



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 PM UTC

PDB ID : 3WXL / pdb_00003wxl
Title : Crystal structure of trypanosoma brucei gambiense glycerol kinase complex with adp, mg2+, and glycerol
Authors : Balogun, E.O.; Inaoka, D.K.; Shiba, T.; Kido, Y.; Tsuge, C.; Nara, T.; Aoki, T.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Michels, P.A.M.; Kita, K.; Harada, S.
Deposited on : 2014-08-01
Resolution : 1.90 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](#) ①) 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

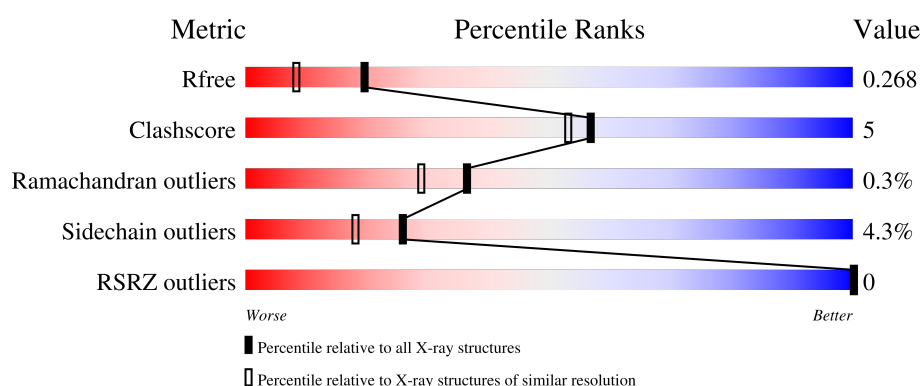
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	518	85% 13% ..
1	B	518	87% 11% ..
1	C	518	86% 11% ..
1	D	518	86% 11% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17079 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 Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3951	2493	694	731	33			
1	B	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	C	513	Total	C	N	O	S	0	0	0
			3957	2499	694	731	33			
1	D	513	Total	C	N	O	S	0	0	0
			3949	2492	694	730	33			

There are 24 discrepancies between the modelled and reference sequences:

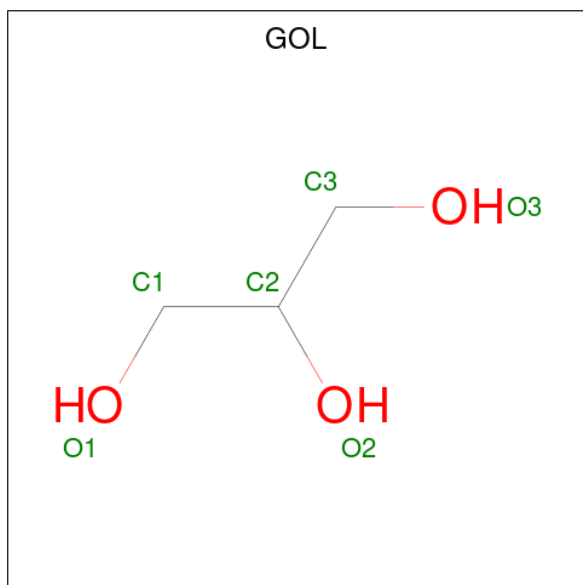
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-5	GLY	-	expression tag	UNP D3KVM3
B	-4	ILE	-	expression tag	UNP D3KVM3
B	-3	ASP	-	expression tag	UNP D3KVM3
B	-2	PRO	-	expression tag	UNP D3KVM3
B	-1	PHE	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3
C	-5	GLY	-	expression tag	UNP D3KVM3
C	-4	ILE	-	expression tag	UNP D3KVM3
C	-3	ASP	-	expression tag	UNP D3KVM3
C	-2	PRO	-	expression tag	UNP D3KVM3
C	-1	PHE	-	expression tag	UNP D3KVM3
C	0	THR	-	expression tag	UNP D3KVM3
D	-5	GLY	-	expression tag	UNP D3KVM3
D	-4	ILE	-	expression tag	UNP D3KVM3
D	-3	ASP	-	expression tag	UNP D3KVM3

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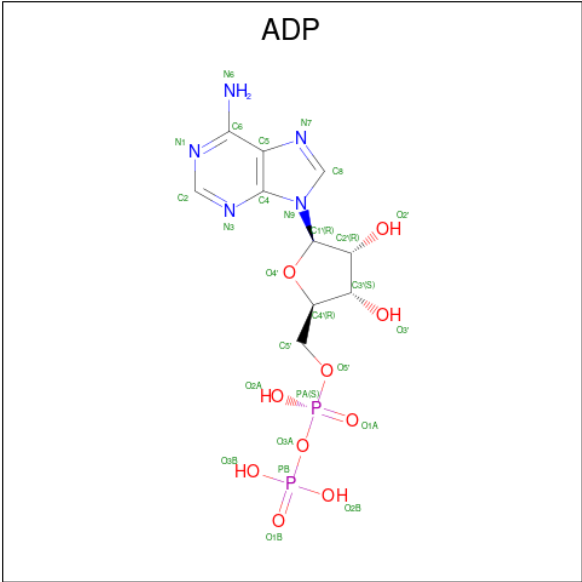
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	PRO	-	expression tag	UNP D3KVM3
D	-1	PHE	-	expression tag	UNP D3KVM3
D	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total	O	0	0
			287	287		
5	B	285	Total	O	0	0
			285	285		

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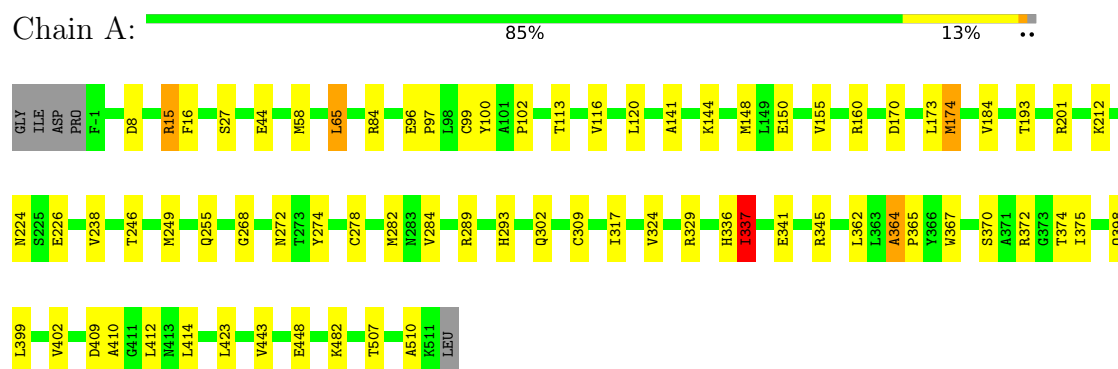
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	261	Total 261	O 261	0	0
5	D	259	Total 259	O 259	0	0

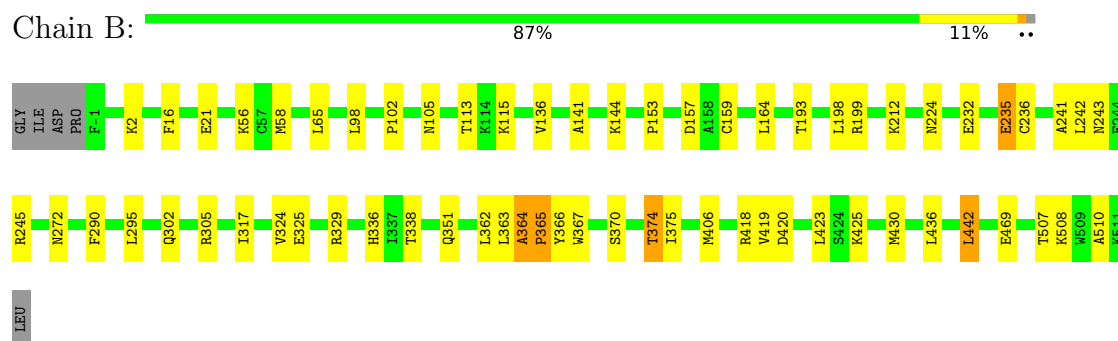
3 Residue-property plots

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.

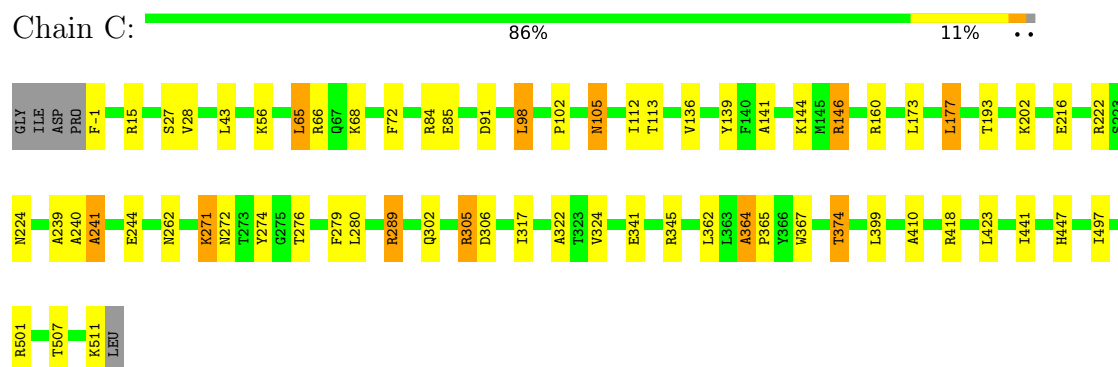
• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



• Molecule 1: Glycerol kinase



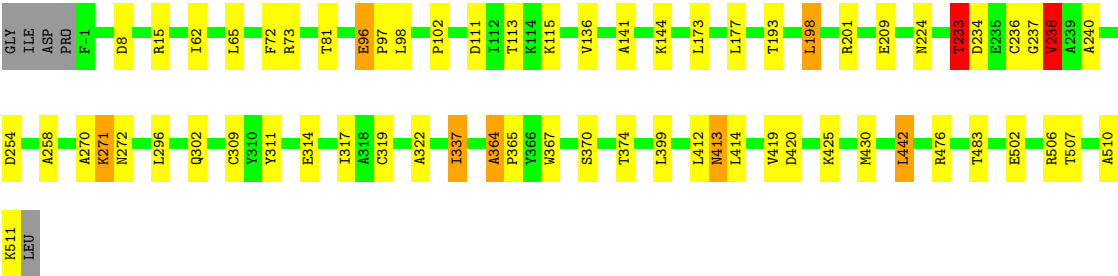
● Molecule 1: Glycerol kinase

Chain D:

86%

11%

..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.12Å 153.84Å 120.10Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 30.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (30.00-1.90) 98.3 (30.00-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.254 0.226 , 0.268	Depositor DCC
R_{free} test set	8665 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.237 for h,-k,-l	Xtriage
Reported twinning fraction	0.515 for H, K, L 0.485 for h,-k,-l	Depositor
Outliers	1 of 173946 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17079	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: GOL, ADP, 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	0.49	1/4032 (0.0%)	0.78	2/5456 (0.0%)
1	B	0.47	2/4039 (0.0%)	0.79	2/5465 (0.0%)
1	C	0.57	5/4039 (0.1%)	0.80	1/5465 (0.0%)
1	D	0.50	1/4030 (0.0%)	0.81	2/5453 (0.0%)
All	All	0.51	9/16140 (0.1%)	0.79	7/21839 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	PHE	C-O	-6.59	1.16	1.24
1	C	241	ALA	CA-CB	-6.40	1.43	1.53
1	B	365	PRO	N-CD	5.81	1.55	1.47
1	C	280	LEU	C-O	-5.78	1.17	1.24
1	C	241	ALA	C-O	-5.46	1.17	1.24
1	A	246	THR	C-O	-5.34	1.19	1.24
1	C	239	ALA	CA-CB	-5.25	1.44	1.53
1	D	238	VAL	C-O	-5.13	1.18	1.24
1	B	241	ALA	CA-CB	-5.06	1.45	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	233	THR	N-CA-C	7.77	119.38	111.07
1	A	238	VAL	N-CA-C	7.42	118.22	110.72
1	A	337	ILE	N-CA-C	6.75	118.31	110.62
1	D	237	GLY	N-CA-C	-6.11	98.70	113.18
1	C	240	ALA	N-CA-C	-6.09	104.92	112.90
1	B	365	PRO	N-CA-C	5.89	124.61	112.47
1	B	242	LEU	N-CA-C	5.33	118.00	111.82

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	3951	0	3963	46	0
1	B	3957	0	3970	30	0
1	C	3957	0	3970	37	0
1	D	3949	0	3958	36	0
2	A	6	0	8	2	0
2	B	6	0	8	0	0
2	C	18	0	24	2	0
2	D	6	0	8	0	0
3	A	27	0	12	1	0
3	B	54	0	24	0	0
3	D	54	0	24	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	287	0	0	0	0
5	B	285	0	0	2	0
5	C	261	0	0	0	0
5	D	259	0	0	1	0
All	All	17079	0	15969	146	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 5.

All (146) 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:C:364:ALA:HB1	1:C:365:PRO:HD2	1.34	1.08
1:D:364:ALA:HB1	1:D:365:PRO:HD2	1.35	1.06
1:A:364:ALA:HB1	1:A:365:PRO:CD	1.98	0.93
1:C:364:ALA:HB1	1:C:365:PRO:CD	1.98	0.93
1:D:236:CYS:SG	1:D:236:CYS:O	2.29	0.91
1:A:364:ALA:HB1	1:A:365:PRO:HD2	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ALA:HB1	1:D:365:PRO:CD	2.03	0.89
1:D:317:ILE:HB	5:D:878:HOH:O	1.78	0.82
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.62	0.81
1:C:364:ALA:CB	1:C:365:PRO:HD2	2.13	0.78
1:D:224:ASN:HD22	1:D:302:GLN:H	1.28	0.78
1:B:224:ASN:HD22	1:B:302:GLN:H	1.31	0.76
1:A:364:ALA:CB	1:A:365:PRO:HD2	2.16	0.76
1:C:289:ARG:HG2	1:C:410:ALA:HA	1.66	0.75
1:A:224:ASN:HD22	1:A:302:GLN:H	1.34	0.75
1:A:364:ALA:CB	1:A:365:PRO:CD	2.66	0.72
1:C:305:ARG:HH11	1:C:305:ARG:HG3	1.56	0.71
1:C:224:ASN:HD22	1:C:302:GLN:H	1.37	0.70
1:B:364:ALA:CB	1:B:365:PRO:CD	2.70	0.69
1:C:113:THR:HG23	1:C:136:VAL:HG12	1.73	0.69
1:C:15:ARG:HH21	1:C:28:VAL:HG21	1.57	0.69
1:A:278:CYS:HB2	1:A:317:ILE:HG12	1.75	0.69
1:C:305:ARG:HG3	1:C:305:ARG:NH1	2.08	0.69
1:A:96:GLU:HG3	1:A:97:PRO:HD2	1.75	0.67
1:C:43:LEU:HD23	1:C:105:ASN:HD21	1.59	0.67
1:D:364:ALA:CB	1:D:365:PRO:HD2	2.19	0.66
1:A:27:SER:HB2	1:A:65:LEU:HG	1.78	0.64
1:D:113:THR:HG23	1:D:136:VAL:HG12	1.80	0.64
1:B:324:VAL:HG21	1:B:423:LEU:HD21	1.79	0.63
1:A:102:PRO:HD3	1:A:148:MET:HE3	1.80	0.63
1:D:374:THR:HG21	1:D:507:THR:HA	1.81	0.63
1:A:374:THR:HG21	1:A:507:THR:HA	1.81	0.63
1:C:105:ASN:HD22	1:C:105:ASN:H	1.47	0.62
1:A:212:LYS:HB2	1:C:306:ASP:OD2	2.00	0.61
1:D:258:ALA:HB3	1:D:271:LYS:HD2	1.82	0.61
1:D:337:ILE:HD13	1:D:337:ILE:H	1.66	0.60
1:C:364:ALA:CB	1:C:365:PRO:CD	2.72	0.60
1:B:351:GLN:HG2	5:B:948:HOH:O	2.03	0.59
1:A:255:GLN:HE22	3:A:602:ADP:HN62	1.51	0.58
1:C:91:ASP:HB2	1:C:98:LEU:HD11	1.86	0.58
1:C:274:TYR:HB3	1:C:423:LEU:HB2	1.84	0.58
1:C:374:THR:HG21	1:C:507:THR:HG22	1.87	0.57
1:B:364:ALA:O	1:B:367:TRP:CZ3	2.58	0.56
1:D:419:VAL:HG21	1:D:430:MET:SD	2.46	0.56
1:A:102:PRO:HB2	1:A:144:LYS:HD3	1.87	0.56
1:A:84:ARG:HH21	2:A:601:GOL:H11	1.70	0.56
1:D:96:GLU:HG3	1:D:97:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:PRO:HB2	1:D:144:LYS:HD3	1.88	0.55
1:D:8:ASP:HB3	1:D:15:ARG:CG	2.37	0.54
1:A:272:ASN:HD21	1:A:278:CYS:HB3	1.73	0.54
1:C:305:ARG:HH11	1:C:305:ARG:CG	2.21	0.54
1:B:199:ARG:HD2	1:B:290:PHE:HZ	1.72	0.54
1:A:102:PRO:CD	1:A:148:MET:HE3	2.38	0.53
1:B:272:ASN:HB3	1:B:419:VAL:HG12	1.90	0.53
1:C:222:ARG:HA	1:C:305:ARG:HH12	1.74	0.53
1:A:99:CYS:SG	1:A:148:MET:HE2	2.48	0.52
1:C:271:LYS:HG2	1:C:272:ASN:N	2.19	0.52
1:A:44:GLU:OE1	1:A:100:TYR:HB2	2.09	0.52
1:A:370:SER:HA	1:A:510:ALA:HB3	1.91	0.52
1:A:289:ARG:HD3	1:A:410:ALA:HA	1.92	0.52
1:A:44:GLU:HG2	1:A:100:TYR:HB2	1.92	0.51
1:C:27:SER:HB2	1:C:65:LEU:HG	1.92	0.51
1:D:370:SER:HA	1:D:510:ALA:HB3	1.92	0.51
1:A:443:VAL:HB	1:A:482:LYS:HB3	1.93	0.51
1:D:296:LEU:HB2	1:D:314:GLU:HB3	1.93	0.51
1:B:364:ALA:HB1	1:B:365:PRO:CD	2.29	0.51
1:C:324:VAL:HG21	1:C:423:LEU:HD21	1.93	0.50
1:D:319:CYS:HA	1:D:322:ALA:HB3	1.93	0.50
1:B:325:GLU:HG3	1:B:329:ARG:HG2	1.94	0.50
1:C:262:ASN:O	1:C:418:ARG:HD3	2.11	0.50
1:A:274:TYR:HB3	1:A:423:LEU:HB2	1.93	0.50
1:B:2:LYS:HG2	1:B:21:GLU:OE2	2.11	0.50
1:A:174:MET:HE3	1:A:184:VAL:HG23	1.94	0.49
1:A:170:ASP:O	1:A:174:MET:HB2	2.13	0.49
1:A:341:GLU:OE2	1:A:345:ARG:NH2	2.43	0.49
1:C:374:THR:CG2	1:C:507:THR:HG22	2.42	0.49
1:A:116:VAL:HG13	1:A:120:LEU:HD12	1.94	0.49
1:B:113:THR:HG23	1:B:136:VAL:HG12	1.94	0.48
1:D:234:ASP:HA	1:D:238:VAL:HA	1.94	0.48
1:D:238:VAL:C	1:D:240:ALA:H	2.21	0.48
1:D:510:ALA:O	1:D:511:LYS:HB2	2.13	0.48
1:B:363:LEU:O	1:B:364:ALA:C	2.55	0.48
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.91	0.48
1:A:398:GLN:O	1:A:402:VAL:HG23	2.13	0.48
1:B:16:PHE:CD2	1:B:58:MET:HA	2.48	0.48
1:D:62:ILE:HG23	1:D:72:PHE:HE1	1.79	0.47
1:A:226:GLU:O	1:A:249:MET:HA	2.15	0.47
1:B:374:THR:HG21	1:B:507:THR:HG22	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:HH21	2:C:601:GOL:H11	1.79	0.47
1:C:224:ASN:ND2	1:C:302:GLN:H	2.10	0.47
1:B:418:ARG:HE	1:B:442:LEU:HD23	1.79	0.47
1:C:66:ARG:NH2	1:C:241:ALA:O	2.47	0.47
1:D:141:ALA:HB3	1:D:193:THR:HA	1.96	0.47
1:D:233:THR:O	1:D:234:ASP:HB2	2.15	0.46
1:D:8:ASP:HB3	1:D:15:ARG:HG3	1.98	0.46
1:D:272:ASN:HB3	1:D:419:VAL:HG12	1.97	0.46
1:A:148:MET:HB3	1:A:155:VAL:HG11	1.98	0.46
1:A:372:ARG:O	1:A:374:THR:HG23	2.16	0.46
1:B:159:CYS:HB2	1:B:164:LEU:HD22	1.98	0.45
1:D:8:ASP:HB3	1:D:15:ARG:HG2	1.97	0.45
1:A:364:ALA:HB1	1:A:402:VAL:HG22	1.99	0.45
1:D:198:LEU:HD22	1:D:311:TYR:HE1	1.82	0.45
1:A:8:ASP:HB3	1:A:15:ARG:HG3	1.98	0.45
1:D:442:LEU:HD12	1:D:483:THR:HG22	1.97	0.45
1:A:84:ARG:HH21	2:A:601:GOL:C1	2.30	0.45
1:B:235:GLU:HA	1:B:236:CYS:HA	1.77	0.45
1:A:324:VAL:HG21	1:A:423:LEU:HD21	1.98	0.45
1:D:111:ASP:O	1:D:115:LYS:HG2	2.17	0.45
1:C:102:PRO:HB2	1:C:144:LYS:HD3	1.99	0.44
1:C:497:ILE:O	1:C:501:ARG:HG2	2.16	0.44
1:A:268:GLY:HA2	1:A:412:LEU:HD13	1.99	0.44
1:A:375:ILE:HD12	1:B:375:ILE:HD12	1.98	0.44
1:C:276:THR:HG23	1:C:322:ALA:HB2	1.99	0.44
1:D:413:ASN:HD22	1:D:414:LEU:H	1.65	0.43
1:D:201:ARG:HD3	1:D:309:CYS:SG	2.58	0.43
1:A:293:HIS:HD2	1:A:409:ASP:OD2	2.00	0.43
1:B:370:SER:HB2	1:B:510:ALA:HB2	2.01	0.42
1:B:374:THR:CG2	1:B:507:THR:HG22	2.50	0.42
1:B:102:PRO:HB2	1:B:144:LYS:HD3	2.01	0.42
1:B:199:ARG:HD3	5:B:701:HOH:O	2.18	0.42
1:C:173:LEU:O	1:C:177:LEU:HB2	2.20	0.42
1:B:364:ALA:HB3	1:B:365:PRO:CD	2.48	0.42
1:A:141:ALA:HB3	1:A:193:THR:HA	2.02	0.42
1:D:198:LEU:HD22	1:D:311:TYR:CE1	2.53	0.42
1:C:85:GLU:HB3	1:C:139:TYR:O	2.19	0.42
1:B:153:PRO:O	1:B:157:ASP:HB2	2.19	0.42
1:B:317:ILE:HD13	1:B:364:ALA:HB2	2.00	0.42
1:C:341:GLU:O	1:C:345:ARG:HG3	2.20	0.42
1:C:85:GLU:OE1	2:C:601:GOL:H12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ALA:HB3	1:C:193:THR:HA	2.02	0.41
1:B:141:ALA:HB3	1:B:193:THR:HA	2.01	0.41
1:D:234:ASP:CA	1:D:238:VAL:HA	2.50	0.41
1:C:65:LEU:HD13	1:C:72:PHE:CG	2.55	0.41
1:D:270:ALA:HB3	1:D:414:LEU:HD11	2.02	0.41
1:A:336:HIS:ND1	1:A:337:ILE:HD13	2.36	0.41
1:B:336:HIS:HD2	1:B:338:THR:H	1.68	0.41
1:A:282:MET:HE2	1:A:414:LEU:HD13	2.03	0.41
1:D:81:THR:OG1	1:D:254:ASP:HA	2.20	0.41
1:A:16:PHE:CD2	1:A:58:MET:HA	2.56	0.41
1:A:201:ARG:HD3	1:A:309:CYS:SG	2.60	0.41
1:A:284:VAL:HB	1:A:289:ARG:HG3	2.03	0.41
1:B:295:LEU:HD13	1:B:406:MET:HG2	2.03	0.41
1:B:419:VAL:HG21	1:B:430:MET:SD	2.61	0.41
1:D:502:GLU:HG3	1:D:506:ARG:HH12	1.84	0.41
1:C:112:ILE:HG21	1:C:146:ARG:HG2	2.02	0.40
1:A:150:GLU:O	1:C:202:LYS:HG3	2.21	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	511/518 (99%)	496 (97%)	14 (3%)	1 (0%)	43	36
1	B	511/518 (99%)	491 (96%)	19 (4%)	1 (0%)	43	36
1	C	511/518 (99%)	495 (97%)	15 (3%)	1 (0%)	43	36
1	D	511/518 (99%)	489 (96%)	19 (4%)	3 (1%)	21	13
All	All	2044/2072 (99%)	1971 (96%)	67 (3%)	6 (0%)	36	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	364	ALA
1	C	364	ALA
1	D	364	ALA
1	D	367	TRP
1	D	238	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	420/425 (99%)	408 (97%)	12 (3%)	37	31
1	B	421/425 (99%)	400 (95%)	21 (5%)	22	14
1	C	421/425 (99%)	399 (95%)	22 (5%)	21	13
1	D	419/425 (99%)	401 (96%)	18 (4%)	26	18
All	All	1681/1700 (99%)	1608 (96%)	73 (4%)	26	18

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	65	LEU
1	A	113	THR
1	A	160	ARG
1	A	173	LEU
1	A	174	MET
1	A	329	ARG
1	A	337	ILE
1	A	362	LEU
1	A	367	TRP
1	A	399	LEU
1	A	448	GLU
1	B	56	LYS
1	B	65	LEU
1	B	98	LEU
1	B	105	ASN

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Mol	Chain	Res	Type
1	B	115	LYS
1	B	198	LEU
1	B	212	LYS
1	B	232	GLU
1	B	235	GLU
1	B	243	ASN
1	B	245	ARG
1	B	305	ARG
1	B	362	LEU
1	B	366	TYR
1	B	374	THR
1	B	420	ASP
1	B	425	LYS
1	B	436	LEU
1	B	442	LEU
1	B	469	GLU
1	B	508	LYS
1	C	-1	PHE
1	C	56	LYS
1	C	65	LEU
1	C	68	LYS
1	C	98	LEU
1	C	105	ASN
1	C	146	ARG
1	C	160	ARG
1	C	177	LEU
1	C	216	GLU
1	C	244	GLU
1	C	271	LYS
1	C	289	ARG
1	C	305	ARG
1	C	317	ILE
1	C	362	LEU
1	C	367	TRP
1	C	374	THR
1	C	399	LEU
1	C	441	ILE
1	C	447	HIS
1	C	511	LYS
1	D	65	LEU
1	D	73	ARG
1	D	96	GLU

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Mol	Chain	Res	Type
1	D	98	LEU
1	D	173	LEU
1	D	177	LEU
1	D	198	LEU
1	D	209	GLU
1	D	233	THR
1	D	271	LYS
1	D	337	ILE
1	D	399	LEU
1	D	412	LEU
1	D	413	ASN
1	D	420	ASP
1	D	425	LYS
1	D	442	LEU
1	D	476	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	36	HIS
1	A	151	ASN
1	A	224	ASN
1	A	243	ASN
1	A	262	ASN
1	A	272	ASN
1	A	293	HIS
1	A	302	GLN
1	A	351	GLN
1	B	23	GLN
1	B	151	ASN
1	B	224	ASN
1	B	262	ASN
1	B	272	ASN
1	B	302	GLN
1	B	336	HIS
1	B	447	HIS
1	C	23	GLN
1	C	29	HIS
1	C	105	ASN
1	C	151	ASN
1	C	224	ASN

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Mol	Chain	Res	Type
1	C	293	HIS
1	C	302	GLN
1	C	336	HIS
1	C	351	GLN
1	D	23	GLN
1	D	29	HIS
1	D	30	GLN
1	D	151	ASN
1	D	224	ASN
1	D	262	ASN
1	D	293	HIS
1	D	302	GLN
1	D	398	GLN
1	D	413	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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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
3	ADP	A	602	-	28,29,29	1.47	4 (14%)	43,45,45	1.87	9 (20%)
2	GOL	D	601	-	5,5,5	0.39	0	5,5,5	0.27	0
2	GOL	B	601	-	5,5,5	0.34	0	5,5,5	0.37	0
2	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.33	0
3	ADP	B	603	4	28,29,29	1.44	5 (17%)	43,45,45	1.80	11 (25%)
2	GOL	C	602	-	5,5,5	0.37	0	5,5,5	0.32	0
3	ADP	B	602	4	28,29,29	1.47	5 (17%)	43,45,45	1.77	8 (18%)
3	ADP	D	602	4	28,29,29	1.45	5 (17%)	43,45,45	1.76	9 (20%)
2	GOL	C	601	-	5,5,5	0.39	0	5,5,5	0.20	0
2	GOL	C	603	-	5,5,5	0.38	0	5,5,5	0.32	0
3	ADP	D	603	4	28,29,29	1.49	5 (17%)	43,45,45	1.81	8 (18%)

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
3	ADP	A	602	-	-	6/16/32/32	0/3/3/3
2	GOL	D	601	-	-	0/4/4/4	-
2	GOL	B	601	-	-	0/4/4/4	-
2	GOL	A	601	-	-	2/4/4/4	-
3	ADP	B	603	4	-	2/16/32/32	0/3/3/3
2	GOL	C	602	-	-	2/4/4/4	-
3	ADP	B	602	4	-	4/16/32/32	0/3/3/3
3	ADP	D	602	4	-	0/16/32/32	0/3/3/3
2	GOL	C	601	-	-	2/4/4/4	-
2	GOL	C	603	-	-	0/4/4/4	-
3	ADP	D	603	4	-	5/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	C5-C4	5.01	1.48	1.39
3	B	602	ADP	C5-C4	4.95	1.47	1.39
3	D	603	ADP	C5-C4	4.94	1.47	1.39
3	D	602	ADP	C5-C4	4.85	1.47	1.39
3	B	603	ADP	C5-C4	4.72	1.47	1.39
3	D	603	ADP	C5-C6	2.92	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	C5-C6	2.88	1.49	1.41
3	B	602	ADP	C5-C6	2.84	1.48	1.41
3	B	603	ADP	C5-C6	2.79	1.48	1.41
3	D	602	ADP	C5-C6	2.79	1.48	1.41
3	D	603	ADP	C8-N7	2.37	1.36	1.31
3	D	602	ADP	C8-N7	2.36	1.36	1.31
3	A	602	ADP	C5-N7	-2.34	1.34	1.39
3	B	603	ADP	C5-N7	-2.30	1.34	1.39
3	B	602	ADP	C8-N7	2.30	1.36	1.31
3	B	603	ADP	C8-N7	2.28	1.36	1.31
3	B	602	ADP	C5-N7	-2.28	1.34	1.39
3	A	602	ADP	C8-N7	2.27	1.36	1.31
3	D	603	ADP	C5-N7	-2.26	1.35	1.39
3	D	603	ADP	PA-O3A	2.20	1.61	1.59
3	D	602	ADP	C5-N7	-2.15	1.35	1.39
3	B	602	ADP	PA-O3A	2.09	1.61	1.59
3	D	602	ADP	PA-O3A	2.06	1.61	1.59
3	B	603	ADP	PA-O3A	2.01	1.61	1.59

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ADP	C5-C4-N3	-6.14	118.26	126.72
3	D	603	ADP	C5-C4-N3	-5.84	118.68	126.72
3	B	602	ADP	C5-C4-N3	-5.83	118.69	126.72
3	B	603	ADP	C5-C4-N3	-5.47	119.18	126.72
3	D	602	ADP	C5-C4-N3	-5.38	119.31	126.72
3	A	602	ADP	N3-C4-N9	4.92	135.54	127.17
3	B	602	ADP	N3-C4-N9	4.70	135.16	127.17
3	D	603	ADP	N3-C4-N9	4.65	135.07	127.17
3	B	603	ADP	N3-C4-N9	4.49	134.80	127.17
3	D	602	ADP	N3-C4-N9	4.32	134.51	127.17
3	A	602	ADP	C2-N3-C4	3.92	121.40	111.83
3	D	603	ADP	C2-N3-C4	3.84	121.20	111.83
3	B	602	ADP	C2-N3-C4	3.79	121.08	111.83
3	B	603	ADP	C2-N3-C4	3.68	120.83	111.83
3	B	603	ADP	N3-C2-N1	-3.66	123.05	128.58
3	D	602	ADP	C2-N3-C4	3.65	120.75	111.83
3	D	602	ADP	N3-C2-N1	-3.58	123.16	128.58
3	D	603	ADP	N3-C2-N1	-3.50	123.28	128.58
3	D	603	ADP	C4-C5-N7	-3.42	106.67	110.58
3	D	602	ADP	C4-C5-N7	-3.42	106.67	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	ADP	N3-C2-N1	-3.41	123.42	128.58
3	B	602	ADP	N3-C2-N1	-3.40	123.44	128.58
3	A	602	ADP	C4-C5-N7	-3.38	106.72	110.58
3	B	603	ADP	C4-C5-N7	-3.26	106.86	110.58
3	B	602	ADP	C4-C5-N7	-3.25	106.87	110.58
3	B	603	ADP	C4-N9-C8	2.89	108.77	105.74
3	D	602	ADP	C4-N9-C8	2.84	108.72	105.74
3	D	603	ADP	C4-N9-C8	2.52	108.38	105.74
3	D	603	ADP	C5-N7-C8	2.51	107.40	103.45
3	A	602	ADP	C5-N7-C8	2.47	107.33	103.45
3	B	603	ADP	C5-N7-C8	2.47	107.33	103.45
3	D	602	ADP	C5-N7-C8	2.46	107.32	103.45
3	A	602	ADP	C3'-C2'-C1'	2.46	106.12	101.46
3	B	602	ADP	C5-N7-C8	2.36	107.16	103.45
3	B	602	ADP	C4-N9-C8	2.34	108.19	105.74
3	D	602	ADP	C6-C5-N7	2.34	136.59	132.09
3	B	603	ADP	C2-N1-C6	2.21	122.36	118.73
3	D	603	ADP	C6-C5-N7	2.19	136.31	132.09
3	D	602	ADP	C2-N1-C6	2.19	122.32	118.73
3	A	602	ADP	C4-N9-C8	2.15	108.00	105.74
3	B	603	ADP	C6-C5-N7	2.14	136.22	132.09
3	B	603	ADP	O4'-C1'-N9	2.10	112.11	108.09
3	B	603	ADP	N9-C8-N7	-2.05	111.03	113.94
3	A	602	ADP	C6-C5-N7	2.05	136.04	132.09
3	B	602	ADP	C6-C5-N7	2.05	136.04	132.09

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
3	A	602	ADP	C5'-O5'-PA-O1A
3	A	602	ADP	C5'-O5'-PA-O3A
3	A	602	ADP	O4'-C4'-C5'-O5'
3	B	602	ADP	PA-O3A-PB-O2B
3	B	603	ADP	C5'-O5'-PA-O2A
3	B	603	ADP	C5'-O5'-PA-O3A
3	D	603	ADP	C5'-O5'-PA-O2A
3	D	603	ADP	C5'-O5'-PA-O3A
2	C	601	GOL	O1-C1-C2-O2
2	A	601	GOL	C1-C2-C3-O3

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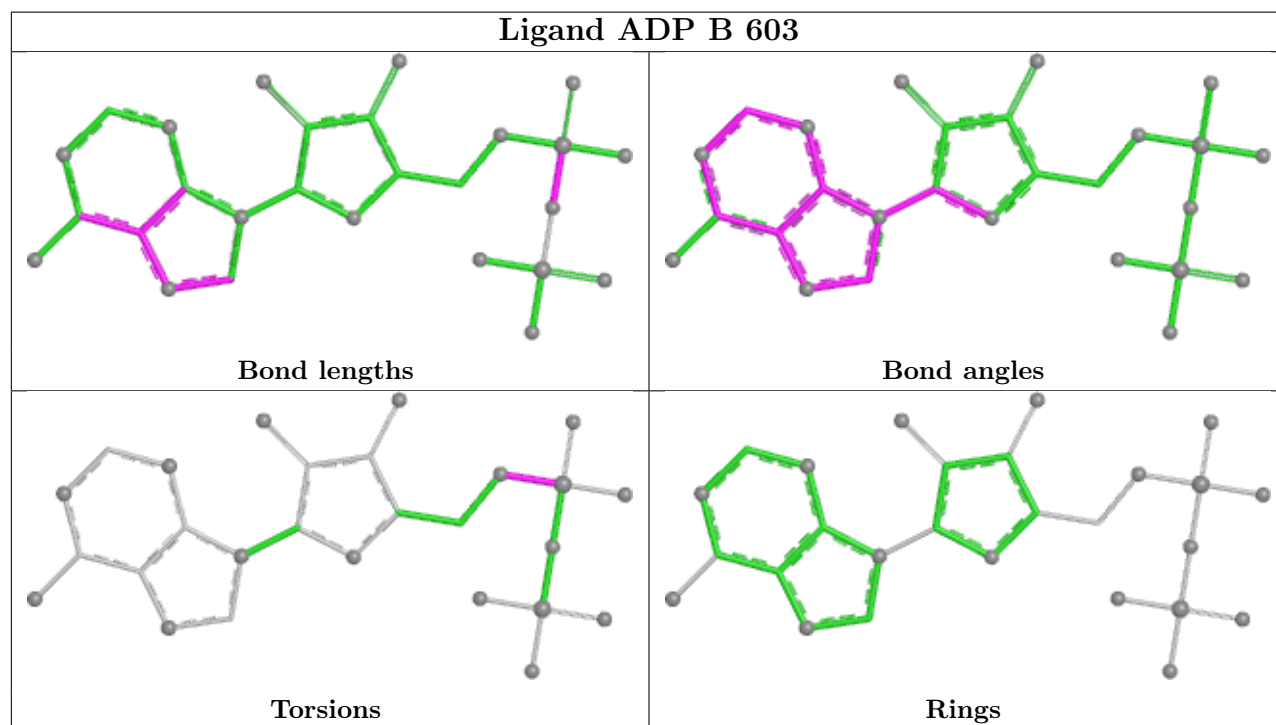
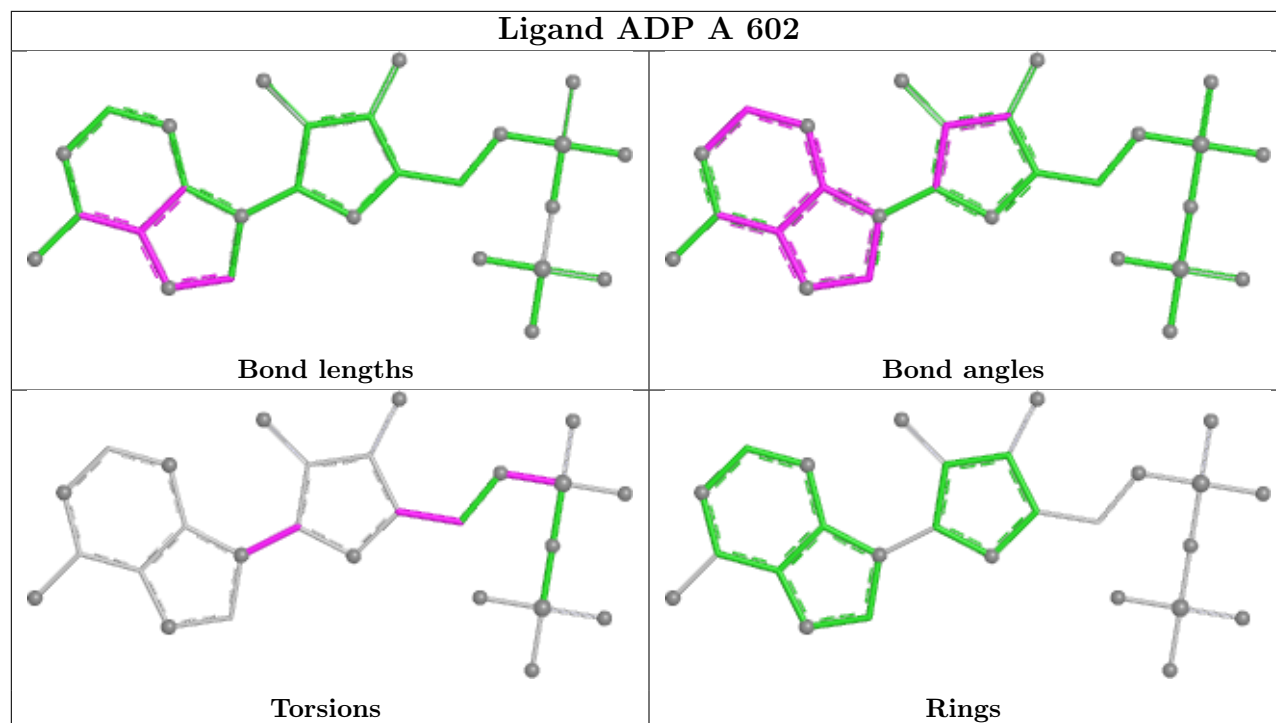
Mol	Chain	Res	Type	Atoms
3	A	602	ADP	C3'-C4'-C5'-O5'
3	B	602	ADP	O4'-C4'-C5'-O5'
3	D	603	ADP	PA-O3A-PB-O1B
2	C	602	GOL	O2-C2-C3-O3
3	B	602	ADP	C3'-C4'-C5'-O5'
2	A	601	GOL	O2-C2-C3-O3
3	D	603	ADP	PA-O3A-PB-O2B
3	A	602	ADP	C5'-O5'-PA-O2A
3	D	603	ADP	C5'-O5'-PA-O1A
3	B	602	ADP	PA-O3A-PB-O3B
3	A	602	ADP	O4'-C1'-N9-C8

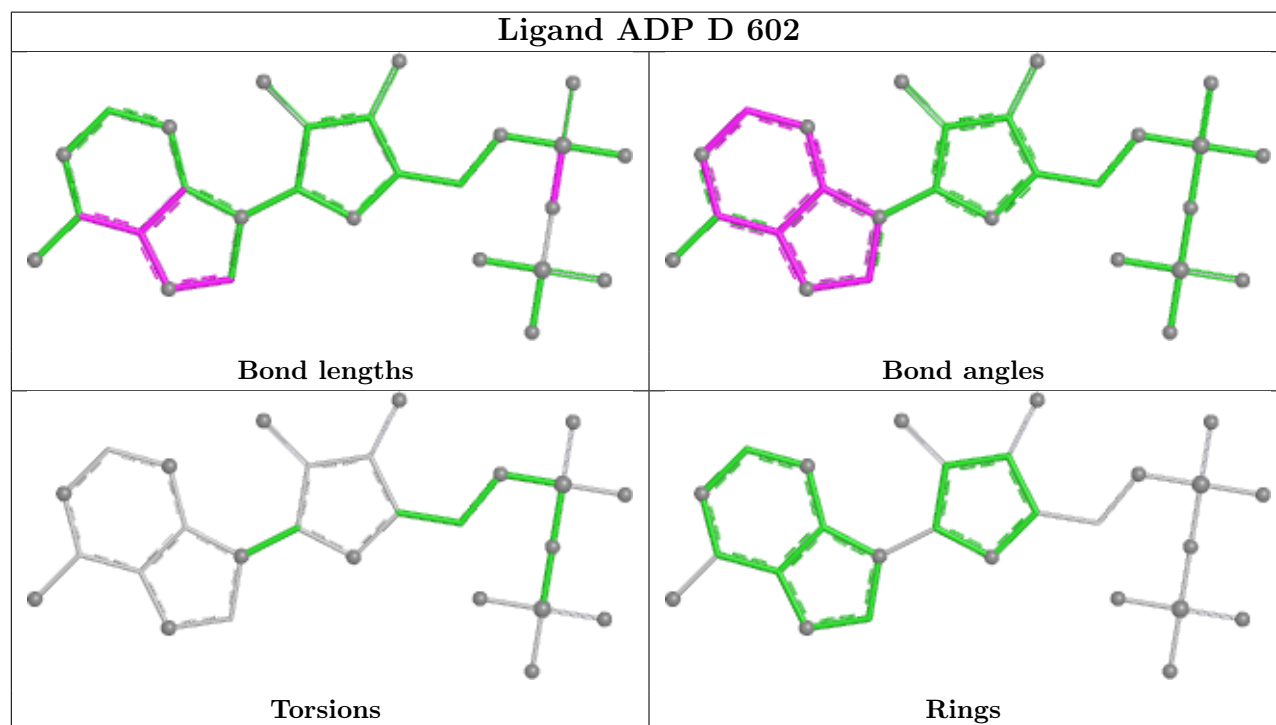
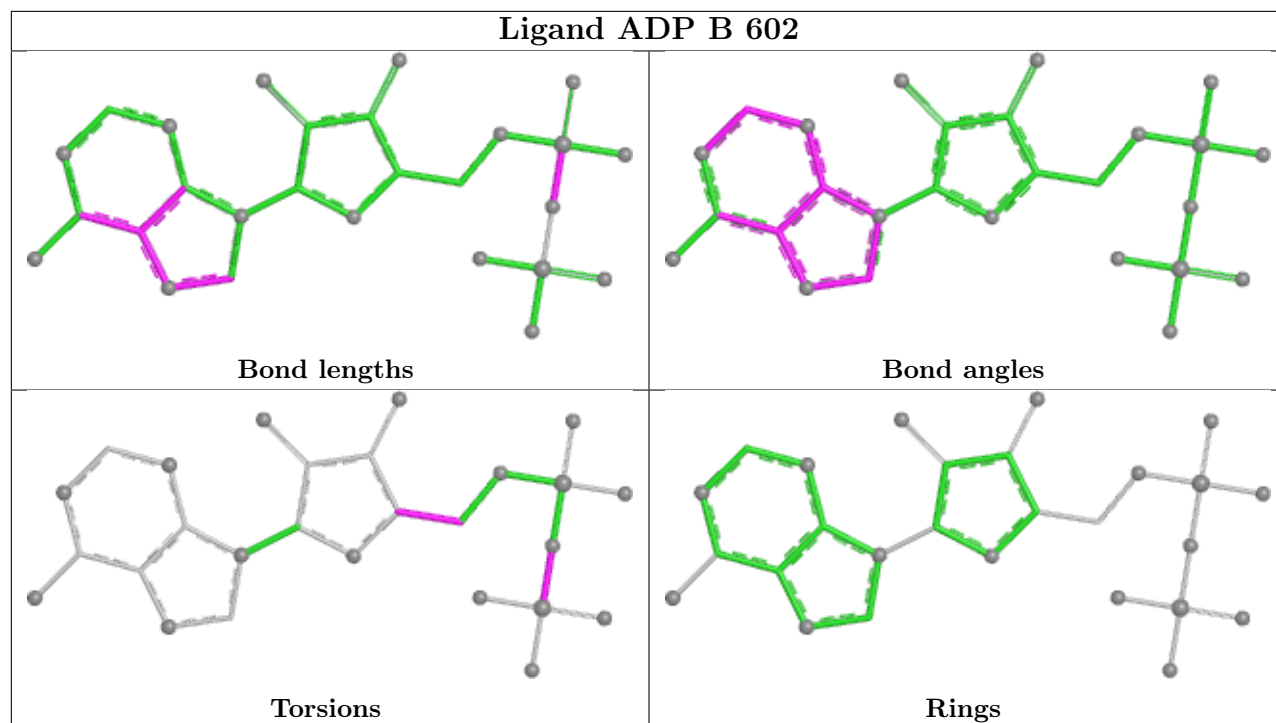
There are no ring outliers.

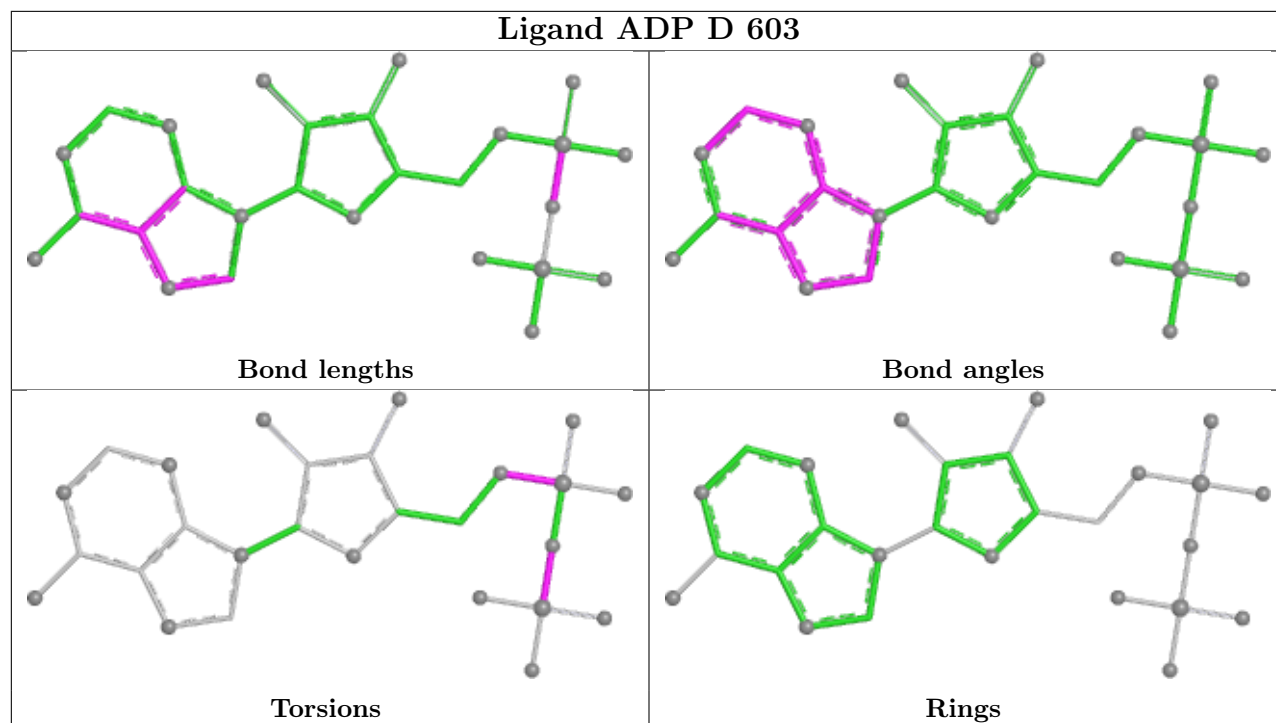
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ADP	1	0
2	A	601	GOL	2	0
2	C	601	GOL	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 [i](#)

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	513/518 (99%)	-1.13	0 100 100	19, 32, 40, 44	1 (0%)
1	B	513/518 (99%)	-1.16	0 100 100	19, 31, 42, 48	1 (0%)
1	C	513/518 (99%)	-1.13	0 100 100	21, 32, 44, 51	1 (0%)
1	D	513/518 (99%)	-1.12	0 100 100	21, 33, 45, 50	1 (0%)
All	All	2052/2072 (99%)	-1.13	0 100 100	19, 32, 42, 51	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	A	602	27/27	0.97	0.05	60,60,61,61	0
2	GOL	C	603	6/6	0.98	0.09	76,76,76,76	0
2	GOL	C	602	6/6	0.98	0.05	49,49,49,49	0
2	GOL	A	601	6/6	0.99	0.05	39,40,41,41	0

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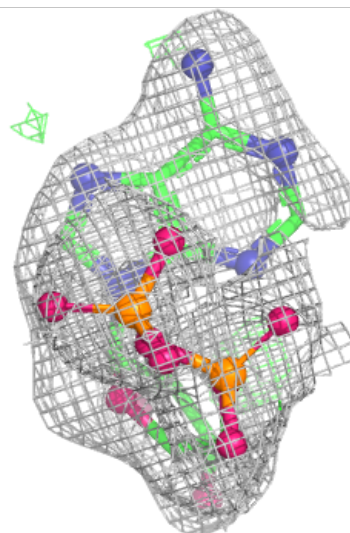
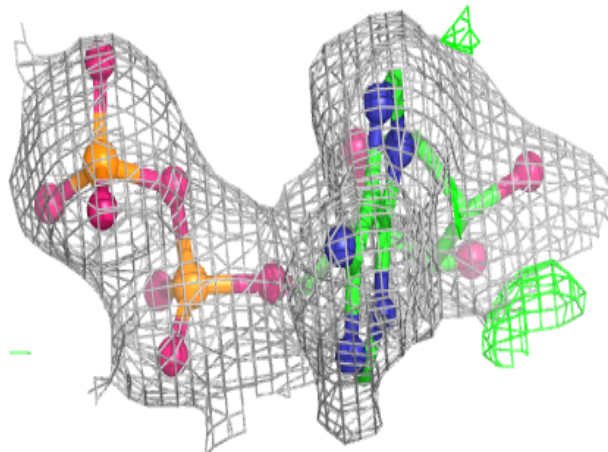
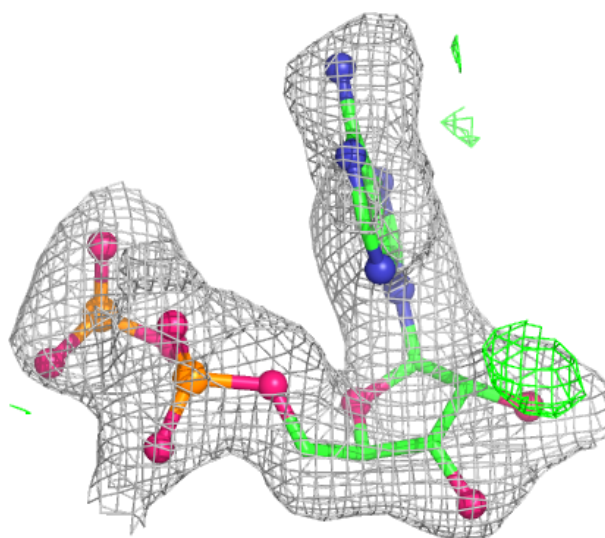
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	601	6/6	0.99	0.03	26,26,26,27	0
2	GOL	D	601	6/6	0.99	0.03	25,26,26,26	0
2	GOL	C	601	6/6	0.99	0.05	56,57,57,57	0
3	ADP	B	602	27/27	0.99	0.04	41,44,45,45	0
3	ADP	B	603	27/27	0.99	0.03	29,29,30,30	0
3	ADP	D	602	27/27	0.99	0.03	33,33,39,40	0
3	ADP	D	603	27/27	0.99	0.04	34,35,36,37	0
4	MG	B	604	1/1	0.99	0.02	32,32,32,32	0
4	MG	D	604	1/1	0.99	0.02	37,37,37,37	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.

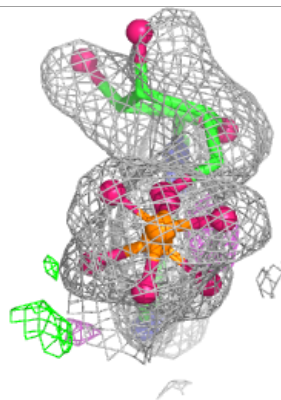
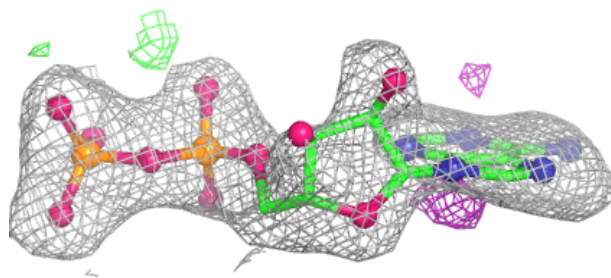
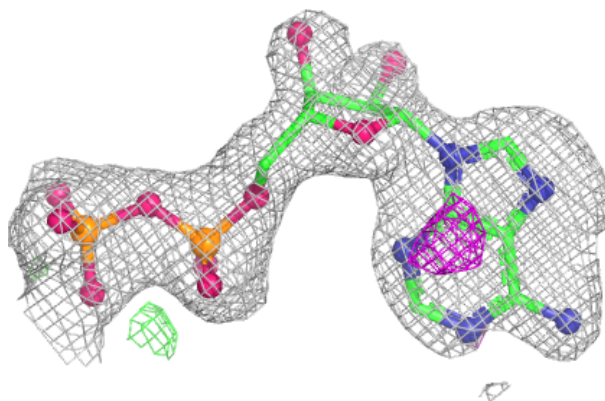
Electron density around ADP A 602:

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



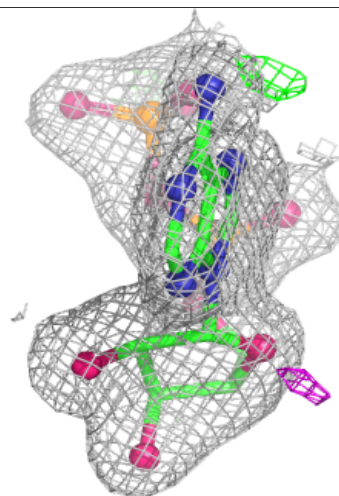
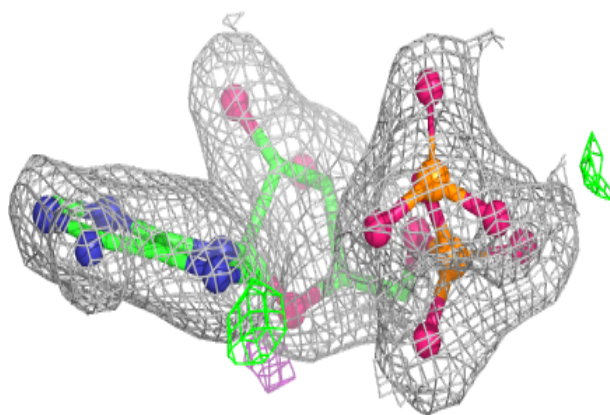
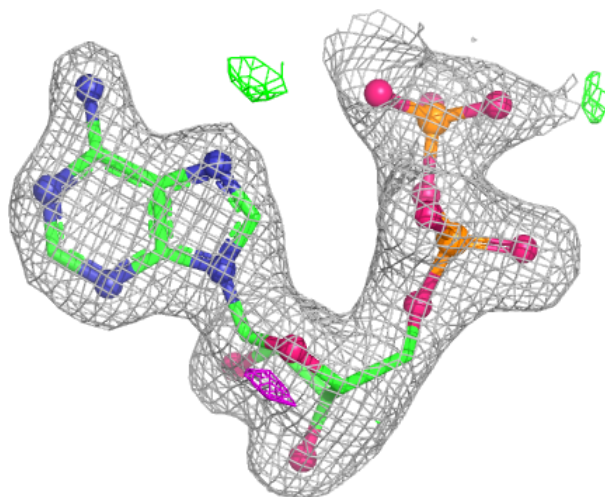
Electron density around ADP B 602:

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



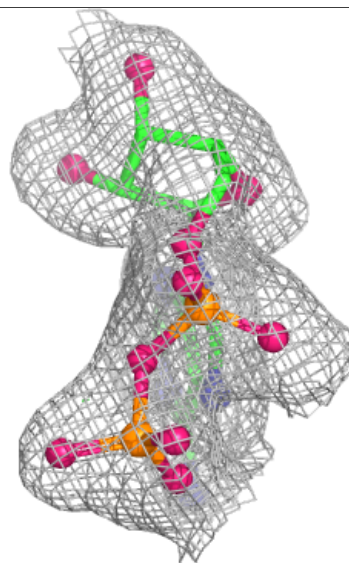
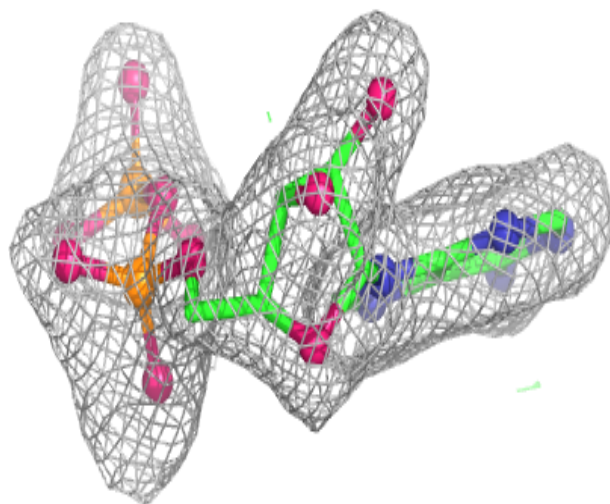
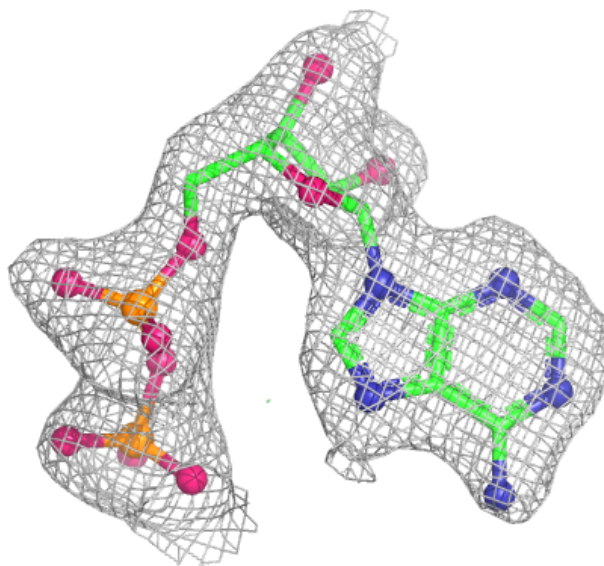
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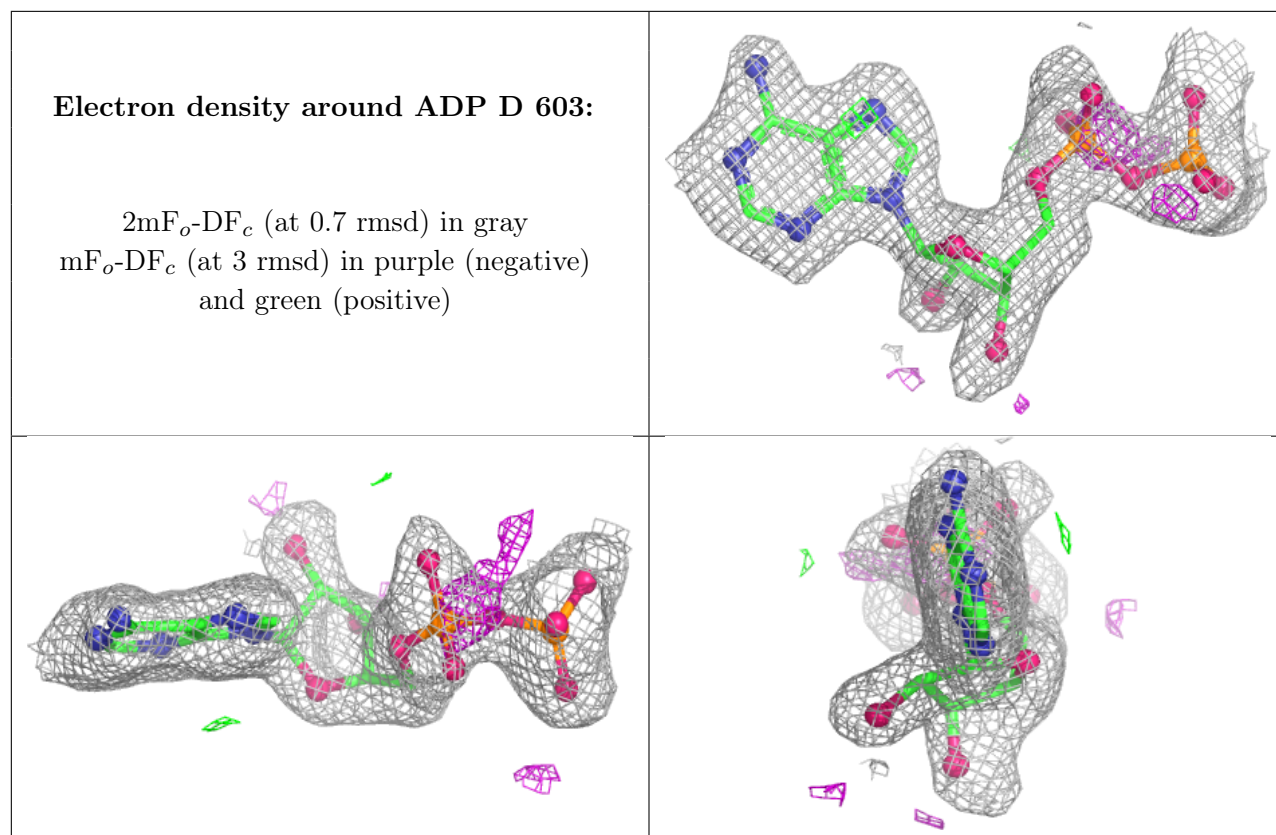
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP D 602:

$2mF_o-DF_c$ (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.