



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:10 AM UTC

PDB ID : 1XJK / pdb_00001xjk
Title : Structural mechanism of allosteric substrate specificity in a ribonucleotide reductase: dGTP-ADP complex
Authors : Larsson, K.-M.; Jordan, A.; Eliasson, R.; Reichard, P.; Logan, D.T.; Nordlund, P.
Deposited on : 2004-09-23
Resolution : 2.12 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

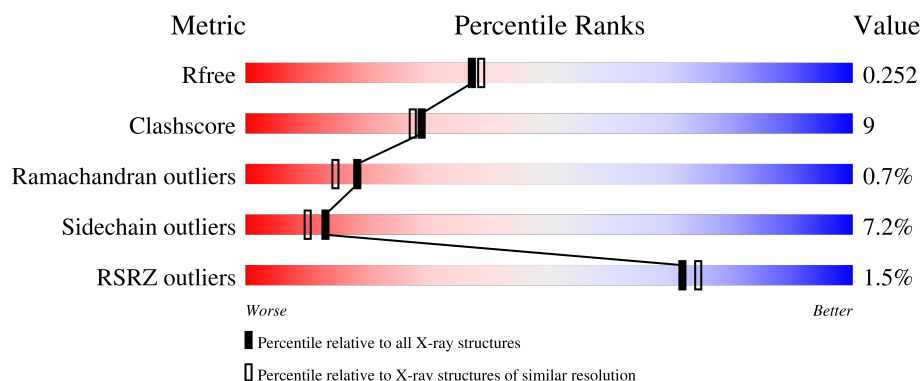
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	644	0% 76% 18% • •
1	B	644	2% 69% 23% • 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10248 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 ribonucleotide reductase, B12-dependent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5005	3208	848	929	20			
1	B	608	Total	C	N	O	S	0	0	0
			4878	3125	830	903	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	TYR	SEE REMARK 999	UNP O33839
A	519	ASP	GLU	conflict	UNP O33839
B	205	SER	TYR	SEE REMARK 999	UNP O33839
B	519	ASP	GLU	conflict	UNP O33839

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

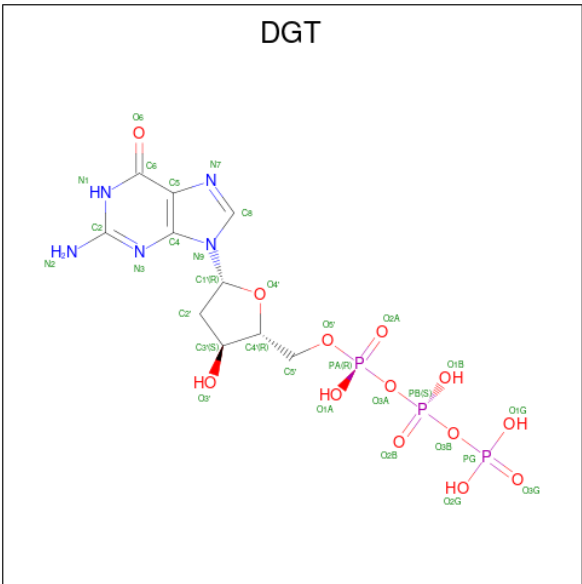
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

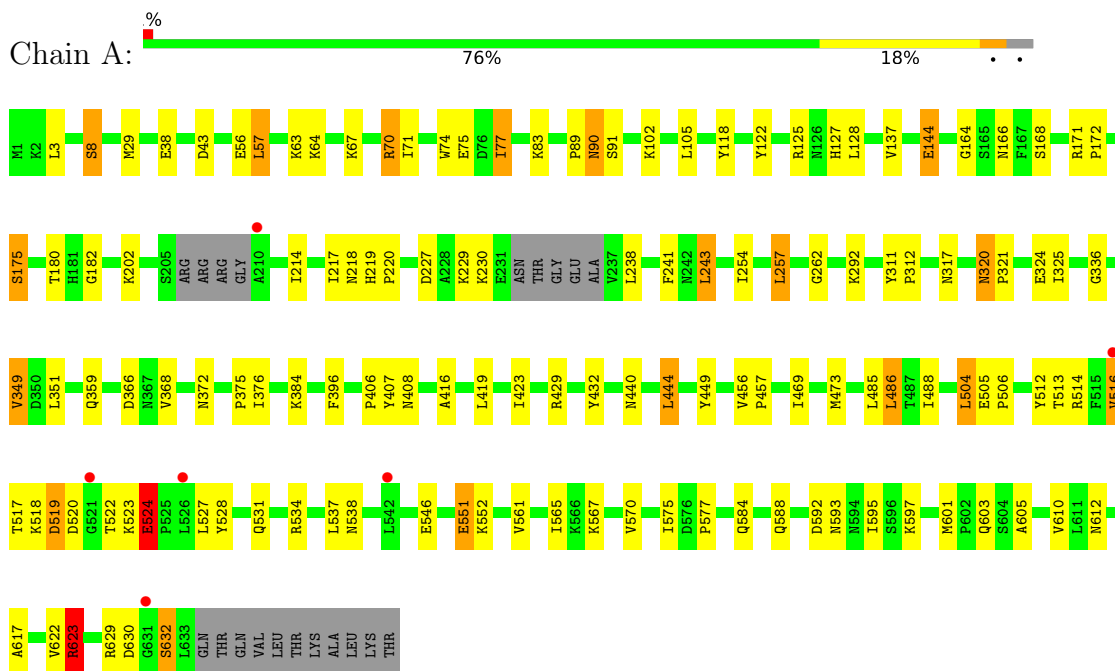
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		
5	B	108	Total	O	0	0
			108	108		

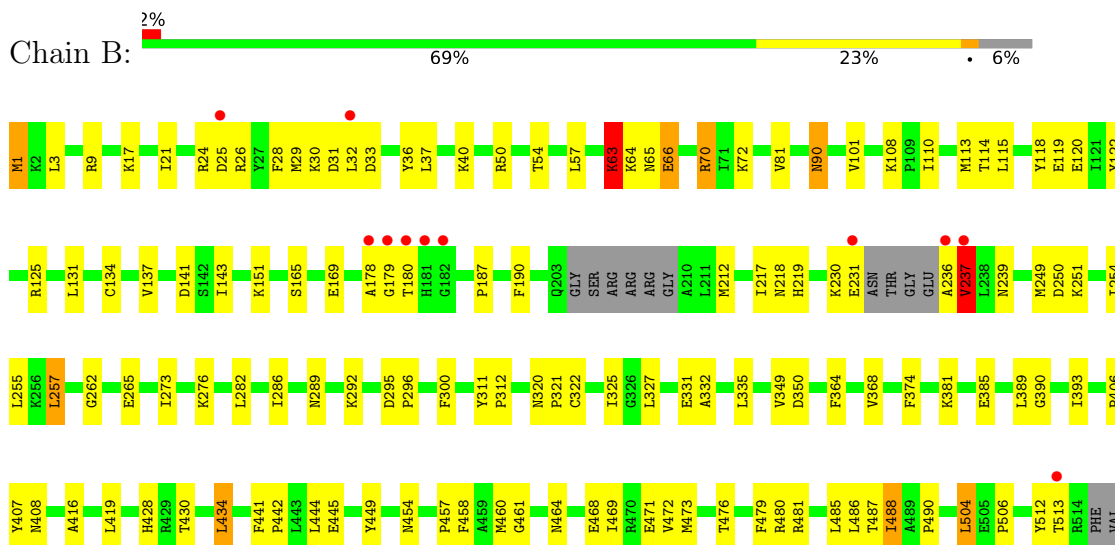
3 Residue-property plots

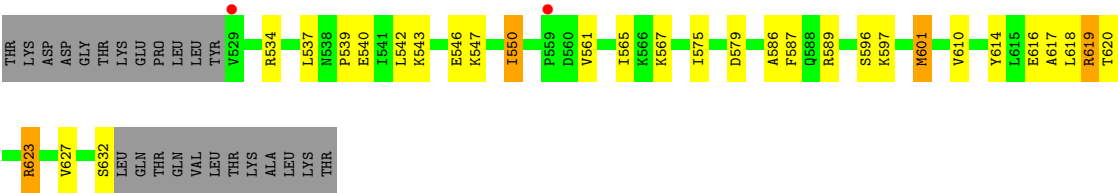
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ribonucleotide reductase, B12-dependent



- Molecule 1: ribonucleotide reductase, B12-dependent





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.12Å 122.86Å 106.06Å 90.00° 103.46° 90.00°	Depositor
Resolution (Å)	22.70 – 2.12 22.70 – 2.12	Depositor EDS
% Data completeness (in resolution range)	97.0 (22.70-2.12) 96.9 (22.70-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.256 (Not available) , 0.252	Depositor DCC
R_{free} test set	4113 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10248	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, DGT, MG

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	1.07	8/5104 (0.2%)	1.17	11/6890 (0.2%)
1	B	1.01	4/4973 (0.1%)	1.15	11/6711 (0.2%)
All	All	1.04	12/10077 (0.1%)	1.16	22/13601 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	456	VAL	CA-CB	6.93	1.59	1.54
1	B	180	THR	CA-CB	6.78	1.65	1.53
1	A	423	ILE	CA-CB	6.61	1.62	1.54
1	A	217	ILE	N-CA	6.33	1.55	1.46
1	A	605	ALA	CA-CB	6.33	1.64	1.53
1	B	101	VAL	CA-CB	5.68	1.61	1.54
1	B	349	VAL	CA-CB	5.62	1.60	1.54
1	A	164	GLY	CA-C	-5.37	1.47	1.52
1	B	586	ALA	CA-CB	5.35	1.61	1.53
1	A	214	ILE	CA-CB	5.22	1.60	1.54
1	A	349	VAL	CA-CB	5.18	1.60	1.54
1	A	456	VAL	CA-C	5.09	1.56	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LYS	N-CA-C	6.05	118.40	111.02
1	B	26	ARG	N-CA-C	6.02	123.06	114.16
1	A	516	VAL	N-CA-C	5.93	116.67	110.62
1	B	461	GLY	N-CA-C	-5.82	106.47	116.01
1	B	374	PHE	CA-C-N	5.77	125.87	119.87
1	B	374	PHE	C-N-CA	5.77	125.87	119.87
1	B	165	SER	N-CA-C	5.72	118.10	109.23
1	A	320	ASN	CA-C-N	5.70	126.96	119.84
1	A	320	ASN	C-N-CA	5.70	126.96	119.84
1	B	137	VAL	CA-C-N	-5.64	114.78	120.31
1	B	137	VAL	C-N-CA	-5.64	114.78	120.31
1	A	105	LEU	N-CA-C	5.60	118.32	111.82
1	B	619	ARG	N-CA-C	5.60	119.28	112.23
1	B	81	VAL	N-CA-C	5.39	116.02	110.36
1	A	91	SER	N-CA-C	5.36	121.66	109.81
1	A	623	ARG	CB-CG-CD	5.36	123.62	111.30
1	A	219	HIS	N-CA-C	-5.32	103.33	109.93
1	A	8	SER	N-CA-C	5.25	117.01	111.28
1	B	190	PHE	N-CA-C	5.16	116.91	111.28
1	A	168	SER	N-CA-C	5.16	117.65	111.71
1	B	218	ASN	N-CA-C	5.10	119.14	113.02
1	A	366	ASP	N-CA-C	-5.09	106.57	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	63	LYS	Peptide

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	5005	0	5057	71	0
1	B	4878	0	4929	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	4	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
5	A	139	0	0	2	0
5	B	108	0	0	2	0
All	All	10248	0	10034	174	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 9.

All (174) 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:B:230:LYS:CA	1:B:231:GLU:HB2	1.72	1.19
1:A:601:MET:HE1	1:A:610:VAL:HG22	1.21	1.09
1:B:230:LYS:HA	1:B:231:GLU:CB	1.84	1.06
1:B:449:TYR:HE1	1:B:473:MET:HE1	1.23	1.01
1:B:428:HIS:CD2	1:B:480:ARG:HH22	1.83	0.96
1:A:457:PRO:HD3	1:A:473:MET:HE2	1.52	0.92
1:B:449:TYR:CE1	1:B:473:MET:HE1	2.06	0.91
1:B:428:HIS:HD2	1:B:480:ARG:HH22	0.91	0.90
1:B:449:TYR:HE1	1:B:473:MET:CE	1.85	0.90
1:B:230:LYS:HA	1:B:231:GLU:HB2	0.90	0.89
1:B:230:LYS:HG3	1:B:231:GLU:HB3	1.56	0.87
1:B:428:HIS:HD2	1:B:480:ARG:NH2	1.74	0.83
1:B:257:LEU:HD22	1:B:262:GLY:HA3	1.61	0.82
1:A:601:MET:CE	1:A:610:VAL:HG22	2.06	0.81
1:B:457:PRO:HD3	1:B:473:MET:HE2	1.62	0.81
1:B:122:TYR:O	1:B:125:ARG:HD3	1.83	0.79
1:B:230:LYS:HG3	1:B:231:GLU:CB	2.16	0.76
1:A:449:TYR:HE1	1:A:473:MET:HE1	1.49	0.76
1:A:320:ASN:HB2	1:A:321:PRO:HD2	1.68	0.76
1:B:1:MET:HB3	1:B:350:ASP:OD1	1.85	0.75
1:B:601:MET:HE1	1:B:610:VAL:HG22	1.68	0.74
1:A:229:LYS:HG3	1:A:243:LEU:HD22	1.70	0.74
1:B:601:MET:CE	1:B:610:VAL:HG22	2.20	0.72
1:A:449:TYR:HE1	1:A:473:MET:CE	2.05	0.70
1:A:516:VAL:CG1	1:A:524:GLU:HB3	2.22	0.69
1:A:457:PRO:HD3	1:A:473:MET:CE	2.22	0.69
1:B:70:ARG:HH11	1:B:70:ARG:HG3	1.58	0.68
1:A:531:GLN:HG3	1:A:534:ARG:HH12	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HG2	1:A:43:ASP:HB3	1.75	0.68
1:A:592:ASP:O	1:A:623:ARG:NH2	2.28	0.67
1:B:449:TYR:CE1	1:B:473:MET:CE	2.72	0.67
1:A:257:LEU:HD22	1:A:262:GLY:HA3	1.77	0.65
1:B:322:CYS:HB2	3:B:1002:ADP:O3'	1.96	0.65
1:A:449:TYR:CE1	1:A:473:MET:HE1	2.31	0.65
1:A:531:GLN:HG3	1:A:534:ARG:NH1	2.12	0.65
1:A:408:ASN:HB3	1:A:575:ILE:HG23	1.79	0.64
1:B:50:ARG:NH2	1:B:108:LYS:O	2.30	0.64
1:B:393:ILE:HD11	1:B:587:PHE:CE1	2.32	0.64
1:B:230:LYS:CG	1:B:231:GLU:HB3	2.28	0.64
1:A:486:LEU:O	1:A:593:ASN:HB2	1.98	0.64
1:A:122:TYR:O	1:A:125:ARG:HD3	1.99	0.62
1:B:230:LYS:CA	1:B:231:GLU:CB	2.60	0.62
1:A:172:PRO:HG3	1:A:220:PRO:HG2	1.81	0.61
1:B:113:MET:HE2	1:B:118:TYR:CE2	2.35	0.61
1:B:54:THR:O	1:B:57:LEU:HB2	2.01	0.60
1:B:534:ARG:HA	1:B:542:LEU:HD11	1.84	0.59
1:B:540:GLU:HA	1:B:543:LYS:HB2	1.83	0.59
1:A:516:VAL:HG11	1:A:524:GLU:HB3	1.83	0.58
1:B:487:THR:O	1:B:488:ILE:HD13	2.02	0.58
1:B:255:LEU:CD2	1:B:619:ARG:HG3	2.33	0.58
1:B:255:LEU:HD21	1:B:619:ARG:HG3	1.83	0.58
1:B:230:LYS:CG	1:B:231:GLU:CB	2.82	0.58
1:A:128:LEU:HD13	1:B:179:GLY:HA2	1.86	0.57
1:B:408:ASN:HB3	1:B:575:ILE:HG23	1.86	0.57
1:A:519:ASP:O	1:A:520:ASP:C	2.48	0.57
1:B:322:CYS:HB2	3:B:1002:ADP:HO3'	1.70	0.56
1:B:504:LEU:CD1	1:B:597:LYS:HD2	2.35	0.56
1:B:546:GLU:O	1:B:550:ILE:HG13	2.04	0.56
1:A:180:THR:C	1:A:182:GLY:H	2.14	0.56
1:B:24:ARG:HA	1:B:28:PHE:CD2	2.42	0.55
1:B:393:ILE:HD11	1:B:587:PHE:HE1	1.71	0.55
1:B:327:LEU:HD22	1:B:331:GLU:HB3	1.88	0.55
1:B:311:TYR:CD1	1:B:312:PRO:HA	2.42	0.54
1:B:31:ASP:HB3	1:B:37:LEU:HD21	1.88	0.54
1:B:212:MET:HB2	1:B:321:PRO:HA	1.88	0.53
1:B:537:LEU:HD13	1:B:565:ILE:HG21	1.91	0.53
1:B:21:ILE:O	1:B:25:ASP:HB2	2.08	0.53
1:B:381:LYS:O	1:B:385:GLU:HG3	2.09	0.53
1:A:171:ARG:HG3	1:A:175:SER:OG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ARG:HH11	1:B:70:ARG:CG	2.21	0.53
1:A:429:ARG:O	1:A:432:TYR:HB3	2.09	0.52
1:A:229:LYS:HD3	1:A:238:LEU:O	2.10	0.52
1:B:63:LYS:HB2	1:B:64:LYS:O	2.10	0.52
1:B:134:CYS:O	1:B:332:ALA:HA	2.09	0.52
1:A:166:ASN:HB2	1:A:317:ASN:O	2.09	0.52
1:B:407:TYR:CZ	1:B:506:PRO:HD3	2.44	0.52
1:B:472:VAL:O	1:B:476:THR:HG23	2.10	0.52
1:B:487:THR:C	1:B:488:ILE:HD13	2.34	0.52
1:B:141:ASP:HB2	1:B:169:GLU:O	2.10	0.51
1:A:537:LEU:HD13	1:A:565:ILE:HG21	1.91	0.51
1:A:74:TRP:HA	1:A:77:ILE:HG22	1.93	0.51
1:B:50:ARG:NH1	1:B:108:LYS:O	2.42	0.51
1:B:428:HIS:CE1	1:B:485:LEU:HD12	2.47	0.50
1:A:488:ILE:HG21	1:A:504:LEU:HG	1.94	0.50
1:B:251:LYS:HE2	1:B:618:LEU:HA	1.93	0.50
1:B:476:THR:HB	1:B:480:ARG:HE	1.77	0.50
1:B:441:PHE:HB3	1:B:481:ARG:O	2.12	0.50
1:A:512:TYR:CE2	1:A:528:TYR:HD2	2.29	0.49
1:B:320:ASN:ND2	3:B:1002:ADP:O3'	2.45	0.49
1:B:616:GLU:O	1:B:620:THR:HG23	2.13	0.49
1:A:128:LEU:HD11	1:B:178:ALA:O	2.13	0.49
1:B:236:ALA:O	1:B:237:VAL:HG13	2.12	0.49
1:A:324:GLU:HG2	1:A:325:ILE:HG12	1.94	0.49
1:B:614:TYR:O	1:B:617:ALA:HB3	2.12	0.49
1:A:375:PRO:C	1:A:376:ILE:HG13	2.39	0.48
1:B:30:LYS:HE2	1:B:36:TYR:CE1	2.48	0.48
1:B:601:MET:HE2	1:B:627:VAL:HB	1.96	0.48
1:A:83:LYS:NZ	5:A:1086:HOH:O	2.46	0.48
1:B:476:THR:HA	1:B:479:PHE:O	2.14	0.48
1:A:320:ASN:ND2	3:A:1001:ADP:O3'	2.46	0.48
1:B:469:ILE:O	1:B:473:MET:HG2	2.14	0.48
1:A:90:ASN:C	1:A:90:ASN:HD22	2.20	0.47
1:B:239:ASN:H	1:B:239:ASN:ND2	2.11	0.47
1:B:539:PRO:O	1:B:540:GLU:HB3	2.13	0.47
1:A:516:VAL:HG13	1:A:518:LYS:H	1.79	0.47
1:B:292:LYS:O	1:B:632:SER:HB2	2.14	0.47
1:A:144:GLU:OE2	1:B:151:LYS:NZ	2.47	0.47
1:A:440:ASN:ND2	1:A:444:LEU:HD12	2.30	0.47
1:B:230:LYS:CB	1:B:231:GLU:HB2	2.41	0.47
1:B:623:ARG:HD2	5:B:1008:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:HB3	1:A:567:LYS:O	2.15	0.47
1:B:131:LEU:HD12	1:B:368:VAL:HG13	1.97	0.47
1:B:286:ILE:HG23	1:B:296:PRO:HG2	1.95	0.47
1:B:504:LEU:HD13	1:B:597:LYS:HD2	1.96	0.47
1:A:227:ASP:O	1:A:230:LYS:HB2	2.14	0.47
1:B:217:ILE:CG2	1:B:249:MET:HE1	2.44	0.47
1:A:588:GLN:O	1:A:588:GLN:HG3	2.16	0.46
1:B:72:LYS:O	1:B:110:ILE:HD11	2.15	0.46
1:B:239:ASN:H	1:B:239:ASN:HD22	1.64	0.46
1:A:584:GLN:HB2	1:A:597:LYS:HG2	1.97	0.46
1:A:320:ASN:HB2	1:A:321:PRO:CD	2.43	0.46
1:A:469:ILE:O	1:A:473:MET:HG2	2.16	0.46
1:A:57:LEU:HD13	1:A:71:ILE:CD1	2.45	0.46
1:A:407:TYR:CZ	1:A:506:PRO:HD3	2.50	0.46
1:A:512:TYR:CE2	1:A:528:TYR:CD2	3.04	0.46
1:A:629:ARG:O	1:A:632:SER:OG	2.34	0.46
1:B:490:PRO:HD2	3:B:1002:ADP:H5'2	1.98	0.45
1:B:230:LYS:HG3	1:B:231:GLU:HB2	1.98	0.45
1:B:90:ASN:HD22	1:B:90:ASN:C	2.25	0.45
1:A:396:PHE:CZ	1:A:416:ALA:HB2	2.52	0.45
1:A:457:PRO:CD	1:A:473:MET:HE2	2.35	0.45
1:A:311:TYR:CD1	1:A:312:PRO:HA	2.53	0.44
1:A:368:VAL:O	1:A:372:ASN:HB2	2.17	0.44
1:A:202:LYS:NZ	3:A:1001:ADP:N1	2.64	0.44
1:B:416:ALA:HB1	1:B:587:PHE:CE2	2.53	0.44
1:B:504:LEU:HD11	1:B:597:LYS:HD2	1.98	0.44
1:B:70:ARG:CG	1:B:70:ARG:NH1	2.80	0.44
1:A:241:PHE:HB3	1:A:243:LEU:HD13	1.99	0.43
1:B:458:PHE:HB2	1:B:589:ARG:O	2.17	0.43
1:B:457:PRO:HD3	1:B:473:MET:CE	2.40	0.43
1:A:70:ARG:HD3	1:A:70:ARG:HA	1.58	0.43
1:A:292:LYS:O	1:A:632:SER:HB3	2.19	0.43
1:B:265:GLU:OE1	1:B:276:LYS:HG3	2.17	0.43
1:A:75:GLU:OE1	1:A:118:TYR:OH	2.29	0.43
1:B:408:ASN:HB2	1:B:579:ASP:OD2	2.18	0.43
1:B:335:LEU:HD22	1:B:390:GLY:HA3	1.99	0.43
1:A:519:ASP:HA	1:A:522:THR:HB	2.01	0.43
1:A:449:TYR:CE1	1:A:473:MET:CE	2.92	0.43
1:B:449:TYR:OH	1:B:457:PRO:HG3	2.19	0.43
1:A:180:THR:C	1:A:182:GLY:N	2.78	0.42
1:B:143:ILE:HD13	1:B:143:ILE:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LEU:HD12	1:B:485:LEU:HD23	2.01	0.42
1:A:56:GLU:HB2	1:A:71:ILE:HG12	2.02	0.42
1:A:89:PRO:HA	1:A:336:GLY:HA2	2.00	0.42
1:B:445:GLU:HG3	5:B:1112:HOH:O	2.18	0.42
1:B:64:LYS:O	1:B:65:ASN:HB2	2.19	0.42
1:B:601:MET:HE3	1:B:610:VAL:HG22	1.98	0.42
1:B:230:LYS:CG	1:B:231:GLU:HB2	2.49	0.42
1:B:187:PRO:HG3	1:B:219:HIS:CE1	2.55	0.42
1:A:440:ASN:CG	1:A:444:LEU:HD12	2.44	0.41
1:A:551:GLU:HG2	1:A:552:LYS:HG3	2.02	0.41
1:B:430:THR:HG22	1:B:434:LEU:HD22	2.02	0.41
1:A:505:GLU:OE2	1:A:597:LYS:HA	2.21	0.41
1:B:441:PHE:O	1:B:442:PRO:C	2.63	0.41
1:A:612:ASN:ND2	5:A:1095:HOH:O	2.54	0.41
1:B:251:LYS:HE3	1:B:300:PHE:CD2	2.56	0.41
1:B:31:ASP:O	1:B:33:ASP:N	2.54	0.41
1:A:349:VAL:O	1:A:351:LEU:N	2.54	0.41
1:B:57:LEU:HD21	1:B:119:GLU:HG3	2.03	0.41
1:B:406:PRO:HB3	1:B:567:LYS:O	2.21	0.40
1:A:617:ALA:HB1	1:A:622:VAL:HG21	2.03	0.40
1:A:127:HIS:CD2	1:A:127:HIS:H	2.38	0.40
1:B:57:LEU:HD21	1:B:119:GLU:HA	2.03	0.40
1:B:364:PHE:C	1:B:364:PHE:CD1	2.98	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	618/644 (96%)	578 (94%)	36 (6%)	4 (1%)	21 18
1	B	600/644 (93%)	562 (94%)	33 (6%)	5 (1%)	16 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1218/1288 (95%)	1140 (94%)	69 (6%)	9 (1%)	18	15

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	GLU
1	A	519	ASP
1	A	523	LYS
1	A	630	ASP
1	B	32	LEU
1	B	513	THR
1	A	524	GLU
1	B	460	MET
1	B	237	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	550/566 (97%)	511 (93%)	39 (7%)	13	10
1	B	535/566 (94%)	496 (93%)	39 (7%)	13	10
All	All	1085/1132 (96%)	1007 (93%)	78 (7%)	13	10

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	8	SER
1	A	29	MET
1	A	57	LEU
1	A	63	LYS
1	A	64	LYS
1	A	70	ARG
1	A	77	ILE
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	102	LYS
1	A	137	VAL
1	A	144	GLU
1	A	175	SER
1	A	218	ASN
1	A	243	LEU
1	A	254	ILE
1	A	257	LEU
1	A	359	GLN
1	A	384	LYS
1	A	419	LEU
1	A	444	LEU
1	A	485	LEU
1	A	486	LEU
1	A	504	LEU
1	A	513	THR
1	A	514	ARG
1	A	517	THR
1	A	524	GLU
1	A	527	LEU
1	A	538	ASN
1	A	546	GLU
1	A	551	GLU
1	A	561	VAL
1	A	570	VAL
1	A	577	PRO
1	A	595	ILE
1	A	603	GLN
1	A	623	ARG
1	A	632	SER
1	B	1	MET
1	B	3	LEU
1	B	9	ARG
1	B	17	LYS
1	B	29	MET
1	B	40	LYS
1	B	63	LYS
1	B	66	GLU
1	B	70	ARG
1	B	90	ASN
1	B	114	THR
1	B	115	LEU

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Mol	Chain	Res	Type
1	B	120	GLU
1	B	237	VAL
1	B	250	ASP
1	B	254	ILE
1	B	257	LEU
1	B	273	ILE
1	B	282	LEU
1	B	289	ASN
1	B	295	ASP
1	B	325	ILE
1	B	419	LEU
1	B	434	LEU
1	B	444	LEU
1	B	454	ASN
1	B	464	ASN
1	B	468	GLU
1	B	471	GLU
1	B	486	LEU
1	B	488	ILE
1	B	504	LEU
1	B	512	TYR
1	B	547	LYS
1	B	550	ILE
1	B	561	VAL
1	B	596	SER
1	B	601	MET
1	B	623	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	90	ASN
1	A	103	HIS
1	A	181	HIS
1	A	239	ASN
1	A	345	ASN
1	A	346	ASN
1	A	355	GLN
1	A	359	GLN
1	A	600	ASN
1	A	612	ASN

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Mol	Chain	Res	Type
1	B	20	GLN
1	B	127	HIS
1	B	239	ASN
1	B	320	ASN
1	B	346	ASN
1	B	428	HIS
1	B	496	ASN
1	B	538	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	DGT	B	1004	2	32,33,33	3.01	7 (21%)	48,52,52	1.89	11 (22%)
4	DGT	A	1003	2	32,33,33	1.99	7 (21%)	48,52,52	1.94	10 (20%)
3	ADP	A	1001	-	28,29,29	1.17	3 (10%)	43,45,45	2.30	11 (25%)
3	ADP	B	1002	-	28,29,29	1.48	8 (28%)	43,45,45	2.37	14 (32%)

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	DGT	B	1004	2	-	1/22/34/34	0/3/3/3
4	DGT	A	1003	2	-	2/22/34/34	0/3/3/3
3	ADP	A	1001	-	-	2/16/32/32	0/3/3/3
3	ADP	B	1002	-	-	4/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1004	DGT	PB-O3A	13.46	1.74	1.59
4	B	1004	DGT	PA-O3A	5.06	1.65	1.59
4	A	1003	DGT	PA-O3A	5.06	1.65	1.59
4	B	1004	DGT	PB-O3B	5.00	1.64	1.59
4	A	1003	DGT	PG-O3G	4.86	1.65	1.50
4	B	1004	DGT	PG-O3G	3.98	1.62	1.50
4	A	1003	DGT	PB-O3B	3.40	1.63	1.59
3	B	1002	ADP	PB-O3B	3.18	1.66	1.54
4	A	1003	DGT	PB-O3A	3.12	1.62	1.59
3	B	1002	ADP	O4'-C1'	2.79	1.48	1.42
4	A	1003	DGT	C5-N7	-2.46	1.34	1.39
3	B	1002	ADP	PB-O2B	2.38	1.63	1.54
4	A	1003	DGT	PG-O1G	-2.36	1.46	1.54
4	B	1004	DGT	C1'-N9	2.35	1.54	1.48
3	A	1001	ADP	PB-O3B	2.33	1.63	1.54
3	B	1002	ADP	O4'-C4'	2.31	1.50	1.45
3	B	1002	ADP	C5-N7	-2.27	1.34	1.39
3	A	1001	ADP	C5-N7	-2.26	1.35	1.39
4	B	1004	DGT	PA-O1A	-2.23	1.45	1.55
3	B	1002	ADP	PA-O5'	2.18	1.67	1.59
3	B	1002	ADP	PA-O2A	2.17	1.65	1.55
3	A	1001	ADP	PA-O3A	2.15	1.61	1.59
4	A	1003	DGT	O4'-C1'	-2.12	1.37	1.42
3	B	1002	ADP	C1'-N9	2.08	1.52	1.46
4	B	1004	DGT	PG-O1G	-2.04	1.47	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	ADP	O2A-PA-O5'	-7.01	75.81	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	DGT	C2-N3-C4	5.99	122.62	112.30
3	A	1001	ADP	O2A-PA-O5'	-5.86	81.02	107.57
3	A	1001	ADP	C5-C4-N3	-5.83	118.68	126.72
3	A	1001	ADP	O5'-PA-O1A	-5.59	86.80	108.94
3	B	1002	ADP	C5-C4-N3	-5.29	119.43	126.72
4	A	1003	DGT	C5-C4-N3	-5.29	119.97	128.39
4	A	1003	DGT	C2-N3-C4	5.00	120.92	112.30
3	B	1002	ADP	N3-C2-N1	-4.79	121.33	128.58
4	A	1003	DGT	C2-N1-C6	-4.73	116.53	125.11
4	B	1004	DGT	C5-C4-N3	-4.52	121.20	128.39
4	A	1003	DGT	N9-C4-N3	4.34	134.63	125.95
3	B	1002	ADP	O5'-PA-O1A	-4.34	91.74	108.94
3	A	1001	ADP	O2A-PA-O3A	4.10	118.36	107.27
3	A	1001	ADP	N3-C2-N1	-4.10	122.38	128.58
3	B	1002	ADP	O4'-C1'-N9	4.06	115.89	108.09
4	A	1003	DGT	O6-C6-C5	-3.99	116.01	126.53
3	A	1001	ADP	C2-N3-C4	3.92	121.41	111.83
4	B	1004	DGT	N1-C2-N3	-3.70	116.54	123.32
3	B	1002	ADP	N3-C4-N9	3.70	133.46	127.17
3	A	1001	ADP	N3-C4-N9	3.65	133.37	127.17
3	B	1002	ADP	C2-N3-C4	3.62	120.66	111.83
3	B	1002	ADP	O2A-PA-O1A	3.55	128.96	112.44
4	B	1004	DGT	N2-C2-N3	3.51	126.53	119.67
3	A	1001	ADP	C4-C5-N7	-3.50	106.58	110.58
4	B	1004	DGT	O2G-PG-O1G	3.42	120.64	107.80
3	B	1002	ADP	O2A-PA-O3A	3.34	116.30	107.27
4	A	1003	DGT	C5-C6-N1	3.23	121.47	113.25
3	A	1001	ADP	C5-N7-C8	3.16	108.42	103.45
4	A	1003	DGT	C2'-C1'-N9	-3.08	106.11	113.81
3	A	1001	ADP	N9-C8-N7	-3.08	109.57	113.94
4	B	1004	DGT	N9-C4-N3	3.06	132.06	125.95
3	A	1001	ADP	O2A-PA-O1A	3.05	126.61	112.44
4	B	1004	DGT	N9-C8-N7	-3.03	107.78	113.40
4	A	1003	DGT	O2G-PG-O1G	2.98	118.97	107.80
3	B	1002	ADP	O2B-PB-O3A	-2.79	95.29	104.64
3	B	1002	ADP	N9-C8-N7	-2.59	110.27	113.94
3	B	1002	ADP	C5-N7-C8	2.51	107.39	103.45
3	B	1002	ADP	C4-C5-N7	-2.46	107.77	110.58
3	B	1002	ADP	O3B-PB-O3A	2.39	112.67	104.64
4	B	1004	DGT	C5-C6-N1	2.39	119.34	113.25
4	A	1003	DGT	C2'-C3'-C4'	-2.39	97.96	102.80
4	A	1003	DGT	O4'-C4'-C5'	-2.31	101.92	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1004	DGT	O1A-PA-O5'	2.18	117.47	107.57
4	B	1004	DGT	O2G-PG-O3G	-2.17	102.38	110.83
4	B	1004	DGT	O6-C6-N1	-2.17	116.04	120.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	ADP	PA-O3A-PB-O3B
3	B	1002	ADP	C5'-O5'-PA-O2A
3	B	1002	ADP	C5'-O5'-PA-O3A
3	B	1002	ADP	O4'-C4'-C5'-O5'
3	B	1002	ADP	C3'-C4'-C5'-O5'
3	A	1001	ADP	PA-O3A-PB-O1B
4	A	1003	DGT	PA-O3A-PB-O2B
4	A	1003	DGT	PA-O3A-PB-O1B
4	B	1004	DGT	PA-O3A-PB-O1B

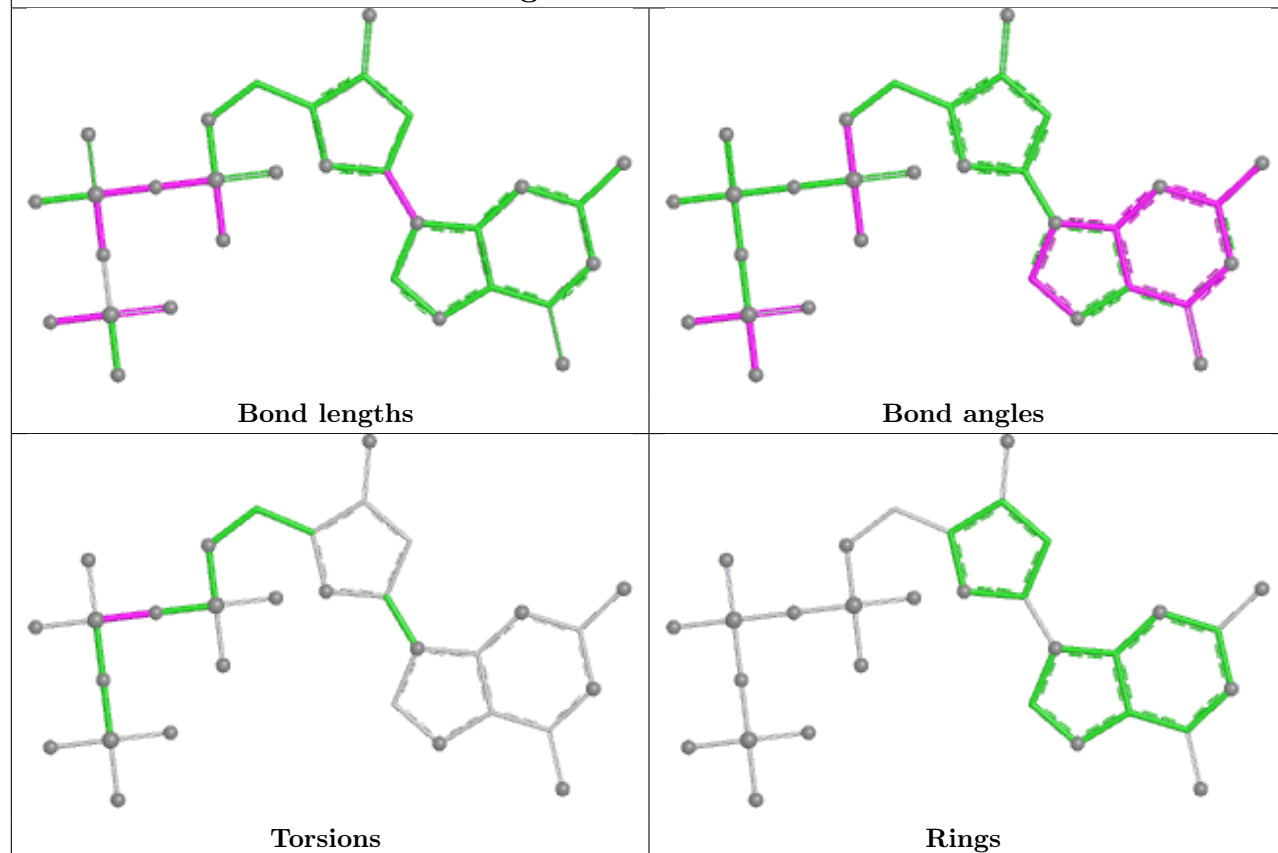
There are no ring outliers.

2 monomers are involved in 6 short contacts:

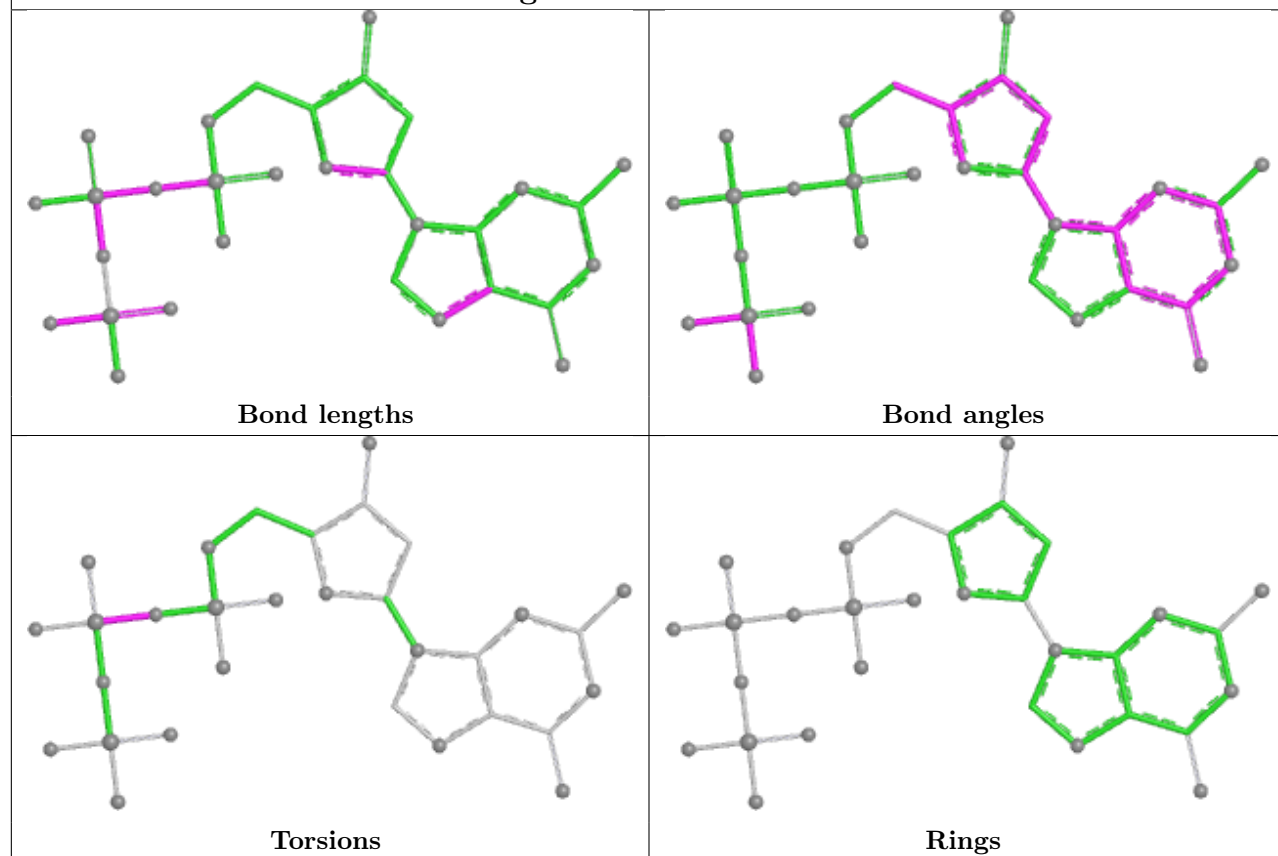
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	ADP	2	0
3	B	1002	ADP	4	0

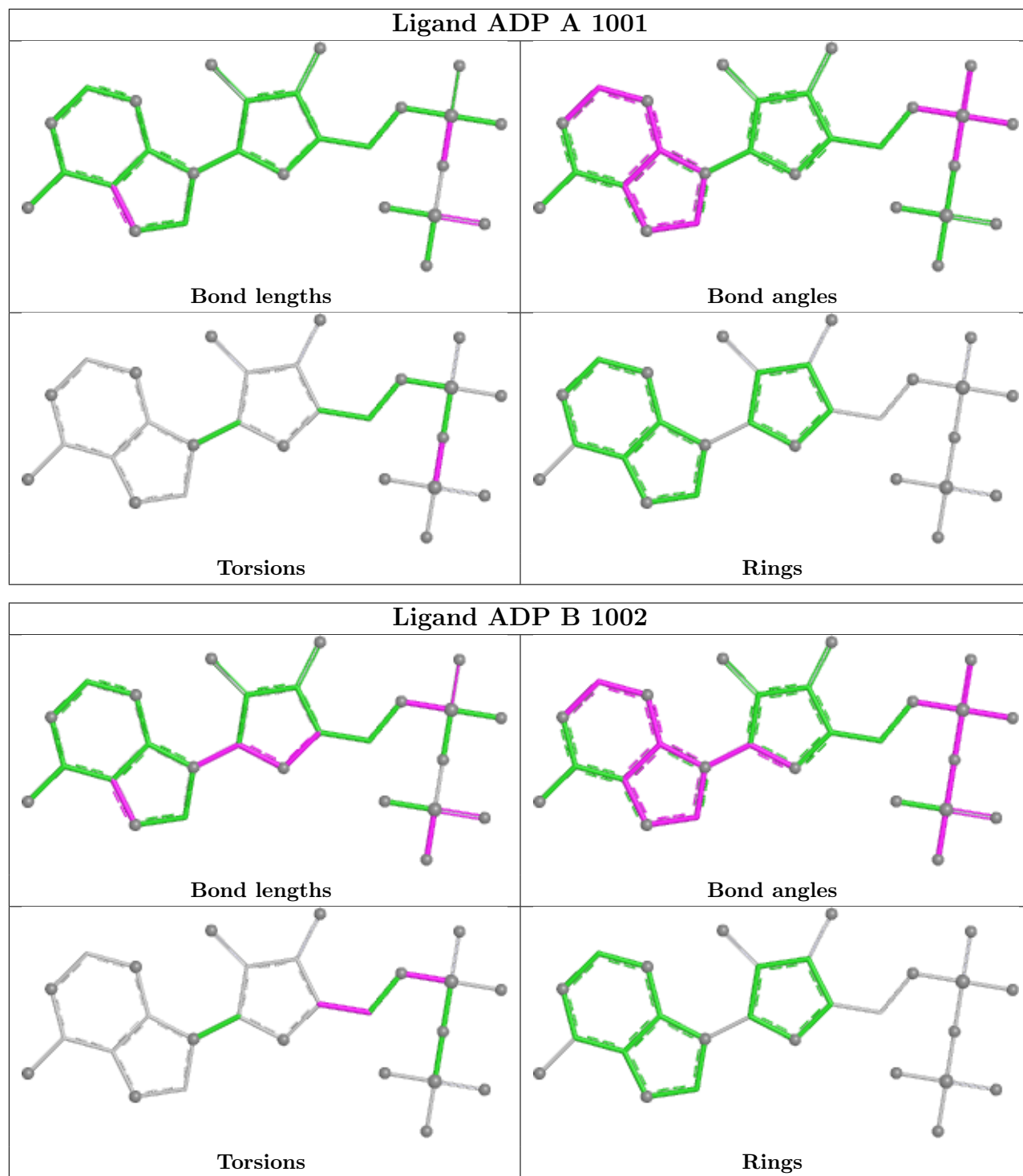
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DGT B 1004



Ligand DGT A 1003





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	624/644 (96%)	-0.02	6 (0%) 79 82	24, 41, 72, 104	0
1	B	608/644 (94%)	0.04	13 (2%) 63 66	27, 43, 73, 91	0
All	All	1232/1288 (95%)	0.01	19 (1%) 72 74	24, 42, 73, 104	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	ALA	4.2
1	B	180	THR	4.2
1	B	181	HIS	3.8
1	B	182	GLY	3.4
1	A	210	ALA	3.3
1	B	237	VAL	3.3
1	B	236	ALA	3.3
1	B	179	GLY	3.1
1	B	513	THR	2.9
1	B	231	GLU	2.7
1	B	559	PRO	2.6
1	A	521	GLY	2.5
1	A	526	LEU	2.4
1	B	32	LEU	2.4
1	A	516	VAL	2.4
1	B	25	ASP	2.3
1	B	529	VAL	2.3
1	A	542	LEU	2.1
1	A	631	GLY	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

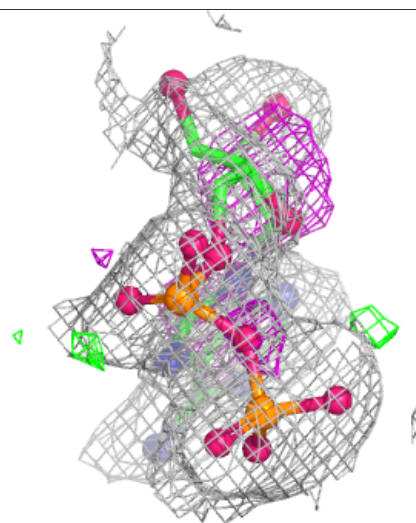
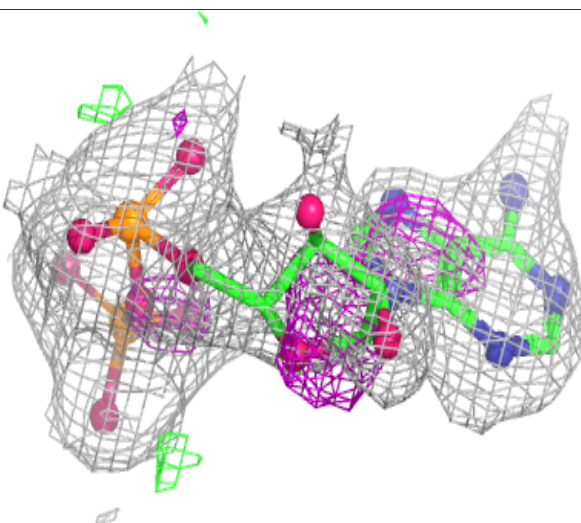
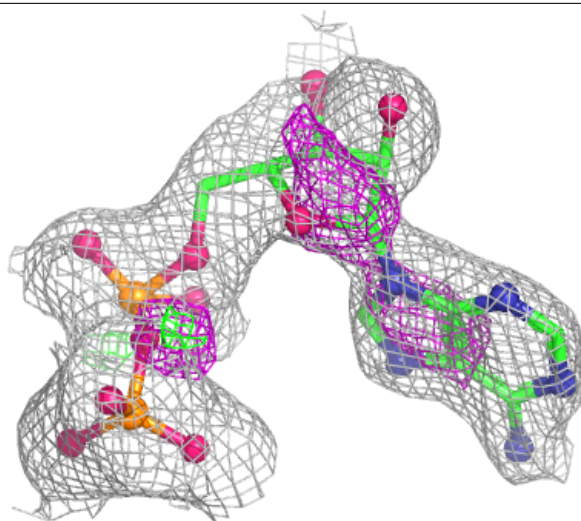
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1005	1/1	0.92	0.10	46,46,46,46	0
3	ADP	B	1002	27/27	0.92	0.10	38,56,66,66	0
3	ADP	A	1001	27/27	0.94	0.09	41,60,65,65	0
4	DGT	B	1004	31/31	0.95	0.06	24,31,52,52	0
4	DGT	A	1003	31/31	0.96	0.06	32,36,49,52	0
2	MG	B	1006	1/1	0.98	0.08	44,44,44,44	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.

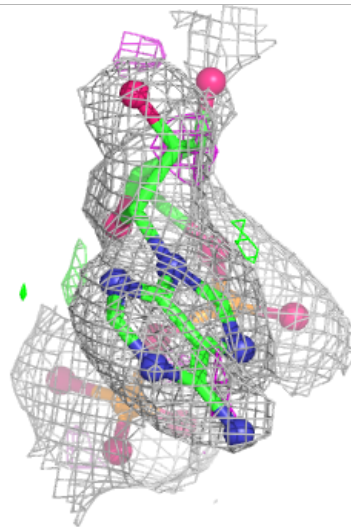
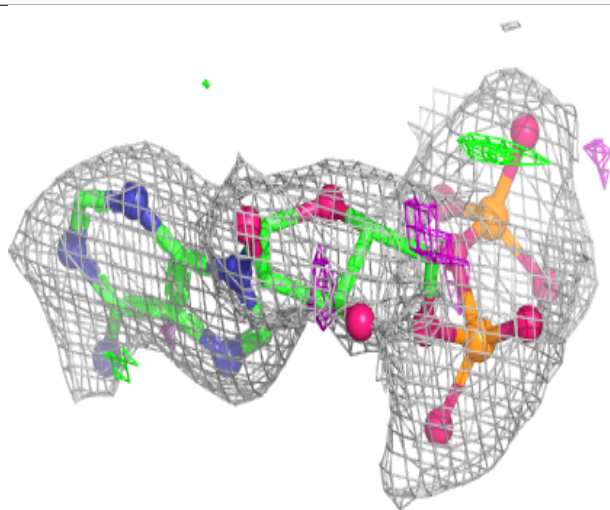
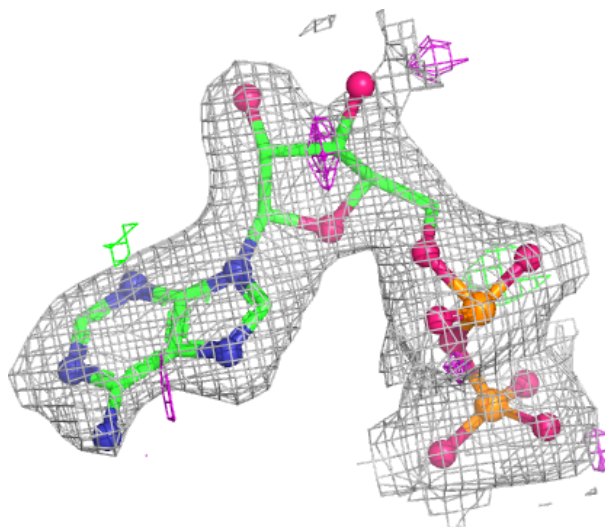
Electron density around ADP B 1002:

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



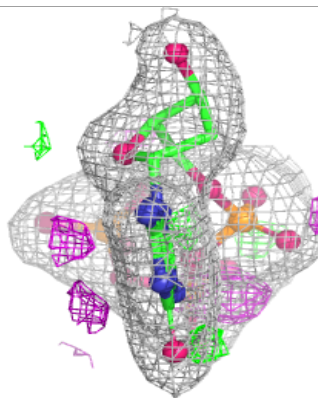
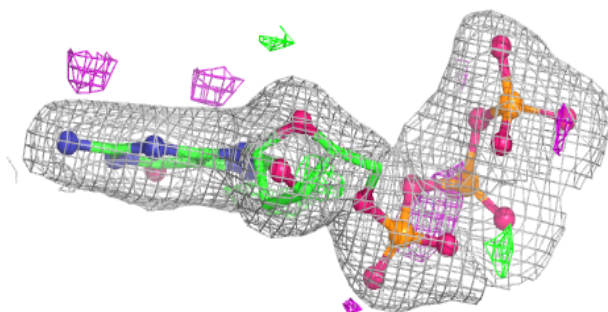
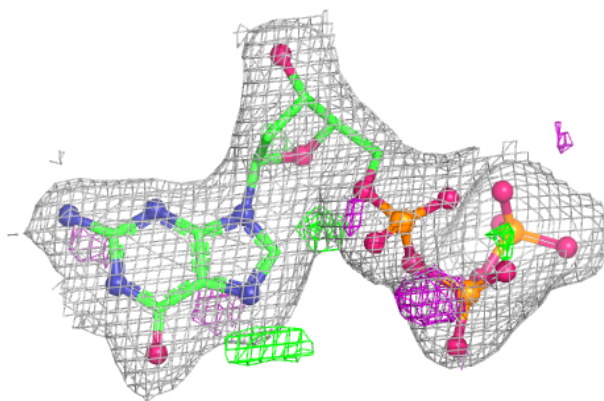
Electron density around ADP A 1001:

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

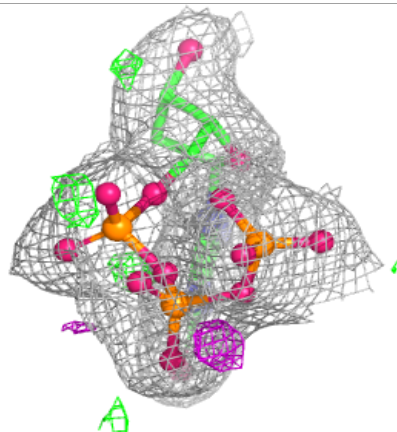
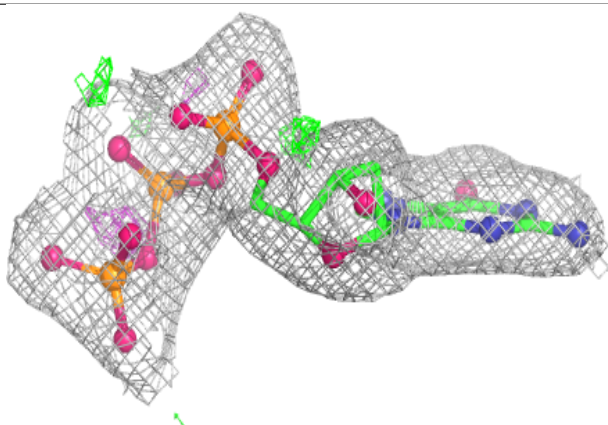
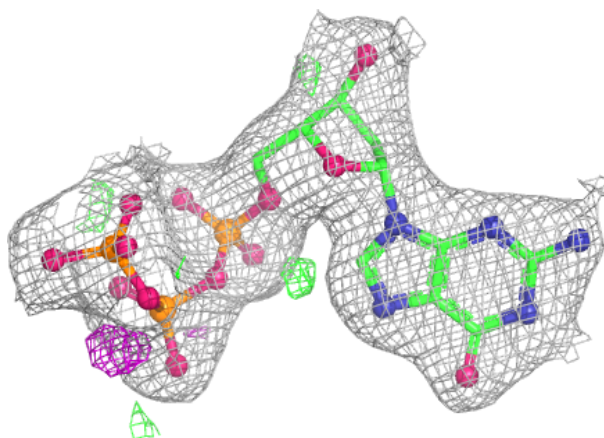


Electron density around DGT B 1004:

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

**Electron density around DGT A 1003:**

$2mF_o-DF_c$ (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.