Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 07:54 PM EDT

PDB ID : 4X20
Title : Discovery of cytotoxic Dolastatin 10 analogs with N-terminal modifications
Authors : Parris, K.D.
Deposited on : 2014-11-25
Resolution : 3.50 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 (i) 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 (i)) were used in the production of this report:

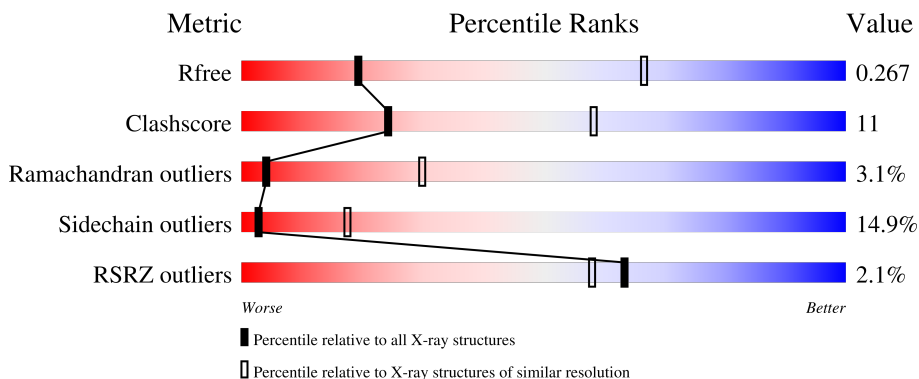|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		11
Ramachandran outliers		3.1%
Sidechain outliers		14.9%
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	3% / 60% / 31% / • / 5%
1	C	451	% / 60% / 30% / • / 5%
2	B	445	2% / 60% / 31% / 5% / •
2	D	445	% / 62% / 30% / • / •
3	E	142	4% / 63% / 19% / • / 13%

2　Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 14717 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total 3363	C 2132	N 572	O 638	S 21	0	0	0
1	C	430	Total 3351	C 2124	N 569	O 635	S 23	0	2	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total 3342	C 2100	N 568	O 649	S 25	0	0	0
2	D	430	Total 3369	C 2112	N 578	O 655	S 24	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total 1008	C 626	N 184	O 195	S 3	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).
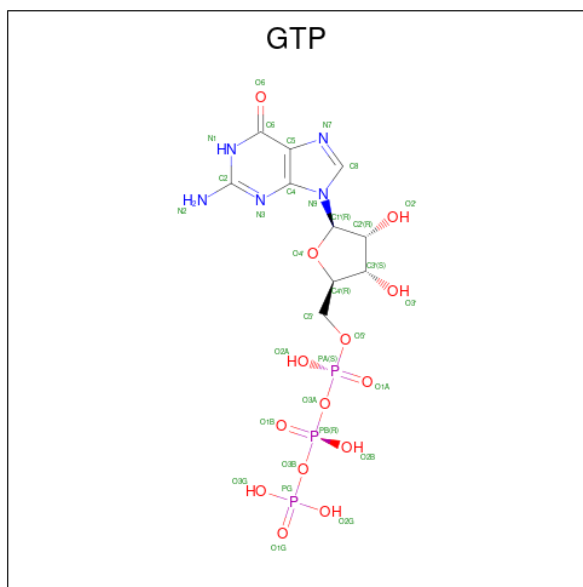
GTP

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
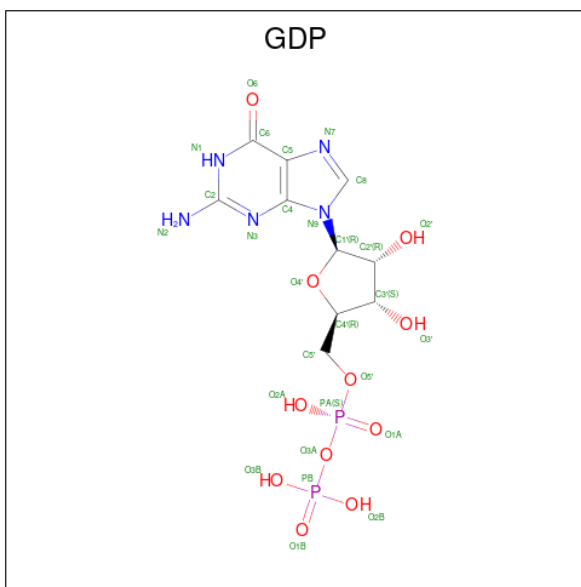
GDP

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

- Molecule 7 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]eth anamide (three-letter code: LOC) (formula: $C_{22}H_{25}NO_6$).
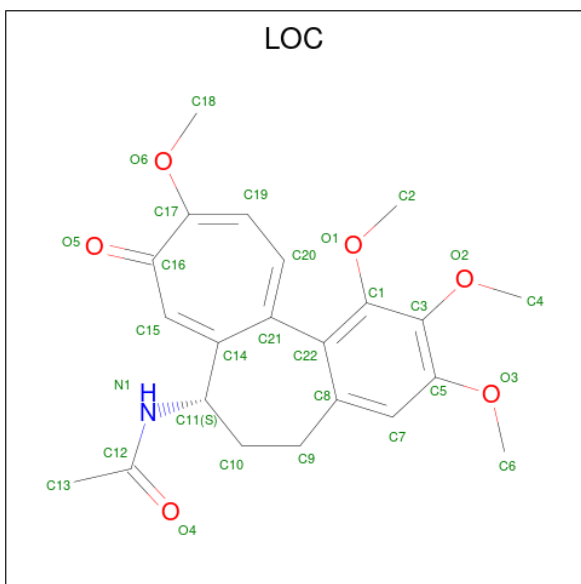
LOC

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

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

- Molecule 8 is 2-methyl-L-prolyl-N-[(3R,4S,5S)-1-{(2S)-2-[(1R,2R)-3-{[(1S)-1-carboxy-2-phe nylethyl]amino}-1-methoxy-2-methyl-3-oxopropyl]pyrrolidin-1-yl}-3-methoxy-5-methyl-1-ox oheptan-4-yl]-N-methyl-L-valinamide (three-letter code: 3WY) (formula: $C_{39}H_{63}N_5O_8$).
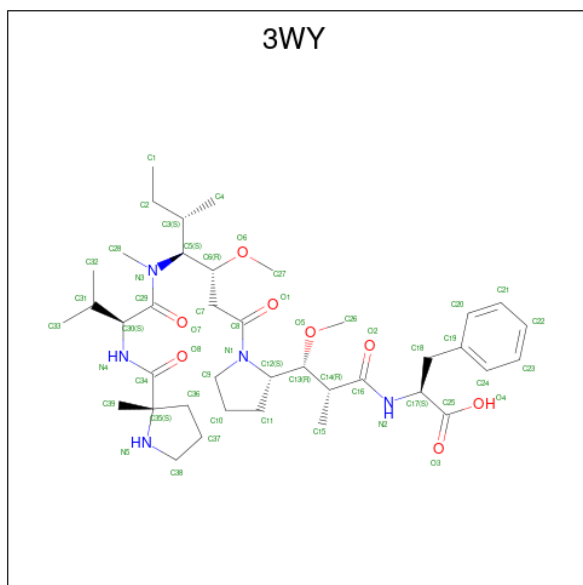

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total 52	C 39	N 5	O 8	0	0
8	D	1	Total 52	C 39	N 5	O 8	0	0

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.
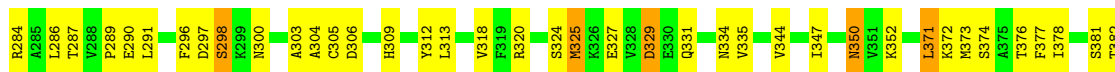
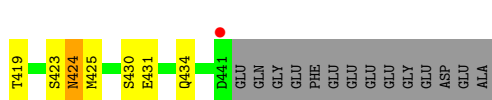- Molecule 1: Tubulin alpha chain
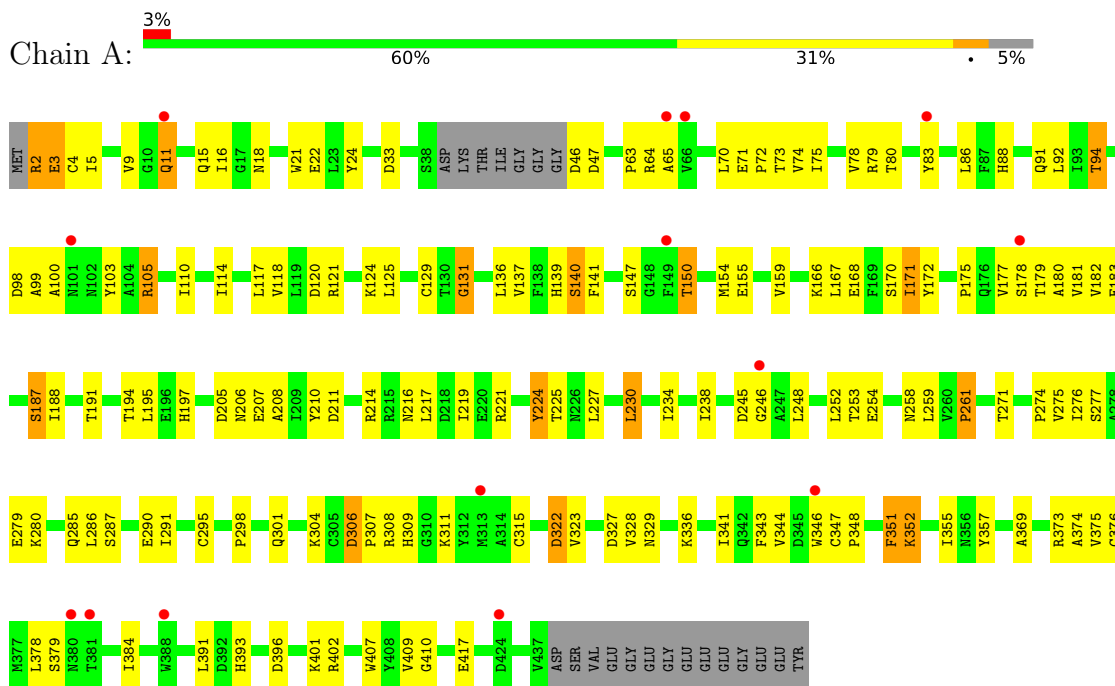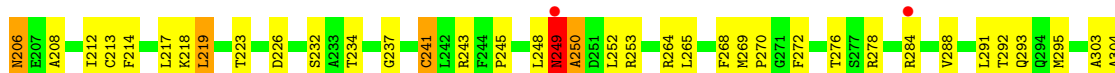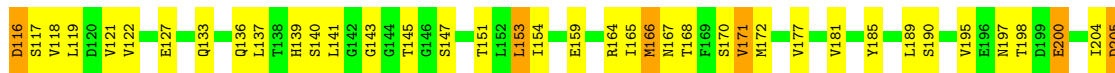

Chain A:

- Molecule 1: Tubulin alpha chain

Chain C:
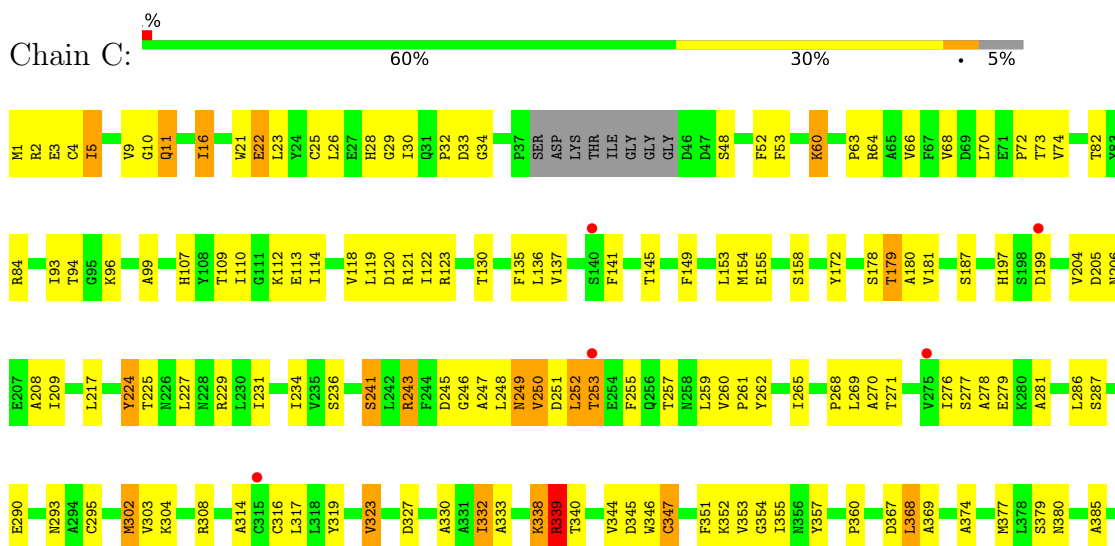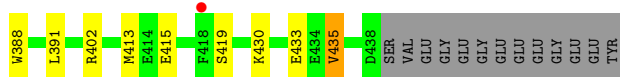
• Molecule 2: Tubulin beta chain

Chain B:

• Molecule 2: Tubulin beta chain

Chain D:
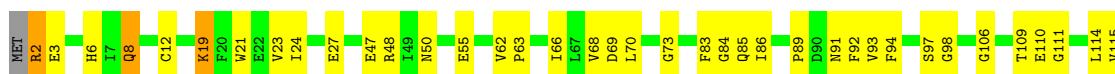
• Molecule 3: Stathmin-4

Chain E:
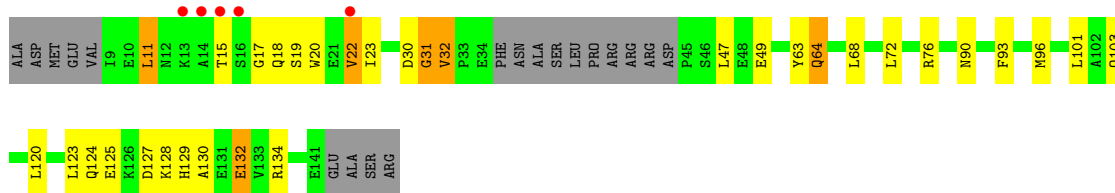
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.24Å 128.27Å 254.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.83 – 3.50 43.32 – 3.29	Depositor EDS
% Data completeness (in resolution range)	90.2 (40.83-3.50) 97.3 (43.32-3.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.252 0.190 , 0.267	Depositor DCC
R_{free} test set	1659 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	120.6	Xtriage
Anisotropy	0.630	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 115.9	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14717	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 3WY, MG, GDP, LOC

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	0.52	0/3440	0.75	0/4671
1	C	0.53	0/3432	0.79	0/4662
2	B	0.53	0/3417	0.81	1/4634 (0.0%)
2	D	0.52	0/3446	0.78	2/4670 (0.0%)
3	E	0.52	0/1019	0.73	0/1355
All	All	0.53	0/14754	0.78	3/19992 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	249	ASN	C-N-CA	6.59	138.17	121.70
2	B	98	GLY	N-CA-C	6.45	129.21	113.10
2	D	248	LEU	C-N-CA	5.47	135.37	121.70

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	3363	0	3274	71	0
1	C	3351	0	3258	80	0
2	B	3342	0	3198	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3369	0	3237	84	0
3	E	1008	0	1022	20	0
4	A	32	0	12	0	0
4	C	32	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	1	0
7	B	29	0	25	1	0
7	D	29	0	25	1	0
8	B	52	0	62	1	0
8	D	52	0	62	4	0
All	All	14717	0	14211	319	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 (319) 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:187:SER:HB3	1:A:391:LEU:HD21	1.43	1.01
1:C:308:ARG:HD2	1:C:340:THR:CG2	1.90	1.01
1:C:308:ARG:HD2	1:C:340:THR:HG21	1.00	0.99
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.30	0.96
1:C:308:ARG:CD	1:C:340:THR:HG21	1.96	0.96
1:C:249:ASN:HB2	1:C:355:ILE:H	1.38	0.88
1:C:217:LEU:HD21	1:C:368:LEU:HG	1.60	0.83
2:B:306:ASP:HB3	2:B:309:HIS:HD2	1.45	0.82
1:A:9:VAL:HB	1:A:150:THR:HG23	1.61	0.81
2:D:133:GLN:HE21	2:D:252:LEU:H	1.25	0.81
1:C:344:VAL:HG23	1:C:347:CYS:HB2	1.63	0.78
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.49	0.77
1:A:276:ILE:HG23	1:A:369:ALA:HB3	1.68	0.75
1:A:259:LEU:O	1:A:261:PRO:HD3	1.85	0.75
2:D:185:TYR:O	2:D:189:LEU:HG	1.88	0.74
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.70	0.74
1:C:231:ILE:HA	1:C:234:ILE:HD12	1.70	0.73
1:C:252:LEU:HD23	1:C:253:THR:H	1.55	0.72
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.70	0.71
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.08	0.71
1:C:119:LEU:HA	1:C:122:ILE:HD12	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:SER:HB2	2:D:190:SER:OG	1.93	0.69
8:D:503:3WY:H9	8:D:503:3WY:H53	1.75	0.69
2:B:382:THR:HA	2:B:432:TYR:HD2	1.57	0.69
1:A:140:SER:HA	1:A:171:ILE:HG22	1.75	0.68
2:B:385:GLN:HB2	2:B:429:VAL:HG13	1.75	0.68
1:A:71:GLU:HG2	1:A:98:ASP:OD1	1.93	0.68
2:B:382:THR:HA	2:B:432:TYR:CD2	2.29	0.67
1:C:319:TYR:HB3	1:C:323:VAL:HG21	1.76	0.67
1:C:70:LEU:HD12	1:C:99:ALA:HB2	1.75	0.67
1:C:137:VAL:HG21	1:C:154:MET:SD	2.35	0.67
1:C:241:SER:HA	1:C:250:VAL:HB	1.78	0.66
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.30	0.66
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.78	0.64
1:C:3:GLU:HG2	1:C:64:ARG:CZ	2.27	0.64
1:C:224:TYR:HA	1:C:227:LEU:HD12	1.80	0.64
3:E:11:LEU:HB2	3:E:20:TRP:HA	1.78	0.64
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.81	0.63
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.33	0.63
2:D:171:VAL:HA	2:D:204:ILE:O	1.98	0.63
1:C:28:HIS:O	1:C:30:ILE:HG13	1.99	0.62
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.81	0.62
2:B:69:ASP:HA	2:B:145:THR:HG21	1.80	0.62
1:A:3:GLU:HG3	1:A:129:CYS:HB3	1.82	0.62
2:B:206:ASN:HD21	6:B:501:GDP:HN22	1.47	0.61
2:B:313:LEU:HA	2:B:344:VAL:HG22	1.81	0.61
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.80	0.61
2:B:179:ASP:HB2	1:C:352:LYS:HG2	1.82	0.61
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.81	0.61
2:D:69:ASP:HB3	2:D:94:PHE:CE1	2.36	0.60
2:D:249:ASN:H	2:D:250:ALA:HB2	1.65	0.60
8:D:503:3WY:H51	8:D:503:3WY:H4	1.82	0.60
2:B:71:GLU:HB3	2:B:98:GLY:HA2	1.83	0.60
2:D:48:ARG:HB2	2:D:243:ARG:O	2.02	0.60
1:A:329:ASN:ND2	3:E:22:VAL:HG11	2.17	0.60
1:C:252:LEU:CD2	1:C:253:THR:H	2.16	0.58
2:D:399:PHE:CE1	2:D:418:PHE:HB3	2.39	0.58
2:B:114:LEU:O	2:B:118:VAL:HG23	2.03	0.58
2:D:89:PRO:HA	2:D:92:PHE:CD1	2.38	0.58
2:D:143:GLY:O	2:D:147:SER:OG	2.22	0.57
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.36	0.57
1:C:72:PRO:HD3	1:C:96:LYS:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:GLY:O	2:B:111:GLY:HA3	2.04	0.57
1:A:177:VAL:HG21	1:A:206:ASN:HB3	1.87	0.57
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.86	0.57
1:C:5:ILE:HD12	1:C:135:PHE:CE2	2.40	0.57
1:A:136:LEU:HD11	1:A:252:LEU:HD21	1.86	0.56
1:A:246:GLY:HA2	3:E:17:GLY:HA3	1.86	0.56
1:A:99:ALA:HA	1:A:105:ARG:HG2	1.87	0.56
2:D:165:ILE:HD11	2:D:253:ARG:HG3	1.88	0.56
2:D:206:ASN:HD21	6:D:501:GDP:HN22	1.54	0.56
1:C:319:TYR:HB2	1:C:355:ILE:HG13	1.87	0.56
1:C:217:LEU:HA	1:C:277:SER:HB2	1.87	0.56
2:D:269:MET:HE1	2:D:381:SER:HB3	1.88	0.55
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.87	0.55
2:D:62:VAL:HG23	2:D:86:ILE:O	2.06	0.55
2:B:30:ILE:HG22	2:B:86:ILE:HD11	1.89	0.55
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.25	0.55
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.88	0.55
2:D:19:LYS:O	2:D:23:VAL:HG23	2.07	0.55
1:C:158:SER:OG	1:C:197:HIS:HB3	2.07	0.55
1:C:204:VAL:HG13	1:C:209:ILE:HD11	1.88	0.54
2:D:151:THR:HA	2:D:154:ILE:HD12	1.90	0.54
1:A:21:TRP:CZ2	1:A:65:ALA:HB2	2.43	0.54
3:E:130:ALA:HB1	3:E:134:ARG:HH12	1.71	0.54
2:B:347:ILE:HG22	2:B:347:ILE:O	2.08	0.54
2:B:371:LEU:H	2:B:371:LEU:HD23	1.71	0.54
1:C:248:LEU:HD12	1:C:248:LEU:H	1.73	0.53
2:B:286:LEU:HD23	2:B:290:GLU:HB3	1.89	0.53
1:C:346:TRP:HZ2	1:C:435:VAL:HG22	1.73	0.53
2:D:291:LEU:O	2:D:295:MET:HB2	2.08	0.53
1:C:248:LEU:O	1:C:249:ASN:ND2	2.42	0.53
2:D:249:ASN:N	2:D:250:ALA:HB2	2.23	0.53
2:D:272:PHE:HD1	2:D:376:THR:HG23	1.73	0.53
1:A:306:ASP:OD2	1:A:309:HIS:ND1	2.38	0.53
1:A:2:ARG:N	1:A:131:GLY:O	2.43	0.52
1:C:259:LEU:HD22	1:C:268:PRO:HB3	1.91	0.52
2:D:137:LEU:HB3	2:D:168:THR:HG22	1.91	0.52
2:B:159:GLU:HA	3:E:72:LEU:HD13	1.92	0.52
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.44	0.52
1:A:410:GLY:HA2	3:E:64:GLN:HE22	1.75	0.52
2:B:172:MET:HB2	2:B:205:ASP:HA	1.90	0.52
2:D:219:LEU:HD13	2:D:226:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:HB3	2:D:94:PHE:CD1	2.45	0.51
1:A:15:GLN:HA	1:A:18:ASN:HD22	1.74	0.51
1:A:214:ARG:HG2	1:A:219:ILE:O	2.10	0.51
1:A:258:ASN:HD22	1:A:352:LYS:HD3	1.75	0.51
1:A:346:TRP:CE3	3:E:32:VAL:HG13	2.46	0.51
2:D:68:VAL:HG22	2:D:93:VAL:HB	1.91	0.51
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.91	0.51
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.93	0.51
2:D:139:HIS:CE1	2:D:170:SER:OG	2.64	0.51
1:A:207:GLU:O	1:A:210:TYR:HB3	2.11	0.51
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.91	0.51
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.46	0.51
2:B:64:ARG:HB2	2:B:64:ARG:HH11	1.76	0.51
1:A:191:THR:O	1:A:195:LEU:HB2	2.11	0.51
2:B:407:TRP:CZ2	1:C:257:THR:HA	2.46	0.51
2:D:214:PHE:O	2:D:218:LYS:HA	2.11	0.50
1:A:375:VAL:HG22	1:A:376:CYS:H	1.76	0.50
1:A:301:GLN:HE22	1:A:307:PRO:HG3	1.76	0.50
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.92	0.50
1:A:248:LEU:HB2	3:E:19:SER:HB3	1.92	0.50
1:A:286:LEU:HD23	1:A:290:GLU:HB3	1.92	0.50
2:B:48:ARG:HH11	2:B:245:PRO:HA	1.77	0.50
2:B:325:MET:O	2:B:329:ASP:HB2	2.10	0.50
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.45	0.50
1:C:249:ASN:CB	1:C:355:ILE:H	2.19	0.50
8:D:503:3WY:H4	8:D:503:3WY:C28	2.40	0.50
2:B:306:ASP:CB	2:B:309:HIS:HD2	2.21	0.50
2:B:331:GLN:O	2:B:335:VAL:HG23	2.11	0.50
1:A:3:GLU:HG3	1:A:129:CYS:CB	2.41	0.50
2:D:291:LEU:HD11	2:D:373:MET:HB3	1.93	0.50
1:C:208:ALA:HB2	1:C:304:LYS:HG3	1.92	0.49
2:D:91:ASN:HA	2:D:121:VAL:HG11	1.93	0.49
2:D:137:LEU:HD22	2:D:154:ILE:HD11	1.94	0.49
1:C:271:THR:HG21	1:C:295:CYS:O	2.12	0.49
2:D:12:CYS:SG	2:D:171:VAL:HG11	2.52	0.49
2:D:106:GLY:O	2:D:111:GLY:HA3	2.12	0.49
2:D:269:MET:HE1	2:D:383:ALA:HB3	1.94	0.49
2:B:240:THR:HB	2:B:318:VAL:HG11	1.95	0.49
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.48	0.49
1:A:298:PRO:HA	1:A:301:GLN:HB2	1.93	0.49
2:B:133:GLN:HG2	2:B:252:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:HIS:HE1	2:B:170:SER:OG	1.96	0.49
1:A:393:HIS:HA	1:A:396:ASP:HB2	1.95	0.48
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.53	0.48
2:D:93:VAL:HG12	2:D:114:LEU:HD11	1.96	0.48
1:A:70:LEU:HD13	1:A:110:ILE:HB	1.95	0.48
1:C:93:ILE:HG21	1:C:118:VAL:HG22	1.94	0.48
2:D:181:VAL:HG21	2:D:404:PHE:CZ	2.48	0.48
2:D:166:MET:HB3	2:D:198:THR:HA	1.95	0.48
2:D:6:HIS:CE1	2:D:8:GLN:NE2	2.78	0.48
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.49	0.48
2:B:75:MET:HG3	2:B:92:PHE:HD2	1.79	0.48
1:C:52:PHE:CD1	1:C:243:ARG:HG2	2.48	0.48
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.59	0.48
3:E:129:HIS:O	3:E:132:GLU:HG3	2.13	0.48
2:B:12:CYS:HB3	2:B:140:SER:HB3	1.96	0.48
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.49	0.48
1:A:154:MET:HG3	1:A:194:THR:HG23	1.95	0.47
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.95	0.47
2:D:292:THR:HG22	2:D:335:VAL:HG21	1.96	0.47
1:A:245:ASP:HB3	3:E:15:THR:HB	1.95	0.47
2:B:31:ASP:O	2:B:33:THR:N	2.46	0.47
2:B:98:GLY:C	2:B:100:GLY:H	2.18	0.47
2:B:313:LEU:HA	2:B:344:VAL:CG2	2.44	0.47
2:D:166:MET:HG3	2:D:198:THR:HG22	1.94	0.47
1:C:260:VAL:HG12	1:C:262:TYR:O	2.14	0.47
1:A:180:ALA:H	1:A:183:GLU:HG3	1.80	0.47
8:B:503:3WY:H16	8:B:503:3WY:H12	1.97	0.47
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.49	0.47
2:D:177:VAL:HA	8:D:503:3WY:H46	1.97	0.47
1:C:430:LYS:O	1:C:433:GLU:HB2	2.15	0.47
2:D:6:HIS:HE1	2:D:8:GLN:NE2	2.12	0.47
2:B:139:HIS:HD2	2:B:146:GLY:O	1.98	0.47
1:A:70:LEU:HB2	1:A:98:ASP:HA	1.96	0.46
1:A:208:ALA:HA	1:A:304:LYS:HE3	1.96	0.46
1:A:315:CYS:HB3	1:A:351:PHE:HB3	1.97	0.46
2:B:165:ILE:HG22	2:B:252:LEU:HD23	1.97	0.46
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.97	0.46
1:C:241:SER:HB2	1:C:252:LEU:H	1.79	0.46
2:D:139:HIS:HE1	2:D:170:SER:OG	1.98	0.46
3:E:125:GLU:O	3:E:128:LYS:HB2	2.15	0.46
2:D:264:ARG:HH12	2:D:424:ASN:HD21	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HA	1:A:94:THR:HG21	1.97	0.46
1:A:329:ASN:HD21	3:E:22:VAL:HG11	1.81	0.46
2:B:54:ASN:HB2	2:B:62:VAL:HG13	1.97	0.46
2:B:79:ARG:HH22	2:B:94:PHE:HE2	1.64	0.46
1:C:302:MET:HA	1:C:302:MET:HE2	1.98	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.98	0.46
2:D:195:VAL:HG22	2:D:264:ARG:HG2	1.98	0.46
2:B:286:LEU:HD22	2:B:291:LEU:HD12	1.97	0.46
1:C:9:VAL:HG12	1:C:145:THR:HG22	1.98	0.46
2:B:55:GLU:HB3	2:B:57:THR:HG23	1.98	0.46
1:C:360:PRO:HG3	1:C:374:ALA:HB2	1.98	0.46
2:D:116:ASP:HA	2:D:119:LEU:HD12	1.97	0.46
2:D:268:PHE:O	2:D:270:PRO:HD3	2.15	0.46
2:B:268:PHE:HB3	2:B:378:ILE:HG23	1.98	0.45
1:C:286:LEU:HD23	1:C:290:GLU:HB3	1.97	0.45
1:C:330:ALA:O	1:C:333:ALA:HB3	2.15	0.45
1:A:155:GLU:HG2	1:A:197:HIS:HE1	1.81	0.45
1:C:265:ILE:HG22	1:C:380:ASN:HD21	1.82	0.45
2:B:259:MET:SD	7:B:502:LOC:H19	2.57	0.45
1:C:107:HIS:HE1	1:C:155:GLU:OE2	1.99	0.45
3:E:125:GLU:HA	3:E:128:LYS:HD2	1.98	0.45
1:A:70:LEU:HD22	1:A:110:ILE:HG22	1.99	0.45
1:A:346:TRP:HB2	3:E:32:VAL:HG22	1.99	0.45
2:D:66:ILE:HG22	2:D:68:VAL:HG23	1.99	0.45
2:D:315:VAL:HB	2:D:351:VAL:HG13	1.99	0.45
1:A:70:LEU:HD21	1:A:114:ILE:HG21	1.98	0.45
1:C:317:LEU:HB2	1:C:353:VAL:HG22	1.98	0.45
2:D:48:ARG:CZ	2:D:245:PRO:HA	2.46	0.45
1:A:78:VAL:C	1:A:80:THR:H	2.20	0.45
1:C:344:VAL:CG2	1:C:347:CYS:HB2	2.42	0.45
2:D:385:GLN:O	2:D:389:LYS:HG3	2.17	0.45
3:E:64:GLN:H	3:E:64:GLN:HG3	1.63	0.45
2:B:404:PHE:CE2	1:C:261:PRO:HA	2.53	0.44
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.52	0.44
2:D:24:ILE:HA	2:D:27:GLU:HB2	1.99	0.44
2:D:226:ASP:OD1	2:D:278:ARG:NH2	2.51	0.44
1:C:317:LEU:HD22	1:C:332:ILE:HD11	1.99	0.44
3:E:31:GLY:O	3:E:32:VAL:HB	2.18	0.44
1:A:329:ASN:HD21	3:E:20:TRP:HE1	1.64	0.44
2:B:114:LEU:HB3	2:B:149:MET:HE3	1.99	0.44
1:C:248:LEU:HD11	1:C:357:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:LEU:HD22	2:B:154:ILE:HD11	1.98	0.44
2:D:48:ARG:NH1	2:D:241:CYS:O	2.45	0.44
1:C:66:VAL:HG12	1:C:68:VAL:HG23	2.00	0.44
1:C:308:ARG:HA	1:C:340:THR:CG2	2.48	0.44
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.99	0.44
1:A:224:TYR:HA	1:A:227:LEU:HD12	2.00	0.44
1:A:274:PRO:HD3	1:A:374:ALA:HA	1.99	0.44
2:B:114:LEU:HB3	2:B:149:MET:CE	2.48	0.44
2:B:271:GLY:HA3	2:B:377:PHE:HB3	1.99	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.43
2:B:404:PHE:O	2:B:407:TRP:HD1	2.01	0.43
2:B:164:ARG:HA	2:B:164:ARG:HH11	1.81	0.43
2:B:182:VAL:O	2:B:185:TYR:HB2	2.18	0.43
2:D:234:THR:HG22	2:D:272:PHE:HB2	2.01	0.43
1:A:285:GLN:HE22	1:A:373:ARG:H	1.66	0.43
2:B:3:GLU:O	2:B:133:GLN:HB2	2.18	0.43
2:B:320:ARG:HB2	2:B:374:SER:HB3	1.99	0.43
1:C:302:MET:HA	1:C:302:MET:CE	2.48	0.43
2:B:115:VAL:HG22	2:B:119:LEU:HD13	2.00	0.43
2:B:189:LEU:O	2:B:192:HIS:HB3	2.19	0.43
2:B:3:GLU:HG2	2:B:129:CYS:HB3	2.00	0.43
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.84	0.43
1:A:291:ILE:HD12	1:A:375:VAL:HB	2.01	0.43
1:C:179:THR:HG22	1:C:180:ALA:H	1.83	0.43
1:A:230:LEU:HD23	1:A:234:ILE:HD11	2.00	0.43
2:B:204:ILE:HD13	2:B:270:PRO:HG2	2.01	0.43
1:C:70:LEU:HD22	1:C:110:ILE:HG22	2.01	0.43
2:D:265:LEU:HD21	2:D:431:GLU:HG2	2.00	0.43
1:A:277:SER:HB3	1:A:280:LYS:HD3	2.01	0.43
2:B:64:ARG:HB2	2:B:64:ARG:NH1	2.34	0.43
2:D:12:CYS:CB	2:D:140:SER:HB3	2.46	0.43
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.01	0.43
2:D:70:LEU:O	2:D:98:GLY:N	2.51	0.43
1:C:16:ILE:HD11	1:C:231:ILE:HD13	2.01	0.42
1:A:11:GLN:HG2	1:A:15:GLN:HE21	1.84	0.42
2:B:425:MET:O	2:B:429:VAL:HG23	2.19	0.42
1:C:261:PRO:HB2	1:C:262:TYR:CD1	2.54	0.42
1:C:234:ILE:HD13	1:C:302:MET:SD	2.60	0.42
1:C:270:ALA:HB3	1:C:302:MET:HB2	2.01	0.42
1:C:287:SER:OG	1:C:290:GLU:HG3	2.20	0.42
1:A:21:TRP:HA	1:A:24:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:THR:HG22	1:C:180:ALA:N	2.34	0.42
2:D:185:TYR:HD1	2:D:408:TYR:HE1	1.68	0.42
1:A:347:CYS:HA	1:A:348:PRO:HD3	1.94	0.42
1:C:22:GLU:O	1:C:26:LEU:HG	2.20	0.42
1:C:346:TRP:CZ2	1:C:435:VAL:HG22	2.53	0.42
2:D:83:PHE:O	2:D:85:GLN:N	2.52	0.42
1:A:238:ILE:HG12	1:A:378:LEU:HD21	2.02	0.42
2:B:244:PHE:HA	2:B:245:PRO:HD3	1.80	0.42
1:C:53:PHE:HA	1:C:63:PRO:HA	2.02	0.42
1:C:179:THR:CG2	1:C:180:ALA:H	2.33	0.42
1:A:287:SER:HA	1:A:373:ARG:HH11	1.84	0.41
2:D:200:GLU:HB2	2:D:268:PHE:CE1	2.55	0.41
1:A:139:HIS:CG	1:A:150:THR:HG21	2.55	0.41
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.38	0.41
2:B:44:LEU:HD23	2:B:49:ILE:HD13	2.02	0.41
1:C:180:ALA:HA	7:D:502:LOC:O5	2.20	0.41
1:C:249:ASN:HB3	1:C:354:GLY:HA2	2.01	0.41
2:D:69:ASP:HB3	2:D:94:PHE:HE1	1.80	0.41
1:C:276:ILE:HD12	1:C:369:ALA:HB3	2.02	0.41
2:D:308:ARG:HD2	2:D:342:TYR:CE2	2.56	0.41
1:A:114:ILE:O	1:A:118:VAL:HG23	2.19	0.41
2:D:133:GLN:NE2	2:D:252:LEU:H	2.03	0.41
2:D:312:TYR:HA	2:D:381:SER:HA	2.01	0.41
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.01	0.41
1:A:137:VAL:HG23	1:A:168:GLU:HA	2.01	0.41
1:A:175:PRO:HA	1:A:179:THR:CG2	2.51	0.41
2:B:305:CYS:SG	2:B:384:ILE:HA	2.60	0.41
1:C:34:GLY:HA3	1:C:60:LYS:HG2	2.02	0.41
2:D:136:GLN:HG3	2:D:167:ASN:HD22	1.86	0.41
2:B:12:CYS:CB	2:B:140:SER:HB3	2.50	0.41
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.55	0.41
2:B:104:ALA:HB2	2:B:413:MET:SD	2.61	0.41
1:C:68:VAL:HG11	1:C:149:PHE:CE1	2.55	0.41
2:D:159:GLU:HG3	3:E:123:LEU:HD13	2.03	0.41
2:D:185:TYR:HD1	2:D:408:TYR:CE1	2.39	0.41
2:D:208:ALA:O	2:D:212:ILE:HD13	2.19	0.41
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.03	0.41
1:A:5:ILE:HD13	1:A:64:ARG:HB3	2.02	0.41
1:C:339:ARG:HD3	1:C:339:ARG:HA	1.82	0.41
2:B:96:GLN:HG3	1:C:1:MET:HE3	2.03	0.40
2:D:2:ARG:O	2:D:2:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ASN:HD22	2:D:206:ASN:HA	1.60	0.40
1:A:328:VAL:HG21	1:A:355:ILE:HD11	2.02	0.40
2:B:141:LEU:HD12	2:B:172:MET:SD	2.62	0.40
1:C:25:CYS:O	1:C:30:ILE:N	2.54	0.40
1:A:407:TRP:CE2	2:B:257:VAL:HA	2.56	0.40
2:B:78:VAL:O	2:B:84:GLY:HA3	2.21	0.40
2:B:177:VAL:HG13	2:B:206:ASN:HB3	2.03	0.40
1:A:18:ASN:O	1:A:22:GLU:HB2	2.20	0.40
1:A:311:LYS:HD3	1:A:344:VAL:HG12	2.03	0.40
1:C:255:PHE:CD2	1:C:316:CYS:HB3	2.56	0.40
2:D:313:LEU:HA	2:D:344:VAL:HG22	2.04	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	425/451 (94%)	364 (86%)	51 (12%)	10 (2%)	6	35
1	C	428/451 (95%)	355 (83%)	51 (12%)	22 (5%)	2	19
2	B	426/445 (96%)	372 (87%)	39 (9%)	15 (4%)	3	27
2	D	429/445 (96%)	374 (87%)	47 (11%)	8 (2%)	8	40
3	E	119/142 (84%)	107 (90%)	10 (8%)	2 (2%)	9	42
All	All	1827/1934 (94%)	1572 (86%)	198 (11%)	57 (3%)	4	30

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ALA
1	A	178	SER
1	A	322	ASP

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Mol	Chain	Res	Type
1	A	341	ILE
2	B	32	PRO
2	B	98	GLY
2	B	178	SER
2	B	350	ASN
1	C	10	GLY
1	C	249	ASN
2	D	84	GLY
2	D	250	ALA
2	D	413	MET
3	E	32	VAL
2	B	73	GLY
2	B	100	GLY
2	B	101	ASN
2	B	144	GLY
2	B	373	MET
1	C	29	GLY
1	C	109	THR
1	C	181	VAL
1	C	250	VAL
2	D	73	GLY
1	A	73	THR
1	A	147	SER
2	B	298	SER
1	C	11	GLN
1	C	279	GLU
1	C	314	ALA
1	C	338	LYS
1	C	413	MET
2	D	47	GLU
2	D	109	THR
2	D	383	ALA
2	B	99	ALA
2	B	214	PHE
2	B	284	ARG
1	C	82	THR
1	C	179	THR
1	C	247	ALA
1	C	281	ALA
1	C	339	ARG
2	D	304	ALA
1	A	11	GLN

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Mol	Chain	Res	Type
1	A	261	PRO
2	B	39	ASP
1	C	32	PRO
1	C	73	THR
1	C	84	ARG
1	C	206	ASN
1	C	241	SER
1	A	131	GLY
3	E	31	GLY
1	C	246	GLY
1	A	306	ASP
2	B	263	PRO

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	362/378 (96%)	305 (84%)	57 (16%)	2	15
1	C	359/378 (95%)	309 (86%)	50 (14%)	3	20
2	B	364/383 (95%)	309 (85%)	55 (15%)	3	17
2	D	369/383 (96%)	317 (86%)	52 (14%)	3	19
3	E	107/125 (86%)	89 (83%)	18 (17%)	2	12
All	All	1561/1647 (95%)	1329 (85%)	232 (15%)	3	17

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	GLU
1	A	4	CYS
1	A	16	ILE
1	A	33	ASP
1	A	46	ASP
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	74	VAL
1	A	75	ILE
1	A	79	ARG
1	A	92	LEU
1	A	94	THR
1	A	103	TYR
1	A	105	ARG
1	A	117	LEU
1	A	120	ASP
1	A	121	ARG
1	A	124	LYS
1	A	125	LEU
1	A	140	SER
1	A	141	PHE
1	A	150	THR
1	A	166	LYS
1	A	167	LEU
1	A	171	ILE
1	A	181	VAL
1	A	182	VAL
1	A	187	SER
1	A	188	ILE
1	A	211	ASP
1	A	216	ASN
1	A	217	LEU
1	A	221	ARG
1	A	224	TYR
1	A	225	THR
1	A	230	LEU
1	A	253	THR
1	A	254	GLU
1	A	271	THR
1	A	275	VAL
1	A	279	GLU
1	A	295	CYS
1	A	308	ARG
1	A	322	ASP
1	A	323	VAL
1	A	327	ASP
1	A	336	LYS
1	A	343	PHE
1	A	351	PHE

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Mol	Chain	Res	Type
1	A	352	LYS
1	A	357	TYR
1	A	379	SER
1	A	384	ILE
1	A	401	LYS
1	A	402	ARG
1	A	409	VAL
1	A	417	GLU
2	B	4	ILE
2	B	35	SER
2	B	42	LEU
2	B	49	ILE
2	B	50	ASN
2	B	62	VAL
2	B	64	ARG
2	B	70	LEU
2	B	75	MET
2	B	86	ILE
2	B	97	SER
2	B	109	THR
2	B	116	ASP
2	B	117	SER
2	B	122	VAL
2	B	127	GLU
2	B	129	CYS
2	B	130	ASP
2	B	133	GLN
2	B	137	LEU
2	B	138	THR
2	B	139	HIS
2	B	153	LEU
2	B	155	SER
2	B	158	ARG
2	B	163	ASP
2	B	164	ARG
2	B	166	MET
2	B	171	VAL
2	B	177	VAL
2	B	179	ASP
2	B	180	THR
2	B	206	ASN
2	B	207	GLU

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Mol	Chain	Res	Type
2	B	214	PHE
2	B	223	THR
2	B	227	LEU
2	B	234	THR
2	B	251	ASP
2	B	296	PHE
2	B	297	ASP
2	B	298	SER
2	B	324	SER
2	B	325	MET
2	B	327	GLU
2	B	329	ASP
2	B	334	ASN
2	B	350	ASN
2	B	352	LYS
2	B	371	LEU
2	B	372	LYS
2	B	376	THR
2	B	390	ARG
2	B	416	MET
2	B	439	THR
1	C	2	ARG
1	C	5	ILE
1	C	11	GLN
1	C	16	ILE
1	C	22	GLU
1	C	23	LEU
1	C	33	ASP
1	C	48	SER
1	C	60	LYS
1	C	74	VAL
1	C	94	THR
1	C	112	LYS
1	C	113	GLU
1	C	114	ILE
1	C	120	ASP
1	C	121	ARG
1	C	123	ARG
1	C	130	THR
1	C	141	PHE
1	C	153	LEU
1	C	178	SER

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Mol	Chain	Res	Type
1	C	199	ASP
1	C	224	TYR
1	C	225	THR
1	C	229	ARG
1	C	236	SER
1	C	243	ARG
1	C	245	ASP
1	C	251	ASP
1	C	252	LEU
1	C	253	THR
1	C	269	LEU
1	C	293	ASN
1	C	302	MET
1	C	323	VAL
1	C	327	ASP
1	C	332	ILE
1	C	338	LYS
1	C	339	ARG
1	C	345	ASP
1	C	347	CYS
1	C	351	PHE
1	C	367	ASP
1	C	368	LEU
1	C	377	MET
1	C	379	SER
1	C	402	ARG
1	C	415	GLU
1	C	419	SER
1	C	435	VAL
2	D	2	ARG
2	D	3	GLU
2	D	8	GLN
2	D	19	LYS
2	D	50	ASN
2	D	55	GLU
2	D	97	SER
2	D	110	GLU
2	D	115	VAL
2	D	116	ASP
2	D	117	SER
2	D	122	VAL
2	D	127	GLU

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Mol	Chain	Res	Type
2	D	141	LEU
2	D	145	THR
2	D	153	LEU
2	D	164	ARG
2	D	166	MET
2	D	171	VAL
2	D	197	ASN
2	D	200	GLU
2	D	205	ASP
2	D	206	ASN
2	D	219	LEU
2	D	223	THR
2	D	241	CYS
2	D	249	ASN
2	D	276	THR
2	D	284	ARG
2	D	288	VAL
2	D	293	GLN
2	D	323	MET
2	D	325	MET
2	D	326	LYS
2	D	333	LEU
2	D	355	VAL
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	384	ILE
2	D	387	LEU
2	D	391	ILE
2	D	402	LYS
2	D	405	LEU
2	D	415	GLU
2	D	416	MET
2	D	419	THR
2	D	423	SER
2	D	424	ASN
2	D	425	MET
2	D	430	SER
2	D	434	GLN
3	E	11	LEU
3	E	18	GLN
3	E	22	VAL

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Mol	Chain	Res	Type
3	E	23	ILE
3	E	30	ASP
3	E	49	GLU
3	E	63	TYR
3	E	64	GLN
3	E	68	LEU
3	E	90	ASN
3	E	93	PHE
3	E	96	MET
3	E	101	LEU
3	E	103	GLN
3	E	120	LEU
3	E	124	GLN
3	E	127	ASP
3	E	132	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	11	GLN
1	A	15	GLN
1	A	28	HIS
1	A	139	HIS
1	A	197	HIS
1	A	233	GLN
1	A	249	ASN
1	A	258	ASN
1	A	301	GLN
1	A	329	ASN
2	B	8	GLN
2	B	11	GLN
2	B	14	ASN
2	B	139	HIS
2	B	206	ASN
2	B	294	GLN
2	B	309	HIS
2	B	334	ASN
2	B	380	ASN
2	B	406	HIS
2	B	433	GLN
2	B	436	GLN

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Mol	Chain	Res	Type
1	C	8	HIS
1	C	11	GLN
1	C	61	HIS
1	C	102	ASN
1	C	107	HIS
1	C	139	HIS
1	C	266	HIS
1	C	300	ASN
1	C	380	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	133	GLN
2	D	136	GLN
2	D	139	HIS
2	D	206	ASN
2	D	249	ASN
2	D	266	HIS
2	D	293	GLN
2	D	300	ASN
2	D	331	GLN
2	D	385	GLN
2	D	424	ASN
2	D	433	GLN
2	D	436	GLN
3	E	64	GLN
3	E	91	ASN
3	E	111	ASN
3	E	129	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 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	#$|Z| > 2$
4	GTP	A	600	5	26,34,34	0.72	1 (3%)	32,54,54	0.71	0
4	GTP	C	600	5	26,34,34	0.72	1 (3%)	32,54,54	0.73	0
6	GDP	B	501	-	24,30,30	0.74	0	30,47,47	0.78	0
8	3WY	B	503	-	53,54,54	0.99	5 (9%)	58,76,76	1.48	9 (15%)
7	LOC	D	502	-	31,31,31	0.49	0	44,44,44	0.74	1 (2%)
8	3WY	D	503	-	53,54,54	1.07	6 (11%)	58,76,76	1.50	13 (22%)
6	GDP	D	501	-	24,30,30	0.95	2 (8%)	30,47,47	0.80	0
7	LOC	B	502	-	31,31,31	0.53	1 (3%)	44,44,44	0.66	1 (2%)

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
4	GTP	A	600	5	-	2/18/38/38	0/3/3/3
4	GTP	C	600	5	-	7/18/38/38	0/3/3/3
6	GDP	B	501	-	-	7/12/32/32	0/3/3/3
8	3WY	B	503	-	-	26/72/91/91	0/3/3/3
7	LOC	D	502	-	-	0/12/25/25	0/3/3/3
8	3WY	D	503	-	-	17/72/91/91	0/3/3/3
6	GDP	D	501	-	-	6/12/32/32	0/3/3/3
7	LOC	B	502	-	-	0/12/25/25	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	503	3WY	C5-N3	4.29	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	503	3WY	C5-N3	3.69	1.55	1.47
8	D	503	3WY	C6-C5	3.47	1.60	1.52
8	B	503	3WY	O3-C25	3.18	1.31	1.22
8	D	503	3WY	O3-C25	2.98	1.31	1.22
8	B	503	3WY	C6-C5	2.94	1.59	1.52
8	B	503	3WY	O4-C25	-2.56	1.22	1.30
6	D	501	GDP	C5-C6	-2.52	1.42	1.47
8	D	503	3WY	O4-C25	-2.44	1.22	1.30
7	B	502	LOC	C11-C14	2.39	1.57	1.53
8	D	503	3WY	C3-C5	2.36	1.59	1.54
8	B	503	3WY	C14-C16	2.25	1.56	1.52
8	D	503	3WY	C14-C16	2.22	1.56	1.52
6	D	501	GDP	C8-N7	-2.17	1.31	1.35
4	C	600	GTP	C8-N7	-2.08	1.31	1.35
4	A	600	GTP	C8-N7	-2.03	1.31	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	503	3WY	C28-N3-C5	-5.44	108.76	119.46
8	B	503	3WY	C28-N3-C5	-4.76	110.09	119.46
8	B	503	3WY	C5-N3-C29	4.71	133.84	120.34
8	B	503	3WY	C4-C3-C5	4.23	122.91	111.20
8	D	503	3WY	C37-C36-C35	3.19	107.12	104.18
8	D	503	3WY	C31-C30-C29	3.08	116.96	110.73
7	B	502	LOC	C14-C11-N1	3.02	116.72	114.34
8	D	503	3WY	C30-C29-N3	2.86	124.65	118.74
8	B	503	3WY	O5-C13-C14	2.82	112.52	105.83
8	D	503	3WY	C14-C16-N2	-2.79	112.22	116.44
8	D	503	3WY	O3-C25-C17	-2.73	113.29	122.26
8	D	503	3WY	O4-C25-C17	2.70	122.38	113.40
7	D	502	LOC	C14-C11-N1	2.70	116.47	114.34
8	B	503	3WY	O4-C25-C17	2.70	122.37	113.40
8	D	503	3WY	C28-N3-C29	2.67	130.95	122.26
8	D	503	3WY	O7-C29-C30	-2.56	115.00	119.99
8	B	503	3WY	O3-C25-C17	-2.55	113.87	122.26
8	B	503	3WY	C30-C29-N3	2.53	123.96	118.74
8	D	503	3WY	C29-C30-N4	2.31	113.46	108.03
8	D	503	3WY	C6-C7-C8	-2.25	108.95	112.42
8	D	503	3WY	C4-C3-C5	2.19	117.26	111.20
8	B	503	3WY	O7-C29-C30	-2.10	115.90	119.99
8	B	503	3WY	C14-C16-N2	-2.06	113.32	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	503	3WY	O2-C16-C14	2.05	124.72	121.02

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	600	GTP	PB-O3B-PG-O3G
4	C	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O2A
6	B	501	GDP	PA-O3A-PB-O2B
6	B	501	GDP	C5'-O5'-PA-O1A
6	B	501	GDP	C5'-O5'-PA-O2A
6	D	501	GDP	C5'-O5'-PA-O1A
6	D	501	GDP	C5'-O5'-PA-O2A
8	B	503	3WY	O8-C34-C35-N5
8	B	503	3WY	N4-C34-C35-N5
8	B	503	3WY	C3-C5-C6-C7
8	B	503	3WY	N3-C5-C6-O6
8	B	503	3WY	C3-C5-C6-O6
8	B	503	3WY	C2-C3-C5-N3
8	B	503	3WY	C4-C3-C5-N3
8	B	503	3WY	C7-C8-N1-C12
8	B	503	3WY	C7-C8-N1-C9
8	B	503	3WY	C14-C13-O5-C26
8	D	503	3WY	N3-C5-C6-C7
8	D	503	3WY	C7-C6-O6-C27
8	B	503	3WY	C35-C34-N4-C30
8	B	503	3WY	C25-C17-C18-C19
8	B	503	3WY	O8-C34-N4-C30
8	B	503	3WY	N2-C17-C18-C19
8	D	503	3WY	C29-C30-C31-C33
8	D	503	3WY	N4-C34-C35-N5
8	B	503	3WY	C1-C2-C3-C4
8	D	503	3WY	C1-C2-C3-C4
8	D	503	3WY	O8-C34-C35-N5
8	D	503	3WY	C1-C2-C3-C5
8	B	503	3WY	C1-C2-C3-C5
8	B	503	3WY	O1-C8-N1-C9
8	B	503	3WY	C17-C18-C19-C20
8	B	503	3WY	C17-C18-C19-C24
8	B	503	3WY	C5-C6-C7-C8
4	C	600	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
6	B	501	GDP	PA-O3A-PB-O3B
6	B	501	GDP	C5'-O5'-PA-O3A
4	A	600	GTP	PB-O3A-PA-O1A
8	B	503	3WY	C3-C5-N3-C29
6	B	501	GDP	C4'-C5'-O5'-PA
8	B	503	3WY	O8-C34-C35-C39
8	B	503	3WY	N4-C34-C35-C39
8	B	503	3WY	N3-C5-C6-C7
8	B	503	3WY	C2-C3-C5-C6
8	D	503	3WY	N2-C17-C25-O3
4	C	600	GTP	PB-O3A-PA-O1A
4	C	600	GTP	C4'-C5'-O5'-PA
6	D	501	GDP	C3'-C4'-C5'-O5'
8	B	503	3WY	C6-C7-C8-N1
8	D	503	3WY	C3-C5-N3-C29
8	D	503	3WY	C29-C30-C31-C32
4	A	600	GTP	PB-O3B-PG-O1G
8	D	503	3WY	N4-C30-C31-C33
6	D	501	GDP	O4'-C4'-C5'-O5'
8	D	503	3WY	O7-C29-C30-C31
8	D	503	3WY	N2-C17-C25-O4
8	D	503	3WY	C5-C6-C7-C8
4	C	600	GTP	C5'-O5'-PA-O3A
6	D	501	GDP	C5'-O5'-PA-O3A
6	D	501	GDP	PB-O3A-PA-O2A
8	D	503	3WY	O8-C34-C35-C39
8	D	503	3WY	N4-C34-C35-C39
6	B	501	GDP	PA-O3A-PB-O1B
8	D	503	3WY	N3-C29-C30-C31

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GDP	1	0
8	B	503	3WY	1	0
7	D	502	LOC	1	0
8	D	503	3WY	4	0
6	D	501	GDP	1	0
7	B	502	LOC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 600

Bond lengths

Bond angles

Torsions

Rings

Ligand GTP C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 3WY B 503

Bond lengths

Bond angles

Torsions

Rings

Ligand LOC D 502

Bond lengths

Bond angles

Torsions

Rings

Ligand 3WY D 503

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand LOC B 502

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	429/451 (95%)	0.08	14 (3%)	46	41	120, 161, 207, 239	0
1	C	430/451 (95%)	-0.26	6 (1%)	75	69	98, 132, 177, 194	1 (0%)
2	B	428/445 (96%)	-0.19	9 (2%)	63	58	108, 144, 187, 212	2 (0%)
2	D	430/445 (96%)	-0.21	4 (0%)	84	79	97, 130, 171, 187	2 (0%)
3	E	123/142 (86%)	-0.30	5 (4%)	37	33	134, 159, 215, 225	0
All	All	1840/1934 (95%)	-0.15	38 (2%)	63	58	97, 144, 194, 239	5 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	MET	6.1
3	E	14	ALA	4.0
1	A	346	TRP	3.9
1	A	83	TYR	3.6
2	D	441	ASP	3.3
3	E	15	THR	3.2
3	E	16	SER	3.1
1	A	178	SER	3.1
1	C	140	SER	3.0
3	E	22	VAL	3.0
2	B	30	ILE	3.0
1	A	380	ASN	3.0
3	E	13	LYS	2.9
1	A	66	VAL	2.9
1	A	11	GLN	2.8
1	A	65	ALA	2.8
2	B	42	LEU	2.7
1	C	199	ASP	2.7
1	A	381	THR	2.6
1	A	424	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	253	THR	2.4
2	D	249	ASN	2.4
2	D	413	MET	2.4
2	B	247	GLN	2.4
1	A	246	GLY	2.3
1	C	418	PHE	2.3
2	D	284	ARG	2.3
1	A	101	ASN	2.2
2	B	36	TYR	2.2
2	B	249	ASN	2.1
1	A	388	TRP	2.1
2	B	250	ALA	2.1
1	C	275	VAL	2.1
2	B	66	ILE	2.1
2	B	251	ASP	2.1
1	A	149	PHE	2.1
1	C	315	CYS	2.0
2	B	188	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	LOC	B	502	29/29	0.86	0.29	155,162,167,168	0
8	3WY	B	503	52/52	0.89	0.23	137,150,161,163	0
8	3WY	D	503	52/52	0.89	0.27	118,147,162,165	0
7	LOC	D	502	29/29	0.90	0.35	138,144,147,150	0
4	GTP	C	600	32/32	0.93	0.35	107,113,119,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GTP	A	600	32/32	0.94	0.47	137,148,154,155	0
6	GDP	B	501	28/28	0.96	0.27	124,130,134,135	0
6	GDP	D	501	28/28	0.96	0.22	112,117,137,138	0
5	MG	A	601	1/1	0.97	0.41	91,91,91,91	0
5	MG	C	601	1/1	0.97	0.41	63,63,63,63	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 LOC B 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
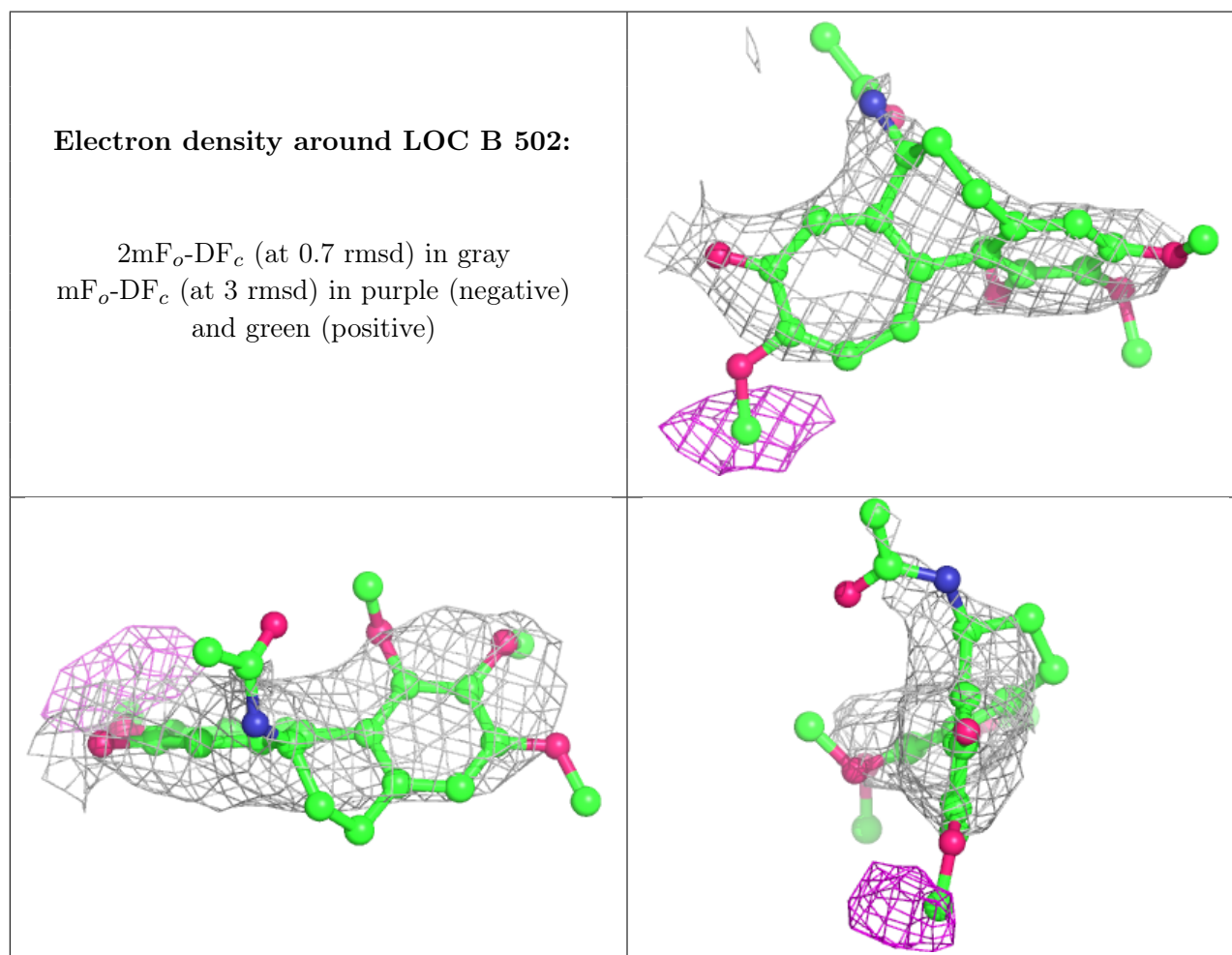
Electron density around 3WY B 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
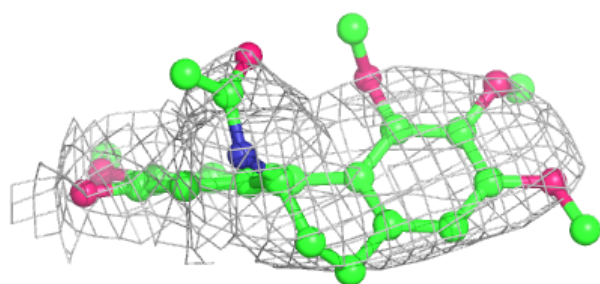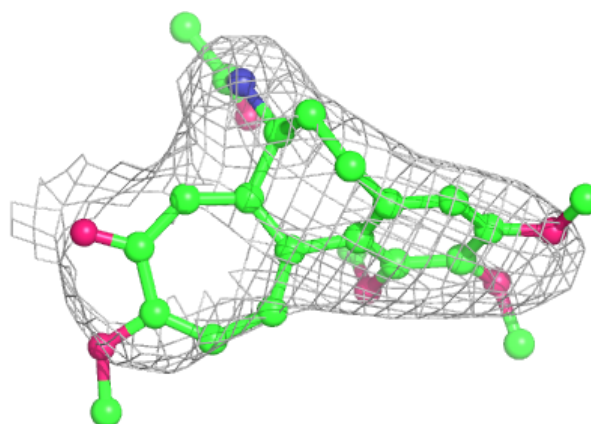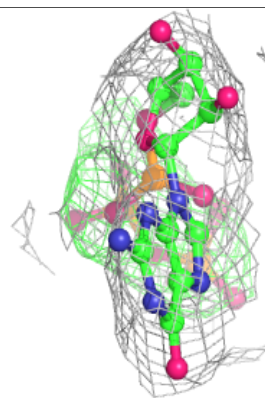and green (positive)
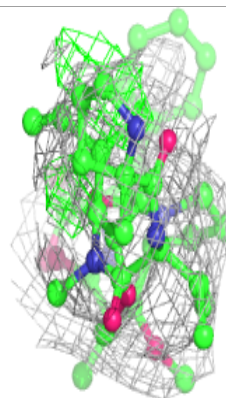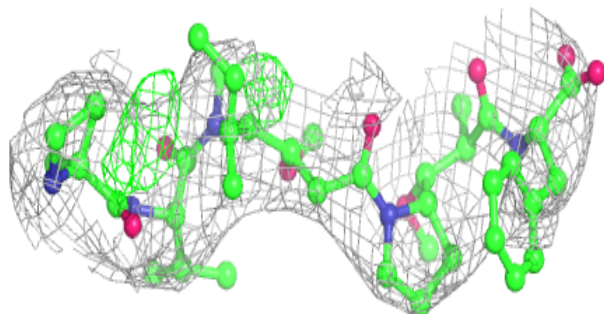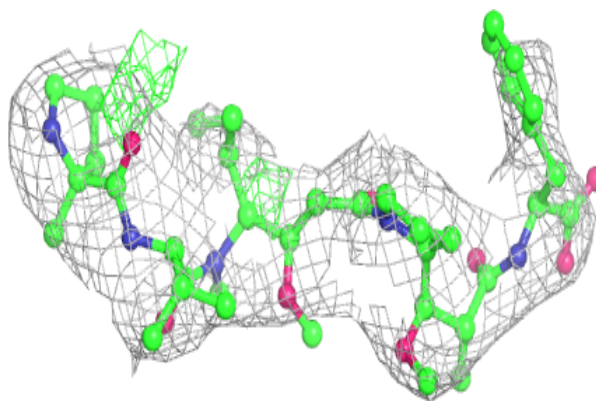
Electron density around 3WY D 503:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
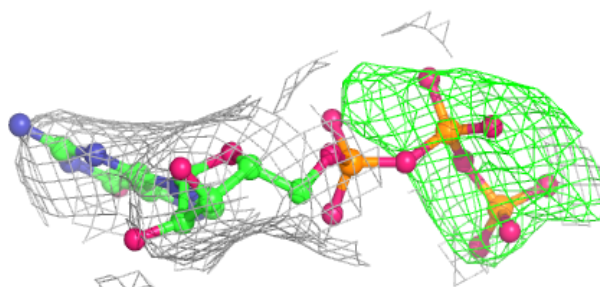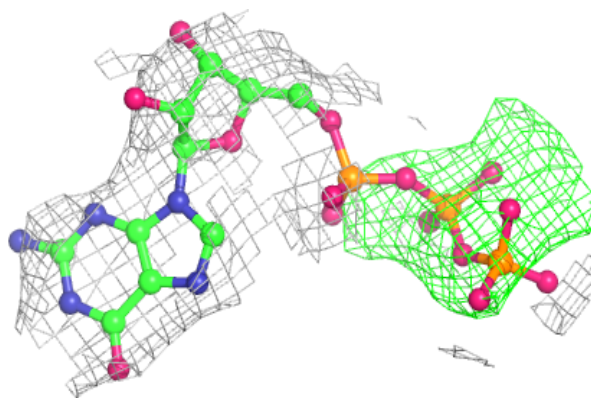mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
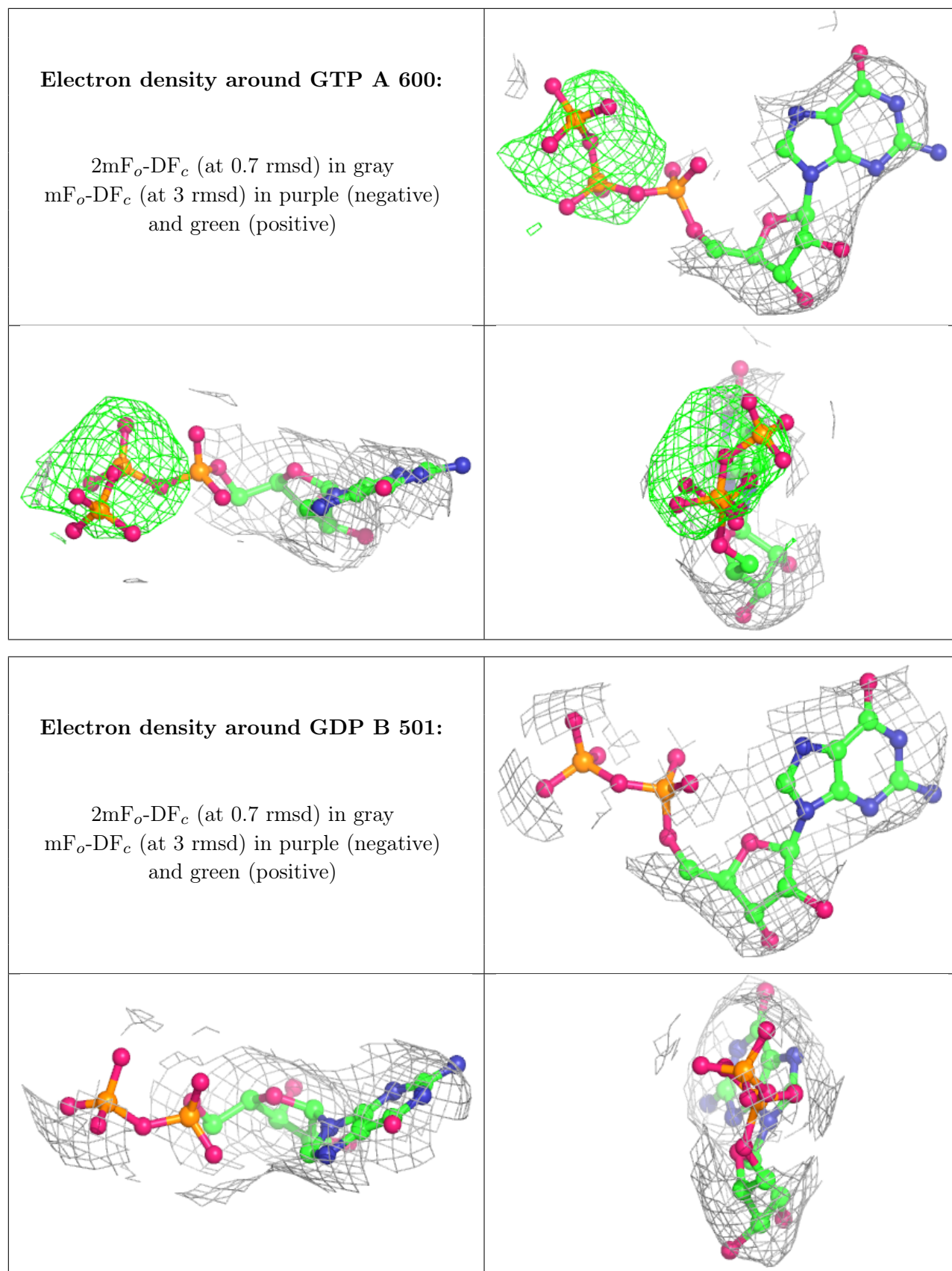and green (positive)
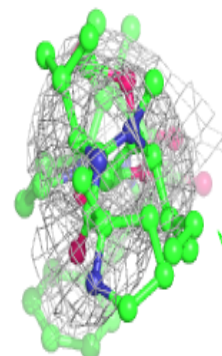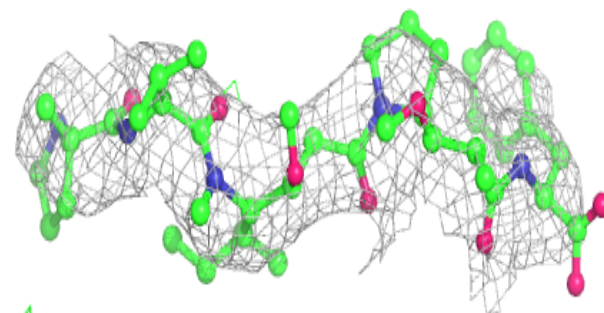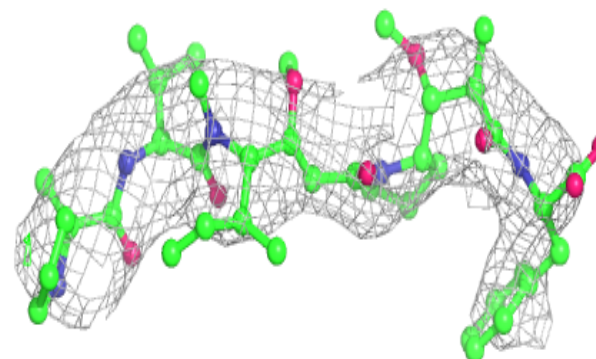
Electron density around LOC D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
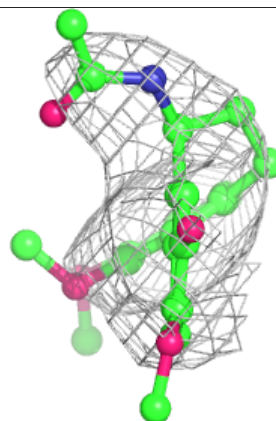
Electron density around GTP C 600:

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

Electron density around GTP A 600:

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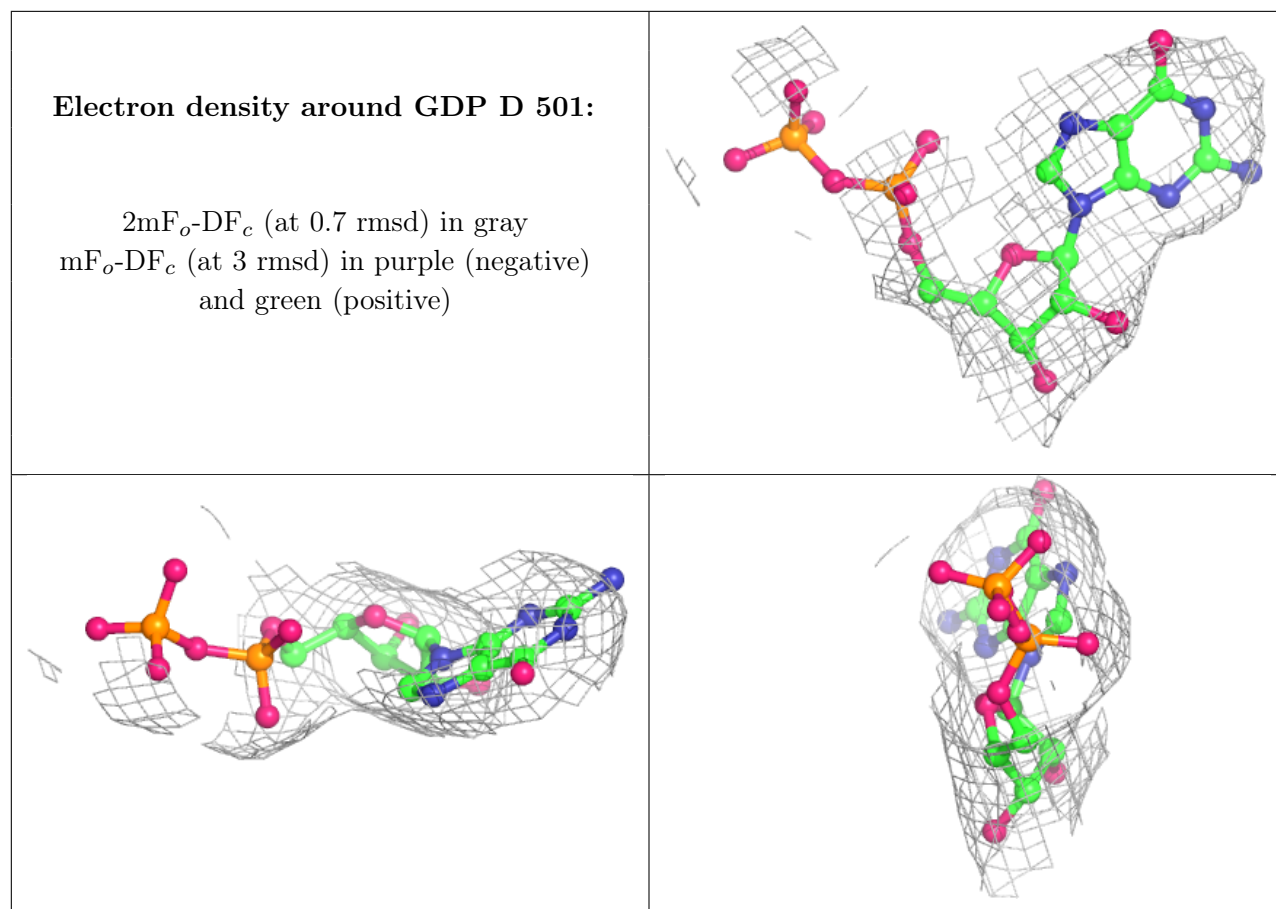

Electron density around GDP B 501:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)

6.5 Other polymers ⓘ

There are no such residues in this entry.