



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:15 AM UTC

PDB ID : 5MPJ / pdb_00005mpj
Title : 1-(2-chloro-[1,1'-biphenyl]-4-yl)-N-methylethanamine
Authors : Brear, P.; De Fusco, C.; Georgiou, K.; Iegre, J.; Sore, H.; Hyvonen, M.; Spring, D.
Deposited on : 2016-12-16
Resolution : 2.14 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

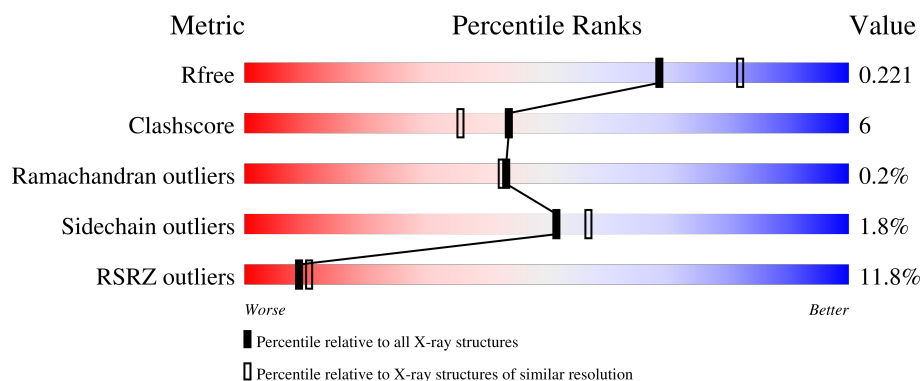
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	352	6% 79% 12% • 7%
1	B	352	16% 78% 13% • 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5820 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	3	0
			2774	1777	487	499	11			
1	B	324	Total	C	N	O	S	0	4	0
			2766	1772	486	497	11			

There are 50 discrepancies between the modelled and reference sequences:

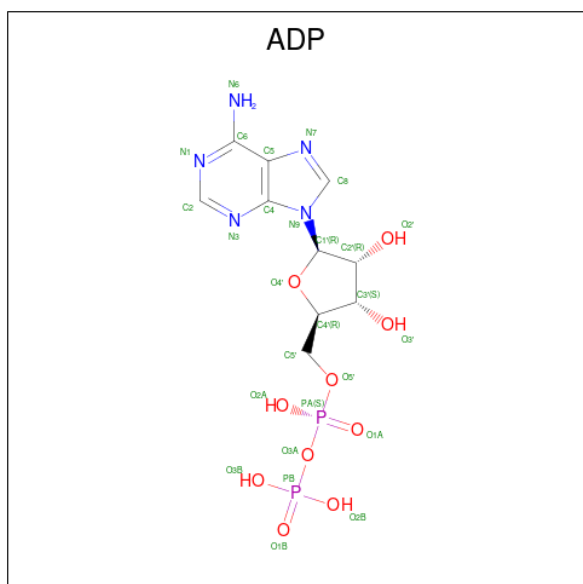
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	GLY	-	expression tag	UNP P68400
A	-21	SER	-	expression tag	UNP P68400
A	-20	MET	-	expression tag	UNP P68400
A	-19	ASP	-	expression tag	UNP P68400
A	-18	ILE	-	expression tag	UNP P68400
A	-17	GLU	-	expression tag	UNP P68400
A	-16	PHE	-	expression tag	UNP P68400
A	-15	ASP	-	expression tag	UNP P68400
A	-14	ASP	-	expression tag	UNP P68400
A	-13	ASP	-	expression tag	UNP P68400
A	-12	ALA	-	expression tag	UNP P68400
A	-11	ASP	-	expression tag	UNP P68400
A	-10	ASP	-	expression tag	UNP P68400
A	-9	ASP	-	expression tag	UNP P68400
A	-8	GLY	-	expression tag	UNP P68400
A	-7	SER	-	expression tag	UNP P68400
A	-6	GLY	-	expression tag	UNP P68400
A	-5	SER	-	expression tag	UNP P68400
A	-4	GLY	-	expression tag	UNP P68400
A	-3	SER	-	expression tag	UNP P68400
A	-2	GLY	-	expression tag	UNP P68400
A	-1	SER	-	expression tag	UNP P68400
A	0	GLY	-	expression tag	UNP P68400
A	1	SER	-	expression tag	UNP P68400
A	21	SER	ARG	engineered mutation	UNP P68400

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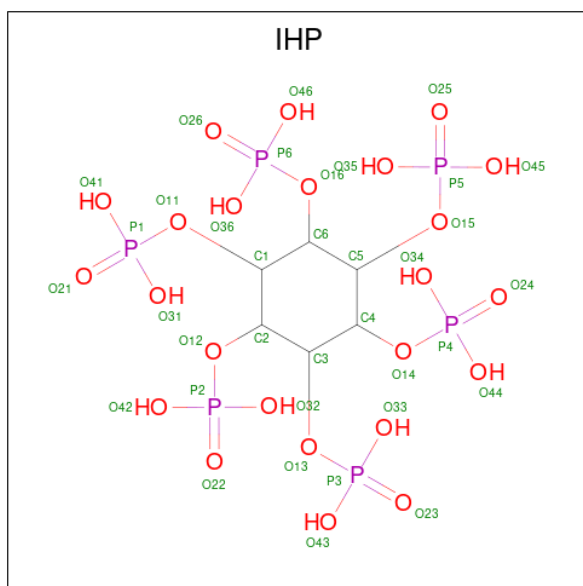
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P68400
B	-21	SER	-	expression tag	UNP P68400
B	-20	MET	-	expression tag	UNP P68400
B	-19	ASP	-	expression tag	UNP P68400
B	-18	ILE	-	expression tag	UNP P68400
B	-17	GLU	-	expression tag	UNP P68400
B	-16	PHE	-	expression tag	UNP P68400
B	-15	ASP	-	expression tag	UNP P68400
B	-14	ASP	-	expression tag	UNP P68400
B	-13	ASP	-	expression tag	UNP P68400
B	-12	ALA	-	expression tag	UNP P68400
B	-11	ASP	-	expression tag	UNP P68400
B	-10	ASP	-	expression tag	UNP P68400
B	-9	ASP	-	expression tag	UNP P68400
B	-8	GLY	-	expression tag	UNP P68400
B	-7	SER	-	expression tag	UNP P68400
B	-6	GLY	-	expression tag	UNP P68400
B	-5	SER	-	expression tag	UNP P68400
B	-4	GLY	-	expression tag	UNP P68400
B	-3	SER	-	expression tag	UNP P68400
B	-2	GLY	-	expression tag	UNP P68400
B	-1	SER	-	expression tag	UNP P68400
B	0	GLY	-	expression tag	UNP P68400
B	1	SER	-	expression tag	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



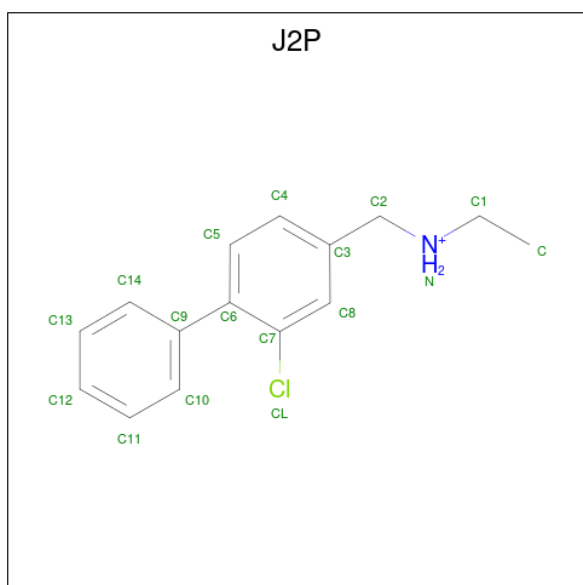
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	
								0
								0

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P		
			36	6	24	6		
							0	0

- Molecule 4 is (3-chloranyl-4-phenyl-phenyl)methyl-ethyl-azanium (CCD ID: J2P) (formula: $C_{15}H_{17}ClN$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	1
			34	30	2	2		

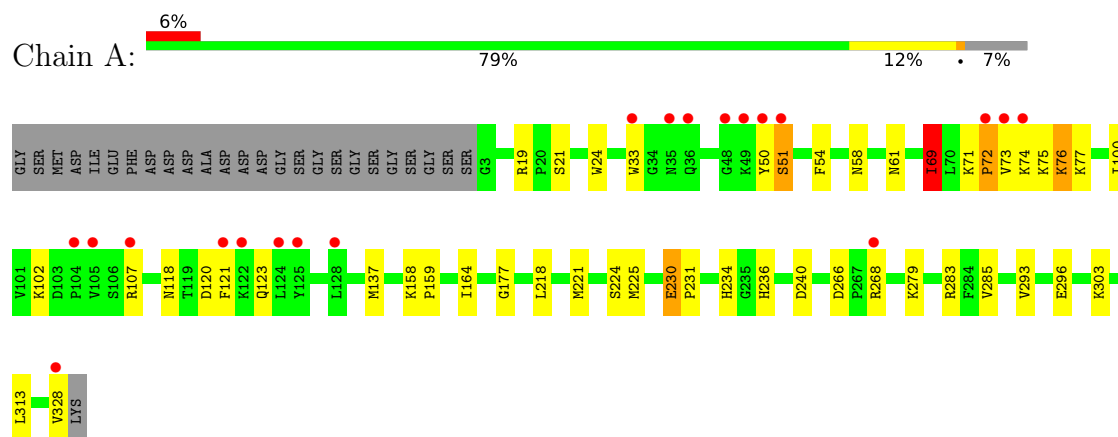
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		
5	B	44	Total	O	0	0
			44	44		

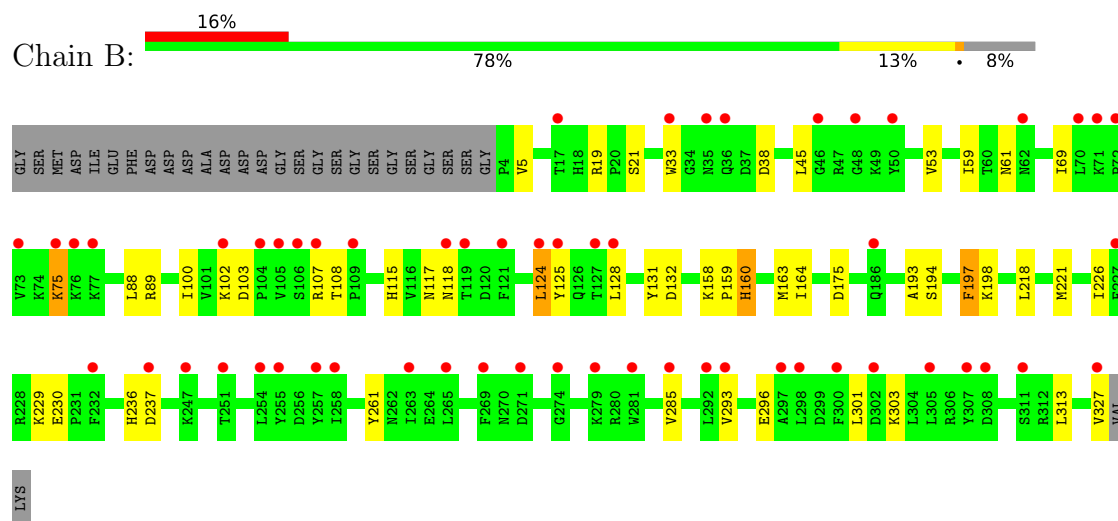
3 Residue-property plots [i](#)

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: Casein kinase II subunit alpha



- Molecule 1: Casein kinase II subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	64.76Å 68.46Å 334.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.29 – 2.14 45.29 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.29-2.14) 99.7 (45.29-2.14)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.212 , 0.241 0.218 , 0.221	Depositor DCC
R_{free} test set	2112 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5820	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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: J2P, IHP, ADP

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	0.98	1/2849 (0.0%)	1.15	4/3855 (0.1%)
1	B	1.08	12/2845 (0.4%)	1.47	29/3850 (0.8%)
All	All	1.03	13/5694 (0.2%)	1.32	33/7705 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	6
All	All	0	8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ILE	C-N	-23.91	0.99	1.33
1	B	88	LEU	C-N	-22.08	1.02	1.33
1	B	89	ARG	C-N	-15.05	1.08	1.33
1	B	197	PHE	C-N	-14.30	1.14	1.33
1	B	230	GLU	C-N	-13.88	1.07	1.34
1	B	198	LYS	C-N	-12.46	1.15	1.33
1	B	194[A]	SER	C-N	-11.94	1.19	1.33
1	B	194[B]	SER	C-N	-11.94	1.19	1.33
1	B	237	ASP	C-N	-8.65	1.21	1.33
1	B	160[A]	HIS	C-O	5.68	1.31	1.24
1	B	160[B]	HIS	C-O	5.68	1.31	1.24
1	B	160[A]	HIS	CA-C	5.09	1.59	1.52
1	B	160[B]	HIS	CA-C	5.09	1.59	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	LYS	CA-C-N	25.74	157.06	122.56
1	B	229	LYS	C-N-CA	25.74	157.06	122.56
1	B	229	LYS	O-C-N	-18.08	99.63	123.14
1	B	230	GLU	O-C-N	14.29	137.37	121.23
1	B	88	LEU	CA-C-N	12.93	146.24	121.54
1	B	88	LEU	C-N-CA	12.93	146.24	121.54
1	B	61	ASN	CB-CA-C	10.97	123.88	109.28
1	B	198	LYS	O-C-N	10.96	135.35	122.96
1	B	160[A]	HIS	CA-C-O	10.68	132.52	119.38
1	B	160[B]	HIS	CA-C-O	10.68	132.52	119.38
1	B	88	LEU	O-C-N	-9.08	109.51	122.41
1	B	197	PHE	O-C-N	-9.03	111.24	122.35
1	B	194[A]	SER	CA-C-N	8.81	132.44	120.54
1	B	194[A]	SER	C-N-CA	8.81	132.44	120.54
1	B	194[B]	SER	CA-C-N	8.81	132.44	120.54
1	B	194[B]	SER	C-N-CA	8.81	132.44	120.54
1	B	160[A]	HIS	N-CA-C	8.60	123.03	112.54
1	B	160[B]	HIS	N-CA-C	8.60	123.03	112.54
1	B	236	HIS	O-C-N	-8.03	111.46	122.46
1	B	237	ASP	O-C-N	-6.85	113.89	122.73
1	B	198	LYS	CA-C-N	-6.62	111.48	121.87
1	B	198	LYS	C-N-CA	-6.62	111.48	121.87
1	B	175	ASP	N-CA-C	5.91	118.40	111.02
1	B	236	HIS	CA-C-N	5.49	131.65	122.20
1	B	236	HIS	C-N-CA	5.49	131.65	122.20
1	A	61	ASN	CB-CA-C	5.38	121.12	110.42
1	A	58	ASN	N-CA-C	-5.32	100.43	108.67
1	B	237	ASP	CA-C-N	5.26	129.57	120.58
1	B	237	ASP	C-N-CA	5.26	129.57	120.58
1	A	51	SER	N-CA-C	5.17	116.15	108.60
1	B	218	LEU	CA-C-N	5.06	125.56	119.94
1	B	218	LEU	C-N-CA	5.06	125.56	119.94
1	A	24	TRP	N-CA-C	5.03	119.56	113.38

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19[A]	ARG	Sidechain
1	A	69	ILE	Mainchain
1	B	160[A]	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	B	160[B]	HIS	Sidechain
1	B	19[A]	ARG	Mainchain
1	B	19[B]	ARG	Mainchain
1	B	193	ALA	Mainchain

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	2774	0	2709	35	4
1	B	2766	0	2694	32	0
2	A	27	0	12	0	0
3	A	36	0	6	1	3
4	A	34	0	0	9	0
5	A	139	0	0	0	0
5	B	44	0	0	0	0
All	All	5820	0	5421	67	4

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 6.

All (67) 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:225:MET:HG3	4:A:403[A]:J2P:C13	1.77	1.12
1:A:225:MET:CG	4:A:403[A]:J2P:C13	2.47	0.91
1:A:71:LYS:HB3	1:A:72:PRO:CD	2.02	0.89
1:A:225:MET:HG3	4:A:403[B]:J2P:C11	2.04	0.86
1:A:71:LYS:HB3	1:A:72:PRO:HD2	1.57	0.86
1:B:124:LEU:C	1:B:124:LEU:HD13	2.01	0.85
1:B:75:LYS:HB3	1:B:75:LYS:NZ	1.90	0.84
1:B:115:HIS:HE1	1:B:117:ASN:OD1	1.60	0.83
1:A:77:LYS:HE2	1:A:177:GLY:O	1.81	0.80
1:A:225:MET:HG3	4:A:403[A]:J2P:C12	2.13	0.78
1:B:118:ASN:CG	1:B:164:ILE:H	1.93	0.77
1:B:75:LYS:HB3	1:B:75:LYS:HZ3	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD13	1:B:124:LEU:O	1.88	0.72
1:B:115:HIS:CE1	1:B:117:ASN:OD1	2.45	0.69
1:A:236:HIS:HE1	3:A:402:IHP:O24	1.79	0.66
1:B:107:ARG:O	1:B:107:ARG:HG3	1.96	0.65
1:B:131:TYR:CE1	1:B:327:VAL:HG12	2.36	0.60
1:A:279:LYS:HD2	1:A:283:ARG:NH1	2.16	0.60
1:B:128:LEU:HD22	1:B:132:ASP:HB3	1.83	0.60
1:A:118:ASN:HD22	1:A:164:ILE:H	1.52	0.58
1:A:279:LYS:HD2	1:A:283:ARG:HH11	1.70	0.56
1:B:124:LEU:C	1:B:124:LEU:CD1	2.74	0.55
1:B:103:ASP:HB3	1:B:108:THR:H	1.72	0.55
1:B:45:LEU:HB2	1:B:53:VAL:HG12	1.88	0.55
1:A:225:MET:CG	4:A:403[B]:J2P:C11	2.79	0.55
1:A:303:LYS:HB3	1:A:313:LEU:HG	1.88	0.53
1:B:303:LYS:HB3	1:B:313:LEU:HG	1.89	0.53
1:A:225:MET:HG2	4:A:403[A]:J2P:C13	2.36	0.53
1:A:51:SER:HA	1:A:71:LYS:HG3	1.91	0.52
1:B:102:LYS:HE3	1:B:107:ARG:HB2	1.90	0.52
1:A:164:ILE:H	4:A:403[B]:J2P:C	2.24	0.51
1:B:159:PRO:HD3	1:B:221:MET:HG2	1.93	0.51
1:B:226:ILE:HD11	1:B:301:LEU:HD22	1.93	0.50
1:B:75:LYS:HB3	1:B:75:LYS:HZ2	1.75	0.49
1:A:159:PRO:HD3	1:A:221:MET:HG2	1.95	0.49
1:B:159:PRO:HD2	1:B:197:PHE:CZ	2.47	0.49
1:B:118:ASN:ND2	1:B:163:MET:HA	2.27	0.48
1:A:118:ASN:ND2	1:A:164:ILE:H	2.12	0.47
1:B:118:ASN:OD1	1:B:164:ILE:N	2.38	0.47
1:A:50:TYR:HD1	1:A:73:VAL:HG11	1.80	0.47
1:A:121:PHE:CD1	4:A:403[B]:J2P:C8	2.98	0.46
1:A:121:PHE:HD1	4:A:403[B]:J2P:C8	2.28	0.46
1:B:69:ILE:HG23	1:B:108:THR:HG21	1.97	0.46
1:B:69:ILE:HG23	1:B:108:THR:CG2	2.46	0.45
1:A:50:TYR:CD1	1:A:73:VAL:HG11	2.52	0.45
1:A:102:LYS:HE2	1:A:107:ARG:O	2.16	0.45
1:B:285:VAL:HG22	1:B:293:VAL:HG11	1.98	0.45
1:B:158:LYS:HB2	1:B:159:PRO:HD2	2.00	0.44
1:B:118:ASN:OD1	1:B:164:ILE:O	2.35	0.44
1:A:285:VAL:HG22	1:A:293:VAL:HG11	1.98	0.44
1:A:54:PHE:CE1	1:A:69:ILE:HD12	2.53	0.43
1:A:76:LYS:HE3	1:A:76:LYS:HB2	1.81	0.43
1:A:230:GLU:HA	1:A:231:PRO:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TRP:CE3	1:B:100:ILE:HG22	2.54	0.43
1:A:266:ASP:OD1	1:A:268:ARG:HG2	2.19	0.42
1:B:124:LEU:HD12	1:B:125:TYR:HD1	1.84	0.42
1:B:197:PHE:CD1	1:B:197:PHE:N	2.87	0.42
1:A:71:LYS:HB3	1:A:72:PRO:HD3	1.95	0.42
1:A:137:MET:HE1	1:A:218:LEU:HG	2.01	0.42
1:A:71:LYS:CB	1:A:72:PRO:CD	2.77	0.41
1:A:224:SER:HB2	1:A:230:GLU:HG2	2.03	0.41
1:B:38:ASP:HA	1:B:59:ILE:HG12	2.02	0.41
1:B:125:TYR:HA	1:B:128:LEU:HD12	2.01	0.41
1:A:158:LYS:HB2	1:A:159:PRO:HD2	2.03	0.40
1:A:120:ASP:HB3	1:A:123:GLN:HB2	2.02	0.40
1:A:33:TRP:CE3	1:A:100:ILE:HG22	2.55	0.40
1:B:5:VAL:HB	1:B:261:TYR:HA	2.04	0.40

All (4) 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:234:HIS:ND1	3:A:402:IHP:O43[4_597]	1.01	1.19
1:A:236:HIS:CD2	1:A:240:ASP:OD2[4_597]	1.92	0.28
1:A:234:HIS:CE1	3:A:402:IHP:O43[4_597]	1.93	0.27
1:A:234:HIS:CG	3:A:402:IHP:O43[4_597]	2.03	0.17

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	327/352 (93%)	311 (95%)	15 (5%)	1 (0%)	36	33
1	B	326/352 (93%)	313 (96%)	13 (4%)	0	100	100
All	All	653/704 (93%)	624 (96%)	28 (4%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	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	303/319 (95%)	296 (98%)	7 (2%)	44	47
1	B	302/319 (95%)	298 (99%)	4 (1%)	61	67
All	All	605/638 (95%)	594 (98%)	11 (2%)	51	57

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	74	LYS
1	A	75	LYS
1	A	76	LYS
1	A	230	GLU
1	A	296	GLU
1	A	328	VAL
1	B	21	SER
1	B	75	LYS
1	B	124	LEU
1	B	296	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	A	117	ASN
1	A	168	HIS
1	A	186	GLN
1	A	236	HIS

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Mol	Chain	Res	Type
1	A	262	ASN
1	B	58	ASN
1	B	115	HIS
1	B	168	HIS
1	B	186	GLN
1	B	262	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	J2P	A	403[B]	-	18,18,18	0.12	0	22,23,23	0.18	0
3	IHP	A	402	-	36,36,36	0.75	0	60,60,60	0.95	0
2	ADP	A	401	-	28,29,29	0.53	0	43,45,45	0.86	2 (4%)
4	J2P	A	403[A]	-	18,18,18	0.14	0	22,23,23	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	J2P	A	403[B]	-	-	5/8/8/8	0/2/2/2
3	IHP	A	402	-	-	7/30/54/54	0/1/1/1
2	ADP	A	401	-	-	1/16/32/32	0/3/3/3
4	J2P	A	403[A]	-	-	0/8/8/8	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADP	O2B-PB-O3A	2.64	113.50	104.64
2	A	401	ADP	O2A-PA-O5'	2.46	118.72	107.57

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	IHP	C2-C1-O11-P1
3	A	402	IHP	C6-C1-O11-P1
3	A	402	IHP	C3-C4-O14-P4
3	A	402	IHP	C5-C4-O14-P4
3	A	402	IHP	C1-C6-O16-P6
4	A	403[B]	J2P	C3-C2-N-C1
4	A	403[B]	J2P	C7-C6-C9-C10
4	A	403[B]	J2P	C7-C6-C9-C14
3	A	402	IHP	C5-C6-O16-P6
4	A	403[B]	J2P	C5-C6-C9-C10
4	A	403[B]	J2P	C5-C6-C9-C14
3	A	402	IHP	C4-O14-P4-O24
2	A	401	ADP	PB-O3A-PA-O2A

There are no ring outliers.

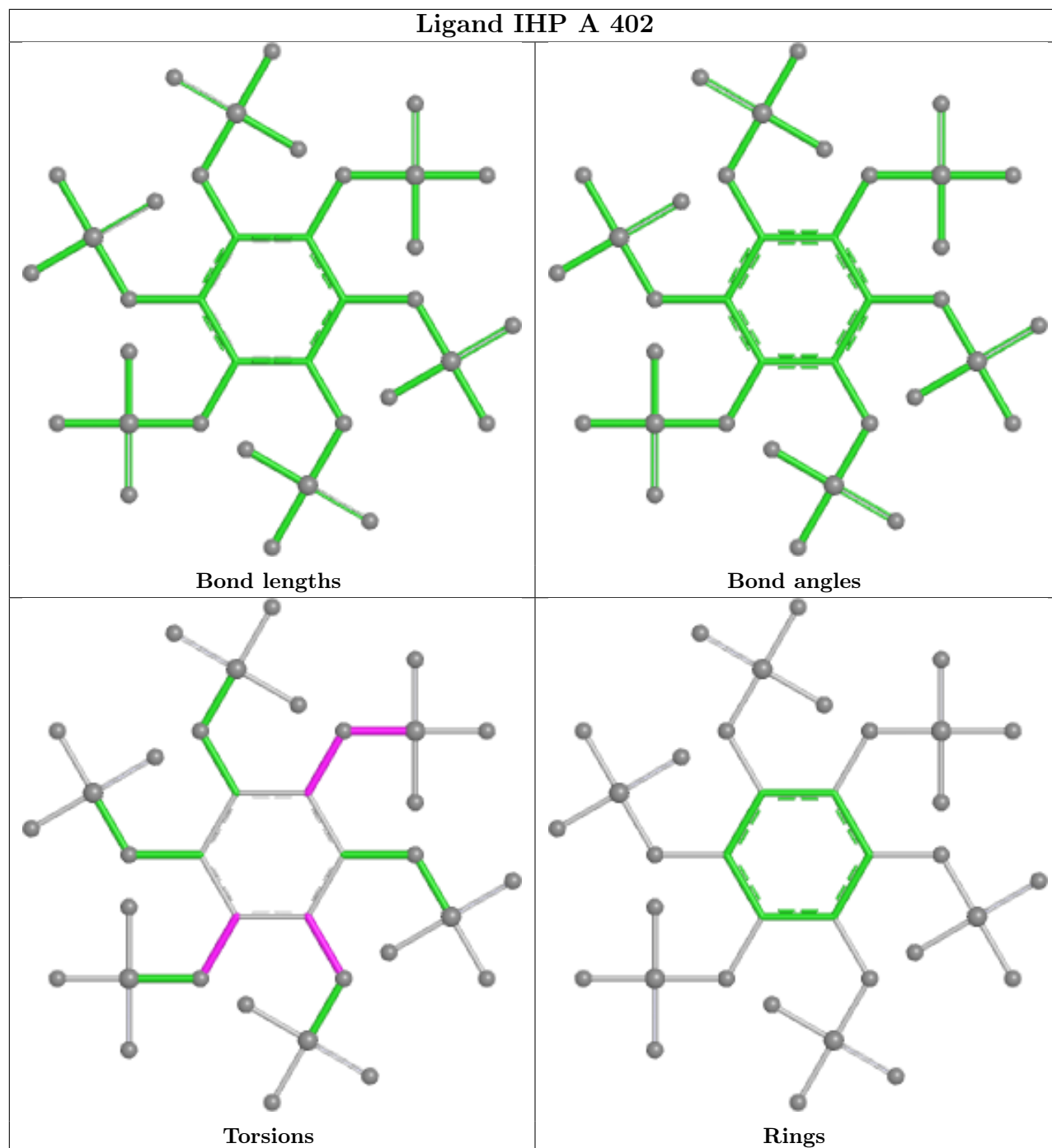
3 monomers are involved in 13 short contacts:

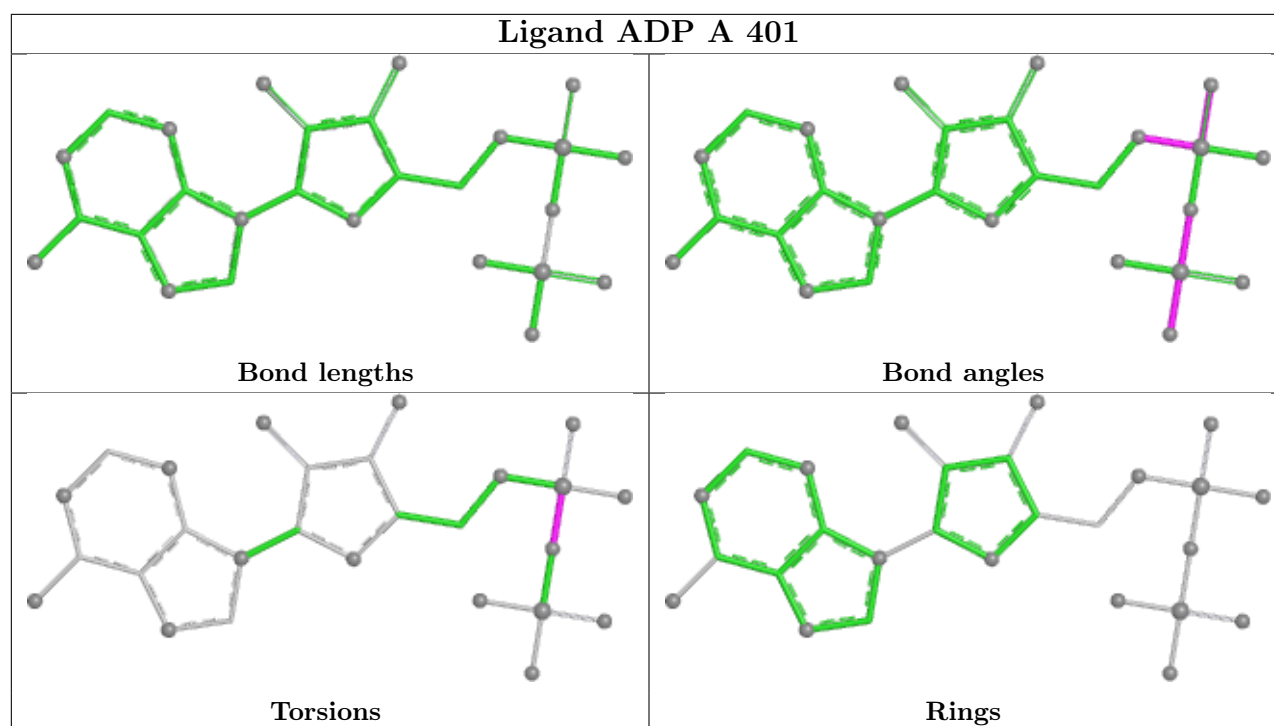
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403[B]	J2P	5	0
3	A	402	IHP	1	3
4	A	403[A]	J2P	4	0

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

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

Ligand IHP A 402





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	7
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	194[A]:SER	C	195:ARG	N	1.19
1	B	194[B]:SER	C	195:ARG	N	1.18
1	B	197:PHE	C	198:LYS	N	1.14
1	B	198:LYS	C	199:GLY	N	1.14
1	B	89:ARG	C	90:GLY	N	1.08
1	B	230:GLU	C	231:PRO	N	1.07
1	B	88:LEU	C	89:ARG	N	1.02
1	A	69:ILE	C	70:LEU	N	0.99

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	326/352 (92%)	0.13	20 (6%) 27 31	11, 35, 79, 107	3 (0%)
1	B	324/352 (92%)	1.15	57 (17%) 4 5	20, 73, 116, 145	4 (1%)
All	All	650/704 (92%)	0.64	77 (11%) 9 11	11, 52, 108, 145	7 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	PRO	4.9
1	B	50	TYR	4.9
1	A	50	TYR	4.8
1	A	121	PHE	4.6
1	B	118	ASN	4.6
1	B	33	TRP	4.4
1	B	327	VAL	4.4
1	B	125	TYR	4.3
1	B	104	PRO	4.1
1	B	105	VAL	4.1
1	B	77	LYS	4.1
1	B	265	LEU	3.9
1	A	33	TRP	3.9
1	A	125	TYR	3.9
1	B	72	PRO	3.9
1	B	258	ILE	3.7
1	B	257	TYR	3.7
1	B	281	TRP	3.6
1	B	121	PHE	3.5
1	B	255	TYR	3.4
1	B	269	PHE	3.4
1	A	124	LEU	3.4
1	B	36	GLN	3.4
1	B	263	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	3.3
1	B	102	LYS	3.2
1	B	254	LEU	3.1
1	A	104	PRO	3.1
1	A	107	ARG	3.1
1	B	73	VAL	3.1
1	B	46	GLY	3.0
1	B	119	THR	3.0
1	A	49	LYS	3.0
1	A	128	LEU	2.9
1	B	307	TYR	2.9
1	B	311[A]	SER	2.8
1	B	292	LEU	2.8
1	A	328	VAL	2.8
1	B	237	ASP	2.7
1	B	128	LEU	2.7
1	A	48	GLY	2.7
1	B	76	LYS	2.7
1	B	107	ARG	2.7
1	B	106	SER	2.6
1	B	232	PHE	2.6
1	B	48	GLY	2.6
1	B	297	ALA	2.6
1	B	62	ASN	2.5
1	B	70	LEU	2.5
1	B	124	LEU	2.5
1	A	74	LYS	2.5
1	B	17	THR	2.5
1	B	227	PHE	2.4
1	A	268	ARG	2.4
1	A	105	VAL	2.4
1	B	127	THR	2.4
1	B	75	LYS	2.3
1	B	247	LYS	2.3
1	B	300	PHE	2.3
1	A	36	GLN	2.3
1	B	285	VAL	2.3
1	B	71	LYS	2.3
1	B	251	THR	2.2
1	B	271	ASP	2.2
1	A	73	VAL	2.2
1	B	308	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	186	GLN	2.2
1	B	279	LYS	2.2
1	B	109	PRO	2.1
1	B	302	ASP	2.2
1	B	305	LEU	2.1
1	A	122	LYS	2.1
1	B	293	VAL	2.1
1	A	35	ASN	2.1
1	B	274	GLY	2.1
1	A	51	SER	2.1
1	B	35	ASN	2.0

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](#)

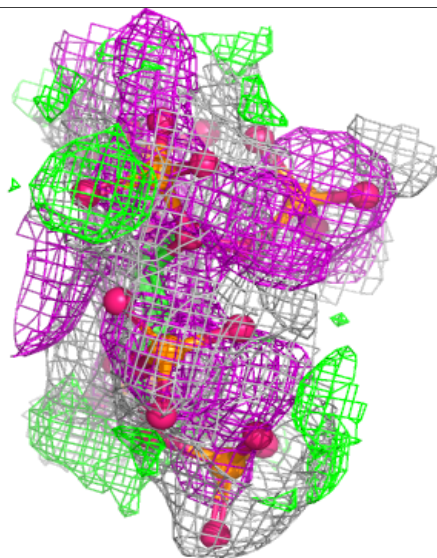
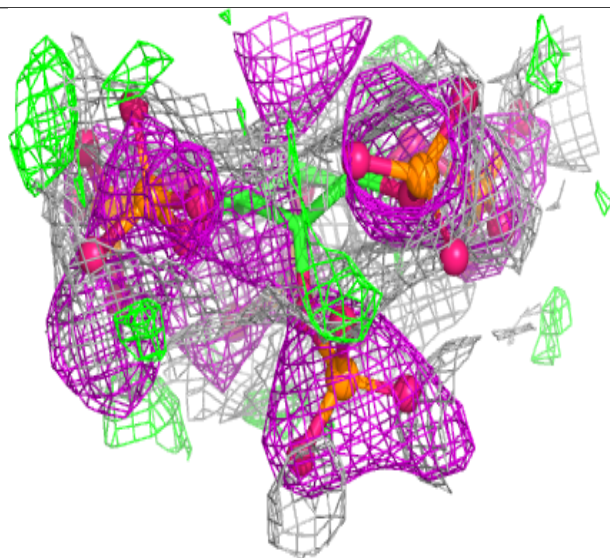
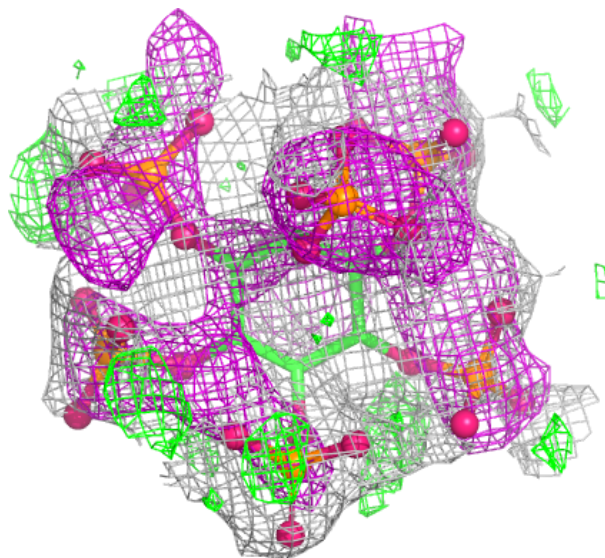
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

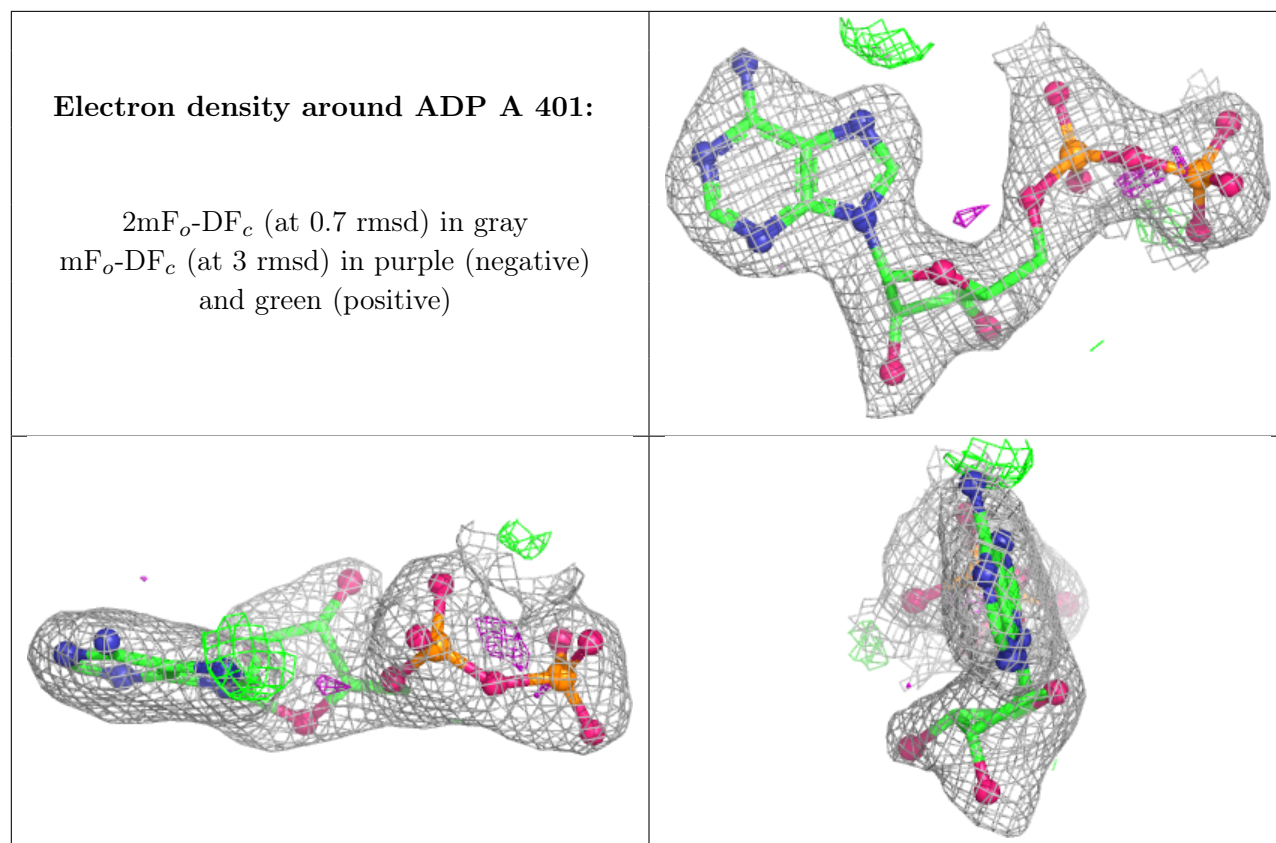
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IHP	A	402	36/36	0.72	0.16	20,20,20,20	36
4	J2P	A	403[A]	17/17	0.74	0.32	61,85,89,96	17
4	J2P	A	403[B]	17/17	0.74	0.32	61,85,89,96	17
2	ADP	A	401	27/27	0.90	0.09	45,57,67,68	0

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 IHP A 402:

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.