Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:58 am BST

PDB ID	:	3VPC
Title	:	ArgX from Sulfolobus tokodaii complexed with ADP
Authors	:	Tomita, T.; Horie, A.; Kuzuyama, T.; Nishiyama, M.
Deposited on	:	2012-02-29
Resolution	:	1.87 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

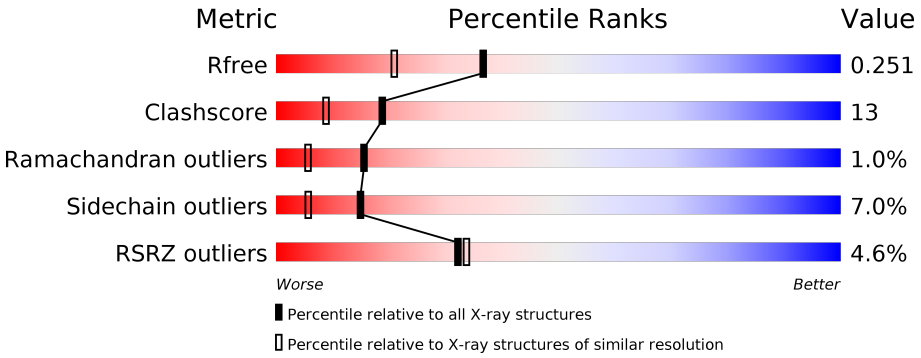
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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	282	5% 78% 18% ·
1	B	282	4% 78% 19% ·
1	C	282	4% 78% 15% · ·
1	D	282	6% 75% 22% ·

2 Entry composition

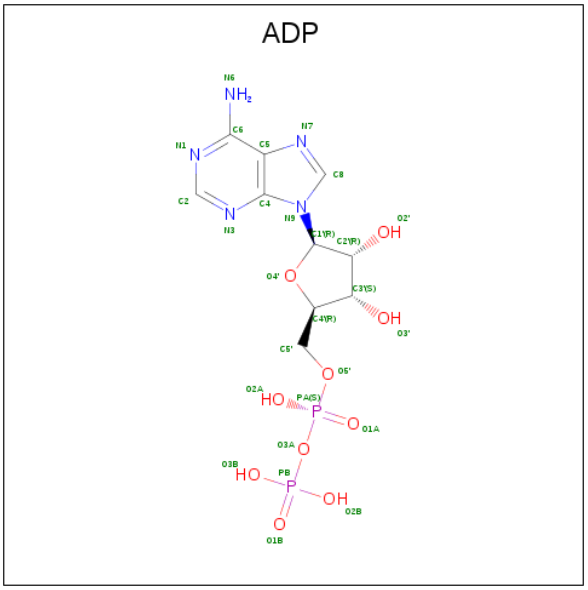
There are 3 unique types of molecules in this entry. The entry contains 10021 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative acetylornithine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	5	0
			2246	1440	382	417	7			
1	B	282	Total	C	N	O	S	0	8	0
			2260	1450	382	421	7			
1	C	275	Total	C	N	O	S	0	7	0
			2213	1420	375	411	7			
1	D	282	Total	C	N	O	S	0	3	0
			2238	1435	379	417	7			

- 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
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 3 is water.

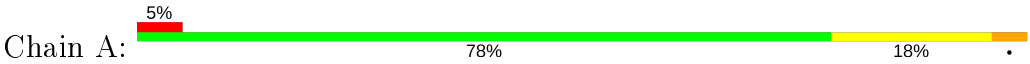
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	270	Total	O	0	0
			270	270		
3	C	221	Total	O	0	0
			221	221		
3	D	218	Total	O	0	0
			218	218		

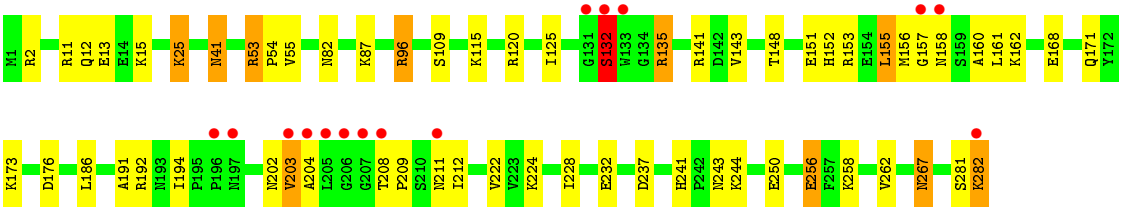
3 Residue-property plots (i)

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: Putative acetylornithine deacetylase

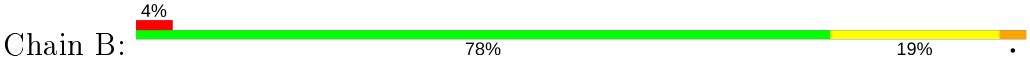
Chain A:

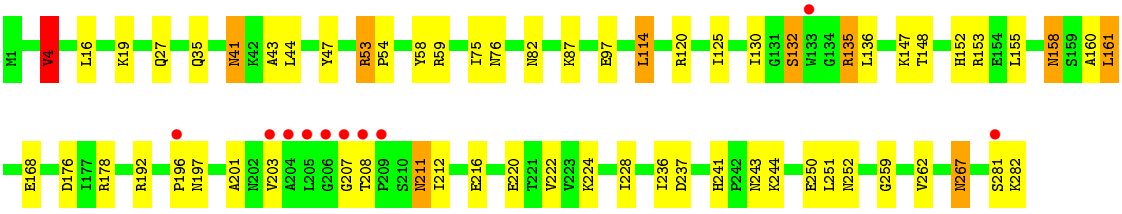




- Molecule 1: Putative acetylornithine deacetylase

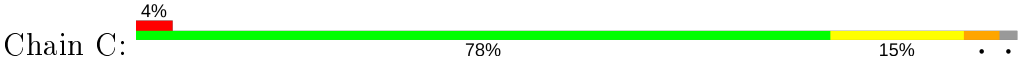
Chain B:

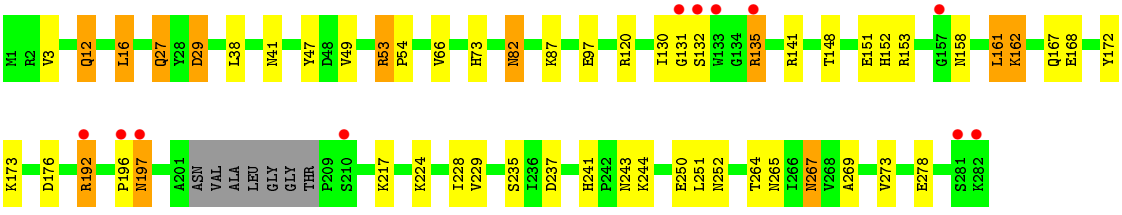




- Molecule 1: Putative acetylornithine deacetylase

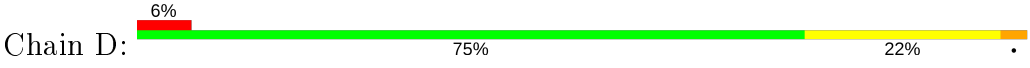
Chain C:

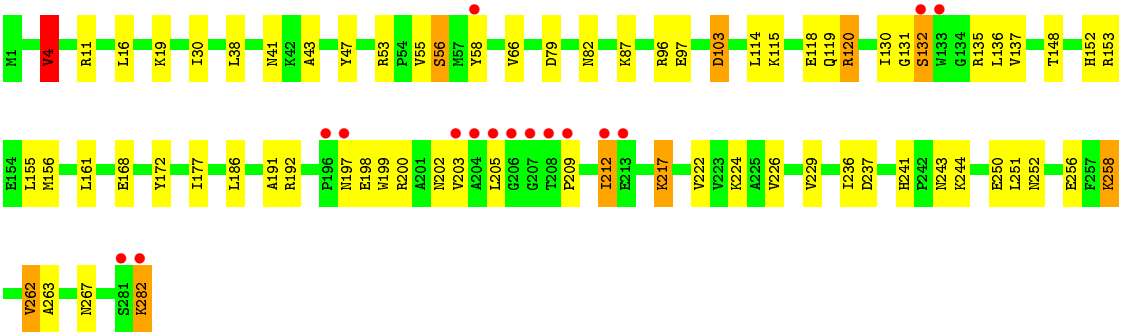




- Molecule 1: Putative acetylornithine deacetylase

Chain D:




M1
V4
R11
L16
K19
I30
L38
N41
K42
A43
Y47
R53
P54
V55
S56
M57
Y58
V66
D79
N82
K87
R96
E97
D103
L114
K115
E118
Q119
R120
L130
G131
S132
W133
G134
R135
L136
V137
T148
H152
R153
E154
L155
M156
L161
E168
Y172
I177
L186
A191
R192
P196
N197
E198
W199
R200
A201
N202
V203
A204
L205
G206
G207
T208
P209
I212
E213
K217
V222
V223
K224
A225
V226
V229
I236
D237
H241
P242
N243
K244
E250
L251
N252
E256
F257
K258
V262
A263
N267
S281
K282

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.27Å 67.84Å 80.03Å 87.77° 75.29° 67.03°	Depositor
Resolution (Å)	34.96 – 1.87 34.96 – 1.87	Depositor EDS
% Data completeness (in resolution range)	95.6 (34.96-1.87) 95.6 (34.96-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.198 , 0.253 0.197 , 0.251	Depositor DCC
R_{free} test set	4707 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10021	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.54	0/2301	0.66	0/3117
1	B	0.56	0/2321	0.69	1/3146 (0.0%)
1	C	0.53	0/2273	0.66	0/3076
1	D	0.55	0/2287	0.69	1/3099 (0.0%)
All	All	0.55	0/9182	0.68	2/12438 (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	4	VAL	CB-CA-C	-5.86	100.27	111.40
1	D	4	VAL	CB-CA-C	-5.33	101.27	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2246	0	2316	70	0
1	B	2260	0	2331	69	0
1	C	2213	0	2282	65	0
1	D	2238	0	2299	61	0
2	A	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
3	A	247	0	0	8	0
3	B	270	0	0	7	0
3	C	221	0	0	7	0
3	D	218	0	0	7	0
All	All	10021	0	9276	241	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 (241) 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:B:135:ARG:HD3	1:B:136:LEU:H	1.10	1.16
1:C:135:ARG:HH21	1:C:135:ARG:HG2	1.06	1.13
1:B:135:ARG:CD	1:B:136:LEU:H	1.67	1.06
1:A:96[A]:ARG:HG2	1:A:96[A]:ARG:HH11	0.89	1.06
1:C:192[B]:ARG:HG2	1:C:192[B]:ARG:HH21	0.90	1.03
1:B:135:ARG:HD3	1:B:136:LEU:N	1.73	1.02
1:A:132:SER:HB3	1:A:135:ARG:HB2	1.43	0.98
1:A:153:ARG:HE	1:D:152:HIS:HE1	1.09	0.96
1:B:87:LYS:NZ	1:B:250:GLU:HG2	1.80	0.96
1:B:152:HIS:HE1	1:C:153:ARG:HE	1.07	0.96
1:C:192[B]:ARG:HG2	1:C:192[B]:ARG:NH2	1.66	0.96
1:A:96[A]:ARG:HG2	1:A:96[A]:ARG:NH1	1.67	0.96
1:C:132:SER:O	1:C:135:ARG:HB2	1.66	0.95
1:A:96[A]:ARG:CG	1:A:96[A]:ARG:HH11	1.80	0.94
1:B:87:LYS:NZ	1:B:250:GLU:CG	2.32	0.92
1:C:192[B]:ARG:CG	1:C:192[B]:ARG:HH21	1.81	0.92
1:A:152:HIS:HE1	1:D:153:ARG:HE	1.13	0.89
1:B:153:ARG:HE	1:C:152:HIS:HE1	1.16	0.89
1:B:41:ASN:HD22	1:B:41:ASN:C	1.79	0.86
1:B:87:LYS:HZ3	1:B:250:GLU:CD	1.79	0.85
1:A:153:ARG:HE	1:D:152:HIS:CE1	1.93	0.85
1:A:132:SER:HB3	1:A:135:ARG:CB	2.07	0.85
1:C:176[A]:ASP:OD2	1:C:192[A]:ARG:NH1	2.09	0.84
1:C:224:LYS:O	1:C:228:ILE:HD13	1.76	0.84
1:C:135:ARG:NH2	1:C:135:ARG:HG2	1.86	0.84
1:B:241:HIS:HD2	1:B:243:ASN:H	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:GLU:HG2	1:D:199:TRP:H	1.43	0.82
1:A:132:SER:O	1:A:135:ARG:HB2	1.79	0.81
1:C:97:GLU:HG2	1:C:228:ILE:HG12	1.62	0.81
1:A:162:LYS:NZ	1:B:59:ARG:HH11	1.78	0.80
1:D:87:LYS:HZ3	1:D:250:GLU:HG2	1.47	0.79
1:A:87:LYS:NZ	1:A:250:GLU:HG2	1.99	0.78
1:A:115:LYS:HE3	1:B:35:GLN:O	1.84	0.78
1:B:241:HIS:CD2	1:B:243:ASN:H	2.01	0.77
1:B:87:LYS:NZ	1:B:250:GLU:CD	2.38	0.76
1:C:135:ARG:CG	1:C:135:ARG:HH21	1.94	0.76
1:B:224:LYS:HD3	3:B:776:HOH:O	1.86	0.76
1:B:152:HIS:CE1	1:C:153:ARG:HE	1.99	0.75
1:B:87:LYS:HZ2	1:B:250:GLU:HG2	1.52	0.75
1:A:87:LYS:HZ3	1:A:250:GLU:HG2	1.51	0.74
1:D:252:ASN:HB2	3:D:608:HOH:O	1.88	0.74
1:A:153:ARG:NE	1:D:152:HIS:HE1	1.85	0.73
1:A:152:HIS:CE1	1:D:153:ARG:HE	2.03	0.73
1:A:12:GLN:HA	1:A:15:LYS:HE2	1.72	0.72
1:D:87:LYS:NZ	1:D:250:GLU:HG2	2.06	0.70
1:D:132:SER:OG	1:D:135:ARG:HB2	1.91	0.70
1:A:168:GLU:OE1	1:A:241:HIS:HE1	1.74	0.70
1:A:241:HIS:CD2	1:A:244:LYS:H	2.11	0.69
1:A:241:HIS:HD2	1:A:244:LYS:H	1.37	0.69
1:D:130:ILE:O	3:D:695:HOH:O	2.10	0.68
1:B:135:ARG:HE	1:C:151:GLU:HG3	1.57	0.68
1:A:162:LYS:HZ2	1:B:59:ARG:NH1	1.91	0.68
1:A:281:SER:O	1:A:282:LYS:HB3	1.93	0.68
1:B:87:LYS:HZ3	1:B:250:GLU:CG	2.00	0.67
1:C:132:SER:HB2	3:C:605:HOH:O	1.95	0.66
1:A:151:GLU:OE2	1:D:135:ARG:HA	1.95	0.66
1:C:73:HIS:HE1	3:C:729:HOH:O	1.77	0.66
1:D:41:ASN:ND2	1:D:43:ALA:HB3	2.11	0.66
1:C:38:LEU:HB3	1:C:66:VAL:HG11	1.78	0.65
1:C:168:GLU:OE1	1:C:241:HIS:HE1	1.80	0.65
1:B:241:HIS:CD2	1:B:244:LYS:H	2.15	0.65
1:B:252:ASN:HB2	3:B:791:HOH:O	1.97	0.65
2:B:500:ADP:O2B	3:B:620:HOH:O	2.15	0.64
1:B:41:ASN:HD21	1:B:44:LEU:H	1.46	0.64
1:B:135:ARG:HD2	1:B:136:LEU:H	1.61	0.63
1:C:12:GLN:HA	1:C:12:GLN:HE21	1.62	0.63
1:A:176[B]:ASP:OD2	2:A:500:ADP:O3'	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:NZ	1:A:250:GLU:CG	2.62	0.62
1:D:87:LYS:NZ	1:D:250:GLU:CG	2.63	0.62
1:A:191:ALA:HB2	1:A:212:ILE:HD12	1.82	0.62
1:B:148:THR:O	1:B:152:HIS:HD2	1.81	0.62
1:D:237:ASP:HB2	1:D:250:GLU:HB2	1.81	0.62
1:B:41:ASN:ND2	1:B:41:ASN:C	2.48	0.61
1:D:241:HIS:HD2	1:D:243:ASN:H	1.50	0.60
1:A:96[A]:ARG:CG	1:A:96[A]:ARG:NH1	2.47	0.60
1:D:241:HIS:CD2	1:D:243:ASN:H	2.20	0.60
1:B:135:ARG:NE	1:C:151:GLU:HG3	2.16	0.60
1:D:87:LYS:HE3	3:D:715:HOH:O	2.02	0.59
1:A:115:LYS:CE	1:B:35:GLN:O	2.50	0.59
1:C:241:HIS:HD2	1:C:243[B]:ASN:H	1.50	0.59
1:A:132:SER:O	1:A:135:ARG:HD3	2.03	0.59
1:A:237:ASP:HB2	1:A:250:GLU:HB2	1.84	0.59
1:B:132:SER:OG	1:B:135:ARG:O	2.20	0.58
1:C:241:HIS:HD2	1:C:243[A]:ASN:H	1.50	0.58
1:D:192:ARG:HH21	1:D:203:VAL:HG23	1.66	0.58
1:D:217:LYS:HE2	1:D:217:LYS:H	1.67	0.58
1:B:135:ARG:HG3	1:C:151:GLU:HB3	1.85	0.58
1:A:258:LYS:O	1:A:262:VAL:HG13	2.03	0.58
1:A:162:LYS:NZ	1:B:59:ARG:NH1	2.46	0.58
1:C:87:LYS:HZ3	1:C:250:GLU:HG2	1.68	0.58
1:D:258:LYS:O	1:D:262:VAL:HG13	2.04	0.58
1:C:241:HIS:CD2	1:C:244:LYS:H	2.22	0.57
1:B:153:ARG:HE	1:C:152:HIS:CE1	2.08	0.57
1:A:202:ASN:HB2	1:A:203:VAL:HA	1.87	0.56
1:A:25:LYS:N	1:A:25:LYS:HD3	2.21	0.56
1:C:241:HIS:HD2	1:C:244:LYS:H	1.54	0.56
3:C:650:HOH:O	1:D:79:ASP:HB3	2.06	0.55
1:C:172:TYR:CD1	1:C:173:LYS:HD2	2.42	0.55
1:A:96[A]:ARG:CZ	3:A:711:HOH:O	2.53	0.55
1:D:132:SER:HG	1:D:135:ARG:HB2	1.70	0.55
1:D:209:PRO:HB2	1:D:263:ALA:HB2	1.87	0.55
1:A:250:GLU:OE1	3:A:823:HOH:O	2.18	0.55
1:D:229:VAL:HG21	1:D:251:LEU:HD22	1.89	0.55
1:D:168:GLU:OE1	1:D:241:HIS:HE1	1.90	0.55
1:C:12:GLN:HG3	1:C:16:LEU:HD22	1.89	0.55
1:B:241:HIS:HD2	1:B:244:LYS:H	1.55	0.55
1:D:41:ASN:HD21	1:D:43:ALA:HB3	1.71	0.55
1:A:87:LYS:HZ1	1:A:250:GLU:CG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASN:ND2	1:B:212:ILE:H	2.04	0.55
1:C:158:ASN:HB3	1:C:161:LEU:HD22	1.88	0.55
1:C:176[B]:ASP:OD2	2:C:500:ADP:O3'	2.25	0.55
1:B:241:HIS:HD2	1:B:243:ASN:N	2.02	0.54
1:B:135:ARG:HG3	1:C:151:GLU:OE1	2.07	0.54
1:B:87:LYS:HZ3	1:B:250:GLU:HG2	1.60	0.54
1:B:135:ARG:CD	1:B:136:LEU:N	2.47	0.54
1:C:29[A]:ASP:OD1	1:C:47:TYR:CE1	2.61	0.53
1:C:237:ASP:HB2	1:C:250:GLU:HB2	1.90	0.53
1:D:222:VAL:HG13	1:D:236:ILE:HD13	1.90	0.53
1:A:13:GLU:OE1	1:A:256:GLU:HG3	2.09	0.53
1:B:152:HIS:HE1	1:C:153:ARG:NE	1.91	0.52
1:C:267:ASN:ND2	3:C:682:HOH:O	2.42	0.52
1:A:155:LEU:HD22	1:D:136:LEU:HD11	1.92	0.52
1:D:282:LYS:HA	3:D:751:HOH:O	2.10	0.52
1:A:162:LYS:HD2	1:B:58:TYR:OH	2.10	0.52
1:C:252:ASN:HB2	3:C:629:HOH:O	2.09	0.51
1:D:241:HIS:HD2	1:D:244:LYS:H	1.57	0.51
1:D:250:GLU:OE1	3:D:760:HOH:O	2.19	0.51
1:A:109:SER:HA	1:A:162:LYS:NZ	2.26	0.51
1:C:73:HIS:CE1	3:C:729:HOH:O	2.57	0.51
1:C:241:HIS:CD2	1:C:243[A]:ASN:H	2.28	0.51
1:C:241:HIS:CD2	1:C:243[B]:ASN:H	2.28	0.51
1:B:87:LYS:HE3	3:B:681:HOH:O	2.11	0.51
1:A:176[A]:ASP:HB3	1:A:192:ARG:HD3	1.93	0.51
1:C:97:GLU:HG2	1:C:228:ILE:CG1	2.38	0.50
1:B:216:GLU:OE1	1:B:220:GLU:OE2	2.29	0.50
1:B:97:GLU:HG3	1:B:228:ILE:HG12	1.93	0.50
1:D:103:ASP:HB3	1:D:120:ARG:HH22	1.77	0.50
1:D:258:LYS:HE2	3:D:777:HOH:O	2.10	0.50
1:D:132:SER:HB3	1:D:135:ARG:O	2.12	0.50
1:A:202:ASN:N	1:A:203:VAL:HB	2.27	0.49
1:B:168:GLU:OE1	1:B:241:HIS:HE1	1.94	0.49
1:A:256:GLU:HG3	3:A:772:HOH:O	2.12	0.49
1:C:87:LYS:NZ	1:C:250:GLU:HG2	2.26	0.49
1:B:41:ASN:OD1	1:B:43:ALA:HB3	2.13	0.49
1:C:130:ILE:HG22	1:C:131:GLY:N	2.27	0.49
1:A:53:ARG:N	1:A:54:PRO:CD	2.76	0.49
1:C:148:THR:O	1:C:152:HIS:HD2	1.96	0.48
1:D:56:SER:OG	1:D:58:TYR:CD1	2.62	0.48
1:D:198:GLU:HG2	1:D:200:ARG:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:VAL:HG13	1:D:47:TYR:CZ	2.48	0.48
1:A:232:GLU:OE1	3:A:679:HOH:O	2.20	0.48
1:D:202:ASN:HB2	1:D:205:LEU:HD23	1.95	0.48
1:C:53:ARG:N	1:C:54:PRO:CD	2.76	0.48
1:B:158:ASN:O	1:B:161:LEU:HB2	2.14	0.48
1:B:222:VAL:HG13	1:B:236:ILE:HG21	1.96	0.48
1:A:162:LYS:HZ2	1:B:59:ARG:HH11	1.46	0.48
1:A:87:LYS:HZ3	1:A:250:GLU:CG	2.25	0.47
1:A:241:HIS:CD2	1:A:243:ASN:H	2.32	0.47
1:D:177:ILE:HG12	1:D:212:ILE:HD12	1.95	0.47
1:A:53:ARG:H	1:A:54:PRO:HD3	1.79	0.47
1:C:229:VAL:HG21	1:C:251:LEU:HD22	1.96	0.47
1:A:11:ARG:CZ	1:A:55:VAL:HG22	2.45	0.47
1:B:158:ASN:HD22	1:B:160:ALA:H	1.62	0.47
1:A:41:ASN:HD22	1:A:41:ASN:C	2.17	0.47
1:B:224:LYS:O	1:B:228:ILE:HD12	2.14	0.47
1:A:156:MET:N	1:A:157:GLY:HA2	2.29	0.47
1:A:241:HIS:HD2	1:A:243:ASN:H	1.63	0.47
1:D:241:HIS:CD2	1:D:244:LYS:H	2.32	0.46
1:D:87:LYS:HZ1	1:D:250:GLU:CG	2.27	0.46
1:D:4:VAL:HG22	1:D:47:TYR:CG	2.51	0.46
1:D:156:MET:SD	1:D:161:LEU:HD23	2.55	0.46
1:C:87:LYS:NZ	1:C:250:GLU:CG	2.79	0.46
1:D:130:ILE:HD11	1:D:161:LEU:HD11	1.98	0.46
1:A:53:ARG:N	1:A:54:PRO:HD3	2.31	0.46
1:D:38:LEU:HB3	1:D:66:VAL:HG11	1.97	0.46
1:B:196:PRO:HA	1:B:197:ASN:HA	1.64	0.45
1:B:207:GLY:HA2	1:B:208:THR:HA	1.61	0.45
1:D:186:LEU:HD13	1:D:222:VAL:HG11	1.98	0.45
1:C:167:GLN:NE2	2:C:500:ADP:HN61	2.15	0.45
1:B:237:ASP:HB2	1:B:250:GLU:HB2	1.99	0.45
1:D:11:ARG:CZ	1:D:55:VAL:HG22	2.46	0.45
1:C:131:GLY:HA3	1:C:132:SER:HB2	1.98	0.44
1:D:137:VAL:O	1:D:199:TRP:HH2	2.00	0.44
1:B:259:GLY:HA2	1:B:262:VAL:HG22	2.00	0.44
1:D:226:VAL:CG1	1:D:236:ILE:HD11	2.47	0.44
1:D:130:ILE:HD12	1:D:131:GLY:H	1.82	0.44
1:D:226:VAL:HG11	1:D:236:ILE:HD11	1.99	0.44
1:C:192[B]:ARG:NH2	1:C:192[B]:ARG:CG	2.51	0.44
1:D:11:ARG:NH1	1:D:256[A]:GLU:OE2	2.51	0.44
1:C:264:THR:O	1:C:265:ASN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ALA:O	1:C:273:VAL:HG12	2.18	0.44
1:A:143:VAL:HG23	3:A:635:HOH:O	2.17	0.44
1:A:171:GLN:NE2	3:A:748:HOH:O	2.50	0.44
1:B:178:ARG:HD3	3:B:777:HOH:O	2.18	0.43
1:D:115:LYS:O	1:D:119:GLN:HG3	2.18	0.43
1:C:53:ARG:H	1:C:54:PRO:HD3	1.83	0.43
1:B:259:GLY:O	1:B:262:VAL:HG22	2.18	0.43
1:B:125:ILE:HG13	2:B:500:ADP:C6	2.52	0.43
1:D:96:ARG:NH2	3:D:748:HOH:O	2.51	0.43
1:A:267:ASN:C	1:A:267:ASN:HD22	2.22	0.43
1:B:267:ASN:ND2	3:B:648:HOH:O	2.48	0.43
1:B:53:ARG:N	1:B:54:PRO:CD	2.81	0.43
1:B:176[A]:ASP:OD2	1:B:201:ALA:HB3	2.19	0.43
1:B:4:VAL:HG13	1:B:47:TYR:CZ	2.54	0.43
1:C:3:VAL:HG22	1:C:49:VAL:HG12	2.01	0.43
1:C:87:LYS:HZ1	1:C:250:GLU:CD	2.22	0.43
1:C:130:ILE:CG2	1:C:131:GLY:N	2.81	0.43
1:C:235:SER:OG	1:C:252:ASN:HB3	2.19	0.43
1:D:198:GLU:CG	1:D:199:TRP:H	2.16	0.43
1:A:281:SER:O	1:A:282:LYS:CB	2.65	0.42
1:A:256:GLU:CG	3:A:772:HOH:O	2.66	0.42
1:B:241:HIS:CE1	1:B:244:LYS:HE2	2.54	0.42
1:A:148:THR:O	1:A:152:HIS:HD2	2.02	0.42
1:A:203:VAL:HG13	1:A:203:VAL:O	2.18	0.42
1:B:135:ARG:HD2	1:C:151:GLU:HB3	2.02	0.42
1:C:120:ARG:HD3	3:C:653:HOH:O	2.20	0.42
1:A:162:LYS:HZ3	1:B:59:ARG:HH11	1.65	0.42
1:A:132:SER:HB3	1:A:135:ARG:HB3	1.96	0.42
1:A:224:LYS:O	1:A:228:ILE:HG12	2.20	0.42
1:C:131:GLY:HA3	1:C:132:SER:CB	2.48	0.42
1:A:160:ALA:HB2	3:B:651:HOH:O	2.20	0.42
1:C:135:ARG:CG	1:C:135:ARG:NH2	2.64	0.42
1:B:75:ILE:HA	1:B:76:ASN:HA	1.83	0.41
1:C:27:GLN:HE21	1:C:27:GLN:HB2	1.66	0.41
1:B:114:LEU:HD11	1:B:147:LYS:HE2	2.01	0.41
1:D:217:LYS:HE2	1:D:217:LYS:N	2.33	0.41
1:B:281:SER:O	1:B:282:LYS:HB2	2.21	0.41
1:D:148:THR:O	1:D:152:HIS:HD2	2.02	0.41
1:A:208:THR:HA	1:A:209:PRO:HD3	1.80	0.41
1:B:87:LYS:HZ1	1:B:250:GLU:CG	2.29	0.41
1:D:87:LYS:HZ1	1:D:250:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:HD11	3:A:756:HOH:O	2.20	0.41
1:D:191:ALA:HB2	1:D:212:ILE:HD11	2.03	0.41
1:B:212:ILE:O	1:B:212:ILE:HG13	2.21	0.41
1:D:114:LEU:O	1:D:118:GLU:HG2	2.19	0.41
1:C:82:ASN:HD22	1:C:82:ASN:HA	1.73	0.41
1:A:186:LEU:HD13	1:A:222:VAL:HG11	2.03	0.40
1:A:87:LYS:HG2	1:A:250:GLU:OE2	2.20	0.40
1:C:196:PRO:HA	1:C:197:ASN:HA	1.61	0.40
1:A:125:ILE:HG13	2:A:500:ADP:C6	2.57	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	285/282 (101%)	272 (95%)	9 (3%)	4 (1%)	11 3
1	B	288/282 (102%)	280 (97%)	5 (2%)	3 (1%)	15 6
1	C	278/282 (99%)	270 (97%)	7 (2%)	1 (0%)	34 22
1	D	283/282 (100%)	274 (97%)	6 (2%)	3 (1%)	14 5
All	All	1134/1128 (100%)	1096 (97%)	27 (2%)	11 (1%)	15 6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	203	VAL
1	A	204	ALA
1	B	132	SER
1	D	132	SER
1	D	172	TYR

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Mol	Chain	Res	Type
1	B	203	VAL
1	A	53	ARG
1	C	53	ARG
1	B	53	ARG
1	D	53	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	247/242 (102%)	229 (93%)	18 (7%)	14	5
1	B	250/242 (103%)	231 (92%)	19 (8%)	13	4
1	C	245/242 (101%)	227 (93%)	18 (7%)	14	5
1	D	245/242 (101%)	226 (92%)	19 (8%)	12	4
All	All	987/968 (102%)	913 (92%)	74 (8%)	15	5

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	25	LYS
1	A	41	ASN
1	A	82	ASN
1	A	96[A]	ARG
1	A	96[B]	ARG
1	A	120	ARG
1	A	132	SER
1	A	135	ARG
1	A	141	ARG
1	A	155	LEU
1	A	158	ASN
1	A	161	LEU
1	A	173	LYS
1	A	211	ASN
1	A	256	GLU

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	282	LYS
1	B	4	VAL
1	B	16[A]	LEU
1	B	16[B]	LEU
1	B	19	LYS
1	B	27	GLN
1	B	41	ASN
1	B	82	ASN
1	B	114	LEU
1	B	120[A]	ARG
1	B	120[B]	ARG
1	B	130	ILE
1	B	135	ARG
1	B	155	LEU
1	B	158	ASN
1	B	161	LEU
1	B	192	ARG
1	B	211	ASN
1	B	251	LEU
1	B	267	ASN
1	C	12	GLN
1	C	16	LEU
1	C	27	GLN
1	C	29[A]	ASP
1	C	29[B]	ASP
1	C	41	ASN
1	C	82	ASN
1	C	135	ARG
1	C	141	ARG
1	C	161	LEU
1	C	162[A]	LYS
1	C	162[B]	LYS
1	C	192[A]	ARG
1	C	192[B]	ARG
1	C	197	ASN
1	C	217	LYS
1	C	267	ASN
1	C	278	GLU
1	D	4	VAL
1	D	16	LEU
1	D	19	LYS

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Mol	Chain	Res	Type
1	D	30	ILE
1	D	56	SER
1	D	82	ASN
1	D	97	GLU
1	D	103	ASP
1	D	120	ARG
1	D	155	LEU
1	D	197	ASN
1	D	212	ILE
1	D	217	LYS
1	D	224[A]	LYS
1	D	224[B]	LYS
1	D	258	LYS
1	D	262	VAL
1	D	267	ASN
1	D	282	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	41	ASN
1	A	82	ASN
1	A	119	GLN
1	A	152	HIS
1	A	211	ASN
1	A	241	HIS
1	A	267	ASN
1	A	270	GLN
1	B	12	GLN
1	B	24	ASN
1	B	41	ASN
1	B	82	ASN
1	B	152	HIS
1	B	158	ASN
1	B	193	ASN
1	B	211	ASN
1	B	241	HIS
1	B	267	ASN
1	B	270	GLN
1	B	279	ASN
1	C	12	GLN

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Mol	Chain	Res	Type
1	C	24	ASN
1	C	27	GLN
1	C	35	GLN
1	C	82	ASN
1	C	152	HIS
1	C	167	GLN
1	C	197	ASN
1	C	211	ASN
1	C	241	HIS
1	C	267	ASN
1	C	270	GLN
1	D	24	ASN
1	D	27	GLN
1	D	82	ASN
1	D	119	GLN
1	D	152	HIS
1	D	193	ASN
1	D	197	ASN
1	D	202	ASN
1	D	241	HIS
1	D	267	ASN
1	D	270	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	B	500	-	24,29,29	0.98	1 (4%)	29,45,45	1.32	2 (6%)
2	ADP	D	500	-	24,29,29	0.98	1 (4%)	29,45,45	1.46	4 (13%)
2	ADP	A	500	-	24,29,29	1.05	2 (8%)	29,45,45	1.25	2 (6%)
2	ADP	C	500	-	24,29,29	1.02	1 (4%)	29,45,45	1.38	4 (13%)

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	B	500	-	-	1/12/32/32	0/3/3/3
2	ADP	D	500	-	-	1/12/32/32	0/3/3/3
2	ADP	A	500	-	-	2/12/32/32	0/3/3/3
2	ADP	C	500	-	-	2/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ADP	C5-C4	2.47	1.47	1.40
2	D	500	ADP	C5-C4	2.44	1.47	1.40
2	C	500	ADP	C5-C4	2.43	1.47	1.40
2	B	500	ADP	C5-C4	2.10	1.46	1.40
2	A	500	ADP	C2-N3	2.05	1.35	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	ADP	N3-C2-N1	-3.94	122.52	128.68
2	C	500	ADP	N3-C2-N1	-3.58	123.08	128.68
2	D	500	ADP	N3-C2-N1	-3.12	123.80	128.68
2	D	500	ADP	C3'-C2'-C1'	3.08	105.62	100.98
2	A	500	ADP	N3-C2-N1	-2.95	124.07	128.68
2	D	500	ADP	PA-O3A-PB	-2.40	124.60	132.83
2	A	500	ADP	C4-C5-N7	-2.30	107.00	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	ADP	PA-O3A-PB	-2.18	125.34	132.83
2	B	500	ADP	C1'-N9-C4	-2.16	122.84	126.64
2	D	500	ADP	C2-N1-C6	2.16	122.45	118.75
2	C	500	ADP	O2'-C2'-C1'	-2.09	103.15	110.85
2	C	500	ADP	O3'-C3'-C4'	-2.04	105.15	111.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ADP	PB-O3A-PA-O2A
2	B	500	ADP	PB-O3A-PA-O2A
2	D	500	ADP	PB-O3A-PA-O2A
2	C	500	ADP	PB-O3A-PA-O2A
2	A	500	ADP	PB-O3A-PA-O1A
2	C	500	ADP	PB-O3A-PA-O1A

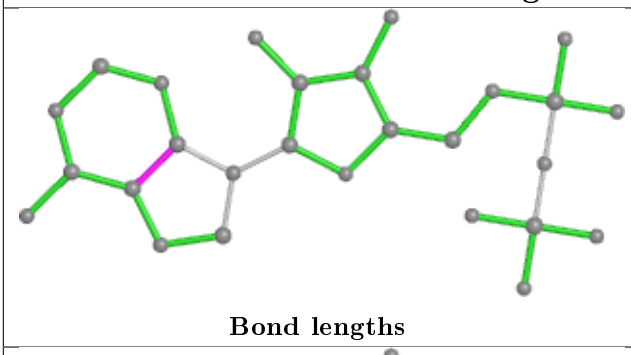
There are no ring outliers.

3 monomers are involved in 6 short contacts:

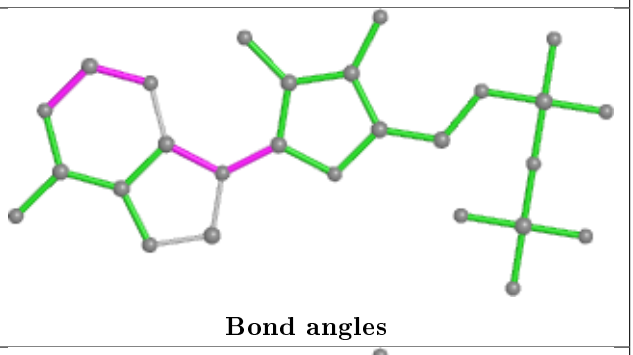
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	ADP	2	0
2	A	500	ADP	2	0
2	C	500	ADP	2	0

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.

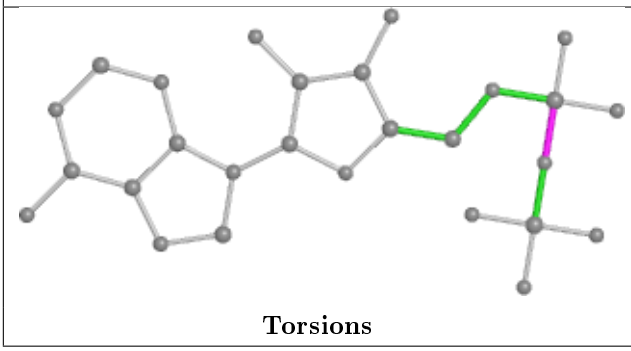
Ligand ADP B 500



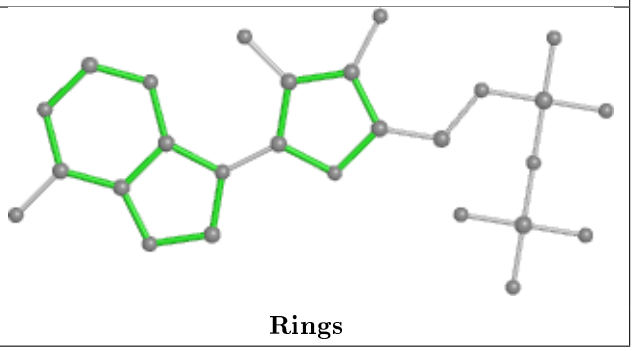
Bond lengths



Bond angles

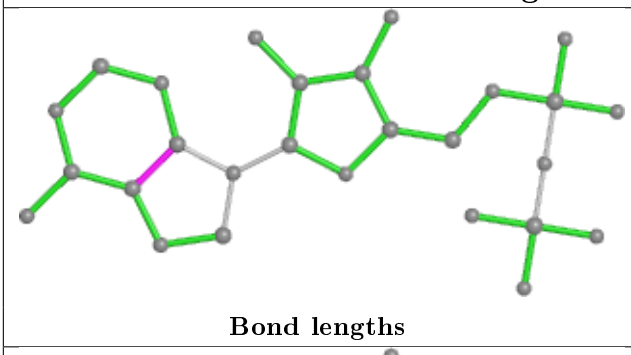


Torsions

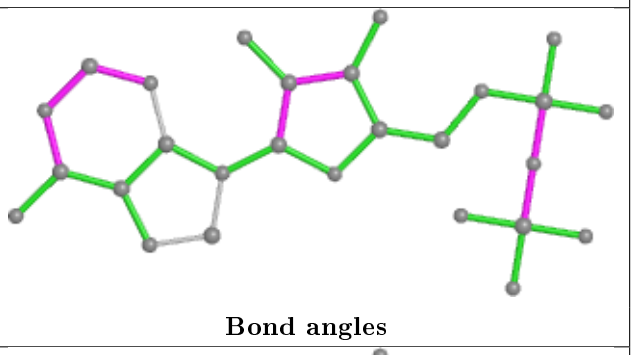


Rings

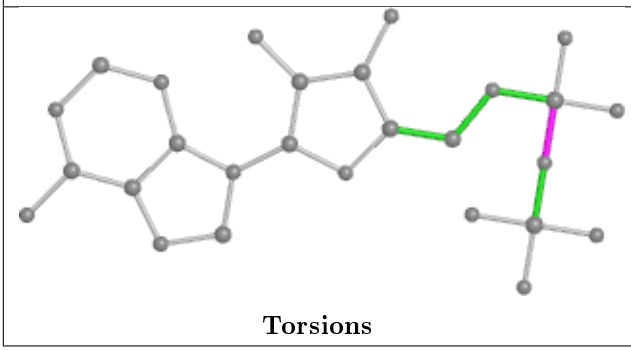
Ligand ADP D 500



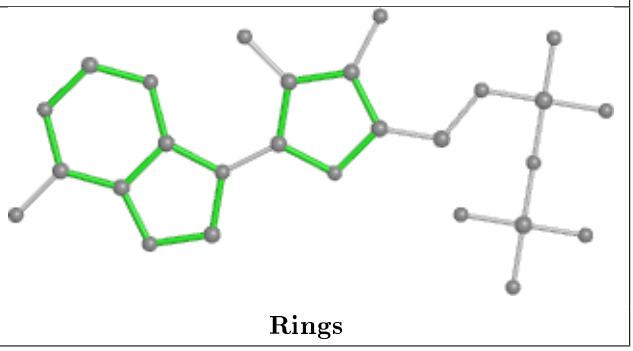
Bond lengths



Bond angles

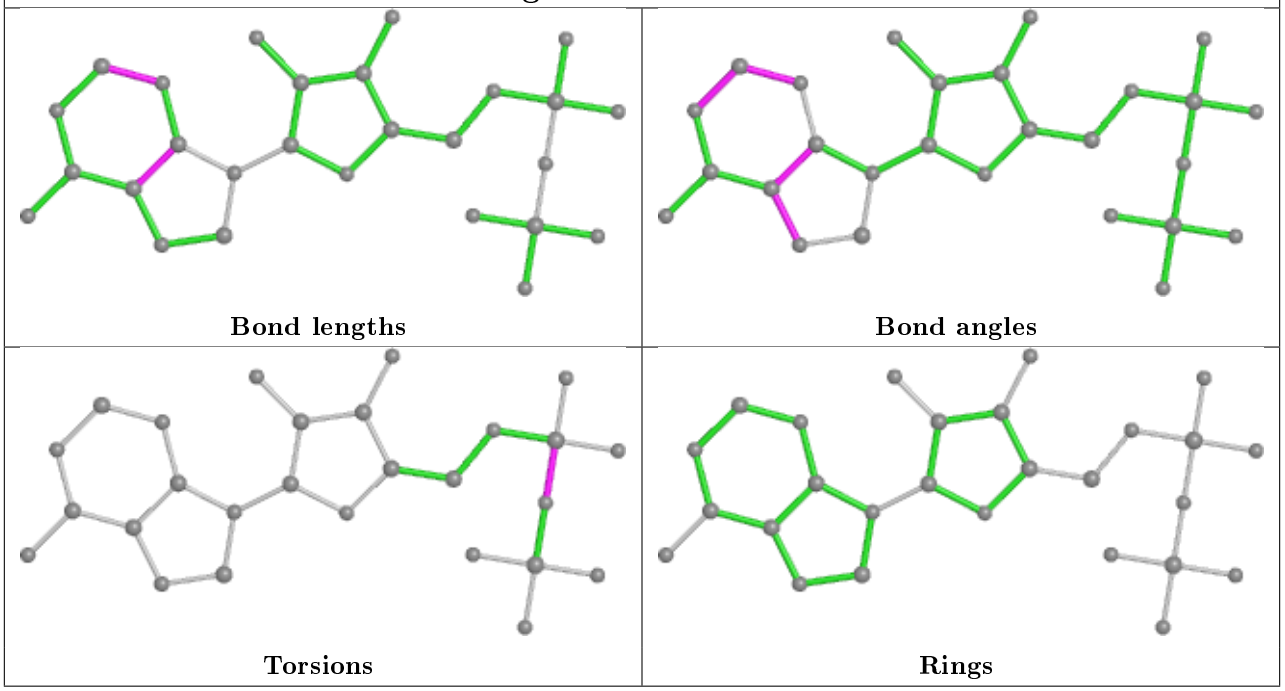


Torsions

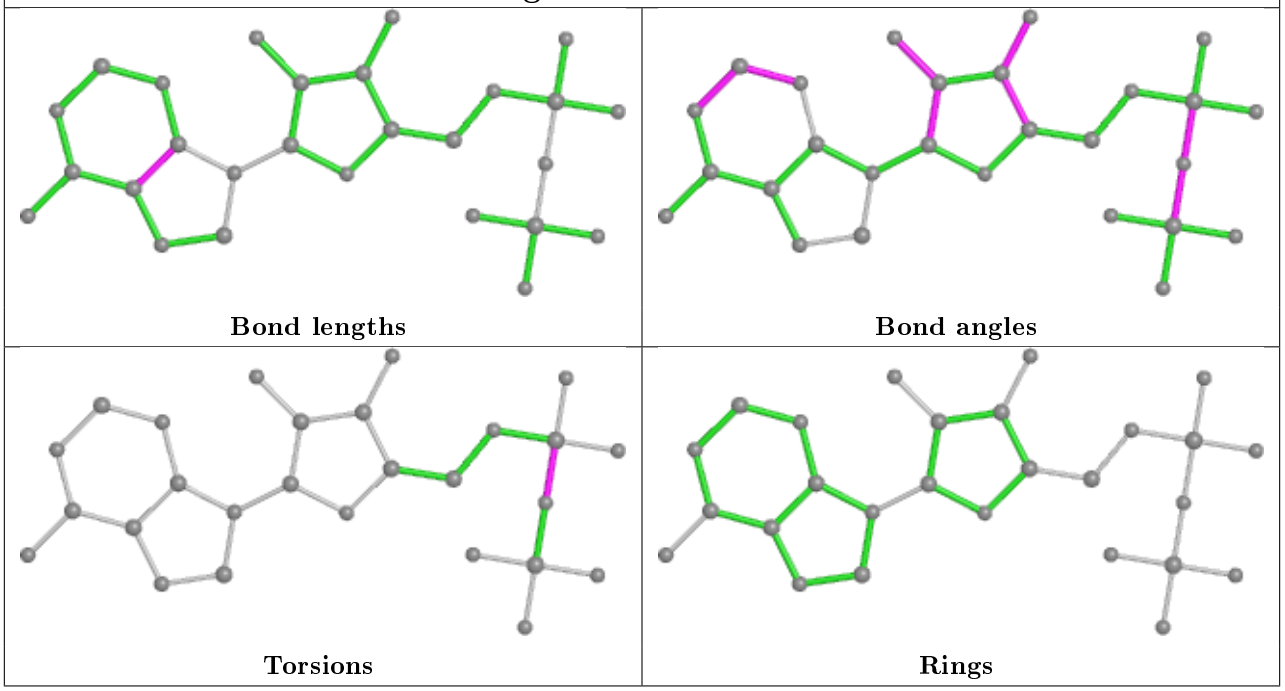


Rings

Ligand ADP A 500



Ligand ADP C 500



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	282/282 (100%)	0.01	15 (5%)	26	28	11, 23, 50, 63	0
1	B	282/282 (100%)	0.05	10 (3%)	44	45	12, 23, 43, 60	0
1	C	275/282 (97%)	0.05	11 (4%)	38	39	12, 26, 46, 55	0
1	D	282/282 (100%)	0.07	16 (5%)	23	25	13, 25, 46, 58	0
All	All	1121/1128 (99%)	0.05	52 (4%)	32	34	11, 24, 47, 63	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	11.0
1	A	205	LEU	9.2
1	C	133	TRP	8.0
1	B	208	THR	8.0
1	A	204	ALA	7.7
1	D	204	ALA	6.5
1	D	203	VAL	6.4
1	B	203	VAL	5.9
1	C	196	PRO	5.5
1	B	205	LEU	5.4
1	B	133	TRP	5.1
1	D	133	TRP	5.0
1	A	207	GLY	4.7
1	C	282	LYS	4.6
1	A	157	GLY	4.0
1	B	204	ALA	3.9
1	C	197	ASN	3.9
1	A	282	LYS	3.7
1	A	133	TRP	3.7
1	B	281	SER	3.6
1	A	208	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	196	PRO	3.2
1	A	197	ASN	3.2
1	A	206	GLY	3.1
1	A	196	PRO	3.0
1	D	196	PRO	3.0
1	D	281	SER	3.0
1	D	208	THR	3.0
1	C	131	GLY	2.9
1	C	210	SER	2.8
1	D	282	LYS	2.7
1	D	209	PRO	2.7
1	D	197	ASN	2.6
1	D	213	GLU	2.6
1	B	206	GLY	2.5
1	A	158	ASN	2.5
1	C	132	SER	2.5
1	C	157	GLY	2.4
1	A	211	ASN	2.4
1	D	207	GLY	2.4
1	C	135	ARG	2.4
1	A	203	VAL	2.4
1	A	132	SER	2.3
1	C	192[A]	ARG	2.3
1	D	132	SER	2.3
1	A	131	GLY	2.3
1	D	206	GLY	2.2
1	D	58	TYR	2.2
1	D	205	LEU	2.2
1	B	209	PRO	2.1
1	C	281	SER	2.1
1	D	212	ILE	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 carbohydrates in this entry.

6.4 Ligands

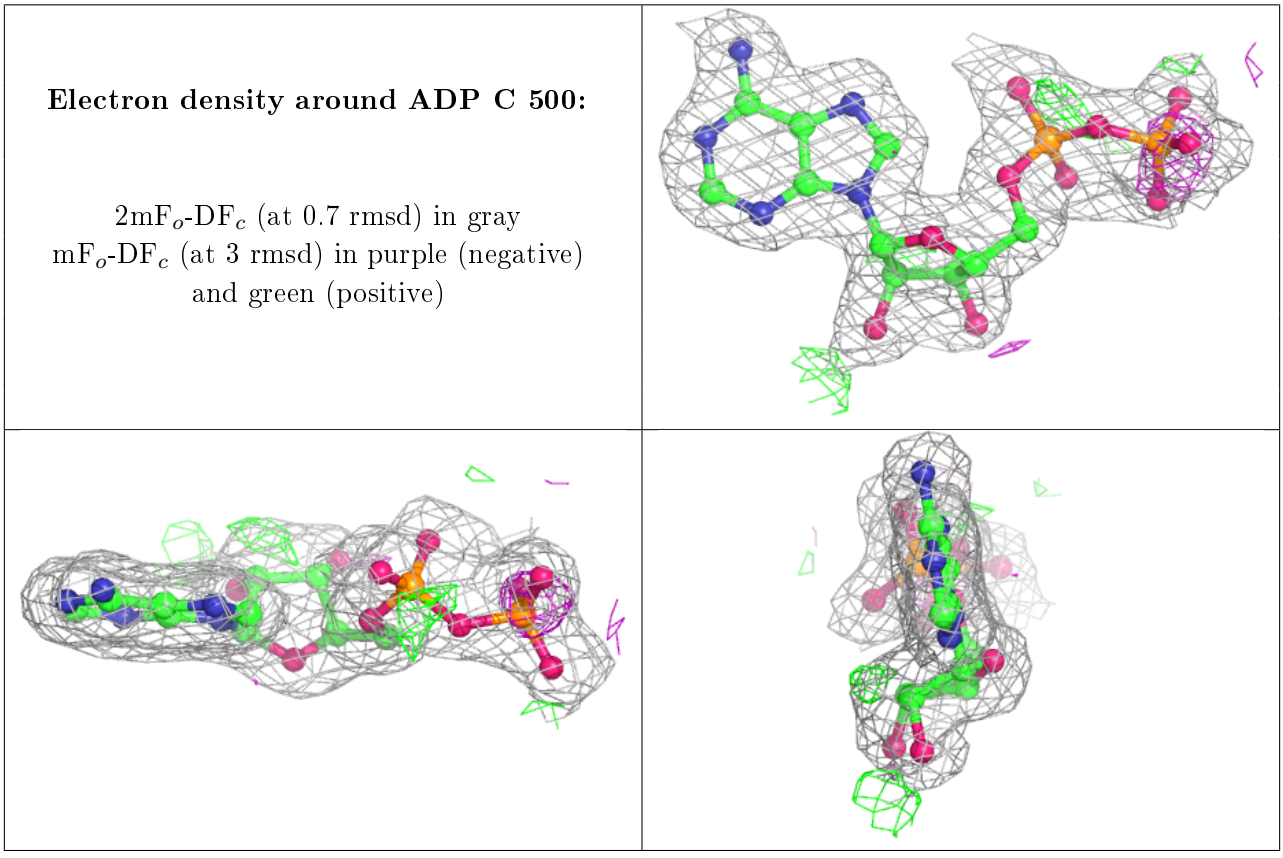
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	C	500	27/27	0.93	0.11	18,25,40,42	0
2	ADP	A	500	27/27	0.94	0.09	17,22,36,38	0
2	ADP	B	500	27/27	0.96	0.09	15,20,33,33	0
2	ADP	D	500	27/27	0.96	0.09	15,22,38,39	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.

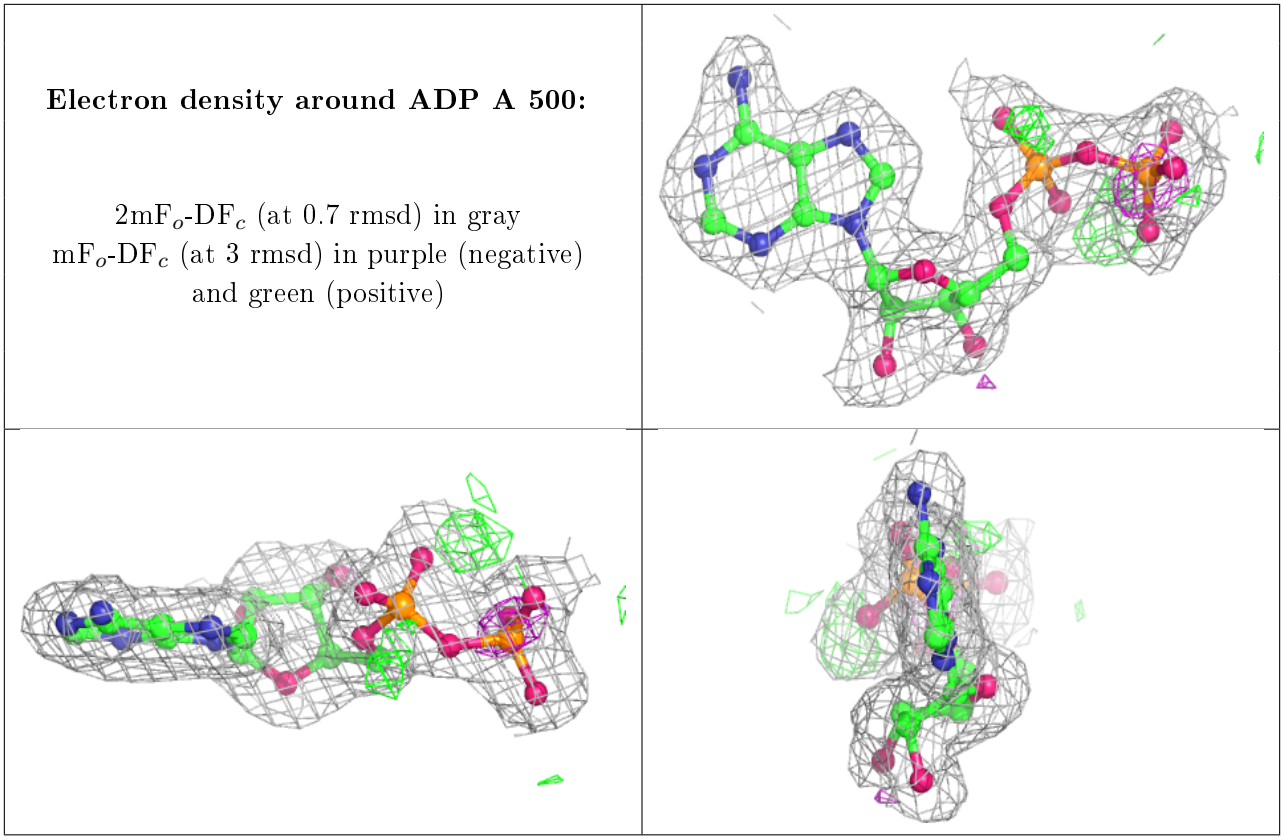
Electron density around ADP C 500:

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



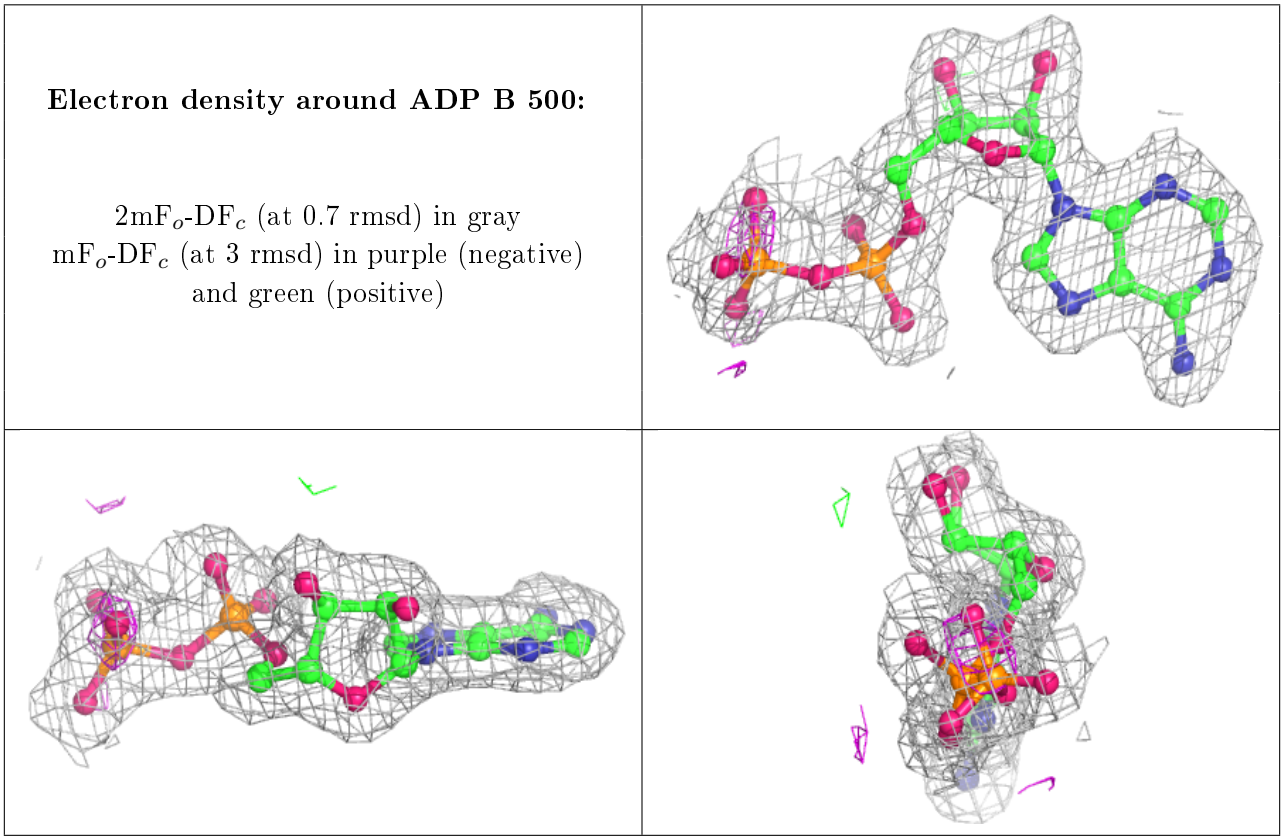
Electron density around ADP A 500:

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



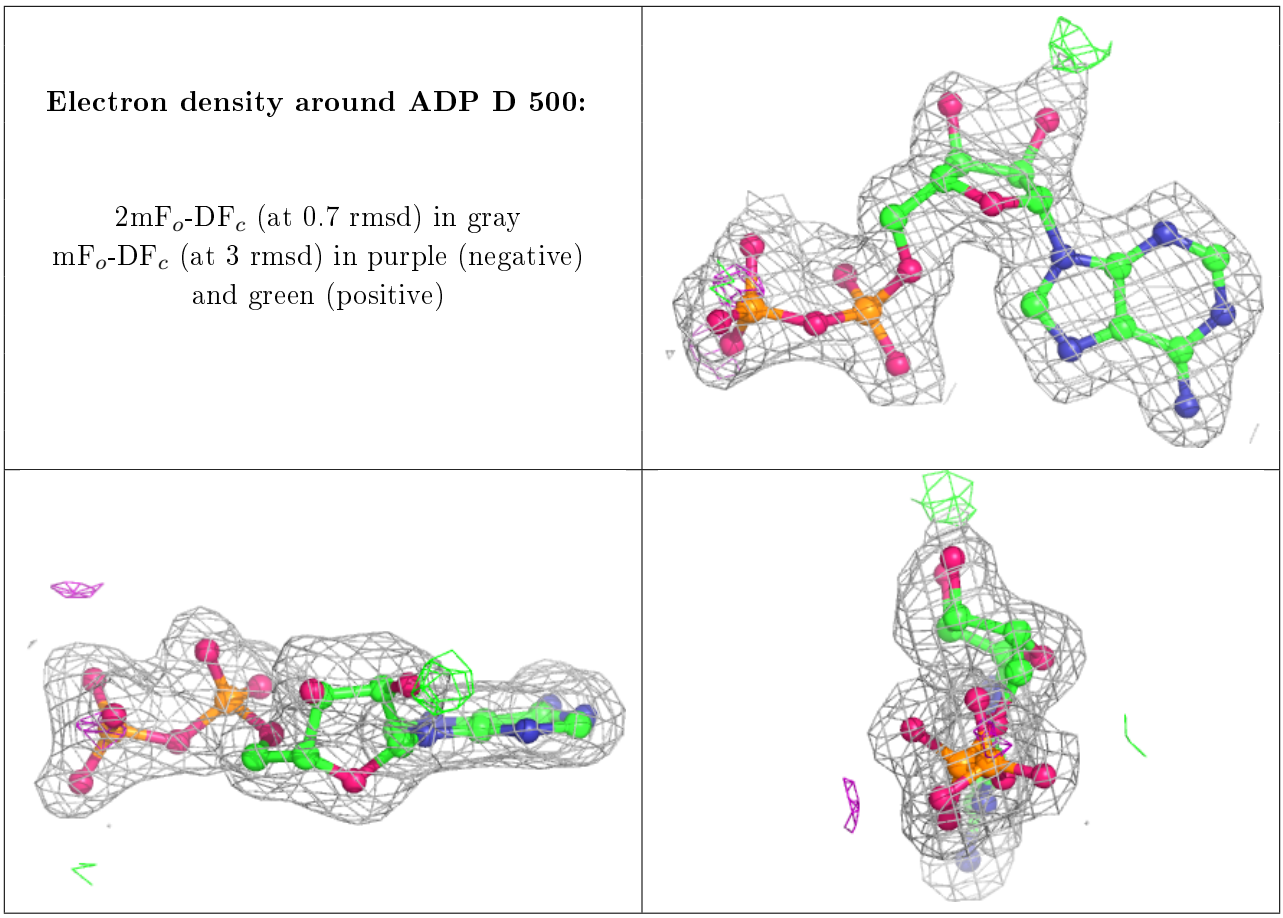
Electron density around ADP B 500:

$2mF_o$-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 D 500:

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



6.5 Other polymers

There are no such residues in this entry.