Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:14 PM EDT

PDB ID	:	3K1J
Title	:	Crystal structure of Lon protease from Thermococcus onnurineus NA1
Authors	:	Cha, S.S.; An, Y.J.
Deposited on	:	2009-09-28
Resolution	:	2.00 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:

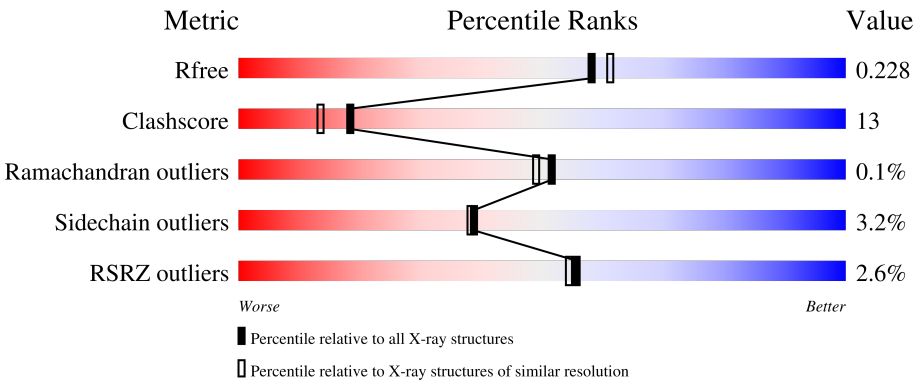
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	604	% 76% 17% • 6%
1	B	604	3% 66% 25% • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9587 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 ATP-dependent protease Lon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	566	4356	2746	765	829	16	0	0	0
1	B	561	4322	2728	760	817	17	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	DELETION	UNP B6YU74
A	?	-	ILE	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	PHE	DELETION	UNP B6YU74
A	?	-	VAL	DELETION	UNP B6YU74
A	?	-	MET	DELETION	UNP B6YU74
A	?	-	PHE	DELETION	UNP B6YU74
A	?	-	THR	DELETION	UNP B6YU74
A	?	-	VAL	DELETION	UNP B6YU74
A	?	-	MET	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	ALA	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	PHE	DELETION	UNP B6YU74
A	?	-	ILE	DELETION	UNP B6YU74
A	?	-	GLU	DELETION	UNP B6YU74
A	?	-	PHE	DELETION	UNP B6YU74
A	?	-	SER	DELETION	UNP B6YU74
A	?	-	ALA	DELETION	UNP B6YU74
A	?	-	THR	DELETION	UNP B6YU74
A	?	-	THR	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	MET	DELETION	UNP B6YU74

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	PHE	DELETION	UNP B6YU74
A	?	-	VAL	DELETION	UNP B6YU74
A	?	-	VAL	DELETION	UNP B6YU74
A	?	-	ILE	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	?	-	THR	DELETION	UNP B6YU74
A	?	-	ILE	DELETION	UNP B6YU74
A	?	-	MET	DELETION	UNP B6YU74
A	?	-	ALA	DELETION	UNP B6YU74
A	?	-	LEU	DELETION	UNP B6YU74
A	523	ALA	SER	ENGINEERED MUTATION	UNP B6YU74
A	566	ALA	LYS	ENGINEERED MUTATION	UNP B6YU74
A	636	HIS	-	EXPRESSION TAG	UNP B6YU74
A	637	HIS	-	EXPRESSION TAG	UNP B6YU74
A	638	HIS	-	EXPRESSION TAG	UNP B6YU74
A	639	HIS	-	EXPRESSION TAG	UNP B6YU74
A	640	HIS	-	EXPRESSION TAG	UNP B6YU74
A	641	HIS	-	EXPRESSION TAG	UNP B6YU74
B	?	-	TYR	DELETION	UNP B6YU74
B	?	-	ILE	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	PHE	DELETION	UNP B6YU74
B	?	-	VAL	DELETION	UNP B6YU74
B	?	-	MET	DELETION	UNP B6YU74
B	?	-	PHE	DELETION	UNP B6YU74
B	?	-	THR	DELETION	UNP B6YU74
B	?	-	VAL	DELETION	UNP B6YU74
B	?	-	MET	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	ALA	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	PHE	DELETION	UNP B6YU74
B	?	-	ILE	DELETION	UNP B6YU74
B	?	-	GLU	DELETION	UNP B6YU74
B	?	-	PHE	DELETION	UNP B6YU74
B	?	-	SER	DELETION	UNP B6YU74
B	?	-	ALA	DELETION	UNP B6YU74
B	?	-	THR	DELETION	UNP B6YU74
B	?	-	THR	DELETION	UNP B6YU74

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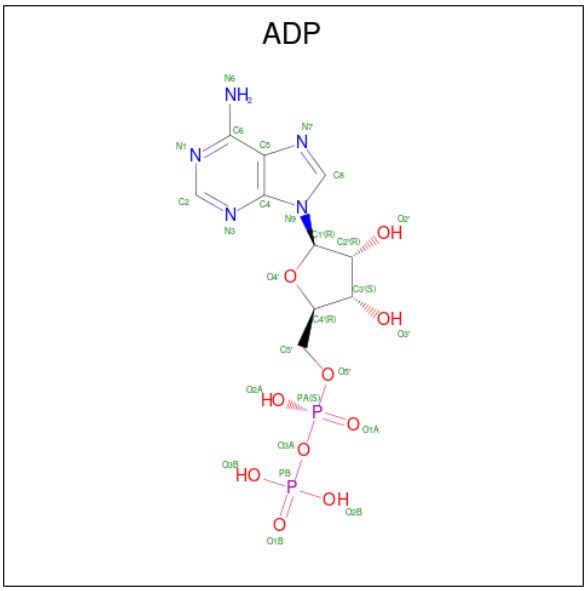
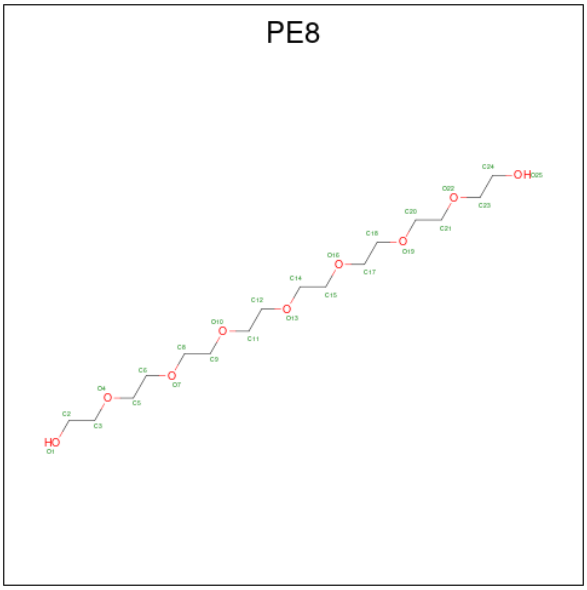
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	MET	DELETION	UNP B6YU74
B	?	-	GLY	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	PHE	DELETION	UNP B6YU74
B	?	-	VAL	DELETION	UNP B6YU74
B	?	-	VAL	DELETION	UNP B6YU74
B	?	-	ILE	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	?	-	THR	DELETION	UNP B6YU74
B	?	-	ILE	DELETION	UNP B6YU74
B	?	-	MET	DELETION	UNP B6YU74
B	?	-	ALA	DELETION	UNP B6YU74
B	?	-	LEU	DELETION	UNP B6YU74
B	523	ALA	SER	ENGINEERED MUTATION	UNP B6YU74
B	566	ALA	LYS	ENGINEERED MUTATION	UNP B6YU74
B	636	HIS	-	EXPRESSION TAG	UNP B6YU74
B	637	HIS	-	EXPRESSION TAG	UNP B6YU74
B	638	HIS	-	EXPRESSION TAG	UNP B6YU74
B	639	HIS	-	EXPRESSION TAG	UNP B6YU74
B	640	HIS	-	EXPRESSION TAG	UNP B6YU74
B	641	HIS	-	EXPRESSION TAG	UNP B6YU74

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



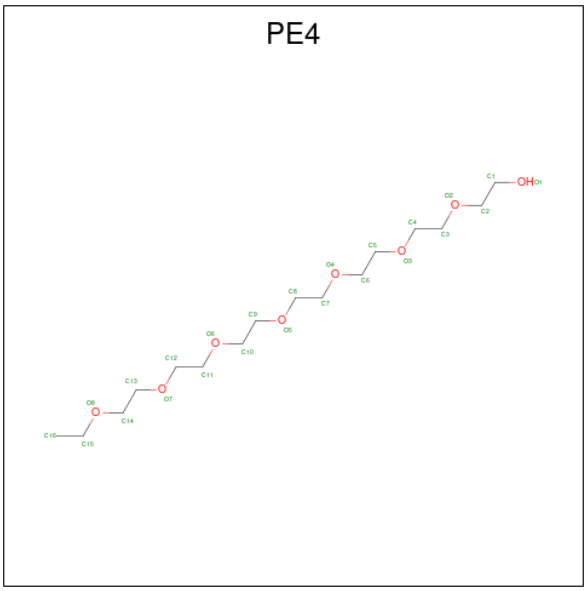
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	B	1	27	10	5	10	2	0	0

- Molecule 3 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	8	5	0	0

- Molecule 4 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0

- Molecule 5 is water.

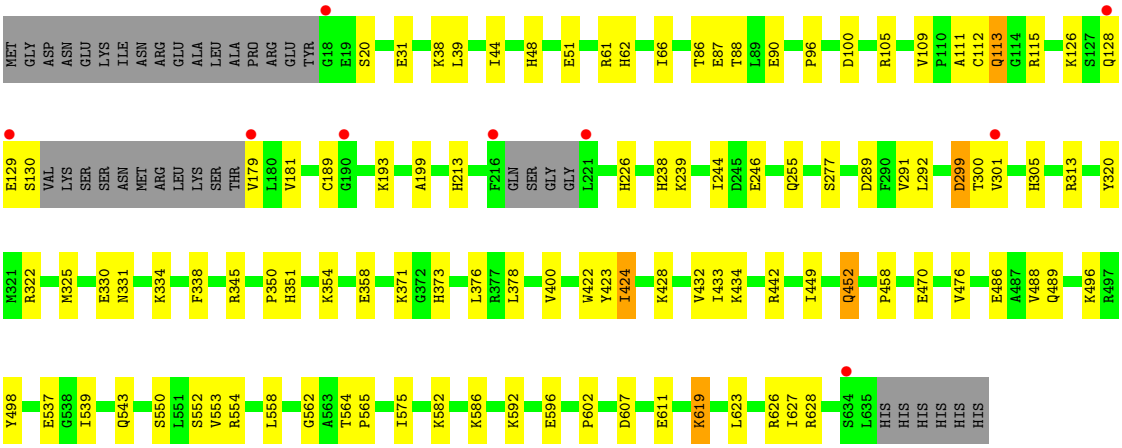
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	471	471	471	0	0
			Total	O		
5	B	364	364	364	0	0

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.

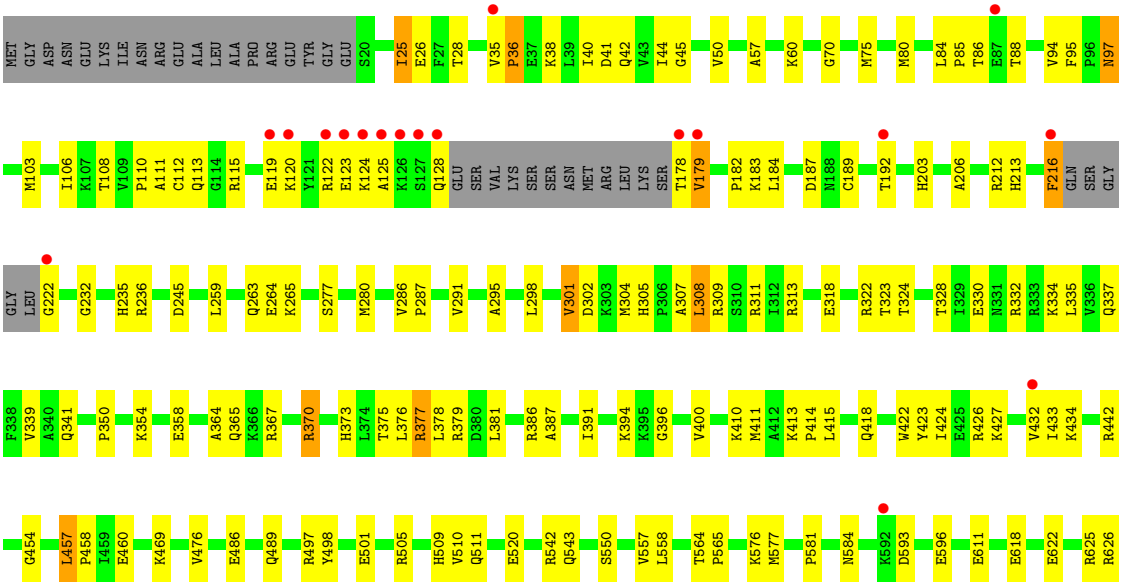
• Molecule 1: ATP-dependent protease Lon

Chain A:



• Molecule 1: ATP-dependent protease Lon

Chain B:



L633
S634
LEU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	121.45Å 121.45Å 195.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.17 – 2.00 30.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.17-2.00) 99.9 (30.87-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.235 0.201 , 0.228	Depositor DCC
R_{free} test set	5516 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.9	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.045 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9587	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.62 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7675e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PE4, PE8, 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	0.38	0/4415	0.65	1/5953 (0.0%)
1	B	0.36	0/4381	0.64	1/5907 (0.0%)
All	All	0.37	0/8796	0.64	2/11860 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	45	GLY	N-CA-C	5.12	125.90	113.10
1	A	291	VAL	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4356	0	4492	110	0
1	B	4322	0	4473	148	0
2	A	27	0	12	1	0
2	B	27	0	12	2	0
3	A	13	0	17	1	0
4	A	7	0	9	0	0
5	A	471	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	364	0	0	17	0
All	All	9587	0	9015	236	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 13.

All (236) 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:313:ARG:HH22	1:B:414:PRO:HG3	1.26	0.99
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.28	0.96
1:A:334:LYS:HE2	5:A:820:HOH:O	1.69	0.92
1:B:213:HIS:HD2	1:B:277:SER:H	1.15	0.92
1:A:62:HIS:HD2	1:A:292:LEU:H	1.16	0.91
1:A:432:VAL:HG12	1:A:442:ARG:HH22	1.36	0.90
1:B:108:THR:HG21	1:B:287:PRO:HG3	1.53	0.89
1:A:238:HIS:HD2	1:A:289:ASP:H	1.22	0.87
1:A:61:ARG:HH12	1:B:386:ARG:HB3	1.41	0.86
1:A:313:ARG:HH12	1:B:414:PRO:HA	1.38	0.85
1:B:120:LYS:O	1:B:123:GLU:HG2	1.76	0.85
1:A:61:ARG:NH1	1:B:386:ARG:HB3	1.93	0.84
1:A:313:ARG:HH22	1:B:414:PRO:CG	1.90	0.84
1:A:452:GLN:O	1:A:452:GLN:HG2	1.78	0.83
1:B:44:ILE:HD12	1:B:334:LYS:HB3	1.59	0.83
1:B:313:ARG:HD2	1:B:318:GLU:OE2	1.79	0.82
1:B:232:GLY:H	1:B:235:HIS:HD2	1.27	0.82
1:A:611:GLU:HB2	5:A:1064:HOH:O	1.80	0.81
1:B:370:ARG:HH11	1:B:370:ARG:CG	1.93	0.80
1:B:124:LYS:HG2	1:B:179:VAL:HG11	1.63	0.80
1:B:298:LEU:HD12	5:B:893:HOH:O	1.81	0.79
1:A:607:ASP:OD2	1:A:628:ARG:NH1	2.17	0.78
1:B:457:LEU:HD23	5:B:830:HOH:O	1.82	0.77
1:A:213:HIS:HD2	1:A:277:SER:H	1.32	0.77
1:B:128:GLN:NE2	1:B:179:VAL:HG13	2.00	0.76
1:A:432:VAL:HG12	1:A:432:VAL:O	1.85	0.75
1:A:313:ARG:NH2	1:B:414:PRO:HG3	2.02	0.75
1:B:277:SER:O	1:B:280:MET:HG2	1.86	0.75
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.52	0.75
1:B:550:SER:HB3	1:B:558:LEU:HB2	1.70	0.74
1:B:213:HIS:CD2	1:B:277:SER:H	2.04	0.74
1:B:377:ARG:HH11	1:B:377:ARG:HG2	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:CB	1:A:539:ILE:HD13	2.18	0.74
1:B:60:LYS:HE2	5:B:716:HOH:O	1.88	0.73
1:B:25:ILE:HD13	1:B:26:GLU:N	2.04	0.72
1:A:179:VAL:HA	5:A:1058:HOH:O	1.90	0.72
1:A:38:LYS:HG2	5:A:785:HOH:O	1.88	0.72
1:A:550:SER:HB3	1:A:558:LEU:HB2	1.72	0.71
1:A:351:HIS:ND1	5:A:817:HOH:O	2.24	0.68
1:B:28:THR:HG23	5:B:782:HOH:O	1.93	0.68
1:B:581:PRO:HG2	1:B:584:ASN:OD1	1.92	0.68
1:B:301:VAL:HG12	5:B:908:HOH:O	1.92	0.68
1:B:350:PRO:HG2	1:B:400:VAL:HG23	1.75	0.67
1:A:62:HIS:CD2	1:A:292:LEU:H	2.06	0.67
1:B:564:THR:HB	1:B:565:PRO:HD3	1.77	0.67
1:B:38:LYS:HG3	5:B:758:HOH:O	1.95	0.66
1:A:255:GLN:HE22	1:A:305:HIS:H	1.42	0.66
1:B:354:LYS:O	1:B:358:GLU:HG3	1.95	0.66
1:A:213:HIS:CD2	1:A:277:SER:H	2.14	0.66
1:A:38:LYS:HD2	5:A:1083:HOH:O	1.95	0.65
1:A:255:GLN:NE2	1:A:305:HIS:H	1.94	0.65
1:B:377:ARG:HG2	1:B:377:ARG:NH1	2.12	0.65
1:A:552:SER:HA	1:B:511:GLN:HE22	1.62	0.64
1:B:323:THR:HG23	1:B:324:THR:HG23	1.79	0.64
1:A:586:LYS:HD3	5:A:151:HOH:O	1.98	0.64
1:B:40:ILE:HD11	1:B:50:VAL:HG13	1.79	0.64
1:B:42:GLN:HA	1:B:337:GLN:HE22	1.62	0.63
1:B:108:THR:CG2	1:B:287:PRO:HG3	2.26	0.63
1:B:85:PRO:HD3	5:B:852:HOH:O	1.98	0.63
1:A:537:GLU:HB2	1:A:539:ILE:HD13	1.80	0.63
1:B:232:GLY:H	1:B:235:HIS:CD2	2.15	0.62
1:B:301:VAL:HG21	1:B:313:ARG:HD3	1.80	0.62
1:A:126:LYS:O	1:A:129:GLU:HG2	1.98	0.62
1:A:432:VAL:O	1:A:432:VAL:CG1	2.48	0.62
1:A:537:GLU:HB3	1:A:539:ILE:HD13	1.82	0.62
1:B:379:ARG:HB3	5:B:841:HOH:O	2.00	0.61
1:B:370:ARG:NH1	1:B:373:HIS:CE1	2.69	0.61
1:A:432:VAL:O	1:A:442:ARG:NH2	2.33	0.61
1:A:105:ARG:HG2	1:A:105:ARG:NH1	2.16	0.61
1:A:371:LYS:O	1:A:373:HIS:HD2	1.85	0.60
1:A:246:GLU:HG3	5:A:140:HOH:O	2.01	0.59
1:B:263:GLN:HG2	1:B:311:ARG:NH1	2.17	0.59
1:B:423:TYR:CZ	1:B:427:LYS:HD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:HD2	5:A:722:HOH:O	1.85	0.59
1:A:354:LYS:O	1:A:358:GLU:HG3	2.03	0.59
1:B:26:GLU:OE1	1:B:26:GLU:HA	2.02	0.59
1:B:124:LYS:HE2	1:B:179:VAL:HG12	1.85	0.58
1:B:422:TRP:O	1:B:426:ARG:HG2	2.02	0.58
1:A:238:HIS:CD2	1:A:289:ASP:H	2.12	0.58
1:A:66:ILE:HG13	1:B:415:LEU:HD22	1.86	0.58
1:B:111:ALA:O	1:B:112:CYS:HB2	2.04	0.58
1:A:325:MET:HE2	1:A:331:ASN:CG	2.25	0.57
1:A:313:ARG:HH22	1:B:414:PRO:CB	2.16	0.57
1:B:611:GLU:HB2	5:B:740:HOH:O	2.04	0.57
1:B:128:GLN:OE1	1:B:178:THR:N	2.38	0.57
1:A:345:ARG:NE	5:A:946:HOH:O	2.37	0.57
1:A:111:ALA:O	1:A:112:CYS:HB2	2.04	0.56
1:B:396:GLY:HA2	5:B:865:HOH:O	2.06	0.56
1:B:128:GLN:HE21	1:B:179:VAL:HG13	1.68	0.56
1:B:432:VAL:HA	5:B:880:HOH:O	2.06	0.56
1:A:325:MET:CE	1:A:331:ASN:CG	2.74	0.56
1:B:557:VAL:HG12	1:B:581:PRO:HB3	1.88	0.56
1:A:476:VAL:HG21	1:A:488:VAL:HG11	1.87	0.55
1:B:112:CYS:HA	1:B:189:CYS:HB2	1.88	0.55
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.73	0.54
1:A:486:GLU:HA	1:A:489:GLN:HE21	1.72	0.54
1:B:36:PRO:HG2	5:B:902:HOH:O	2.06	0.54
1:B:593:ASP:O	1:B:596:GLU:HG2	2.08	0.54
1:A:564:THR:HB	1:A:565:PRO:HD3	1.90	0.54
1:A:181:VAL:O	1:A:226:HIS:HE1	1.90	0.53
1:A:299:ASP:OD1	1:A:300:THR:N	2.41	0.53
1:A:301:VAL:HB	5:A:840:HOH:O	2.08	0.53
1:B:97:ASN:C	1:B:97:ASN:HD22	2.11	0.53
1:A:452:GLN:O	1:A:452:GLN:CG	2.53	0.53
1:A:470:GLU:O	1:B:469:LYS:HG2	2.09	0.53
1:A:619:LYS:NZ	5:A:784:HOH:O	2.41	0.53
1:B:44:ILE:CD1	1:B:334:LYS:HB3	2.36	0.53
1:B:128:GLN:HE22	1:B:179:VAL:H	1.57	0.53
1:A:112:CYS:HA	1:A:189:CYS:HB2	1.91	0.53
1:B:305:HIS:CD2	1:B:307:ALA:H	2.27	0.53
1:A:322:ARG:NH1	5:A:923:HOH:O	2.42	0.52
1:B:330:GLU:O	1:B:334:LYS:HG2	2.10	0.52
1:B:106:ILE:HG13	1:B:286:VAL:HG22	1.91	0.52
1:B:458:PRO:HD2	5:B:830:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:VAL:O	1:B:442:ARG:NH2	2.43	0.52
1:B:476:VAL:HG22	1:B:510:VAL:HB	1.92	0.52
1:B:245:ASP:HA	1:B:295:ALA:HB3	1.92	0.51
1:A:320:TYR:H	1:B:418:GLN:HE22	1.58	0.51
1:B:203:HIS:CE1	1:B:206:ALA:HB2	2.45	0.51
1:A:626:ARG:HG2	5:A:990:HOH:O	2.09	0.51
1:A:88:THR:O	1:A:239:LYS:HE2	2.10	0.51
1:A:424:ILE:HG23	1:A:428:LYS:HE3	1.93	0.51
1:B:370:ARG:CG	1:B:370:ARG:NH1	2.61	0.51
1:B:38:LYS:HB2	1:B:41:ASP:OD2	2.10	0.51
1:B:128:GLN:NE2	1:B:179:VAL:H	2.09	0.51
1:A:100:ASP:OD2	1:B:212:ARG:HD2	2.11	0.50
1:B:505:ARG:NH1	1:B:505:ARG:HG3	2.26	0.50
1:A:31:GLU:HB2	1:A:351:HIS:CD2	2.47	0.50
1:B:432:VAL:HG12	1:B:442:ARG:HH22	1.77	0.50
1:A:553:VAL:H	1:B:511:GLN:NE2	2.10	0.50
1:A:87:GLU:H	1:A:87:GLU:CD	2.15	0.50
1:B:80:MET:HE1	1:B:291:VAL:CG1	2.42	0.50
1:B:57:ALA:HB2	1:B:80:MET:HG3	1.93	0.50
1:A:539:ILE:N	1:A:539:ILE:HD12	2.27	0.49
1:A:433:ILE:HD11	1:A:458:PRO:HD3	1.94	0.49
1:B:94:VAL:CG1	1:B:183:LYS:HB3	2.43	0.49
1:B:633:LEU:O	1:B:634:SER:C	2.51	0.49
1:B:365:GLN:HG2	5:B:800:HOH:O	2.13	0.49
1:B:110:PRO:O	1:B:113:GLN:HB3	2.13	0.49
1:B:301:VAL:O	1:B:309:ARG:HD3	2.12	0.49
1:B:576:LYS:HG3	5:B:715:HOH:O	2.13	0.49
1:A:424:ILE:HD11	1:A:449:ILE:CG1	2.42	0.48
1:B:119:GLU:HA	1:B:122:ARG:HB3	1.95	0.48
1:B:123:GLU:CG	1:B:124:LYS:N	2.75	0.48
1:B:486:GLU:HA	1:B:489:GLN:HE21	1.78	0.48
1:B:179:VAL:CG2	1:B:179:VAL:O	2.61	0.48
1:B:301:VAL:CG2	1:B:313:ARG:HD3	2.44	0.48
1:B:305:HIS:HD2	1:B:307:ALA:H	1.61	0.48
1:A:90:GLU:OE1	1:A:238:HIS:HE1	1.96	0.48
1:B:44:ILE:HD13	1:B:334:LYS:HE3	1.96	0.48
1:A:51:GLU:OE1	1:B:394:LYS:NZ	2.39	0.47
1:A:496:LYS:HZ1	1:B:509:HIS:CE1	2.32	0.47
1:A:320:TYR:H	1:B:418:GLN:NE2	2.11	0.47
1:B:125:ALA:HA	1:B:179:VAL:CG2	2.44	0.47
1:A:623:LEU:CD1	1:A:627:ILE:HD12	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:HIS:HD2	1:B:307:ALA:N	2.13	0.47
1:B:622:GLU:OE1	1:B:622:GLU:HA	2.15	0.47
1:A:378:LEU:HD12	2:A:642:ADP:C6	2.50	0.47
1:A:325:MET:CE	1:A:331:ASN:OD1	2.63	0.47
1:B:42:GLN:HA	1:B:337:GLN:NE2	2.28	0.47
1:B:42:GLN:HB3	1:B:341:GLN:HE22	1.81	0.46
1:B:103:MET:O	1:B:103:MET:HG2	2.16	0.46
1:B:364:ALA:HA	1:B:375:THR:HG22	1.98	0.46
1:A:51:GLU:CD	1:B:394:LYS:HZ1	2.16	0.46
1:B:304:MET:HE3	1:B:308:LEU:HD22	1.98	0.45
1:A:66:ILE:HG13	1:B:415:LEU:CD2	2.47	0.45
1:A:582:LYS:HA	1:A:602:PRO:HB2	1.98	0.45
1:B:305:HIS:CD2	1:B:307:ALA:HB3	2.51	0.45
1:B:505:ARG:HG3	1:B:505:ARG:HH11	1.82	0.45
1:A:109:VAL:CG2	1:A:113:GLN:HB3	2.46	0.45
1:A:193:LYS:HD3	5:A:1057:HOH:O	2.16	0.45
1:A:496:LYS:NZ	1:B:509:HIS:HE1	2.15	0.45
1:B:497:ARG:NH1	5:B:849:HOH:O	2.50	0.45
1:B:97:ASN:C	1:B:97:ASN:ND2	2.70	0.44
1:B:387:ALA:O	1:B:391:ILE:HG13	2.18	0.44
1:A:115:ARG:NH1	1:A:189:CYS:HB3	2.33	0.44
1:A:325:MET:HE1	1:A:331:ASN:OD1	2.17	0.44
1:B:542:ARG:NH2	1:B:577:MET:HE1	2.33	0.44
1:A:496:LYS:HZ1	1:B:509:HIS:HE1	1.65	0.44
1:A:554:ARG:HD3	1:B:460:GLU:CD	2.38	0.44
1:B:80:MET:CE	1:B:291:VAL:HG11	2.47	0.44
1:B:95:PHE:CD1	1:B:182:PRO:HB3	2.53	0.44
1:A:44:ILE:CD1	1:A:338:PHE:HB2	2.48	0.44
1:A:129:GLU:O	1:A:130:SER:C	2.55	0.44
1:A:130:SER:HA	5:A:775:HOH:O	2.17	0.44
1:A:299:ASP:HB3	5:A:653:HOH:O	2.18	0.43
1:B:434:LYS:HB2	1:B:543:GLN:HE21	1.84	0.43
1:A:423:TYR:OH	3:A:643:PE8:H21	2.18	0.43
1:B:264:GLU:O	1:B:265:LYS:HB2	2.19	0.43
1:B:423:TYR:O	1:B:427:LYS:HG3	2.19	0.43
1:A:20:SER:HB2	1:A:358:GLU:OE2	2.19	0.43
1:B:424:ILE:HD13	1:B:454:GLY:O	2.19	0.43
1:A:537:GLU:HB3	1:A:539:ILE:CD1	2.48	0.43
1:A:44:ILE:HD13	1:A:338:PHE:HB2	2.01	0.43
1:B:427:LYS:HE2	1:B:427:LYS:HB3	1.83	0.43
1:A:86:THR:CG2	1:A:193:LYS:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HG21	1:B:192:THR:O	2.18	0.42
1:B:184:LEU:HD21	1:B:187:ASP:HB2	2.01	0.42
1:A:330:GLU:O	1:A:334:LYS:HG3	2.19	0.42
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.92	0.42
1:B:625:ARG:HG2	1:B:625:ARG:HH11	1.84	0.42
1:A:213:HIS:HD2	1:A:277:SER:N	2.09	0.42
1:A:128:GLN:C	1:A:130:SER:H	2.22	0.42
1:A:424:ILE:HD11	1:A:449:ILE:HG13	2.02	0.42
1:B:124:LYS:HE2	1:B:179:VAL:CG1	2.49	0.42
1:B:75:MET:HE3	2:B:642:ADP:H3'	2.02	0.42
1:B:236:ARG:HD2	5:B:861:HOH:O	2.20	0.42
1:B:378:LEU:HD12	2:B:642:ADP:C6	2.54	0.42
1:A:325:MET:HE1	1:A:331:ASN:CG	2.39	0.42
1:B:263:GLN:HG2	1:B:311:ARG:HH12	1.83	0.42
1:A:562:GLY:C	1:A:565:PRO:HD2	2.41	0.41
1:A:592:LYS:O	1:A:596:GLU:HG3	2.20	0.41
1:B:381:LEU:HD23	1:B:381:LEU:HA	1.79	0.41
1:A:48:HIS:HE1	5:A:874:HOH:O	2.01	0.41
1:A:96:PRO:HB3	1:A:226:HIS:CD2	2.55	0.41
1:B:410:LYS:O	1:B:413:LYS:HG2	2.19	0.41
1:A:434:LYS:HB2	1:A:543:GLN:HE21	1.85	0.41
5:A:723:HOH:O	1:B:411:MET:HE1	2.18	0.41
1:B:25:ILE:HD13	1:B:26:GLU:H	1.82	0.41
1:B:70:GLY:HA3	1:B:379:ARG:HB2	2.02	0.41
1:B:304:MET:CE	1:B:308:LEU:HD22	2.50	0.41
1:B:179:VAL:O	1:B:179:VAL:HG23	2.20	0.41
1:B:216:PHE:HB3	1:B:222:GLY:CA	2.50	0.41
1:B:328:THR:O	1:B:332:ARG:HG3	2.20	0.41
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.90	0.41
1:A:623:LEU:HD11	1:A:627:ILE:HD12	2.03	0.41
1:B:44:ILE:CD1	1:B:334:LYS:HE3	2.50	0.41
1:B:57:ALA:HB2	1:B:80:MET:CG	2.51	0.41
1:B:125:ALA:N	1:B:179:VAL:HG21	2.36	0.41
1:B:335:LEU:O	1:B:339:VAL:HG23	2.21	0.41
1:A:313:ARG:HG3	1:A:313:ARG:NH1	2.34	0.40
1:B:115:ARG:NH1	1:B:189:CYS:SG	2.94	0.40
1:B:432:VAL:O	1:B:433:ILE:HD13	2.21	0.40
1:A:199:ALA:HB3	1:A:244:ILE:HG12	2.02	0.40
1:A:350:PRO:HG2	1:A:400:VAL:HG23	2.04	0.40
1:A:100:ASP:CG	1:B:212:ARG:HD2	2.42	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	560/604 (93%)	547 (98%)	13 (2%)	0	100	100
1	B	555/604 (92%)	540 (97%)	14 (2%)	1 (0%)	47	44
All	All	1115/1208 (92%)	1087 (98%)	27 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	466/504 (92%)	457 (98%)	9 (2%)	57	61
1	B	463/504 (92%)	442 (96%)	21 (4%)	27	24
All	All	929/1008 (92%)	899 (97%)	30 (3%)	39	38

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	113	GLN
1	A	299	ASP
1	A	422	TRP
1	A	424	ILE

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Mol	Chain	Res	Type
1	A	452	GLN
1	A	498	TYR
1	A	575	ILE
1	A	619	LYS
1	B	25	ILE
1	B	35	VAL
1	B	84	LEU
1	B	88	THR
1	B	97	ASN
1	B	179	VAL
1	B	216	PHE
1	B	259	LEU
1	B	301	VAL
1	B	302	ASP
1	B	308	LEU
1	B	322	ARG
1	B	367	ARG
1	B	370	ARG
1	B	377	ARG
1	B	457	LEU
1	B	498	TYR
1	B	501	GLU
1	B	520	GLU
1	B	618	GLU
1	B	626	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	62	HIS
1	A	203	HIS
1	A	213	HIS
1	A	226	HIS
1	A	238	HIS
1	A	255	GLN
1	A	272	GLN
1	A	351	HIS
1	A	373	HIS
1	A	418	GLN
1	A	489	GLN
1	A	543	GLN

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	128	GLN
1	B	203	HIS
1	B	213	HIS
1	B	226	HIS
1	B	235	HIS
1	B	256	GLN
1	B	263	GLN
1	B	272	GLN
1	B	305	HIS
1	B	331	ASN
1	B	341	GLN
1	B	351	HIS
1	B	365	GLN
1	B	418	GLN
1	B	431	GLN
1	B	489	GLN
1	B	509	HIS
1	B	511	GLN
1	B	543	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	ADP	A	642	-	24,29,29	2.14	5 (20%)	29,45,45	3.30	6 (20%)
2	ADP	B	642	-	24,29,29	2.00	6 (25%)	29,45,45	3.47	6 (20%)
4	PE4	A	644	-	6,6,23	0.49	0	5,5,22	0.30	0
3	PE8	A	643	-	12,12,24	0.62	0	11,11,23	0.71	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	642	-	-	5/12/32/32	0/3/3/3
2	ADP	B	642	-	-	3/12/32/32	0/3/3/3
4	PE4	A	644	-	-	2/4/4/21	-
3	PE8	A	643	-	-	1/10/10/22	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	642	ADP	O4'-C1'	7.64	1.50	1.40
2	B	642	ADP	O4'-C1'	7.09	1.50	1.40
2	A	642	ADP	C2-N3	3.24	1.37	1.32
2	B	642	ADP	C2-N3	3.03	1.36	1.32
2	A	642	ADP	PA-O3A	2.79	1.62	1.59
2	B	642	ADP	C1'-N9	2.62	1.56	1.49
2	B	642	ADP	PA-O3A	2.56	1.62	1.59
2	A	642	ADP	O2'-C2'	-2.33	1.37	1.43
2	A	642	ADP	PA-O2A	-2.33	1.44	1.55
2	B	642	ADP	O2'-C2'	-2.25	1.37	1.43
2	B	642	ADP	PB-O3B	-2.25	1.46	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	642	ADP	O4'-C1'-N9	-15.43	88.28	108.75
2	A	642	ADP	O4'-C1'-N9	-14.35	89.71	108.75
2	A	642	ADP	C1'-N9-C4	-8.15	112.32	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	642	ADP	C1'-N9-C4	-8.12	112.38	126.64
2	A	642	ADP	O4'-C4'-C3'	-2.96	99.27	105.15
2	B	642	ADP	O4'-C4'-C5'	-2.90	100.06	109.33
2	B	642	ADP	O3'-C3'-C2'	2.73	120.56	111.82
2	B	642	ADP	C5-C6-N6	2.65	124.35	120.31
2	A	642	ADP	O4'-C4'-C5'	-2.52	101.25	109.33
2	A	642	ADP	O3'-C3'-C2'	2.48	119.77	111.82
2	A	642	ADP	C5-C6-N6	2.30	123.82	120.31
2	B	642	ADP	O4'-C4'-C3'	-2.20	100.78	105.15

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	642	ADP	PA-O3A-PB-O2B
2	A	642	ADP	C5'-O5'-PA-O1A
2	A	642	ADP	C5'-O5'-PA-O2A
2	A	642	ADP	C5'-O5'-PA-O3A
2	B	642	ADP	C5'-O5'-PA-O1A
2	B	642	ADP	C5'-O5'-PA-O2A
2	B	642	ADP	C5'-O5'-PA-O3A
4	A	644	PE4	O1-C1-C2-O2
3	A	643	PE8	O10-C11-C12-O13
4	A	644	PE4	C1-C2-O2-C3
2	A	642	ADP	PA-O3A-PB-O1B

There are no ring outliers.

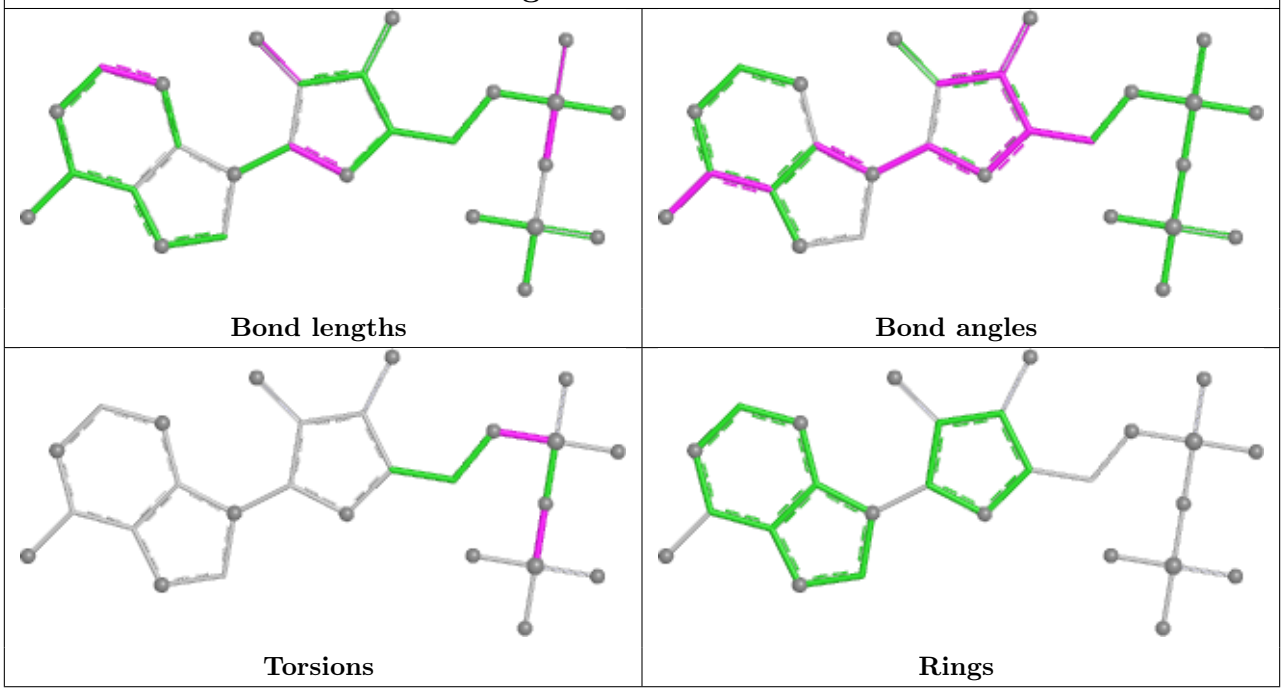
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	642	ADP	1	0
2	B	642	ADP	2	0
3	A	643	PE8	1	0

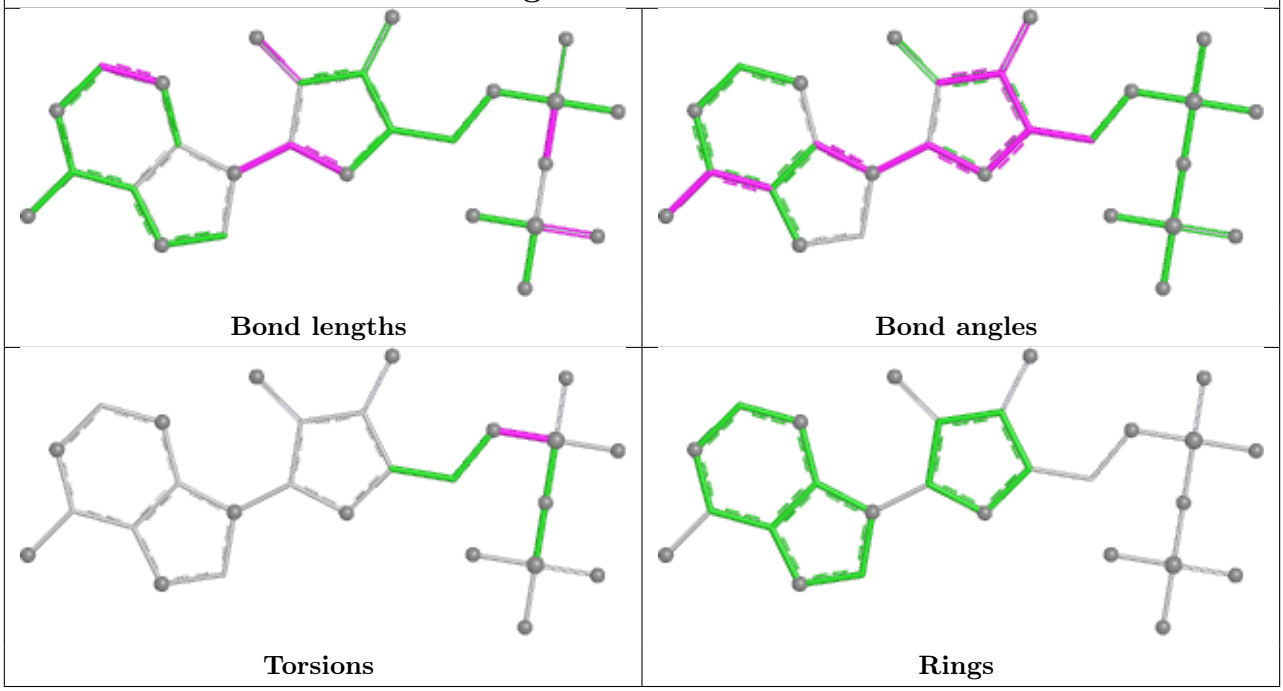
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

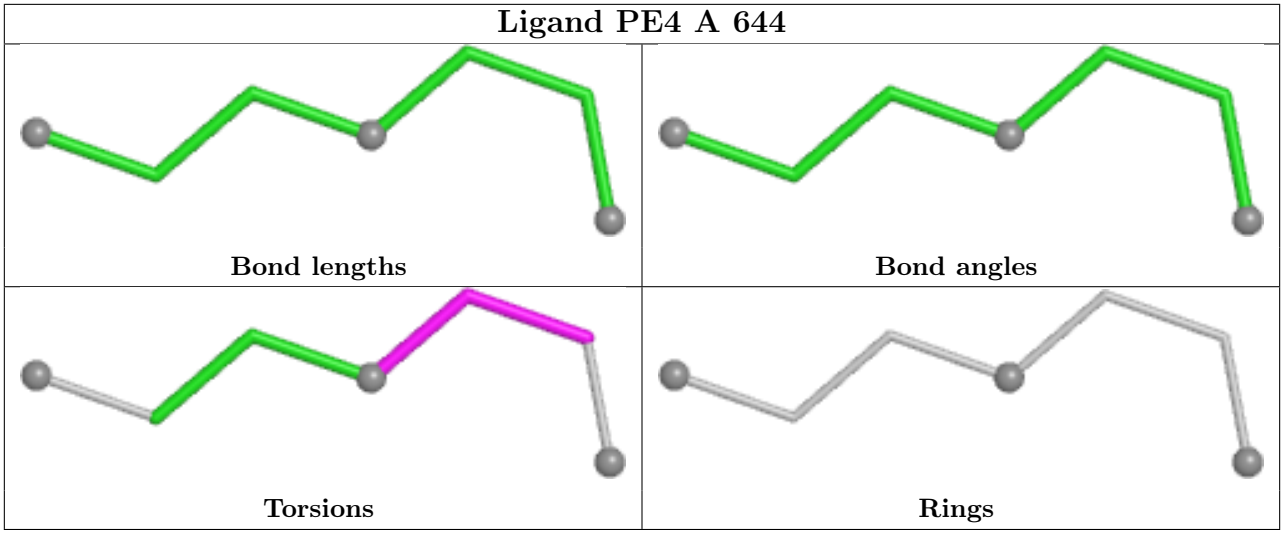
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

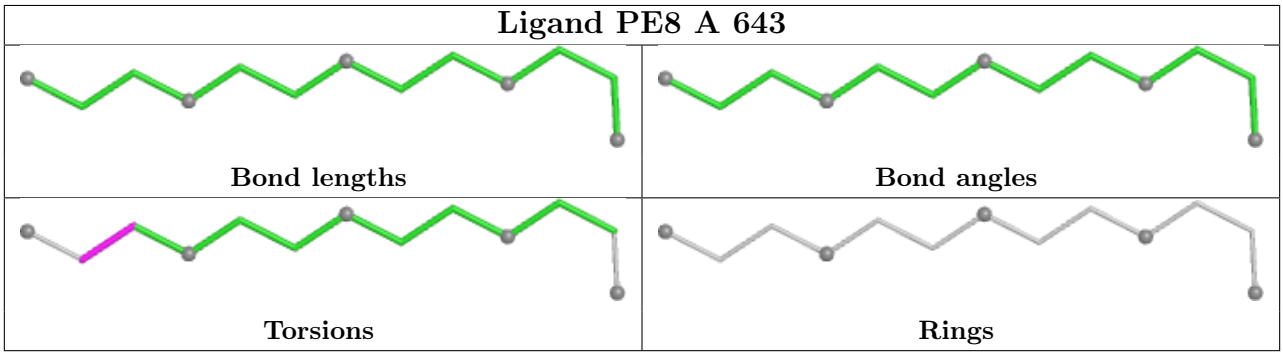
Ligand ADP A 642



Ligand ADP B 642







5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	566/604 (93%)	-0.47	9 (1%)	72	70	12, 24, 44, 66	0
1	B	561/604 (92%)	-0.22	20 (3%)	42	42	13, 29, 55, 91	0
All	All	1127/1208 (93%)	-0.35	29 (2%)	56	54	12, 26, 49, 91	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	PHE	8.7
1	B	634	SER	6.9
1	B	179	VAL	6.4
1	B	125	ALA	5.4
1	A	18	GLY	5.4
1	B	178	THR	4.6
1	B	123	GLU	4.6
1	B	126	LYS	4.5
1	A	179	VAL	4.4
1	B	124	LYS	4.4
1	B	127	SER	3.9
1	B	128	GLN	3.7
1	B	222	GLY	3.7
1	B	87	GLU	3.2
1	A	301	VAL	3.1
1	A	129	GLU	2.9
1	A	221	LEU	2.8
1	B	119	GLU	2.7
1	A	634	SER	2.7
1	B	633	LEU	2.7
1	B	35	VAL	2.6
1	B	592	LYS	2.6
1	A	128	GLN	2.5
1	A	216	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	190	GLY	2.2
1	B	432	VAL	2.2
1	B	192	THR	2.2
1	B	120	LYS	2.1
1	B	122	ARG	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

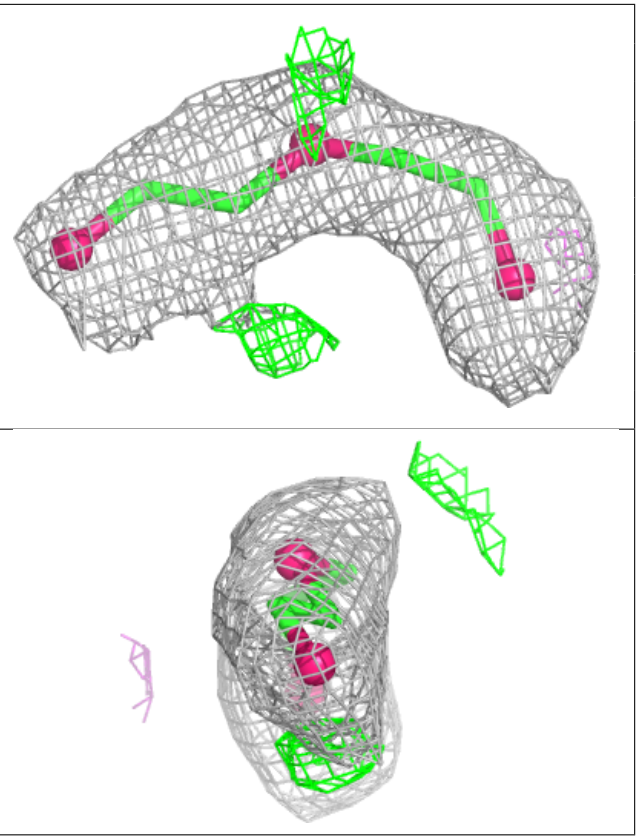
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PE4	A	644	7/24	0.91	0.11	41,42,46,50	0
2	ADP	B	642	27/27	0.93	0.12	36,47,51,54	0
3	PE8	A	643	13/25	0.94	0.09	28,31,33,34	0
2	ADP	A	642	27/27	0.98	0.11	14,19,25,26	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.

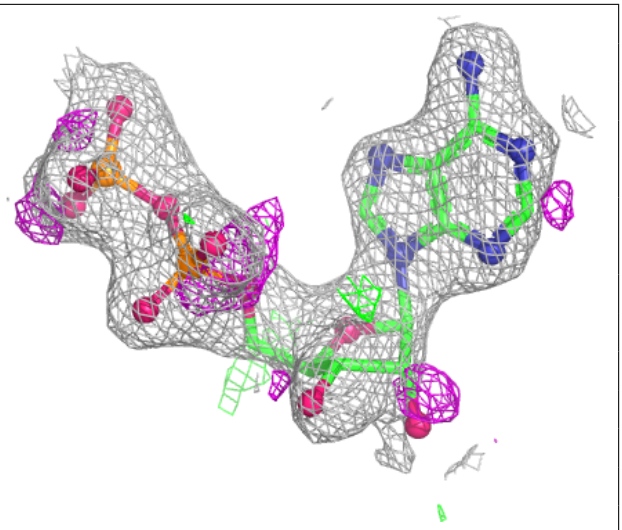
Electron density around PE4 A 644:

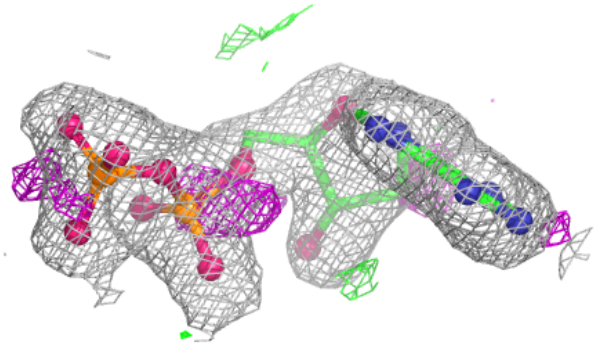
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

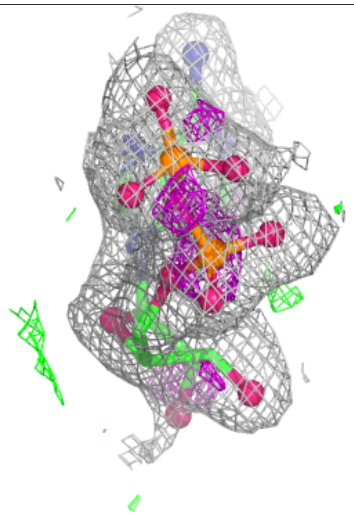


Electron density around ADP B 642:

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

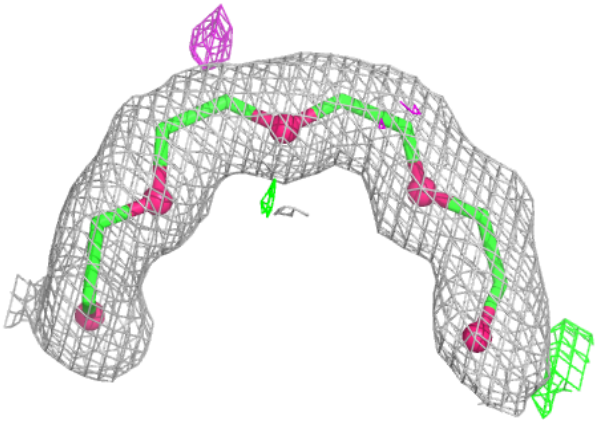


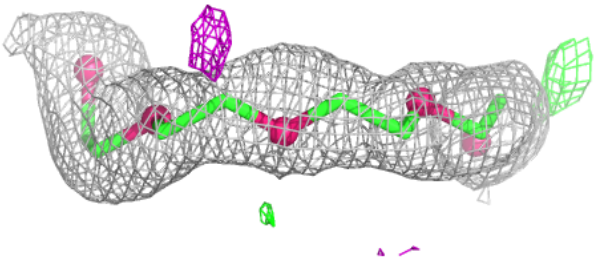


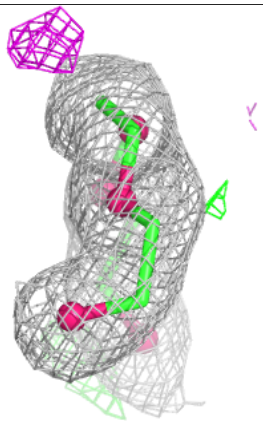


Electron density around PE8 A 643:

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

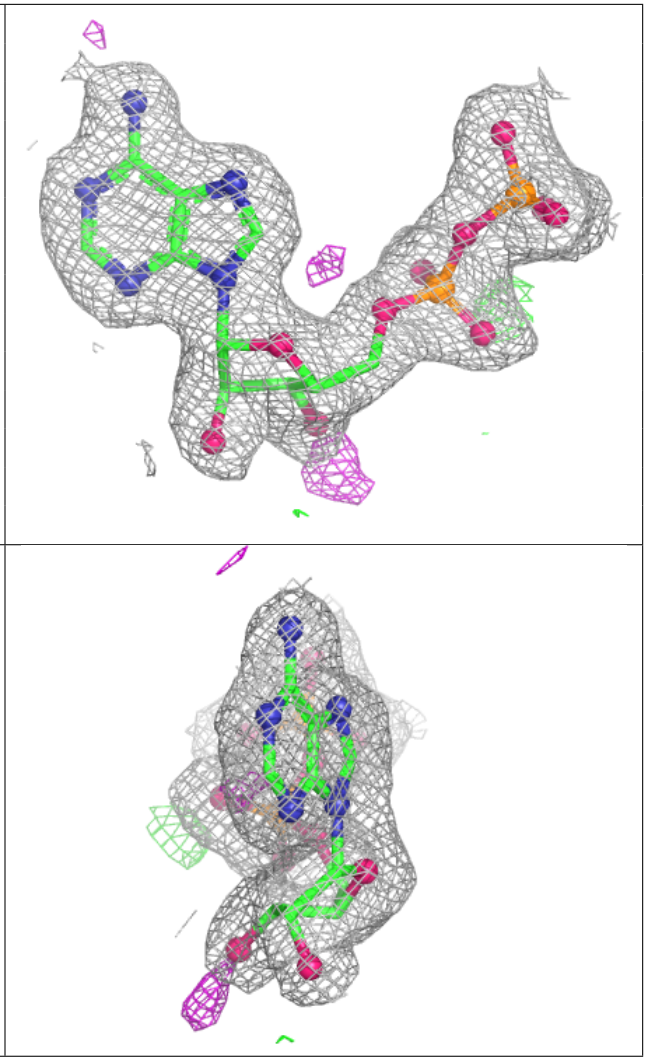






Electron density around ADP A 642:

$2mF_o$-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.