Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 08:57 PM EDT

PDB ID	:	4LV7
Title	:	Crystal structure of inositol 1,3,4,5,6-pentakisphosphate 2-kinase E82C/S142C
Authors	:	Gosein, V.; Miller, G.J.
Deposited on	:	2013-07-26
Resolution	:	2.60 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:

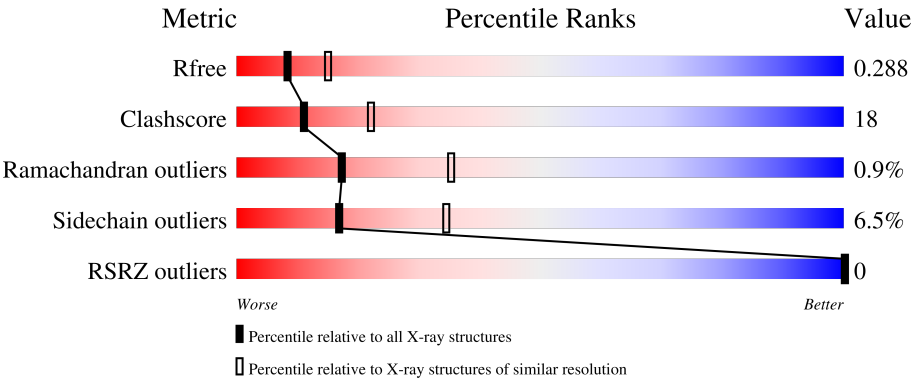
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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% 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	47% 30% . 21%
1	B	493	51% 26% . 20%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6380 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	390	Total	C	N	O	S	0	0	0
			3114	1992	526	582	14			
1	B	394	Total	C	N	O	S	0	0	0
			3136	2003	528	591	14			

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	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	82	CYS	GLU	engineered mutation	UNP Q93YN9
A	90	GLN	LYS	conflict	UNP Q93YN9
A	142	CYS	SER	engineered mutation	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	-	initiating methionine	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

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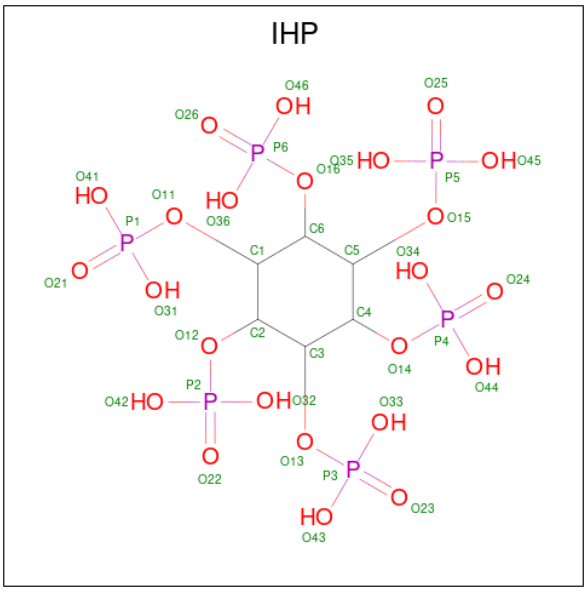
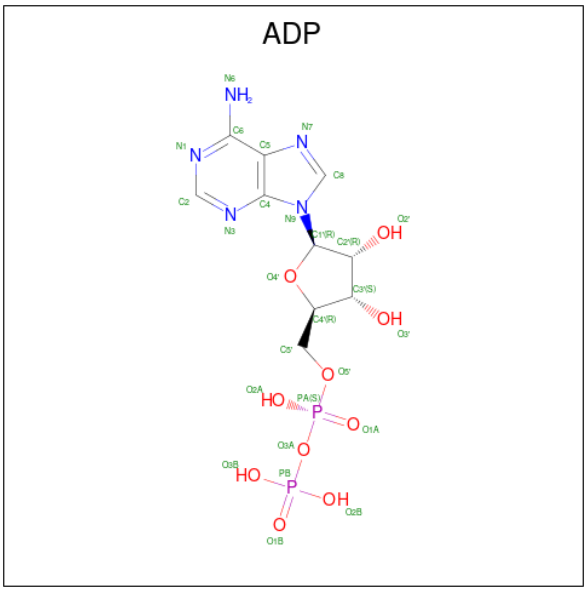
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	VAL	-	expression tag	UNP Q93YN9
B	-18	PRO	-	expression tag	UNP Q93YN9
B	-17	ARG	-	expression tag	UNP Q93YN9
B	-16	GLY	-	expression tag	UNP Q93YN9
B	-15	SER	-	expression tag	UNP Q93YN9
B	-14	HIS	-	expression tag	UNP Q93YN9
B	-13	MET	-	expression tag	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	82	CYS	GLU	engineered mutation	UNP Q93YN9
B	90	GLN	LYS	conflict	UNP Q93YN9
B	142	CYS	SER	engineered mutation	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 INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- 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	C	N	O	P	0	0
			27	10	5	10	2		

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

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

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

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

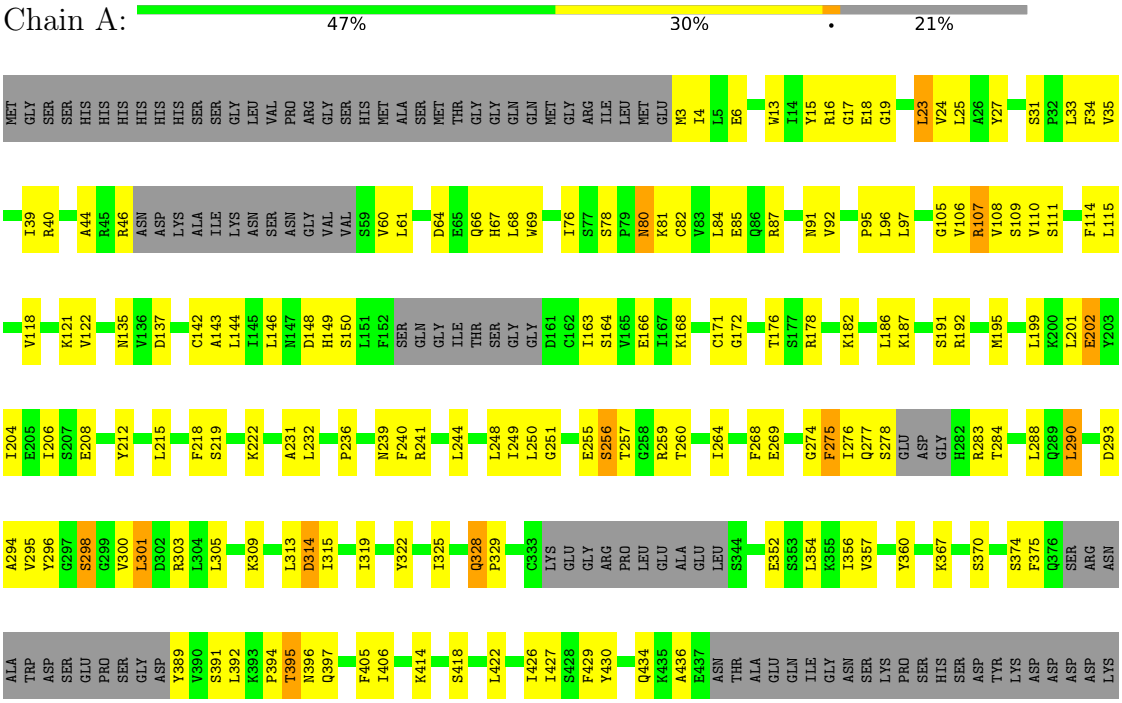
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

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.

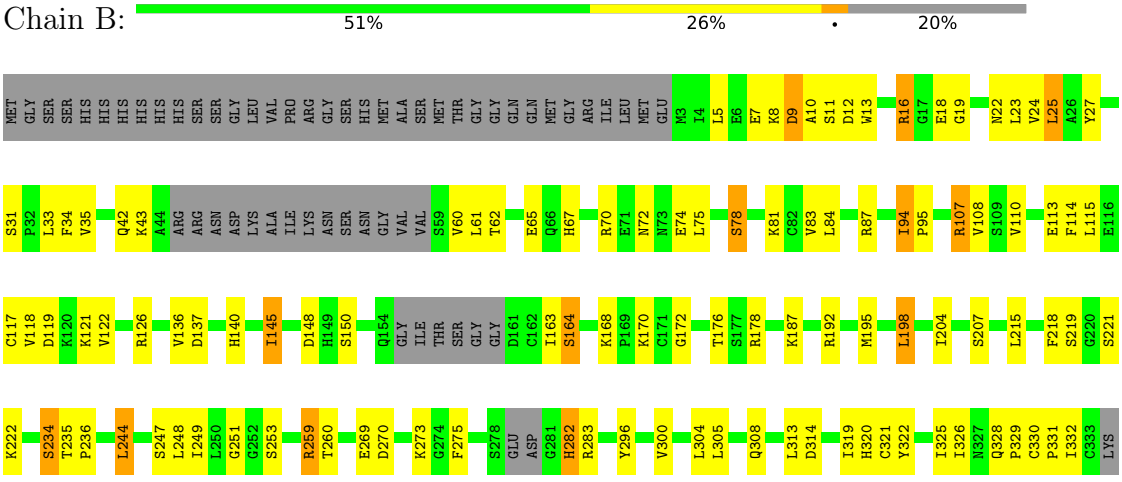
• Molecule 1: Inositol-pentakisphosphate 2-kinase

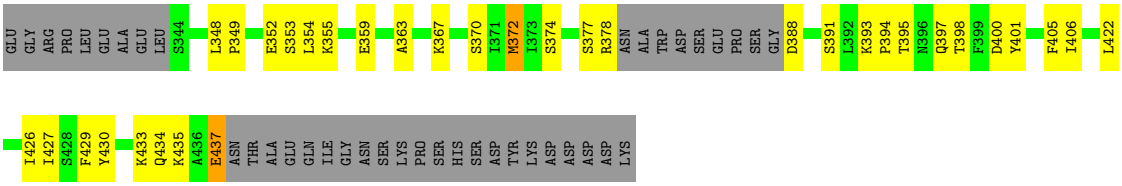
Chain A:



• Molecule 1: Inositol-pentakisphosphate 2-kinase

Chain B:




GLU GLY ARG PRO LEU GLU ALA GLU LEU S344 L348 P349 E352 S353 L354 K355 E359 A363 K367 S370 I371 M372 I373 S374 S377 R378 ASN ALA TRP ASP SER GLU PRO SER GLY D388 S391 L392 K393 P394 T395 N396 Q397 T398 F399 D400 Y401 F405 I406 L422
I426 I427 S428 F429 Y430 K433 Q434 K435 A436 E437 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	59.76Å 59.35Å 82.23Å 83.01° 89.92° 63.41°	Depositor
Resolution (Å)	34.55 – 2.60 34.55 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.4 (34.55-2.60) 90.7 (34.55-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.6.3_473	Depositor
R, R_{free}	0.224 , 0.294 0.216 , 0.288	Depositor DCC
R_{free} test set	1990 reflections (6.04%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 7.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6380	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.91% 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

5.1 Standard geometry

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

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	0.44	0/3170	0.60	0/4271
1	B	0.45	0/3192	0.58	0/4301
All	All	0.45	0/6362	0.59	0/8572

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

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	3114	0	3150	119	0
1	B	3136	0	3162	110	0
2	A	36	0	6	0	0
2	B	36	0	6	0	0
3	A	27	0	12	3	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	6380	0	6348	229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (229) 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:82:CYS:HB2	1:A:107:ARG:HE	0.99	1.07
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.18	1.04
1:A:82:CYS:HB2	1:A:107:ARG:NE	1.76	1.01
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.32	0.93
1:A:275:PHE:HD1	1:A:276:ILE:HD12	1.40	0.87
1:A:422:LEU:O	1:A:426:ILE:HG12	1.78	0.83
1:A:107:ARG:NH2	1:A:142:CYS:SG	2.51	0.83
1:B:5:LEU:HB2	1:B:110:VAL:HG12	1.60	0.83
1:A:107:ARG:HG3	1:A:107:ARG:NH1	1.93	0.80
1:B:150:SER:HA	1:B:164:SER:OG	1.82	0.79
1:B:187:LYS:HG3	1:B:427:ILE:HD13	1.65	0.78
1:A:187:LYS:HA	1:A:195:MET:HE1	1.64	0.78
1:A:82:CYS:CB	1:A:107:ARG:HE	1.89	0.77
1:B:172:GLY:HA3	1:B:218:PHE:CD2	2.20	0.77
1:B:355:LYS:O	1:B:359:GLU:HG3	1.85	0.76
1:A:275:PHE:CD1	1:A:276:ILE:HD12	2.20	0.76
1:B:27:TYR:CD2	1:B:34:PHE:HB2	2.20	0.75
1:B:74:GLU:HG2	1:B:75:LEU:N	2.04	0.73
1:B:248:LEU:HD21	1:B:251:GLY:O	1.89	0.73
1:A:31:SER:O	1:A:35:VAL:HG23	1.91	0.71
1:B:31:SER:O	1:B:35:VAL:HG23	1.91	0.71
1:B:107:ARG:HH11	1:B:107:ARG:CG	2.04	0.70
1:A:80:ASN:OD1	1:A:107:ARG:NH2	2.25	0.69
1:B:150:SER:HA	1:B:164:SER:HG	1.55	0.69
1:A:260:THR:HG23	1:A:264:ILE:CG2	2.22	0.69
1:B:244:LEU:HB2	1:B:249:ILE:HD13	1.75	0.69
1:A:204:ILE:HG22	1:A:204:ILE:O	1.91	0.68
1:B:273:LYS:HA	1:B:283:ARG:NH1	2.08	0.68
1:B:18:GLU:OE1	1:B:126:ARG:HD2	1.93	0.68
1:A:110:VAL:HG21	1:A:115:LEU:HD21	1.75	0.67
1:A:395:THR:OG1	1:A:397:GLN:HG3	1.94	0.67
1:B:325:ILE:HD12	1:B:354:LEU:HD23	1.77	0.66
1:B:269:GLU:OE2	1:B:283:ARG:HB2	1.96	0.66
1:A:66:GLN:HA	1:A:76:ILE:HD12	1.78	0.65
1:A:178:ARG:HG3	1:A:178:ARG:HH11	1.61	0.65
1:A:15:TYR:CZ	1:A:17:GLY:HA2	2.31	0.65
1:B:326:ILE:HG13	1:B:328:GLN:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:HG3	1:A:256:SER:O	1.96	0.65
1:A:172:GLY:HA3	1:A:218:PHE:CD2	2.32	0.64
1:B:108:VAL:HG11	1:B:145:ILE:HD12	1.78	0.64
1:B:222:LYS:HB3	1:B:296:TYR:CZ	2.31	0.64
1:B:282:HIS:N	1:B:282:HIS:CD2	2.65	0.64
1:A:13:TRP:O	1:A:121:LYS:HE2	1.97	0.64
1:B:422:LEU:O	1:B:426:ILE:HG12	1.97	0.64
1:B:325:ILE:HD12	1:B:354:LEU:CD2	2.28	0.64
1:B:429:PHE:CZ	1:B:433:LYS:HD2	2.32	0.64
1:B:430:TYR:O	1:B:434:GLN:HG2	1.98	0.64
1:B:235:THR:HG22	1:B:259:ARG:HB2	1.80	0.63
1:A:325:ILE:HD11	1:A:354:LEU:HA	1.81	0.63
1:B:348:LEU:HD22	1:B:352:GLU:HG2	1.79	0.62
1:B:378:ARG:HD2	1:B:400:ASP:OD1	1.98	0.62
1:A:222:LYS:NZ	1:A:293:ASP:HA	2.14	0.62
1:B:374:SER:O	1:B:401:TYR:HA	2.00	0.62
1:A:260:THR:HG23	1:A:264:ILE:HG22	1.81	0.62
1:A:106:VAL:HG12	1:A:107:ARG:N	2.14	0.61
1:A:107:ARG:NH1	1:A:107:ARG:CG	2.59	0.61
1:B:12:ASP:HB3	1:B:27:TYR:CE1	2.36	0.61
1:A:19:GLY:HA3	3:A:502:ADP:O2B	2.01	0.61
1:A:430:TYR:O	1:A:434:GLN:HG2	2.01	0.60
1:B:300:VAL:HG22	1:B:405:PHE:CZ	2.37	0.60
1:B:304:LEU:O	1:B:308:GLN:HG3	2.01	0.60
1:B:273:LYS:HA	1:B:283:ARG:CZ	2.32	0.59
1:A:149:HIS:O	1:A:374:SER:OG	2.21	0.59
1:B:12:ASP:HB3	1:B:27:TYR:HE1	1.66	0.58
1:B:363:ALA:O	1:B:367:LYS:HG3	2.03	0.58
1:A:69:TRP:HB2	1:A:76:ILE:HD11	1.84	0.58
1:A:46:ARG:HH21	1:A:135:ASN:CG	2.06	0.57
1:A:66:GLN:HA	1:A:76:ILE:CD1	2.34	0.57
1:B:62:THR:OG1	1:B:65:GLU:HG3	2.04	0.57
1:A:18:GLU:HB3	1:A:23:LEU:HD12	1.86	0.57
1:B:94:ILE:HG22	1:B:95:PRO:HD3	1.86	0.57
1:A:215:LEU:O	1:A:219:SER:HB3	2.05	0.57
1:A:3:MET:CE	1:A:33:LEU:HD13	2.35	0.57
1:B:378:ARG:HD3	1:B:398:THR:HG22	1.87	0.56
1:B:218:PHE:CD1	1:B:305:LEU:HD13	2.41	0.56
1:B:107:ARG:HG3	1:B:107:ARG:NH1	2.13	0.56
1:B:215:LEU:O	1:B:219:SER:HB3	2.06	0.55
1:A:44:ALA:HB2	1:A:137:ASP:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:HIS:O	1:B:70:ARG:HD3	2.06	0.55
1:A:106:VAL:CG1	1:A:107:ARG:N	2.70	0.55
1:A:202:GLU:HG2	1:A:429:PHE:CZ	2.41	0.55
1:B:23:LEU:HD21	1:B:122:VAL:HG21	1.89	0.54
1:A:276:ILE:HG22	1:A:283:ARG:HG2	1.89	0.54
1:B:319:ILE:O	1:B:322:TYR:HB3	2.08	0.54
1:A:275:PHE:HD1	1:A:276:ILE:CD1	2.15	0.54
1:B:74:GLU:HG2	1:B:75:LEU:H	1.73	0.54
1:B:83:VAL:HG12	1:B:87:ARG:HD2	1.89	0.54
1:A:352:GLU:O	1:A:356:ILE:HG13	2.08	0.54
1:A:40:ARG:NH1	1:A:85:GLU:OE2	2.42	0.53
1:B:27:TYR:CE2	1:B:34:PHE:HB2	2.43	0.53
1:B:195:MET:HG2	1:B:430:TYR:CD1	2.43	0.53
1:B:72:ASN:HB3	1:B:74:GLU:OE2	2.10	0.52
1:A:81:LYS:O	1:A:84:LEU:HB3	2.10	0.52
1:A:232:LEU:HB3	1:A:240:PHE:CD1	2.44	0.52
1:B:114:PHE:O	1:B:118:VAL:HG23	2.10	0.52
1:A:60:VAL:HG11	1:A:78:SER:O	2.10	0.51
1:A:222:LYS:HZ1	1:A:293:ASP:HA	1.75	0.51
1:A:319:ILE:O	1:A:322:TYR:HB3	2.10	0.51
1:A:222:LYS:HA	1:A:296:TYR:CD1	2.45	0.51
1:A:290:LEU:HD12	1:A:290:LEU:O	2.11	0.51
1:A:199:LEU:HD22	1:A:426:ILE:HD13	1.93	0.51
1:A:296:TYR:C	1:A:296:TYR:CD2	2.84	0.51
1:A:300:VAL:HG22	1:A:405:PHE:CZ	2.46	0.51
1:A:187:LYS:HG3	1:A:427:ILE:HD13	1.92	0.51
1:A:13:TRP:HB3	1:A:25:LEU:HB3	1.93	0.50
1:B:107:ARG:CG	1:B:107:ARG:NH1	2.67	0.50
1:B:7:GLU:HB2	1:B:113:GLU:HB3	1.92	0.50
1:B:74:GLU:CG	1:B:75:LEU:N	2.74	0.50
1:A:328:GLN:HG2	1:A:329:PRO:HD2	1.94	0.50
1:B:22:ASN:ND2	1:B:42:GLN:HG3	2.26	0.50
1:A:168:LYS:HB3	1:A:239:ASN:HA	1.93	0.50
1:A:300:VAL:HG23	1:A:303:ARG:HH22	1.76	0.50
1:A:25:LEU:HB2	1:A:39:ILE:HG22	1.94	0.50
1:A:15:TYR:CE2	1:A:17:GLY:HA2	2.48	0.49
1:B:393:LYS:HB3	1:B:393:LYS:NZ	2.27	0.49
1:B:329:PRO:O	1:B:331:PRO:HD3	2.13	0.49
1:A:248:LEU:HD11	1:A:250:LEU:O	2.12	0.49
1:A:325:ILE:HD12	1:A:357:VAL:HG21	1.95	0.49
1:A:4:ILE:HG12	1:A:109:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HH11	1:A:178:ARG:CG	2.24	0.49
1:B:25:LEU:HD21	1:B:118:VAL:CG1	2.42	0.49
1:A:315:ILE:HB	1:A:360:TYR:OH	2.13	0.48
1:A:3:MET:HE3	1:A:33:LEU:HD13	1.95	0.48
1:A:269:GLU:OE2	1:A:283:ARG:HB2	2.13	0.48
1:B:325:ILE:CD1	1:B:354:LEU:HD23	2.43	0.48
1:B:435:LYS:C	1:B:437:GLU:H	2.16	0.48
1:A:96:LEU:N	1:A:96:LEU:CD1	2.77	0.48
1:B:321:CYS:O	1:B:325:ILE:HG12	2.13	0.48
1:B:395:THR:HB	1:B:397:GLN:HG3	1.95	0.48
1:A:212:TYR:N	1:A:231:ALA:HB1	2.29	0.48
1:A:305:LEU:O	1:A:309:LYS:HG3	2.13	0.48
1:B:163:ILE:CD1	1:B:244:LEU:HG	2.43	0.48
1:A:107:ARG:CZ	1:A:142:CYS:HB2	2.43	0.47
1:A:61:LEU:HD13	1:A:76:ILE:HD13	1.96	0.47
1:A:148:ASP:OD1	1:A:150:SER:OG	2.23	0.47
1:B:137:ASP:CG	1:B:140:HIS:HD2	2.18	0.47
1:B:395:THR:OG1	1:B:397:GLN:HG3	2.15	0.47
1:A:40:ARG:NH2	3:A:502:ADP:O1B	2.47	0.47
1:B:222:LYS:HB3	1:B:296:TYR:CE2	2.49	0.47
1:A:60:VAL:HG23	1:A:61:LEU:N	2.30	0.47
1:A:16:ARG:HB3	1:A:24:VAL:O	2.14	0.47
1:B:81:LYS:HA	1:B:84:LEU:HB3	1.96	0.47
1:A:19:GLY:HA3	3:A:502:ADP:PB	2.55	0.47
1:A:92:VAL:O	1:A:96:LEU:HD13	2.13	0.47
1:B:395:THR:CB	1:B:397:GLN:HG3	2.44	0.47
1:A:290:LEU:HD11	1:A:375:PHE:CE2	2.50	0.47
1:B:259:ARG:CG	1:B:260:THR:N	2.78	0.47
1:B:25:LEU:HD21	1:B:118:VAL:HG11	1.96	0.46
1:A:166:GLU:HB3	1:A:241:ARG:HB2	1.98	0.46
1:A:68:LEU:O	1:A:68:LEU:HG	2.15	0.46
1:B:16:ARG:HB3	1:B:24:VAL:O	2.15	0.46
1:A:96:LEU:N	1:A:96:LEU:HD12	2.30	0.46
1:B:330:CYS:SG	1:B:332:ILE:HB	2.55	0.46
1:B:168:LYS:HE2	1:B:170:LYS:HD3	1.98	0.46
1:B:195:MET:HG2	1:B:430:TYR:CG	2.51	0.46
1:A:171:CYS:HB2	1:A:367:LYS:HG2	1.97	0.46
1:B:372:MET:HG3	1:B:406:ILE:HD13	1.96	0.46
1:A:204:ILE:O	1:A:204:ILE:CG2	2.64	0.46
1:B:234:SER:O	1:B:236:PRO:HD3	2.16	0.46
1:B:10:ALA:HB3	1:B:117:CYS:SG	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:VAL:HG12	1:A:296:TYR:N	2.31	0.45
1:B:19:GLY:HA3	3:B:502:ADP:O2B	2.14	0.45
1:B:222:LYS:HB2	1:B:222:LYS:HE3	1.71	0.45
1:B:23:LEU:HD11	1:B:126:ARG:HD3	1.98	0.45
1:A:370:SER:HB2	1:A:406:ILE:HG13	1.98	0.45
1:B:313:LEU:O	1:B:314:ASP:HB3	2.16	0.45
1:A:236:PRO:HB3	1:A:240:PHE:HB3	1.97	0.45
1:A:295:VAL:HG13	1:A:301:LEU:HD22	1.99	0.45
1:B:192:ARG:O	1:B:192:ARG:HD3	2.17	0.45
1:A:78:SER:OG	1:A:87:ARG:HD2	2.17	0.45
1:B:349:PRO:HG2	1:B:352:GLU:HB2	1.99	0.45
1:B:8:LYS:HG3	1:B:9:ASP:N	2.31	0.44
1:A:105:GLY:HA3	1:A:146:LEU:HD23	1.99	0.44
1:A:108:VAL:HG12	1:A:143:ALA:O	2.18	0.44
1:B:119:ASP:HB2	1:B:136:VAL:CG1	2.48	0.44
1:B:393:LYS:N	1:B:394:PRO:HD2	2.32	0.44
1:A:85:GLU:HB3	1:A:144:LEU:HD11	1.99	0.44
1:A:201:LEU:HD12	1:A:206:ILE:HG13	1.99	0.44
1:A:91:ASN:O	1:A:95:PRO:HG2	2.17	0.44
1:A:259:ARG:HG2	1:A:260:THR:N	2.32	0.44
1:A:64:ASP:O	1:A:67:HIS:HB3	2.18	0.44
1:B:204:ILE:O	1:B:204:ILE:HG22	2.18	0.44
1:A:61:LEU:CD1	1:A:76:ILE:HD13	2.48	0.43
1:B:198:LEU:CD2	1:B:433:LYS:HD3	2.48	0.43
1:A:27:TYR:CD2	1:A:34:PHE:HB2	2.53	0.43
1:B:18:GLU:OE2	1:B:43:LYS:NZ	2.42	0.43
1:A:82:CYS:HB2	1:A:107:ARG:CZ	2.43	0.43
1:A:166:GLU:OE1	1:A:241:ARG:HD2	2.19	0.43
1:B:137:ASP:CG	1:B:140:HIS:CD2	2.92	0.43
1:A:249:ILE:HG13	1:A:268:PHE:CE1	2.53	0.43
1:B:325:ILE:HD11	1:B:353:SER:HB2	2.00	0.43
1:B:119:ASP:HB2	1:B:136:VAL:HG13	2.00	0.42
1:A:6:GLU:O	1:A:114:PHE:HD1	2.02	0.42
1:B:282:HIS:N	1:B:282:HIS:HD2	2.16	0.42
1:B:378:ARG:HD3	1:B:398:THR:CG2	2.49	0.42
1:A:248:LEU:HD21	1:A:251:GLY:O	2.19	0.42
1:B:60:VAL:HG21	1:B:78:SER:O	2.20	0.42
1:B:163:ILE:HD13	1:B:244:LEU:HG	2.00	0.42
1:A:277:GLN:HA	1:A:277:GLN:OE1	2.20	0.42
1:A:284:THR:O	1:A:288:LEU:HG	2.20	0.42
1:A:313:LEU:O	1:A:314:ASP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:O	1:B:121:LYS:HE2	2.20	0.42
1:B:27:TYR:OH	1:B:31:SER:HB3	2.20	0.42
1:B:110:VAL:HG21	1:B:115:LEU:HD21	2.02	0.42
1:A:27:TYR:CE2	1:A:34:PHE:HB2	2.55	0.41
1:A:218:PHE:CE1	1:A:301:LEU:HG	2.55	0.41
1:A:392:LEU:O	1:A:396:ASN:HA	2.20	0.41
1:B:16:ARG:NH2	1:B:150:SER:OG	2.52	0.41
1:A:274:GLY:O	1:A:275:PHE:C	2.58	0.41
1:B:198:LEU:HD22	1:B:433:LYS:HD3	2.02	0.41
1:A:414:LYS:O	1:A:414:LYS:HG3	2.20	0.41
1:B:319:ILE:HG23	1:B:320:HIS:N	2.34	0.41
1:A:97:LEU:O	1:A:303:ARG:NE	2.53	0.41
1:A:294:ALA:O	1:A:298:SER:HB3	2.21	0.41
1:B:163:ILE:HG13	1:B:275:PHE:CE1	2.55	0.41
1:A:118:VAL:O	1:A:122:VAL:HG22	2.20	0.41
1:A:298:SER:OG	1:A:300:VAL:HB	2.19	0.41
1:A:259:ARG:CG	1:A:260:THR:N	2.84	0.41
1:A:389:TYR:CD1	1:A:389:TYR:C	2.94	0.41
1:B:74:GLU:CG	1:B:75:LEU:H	2.33	0.41
1:A:6:GLU:HA	1:A:111:SER:OG	2.20	0.41
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.88	0.41
1:B:437:GLU:HG2	1:B:437:GLU:O	2.21	0.41
1:B:395:THR:C	1:B:397:GLN:H	2.24	0.41
1:B:60:VAL:HG13	1:B:61:LEU:N	2.35	0.40
1:B:329:PRO:O	1:B:331:PRO:CD	2.69	0.40
1:A:251:GLY:HA2	1:A:257:THR:HG21	2.03	0.40
1:B:330:CYS:HA	1:B:331:PRO:HD2	1.93	0.40
1:B:148:ASP:C	1:B:148:ASP:OD1	2.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/493 (77%)	350 (93%)	23 (6%)	5 (1%)	12	24
1	B	382/493 (78%)	356 (93%)	24 (6%)	2 (0%)	29	52
All	All	760/986 (77%)	706 (93%)	47 (6%)	7 (1%)	17	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	394	PRO
1	A	182	LYS
1	A	314	ASP
1	A	436	ALA
1	B	234	SER
1	A	275	PHE
1	B	178	ARG

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	350/434 (81%)	329 (94%)	21 (6%)	19	39
1	B	353/434 (81%)	328 (93%)	25 (7%)	14	29
All	All	703/868 (81%)	657 (94%)	46 (6%)	17	34

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	80	ASN
1	A	107	ARG
1	A	163	ILE
1	A	164	SER
1	A	176	THR
1	A	186	LEU
1	A	191	SER
1	A	192	ARG

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Mol	Chain	Res	Type
1	A	202	GLU
1	A	208	GLU
1	A	244	LEU
1	A	256	SER
1	A	278	SER
1	A	290	LEU
1	A	298	SER
1	A	301	LEU
1	A	328	GLN
1	A	391	SER
1	A	395	THR
1	A	418	SER
1	B	9	ASP
1	B	11	SER
1	B	16	ARG
1	B	25	LEU
1	B	78	SER
1	B	94	ILE
1	B	107	ARG
1	B	145	ILE
1	B	164	SER
1	B	176	THR
1	B	198	LEU
1	B	207	SER
1	B	221	SER
1	B	244	LEU
1	B	247	SER
1	B	253	SER
1	B	259	ARG
1	B	270	ASP
1	B	282	HIS
1	B	370	SER
1	B	372	MET
1	B	377	SER
1	B	388	ASP
1	B	391	SER
1	B	437	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS

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Mol	Chain	Res	Type
1	A	147	ASN
1	A	196	HIS
1	B	72	ASN
1	B	140	HIS
1	B	147	ASN
1	B	196	HIS
1	B	282	HIS

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	$\#\|Z\| > 2$
2	IHP	B	501	4	36,36,36	1.06	1 (2%)	54,60,60	1.23	5 (9%)
2	IHP	A	501	-	36,36,36	1.11	1 (2%)	54,60,60	1.25	6 (11%)
3	ADP	B	502	4	24,29,29	1.07	2 (8%)	29,45,45	1.25	3 (10%)
3	ADP	A	502	4	24,29,29	1.05	2 (8%)	29,45,45	1.43	5 (17%)

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	IHP	B	501	4	-	5/30/54/54	0/1/1/1
2	IHP	A	501	-	-	4/30/54/54	0/1/1/1
3	ADP	B	502	4	-	2/12/32/32	0/3/3/3
3	ADP	A	502	4	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ADP	C5-C4	2.75	1.48	1.40
3	A	502	ADP	C5-C4	2.75	1.48	1.40
3	B	502	ADP	O4'-C1'	2.74	1.44	1.41
3	A	502	ADP	O4'-C1'	2.50	1.44	1.41
2	B	501	IHP	C2-C1	-2.18	1.47	1.52
2	A	501	IHP	O12-C2	-2.04	1.36	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	IHP	C4-C3-C2	-4.15	101.33	110.41
2	B	501	IHP	O11-C1-C6	3.88	117.83	108.69
2	A	501	IHP	C6-C1-C2	-3.82	102.06	110.41
2	B	501	IHP	C6-C1-C2	-3.64	102.43	110.41
2	B	501	IHP	C4-C3-C2	-3.43	102.90	110.41
3	A	502	ADP	C3'-C2'-C1'	3.20	105.80	100.98
3	B	502	ADP	N3-C2-N1	-3.06	123.90	128.68
3	A	502	ADP	N3-C2-N1	-3.02	123.97	128.68
3	B	502	ADP	PA-O3A-PB	-3.01	122.50	132.83
3	A	502	ADP	PA-O3A-PB	-2.87	122.98	132.83
2	A	501	IHP	C3-C2-C1	-2.59	104.75	110.41
2	A	501	IHP	O14-C4-C5	2.40	114.35	108.69
2	B	501	IHP	C6-C5-C4	2.39	115.65	110.41
2	A	501	IHP	C6-C5-C4	2.30	115.44	110.41
2	B	501	IHP	O12-C2-C3	2.27	114.03	108.69
3	A	502	ADP	O3B-PB-O3A	2.24	112.16	104.64
3	A	502	ADP	C4-C5-N7	-2.20	107.10	109.40
3	B	502	ADP	C4-C5-N7	-2.17	107.14	109.40
2	A	501	IHP	O13-C3-C2	2.14	113.72	108.69

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	ADP	C5'-O5'-PA-O1A
2	A	501	IHP	C3-O13-P3-O23
2	B	501	IHP	C3-O13-P3-O23
3	B	502	ADP	C5'-O5'-PA-O3A
2	A	501	IHP	C4-O14-P4-O24
2	B	501	IHP	C4-O14-P4-O24
2	A	501	IHP	C2-O12-P2-O32
2	A	501	IHP	C4-O14-P4-O44
2	B	501	IHP	C2-O12-P2-O32
2	B	501	IHP	C3-O13-P3-O33
2	B	501	IHP	C4-O14-P4-O44

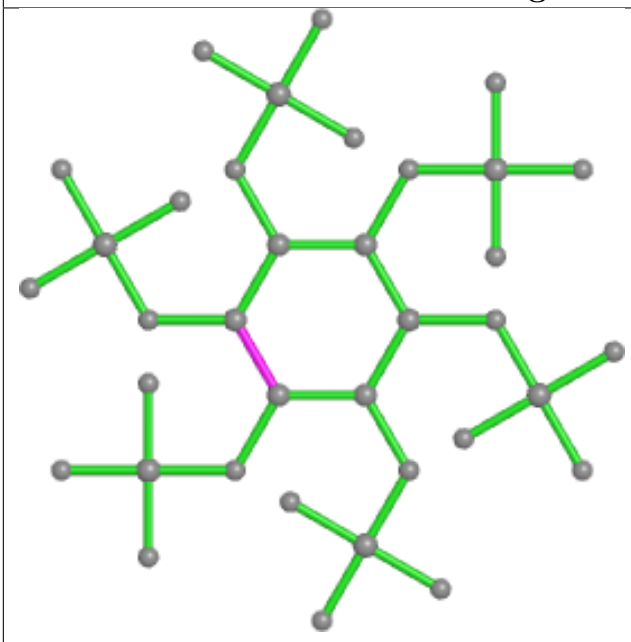
There are no ring outliers.

2 monomers are involved in 4 short contacts:

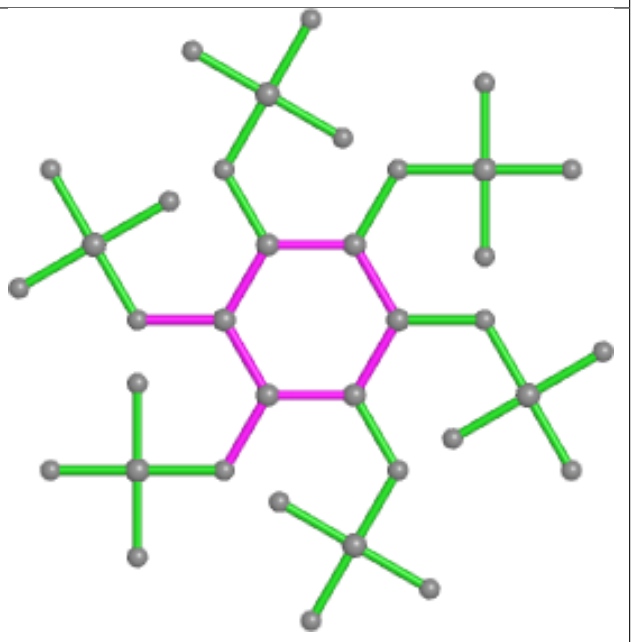
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	ADP	1	0
3	A	502	ADP	3	0

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.

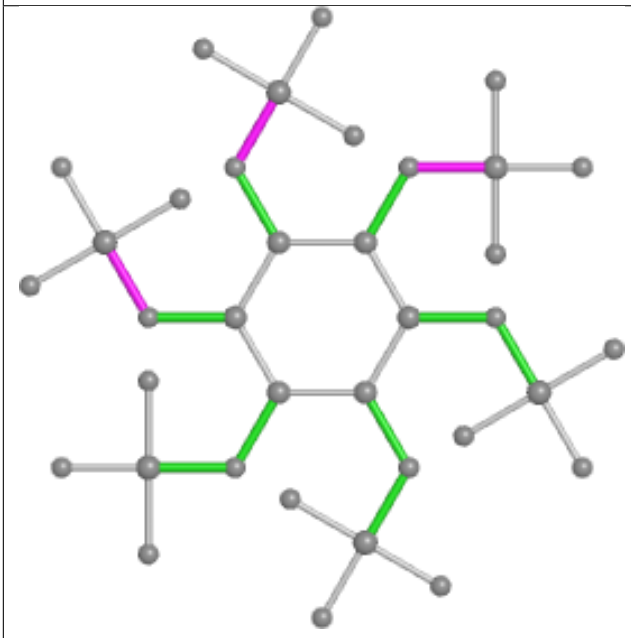
Ligand IHP B 501



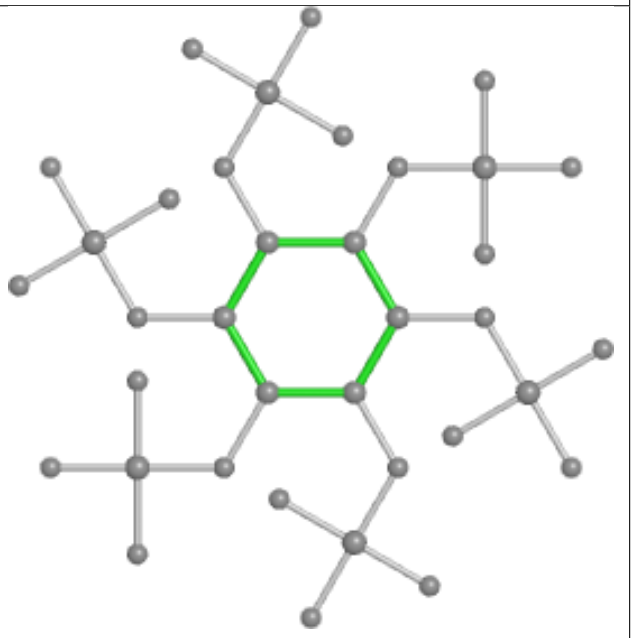
Bond lengths



Bond angles

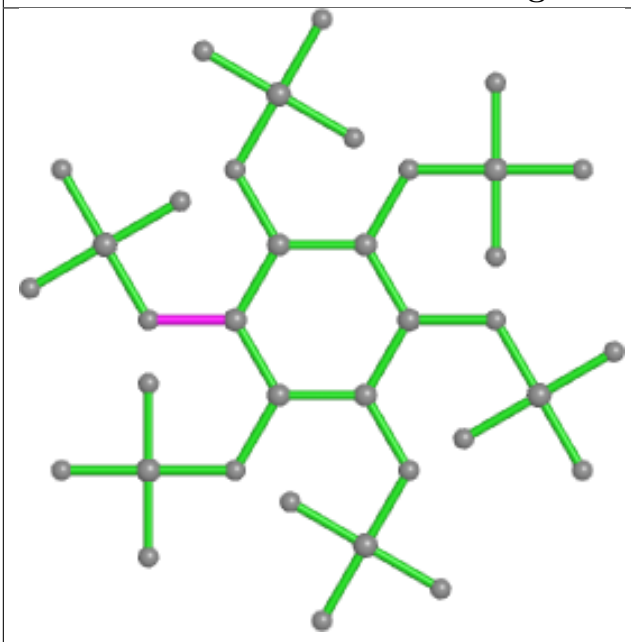


Torsions

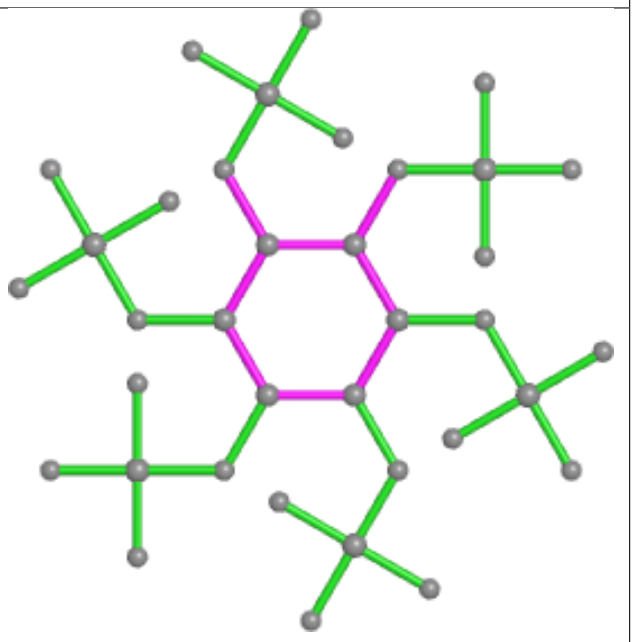


Rings

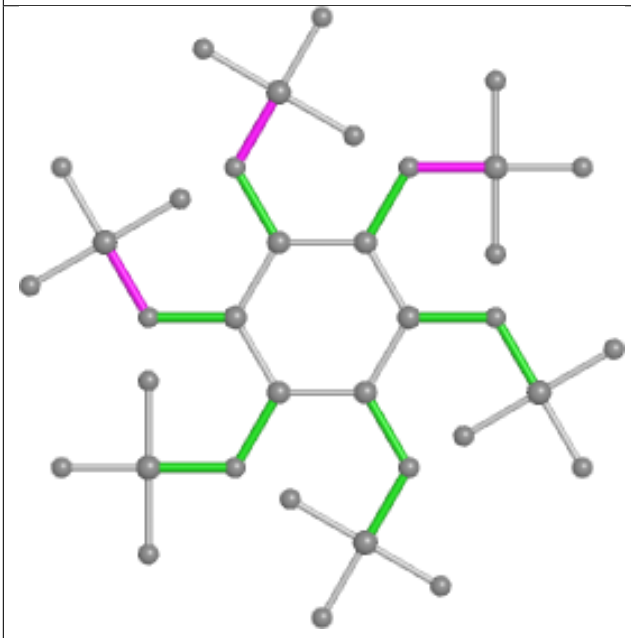
Ligand IHP A 501



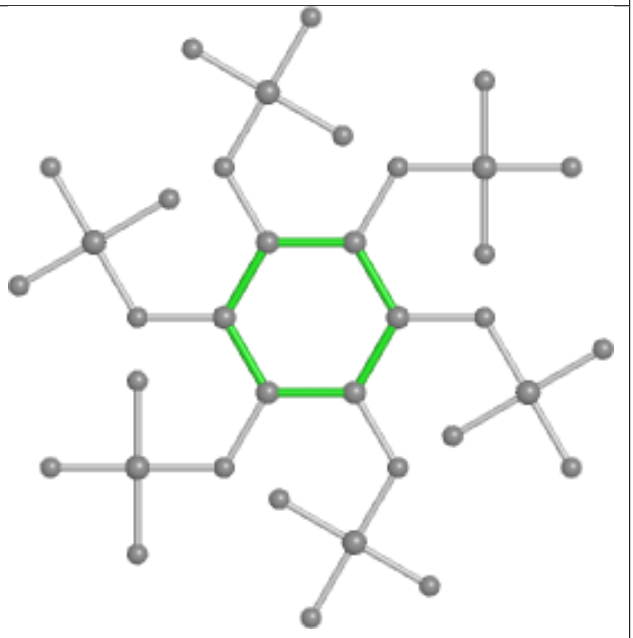
Bond lengths



Bond angles

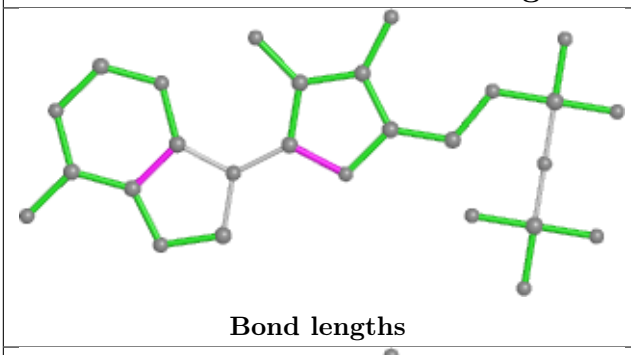


Torsions

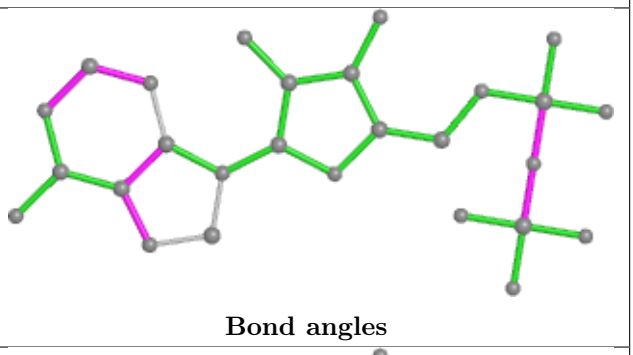


Rings

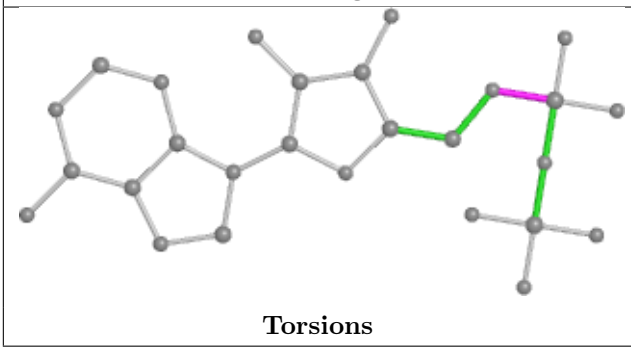
Ligand ADP B 502



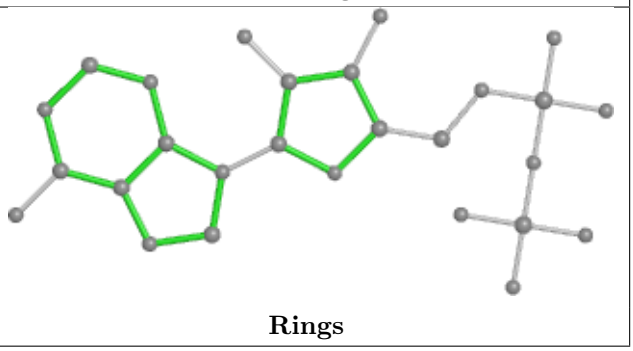
Bond lengths



Bond angles

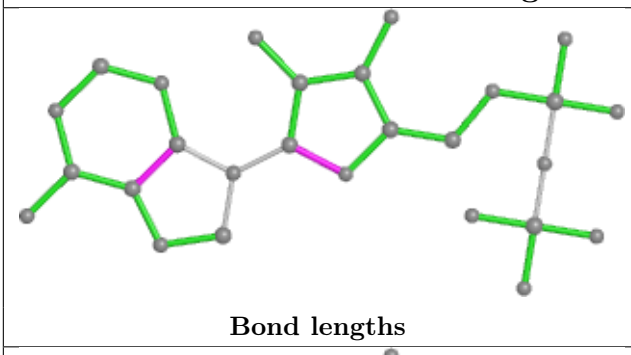


Torsions

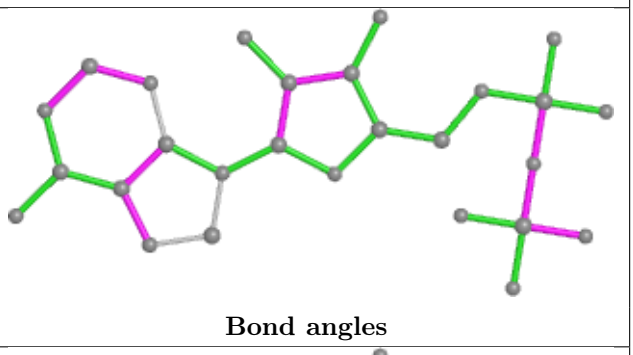


Rings

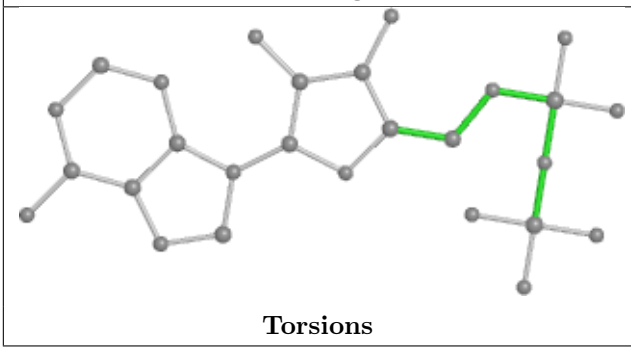
Ligand ADP A 502



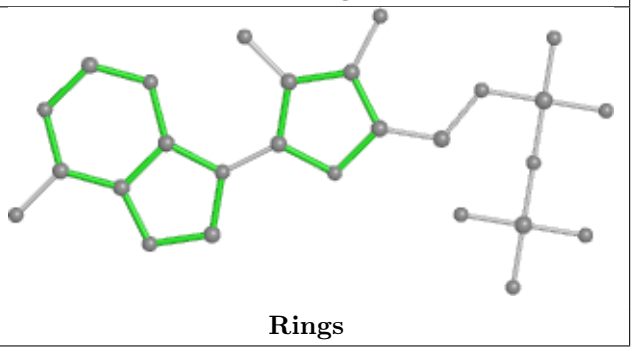
Bond lengths



Bond angles



Torsions



Rings

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

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, 95^{th} 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	390/493 (79%)	-0.73	0	100	100	13, 32, 56, 80	0
1	B	394/493 (79%)	-0.76	0	100	100	13, 29, 54, 82	0
All	All	784/986 (79%)	-0.74	0	100	100	13, 31, 55, 82	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	502	27/27	0.92	0.14	23,33,45,53	0
3	ADP	B	502	27/27	0.93	0.13	19,27,38,42	0
4	MG	A	503	1/1	0.98	0.12	29,29,29,29	0
4	MG	B	503	1/1	0.98	0.10	29,29,29,29	0
2	IHP	A	501	36/36	0.99	0.09	13,19,27,32	0
2	IHP	B	501	36/36	0.99	0.10	11,20,31,32	0
5	ZN	A	504	1/1	0.99	0.10	23,23,23,23	0

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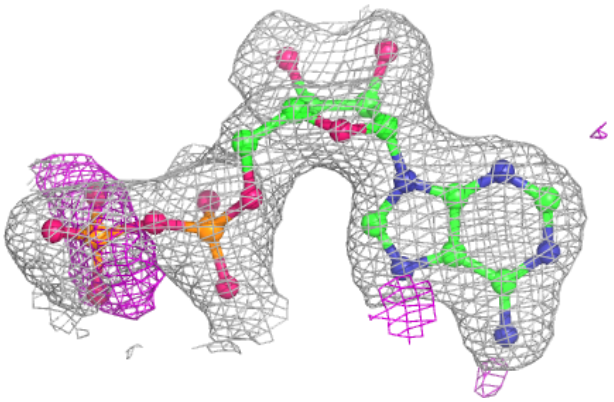
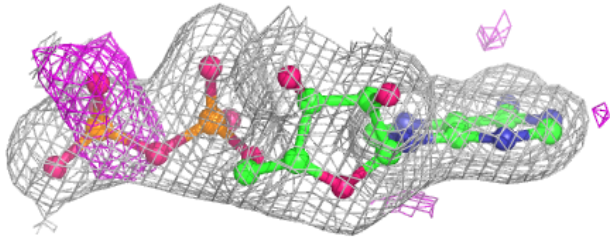
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	B	504	1/1	0.99	0.11	27,27,27,27	0

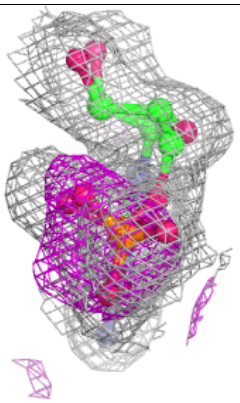
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 502:

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

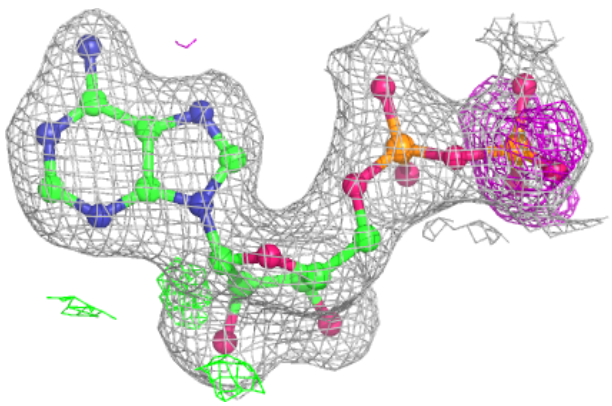


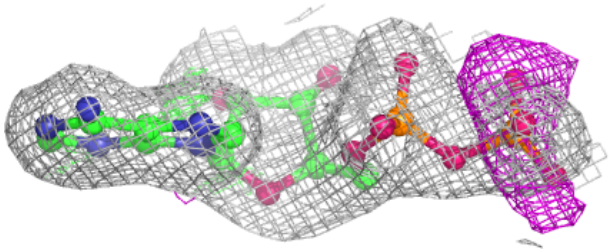


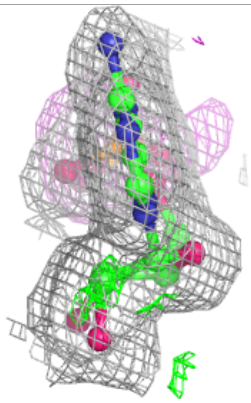


Electron density around ADP B 502:

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

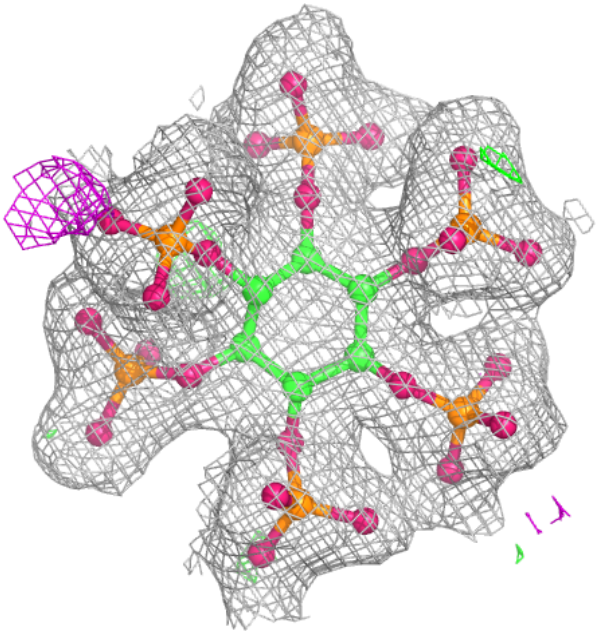


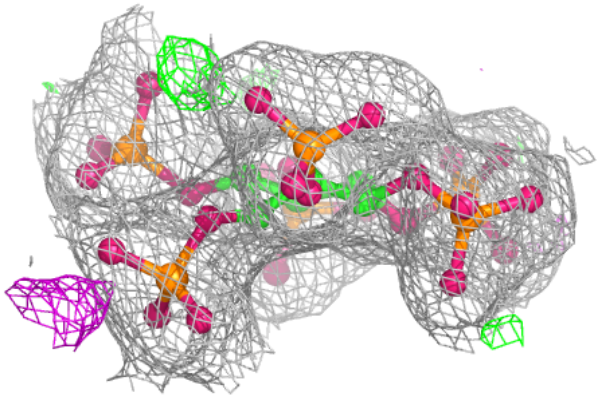


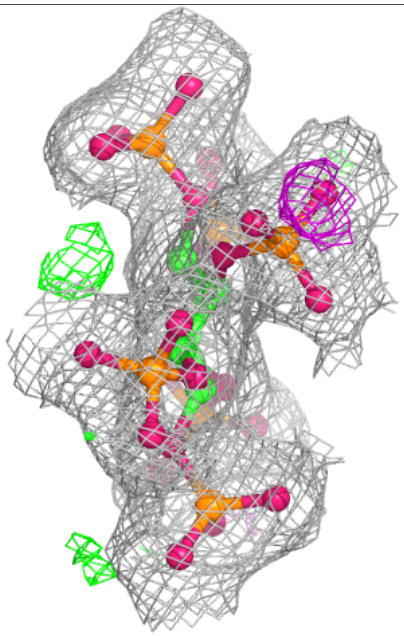


Electron density around IHP A 501:

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

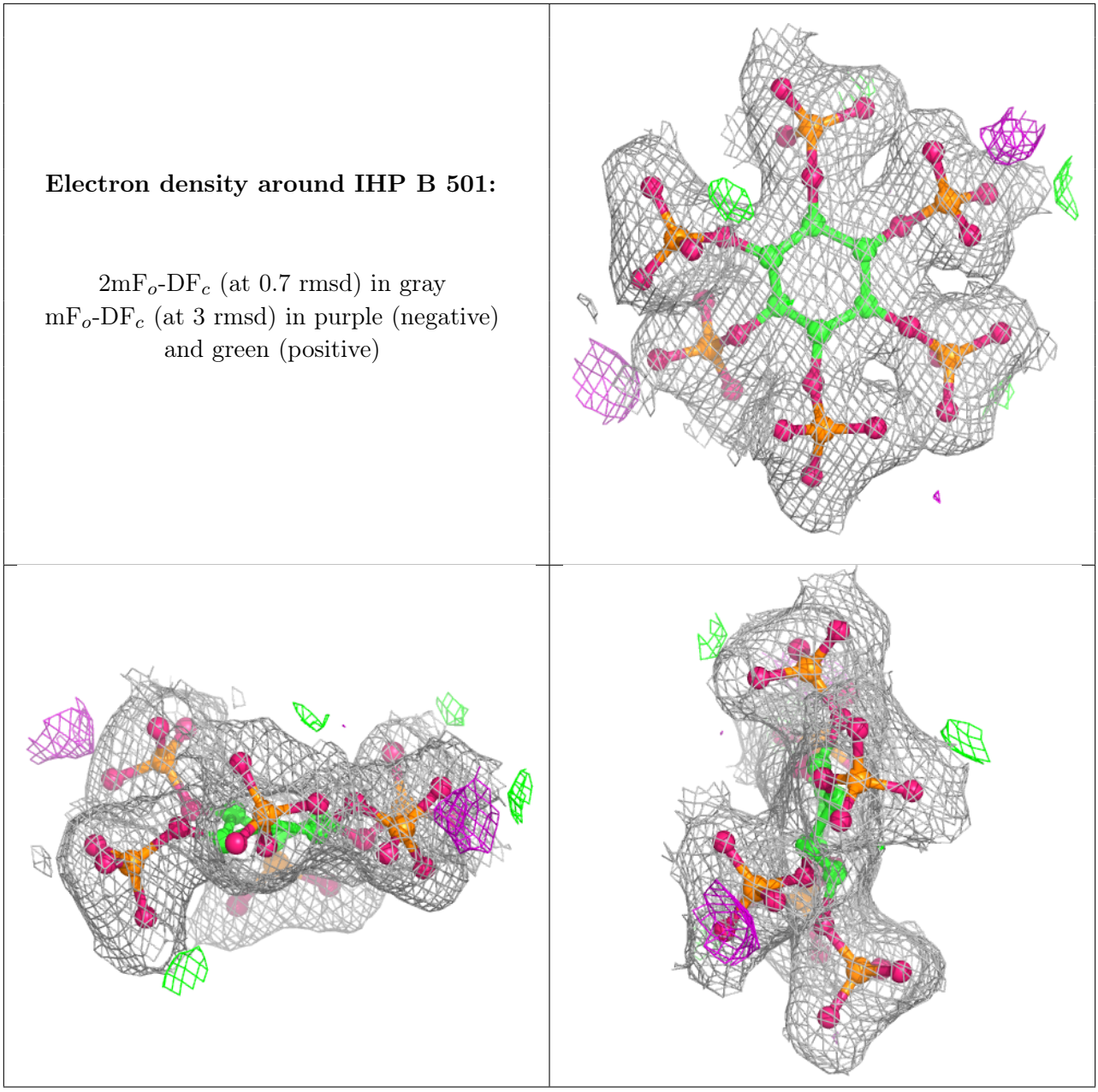






Electron density around IHP B 501:

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



6.5 Other polymers

There are no such residues in this entry.