG	2.4
1	A	66	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	315	CYS	2.3
2	D	305	CYS	2.3
4	F	169	LEU	2.3
1	C	179	THR	2.3
2	D	128	SER	2.3
2	B	284	ARG	2.2
2	B	425	MET	2.2
2	D	1	MET	2.2
4	F	328	TRP	2.2
2	D	42	LEU	2.2
2	B	220	THR	2.2
4	F	179	VAL	2.2
1	A	202	PHE	2.2
1	A	18	ASN	2.2
2	D	179	ASP	2.2
1	A	262	TYR	2.2
3	E	139	LEU	2.2
4	F	160	ILE	2.2
1	C	362	VAL	2.2
4	F	315	PHE	2.2
2	D	57	THR	2.2
1	A	265	ILE	2.1
3	E	15	THR	2.1
2	D	66	ILE	2.1
4	F	240	LEU	2.1
1	A	77	GLU	2.1
2	B	42	LEU	2.1
2	D	405	LEU	2.1
4	F	235	ASP	2.1
2	B	2	ARG	2.1
2	D	278	ARG	2.1
3	E	52	LYS	2.0
4	F	167	SER	2.0
1	C	218	ASP	2.0
4	F	213	ILE	2.0
1	A	149	PHE	2.0
2	D	135	PHE	2.0
1	A	71	GLU	2.0
2	B	172	MET	2.0
2	B	282	GLN	2.0
2	D	275	LEU	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](#)

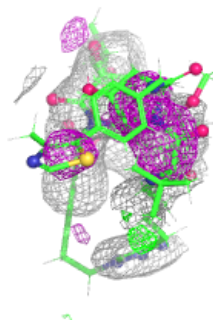
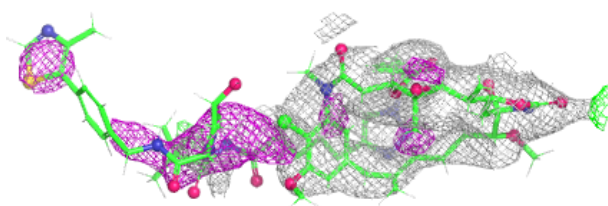
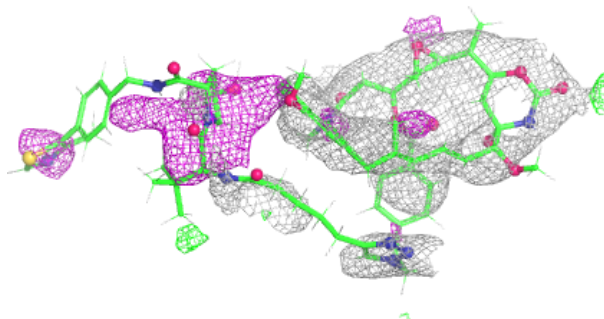
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	A1ISE	D	503	90/90	0.53	0.16	114,158,199,215	0
6	MG	F	402	1/1	0.55	0.18	125,125,125,125	0
7	CA	B	503	1/1	0.72	0.13	108,108,108,108	0
11	ACP	F	401	31/31	0.89	0.09	109,125,132,137	0
7	CA	E	201	1/1	0.90	0.09	120,120,120,120	0
9	MES	B	504	12/12	0.92	0.10	62,71,85,89	0
6	MG	D	502	1/1	0.92	0.07	107,107,107,107	0
8	GDP	D	501	28/28	0.92	0.12	89,96,108,117	0
7	CA	A	503	1/1	0.94	0.06	95,95,95,95	0
6	MG	A	502	1/1	0.96	0.06	60,60,60,60	0
5	GTP	A	501	32/32	0.97	0.07	50,62,67,68	0
8	GDP	B	501	28/28	0.97	0.07	48,59,64,68	0
5	GTP	C	501	32/32	0.98	0.06	50,55,60,63	0
6	MG	B	502	1/1	0.99	0.02	49,49,49,49	0
6	MG	C	502	1/1	0.99	0.02	57,57,57,57	0
7	CA	C	503	1/1	0.99	0.04	83,83,83,83	0

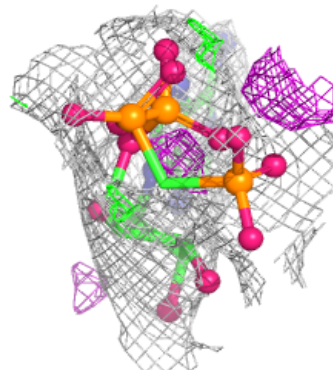
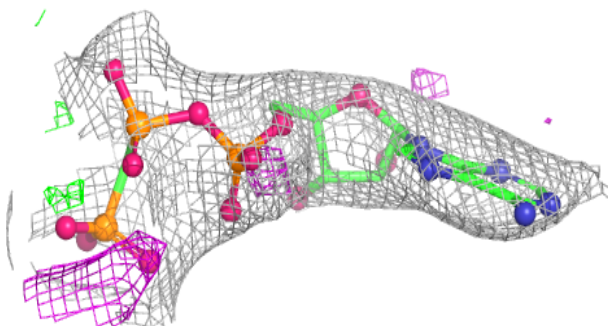
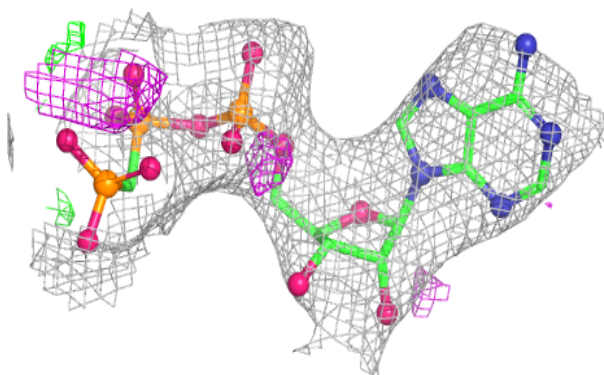
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1ISE D 503:

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

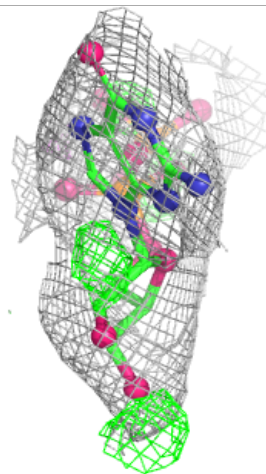
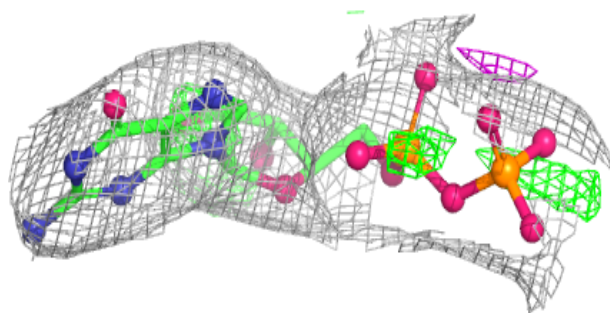
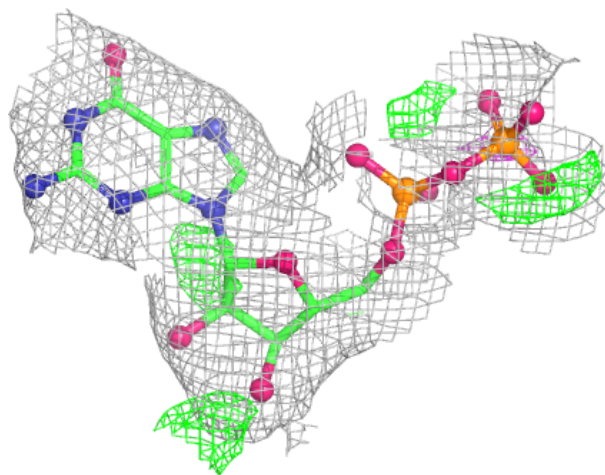
**Electron density around ACP F 401:**

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



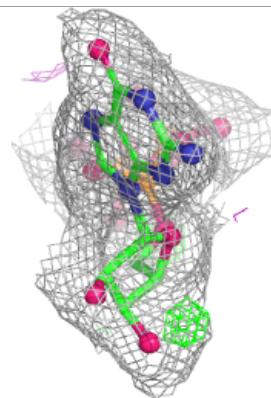
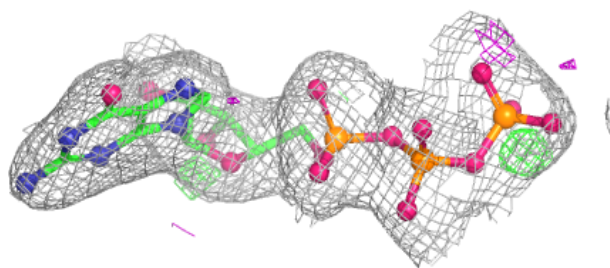
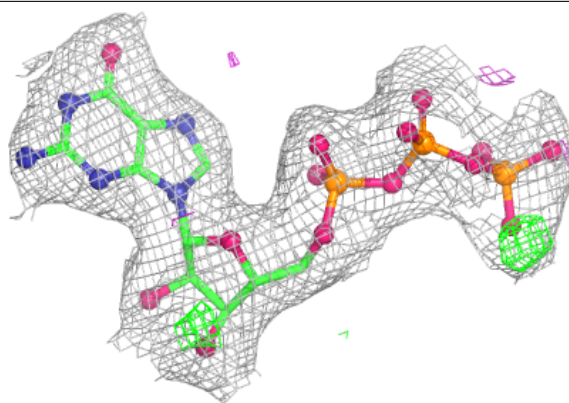
Electron density around GDP D 501:

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



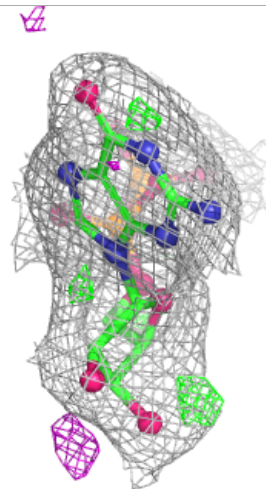
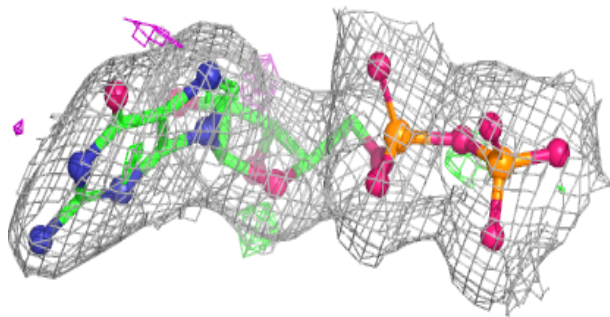
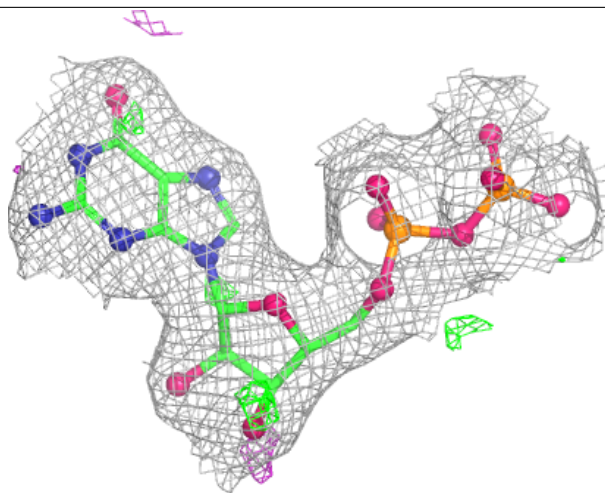
Electron density around GTP A 501:

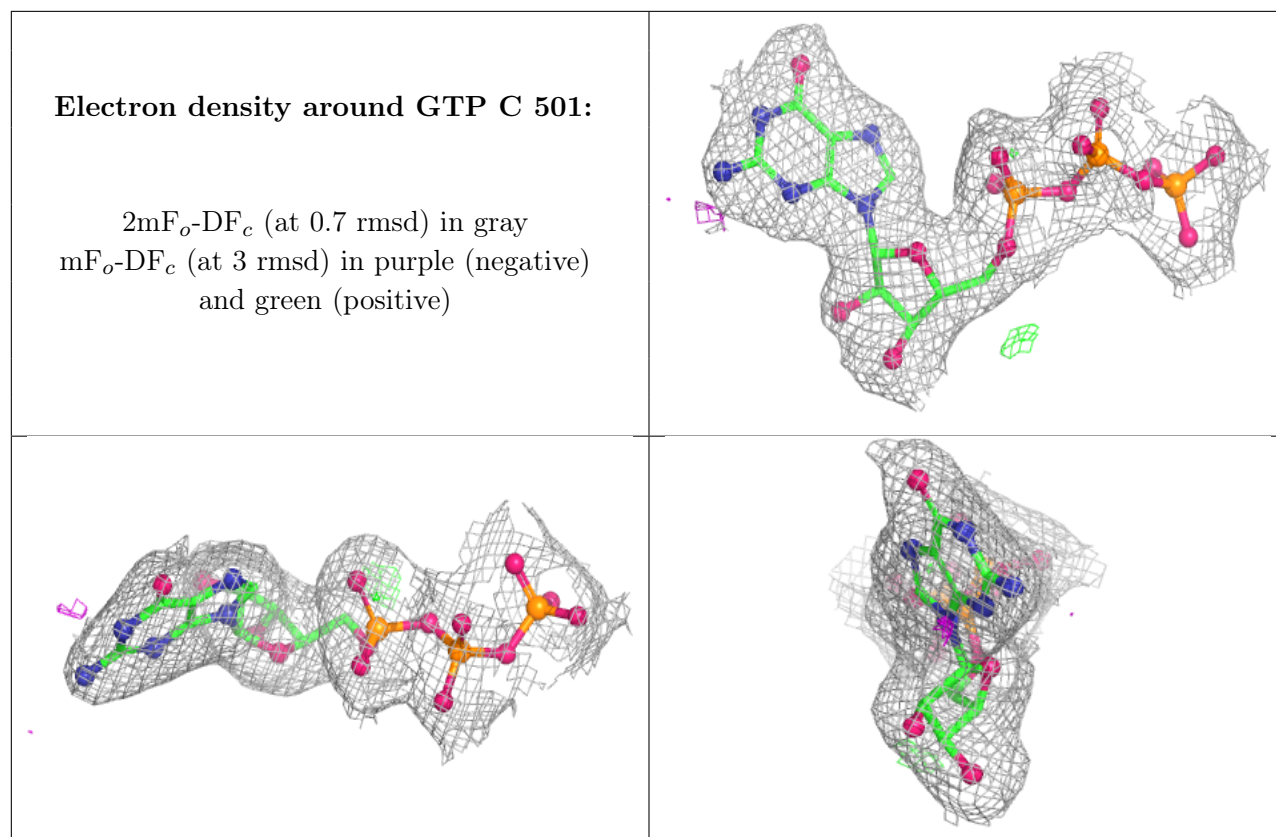
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.