Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 06:16 am BST

PDB ID	:	4H0X
Title	:	Crystal structure of NAD+-Ia(E380A)-actin complex
Authors	:	Tsurumura, T.; Oda, M.; Nagahama, M.; Tsuge, H.
Deposited on	:	2012-09-10
Resolution	:	2.33 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 following versions of software and data (see references (i)) were used in the production of this report:

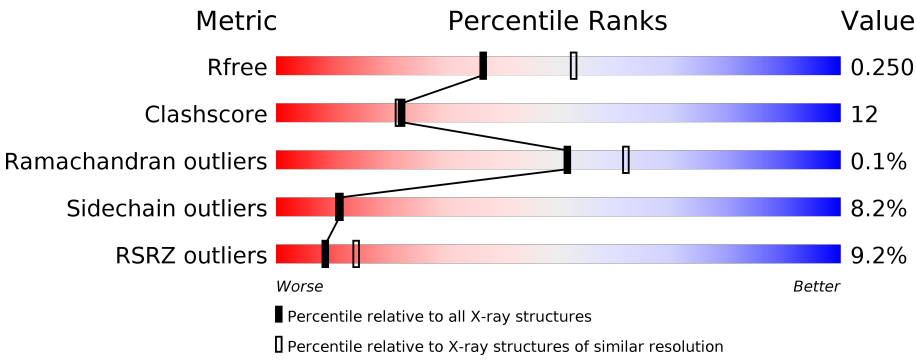
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 on 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	418	11% 75% 21% • •
2	B	375	7% 73% 18% 5% 5%

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
5	EDO	A	511	-	-	X	X
5	EDO	B	407	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6567 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 Iota toxin component Ia.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3360	2144	553	660	3	0	0	0

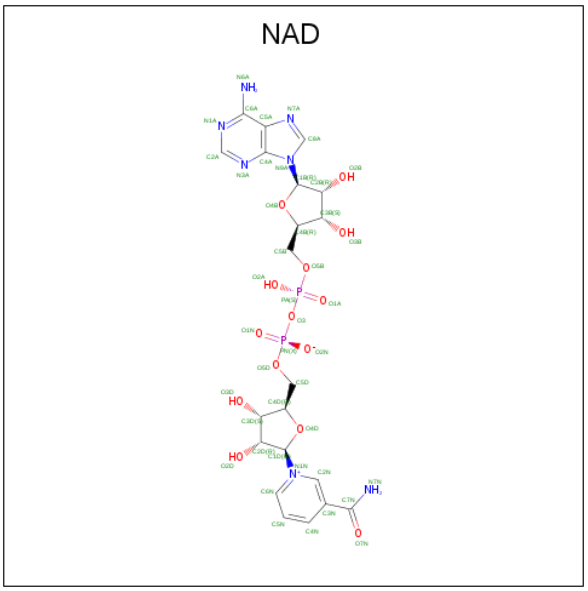
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	ARG	-	EXPRESSION TAG	UNP Q46220
A	-3	GLY	-	EXPRESSION TAG	UNP Q46220
A	-2	SER	-	EXPRESSION TAG	UNP Q46220
A	-1	HIS	-	EXPRESSION TAG	UNP Q46220
A	0	MET	-	EXPRESSION TAG	UNP Q46220
A	380	ALA	GLU	ENGINEERED MUTATION	UNP Q46220

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

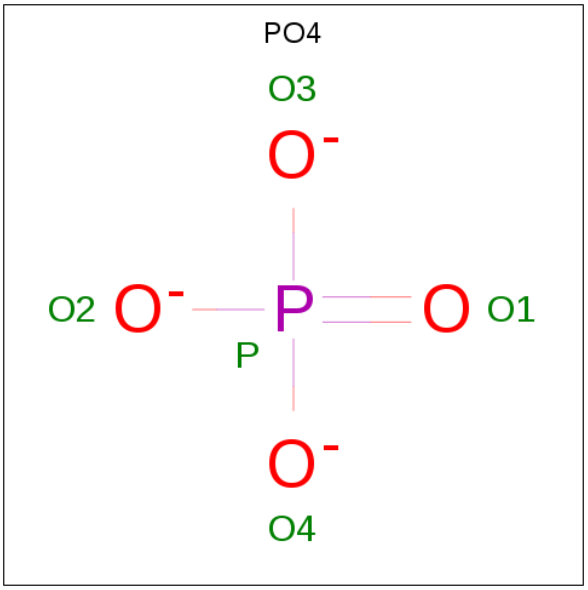
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	358	2799	1774	469	537	19	0	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



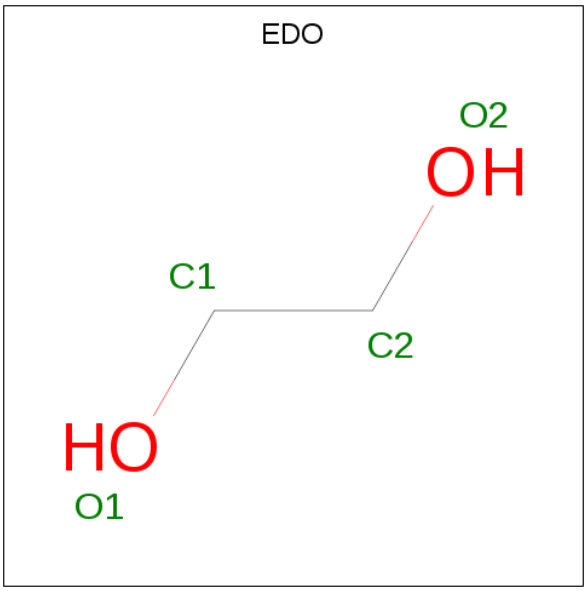
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	44	21	7	14	2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	A	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0

Continued on next page...

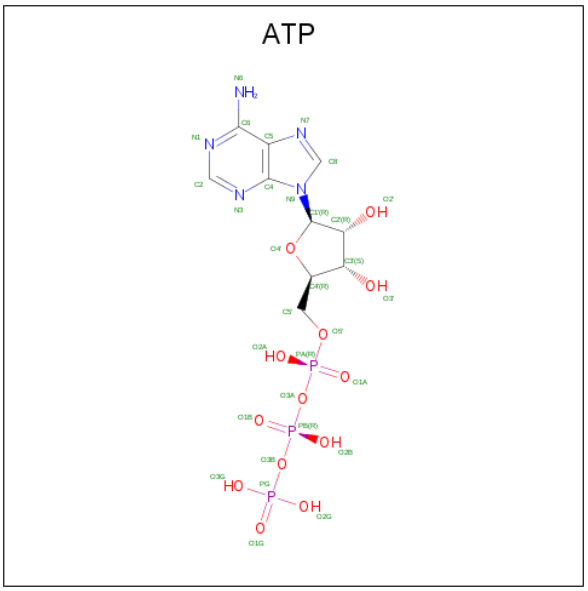
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0
			Total	C	O		
5	B	1	4	2	2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

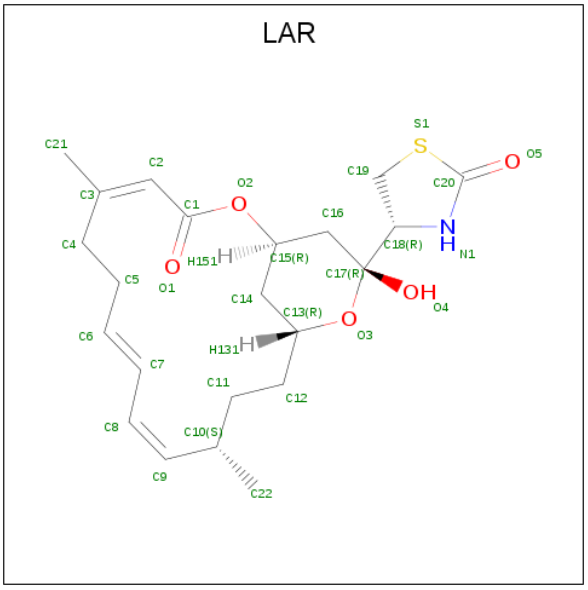
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	B	1	1	1	0	0

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	B	1	31	10	5	13	3	0	0

- Molecule 8 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	B	1	29	22	1	5	1	0	0

- Molecule 9 is water.

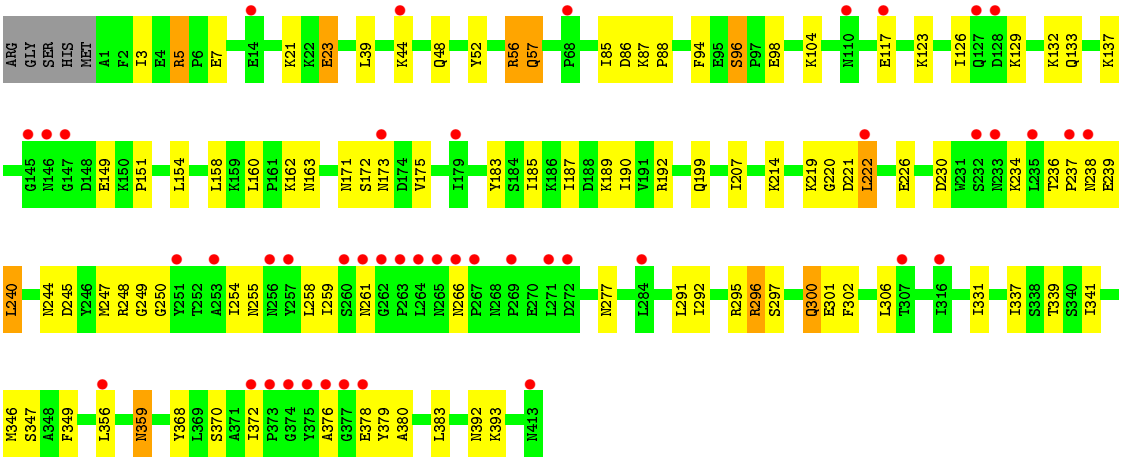
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	110	110	110	0	0
			Total	O		
9	B	100	100	100	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

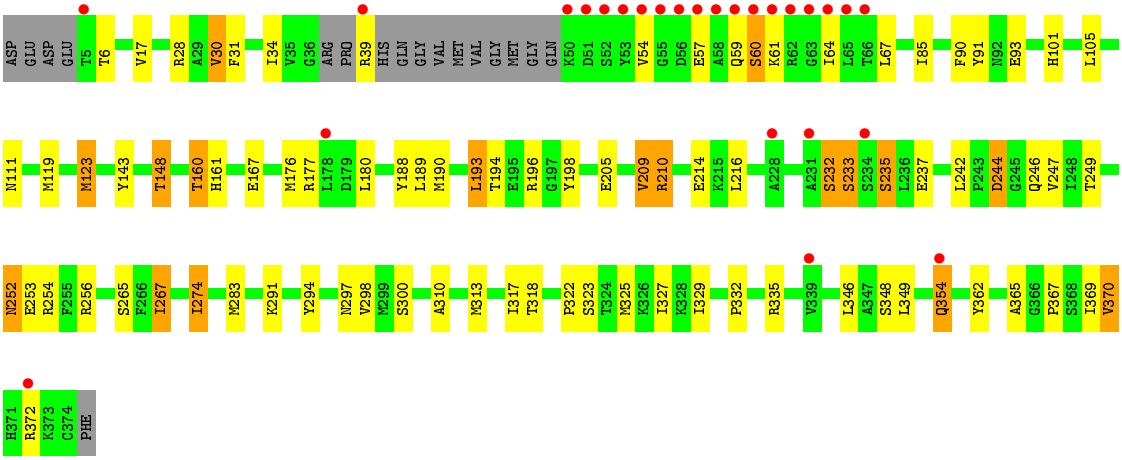
- Molecule 1: Iota toxin component Ia

Chain A:



- Molecule 2: Actin, alpha skeletal muscle

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.08Å 134.65Å 152.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.58 – 2.33 28.58 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.58-2.33) 97.3 (28.58-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.77 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.224 , 0.251 0.229 , 0.250	Depositor DCC
R_{free} test set	2394 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: NAD, PO4, EDO, ATP, CA, LAR

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	0.46	1/3429 (0.0%)	0.61	0/4632
2	B	0.52	2/2857 (0.1%)	0.61	0/3870
All	All	0.49	3/6286 (0.0%)	0.61	0/8502

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	60	SER	CB-OG	7.29	1.51	1.42
1	A	96	SER	CB-OG	5.61	1.49	1.42
2	B	235	SER	CB-OG	5.30	1.49	1.42

There are no bond angle outliers.

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	3360	0	3345	76	0
2	B	2799	0	2772	74	1
3	A	44	0	26	2	0
4	A	5	0	0	0	0
5	A	36	0	54	5	0
5	B	52	0	78	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
7	B	31	0	12	1	0
8	B	29	0	31	0	0
9	A	110	0	0	1	0
9	B	100	0	0	3	1
All	All	6567	0	6318	148	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (148) 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:245:ASP:O	1:A:249:GLY:HA3	1.51	1.11
1:A:236:THR:OG1	1:A:239:GLU:HG3	1.57	1.02
1:A:292:ILE:CD1	1:A:359:ASN:ND2	2.35	0.89
1:A:245:ASP:O	1:A:249:GLY:CA	2.21	0.88
1:A:236:THR:HB	1:A:237:PRO:HD2	1.56	0.85
2:B:291:LYS:HA	2:B:325:MET:HE1	1.62	0.81
1:A:370:SER:HA	1:A:376:ALA:HA	1.61	0.80
2:B:160:THR:HG23	2:B:180:LEU:O	1.82	0.80
2:B:310:ALA:HB1	2:B:329:ILE:HD13	1.65	0.78
2:B:216:LEU:O	2:B:254:ARG:HD2	1.83	0.78
1:A:347:SER:HB2	2:B:176:MET:CE	2.16	0.76
1:A:247:MET:CE	1:A:372:ILE:HG21	2.18	0.73
2:B:210:ARG:HD3	2:B:214:GLU:OE1	1.88	0.72
2:B:190:MET:HG2	2:B:209:VAL:HG11	1.72	0.72
1:A:57:GLN:HG2	1:A:214:LYS:HD3	1.70	0.72
2:B:148:THR:HG23	2:B:167:GLU:HA	1.72	0.72
2:B:244:ASP:OD2	2:B:246:GLN:NE2	2.15	0.71
2:B:332:PRO:HG2	5:B:406:EDO:H12	1.72	0.71
1:A:370:SER:CA	1:A:376:ALA:HA	2.22	0.69
1:A:52:TYR:CZ	1:A:56:ARG:HG3	2.29	0.68
1:A:292:ILE:CD1	1:A:359:ASN:HD22	2.06	0.68
1:A:292:ILE:HD12	1:A:359:ASN:ND2	2.07	0.67
2:B:354:GLN:OE1	2:B:354:GLN:HA	1.95	0.67
2:B:61:LYS:HD3	2:B:64:ILE:HG22	1.77	0.67
1:A:238:ASN:HB3	1:A:277:ASN:ND2	2.10	0.66
1:A:247:MET:HE3	1:A:372:ILE:HG21	1.76	0.66
2:B:362:TYR:O	2:B:365:ALA:O	2.15	0.65
1:A:337:ILE:HG23	1:A:383:LEU:HB2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:THR:CG2	2:B:180:LEU:O	2.44	0.64
1:A:372:ILE:HG22	1:A:372:ILE:O	1.97	0.64
1:A:370:SER:O	1:A:376:ALA:HB1	1.98	0.64
2:B:274:ILE:HG23	2:B:313:MET:HE1	1.80	0.64
1:A:370:SER:CB	1:A:376:ALA:HA	2.27	0.64
2:B:274:ILE:HG23	2:B:313:MET:CE	2.28	0.64
2:B:329:ILE:O	2:B:329:ILE:HD12	1.98	0.63
1:A:236:THR:HB	1:A:237:PRO:CD	2.28	0.62
2:B:111:ASN:HD21	2:B:119:MET:CE	2.13	0.61
1:A:132:LYS:HE3	1:A:359:ASN:ND2	2.15	0.61
1:A:292:ILE:HD12	1:A:359:ASN:HD22	1.66	0.60
2:B:210:ARG:HH11	2:B:210:ARG:HG3	1.66	0.60
1:A:96:SER:HB3	1:A:98:GLU:OE2	2.00	0.60
2:B:188:TYR:CD1	2:B:267:ILE:HD11	2.37	0.60
1:A:296:ARG:H	3:A:501:NAD:H72N	1.49	0.59
2:B:323:SER:HA	5:B:408:EDO:H22	1.84	0.59
1:A:244:ASN:HA	1:A:247:MET:HB2	1.83	0.59
2:B:196:ARG:HH21	2:B:249:THR:HG22	1.67	0.59
2:B:300:SER:HA	2:B:335:ARG:HG2	1.82	0.59
1:A:292:ILE:CD1	1:A:359:ASN:HD21	2.12	0.59
2:B:232:SER:OG	2:B:233:SER:N	2.35	0.58
1:A:302:PHE:HZ	1:A:356:LEU:HD11	1.67	0.58
2:B:367:PRO:O	2:B:370:VAL:HG22	2.04	0.58
2:B:105:LEU:HD21	2:B:123:MET:HE1	1.85	0.58
1:A:347:SER:CB	2:B:176:MET:CE	2.80	0.58
1:A:236:THR:OG1	1:A:239:GLU:CG	2.43	0.57
1:A:5:ARG:NH2	1:A:88:PRO:O	2.35	0.57
1:A:183:TYR:HA	5:A:511:EDO:H12	1.87	0.57
2:B:294:TYR:HE2	5:B:407:EDO:HO2	1.53	0.57
2:B:34:ILE:HD12	2:B:67:LEU:HD22	1.88	0.55
2:B:54:VAL:HG13	2:B:85:ILE:HD13	1.88	0.55
2:B:283:MET:HE1	5:B:407:EDO:O2	2.06	0.55
1:A:247:MET:HE1	1:A:372:ILE:HG21	1.87	0.55
1:A:302:PHE:CZ	1:A:356:LEU:HD11	2.43	0.54
2:B:210:ARG:CD	2:B:214:GLU:OE1	2.54	0.54
1:A:172:SER:OG	1:A:173:ASN:N	2.37	0.54
2:B:298:VAL:CG1	5:B:406:EDO:H21	2.37	0.54
2:B:237:GLU:HG2	2:B:249:THR:HG23	1.89	0.53
1:A:300:GLN:NE2	3:A:501:NAD:O3B	2.42	0.53
1:A:183:TYR:CA	5:A:511:EDO:H12	2.39	0.53
1:A:292:ILE:HD11	1:A:359:ASN:HD21	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLY:HA3	1:A:341:ILE:HD13	1.91	0.53
1:A:306:LEU:HD21	2:B:265:SER:HB2	1.91	0.52
2:B:188:TYR:HB2	2:B:267:ILE:HD11	1.91	0.52
2:B:6:THR:O	2:B:101:HIS:HD2	1.92	0.52
1:A:347:SER:CB	2:B:176:MET:HE2	2.40	0.52
1:A:255:ASN:O	1:A:259:ILE:HG12	2.09	0.52
2:B:369:ILE:HD12	2:B:372:ARG:HD3	1.92	0.52
2:B:283:MET:CE	5:B:407:EDO:O2	2.58	0.51
1:A:85:ILE:HD12	1:A:87:LYS:O	2.10	0.51
1:A:370:SER:O	1:A:376:ALA:CB	2.59	0.50
5:A:504:EDO:H21	2:B:176:MET:HE3	1.93	0.50
5:A:511:EDO:H21	9:A:673:HOH:O	2.11	0.49
1:A:192:ARG:HD2	1:A:199:GLN:OE1	2.12	0.49
2:B:111:ASN:ND2	2:B:119:MET:CE	2.76	0.49
2:B:190:MET:HG2	2:B:209:VAL:CG1	2.42	0.49
2:B:318:THR:HG23	5:B:408:EDO:H21	1.95	0.49
1:A:133:GLN:HG3	1:A:185:ILE:HG12	1.94	0.48
1:A:295:ARG:HB2	1:A:339:THR:HG22	1.95	0.48
2:B:148:THR:H	5:B:409:EDO:H12	1.78	0.48
2:B:143:TYR:OH	2:B:349:LEU:HD11	2.14	0.48
2:B:252:ASN:HD22	2:B:253:GLU:N	2.12	0.47
1:A:52:TYR:CE2	1:A:56:ARG:HG3	2.49	0.47
2:B:317:ILE:HG22	2:B:327:ILE:HD13	1.97	0.47
2:B:111:ASN:HD21	2:B:119:MET:HE3	1.79	0.47
2:B:252:ASN:ND2	2:B:256:ARG:HH21	2.12	0.47
1:A:250:GLY:O	1:A:254:ILE:HD12	2.14	0.46
1:A:346:MET:HG3	1:A:349:PHE:CE1	2.51	0.46
1:A:126:ILE:HD11	1:A:190:ILE:HG21	1.97	0.46
2:B:61:LYS:HD3	2:B:64:ILE:CG2	2.46	0.46
1:A:222:LEU:O	1:A:226:GLU:HB2	2.16	0.46
1:A:378:GLU:HB2	1:A:380:ALA:HB2	1.97	0.46
1:A:346:MET:HG3	1:A:349:PHE:CZ	2.50	0.45
5:B:404:EDO:H11	9:B:581:HOH:O	2.16	0.45
2:B:194:THR:HA	2:B:198:TYR:O	2.16	0.45
2:B:332:PRO:O	2:B:335:ARG:HB2	2.16	0.45
1:A:192:ARG:HD2	1:A:199:GLN:CD	2.37	0.45
2:B:54:VAL:O	2:B:57:GLU:HB2	2.17	0.45
1:A:292:ILE:HD11	5:A:511:EDO:H22	1.99	0.45
2:B:267:ILE:HA	2:B:267:ILE:HD13	1.68	0.45
2:B:30:VAL:HG21	9:B:557:HOH:O	2.16	0.45
1:A:297:SER:HB2	1:A:301:GLU:CD	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:SER:HA	1:A:376:ALA:CA	2.39	0.44
1:A:160:LEU:HD23	1:A:207:ILE:HD12	1.99	0.43
2:B:244:ASP:CG	2:B:246:GLN:HE22	2.12	0.43
1:A:292:ILE:HD11	1:A:359:ASN:ND2	2.25	0.43
1:A:94:PHE:CG	1:A:151:PRO:HD2	2.54	0.43
2:B:188:TYR:CD1	2:B:267:ILE:CD1	3.01	0.43
2:B:205:GLU:O	2:B:209:VAL:HG12	2.18	0.43
2:B:313:MET:HG3	2:B:317:ILE:HD12	1.99	0.43
1:A:162:LYS:O	1:A:163:ASN:HB2	2.19	0.43
1:A:5:ARG:HH21	1:A:7:GLU:HA	1.84	0.43
2:B:274:ILE:HG23	2:B:313:MET:HE2	1.99	0.43
2:B:210:ARG:HD2	2:B:214:GLU:CD	2.39	0.42
2:B:31:PHE:CE2	2:B:93:GLU:HG3	2.55	0.42
2:B:105:LEU:HD21	2:B:123:MET:CE	2.47	0.42
2:B:210:ARG:HH11	2:B:210:ARG:CG	2.30	0.42
5:B:415:EDO:H22	5:B:416:EDO:H12	2.02	0.42
2:B:91:TYR:HA	9:B:548:HOH:O	2.19	0.41
1:A:23:GLU:OE2	1:A:23:GLU:HA	2.21	0.41
1:A:337:ILE:CG2	1:A:383:LEU:HB2	2.47	0.41
1:A:21:LYS:HG3	1:A:175:VAL:HG21	2.01	0.41
1:A:57:GLN:HG2	1:A:214:LYS:HB3	2.01	0.41
1:A:123:LYS:HB2	1:A:190:ILE:HD11	2.02	0.41
1:A:249:GLY:HA3	1:A:250:GLY:HA3	1.61	0.41
2:B:214:GLU:HG2	7:B:402:ATP:C5	2.56	0.41
1:A:372:ILE:CG2	1:A:372:ILE:O	2.66	0.41
1:A:129:LYS:HG2	1:A:392:ASN:HD22	1.84	0.41
1:A:238:ASN:HB3	1:A:277:ASN:HD22	1.80	0.41
1:A:368:TYR:CZ	1:A:370:SER:HB2	2.56	0.41
2:B:90:PHE:CZ	2:B:123:MET:HE3	2.56	0.41
2:B:161:HIS:CD2	2:B:177:ARG:HB2	2.56	0.41
2:B:189:LEU:O	2:B:193:LEU:HB2	2.21	0.41
1:A:347:SER:OG	2:B:176:MET:CE	2.69	0.41
2:B:322:PRO:HG2	5:B:407:EDO:H21	2.03	0.40
1:A:126:ILE:HD12	1:A:187:ILE:HD13	2.03	0.40
1:A:221:ASP:HB2	1:A:379:TYR:CE1	2.56	0.40
2:B:17:VAL:O	2:B:30:VAL:HA	2.21	0.40
1:A:240:LEU:HD22	1:A:240:LEU:HA	1.91	0.40
2:B:298:VAL:HG12	5:B:406:EDO:H21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:GLN:NE2	9:B:548:HOH:O[4_445]	1.94	0.26

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	411/418 (98%)	390 (95%)	20 (5%)	1 (0%)	47	55
2	B	353/375 (94%)	343 (97%)	10 (3%)	0	100	100
All	All	764/793 (96%)	733 (96%)	30 (4%)	1 (0%)	51	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	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	375/379 (99%)	344 (92%)	31 (8%)	11	11
2	B	304/318 (96%)	279 (92%)	25 (8%)	11	11
All	All	679/697 (97%)	623 (92%)	56 (8%)	11	11

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	5	ARG
1	A	23	GLU
1	A	39	LEU
1	A	44	LYS
1	A	48	GLN
1	A	57	GLN
1	A	86	ASP
1	A	104	LYS
1	A	117	GLU
1	A	137	LYS
1	A	149	GLU
1	A	154	LEU
1	A	158	LEU
1	A	171	ASN
1	A	189	LYS
1	A	219	LYS
1	A	222	LEU
1	A	230	ASP
1	A	234	LYS
1	A	240	LEU
1	A	248	ARG
1	A	258	LEU
1	A	261	ASN
1	A	266	ASN
1	A	291	LEU
1	A	296	ARG
1	A	300	GLN
1	A	331	ILE
1	A	359	ASN
1	A	393	LYS
2	B	28	ARG
2	B	30	VAL
2	B	39	ARG
2	B	59	GLN
2	B	60	SER
2	B	123	MET
2	B	148	THR
2	B	160	THR
2	B	193	LEU
2	B	209	VAL
2	B	210	ARG
2	B	232	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	233	SER
2	B	235	SER
2	B	242	LEU
2	B	244	ASP
2	B	247	VAL
2	B	252	ASN
2	B	267	ILE
2	B	274	ILE
2	B	297	ASN
2	B	346	LEU
2	B	348	SER
2	B	354	GLN
2	B	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	51	ASN
1	A	78	ASN
1	A	90	ASN
1	A	120	ASN
1	A	146	ASN
1	A	157	HIS
1	A	171	ASN
1	A	209	ASN
1	A	256	ASN
1	A	261	ASN
1	A	266	ASN
1	A	277	ASN
1	A	280	ASN
1	A	300	GLN
1	A	359	ASN
1	A	392	ASN
2	B	88	HIS
2	B	101	HIS
2	B	111	ASN
2	B	128	ASN
2	B	162	ASN
2	B	252	ASN
2	B	263	GLN
2	B	297	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	$\#\|Z\| > 2$
4	PO4	A	502	-	4,4,4	0.81	0	6,6,6	0.53	0
5	EDO	B	416	-	3,3,3	0.48	0	2,2,2	0.40	0
8	LAR	B	403	-	30,31,31	1.65	3 (10%)	32,43,43	2.31	7 (21%)
5	EDO	A	505	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	A	504	-	3,3,3	0.51	0	2,2,2	0.35	0
5	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	407	-	3,3,3	0.65	0	2,2,2	0.31	0
5	EDO	B	415	-	3,3,3	0.50	0	2,2,2	0.16	0
5	EDO	A	506	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	B	405	-	3,3,3	0.57	0	2,2,2	0.23	0
7	ATP	B	402	-	26,33,33	0.92	1 (3%)	31,52,52	1.28	4 (12%)
5	EDO	B	409	-	3,3,3	0.50	0	2,2,2	0.35	0
5	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.39	0
5	EDO	B	413	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	A	508	-	3,3,3	0.50	0	2,2,2	0.41	0
5	EDO	B	404	-	3,3,3	0.51	0	2,2,2	0.30	0
5	EDO	A	503	-	3,3,3	0.65	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	B	408	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	B	411	-	3,3,3	0.47	0	2,2,2	0.33	0
5	EDO	B	412	-	3,3,3	0.54	0	2,2,2	0.38	0
5	EDO	B	410	-	3,3,3	0.48	0	2,2,2	0.36	0
5	EDO	A	507	-	3,3,3	0.47	0	2,2,2	0.36	0
5	EDO	B	414	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	B	406	-	3,3,3	0.50	0	2,2,2	0.38	0
5	EDO	A	511	-	3,3,3	0.59	0	2,2,2	0.41	0
3	NAD	A	501	-	42,48,48	0.84	2 (4%)	50,73,73	1.30	5 (10%)

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
5	EDO	B	416	-	-	1/1/1/1	-
8	LAR	B	403	-	-	5/23/51/51	0/2/3/3
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	A	504	-	-	0/1/1/1	-
5	EDO	A	510	-	-	1/1/1/1	-
5	EDO	B	407	-	-	1/1/1/1	-
5	EDO	B	415	-	-	1/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
5	EDO	B	405	-	-	1/1/1/1	-
7	ATP	B	402	-	-	4/18/38/38	0/3/3/3
5	EDO	B	409	-	-	1/1/1/1	-
5	EDO	A	509	-	-	0/1/1/1	-
5	EDO	B	413	-	-	0/1/1/1	-
5	EDO	A	508	-	-	1/1/1/1	-
5	EDO	B	404	-	-	1/1/1/1	-
5	EDO	A	503	-	-	0/1/1/1	-
5	EDO	B	408	-	-	1/1/1/1	-
5	EDO	B	411	-	-	1/1/1/1	-
5	EDO	B	412	-	-	0/1/1/1	-
5	EDO	B	410	-	-	0/1/1/1	-
5	EDO	A	507	-	-	0/1/1/1	-
5	EDO	B	414	-	-	1/1/1/1	-
5	EDO	B	406	-	-	1/1/1/1	-
5	EDO	A	511	-	-	0/1/1/1	-
3	NAD	A	501	-	-	12/26/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	403	LAR	O2-C1	6.21	1.47	1.34
8	B	403	LAR	C20-S1	-4.93	1.66	1.77
3	A	501	NAD	C5A-C4A	2.45	1.47	1.40
7	B	402	ATP	C5-C4	2.44	1.47	1.40
3	A	501	NAD	O4D-C1D	2.07	1.44	1.41
8	B	403	LAR	O4-C17	2.06	1.44	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	403	LAR	C4-C5-C6	-7.35	96.71	112.59
8	B	403	LAR	O2-C1-C2	5.29	123.68	111.27
8	B	403	LAR	C8-C7-C6	-4.48	99.76	125.51
3	A	501	NAD	N3A-C2A-N1A	-3.81	122.73	128.68
3	A	501	NAD	PN-O3-PA	-3.63	120.38	132.83
7	B	402	ATP	N3-C2-N1	-3.54	123.15	128.68
8	B	403	LAR	O1-C1-C2	-3.23	118.09	126.23
8	B	403	LAR	O2-C1-O1	-3.15	118.23	123.35
8	B	403	LAR	C19-S1-C20	2.98	93.60	92.00
3	A	501	NAD	C4A-C5A-N7A	-2.69	106.59	109.40
8	B	403	LAR	O5-C20-N1	-2.56	124.01	126.81
3	A	501	NAD	C1B-N9A-C4A	-2.55	122.17	126.64
3	A	501	NAD	C6N-N1N-C2N	-2.52	119.67	121.97
7	B	402	ATP	C2-N1-C6	2.17	122.46	118.75
7	B	402	ATP	C4-C5-N7	-2.13	107.17	109.40
7	B	402	ATP	PA-O3A-PB	-2.03	125.85	132.83

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	403	LAR	O3-C17-C18-C19
3	A	501	NAD	C5D-O5D-PN-O1N
3	A	501	NAD	O4D-C4D-C5D-O5D
3	A	501	NAD	C3D-C4D-C5D-O5D
5	B	416	EDO	O1-C1-C2-O2
5	A	510	EDO	O1-C1-C2-O2
5	B	404	EDO	O1-C1-C2-O2
5	B	411	EDO	O1-C1-C2-O2
3	A	501	NAD	C2N-C3N-C7N-N7N
7	B	402	ATP	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	501	NAD	C5D-O5D-PN-O3
3	A	501	NAD	C2N-C3N-C7N-O7N
3	A	501	NAD	C4D-C5D-O5D-PN
3	A	501	NAD	C5D-O5D-PN-O2N
8	B	403	LAR	O2-C1-C2-C3
5	A	508	EDO	O1-C1-C2-O2
5	B	408	EDO	O1-C1-C2-O2
3	A	501	NAD	C4N-C3N-C7N-N7N
8	B	403	LAR	C3-C4-C5-C6
5	B	405	EDO	O1-C1-C2-O2
3	A	501	NAD	C4N-C3N-C7N-O7N
7	B	402	ATP	PG-O3B-PB-O1B
3	A	501	NAD	PA-O3-PN-O1N
5	B	415	EDO	O1-C1-C2-O2
8	B	403	LAR	O1-C1-C2-C3
5	B	407	EDO	O1-C1-C2-O2
5	B	409	EDO	O1-C1-C2-O2
5	B	406	EDO	O1-C1-C2-O2
8	B	403	LAR	C4-C5-C6-C7
7	B	402	ATP	PB-O3B-PG-O2G
7	B	402	ATP	PG-O3B-PB-O2B
3	A	501	NAD	PA-O3-PN-O2N
5	B	414	EDO	O1-C1-C2-O2

There are no ring outliers.

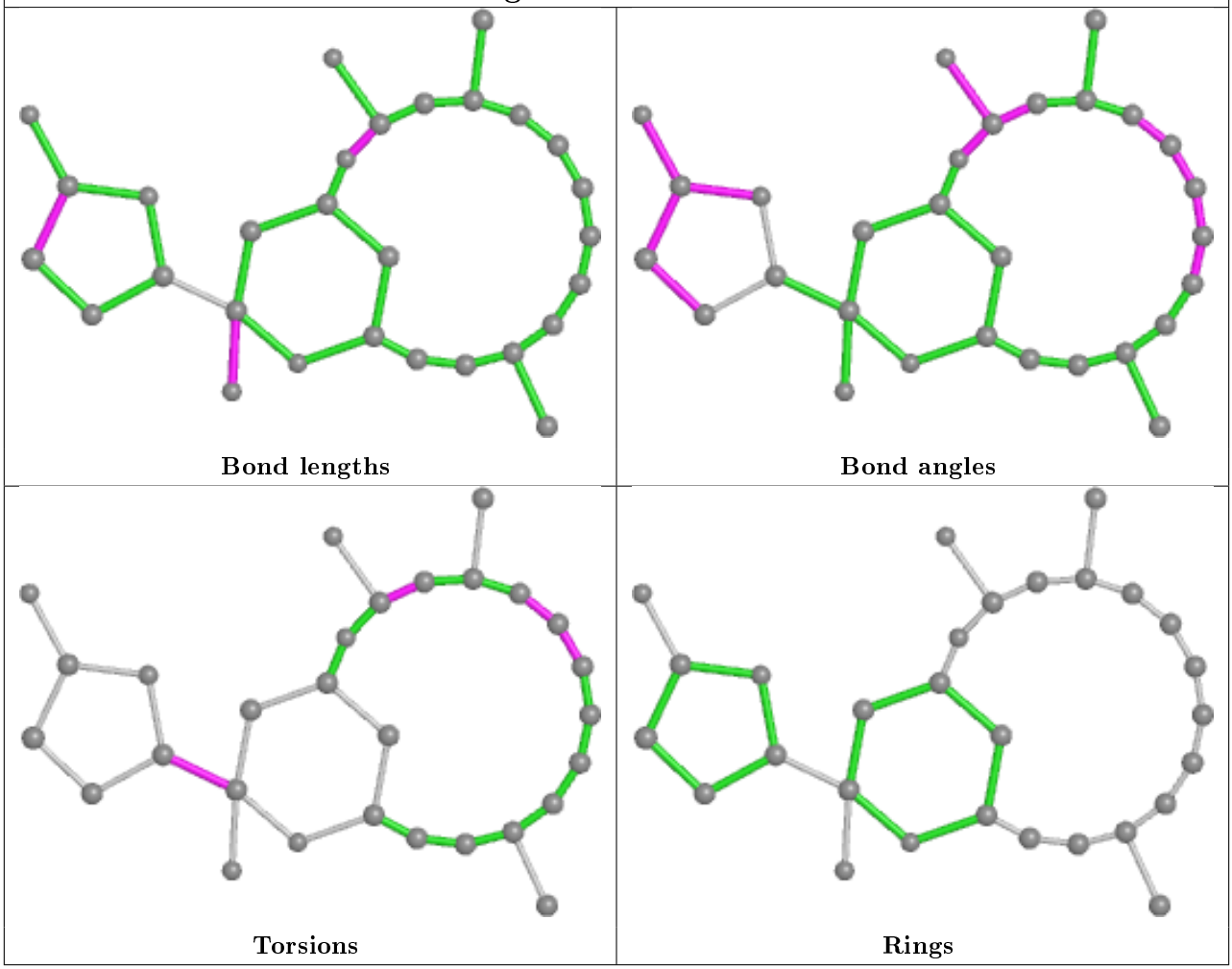
11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	416	EDO	1	0
5	A	504	EDO	1	0
5	B	407	EDO	4	0
5	B	415	EDO	1	0
7	B	402	ATP	1	0
5	B	409	EDO	1	0
5	B	404	EDO	1	0
5	B	408	EDO	2	0
5	B	406	EDO	3	0
5	A	511	EDO	4	0
3	A	501	NAD	2	0

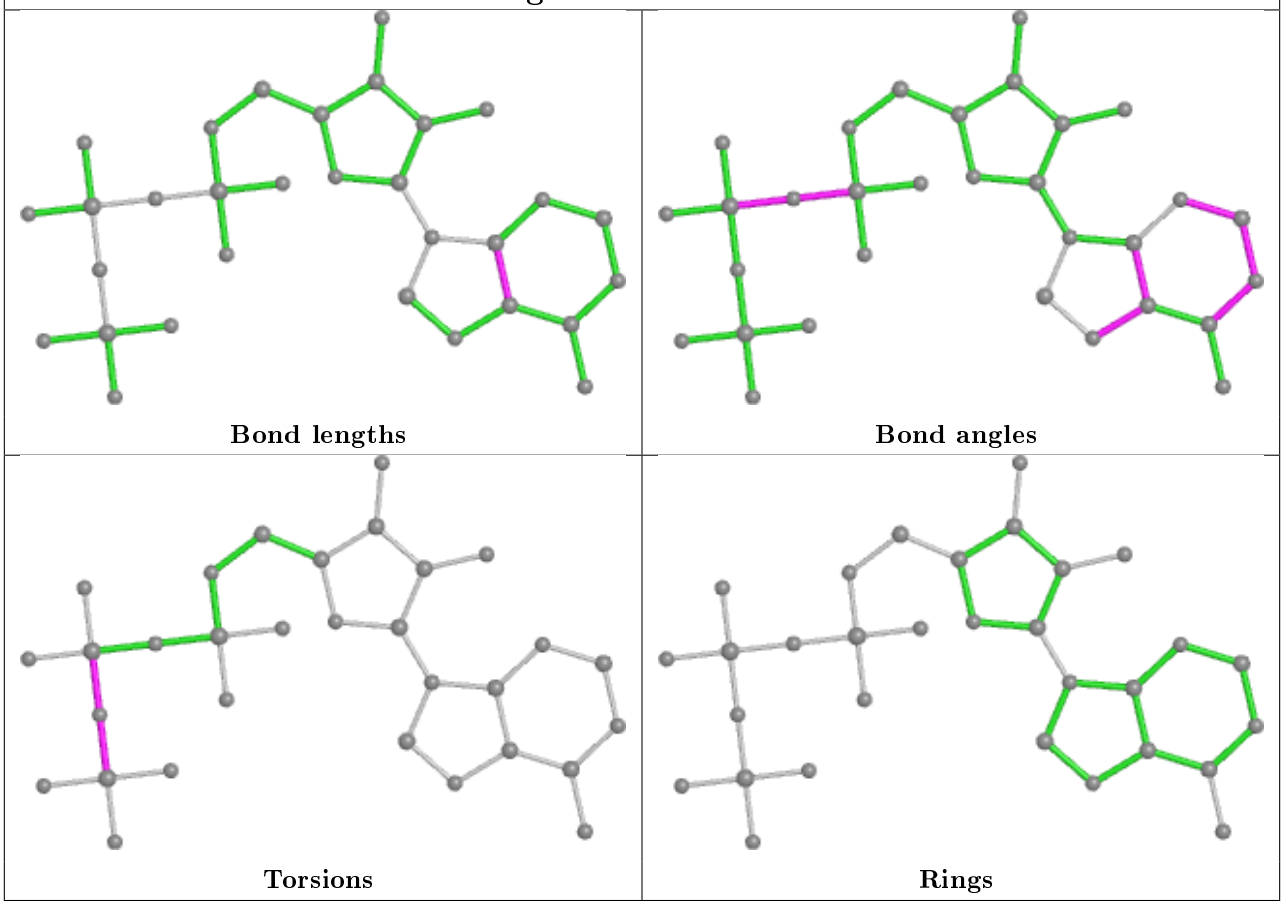
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

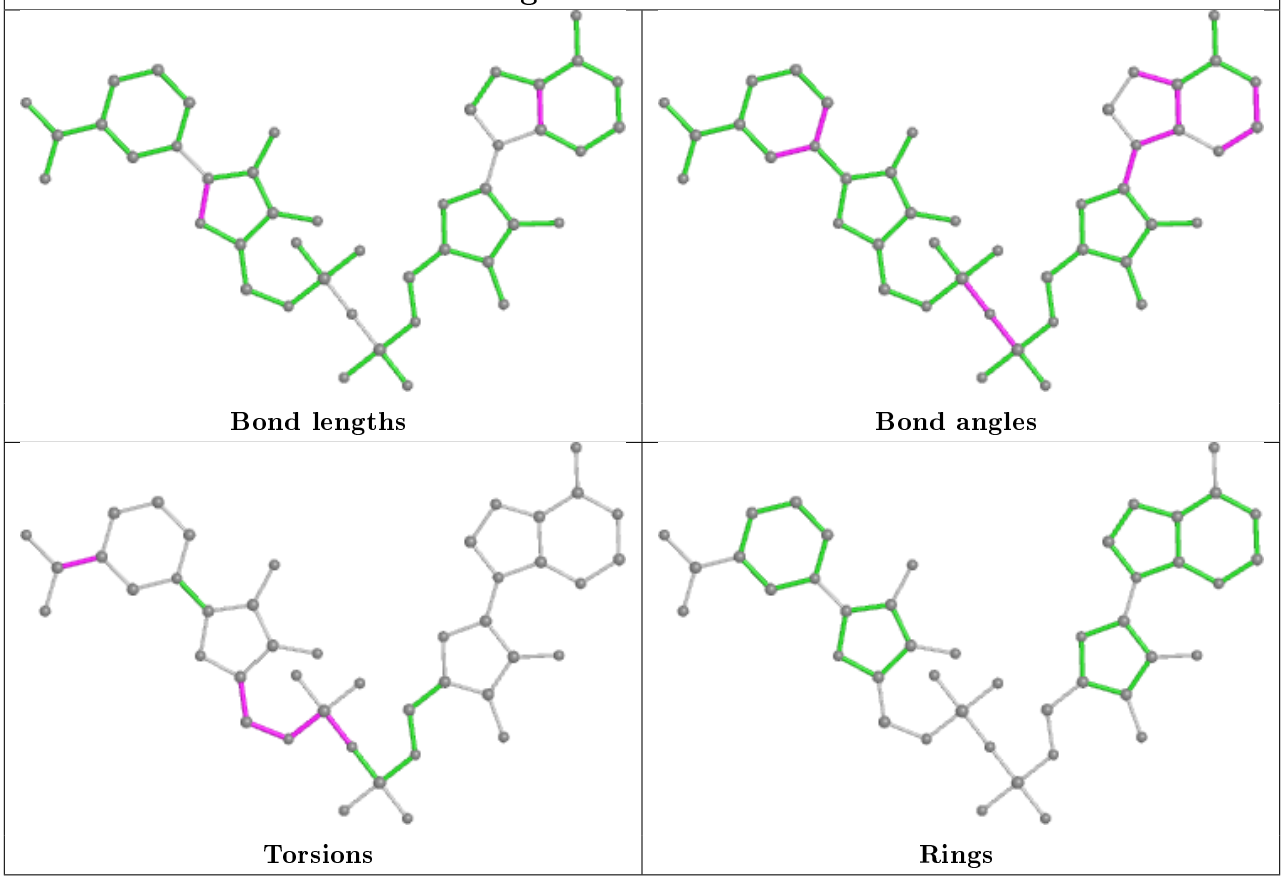
Ligand LAR B 403



Ligand ATP B 402



Ligand NAD A 501



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	413/418 (98%)	0.65	45 (10%) 5 9	28, 46, 83, 101	0
2	B	358/375 (95%)	0.52	26 (7%) 15 22	19, 28, 73, 141	0
All	All	771/793 (97%)	0.59	71 (9%) 9 14	19, 37, 81, 141	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	60	SER	14.6
1	A	376	ALA	11.3
2	B	50	LYS	11.0
2	B	51	ASP	10.4
2	B	39	ARG	10.4
2	B	52	SER	8.6
2	B	64	ILE	7.5
2	B	53	TYR	7.3
2	B	57	GLU	6.7
2	B	62	ARG	6.3
2	B	63	GLY	5.9
1	A	233	ASN	5.6
1	A	264	LEU	5.3
1	A	375	TYR	5.3
2	B	59	GLN	5.2
2	B	56	ASP	4.9
2	B	61	LYS	4.7
1	A	372	ILE	4.6
1	A	269	PRO	4.5
1	A	232	SER	4.1
1	A	173	ASN	4.0
2	B	66	THR	3.9
1	A	263	PRO	3.8
1	A	284	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	65	LEU	3.7
2	B	54	VAL	3.6
1	A	272	ASP	3.4
2	B	234	SER	3.4
1	A	237	PRO	3.3
1	A	267	PRO	3.3
1	A	266	ASN	3.3
1	A	128	ASP	3.3
1	A	238	ASN	3.2
1	A	253	ALA	3.1
1	A	260	SER	3.1
1	A	257	TYR	3.1
1	A	179	ILE	3.1
1	A	271	LEU	3.0
2	B	58	ALA	2.9
1	A	117	GLU	2.9
2	B	55	GLY	2.9
1	A	68	PRO	2.9
1	A	146	ASN	2.8
2	B	5	THR	2.7
1	A	145	GLY	2.6
2	B	354	GLN	2.6
1	A	265	ASN	2.6
1	A	374	GLY	2.5
1	A	222	LEU	2.5
1	A	373	PRO	2.4
1	A	262	GLY	2.4
1	A	378	GLU	2.4
1	A	127	GLN	2.4
1	A	235	LEU	2.4
1	A	110	ASN	2.4
1	A	147	GLY	2.4
1	A	413	ASN	2.3
1	A	14	GLU	2.3
1	A	44	LYS	2.3
1	A	261	ASN	2.3
1	A	316	ILE	2.3
1	A	377	GLY	2.2
1	A	251	TYR	2.2
2	B	339	VAL	2.2
1	A	256	ASN	2.2
2	B	372	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	178	LEU	2.1
2	B	228	ALA	2.1
1	A	356	LEU	2.1
1	A	307	THR	2.1
2	B	231	ALA	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 carbohydrates 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
5	EDO	A	511	4/4	0.58	0.60	43,43,43,44	0
5	EDO	A	504	4/4	0.76	0.26	35,35,35,35	0
5	EDO	B	407	4/4	0.77	0.24	38,38,39,39	0
5	EDO	B	404	4/4	0.78	0.26	37,39,39,40	0
5	EDO	B	405	4/4	0.80	0.40	49,49,49,50	0
5	EDO	A	509	4/4	0.80	0.24	46,46,46,47	0
5	EDO	B	409	4/4	0.81	0.20	40,40,41,49	0
5	EDO	B	406	4/4	0.83	0.25	26,27,28,29	0
5	EDO	A	510	4/4	0.83	0.23	44,44,45,45	0
5	EDO	A	508	4/4	0.85	0.23	40,41,41,41	0
5	EDO	B	415	4/4	0.87	0.33	39,40,45,46	0
3	NAD	A	501	44/44	0.87	0.21	59,70,74,77	0
5	EDO	B	416	4/4	0.89	0.14	36,36,37,38	0
5	EDO	A	506	4/4	0.90	0.18	38,38,39,39	0
8	LAR	B	403	29/29	0.92	0.13	29,31,34,34	0
5	EDO	B	408	4/4	0.92	0.37	37,38,39,39	0
5	EDO	B	411	4/4	0.92	0.33	48,49,49,50	0
5	EDO	B	414	4/4	0.93	0.18	27,28,28,28	0

Continued on next page...

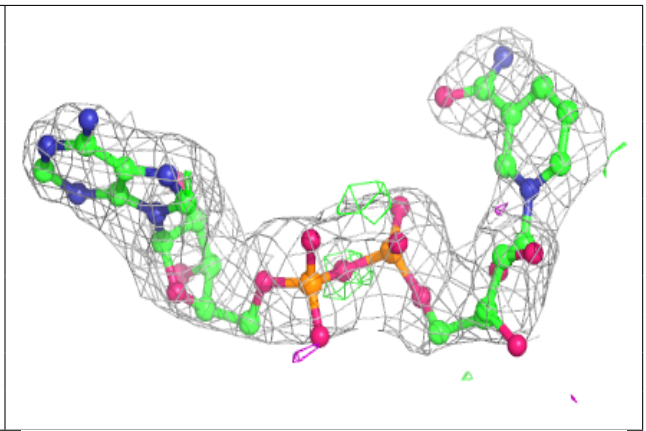
Continued from previous page...

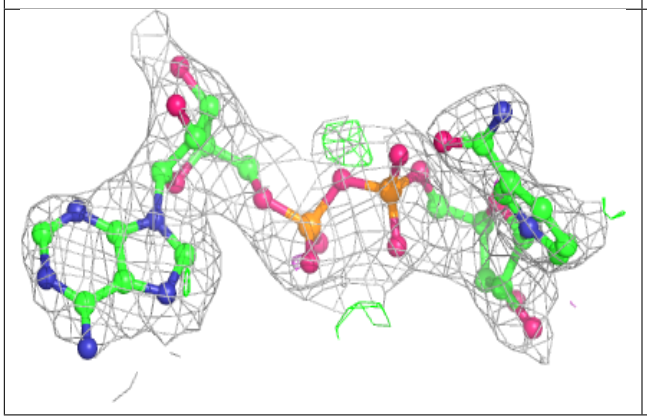
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	505	4/4	0.93	0.19	38,39,39,39	0
5	EDO	A	503	4/4	0.94	0.19	39,39,39,40	0
5	EDO	B	410	4/4	0.94	0.13	38,38,38,39	0
5	EDO	B	413	4/4	0.94	0.16	38,38,38,39	0
4	PO4	A	502	5/5	0.95	0.24	56,57,57,60	0
5	EDO	A	507	4/4	0.95	0.19	43,43,44,44	0
5	EDO	B	412	4/4	0.95	0.16	34,34,34,35	0
7	ATP	B	402	31/31	0.98	0.13	20,20,21,21	0
6	CA	B	401	1/1	0.99	0.11	21,21,21,21	0

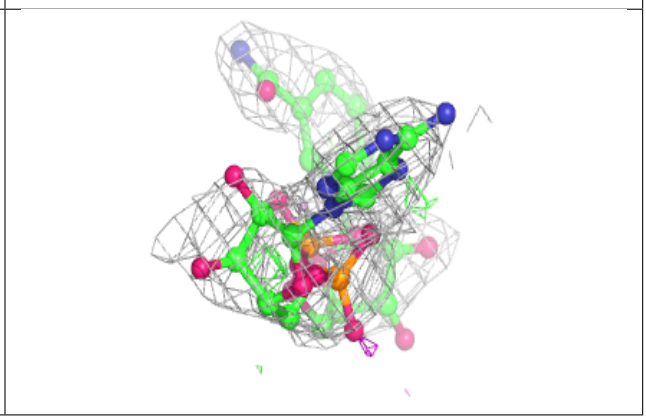
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAD 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)

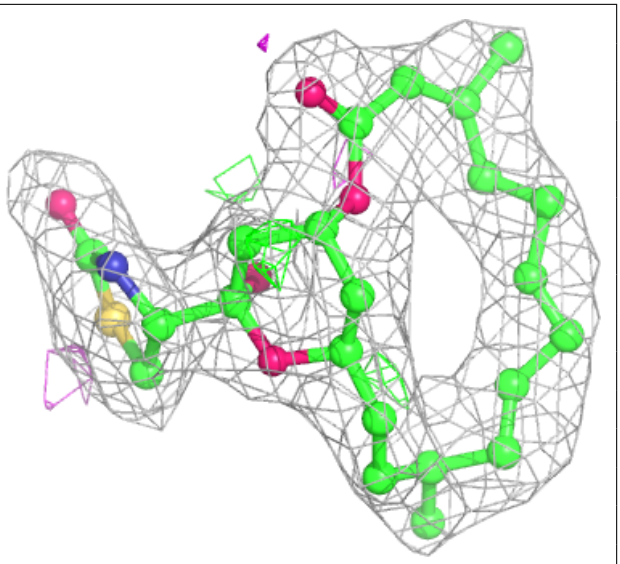


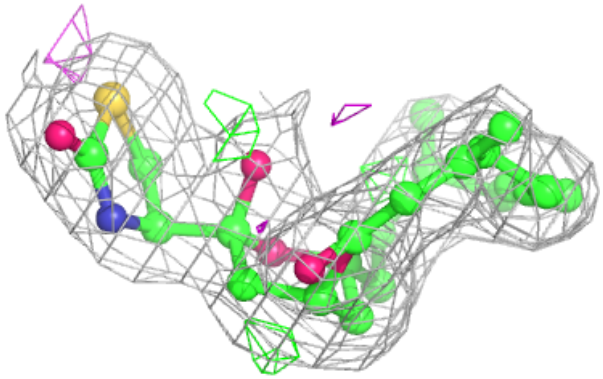


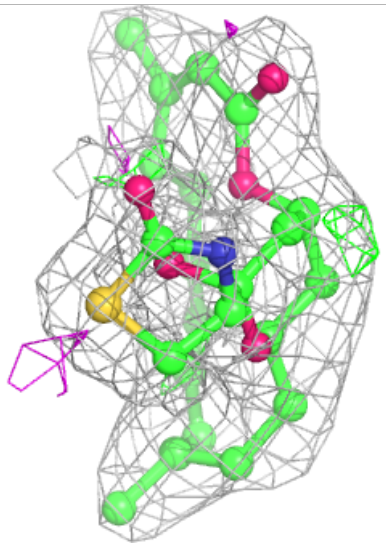


Electron density around LAR B 403:

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

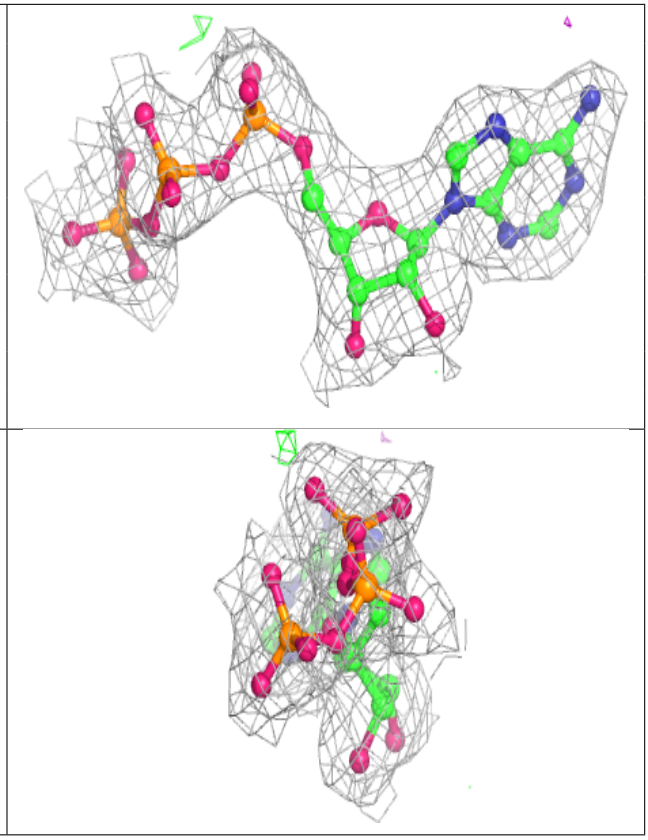






Electron density around ATP B 402:

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



6.5 Other polymers (i)

There are no such residues in this entry.