Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 10:34 pm GMT

PDB ID	:	2V7Y
Title	:	Crystal structure of the molecular chaperone DnaK from Geobacillus kaustophilus HTA426 in post-ATP hydrolysis state
Authors	:	Chang, Y.-W.; Sun, Y.-J.; Wang, C.; Hsiao, C.-D.
Deposited on	:	2007-08-02
Resolution	:	2.37 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:

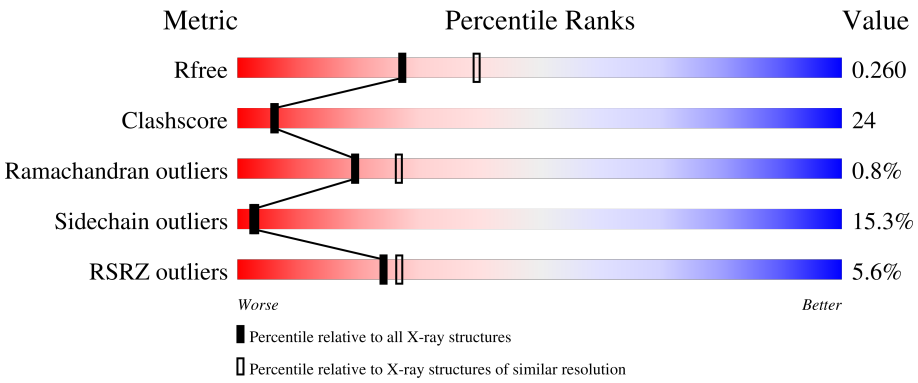
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

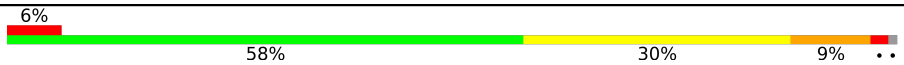
The reported resolution of this entry is 2.37 Å.

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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	509	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	1507	-	-	-	X

2 Entry composition (i)

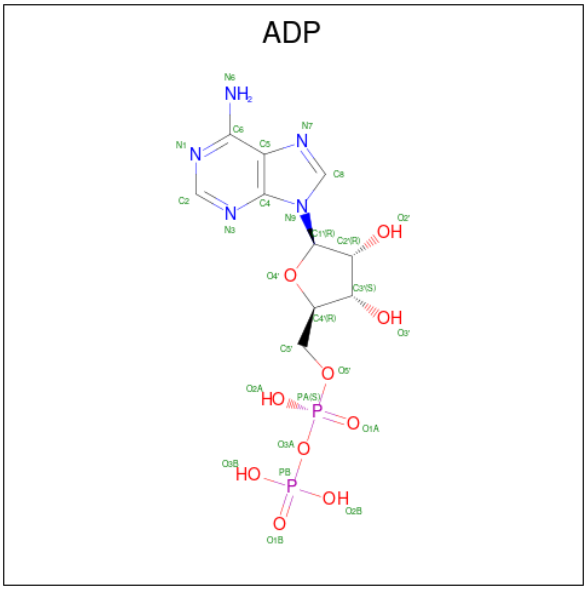
There are 5 unique types of molecules in this entry. The entry contains 3919 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHAPERONE PROTEIN DNAK.

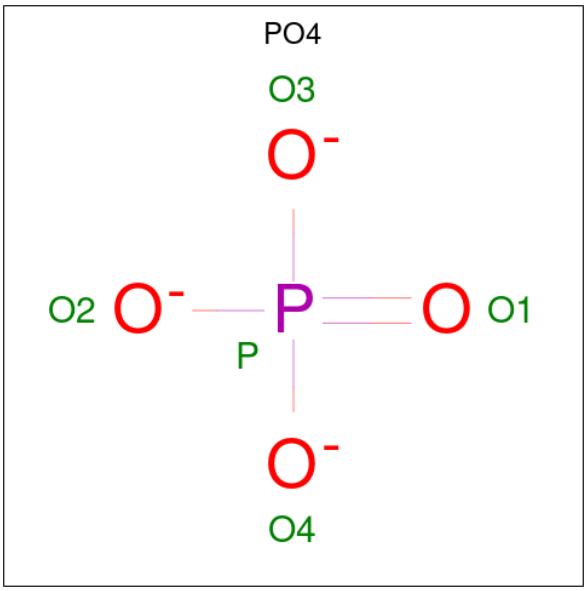
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	504	3720	2330	644	738	8	0	0	0

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



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

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

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

- Molecule 5 is water.

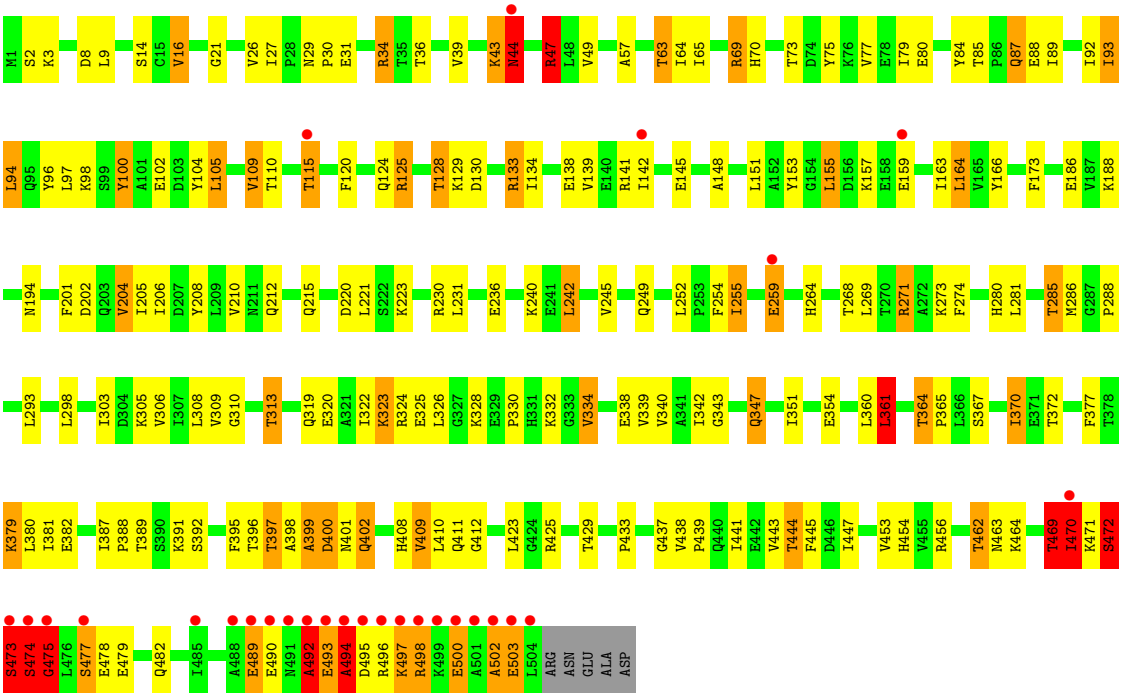
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	166	Total O 166 166	0	0

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: CHAPERONE PROTEIN DNAK

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.75Å 71.45Å 183.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.58 – 2.37 29.58 – 2.37	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.58-2.37) 89.3 (29.58-2.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.36Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.270 0.217 , 0.260	Depositor DCC
R_{free} test set	1351 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3919	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, PO4

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	0.66	8/3770 (0.2%)	1.12	48/5122 (0.9%)

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	1	21

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	ALA	C-N	-9.68	1.11	1.34
1	A	492	ALA	C-N	8.70	1.54	1.34
1	A	201	PHE	C-N	-8.14	1.15	1.34
1	A	204	VAL	C-N	-7.67	1.16	1.34
1	A	43	LYS	C-N	6.93	1.50	1.34
1	A	503	GLU	C-N	-6.03	1.20	1.34
1	A	44	ASN	C-N	5.96	1.43	1.33
1	A	93	ILE	C-N	-5.40	1.21	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	VAL	O-C-N	-11.60	104.15	122.70
1	A	44	ASN	CA-C-N	-10.71	94.79	116.20
1	A	69	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	A	502	ALA	C-N-CA	10.31	147.48	121.70
1	A	125	ARG	NE-CZ-NH2	10.24	125.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	GLN	CB-CA-C	9.99	130.39	110.40
1	A	43	LYS	C-N-CA	-9.13	98.87	121.70
1	A	44	ASN	CA-C-O	8.95	138.89	120.10
1	A	473	SER	C-N-CA	8.92	143.99	121.70
1	A	472	SER	C-N-CA	8.89	143.93	121.70
1	A	492	ALA	C-N-CA	-8.88	99.51	121.70
1	A	202	ASP	CB-CG-OD1	8.79	126.21	118.30
1	A	494	ALA	C-N-CA	8.18	142.16	121.70
1	A	96	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	A	474	SER	CA-C-N	-7.74	100.71	116.20
1	A	470	ILE	CA-C-N	-7.30	101.14	117.20
1	A	470	ILE	C-N-CA	-7.24	103.60	121.70
1	A	473	SER	CA-C-N	-7.12	101.54	117.20
1	A	503	GLU	C-N-CA	6.93	139.02	121.70
1	A	47	ARG	O-C-N	-6.68	112.01	122.70
1	A	204	VAL	CA-CB-CG2	6.53	120.69	110.90
1	A	496	ARG	C-N-CA	6.40	137.70	121.70
1	A	475	GLY	C-N-CA	-6.21	106.19	121.70
1	A	400	ASP	CB-CG-OD1	6.18	123.87	118.30
1	A	493	GLU	O-C-N	-6.17	112.83	122.70
1	A	473	SER	O-C-N	6.14	132.52	122.70
1	A	47	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	469	THR	CA-CB-OG1	6.07	121.74	109.00
1	A	498	ARG	O-C-N	-5.96	113.17	122.70
1	A	402	GLN	O-C-N	5.95	132.22	122.70
1	A	492	ALA	CA-C-N	-5.88	104.26	117.20
1	A	125	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	361	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	478	GLU	CA-C-N	-5.65	104.77	117.20
1	A	21	GLY	N-CA-C	-5.62	99.05	113.10
1	A	470	ILE	O-C-N	5.51	131.52	122.70
1	A	69	ARG	CD-NE-CZ	5.48	131.27	123.60
1	A	469	THR	CA-CB-CG2	5.43	120.00	112.40
1	A	498	ARG	C-N-CA	5.37	135.13	121.70
1	A	204	VAL	CA-C-N	5.37	129.02	117.20
1	A	63	THR	N-CA-C	-5.37	96.51	111.00
1	A	204	VAL	CA-CB-CG1	5.35	118.93	110.90
1	A	402	GLN	C-N-CA	5.34	135.05	121.70
1	A	479	GLU	CA-C-N	-5.26	105.63	117.20
1	A	479	GLU	O-C-N	5.25	131.09	122.70
1	A	204	VAL	CG1-CB-CG2	5.24	119.28	110.90
1	A	502	ALA	CA-C-N	-5.13	105.91	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	477	SER	N-CA-CB	5.11	118.16	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	ILE	CB

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Mainchain
1	A	204	VAL	Mainchain
1	A	44	ASN	Mainchain
1	A	47	ARG	Mainchain
1	A	470	ILE	Peptide
1	A	472	SER	Mainchain,Peptide
1	A	473	SER	Peptide
1	A	474	SER	Mainchain
1	A	475	GLY	Mainchain
1	A	492	ALA	Mainchain,Peptide
1	A	493	GLU	Mainchain,Peptide
1	A	494	ALA	Mainchain,Peptide
1	A	495	ASP	Mainchain,Peptide
1	A	498	ARG	Mainchain
1	A	503	GLU	Mainchain,Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3720	0	3674	182	0
2	A	27	0	12	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	166	0	0	1	0
All	All	3919	0	3686	182	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 24.

All (182) 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:472:SER:HA	1:A:474:SER:CB	1.41	1.51
1:A:47:ARG:CG	1:A:47:ARG:HH11	1.33	1.32
1:A:472:SER:HA	1:A:474:SER:CA	1.63	1.29
1:A:472:SER:CA	1:A:474:SER:CB	2.18	1.20
1:A:47:ARG:HH11	1:A:47:ARG:HG2	0.95	1.11
1:A:47:ARG:HG2	1:A:47:ARG:NH1	1.55	1.03
1:A:286:MET:SD	1:A:325:GLU:HG3	2.04	0.98
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.28	0.96
1:A:472:SER:CB	1:A:474:SER:CB	2.44	0.94
1:A:129:LYS:NZ	1:A:142:ILE:HD13	1.82	0.94
1:A:285:THR:HG22	1:A:286:MET:HE2	1.53	0.91
1:A:87:GLN:H	1:A:87:GLN:HE21	0.96	0.88
1:A:70:HIS:O	1:A:73:THR:HB	1.72	0.88
1:A:73:THR:HG22	1:A:75:TYR:H	1.40	0.85
1:A:47:ARG:CG	1:A:47:ARG:NH1	2.09	0.85
1:A:401:ASN:OD1	1:A:433:PRO:HB3	1.76	0.84
1:A:471:LYS:O	1:A:474:SER:HA	1.79	0.83
1:A:472:SER:HA	1:A:474:SER:HA	1.61	0.82
1:A:254:PHE:H	1:A:264:HIS:CD2	1.99	0.81
1:A:129:LYS:HZ2	1:A:142:ILE:HD13	1.46	0.80
1:A:166:TYR:OH	1:A:285:THR:HG21	1.81	0.80
1:A:444:THR:HG21	1:A:456:ARG:HH21	1.44	0.79
1:A:249:GLN:NE2	1:A:268:THR:HB	1.98	0.79
1:A:87:GLN:HE21	1:A:87:GLN:N	1.78	0.78
1:A:133:ARG:CG	1:A:133:ARG:HH21	1.96	0.78
1:A:205:ILE:HD11	1:A:274:PHE:CD1	2.18	0.78
1:A:254:PHE:H	1:A:264:HIS:HD2	1.32	0.78
1:A:87:GLN:H	1:A:87:GLN:NE2	1.77	0.78
1:A:155:LEU:HD23	1:A:163:ILE:HD13	1.67	0.76
1:A:379:LYS:HB3	1:A:379:LYS:HZ3	1.50	0.76
1:A:411:GLN:HB2	1:A:423:LEU:HD11	1.68	0.74
1:A:129:LYS:HZ3	1:A:142:ILE:HD13	1.54	0.73
1:A:129:LYS:HG3	1:A:142:ILE:HD11	1.70	0.71
1:A:206:ILE:O	1:A:210:VAL:HG13	1.90	0.71
1:A:379:LYS:HB3	1:A:379:LYS:NZ	2.06	0.71
1:A:39:VAL:HB	1:A:65:ILE:HD13	1.71	0.70
1:A:454:HIS:HD2	1:A:469:THR:HG22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:LEU:HB3	1:A:470:ILE:HG13	1.75	0.68
1:A:389:THR:HG23	1:A:447:ILE:HD13	1.75	0.68
1:A:472:SER:CA	1:A:474:SER:CA	2.57	0.68
1:A:102:GLU:CG	1:A:109:VAL:HG13	2.24	0.67
1:A:389:THR:CG2	1:A:447:ILE:HD13	2.24	0.67
1:A:26:VAL:CG2	1:A:342:ILE:HD11	2.25	0.67
1:A:89:ILE:O	1:A:93:ILE:HD12	1.94	0.67
1:A:489:GLU:O	1:A:492:ALA:HB2	1.95	0.67
1:A:64:ILE:CD1	1:A:77:VAL:HG21	2.26	0.66
1:A:462:THR:HG22	1:A:464:LYS:H	1.60	0.66
1:A:133:ARG:HH21	1:A:133:ARG:HG3	1.60	0.65
1:A:115:THR:HG23	1:A:145:GLU:CG	2.27	0.64
1:A:64:ILE:HD12	1:A:77:VAL:HG21	1.80	0.64
1:A:367:SER:CB	1:A:379:LYS:HE2	2.28	0.63
1:A:102:GLU:HG2	1:A:109:VAL:HG13	1.80	0.63
1:A:447:ILE:N	1:A:447:ILE:HD12	2.14	0.63
1:A:220:ASP:OD2	1:A:223:LYS:HG3	2.00	0.62
1:A:361:LEU:O	1:A:361:LEU:HD13	2.00	0.62
1:A:205:ILE:HD11	1:A:274:PHE:HD1	1.63	0.62
1:A:205:ILE:HD12	1:A:269:LEU:HD21	1.81	0.61
1:A:249:GLN:HE22	1:A:268:THR:HB	1.64	0.60
1:A:153:TYR:CZ	1:A:334:VAL:HG13	2.37	0.60
1:A:186:GLU:HG2	1:A:188:LYS:HE2	1.84	0.60
1:A:285:THR:HG22	1:A:286:MET:CE	2.27	0.60
1:A:308:LEU:HB3	1:A:313:THR:HG21	1.83	0.60
1:A:115:THR:HG21	1:A:340:VAL:HG11	1.84	0.60
1:A:164:LEU:HD23	1:A:303:ILE:HD11	1.83	0.60
1:A:423:LEU:HB3	1:A:470:ILE:CG1	2.32	0.60
1:A:347:GLN:HE21	1:A:347:GLN:HA	1.67	0.59
1:A:381:ILE:HD11	1:A:391:LYS:HB2	1.84	0.59
1:A:379:LYS:NZ	1:A:379:LYS:CB	2.65	0.59
1:A:73:THR:HG22	1:A:75:TYR:N	2.14	0.59
1:A:115:THR:HG21	1:A:340:VAL:CG1	2.34	0.58
1:A:16:VAL:HG22	1:A:27:ILE:HD12	1.84	0.57
1:A:221:LEU:HD22	1:A:255:ILE:HD12	1.86	0.57
1:A:367:SER:HB3	1:A:379:LYS:HE2	1.85	0.57
1:A:102:GLU:HG3	1:A:109:VAL:HG13	1.87	0.56
1:A:494:ALA:O	1:A:497:LYS:CB	2.53	0.56
1:A:367:SER:HB3	1:A:379:LYS:NZ	2.21	0.56
1:A:320:GLU:OE2	1:A:324:ARG:HD2	2.05	0.56
1:A:293:LEU:HD21	1:A:303:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:HG2	1:A:330:PRO:HD3	1.88	0.56
1:A:462:THR:O	1:A:463:ASN:HB2	2.05	0.56
1:A:29:ASN:HB2	1:A:30:PRO:CD	2.36	0.55
1:A:409:VAL:HG22	1:A:423:LEU:HB2	1.87	0.55
1:A:115:THR:HG23	1:A:145:GLU:HG3	1.87	0.55
1:A:367:SER:HB2	1:A:412:GLY:O	2.06	0.54
1:A:29:ASN:HB2	1:A:30:PRO:HD2	1.90	0.54
1:A:381:ILE:HD11	1:A:391:LYS:CB	2.37	0.54
1:A:159:GLU:CD	1:A:159:GLU:H	2.11	0.53
1:A:361:LEU:O	1:A:361:LEU:CD1	2.56	0.53
1:A:462:THR:HG22	1:A:464:LYS:N	2.23	0.53
1:A:115:THR:HG23	1:A:145:GLU:HG2	1.89	0.53
1:A:26:VAL:HG22	1:A:342:ILE:HD11	1.91	0.53
1:A:306:VAL:HG21	1:A:326:LEU:HD23	1.91	0.53
1:A:9:LEU:HD13	1:A:94:LEU:HD13	1.91	0.52
1:A:398:ALA:N	1:A:402:GLN:OE1	2.40	0.52
1:A:392:SER:OG	1:A:444:THR:HB	2.10	0.52
1:A:133:ARG:HG3	1:A:133:ARG:NH2	2.23	0.52
1:A:133:ARG:HH21	1:A:133:ARG:HG2	1.74	0.52
1:A:454:HIS:HD2	1:A:469:THR:CG2	2.21	0.52
1:A:57:ALA:HA	1:A:63:THR:HG21	1.92	0.51
1:A:367:SER:HB3	1:A:379:LYS:CE	2.41	0.51
1:A:347:GLN:O	1:A:351:ILE:HG12	2.10	0.51
1:A:164:LEU:HD23	1:A:303:ILE:CD1	2.40	0.51
1:A:443:VAL:HA	1:A:456:ARG:O	2.11	0.51
1:A:69:ARG:NH2	1:A:194:ASN:O	2.37	0.50
1:A:104:TYR:HD1	1:A:105:LEU:HD13	1.77	0.50
1:A:139:VAL:HG11	1:A:142:ILE:HD11	1.92	0.49
1:A:242:LEU:O	1:A:271:ARG:HD2	2.12	0.49
1:A:328:LYS:NZ	1:A:328:LYS:HB3	2.27	0.49
1:A:186:GLU:HG2	1:A:188:LYS:HD3	1.94	0.49
1:A:306:VAL:CG2	1:A:326:LEU:HD23	2.42	0.49
1:A:286:MET:SD	1:A:325:GLU:CG	2.91	0.49
1:A:380:LEU:O	1:A:391:LYS:HG2	2.11	0.49
1:A:26:VAL:HG23	1:A:342:ILE:HD11	1.94	0.49
1:A:115:THR:CG2	1:A:145:GLU:HG2	2.43	0.49
1:A:79:ILE:HD12	1:A:79:ILE:N	2.28	0.48
1:A:319:GLN:HE22	1:A:332:LYS:NZ	2.11	0.48
1:A:64:ILE:HD11	1:A:77:VAL:HG21	1.95	0.48
1:A:85:THR:O	1:A:89:ILE:HD12	2.13	0.48
1:A:308:LEU:CD1	1:A:330:PRO:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:CD	1:A:259:GLU:H	2.15	0.48
1:A:396:THR:CG2	1:A:437:GLY:HA2	2.44	0.47
1:A:133:ARG:HH12	1:A:138:GLU:CD	2.17	0.47
1:A:84:TYR:HB2	1:A:89:ILE:HD11	1.95	0.47
1:A:84:TYR:CB	1:A:89:ILE:HD11	2.44	0.47
1:A:441:ILE:N	1:A:441:ILE:HD12	2.29	0.47
1:A:254:PHE:N	1:A:264:HIS:HD2	2.06	0.47
1:A:208:TYR:O	1:A:212:GLN:HG2	2.14	0.47
1:A:153:TYR:CE2	1:A:334:VAL:HG13	2.49	0.46
1:A:472:SER:HA	1:A:474:SER:N	2.27	0.46
1:A:133:ARG:CG	1:A:133:ARG:NH2	2.65	0.46
1:A:280:HIS:H	1:A:280:HIS:CD2	2.34	0.46
1:A:308:LEU:HD13	1:A:330:PRO:HB3	1.97	0.46
1:A:310:GLY:O	1:A:313:THR:HB	2.16	0.46
1:A:208:TYR:CE2	1:A:273:LYS:HE2	2.51	0.45
1:A:148:ALA:O	1:A:343:GLY:HA3	2.15	0.45
1:A:377:PHE:CE1	1:A:410:LEU:HB2	2.52	0.45
1:A:124:GLN:O	1:A:128:THR:HG23	2.16	0.45
1:A:255:ILE:HD13	1:A:255:ILE:O	2.16	0.45
1:A:129:LYS:O	1:A:133:ARG:HD2	2.17	0.45
1:A:380:LEU:HD22	1:A:445:PHE:CD2	2.52	0.44
1:A:129:LYS:NZ	1:A:142:ILE:CD1	2.68	0.44
1:A:379:LYS:HZ1	1:A:382:GLU:HA	1.82	0.44
1:A:494:ALA:O	1:A:497:LYS:N	2.51	0.44
1:A:381:ILE:CD1	1:A:391:LYS:HB2	2.47	0.44
1:A:30:PRO:HD3	1:A:100:TYR:CD1	2.53	0.44
1:A:347:GLN:HE21	1:A:347:GLN:CA	2.31	0.44
1:A:408:HIS:CE1	1:A:410:LEU:HD21	2.53	0.43
1:A:473:SER:C	1:A:475:GLY:N	2.62	0.43
1:A:47:ARG:NH1	1:A:47:ARG:HG3	2.06	0.43
1:A:236:GLU:HG2	1:A:240:LYS:HE3	1.99	0.43
1:A:370:ILE:HD12	1:A:443:VAL:HG21	2.00	0.43
1:A:367:SER:HB3	1:A:379:LYS:HZ3	1.84	0.42
1:A:387:ILE:HA	1:A:388:PRO:C	2.40	0.42
1:A:124:GLN:O	1:A:128:THR:CG2	2.68	0.42
1:A:497:LYS:O	1:A:500:GLU:CB	2.67	0.42
1:A:98:LYS:HE3	5:A:2056:HOH:O	2.19	0.42
1:A:80:GLU:HA	1:A:80:GLU:OE1	2.20	0.42
1:A:130:ASP:O	1:A:134:ILE:HG12	2.20	0.41
1:A:8:ASP:O	1:A:14:SER:HA	2.20	0.41
1:A:364:THR:HA	1:A:365:PRO:HD2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:VAL:HG22	1:A:339:VAL:HG11	2.02	0.41
1:A:141:ARG:NH1	1:A:351:ILE:HD12	2.36	0.41
1:A:173:PHE:HE2	1:A:288:PRO:HB2	1.85	0.41
1:A:142:ILE:HD12	1:A:142:ILE:N	2.36	0.41
1:A:88:GLU:O	1:A:92:ILE:HD12	2.21	0.41
1:A:370:ILE:CD1	1:A:443:VAL:HG21	2.50	0.41
1:A:367:SER:CB	1:A:379:LYS:CE	2.98	0.41
1:A:500:GLU:C	1:A:502:ALA:H	2.24	0.41
1:A:14:SER:HB3	1:A:97:LEU:HD21	2.02	0.41
1:A:444:THR:HG21	1:A:456:ARG:NH2	2.22	0.41
1:A:470:ILE:C	1:A:470:ILE:HD13	2.41	0.41
1:A:397:THR:OG1	1:A:402:GLN:HB2	2.20	0.40
1:A:399:ALA:O	1:A:400:ASP:C	2.58	0.40
1:A:29:ASN:HA	1:A:100:TYR:CD2	2.56	0.40
1:A:129:LYS:HZ3	1:A:142:ILE:CD1	2.26	0.40
1:A:205:ILE:HD12	1:A:269:LEU:CD2	2.47	0.40
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.95	0.40
1:A:395:PHE:CD1	1:A:443:VAL:HG13	2.56	0.40
1:A:34:ARG:CZ	1:A:338:GLU:OE2	2.70	0.40
1:A:34:ARG:HG2	1:A:34:ARG:HH11	1.87	0.40
1:A:389:THR:HG22	1:A:447:ILE:HD13	2.03	0.40
1:A:438:VAL:HB	1:A:439:PRO:HD3	2.03	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	502/509 (99%)	468 (93%)	30 (6%)	4 (1%)	19 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	LYS
1	A	490	GLU
1	A	500	GLU
1	A	2	SER

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	385/418 (92%)	326 (85%)	59 (15%)	2 3

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	16	VAL
1	A	31	GLU
1	A	34	ARG
1	A	36	THR
1	A	43	LYS
1	A	44	ASN
1	A	47	ARG
1	A	49	VAL
1	A	87	GLN
1	A	94	LEU
1	A	100	TYR
1	A	105	LEU
1	A	109	VAL
1	A	110	THR
1	A	115	THR
1	A	120	PHE
1	A	128	THR
1	A	133	ARG
1	A	151	LEU
1	A	155	LEU
1	A	157	LYS
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	215	GLN
1	A	230	ARG
1	A	231	LEU
1	A	242	LEU
1	A	245	VAL
1	A	252	LEU
1	A	255	ILE
1	A	259	GLU
1	A	271	ARG
1	A	281	LEU
1	A	285	THR
1	A	298	LEU
1	A	305	LYS
1	A	313	THR
1	A	322	ILE
1	A	323	LYS
1	A	334	VAL
1	A	347	GLN
1	A	354	GLU
1	A	360	LEU
1	A	361	LEU
1	A	364	THR
1	A	370	ILE
1	A	372	THR
1	A	379	LYS
1	A	397	THR
1	A	409	VAL
1	A	425	ARG
1	A	429	THR
1	A	444	THR
1	A	453	VAL
1	A	462	THR
1	A	469	THR
1	A	470	ILE
1	A	477	SER
1	A	489	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	83	GLN

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Mol	Chain	Res	Type
1	A	87	GLN
1	A	161	GLN
1	A	211	ASN
1	A	249	GLN
1	A	264	HIS
1	A	280	HIS
1	A	319	GLN
1	A	347	GLN
1	A	384	ASN
1	A	454	HIS
1	A	463	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ADP	A	1505	4	24,29,29	1.23	4 (16%)	29,45,45	1.96	7 (24%)
3	PO4	A	1506	4	4,4,4	0.42	0	6,6,6	1.30	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
2	ADP	A	1505	4	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1505	ADP	C2-N1	-2.26	1.29	1.33
2	A	1505	ADP	O5'-C5'	-2.22	1.36	1.44
2	A	1505	ADP	C2'-C3'	-2.10	1.47	1.53
2	A	1505	ADP	PB-O3B	-2.01	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1505	ADP	N3-C2-N1	-6.28	118.87	128.68
2	A	1505	ADP	PA-O3A-PB	3.08	143.38	132.83
2	A	1505	ADP	C1'-N9-C4	-3.05	121.29	126.64
2	A	1505	ADP	O2B-PB-O3A	2.73	113.80	104.64
2	A	1505	ADP	O3B-PB-O2B	2.67	117.84	107.64
2	A	1505	ADP	O3B-PB-O1B	-2.07	102.58	110.68
2	A	1505	ADP	O5'-PA-O1A	2.05	117.07	109.07

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1505	ADP	PA-O3A-PB-O1B
2	A	1505	ADP	PB-O3A-PA-O1A

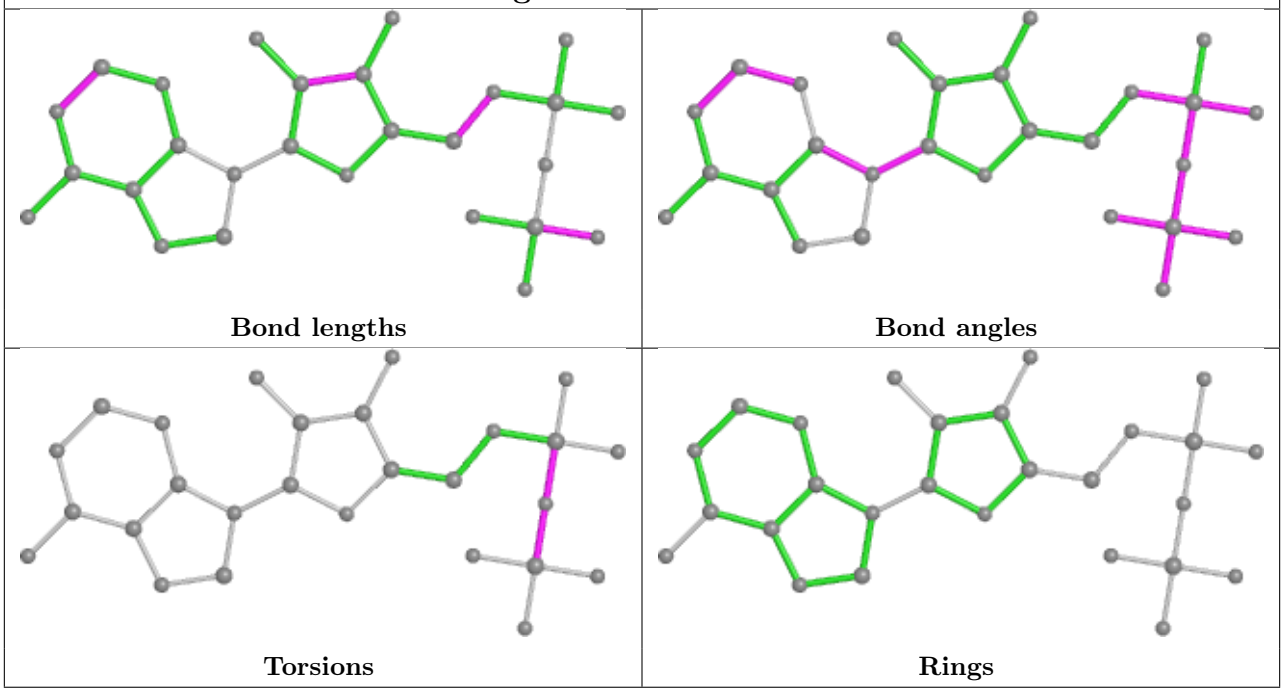
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1505



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	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	503:GLU	C	504:LEU	N	1.20
1	A	204:VAL	C	205:ILE	N	1.16
1	A	201:PHE	C	202:ASP	N	1.15
1	A	399:ALA	C	400:ASP	N	1.11

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	504/509 (99%)	0.27	28 (5%) 24 27	17, 40, 95, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	492	ALA	8.0
1	A	501	ALA	6.0
1	A	488	ALA	5.5
1	A	475	GLY	5.5
1	A	491	ASN	4.4
1	A	494	ALA	3.9
1	A	504	LEU	3.8
1	A	44	ASN	3.8
1	A	485	ILE	3.7
1	A	495	ASP	3.7
1	A	489	GLU	3.5
1	A	499	LYS	3.4
1	A	497	LYS	3.3
1	A	496	ARG	3.3
1	A	493	GLU	3.0
1	A	259	GLU	3.0
1	A	474	SER	2.9
1	A	490	GLU	2.9
1	A	498	ARG	2.8
1	A	500	GLU	2.7
1	A	477	SER	2.6
1	A	503	GLU	2.5
1	A	470	ILE	2.4
1	A	142	ILE	2.3
1	A	473	SER	2.3
1	A	502	ALA	2.2
1	A	115	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

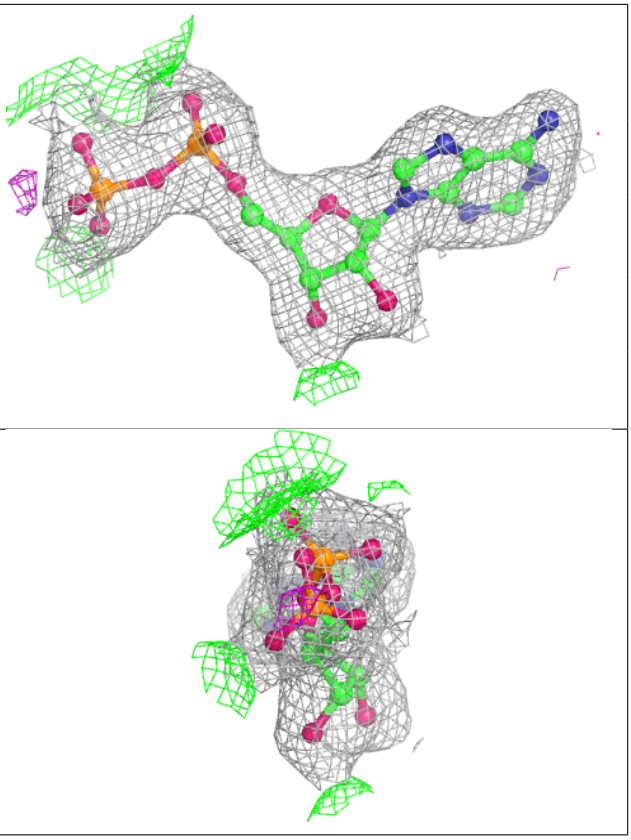
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

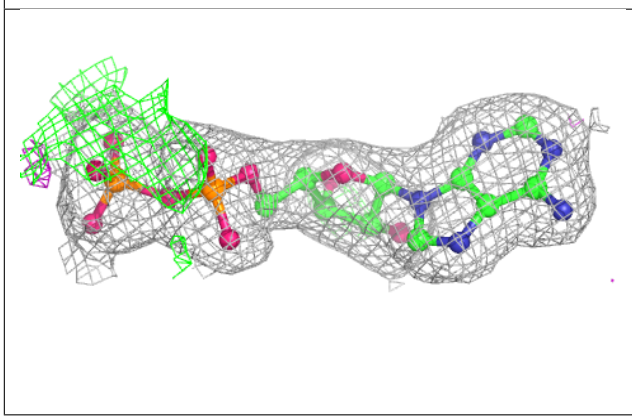
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	A	1507	1/1	0.71	0.67	55,55,55,55	0
2	ADP	A	1505	27/27	0.98	0.15	19,26,32,34	0
3	PO4	A	1506	5/5	0.99	0.14	24,26,31,34	0

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 1505:

$2mF_o$-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.