Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 07:14 PM EST

PDB ID	:	3UDT
Title	:	Inositol 1,3,4,5,6-pentakisphosphate 2-kinase from A. thaliana in complex with ADP and IP5.
Authors	:	Gosein, V.; Leung, T.-F.; Krajden, O.; Miller, G.J.
Deposited on	:	2011-10-28
Resolution	:	3.10 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:

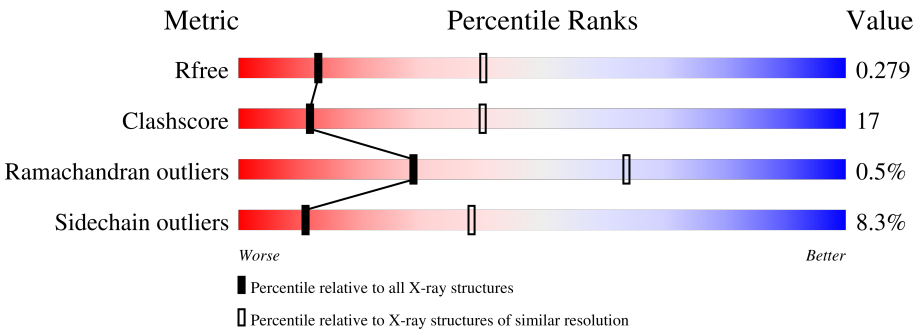
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	493	53% 23% • 22%
1	B	493	49% 26% • 22%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6267 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 Inositol-pentakisphosphate 2-kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	3072	1963	518	580	11	0	0	0
1	B	385	3073	1964	518	580	11	0	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	expression tag	UNP Q93YN9
A	-32	GLY	-	expression tag	UNP Q93YN9
A	-31	SER	-	expression tag	UNP Q93YN9
A	-30	SER	-	expression tag	UNP Q93YN9
A	-29	HIS	-	expression tag	UNP Q93YN9
A	-28	HIS	-	expression tag	UNP Q93YN9
A	-27	HIS	-	expression tag	UNP Q93YN9
A	-26	HIS	-	expression tag	UNP Q93YN9
A	-25	HIS	-	expression tag	UNP Q93YN9
A	-24	HIS	-	expression tag	UNP Q93YN9
A	-23	SER	-	expression tag	UNP Q93YN9
A	-22	SER	-	expression tag	UNP Q93YN9
A	-21	GLY	-	expression tag	UNP Q93YN9
A	-20	LEU	-	expression tag	UNP Q93YN9
A	-19	VAL	-	expression tag	UNP Q93YN9
A	-18	PRO	-	expression tag	UNP Q93YN9
A	-17	ARG	-	expression tag	UNP Q93YN9
A	-16	GLY	-	expression tag	UNP Q93YN9
A	-15	SER	-	expression tag	UNP Q93YN9
A	-14	HIS	-	expression tag	UNP Q93YN9
A	-13	MET	-	expression tag	UNP Q93YN9
A	-12	ALA	-	expression tag	UNP Q93YN9
A	-11	SER	-	expression tag	UNP Q93YN9
A	-10	MET	-	expression tag	UNP Q93YN9
A	-9	THR	-	expression tag	UNP Q93YN9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q93YN9
A	-7	GLY	-	expression tag	UNP Q93YN9
A	-6	GLN	-	expression tag	UNP Q93YN9
A	-5	GLN	-	expression tag	UNP Q93YN9
A	-4	MET	-	expression tag	UNP Q93YN9
A	-3	GLY	-	expression tag	UNP Q93YN9
A	-2	ARG	-	expression tag	UNP Q93YN9
A	-1	ILE	-	expression tag	UNP Q93YN9
A	0	LEU	-	expression tag	UNP Q93YN9
A	54	SER	ALA	conflict	UNP Q93YN9
A	90	GLN	LYS	conflict	UNP Q93YN9
A	157	THR	SER	conflict	UNP Q93YN9
A	185	ILE	MET	conflict	UNP Q93YN9
A	204	ILE	ASN	conflict	UNP Q93YN9
A	224	ARG	SER	conflict	UNP Q93YN9
A	321	CYS	SER	conflict	UNP Q93YN9
A	325	ILE	LEU	conflict	UNP Q93YN9
A	337	ARG	LYS	conflict	UNP Q93YN9
A	452	ASP	-	expression tag	UNP Q93YN9
A	453	TYR	-	expression tag	UNP Q93YN9
A	454	LYS	-	expression tag	UNP Q93YN9
A	455	ASP	-	expression tag	UNP Q93YN9
A	456	ASP	-	expression tag	UNP Q93YN9
A	457	ASP	-	expression tag	UNP Q93YN9
A	458	ASP	-	expression tag	UNP Q93YN9
A	459	LYS	-	expression tag	UNP Q93YN9
B	-33	MET	-	expression tag	UNP Q93YN9
B	-32	GLY	-	expression tag	UNP Q93YN9
B	-31	SER	-	expression tag	UNP Q93YN9
B	-30	SER	-	expression tag	UNP Q93YN9
B	-29	HIS	-	expression tag	UNP Q93YN9
B	-28	HIS	-	expression tag	UNP Q93YN9
B	-27	HIS	-	expression tag	UNP Q93YN9
B	-26	HIS	-	expression tag	UNP Q93YN9
B	-25	HIS	-	expression tag	UNP Q93YN9
B	-24	HIS	-	expression tag	UNP Q93YN9
B	-23	SER	-	expression tag	UNP Q93YN9
B	-22	SER	-	expression tag	UNP Q93YN9
B	-21	GLY	-	expression tag	UNP Q93YN9
B	-20	LEU	-	expression tag	UNP Q93YN9
B	-19	VAL	-	expression tag	UNP Q93YN9
B	-18	PRO	-	expression tag	UNP Q93YN9

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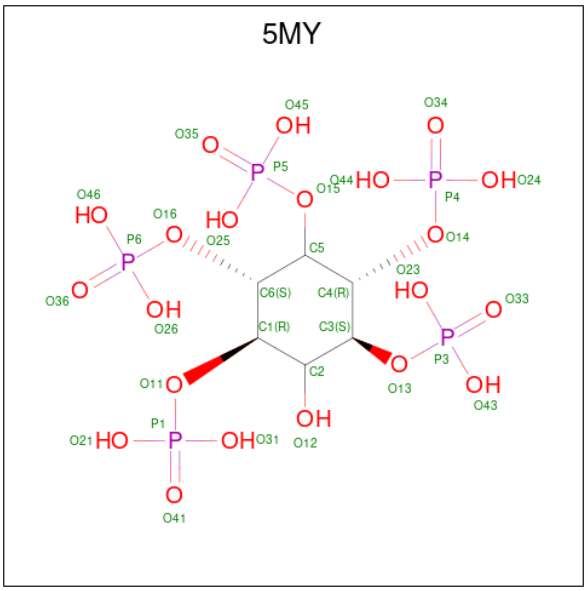
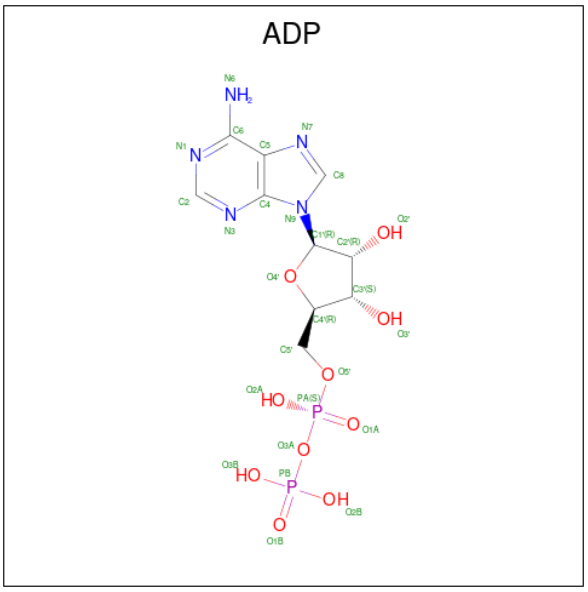
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	ARG	-	expression tag	UNP Q93YN9
B	-16	GLY	-	expression tag	UNP Q93YN9
B	-15	SER	-	expression tag	UNP Q93YN9
B	-14	HIS	-	expression tag	UNP Q93YN9
B	-13	MET	-	expression tag	UNP Q93YN9
B	-12	ALA	-	expression tag	UNP Q93YN9
B	-11	SER	-	expression tag	UNP Q93YN9
B	-10	MET	-	expression tag	UNP Q93YN9
B	-9	THR	-	expression tag	UNP Q93YN9
B	-8	GLY	-	expression tag	UNP Q93YN9
B	-7	GLY	-	expression tag	UNP Q93YN9
B	-6	GLN	-	expression tag	UNP Q93YN9
B	-5	GLN	-	expression tag	UNP Q93YN9
B	-4	MET	-	expression tag	UNP Q93YN9
B	-3	GLY	-	expression tag	UNP Q93YN9
B	-2	ARG	-	expression tag	UNP Q93YN9
B	-1	ILE	-	expression tag	UNP Q93YN9
B	0	LEU	-	expression tag	UNP Q93YN9
B	54	SER	ALA	conflict	UNP Q93YN9
B	90	GLN	LYS	conflict	UNP Q93YN9
B	157	THR	SER	conflict	UNP Q93YN9
B	185	ILE	MET	conflict	UNP Q93YN9
B	204	ILE	ASN	conflict	UNP Q93YN9
B	224	ARG	SER	conflict	UNP Q93YN9
B	321	CYS	SER	conflict	UNP Q93YN9
B	325	ILE	LEU	conflict	UNP Q93YN9
B	337	ARG	LYS	conflict	UNP Q93YN9
B	452	ASP	-	expression tag	UNP Q93YN9
B	453	TYR	-	expression tag	UNP Q93YN9
B	454	LYS	-	expression tag	UNP Q93YN9
B	455	ASP	-	expression tag	UNP Q93YN9
B	456	ASP	-	expression tag	UNP Q93YN9
B	457	ASP	-	expression tag	UNP Q93YN9
B	458	ASP	-	expression tag	UNP Q93YN9
B	459	LYS	-	expression tag	UNP Q93YN9

- Molecule 2 is MYO-INOSITOL-(1,3,4,5,6)-PENTAKISPHOSPHATE (three-letter code: 5MY) (formula: $C_6H_{17}O_{21}P_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 32	C 6	O 21	P 5	0	0
2	B	1	Total 32	C 6	O 21	P 5	0	0

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



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

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

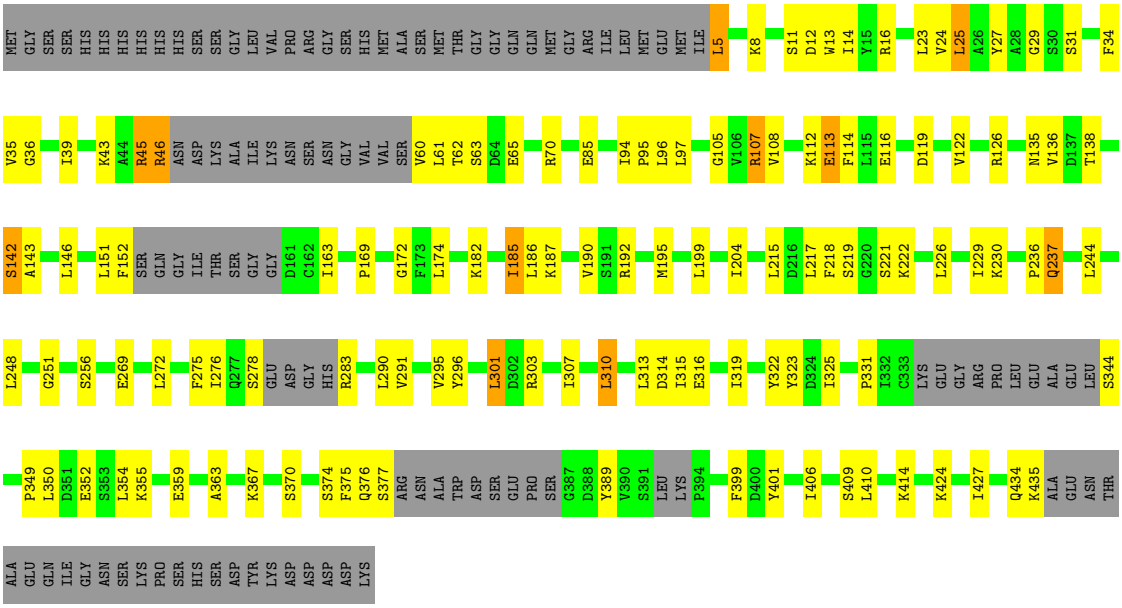
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

3 Residue-property plots (i)

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. 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. 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.

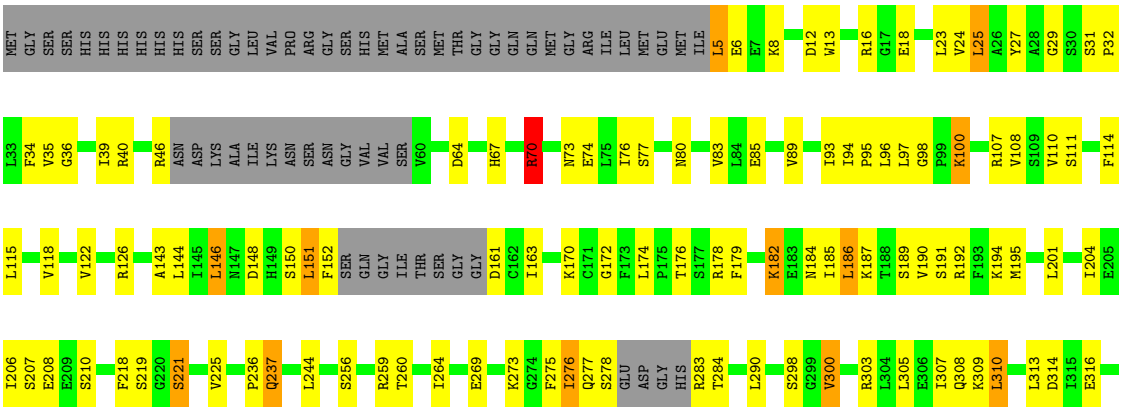
- Molecule 1: Inositol-pentakisphosphate 2-kinase

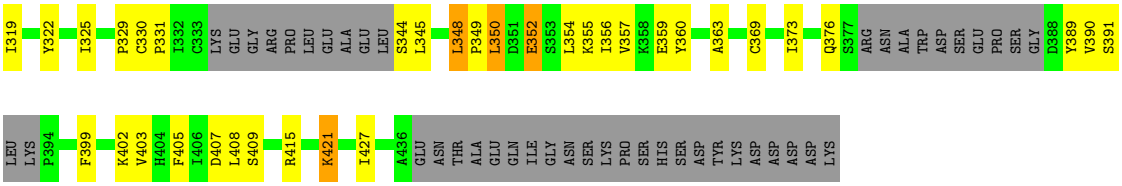
Chain A: 53% 23% • 22%



- Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain B: 49% 26% • 22%




I319 Y322 I325 P329 C330 P331 I332 C333 LYS GLU GLY ARG PRO LEU GLU ALA GLU LEU S344 L345 L348 P349 L350 D351 E352 S353 L354 K355 I356 V357 K358 E359 Y360 A363 C369 I373 Q376 S377 ARG ASN ALA TRP ASP SER GLU PRO SER GLY D388 Y389 V390 S391
LEU LYS P394 F399 K402 V403 H404 F405 I406 D407 L408 S409 R415 K421 I427 A436 GLU ASN THR ALA GLU GLN ILE GLY ASN SER LYS PRO SER HIS SER ASP TYR LYS ASP ASP ASP ASP LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.36Å 59.91Å 83.15Å 90.02° 97.04° 116.81°	Depositor
Resolution (Å)	44.63 – 3.10 44.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (44.63-3.10) 85.9 (44.63-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.6.3_473	Depositor
R, R_{free}	0.210 , 0.276 0.210 , 0.279	Depositor DCC
R_{free} test set	1642 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 3.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6267	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MY, ADP, MG, ZN

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	0.47	0/3126	0.62	0/4210
1	B	0.46	0/3127	0.61	0/4212
All	All	0.46	0/6253	0.61	0/8422

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3072	0	3098	105	1
1	B	3073	0	3100	122	1
2	A	32	0	7	0	0
2	B	32	0	7	1	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	6267	0	6236	218	1

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 17.

All (218) 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:46:ARG:HB2	1:B:185:ILE:HG12	1.30	1.08
1:B:100:LYS:H	1:B:100:LYS:HD3	1.31	0.95
1:A:46:ARG:HB2	1:B:185:ILE:CG1	2.00	0.91
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.35	0.88
1:A:307:ILE:O	1:A:310:LEU:HB2	1.78	0.84
1:A:355:LYS:O	1:A:359:GLU:HG3	1.80	0.81
1:A:45:ARG:HH11	1:A:45:ARG:CG	1.95	0.79
1:A:31:SER:O	1:A:35:VAL:HG23	1.85	0.77
1:A:204:ILE:HG22	1:A:204:ILE:O	1.85	0.74
1:A:172:GLY:HA3	1:A:218:PHE:CD2	2.21	0.74
1:A:45:ARG:HG2	1:A:45:ARG:NH1	2.04	0.72
1:A:36:GLY:HA2	1:A:151:LEU:HD13	1.72	0.71
1:A:269:GLU:OE2	1:A:283:ARG:HB2	1.91	0.71
1:A:60:VAL:HG13	1:A:61:LEU:H	1.56	0.70
1:B:269:GLU:OE2	1:B:283:ARG:HB2	1.91	0.70
1:B:276:ILE:HD11	1:B:283:ARG:HA	1.72	0.69
1:B:25:LEU:HB2	1:B:39:ILE:HG22	1.74	0.68
1:B:307:ILE:O	1:B:310:LEU:HB2	1.93	0.68
1:A:107:ARG:HD2	1:A:142:SER:OG	1.95	0.67
1:B:276:ILE:HG12	1:B:283:ARG:HG2	1.76	0.67
1:B:204:ILE:O	1:B:204:ILE:HG22	1.95	0.66
1:B:201:LEU:HD12	1:B:206:ILE:HG13	1.78	0.65
1:B:27:TYR:CZ	1:B:29:GLY:HA3	2.32	0.65
1:B:100:LYS:H	1:B:100:LYS:CD	2.08	0.65
1:A:46:ARG:HD3	1:B:185:ILE:HG12	1.78	0.64
1:B:80:ASN:OD1	1:B:83:VAL:HG23	1.99	0.63
1:B:5:LEU:HD23	1:B:114:PHE:CZ	2.34	0.63
1:B:110:VAL:HG21	1:B:115:LEU:HD21	1.81	0.62
1:A:46:ARG:HH12	1:B:182:LYS:CB	2.12	0.62
1:B:276:ILE:CG1	1:B:283:ARG:HG2	2.30	0.61
1:A:27:TYR:CZ	1:A:29:GLY:HA3	2.36	0.61
1:A:62:THR:OG1	1:A:65:GLU:HG3	2.01	0.61
1:B:152:PHE:CD1	1:B:376:GLN:HG2	2.36	0.60
1:B:100:LYS:HE2	1:B:303:ARG:NH1	2.17	0.60
1:B:13:TRP:CZ3	1:B:27:TYR:HB2	2.36	0.59
1:B:277:GLN:O	1:B:278:SER:HB2	2.03	0.59
1:A:23:LEU:HD21	1:A:122:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:HD1	1:A:276:ILE:HD12	1.67	0.59
1:B:76:ILE:HD12	1:B:77:SER:N	2.17	0.59
1:B:93:ILE:HG21	1:B:408:LEU:HD13	1.83	0.59
1:B:6:GLU:O	1:B:114:PHE:HD1	1.86	0.58
1:B:118:VAL:O	1:B:122:VAL:HG13	2.03	0.58
1:A:94:ILE:HB	1:A:95:PRO:HD3	1.84	0.58
1:B:313:LEU:O	1:B:314:ASP:HB3	2.02	0.58
1:A:185:ILE:HG13	1:A:185:ILE:O	2.03	0.58
1:A:313:LEU:O	1:A:314:ASP:HB3	2.04	0.58
1:A:85:GLU:OE1	1:A:409:SER:HA	2.04	0.57
1:B:355:LYS:O	1:B:359:GLU:HG3	2.04	0.57
1:B:36:GLY:HA2	1:B:151:LEU:HD23	1.86	0.57
1:B:40:ARG:NH1	3:B:912:ADP:O2A	2.37	0.57
1:A:46:ARG:CD	1:B:185:ILE:HG12	2.33	0.57
1:A:25:LEU:HB2	1:A:39:ILE:HG22	1.87	0.57
1:B:144:LEU:HD23	1:B:146:LEU:HD21	1.87	0.57
1:A:27:TYR:OH	1:A:31:SER:HB3	2.05	0.57
1:B:97:LEU:O	1:B:303:ARG:NH1	2.38	0.56
1:B:190:VAL:HB	1:B:195:MET:HE3	1.87	0.56
1:A:46:ARG:HH12	1:B:182:LYS:HB2	1.69	0.56
1:B:67:HIS:O	1:B:70:ARG:HB2	2.05	0.56
1:A:376:GLN:O	1:A:376:GLN:HG3	2.05	0.56
1:A:186:LEU:O	1:A:195:MET:CE	2.54	0.55
1:A:222:LYS:NZ	1:A:222:LYS:HB3	2.20	0.55
1:A:46:ARG:CB	1:B:185:ILE:HG12	2.20	0.55
1:A:122:VAL:HG23	1:A:126:ARG:HD3	1.88	0.55
1:B:67:HIS:HA	1:B:70:ARG:HH11	1.72	0.55
1:B:186:LEU:HB3	1:B:195:MET:HE1	1.89	0.55
1:B:83:VAL:HG22	1:B:107:ARG:HD2	1.89	0.54
1:A:119:ASP:HB2	1:A:136:VAL:HG21	1.89	0.54
1:A:187:LYS:HG3	1:A:427:ILE:HD13	1.90	0.54
1:B:179:PHE:CE2	1:B:345:LEU:HG	2.43	0.53
1:B:190:VAL:HB	1:B:195:MET:CE	2.39	0.53
1:A:349:PRO:HG2	1:A:352:GLU:HB2	1.91	0.53
1:A:434:GLN:O	1:A:435:LYS:HB3	2.09	0.53
1:A:190:VAL:HB	1:A:195:MET:CE	2.39	0.53
1:A:222:LYS:HB2	1:A:296:TYR:CE2	2.44	0.53
1:A:248:LEU:HD21	1:A:251:GLY:O	2.09	0.53
1:A:60:VAL:HG13	1:A:61:LEU:N	2.22	0.52
1:B:208:GLU:OE2	1:B:259:ARG:NE	2.34	0.52
1:B:67:HIS:HA	1:B:70:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLN:O	1:A:435:LYS:CB	2.58	0.52
1:B:97:LEU:HG	1:B:307:ILE:CD1	2.39	0.52
1:B:31:SER:O	1:B:35:VAL:HG23	2.09	0.52
1:A:204:ILE:O	1:A:204:ILE:CG2	2.58	0.52
1:B:186:LEU:O	1:B:189:SER:N	2.34	0.52
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.65	0.51
1:B:325:ILE:HD12	1:B:357:VAL:HG21	1.91	0.51
1:A:434:GLN:O	1:A:435:LYS:CE	2.58	0.51
1:B:259:ARG:CG	1:B:260:THR:N	2.73	0.51
1:B:275:PHE:CD2	1:B:276:ILE:HG22	2.45	0.51
1:A:97:LEU:O	1:A:303:ARG:NH1	2.44	0.51
1:B:25:LEU:HD11	1:B:122:VAL:HG11	1.94	0.50
1:B:97:LEU:HG	1:B:307:ILE:HD11	1.91	0.50
1:A:363:ALA:O	1:A:367:LYS:HG3	2.12	0.50
1:A:370:SER:HB2	1:A:406:ILE:HG13	1.94	0.50
1:A:119:ASP:HB2	1:A:136:VAL:CG2	2.42	0.50
1:A:169:PRO:HB2	1:A:218:PHE:CZ	2.46	0.50
1:B:360:TYR:O	1:B:363:ALA:HB3	2.12	0.50
1:A:204:ILE:N	1:A:204:ILE:HD12	2.27	0.50
1:B:40:ARG:HH12	1:B:407:ASP:HA	1.77	0.50
1:A:16:ARG:HB3	1:A:24:VAL:O	2.10	0.49
1:B:325:ILE:HD11	1:B:354:LEU:HA	1.93	0.49
1:A:12:ASP:HB3	1:A:27:TYR:CE1	2.47	0.49
1:A:204:ILE:HD11	1:B:356:ILE:HD11	1.93	0.49
1:B:172:GLY:HA3	1:B:218:PHE:CD2	2.47	0.49
1:B:100:LYS:HE2	1:B:303:ARG:HH12	1.77	0.49
1:B:221:SER:O	1:B:225:VAL:HG23	2.13	0.49
1:B:276:ILE:HD11	1:B:283:ARG:CA	2.42	0.49
1:A:108:VAL:HG12	1:A:143:ALA:O	2.13	0.48
1:B:300:VAL:HG21	1:B:403:VAL:HG11	1.95	0.48
1:B:319:ILE:O	1:B:322:TYR:HB3	2.13	0.48
1:B:390:VAL:HG12	1:B:391:SER:N	2.28	0.48
1:A:272:LEU:HB3	1:A:283:ARG:HD2	1.95	0.48
1:B:94:ILE:C	1:B:96:LEU:H	2.16	0.48
1:A:105:GLY:HA3	1:A:146:LEU:HD23	1.95	0.48
1:A:295:VAL:HG12	1:A:296:TYR:N	2.29	0.48
1:B:108:VAL:HG12	1:B:143:ALA:O	2.13	0.47
1:A:70:ARG:NH1	1:A:70:ARG:HG2	2.29	0.47
1:B:18:GLU:OE2	1:B:126:ARG:NH1	2.47	0.47
1:B:163:ILE:HD11	1:B:244:LEU:HD13	1.96	0.47
1:B:260:THR:HG23	1:B:264:ILE:CG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:VAL:HB	1:A:195:MET:HE2	1.97	0.47
1:A:12:ASP:HB3	1:A:27:TYR:HE1	1.79	0.47
1:B:187:LYS:NZ	1:B:316:GLU:HG3	2.30	0.47
1:A:25:LEU:HB2	1:A:39:ILE:CG2	2.45	0.47
1:B:182:LYS:HB3	1:B:182:LYS:HE2	1.62	0.47
1:B:275:PHE:HD2	1:B:276:ILE:HG22	1.80	0.47
1:A:107:ARG:CD	1:A:142:SER:OG	2.62	0.46
1:A:185:ILE:HG23	1:A:186:LEU:HD22	1.96	0.46
1:B:345:LEU:O	1:B:348:LEU:HB2	2.15	0.46
1:B:25:LEU:HB2	1:B:39:ILE:CG2	2.43	0.46
1:B:219:SER:C	1:B:221:SER:H	2.19	0.46
1:B:348:LEU:HA	1:B:349:PRO:HD2	1.78	0.46
1:A:323:TYR:CD2	1:A:331:PRO:HD2	2.51	0.46
1:A:374:SER:O	1:A:401:TYR:HA	2.16	0.46
1:B:76:ILE:HD12	1:B:76:ILE:C	2.36	0.46
1:B:303:ARG:NH2	1:B:405:PHE:HE1	2.14	0.46
1:B:300:VAL:HG22	1:B:405:PHE:CZ	2.51	0.45
1:A:275:PHE:HD1	1:A:276:ILE:CD1	2.27	0.45
1:B:85:GLU:O	1:B:89:VAL:HG23	2.16	0.45
1:A:163:ILE:O	1:A:375:PHE:HB2	2.17	0.45
1:A:187:LYS:NZ	1:A:316:GLU:HG3	2.32	0.45
1:A:315:ILE:HG23	1:A:316:GLU:N	2.31	0.45
1:A:27:TYR:CE2	1:A:34:PHE:HB2	2.51	0.45
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.60	0.45
1:A:435:LYS:HB3	1:A:435:LYS:HE2	1.56	0.45
1:B:260:THR:HG23	1:B:264:ILE:HB	1.99	0.45
1:A:70:ARG:HG2	1:A:70:ARG:HH11	1.81	0.45
1:A:136:VAL:HG23	1:A:138:THR:HG23	1.99	0.45
1:B:31:SER:HA	1:B:32:PRO:HD2	1.82	0.45
1:A:186:LEU:C	1:A:195:MET:HE1	2.37	0.45
1:B:114:PHE:O	1:B:118:VAL:HG23	2.17	0.45
1:B:415:ARG:NH1	2:B:911:5MY:O33	2.43	0.44
1:B:6:GLU:HA	1:B:111:SER:OG	2.17	0.44
1:B:126:ARG:HH11	1:B:126:ARG:HG2	1.82	0.44
1:B:64:ASP:O	1:B:67:HIS:HB3	2.18	0.44
1:B:308:GLN:C	1:B:310:LEU:H	2.20	0.44
1:B:27:TYR:CE2	1:B:34:PHE:HB2	2.52	0.44
1:B:210:SER:HB2	1:B:237:GLN:NE2	2.33	0.44
1:B:298:SER:OG	1:B:300:VAL:HB	2.18	0.44
1:A:217:LEU:HG	1:A:301:LEU:HD21	1.99	0.44
1:B:352:GLU:OE1	1:B:352:GLU:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:CD1	1:A:276:ILE:HD12	2.51	0.44
1:A:290:LEU:HD12	1:A:290:LEU:O	2.17	0.44
1:A:310:LEU:HG	1:A:359:GLU:HB3	1.98	0.44
1:B:186:LEU:HD12	1:B:186:LEU:HA	1.78	0.43
1:B:73:ASN:O	1:B:74:GLU:C	2.57	0.43
1:A:215:LEU:O	1:A:219:SER:HB3	2.18	0.43
1:A:236:PRO:O	1:A:237:GLN:C	2.56	0.43
1:B:73:ASN:OD1	1:B:76:ILE:HD11	2.19	0.43
1:B:25:LEU:HD22	1:B:25:LEU:N	2.34	0.43
1:A:112:LYS:O	1:A:116:GLU:HG3	2.18	0.43
1:B:310:LEU:HG	1:B:359:GLU:HB3	2.01	0.43
1:A:204:ILE:HD13	1:B:313:LEU:HD21	2.01	0.43
1:A:434:GLN:O	1:A:435:LYS:HE2	2.19	0.43
1:B:373:ILE:HA	1:B:402:LYS:O	2.19	0.43
1:A:199:LEU:HD12	1:A:199:LEU:HA	1.73	0.42
1:B:89:VAL:O	1:B:94:ILE:HG13	2.19	0.42
1:A:27:TYR:OH	1:A:31:SER:CB	2.67	0.42
1:B:184:ASN:HB3	1:B:427:ILE:HG12	2.00	0.42
1:B:236:PRO:O	1:B:237:GLN:C	2.57	0.42
1:B:16:ARG:HB3	1:B:24:VAL:O	2.19	0.42
1:B:152:PHE:CE1	1:B:376:GLN:HG2	2.54	0.42
1:B:305:LEU:HG	1:B:309:LYS:HD2	2.01	0.42
1:B:329:PRO:O	1:B:331:PRO:HD3	2.20	0.42
1:B:421:LYS:HE3	1:B:421:LYS:HB2	1.30	0.42
1:A:16:ARG:O	1:A:16:ARG:HD3	2.19	0.42
1:A:319:ILE:O	1:A:322:TYR:HB3	2.19	0.42
1:B:122:VAL:HG23	1:B:126:ARG:HD3	2.02	0.42
1:A:113:GLU:CD	1:A:113:GLU:H	2.23	0.42
1:B:85:GLU:OE1	1:B:409:SER:HA	2.19	0.42
1:B:259:ARG:HG2	1:B:260:THR:N	2.35	0.42
1:B:273:LYS:HA	1:B:283:ARG:NH1	2.35	0.42
1:A:5:LEU:HD23	1:A:114:PHE:CZ	2.55	0.42
1:A:152:PHE:CE1	1:A:376:GLN:HG2	2.55	0.41
1:A:8:LYS:HA	1:A:8:LYS:HD3	1.87	0.41
1:A:136:VAL:HG23	1:A:138:THR:CG2	2.50	0.41
1:A:313:LEU:O	1:A:314:ASP:CB	2.68	0.41
1:A:43:LYS:HG2	1:A:135:ASN:O	2.20	0.41
1:B:98:GLY:HA3	1:B:100:LYS:NZ	2.36	0.41
1:B:201:LEU:CD1	1:B:206:ILE:HG13	2.49	0.41
1:B:170:LYS:HA	1:B:170:LYS:HD2	1.96	0.41
1:A:229:ILE:HD12	1:A:291:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:TRP:CZ3	1:A:27:TYR:HB2	2.56	0.41
1:B:350:LEU:HD23	1:B:350:LEU:HA	1.87	0.41
1:A:27:TYR:CD2	1:A:34:PHE:HB2	2.56	0.41
1:A:190:VAL:HB	1:A:195:MET:HE3	2.02	0.41
1:A:226:LEU:HG	1:A:230:LYS:HE3	2.03	0.41
1:B:36:GLY:HA2	1:B:151:LEU:CD2	2.50	0.41
1:B:148:ASP:OD1	1:B:150:SER:OG	2.33	0.41
1:B:290:LEU:HD12	1:B:290:LEU:O	2.20	0.41
1:B:369:CYS:CB	1:B:408:LEU:HD23	2.51	0.40
1:A:107:ARG:NH1	1:A:142:SER:OG	2.41	0.40
1:B:389:TYR:HA	1:B:399:PHE:O	2.22	0.40
1:A:325:ILE:HD12	1:A:354:LEU:CD2	2.51	0.40
1:A:269:GLU:O	1:A:272:LEU:HB2	2.22	0.40
1:B:24:VAL:HG22	1:B:40:ARG:HG3	2.04	0.40
1:B:204:ILE:O	1:B:204:ILE:CG2	2.65	0.40
1:B:330:CYS:HA	1:B:331:PRO:HD2	1.91	0.40
1:A:389:TYR:HA	1:A:399:PHE:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:CD1	1:B:46:ARG:CB[1_565]	1.44	0.76

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	371/493 (75%)	349 (94%)	21 (6%)	1 (0%)	41 73
1	B	371/493 (75%)	352 (95%)	16 (4%)	3 (1%)	19 54
All	All	742/986 (75%)	701 (94%)	37 (5%)	4 (0%)	29 64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	B	237	GLN
1	B	70	ARG
1	B	95	PRO

5.3.2 Protein sidechains (i)

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	345/434 (80%)	318 (92%)	27 (8%)	12	40
1	B	345/434 (80%)	315 (91%)	30 (9%)	10	36
All	All	690/868 (80%)	633 (92%)	57 (8%)	11	38

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	11	SER
1	A	14	ILE
1	A	25	LEU
1	A	45	ARG
1	A	46	ARG
1	A	63	SER
1	A	96	LEU
1	A	107	ARG
1	A	113	GLU
1	A	142	SER
1	A	174	LEU
1	A	182	LYS
1	A	185	ILE
1	A	192	ARG
1	A	221	SER
1	A	244	LEU
1	A	256	SER
1	A	278	SER

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Mol	Chain	Res	Type
1	A	301	LEU
1	A	310	LEU
1	A	344	SER
1	A	350	LEU
1	A	377	SER
1	A	410	LEU
1	A	414	LYS
1	A	424	LYS
1	B	5	LEU
1	B	8	LYS
1	B	12	ASP
1	B	23	LEU
1	B	25	LEU
1	B	70	ARG
1	B	100	LYS
1	B	146	LEU
1	B	151	LEU
1	B	161	ASP
1	B	174	LEU
1	B	176	THR
1	B	178	ARG
1	B	182	LYS
1	B	186	LEU
1	B	191	SER
1	B	192	ARG
1	B	194	LYS
1	B	207	SER
1	B	221	SER
1	B	256	SER
1	B	276	ILE
1	B	284	THR
1	B	300	VAL
1	B	310	LEU
1	B	344	SER
1	B	348	LEU
1	B	350	LEU
1	B	352	GLU
1	B	421	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	196	HIS
1	B	72	ASN
1	B	125	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
3	ADP	A	912	4	24,29,29	1.00	2 (8%)	29,45,45	1.31	2 (6%)
3	ADP	B	912	4	24,29,29	1.03	2 (8%)	29,45,45	1.29	2 (6%)
2	5MY	B	911	-	32,32,32	0.90	2 (6%)	48,53,53	0.89	2 (4%)
2	5MY	A	911	-	32,32,32	0.96	0	48,53,53	0.88	2 (4%)

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	912	4	-	2/12/32/32	0/3/3/3
3	ADP	B	912	4	-	3/12/32/32	0/3/3/3
2	5MY	B	911	-	-	3/25/49/49	0/1/1/1
2	5MY	A	911	-	-	5/25/49/49	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	912	ADP	C5-C4	2.59	1.47	1.40
3	B	912	ADP	C5-C4	2.56	1.47	1.40
3	A	912	ADP	O4'-C1'	2.27	1.44	1.41
3	B	912	ADP	O4'-C1'	2.25	1.44	1.41
2	B	911	5MY	P1-O41	2.24	1.57	1.50
2	B	911	5MY	P6-O36	2.02	1.57	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	912	ADP	N3-C2-N1	-3.22	123.64	128.68
3	B	912	ADP	N3-C2-N1	-3.04	123.93	128.68
2	A	911	5MY	C2-C1-C6	2.39	117.11	111.66
3	B	912	ADP	PA-O3A-PB	-2.19	125.31	132.83
2	B	911	5MY	C2-C3-C4	2.17	116.62	111.66
2	A	911	5MY	C2-C3-C4	2.07	116.40	111.66
3	A	912	ADP	C1'-N9-C4	-2.06	123.02	126.64
2	B	911	5MY	C2-C1-C6	2.06	116.36	111.66

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	911	5MY	C6-O16-P6-O36
3	A	912	ADP	C5'-O5'-PA-O3A
3	B	912	ADP	C5'-O5'-PA-O3A
2	A	911	5MY	C3-O13-P3-O33
2	A	911	5MY	C4-O14-P4-O24
3	B	912	ADP	C5'-O5'-PA-O1A
3	B	912	ADP	C5'-O5'-PA-O2A
2	B	911	5MY	C4-O14-P4-O34
2	A	911	5MY	C1-O11-P1-O31
2	A	911	5MY	C2-C3-O13-P3

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Mol	Chain	Res	Type	Atoms
2	A	911	5MY	C4-O14-P4-O44
2	B	911	5MY	C4-O14-P4-O24
3	A	912	ADP	C5'-O5'-PA-O1A

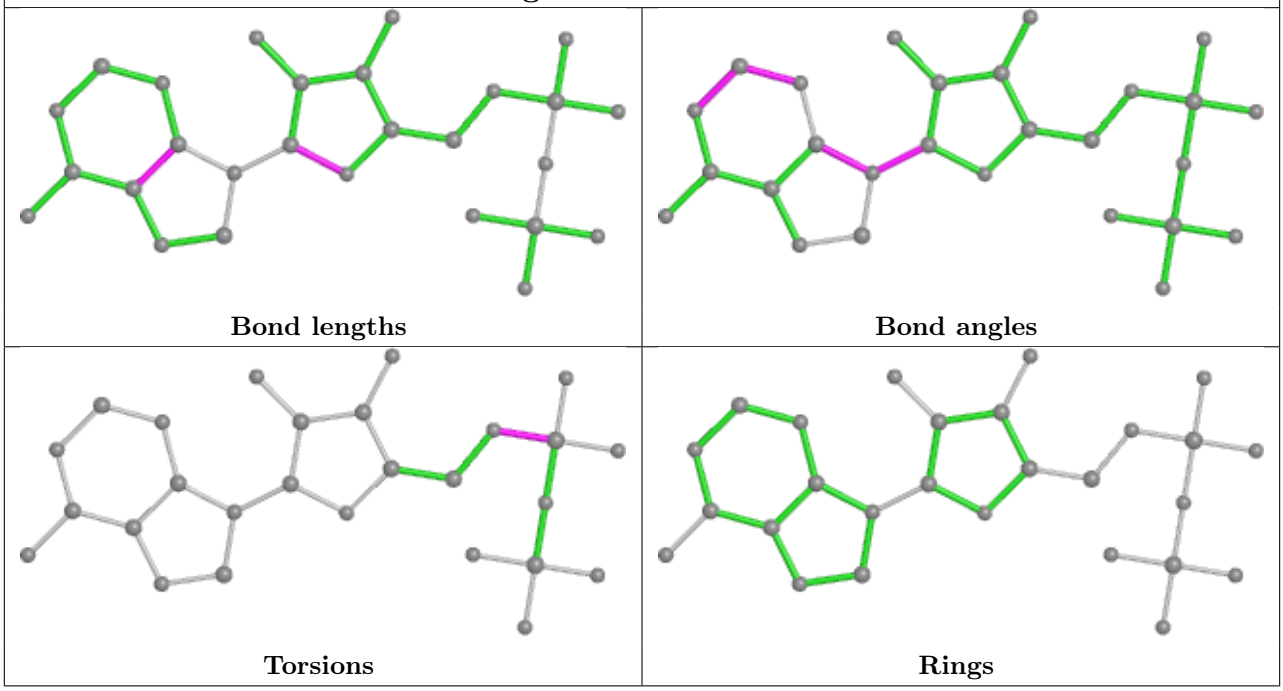
There are no ring outliers.

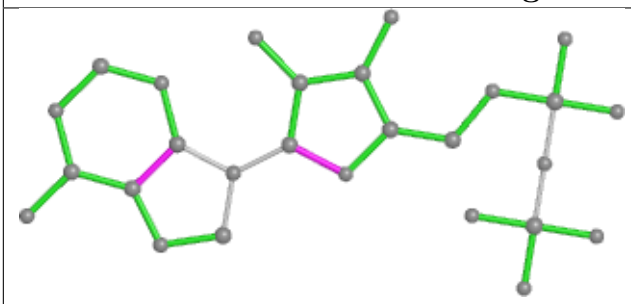
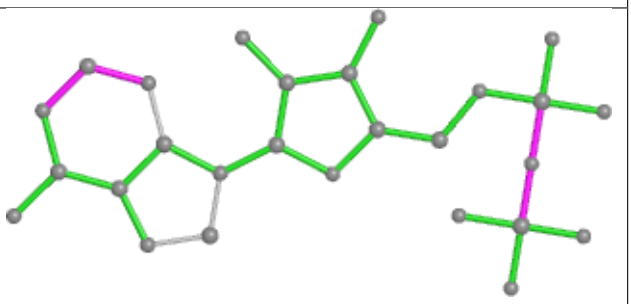
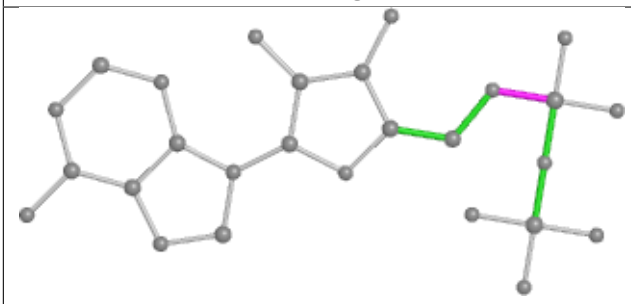
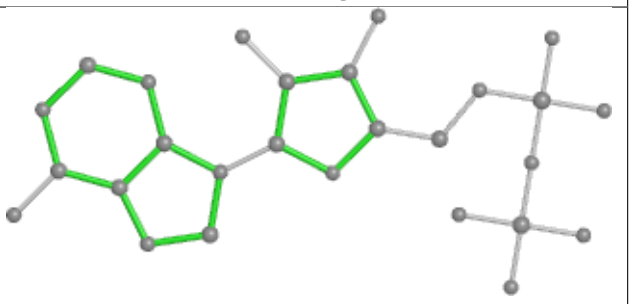
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	912	ADP	1	0
2	B	911	5MY	1	0

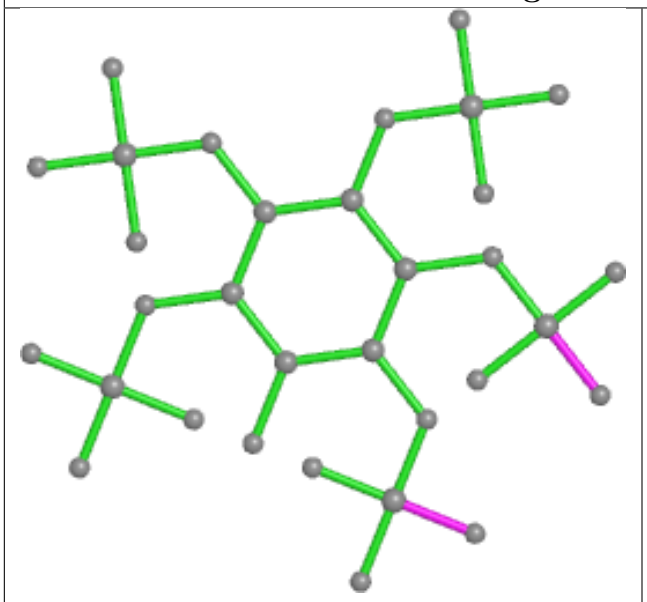
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ADP A 912

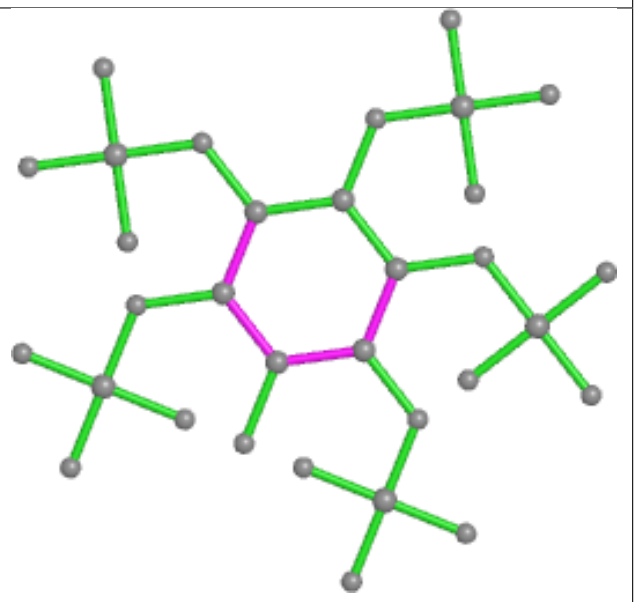


Ligand ADP B 912	
 Bond lengths	 Bond angles
 Torsions	 Rings

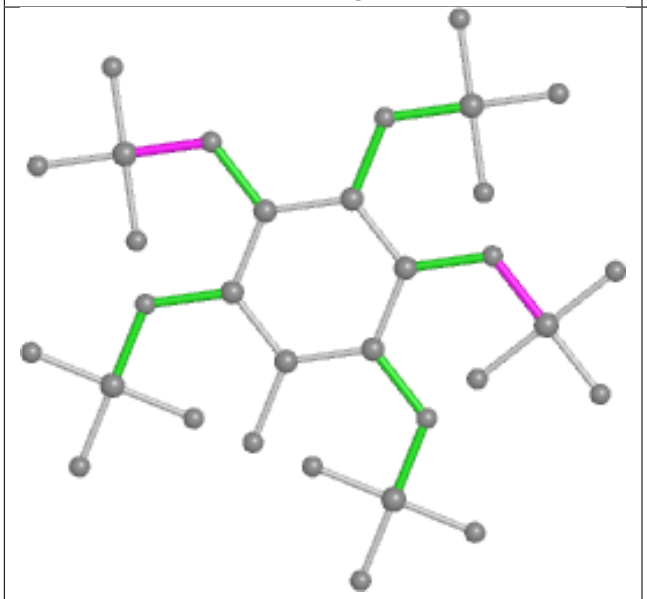
Ligand 5MY B 911



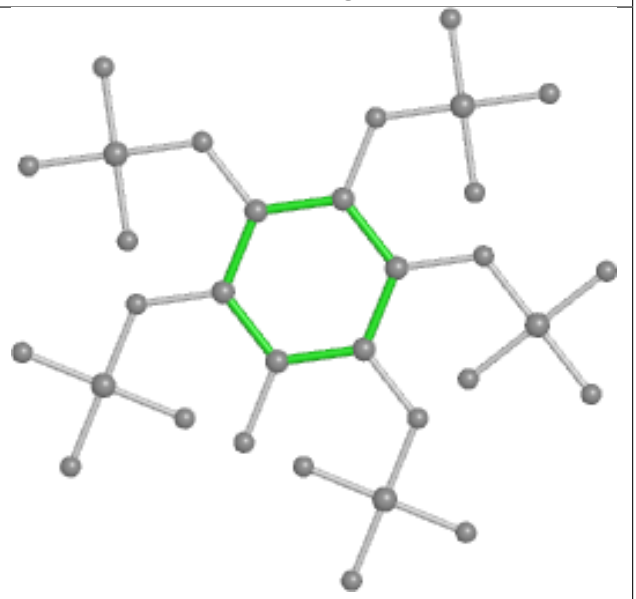
Bond lengths



Bond angles

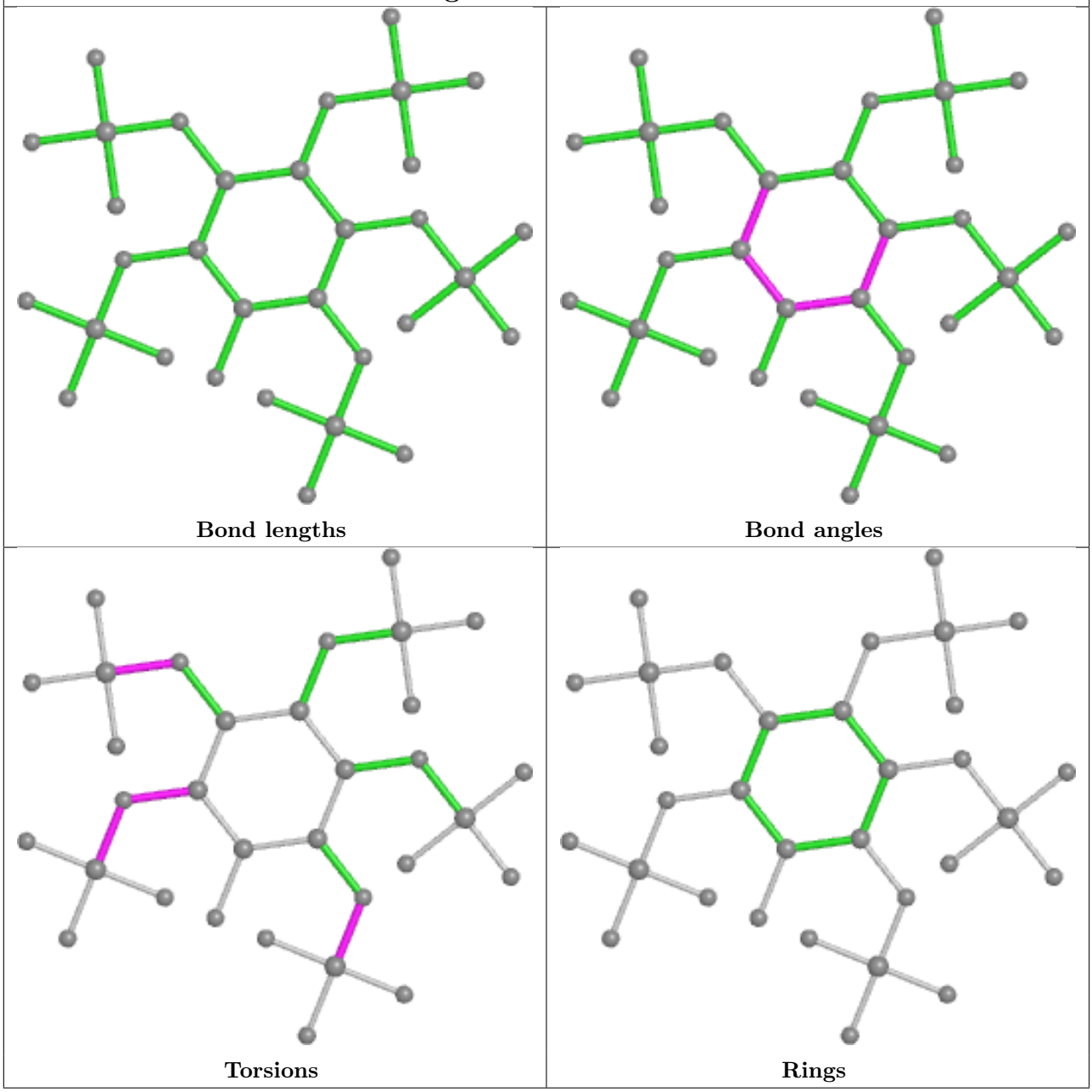


Torsions



Rings

Ligand 5MY A 911



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

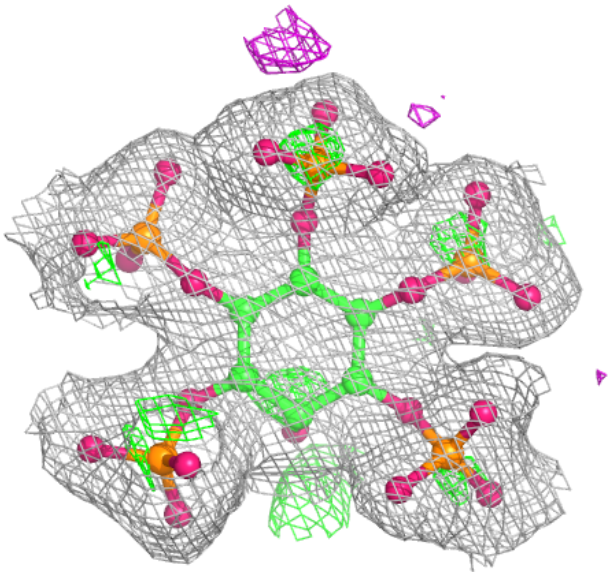
6.4 Ligands (i)

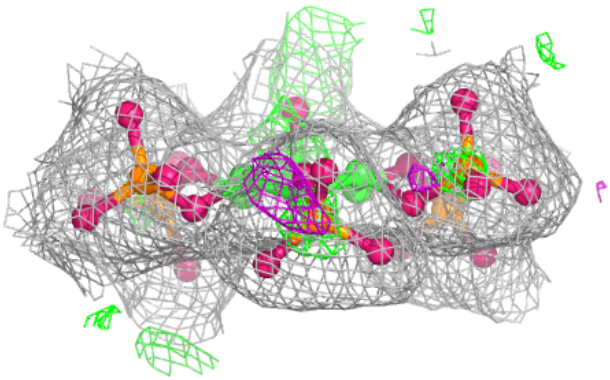
Unable to reproduce the depositors R factor - this section is therefore empty.

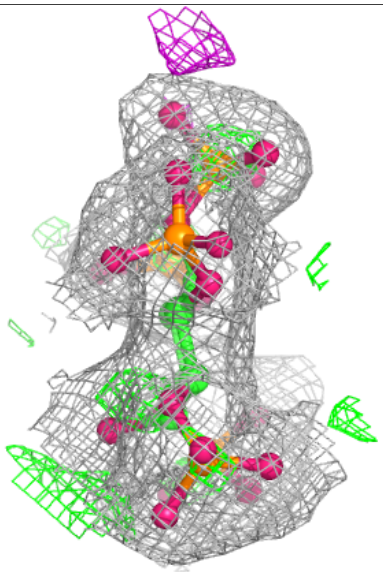
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5MY A 911:

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

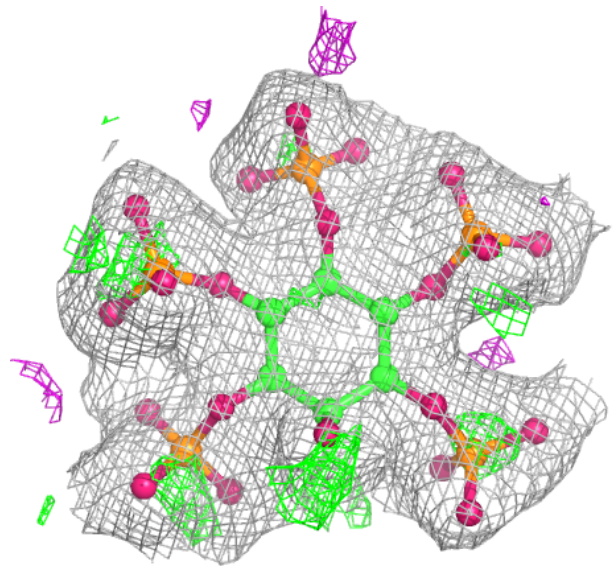


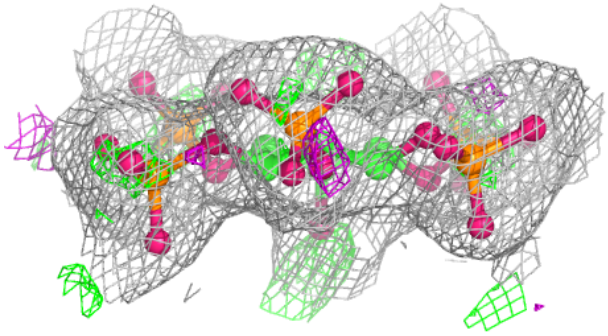


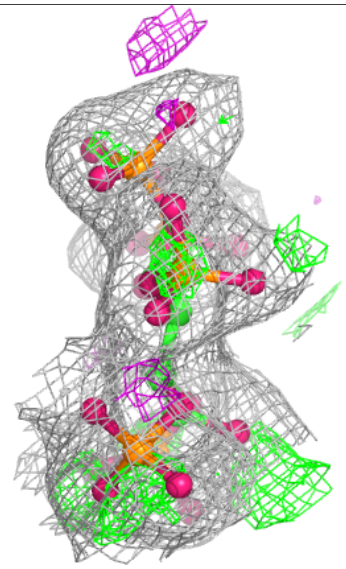


Electron density around 5MY B 911:

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

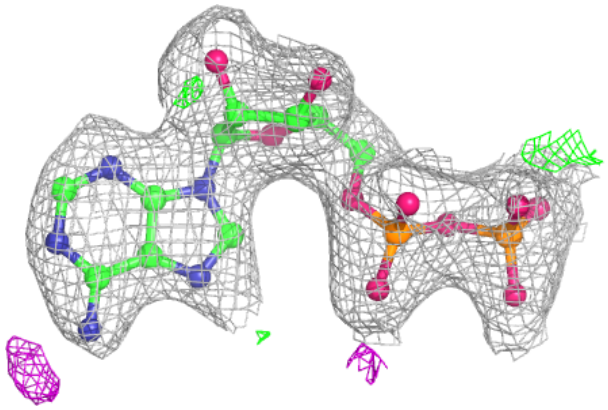


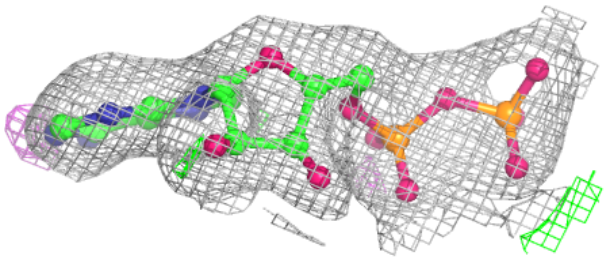


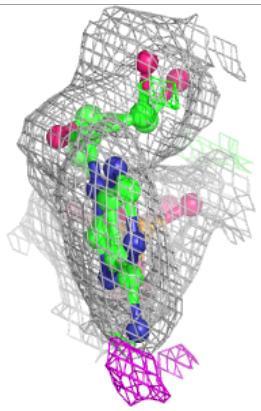


Electron density around ADP A 912:

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

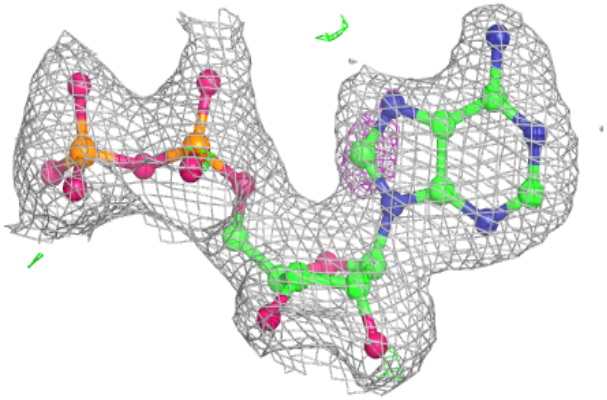


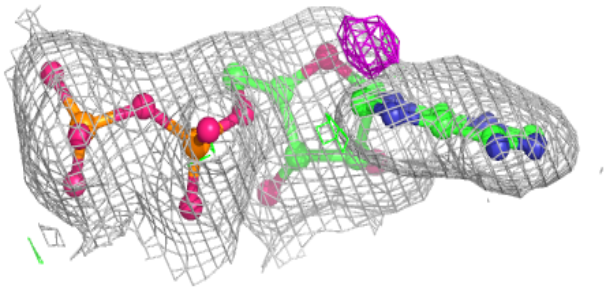


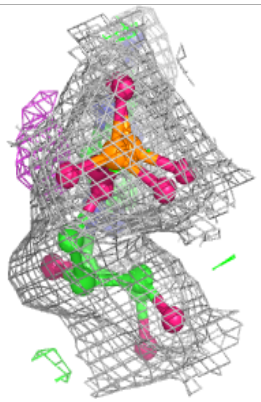


Electron density around ADP B 912:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.