



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:59 PM UTC

PDB ID : 3UDT / pdb_00003udt
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 ⓘ 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

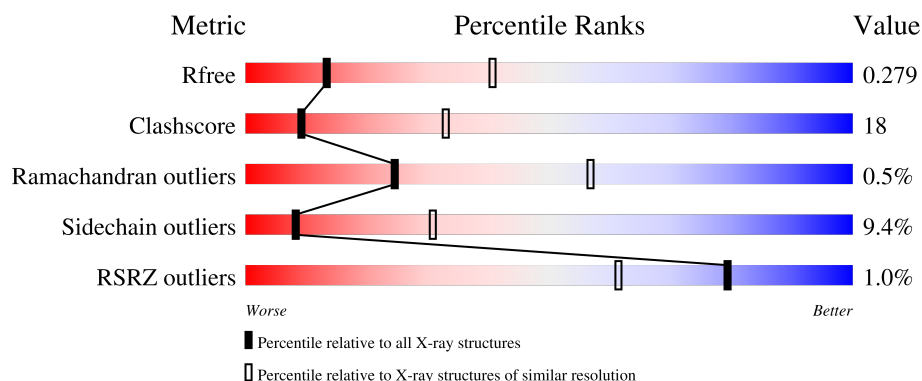
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. 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	493	50% 25% • 22%
1	B	493	47% 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
1	A	385	Total	C	N	O	S	0	0	0
			3072	1963	518	580	11			
1	B	385	Total	C	N	O	S	0	0	0
			3073	1964	518	580	11			

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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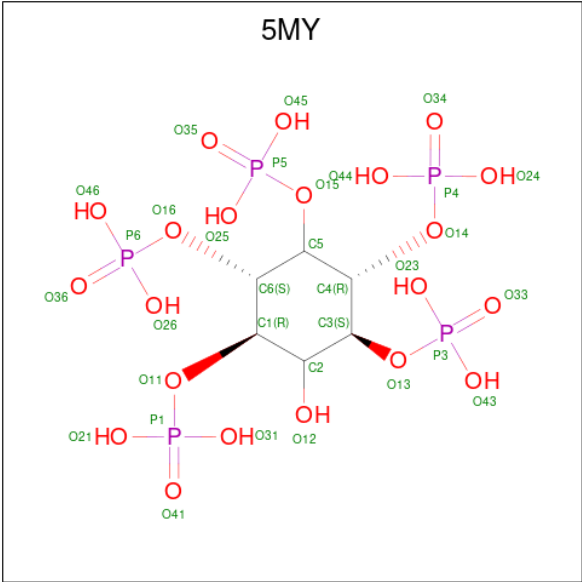
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP Q93YN9
A	-7	GLY	-	expression tag	UNP Q93YN9
A	-6	GLN	-	expression tag	UNP Q93YN9
A	-5	GLN	-	expression tag	UNP Q93YN9
A	-4	MET	-	expression tag	UNP Q93YN9
A	-3	GLY	-	expression tag	UNP Q93YN9
A	-2	ARG	-	expression tag	UNP Q93YN9
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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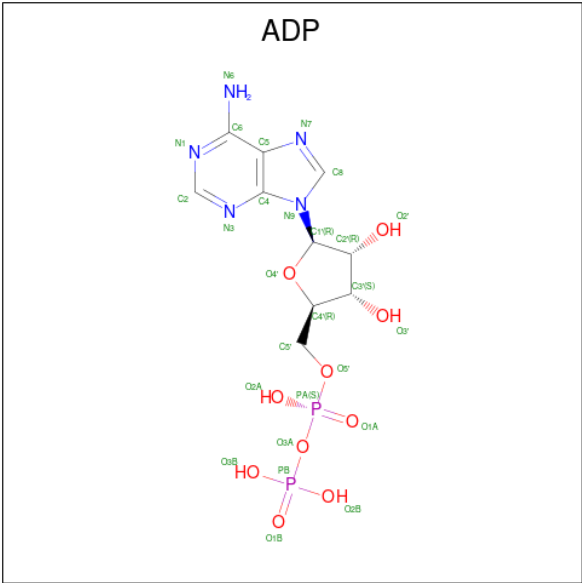
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	ARG	-	expression tag	UNP Q93YN9
B	-16	GLY	-	expression tag	UNP Q93YN9
B	-15	SER	-	expression tag	UNP Q93YN9
B	-14	HIS	-	expression tag	UNP Q93YN9
B	-13	MET	-	expression tag	UNP Q93YN9
B	-12	ALA	-	expression tag	UNP Q93YN9
B	-11	SER	-	expression tag	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 (CCD ID: 5MY) (formula: C₆H₁₇O₂₁P₅).



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

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

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

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

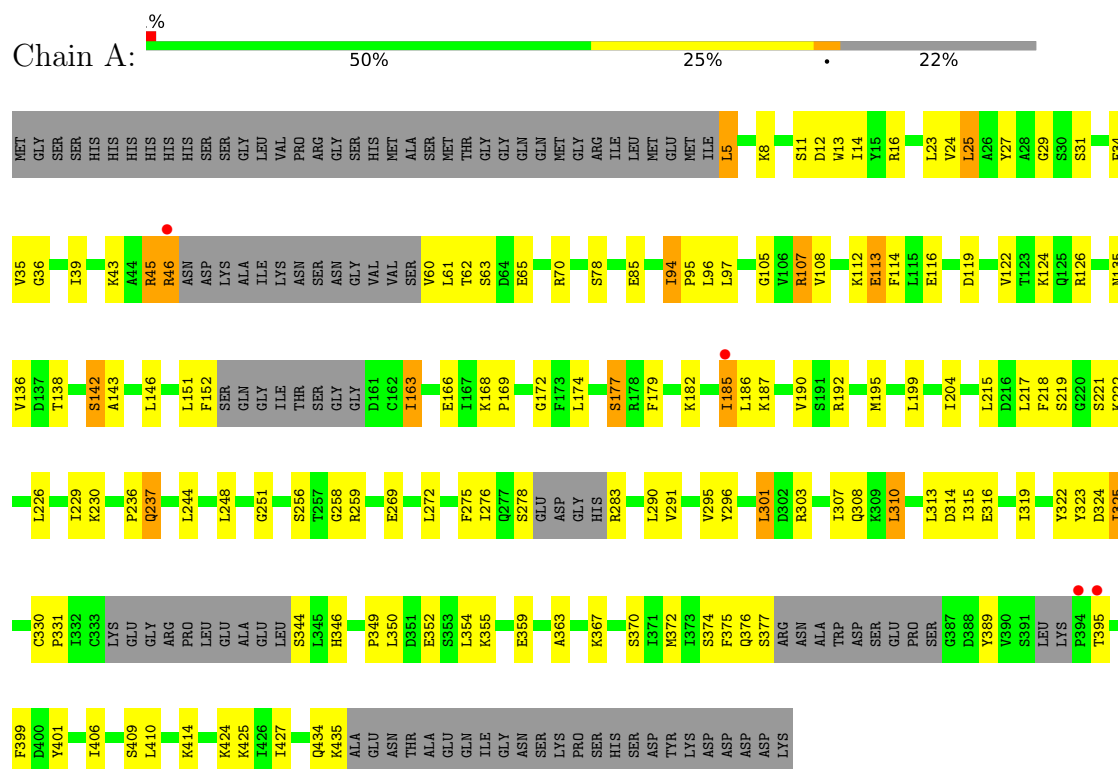
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

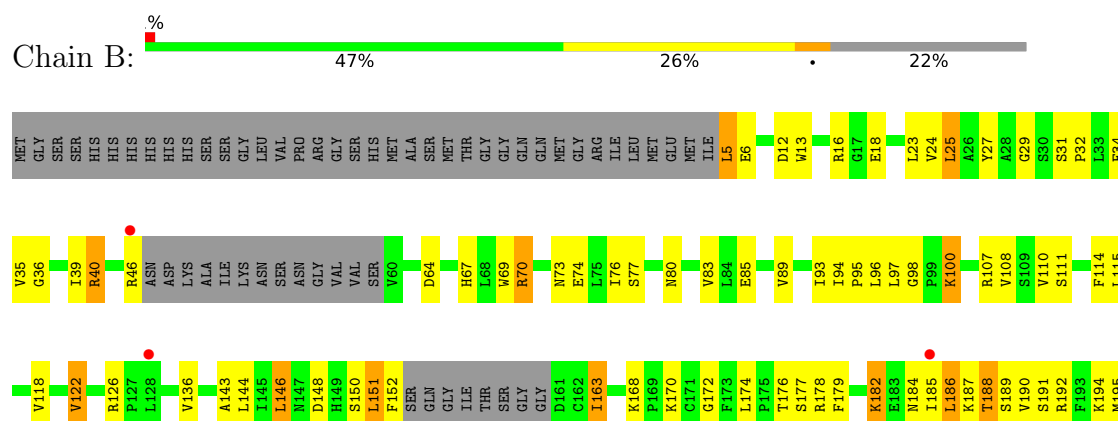
3 Residue-property plots [i](#)

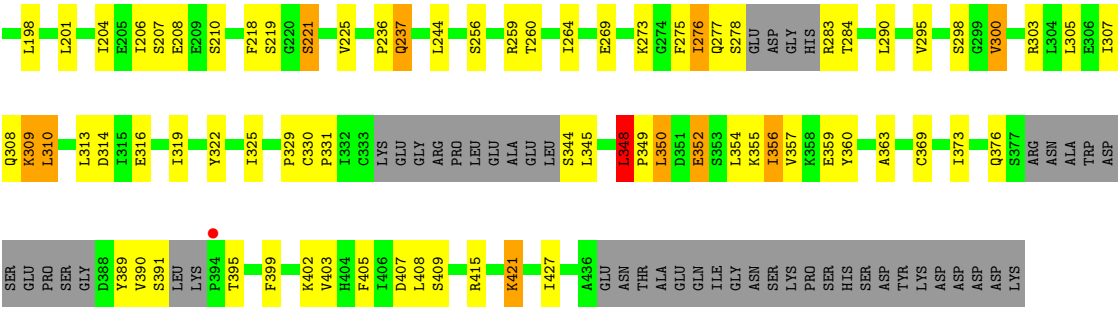
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Inositol-pentakisphosphate 2-kinase



• Molecule 1: Inositol-pentakisphosphate 2-kinase





4 Data and refinement statistics

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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.4 (44.63-3.10) 96.5 (44.63-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.6.3_473	Depositor
R, R_{free}	0.210 , 0.276 0.211 , 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 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

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: MG, 5MY, ADP, 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	0.56	0/3126	0.95	9/4210 (0.2%)
1	B	0.56	0/3127	0.95	8/4212 (0.2%)
All	All	0.56	0/6253	0.95	17/8422 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	SER	CA-C-N	9.70	129.47	119.19
1	A	78	SER	C-N-CA	9.70	129.47	119.19
1	B	168	LYS	CA-C-N	7.99	127.92	119.05
1	B	168	LYS	C-N-CA	7.99	127.92	119.05
1	B	177	SER	N-CA-C	7.11	120.26	110.24
1	A	94	ILE	CB-CA-C	-6.97	107.08	113.70
1	B	395	THR	N-CA-C	-6.91	102.98	113.89
1	A	177	SER	N-CA-C	6.68	119.70	110.35
1	A	168	LYS	CA-C-N	5.60	125.12	119.19
1	A	168	LYS	C-N-CA	5.60	125.12	119.19
1	B	356	ILE	N-CA-C	5.51	116.24	110.62
1	A	330	CYS	CA-C-N	5.48	125.00	119.19
1	A	330	CYS	C-N-CA	5.48	125.00	119.19
1	B	348	LEU	CA-C-N	5.22	125.22	119.90
1	B	348	LEU	C-N-CA	5.22	125.22	119.90
1	B	295	VAL	N-CA-C	5.16	115.78	110.36
1	A	395	THR	N-CA-C	-5.07	107.04	113.18

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	3072	0	3098	110	1
1	B	3073	0	3100	126	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	227	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 18.

All (227) 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:B:190:VAL:HB	1:B:195:MET:HE3	1.64	0.79
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:166:GLU:HB2	1:A:372:MET:HE3	1.69	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:46:ARG:HH12	1:B:182:LYS:HB2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:94:ILE:C	1:B:96:LEU:H	2.16	0.52
1:B:67:HIS:HA	1:B:70:ARG:NH1	2.25	0.52
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:B:219:SER:C	1:B:221:SER:H	2.19	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:B:76:ILE:HD12	1:B:76:ILE:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HH12	1:B:407:ASP:HA	1.77	0.50
1:A:186:LEU:C	1:A:195:MET:HE1	2.36	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:190:VAL:HB	1:A:195:MET:HE3	1.94	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:B:308:GLN:C	1:B:310:LEU:H	2.20	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:73:ASN:O	1:B:74:GLU:C	2.57	0.48
1:A:105:GLY:HA3	1:A:146:LEU:HD23	1.95	0.48
1:A:236:PRO:O	1:A:237:GLN:C	2.56	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
1:B:236:PRO:O	1:B:237:GLN:C	2.57	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:B:190:VAL:HB	1:B:195:MET:CE	2.39	0.47
1:A:25:LEU:HB2	1:A:39:ILE:CG2	2.45	0.47
1:A:113:GLU:CD	1:A:113:GLU:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:A:308:GLN:C	1:A:310:LEU:H	2.26	0.43
1:B:186:LEU:HD12	1:B:186:LEU:HA	1.78	0.43
1:A:215:LEU:O	1:A:219:SER:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:C	1:A:179:PHE:H	2.26	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:186:LEU:O	1:A:195:MET:HE1	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: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:B:24:VAL:C	1:B:25:LEU:HD22	2.45	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
1:B:94:ILE:C	1:B:96:LEU:N	2.77	0.41
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: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:A:258:GLY:O	1:A:259:ARG:C	2.64	0.40
1:B:69:TRP:O	1:B:70:ARG:C	2.63	0.40
1:B:186:LEU:C	1:B:188:THR:N	2.76	0.40
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:A:324:ASP:CG	1:A:346:HIS:HD1	2.30	0.40
1:B:219:SER:C	1:B:221:SER:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

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	371/493 (75%)	349 (94%)	21 (6%)	1 (0%)	36	67
1	B	371/493 (75%)	352 (95%)	16 (4%)	3 (1%)	16	47
All	All	742/986 (75%)	701 (94%)	37 (5%)	4 (0%)	24	57

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 ⓘ

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%)	314 (91%)	31 (9%)	9	33
1	B	345/434 (80%)	311 (90%)	34 (10%)	7	29
All	All	690/868 (80%)	625 (91%)	65 (9%)	8	31

All (65) 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	124	LYS
1	A	142	SER
1	A	163	ILE
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
1	A	301	LEU
1	A	310	LEU
1	A	325	ILE
1	A	344	SER
1	A	350	LEU
1	A	377	SER

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Mol	Chain	Res	Type
1	A	410	LEU
1	A	414	LYS
1	A	424	LYS
1	A	425	LYS
1	B	5	LEU
1	B	12	ASP
1	B	23	LEU
1	B	25	LEU
1	B	40	ARG
1	B	100	LYS
1	B	122	VAL
1	B	136	VAL
1	B	146	LEU
1	B	151	LEU
1	B	163	ILE
1	B	174	LEU
1	B	176	THR
1	B	178	ARG
1	B	182	LYS
1	B	186	LEU
1	B	188	THR
1	B	191	SER
1	B	192	ARG
1	B	194	LYS
1	B	198	LEU
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	309	LYS
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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	90	GLN
1	A	196	HIS
1	A	277	GLN
1	B	66	GLN
1	B	72	ASN
1	B	125	GLN
1	B	376	GLN
1	B	434	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 oligosaccharides 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	$\# Z > 2$
2	5MY	B	911	-	32,32,32	0.96	2 (6%)	53,53,53	0.94	3 (5%)
2	5MY	A	911	-	32,32,32	1.03	2 (6%)	53,53,53	0.97	3 (5%)
3	ADP	B	912	4	28,29,29	1.55	5 (17%)	43,45,45	1.82	8 (18%)
3	ADP	A	912	4	28,29,29	1.55	5 (17%)	43,45,45	1.80	10 (23%)

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
2	5MY	B	911	-	-	3/25/49/49	0/1/1/1
2	5MY	A	911	-	-	2/25/49/49	0/1/1/1
3	ADP	B	912	4	-	3/16/32/32	0/3/3/3
3	ADP	A	912	4	-	1/16/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	912	ADP	C5-C4	4.88	1.47	1.39
3	B	912	ADP	C5-C4	4.82	1.47	1.39
3	A	912	ADP	PA-O3A	3.85	1.63	1.59
3	B	912	ADP	PA-O3A	3.59	1.63	1.59
3	B	912	ADP	C5-C6	2.69	1.48	1.41
3	A	912	ADP	C5-C6	2.68	1.48	1.41
3	B	912	ADP	C8-N7	2.55	1.36	1.31
3	A	912	ADP	C8-N7	2.44	1.36	1.31
2	B	911	5MY	P1-O41	2.35	1.57	1.50
2	B	911	5MY	P6-O36	2.12	1.57	1.50
3	A	912	ADP	C4-N9	-2.10	1.33	1.37
2	A	911	5MY	P5-O35	2.08	1.56	1.50
3	B	912	ADP	C4-N9	-2.06	1.33	1.37
2	A	911	5MY	P3-O13	-2.02	1.56	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	912	ADP	C5-C4-N3	-5.04	119.77	126.72
3	A	912	ADP	C5-C4-N3	-4.75	120.18	126.72
3	B	912	ADP	C2'-C1'-N9	-4.25	102.74	113.30
3	B	912	ADP	N3-C4-N9	4.23	134.37	127.17
3	A	912	ADP	N3-C4-N9	4.06	134.07	127.17
3	A	912	ADP	C2'-C1'-N9	-3.83	103.80	113.30
3	B	912	ADP	C2-N3-C4	3.34	120.00	111.83
3	A	912	ADP	C2-N3-C4	3.30	119.88	111.83
3	A	912	ADP	N3-C2-N1	-3.26	123.64	128.58
3	A	912	ADP	C4-N9-C8	3.15	109.05	105.74
3	B	912	ADP	C4-N9-C8	3.10	109.00	105.74
3	B	912	ADP	N3-C2-N1	-3.07	123.93	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	912	ADP	C4-C5-N7	-2.86	107.32	110.58
3	A	912	ADP	C4-C5-N7	-2.77	107.42	110.58
2	A	911	5MY	C2-C1-C6	2.40	117.11	111.72
3	A	912	ADP	C6-C5-N7	2.23	136.38	132.09
2	B	911	5MY	O45-P5-O15	2.18	114.36	105.85
2	B	911	5MY	C2-C3-C4	2.18	116.62	111.72
2	A	911	5MY	C2-C3-C4	2.08	116.40	111.72
3	B	912	ADP	C5-N7-C8	2.07	106.71	103.45
2	B	911	5MY	C2-C1-C6	2.06	116.36	111.72
3	A	912	ADP	C2-N1-C6	2.04	122.08	118.73
3	A	912	ADP	C5-N7-C8	2.01	106.61	103.45
2	A	911	5MY	O45-P5-O15	2.01	113.67	105.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	912	ADP	C5'-O5'-PA-O3A
2	B	911	5MY	C6-O16-P6-O36
2	B	911	5MY	C4-O14-P4-O34
3	B	912	ADP	C5'-O5'-PA-O1A
3	B	912	ADP	C5'-O5'-PA-O2A
3	B	912	ADP	C5'-O5'-PA-O3A
2	A	911	5MY	C2-C3-O13-P3
2	B	911	5MY	C4-O14-P4-O44
2	A	911	5MY	C3-O13-P3-O33

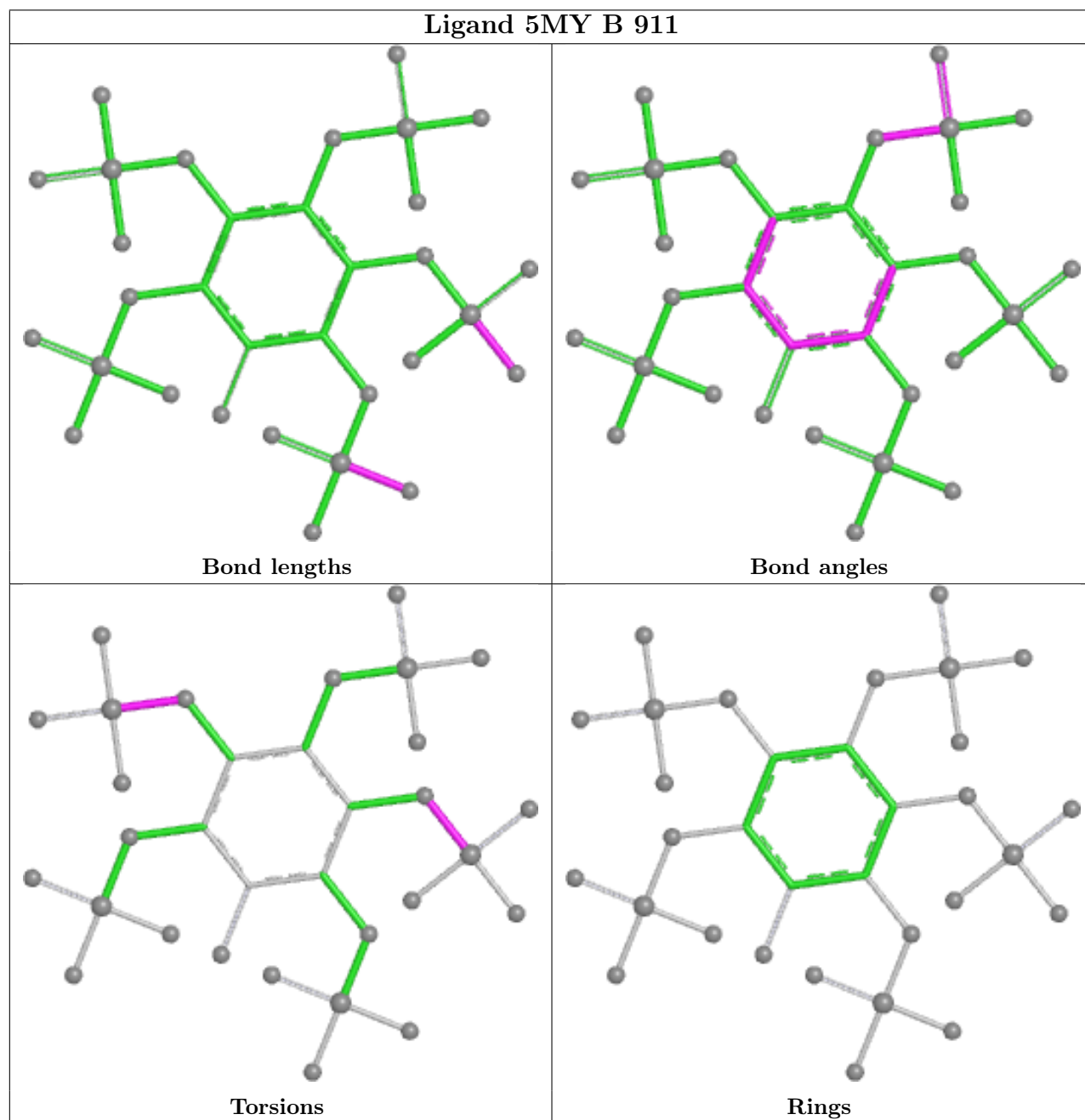
There are no ring outliers.

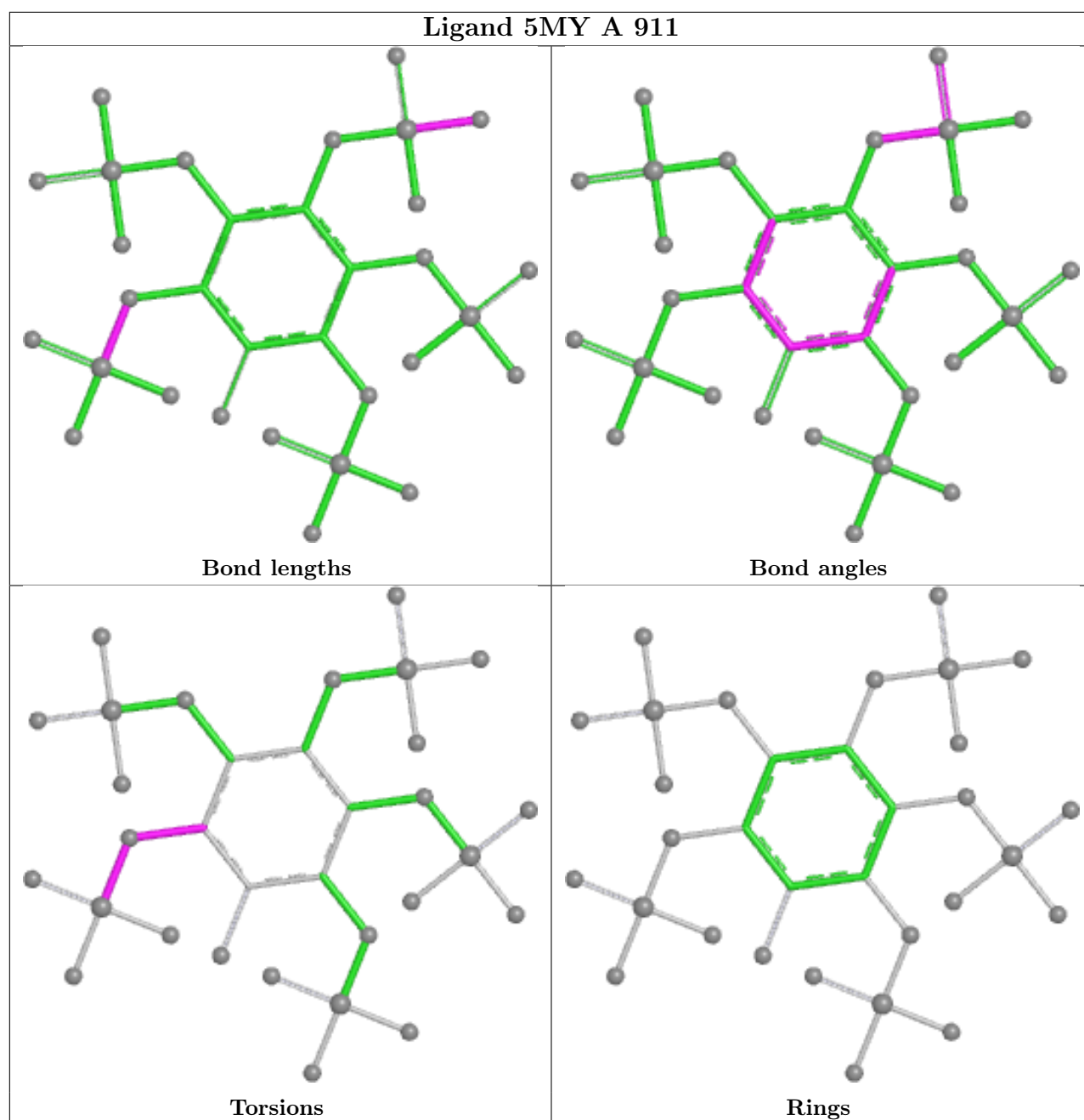
2 monomers are involved in 2 short contacts:

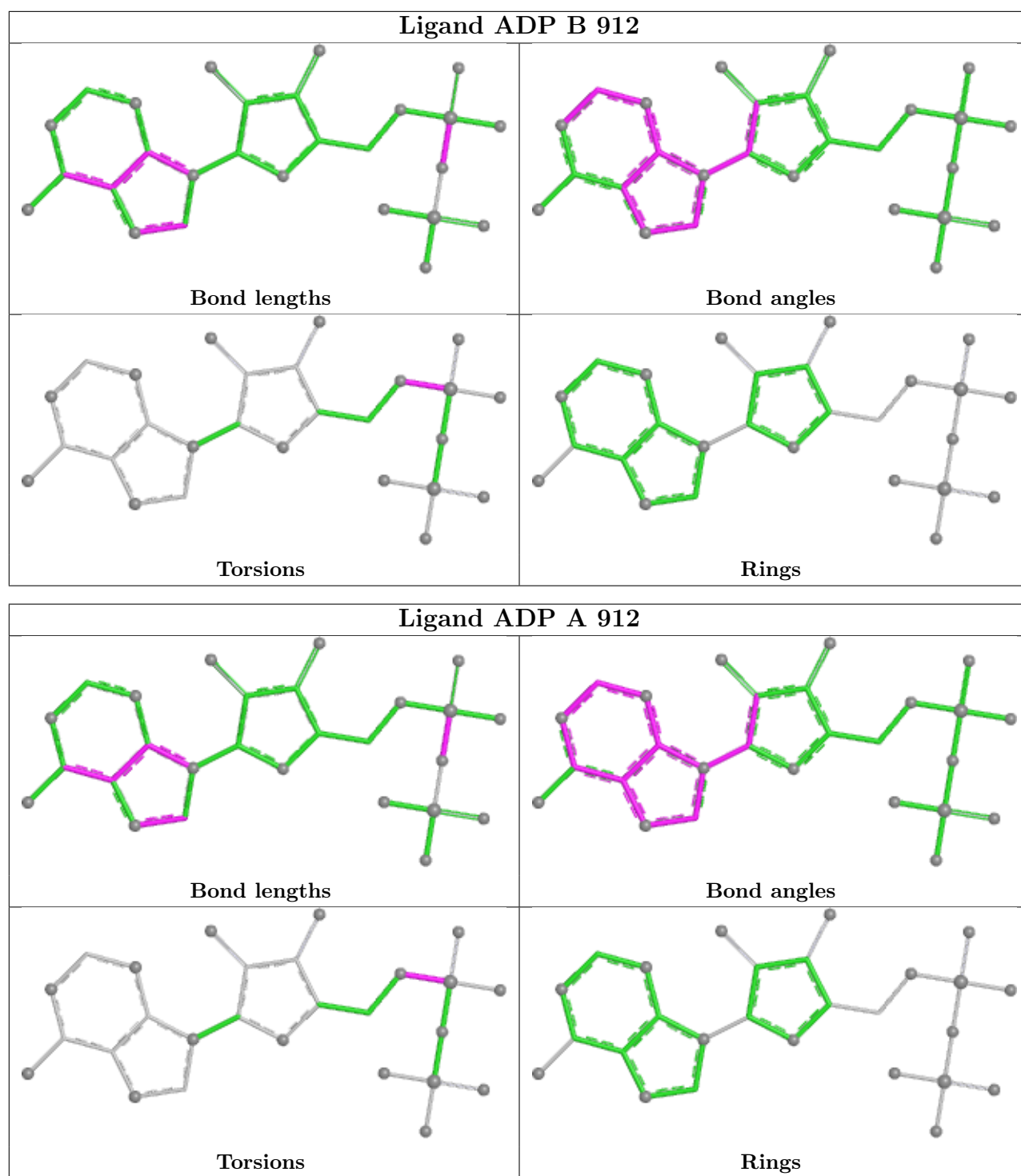
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	911	5MY	1	0
3	B	912	ADP	1	0

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 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 ⓘ

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	385/493 (78%)	0.03	4 (1%) 79 61	10, 23, 45, 62	0
1	B	385/493 (78%)	0.03	4 (1%) 79 61	9, 24, 52, 60	0
All	All	770/986 (78%)	0.03	8 (1%) 79 61	9, 24, 48, 62	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	ILE	5.0
1	B	185	ILE	3.7
1	B	394	PRO	2.6
1	A	394	PRO	2.6
1	B	128	LEU	2.5
1	A	46	ARG	2.4
1	B	46	ARG	2.1
1	A	395	THR	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.

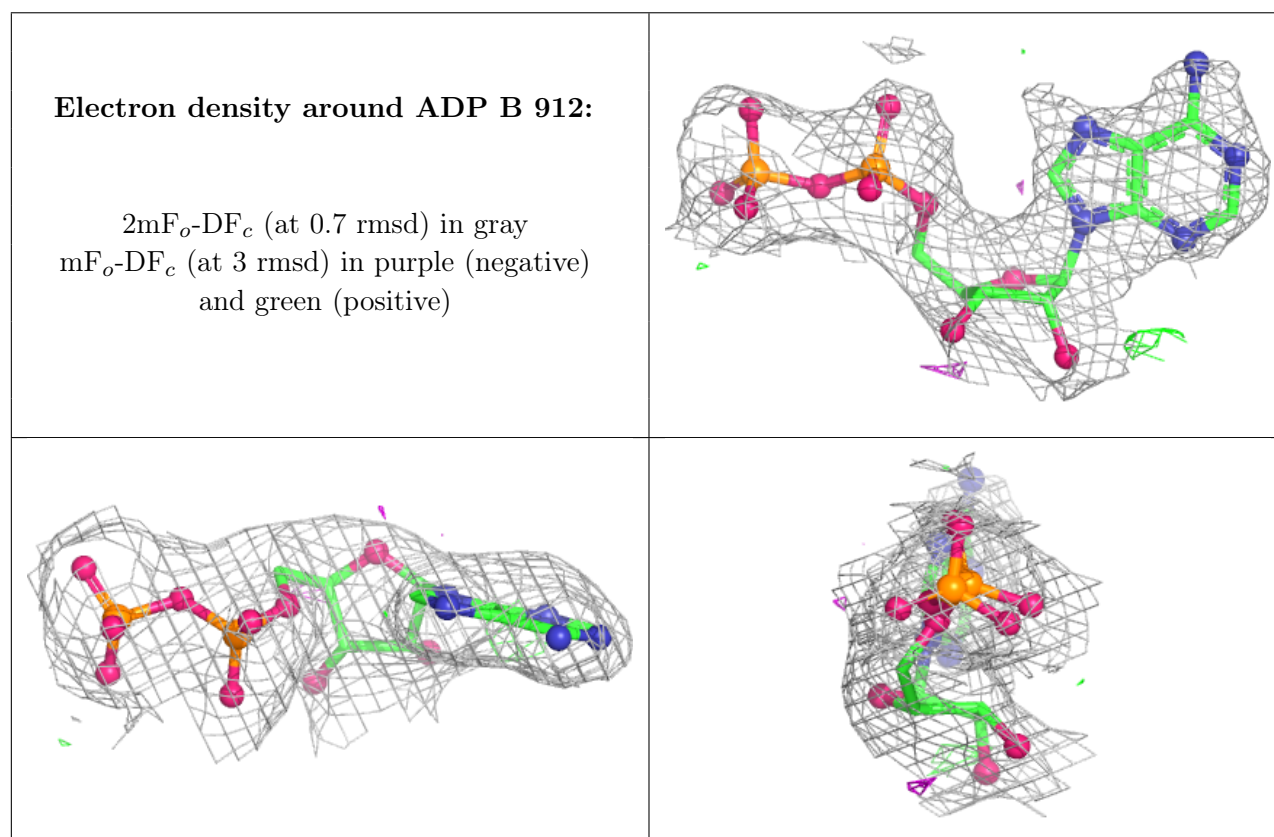
6.4 Ligands [i](#)

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.

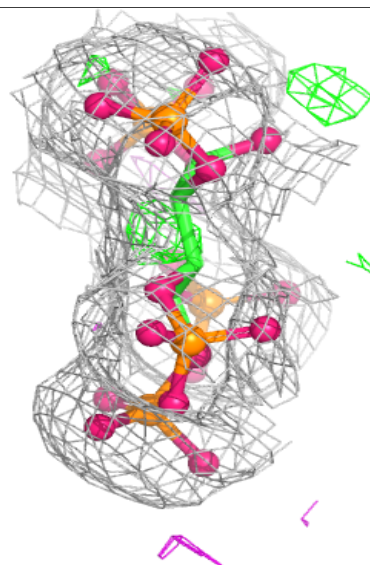
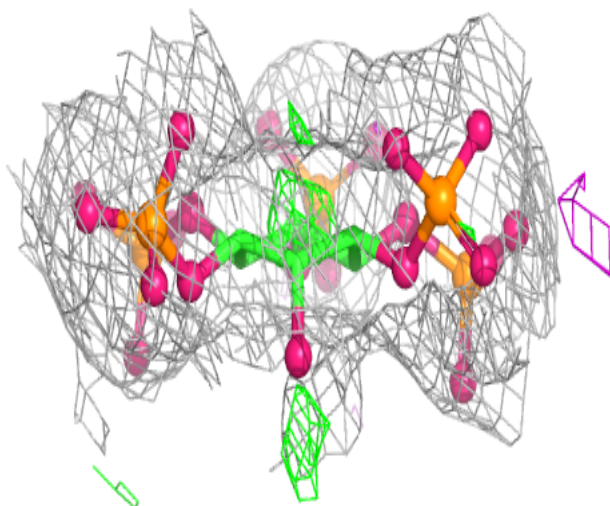
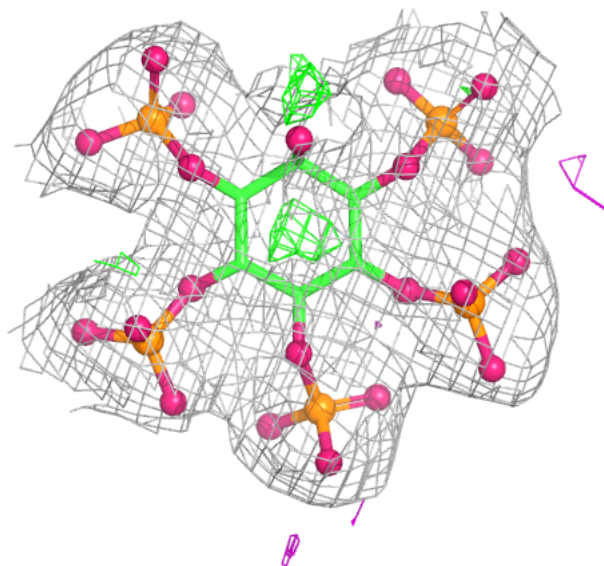
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	A	913	1/1	0.92	0.14	31,31,31,31	0
4	MG	B	913	1/1	0.92	0.17	40,40,40,40	0
3	ADP	B	912	27/27	0.93	0.11	29,40,43,53	0
2	5MY	B	911	32/32	0.93	0.11	20,32,43,49	0
3	ADP	A	912	27/27	0.93	0.12	23,40,46,49	0
2	5MY	A	911	32/32	0.94	0.10	23,30,42,46	0
5	ZN	B	914	1/1	0.99	0.08	33,33,33,33	0
5	ZN	A	914	1/1	1.00	0.09	39,39,39,39	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.



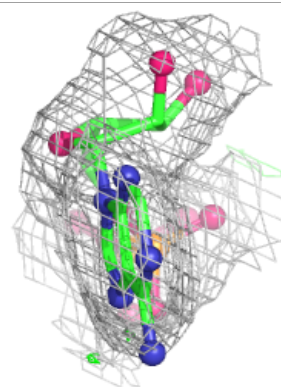
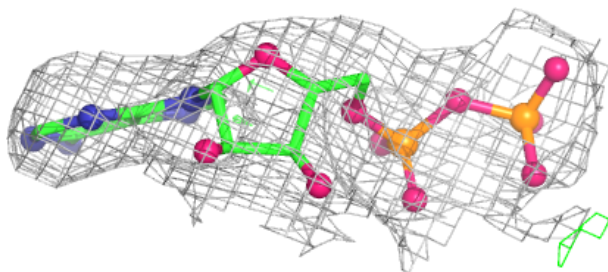
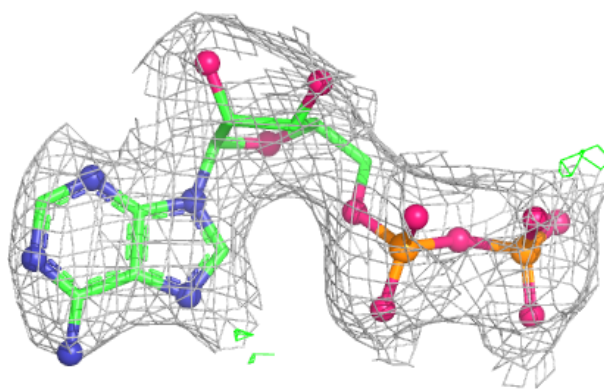
Electron density around 5MY B 911:

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



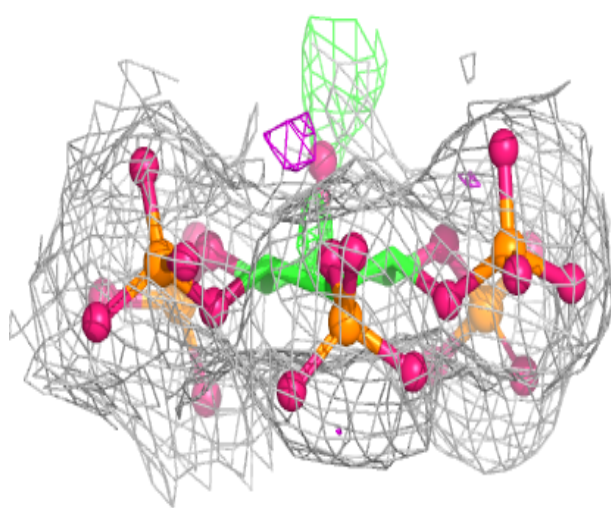
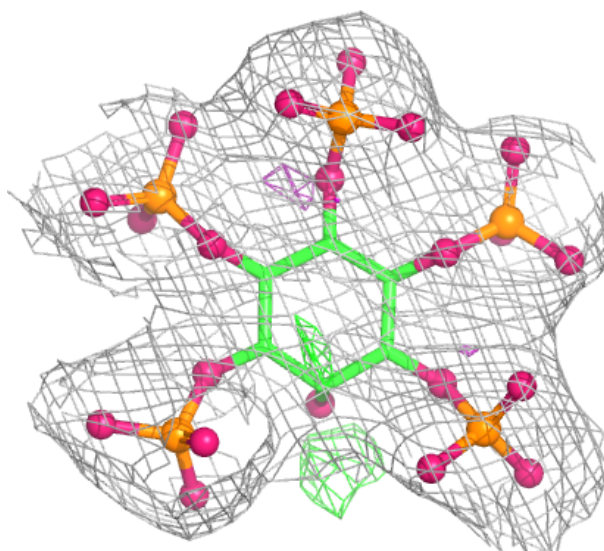
Electron density around ADP A 912:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.