Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 12:14 AM EDT

PDB ID	:	2YZN
Title	:	Crystal structure of D-alanine:D-Alanine Ligase with AMPPNP from Thermus thermophilus HB8.
Authors	:	Kitamuta, Y.; Yokoyama, S.; Kuramitsu, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-05-06
Resolution	:	2.60 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

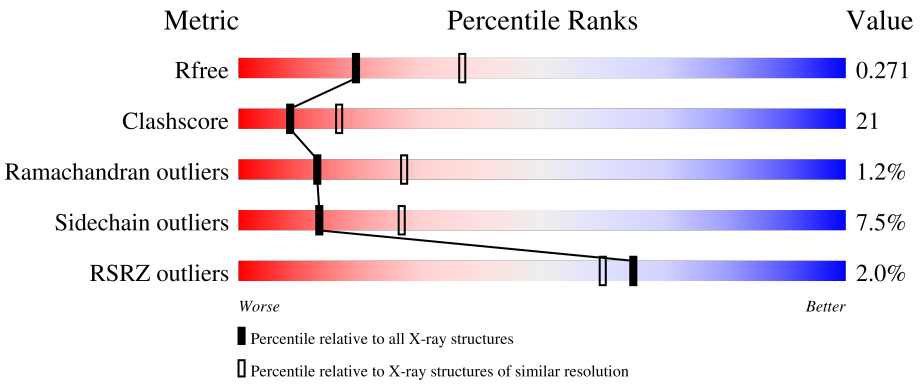
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	66% 31% • •
1	B	319	3% 62% 30% 6% •
1	C	319	3% 60% 33% • •

2 Entry composition (i)

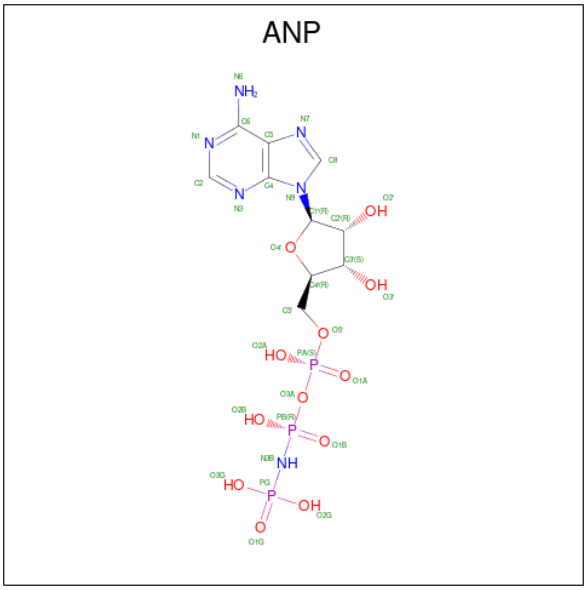
There are 3 unique types of molecules in this entry. The entry contains 7372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-alanine-D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	2443	1588	404	446	5	0	0	0
1	B	313	2396	1556	399	436	5	0	0	0
1	C	309	2359	1529	395	430	5	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	6	12	3	0	0
2	B	1	31	10	6	12	3	0	0
2	C	1	31	10	6	12	3	0	0

- Molecule 3 is water.

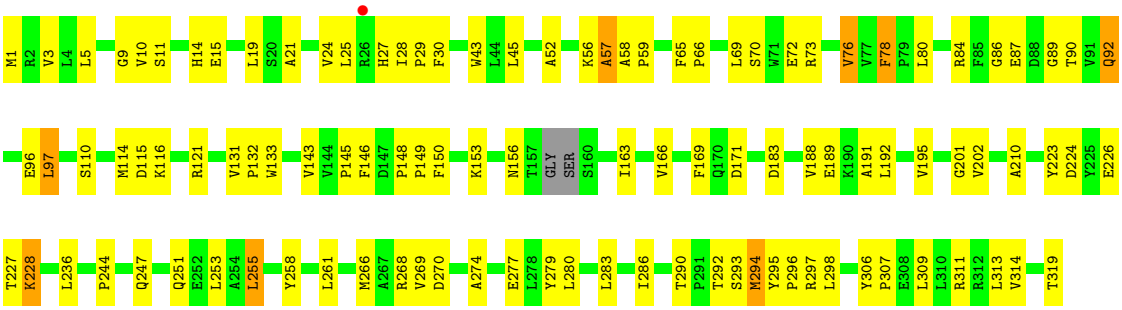
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	24	24	24	0	0
			Total	O		
3	B	22	22	22	0	0
			Total	O		
3	C	35	35	35	0	0

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.

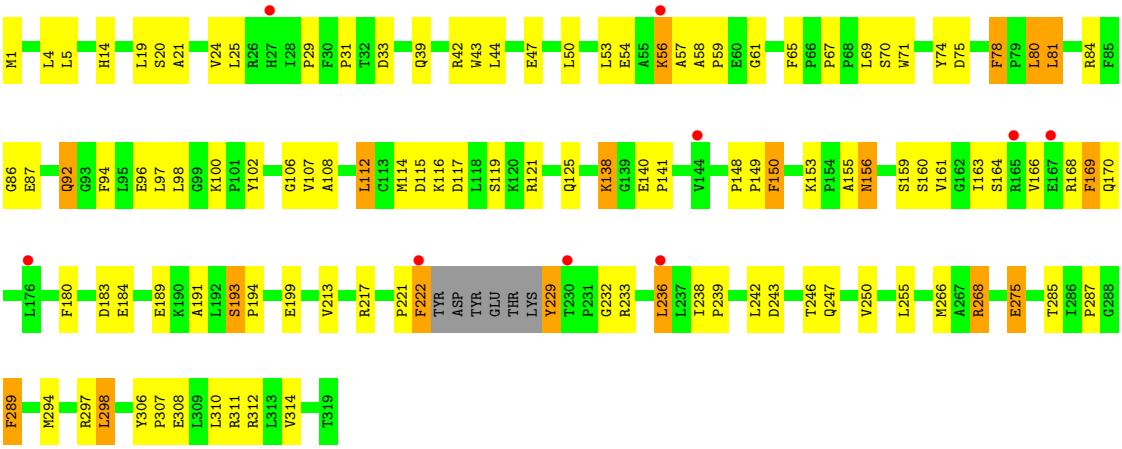
- Molecule 1: D-alanine-D-alanine ligase

Chain A:



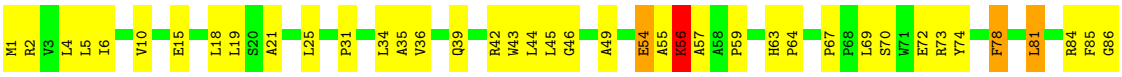
- Molecule 1: D-alanine-D-alanine ligase

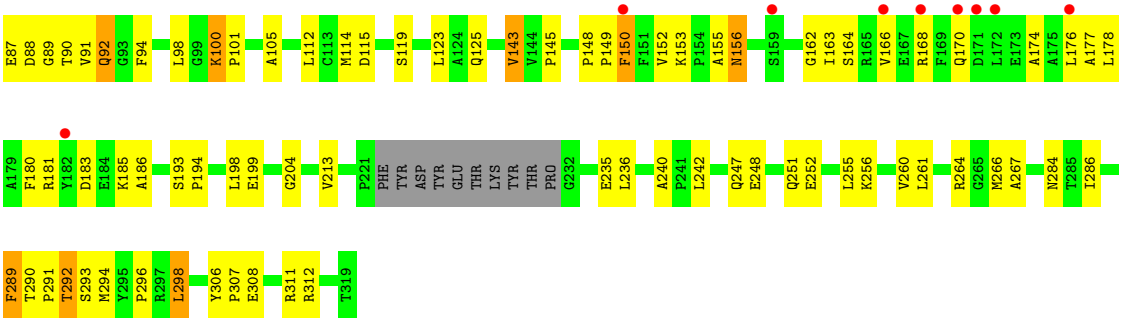
Chain B:



- Molecule 1: D-alanine-D-alanine ligase

Chain C:




E87
D88
G89
T90
V91
Q92
G93
F94
L98
G99
K100
P101
A105
L112
C113
M114
D115
S119
L123
A124
Q125
V143
V144
P145
P148
P149
F150
F151
V152
K153
P154
A155
N156
S159
G162
I163
S164
R165
V166
E167
R168
F169
Q170
D171
L172
E173
A174
A175
L176
A177
L178
A179
F180
R181
Y182
D183
E184
K185
A186
S193
P194
L198
E199
G204
V213
P221
PHE
TYR
ASP
TYR
GLU
THR
LYS
TYR
THR
PRO
G232
E235
L236
A240
P241
L242
Q247
E248
Q251
E252
L255
K256
V260
L261
R264
G265
M266
A267
N284
T285
I286
F289
T290
P291
T292
S293
M294
Y295
P296
R297
L298
Y306
P307
E308
R311
R312
T319

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.72Å 56.71Å 141.83Å 90.00° 108.56° 90.00°	Depositor
Resolution (Å)	47.91 – 2.60 47.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.91-2.60) 96.5 (47.91-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.280 0.219 , 0.271	Depositor DCC
R_{free} test set	3856 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7372	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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: ANP

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	0.41	0/2507	0.66	0/3418
1	B	0.38	0/2458	0.62	0/3351
1	C	0.42	0/2418	0.67	1/3295 (0.0%)
All	All	0.41	0/7383	0.65	1/10064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	105	ALA	N-CA-C	5.29	125.27	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	2443	0	2461	99	0
1	B	2396	0	2421	115	0
1	C	2359	0	2389	95	0
2	A	31	0	13	1	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
3	A	24	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	0	0	0
3	C	35	0	0	2	0
All	All	7372	0	7310	303	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 21.

All (303) 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:C:85:PHE:HA	1:C:90:THR:HG21	1.34	1.08
1:C:89:GLY:HA2	1:C:92:GLN:HG3	1.42	1.01
1:C:290:THR:HG22	1:C:292:THR:H	1.29	0.97
1:A:89:GLY:HA2	1:A:92:GLN:HE21	1.34	0.93
1:C:55:ALA:O	1:C:56:LYS:HD3	1.68	0.92
1:A:70:SER:HB2	1:A:73:ARG:HD3	1.55	0.87
1:A:195:VAL:HG12	1:A:274:ALA:HB2	1.58	0.85
1:B:236:LEU:HD22	1:B:297:ARG:HE	1.42	0.85
1:B:92:GLN:H	1:B:92:GLN:NE2	1.80	0.79
1:B:153:LYS:HB3	1:B:163:ILE:HG12	1.64	0.79
1:C:85:PHE:HA	1:C:90:THR:CG2	2.09	0.79
1:A:224:ASP:HB3	1:A:227:THR:HB	1.63	0.78
1:A:19:LEU:HG	1:A:56:LYS:HZ1	1.46	0.78
1:B:5:LEU:HD12	1:B:78:PHE:HB3	1.65	0.77
1:B:236:LEU:HD22	1:B:297:ARG:NE	2.00	0.77
1:A:89:GLY:HA2	1:A:92:GLN:NE2	1.99	0.76
1:C:115:ASP:HA	1:C:156:ASN:HB3	1.67	0.75
1:B:115:ASP:HA	1:B:156:ASN:HB3	1.67	0.75
1:A:3:VAL:HG22	1:A:76:VAL:HG13	1.69	0.75
1:B:87:GLU:HG3	1:B:114:MET:CE	2.18	0.74
1:B:138:LYS:HD3	1:B:138:LYS:N	2.03	0.74
1:C:168:ARG:NH2	1:C:168:ARG:HB2	2.03	0.74
1:A:290:THR:HG22	1:A:292:THR:H	1.54	0.71
1:B:114:MET:HE2	1:B:114:MET:HA	1.73	0.71
1:B:14:HIS:CE1	1:B:58:ALA:H	2.10	0.70
1:B:199:GLU:HG3	1:B:294:MET:SD	2.31	0.70
1:A:24:VAL:HG21	1:A:80:LEU:HD11	1.74	0.69
1:A:319:THR:HG22	1:A:319:THR:O	1.92	0.69
1:A:224:ASP:CB	1:A:227:THR:HB	2.22	0.69
1:A:306:TYR:HB3	1:A:307:PRO:HD3	1.73	0.69
1:B:100:LYS:HA	1:B:100:LYS:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:TYR:HB3	1:B:307:PRO:HD3	1.75	0.68
1:A:236:LEU:HD22	1:A:297:ARG:HH21	1.58	0.68
1:B:42:ARG:HG3	1:B:42:ARG:HH11	1.58	0.68
1:C:89:GLY:CA	1:C:92:GLN:HG3	2.23	0.67
1:A:19:LEU:HG	1:A:56:LYS:NZ	2.09	0.67
1:A:45:LEU:HD22	1:A:69:LEU:HD21	1.75	0.66
1:B:153:LYS:CB	1:B:163:ILE:HG12	2.26	0.66
1:A:153:LYS:HG2	1:A:163:ILE:HG23	1.78	0.66
1:A:14:HIS:HE1	1:A:58:ALA:H	1.42	0.65
1:B:222:PHE:CE1	1:B:232:GLY:HA2	2.32	0.65
1:B:308:GLU:O	1:B:312:ARG:HG3	1.96	0.65
1:C:153:LYS:HB3	1:C:163:ILE:HG12	1.77	0.65
1:A:116:LYS:HE2	1:A:153:LYS:HD2	1.77	0.65
1:B:24:VAL:HG13	1:B:310:LEU:HD22	1.79	0.65
1:A:76:VAL:HG11	1:A:314:VAL:HG13	1.78	0.64
1:C:74:TYR:O	1:C:100:LYS:HE3	1.99	0.63
1:A:227:THR:O	1:A:228:LYS:HB2	1.98	0.63
1:C:90:THR:HG23	1:C:91:VAL:N	2.14	0.62
1:B:163:ILE:HG22	1:B:164:SER:N	2.15	0.62
1:A:9:GLY:O	1:A:14:HIS:HD2	1.82	0.62
1:B:94:PHE:CZ	1:B:98:LEU:HD11	2.35	0.61
1:A:153:LYS:HB3	1:A:163:ILE:HG12	1.81	0.61
1:B:161:VAL:O	1:B:161:VAL:HG13	2.01	0.61
1:B:69:LEU:HD23	1:B:70:SER:N	2.15	0.61
1:B:236:LEU:HD22	1:B:297:ARG:NH2	2.15	0.61
1:C:290:THR:HG21	1:C:292:THR:HG22	1.83	0.61
1:C:6:ILE:HG22	1:C:81:LEU:HD21	1.81	0.61
1:A:150:PHE:HB2	1:A:189:GLU:O	2.01	0.60
1:B:1:MET:HA	1:B:75:ASP:OD2	2.02	0.60
1:B:222:PHE:N	1:B:222:PHE:HD1	2.00	0.60
1:B:238:ILE:HD12	1:B:298:LEU:HD12	1.83	0.60
1:A:70:SER:CB	1:A:73:ARG:HD3	2.29	0.60
1:A:149:PRO:HG2	1:A:191:ALA:HB3	1.83	0.60
1:A:89:GLY:CA	1:A:92:GLN:HE21	2.11	0.60
1:B:87:GLU:HG3	1:B:114:MET:HE3	1.82	0.60
1:A:192:LEU:HB3	1:A:195:VAL:HG11	1.84	0.59
1:B:236:LEU:HD22	1:B:297:ARG:HH21	1.65	0.59
1:B:14:HIS:HE1	1:B:58:ALA:H	1.50	0.59
1:B:236:LEU:HD12	1:B:236:LEU:H	1.67	0.59
1:B:29:PRO:HG3	1:B:311:ARG:HB2	1.84	0.59
1:B:42:ARG:HG3	1:B:42:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:MET:HB2	3:A:404:HOH:O	2.03	0.59
1:B:71:TRP:HB3	1:B:100:LYS:HD2	1.84	0.59
1:A:294:MET:HG3	1:A:298:LEU:HD13	1.85	0.58
1:C:236:LEU:HG	1:C:294:MET:CE	2.33	0.58
1:B:92:GLN:H	1:B:92:GLN:HE21	1.51	0.58
1:C:2:ARG:HD2	1:C:73:ARG:O	2.03	0.58
1:B:138:LYS:HD2	1:B:184:GLU:HB3	1.84	0.58
1:A:21:ALA:O	1:A:25:LEU:HB2	2.04	0.57
1:B:222:PHE:N	1:B:222:PHE:CD1	2.71	0.57
1:B:236:LEU:HD13	1:B:297:ARG:NH2	2.18	0.57
1:A:266:MET:HB3	1:A:313:LEU:HD21	1.86	0.57
1:B:108:ALA:O	1:B:112:LEU:HD22	2.04	0.57
1:A:27:HIS:HD2	1:A:306:TYR:HE2	1.53	0.57
1:B:138:LYS:HD3	1:B:138:LYS:H	1.69	0.57
1:B:268:ARG:HB2	1:B:287:PRO:HB3	1.86	0.57
1:B:78:PHE:CE1	1:B:80:LEU:HD13	2.39	0.57
1:A:65:PHE:HD1	1:B:98:LEU:HD23	1.70	0.56
1:B:236:LEU:HD22	1:B:297:ARG:CZ	2.34	0.56
1:B:238:ILE:HA	1:B:239:PRO:C	2.24	0.56
1:B:87:GLU:HG3	1:B:114:MET:HE1	1.85	0.56
1:A:277:GLU:OE2	1:A:277:GLU:HA	2.05	0.56
1:C:256:LYS:O	1:C:260:VAL:HG23	2.06	0.56
1:A:148:PRO:HG3	1:A:150:PHE:CE2	2.41	0.56
1:B:233:ARG:NH2	1:B:233:ARG:HB2	2.20	0.56
1:C:156:ASN:O	1:C:156:ASN:ND2	2.38	0.56
1:C:168:ARG:HH22	1:C:170:GLN:HB2	1.70	0.55
1:C:181:ARG:HG3	1:C:181:ARG:HH11	1.70	0.55
1:B:233:ARG:HB2	1:B:233:ARG:HH21	1.70	0.55
1:A:268:ARG:HH21	1:A:268:ARG:HG3	1.71	0.55
1:A:121:ARG:O	1:B:125:GLN:HG3	2.07	0.55
1:A:56:LYS:HZ3	1:A:56:LYS:HB3	1.71	0.54
1:C:1:MET:O	1:C:31:PRO:HD2	2.07	0.54
1:B:4:LEU:HB2	1:B:74:TYR:CD2	2.42	0.54
1:B:50:LEU:HD12	1:B:50:LEU:H	1.71	0.54
1:A:293:SER:O	1:A:297:ARG:HG3	2.07	0.54
1:C:55:ALA:C	1:C:56:LYS:HD3	2.28	0.54
1:B:117:ASP:O	1:B:121:ARG:HG3	2.08	0.54
1:C:248:GLU:HA	1:C:251:GLN:HE21	1.72	0.54
1:B:116:LYS:HG3	1:B:155:ALA:O	2.07	0.54
1:C:5:LEU:HD12	1:C:78:PHE:HB3	1.89	0.54
1:B:20:SER:O	1:B:24:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ALA:O	1:C:56:LYS:CD	2.51	0.54
1:C:87:GLU:HB3	1:C:286:ILE:HD12	1.90	0.54
1:A:56:LYS:O	1:A:57:ALA:HB2	2.08	0.53
1:B:236:LEU:HD13	1:B:297:ARG:HH21	1.73	0.53
1:A:14:HIS:CE1	1:A:58:ALA:H	2.23	0.53
1:C:56:LYS:HD3	1:C:56:LYS:C	2.27	0.53
1:B:5:LEU:CD1	1:B:78:PHE:HB3	2.38	0.53
1:C:56:LYS:HZ2	1:C:57:ALA:HB2	1.74	0.53
1:A:87:GLU:O	1:A:110:SER:HB3	2.08	0.53
1:C:155:ALA:HB3	1:C:183:ASP:OD1	2.09	0.53
1:C:89:GLY:HA2	1:C:92:GLN:CG	2.26	0.53
1:B:221:PRO:HB3	1:B:229:TYR:HE1	1.72	0.52
1:B:50:LEU:HD12	1:B:50:LEU:N	2.23	0.52
1:A:89:GLY:CA	1:A:92:GLN:NE2	2.70	0.52
1:A:227:THR:O	1:A:228:LYS:CB	2.58	0.52
1:C:6:ILE:CG2	1:C:81:LEU:HD21	2.39	0.52
1:C:162:GLY:HA2	1:C:178:LEU:HG	1.92	0.52
1:A:143:VAL:O	1:A:145:PRO:HD3	2.10	0.52
1:C:266:MET:SD	1:C:289:PHE:HE2	2.33	0.52
1:B:148:PRO:HB3	1:B:149:PRO:HA	1.92	0.51
1:A:114:MET:HG3	1:A:114:MET:O	2.09	0.51
1:C:10:VAL:HG23	1:C:39:GLN:O	2.10	0.51
1:A:116:LYS:HD2	2:A:401:ANP:O1G	2.11	0.51
1:C:4:LEU:HB2	1:C:74:TYR:CD2	2.46	0.51
1:A:268:ARG:NE	1:A:270:ASP:OD2	2.43	0.51
1:A:27:HIS:HD2	1:A:306:TYR:CE2	2.29	0.50
1:B:246:THR:O	1:B:250:VAL:HG23	2.12	0.50
1:A:150:PHE:HA	1:A:191:ALA:HB2	1.93	0.50
1:B:112:LEU:O	1:B:119:SER:HB3	2.10	0.50
1:B:233:ARG:HH21	1:B:233:ARG:CB	2.24	0.50
1:A:10:VAL:HG21	1:A:84:ARG:NH1	2.26	0.50
1:C:148:PRO:HG3	1:C:150:PHE:CE1	2.46	0.50
1:B:50:LEU:O	1:B:54:GLU:HG3	2.12	0.50
1:A:251:GLN:O	1:A:255:LEU:HD22	2.12	0.49
1:C:36:VAL:HG23	1:C:49:ALA:HB1	1.93	0.49
1:A:56:LYS:O	1:A:57:ALA:CB	2.60	0.49
1:B:236:LEU:CD2	1:B:297:ARG:HE	2.21	0.49
1:C:88:ASP:OD2	1:C:90:THR:HG22	2.12	0.49
1:C:39:GLN:HE21	1:C:59:PRO:HA	1.77	0.49
1:C:290:THR:CG2	1:C:292:THR:HG22	2.42	0.49
1:A:148:PRO:HB3	1:A:149:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:O	1:C:49:ALA:HB2	2.13	0.49
1:A:73:ARG:HG2	1:A:73:ARG:HH11	1.78	0.49
1:A:290:THR:O	1:A:296:PRO:HG3	2.12	0.49
1:B:193:SER:HA	1:B:194:PRO:C	2.32	0.49
1:B:92:GLN:O	1:B:96:GLU:HG2	2.12	0.48
1:A:210:ALA:HB2	1:A:255:LEU:HD21	1.94	0.48
1:C:149:PRO:HA	1:C:166:VAL:O	2.14	0.48
1:B:21:ALA:O	1:B:25:LEU:HB2	2.14	0.48
1:B:33:ASP:HB2	1:B:74:TYR:CE2	2.49	0.48
1:C:168:ARG:HB2	1:C:168:ARG:HH21	1.78	0.48
1:A:27:HIS:CD2	1:A:306:TYR:CE2	3.01	0.48
1:B:81:LEU:HD13	1:B:81:LEU:N	2.28	0.48
1:B:138:LYS:H	1:B:138:LYS:CD	2.27	0.48
1:C:43:TRP:CE3	1:C:67:PRO:HG3	2.48	0.48
1:B:150:PHE:CE2	1:B:166:VAL:HB	2.49	0.48
1:C:15:GLU:O	1:C:19:LEU:HG	2.14	0.47
1:C:90:THR:CG2	1:C:91:VAL:N	2.78	0.47
1:C:193:SER:HA	1:C:194:PRO:C	2.33	0.47
1:C:312:ARG:HD2	3:C:419:HOH:O	2.13	0.47
1:A:290:THR:HB	1:A:293:SER:OG	2.14	0.47
1:B:138:LYS:N	1:B:138:LYS:CD	2.75	0.47
1:C:88:ASP:OD2	1:C:88:ASP:C	2.52	0.47
1:C:213:VAL:CG2	1:C:247:GLN:HG3	2.45	0.47
1:C:290:THR:O	1:C:296:PRO:HG3	2.14	0.47
1:C:290:THR:HG23	1:C:291:PRO:HD2	1.95	0.47
1:A:311:ARG:HG2	1:A:311:ARG:HH11	1.80	0.47
1:C:90:THR:HG23	1:C:91:VAL:H	1.77	0.47
1:B:150:PHE:HA	1:B:191:ALA:HB2	1.96	0.47
1:B:150:PHE:HB2	1:B:189:GLU:O	2.15	0.47
1:C:100:LYS:HE2	3:C:424:HOH:O	2.14	0.47
1:C:294:MET:HG3	1:C:298:LEU:HD22	1.96	0.47
1:C:168:ARG:HB2	1:C:168:ARG:CZ	2.45	0.47
1:A:56:LYS:HE2	1:A:56:LYS:HA	1.95	0.46
1:A:269:VAL:HG22	1:A:283:LEU:HG	1.97	0.46
1:B:163:ILE:CG2	1:B:164:SER:N	2.78	0.46
1:C:56:LYS:NZ	1:C:57:ALA:HB2	2.28	0.46
1:B:236:LEU:HD12	1:B:236:LEU:N	2.28	0.46
1:C:152:VAL:CG1	1:C:176:LEU:HD23	2.45	0.46
1:C:199:GLU:OE1	1:C:294:MET:HG2	2.15	0.46
1:A:1:MET:HG2	1:A:30:PHE:CD2	2.51	0.46
1:B:47:GLU:CD	1:C:181:ARG:HG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:HB	1:C:293:SER:OG	2.15	0.46
1:C:70:SER:HB3	1:C:72:GLU:OE2	2.15	0.46
1:C:84:ARG:NH1	1:C:84:ARG:HB3	2.31	0.46
1:C:240:ALA:O	1:C:242:LEU:N	2.46	0.45
1:A:28:ILE:HD12	1:A:29:PRO:HD2	1.97	0.45
1:B:160:SER:HA	1:B:163:ILE:HD12	1.98	0.45
1:C:4:LEU:HD21	1:C:69:LEU:HD21	1.99	0.45
1:C:54:GLU:C	1:C:56:LYS:H	2.18	0.45
1:C:213:VAL:HG23	1:C:247:GLN:HG3	1.99	0.45
1:C:155:ALA:HB1	1:C:185:LYS:HE3	1.98	0.45
1:C:306:TYR:HB3	1:C:307:PRO:HD3	1.97	0.45
1:A:56:LYS:NZ	1:A:56:LYS:HB3	2.31	0.45
1:A:311:ARG:HG2	1:A:311:ARG:NH1	2.32	0.45
1:B:114:MET:HE2	1:B:114:MET:CA	2.43	0.45
1:B:213:VAL:HB	1:B:247:GLN:HG3	1.99	0.45
1:C:204:GLY:O	1:C:264:ARG:O	2.35	0.45
1:B:33:ASP:HB2	1:B:74:TYR:HE2	1.81	0.45
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.29	0.45
1:C:91:VAL:O	1:C:94:PHE:HB3	2.17	0.45
1:A:148:PRO:HD3	1:A:169:PHE:CE1	2.51	0.45
1:A:268:ARG:HG3	1:A:268:ARG:NH2	2.32	0.45
1:C:236:LEU:HG	1:C:294:MET:HE2	1.99	0.45
1:A:156:ASN:HB2	1:A:183:ASP:OD2	2.17	0.44
1:B:24:VAL:HG21	1:B:80:LEU:HD21	1.98	0.44
1:C:148:PRO:HB3	1:C:149:PRO:HA	1.98	0.44
1:C:5:LEU:CD2	1:C:25:LEU:HD13	2.47	0.44
1:C:42:ARG:HG2	1:C:64:PRO:HA	1.99	0.44
1:C:155:ALA:H	1:C:186:ALA:HA	1.81	0.44
1:A:192:LEU:HB3	1:A:195:VAL:CG1	2.47	0.44
1:B:53:LEU:HD13	1:B:53:LEU:O	2.18	0.44
1:B:156:ASN:ND2	1:B:183:ASP:OD1	2.51	0.44
1:B:148:PRO:HD3	1:B:169:PHE:CD2	2.53	0.44
1:B:294:MET:O	1:B:298:LEU:HD22	2.17	0.44
1:A:166:VAL:HG13	1:A:171:ASP:HB2	1.98	0.43
1:B:242:LEU:N	1:B:242:LEU:HD22	2.33	0.43
1:A:156:ASN:N	1:A:183:ASP:OD2	2.51	0.43
1:B:4:LEU:HD21	1:B:69:LEU:HD11	1.99	0.43
1:C:84:ARG:HG2	1:C:85:PHE:CD2	2.53	0.43
1:A:52:ALA:HB1	1:A:58:ALA:HB2	2.01	0.43
1:B:150:PHE:CD2	1:B:166:VAL:HB	2.53	0.43
1:A:90:THR:HG22	1:B:107:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ILE:O	1:A:286:ILE:HG22	2.18	0.43
1:C:90:THR:CG2	1:C:91:VAL:H	2.32	0.43
1:C:94:PHE:CZ	1:C:98:LEU:HD11	2.54	0.43
1:A:192:LEU:HD21	1:A:279:TYR:CD2	2.53	0.43
1:C:21:ALA:O	1:C:25:LEU:HB2	2.19	0.43
1:C:174:ALA:O	1:C:177:ALA:HB3	2.18	0.43
1:C:180:PHE:HA	1:C:183:ASP:O	2.18	0.43
1:C:198:LEU:HD13	1:C:242:LEU:HD11	2.01	0.43
1:B:87:GLU:HB2	1:B:285:THR:OG1	2.18	0.43
1:B:310:LEU:O	1:B:314:VAL:HG23	2.18	0.43
1:B:1:MET:O	1:B:31:PRO:HD2	2.19	0.42
1:C:143:VAL:O	1:C:145:PRO:HD3	2.18	0.42
1:A:115:ASP:OD2	1:A:115:ASP:C	2.57	0.42
1:A:133:TRP:HA	1:A:188:VAL:O	2.18	0.42
1:A:224:ASP:CG	1:A:227:THR:HB	2.39	0.42
1:A:236:LEU:HD12	1:A:236:LEU:N	2.34	0.42
1:B:275:GLU:OE1	1:B:275:GLU:HA	2.19	0.42
1:C:63:HIS:HA	1:C:64:PRO:HD3	1.80	0.42
1:A:210:ALA:HB2	1:A:255:LEU:CD2	2.50	0.42
1:B:297:ARG:HG2	1:B:297:ARG:HH11	1.85	0.42
1:C:5:LEU:HD23	1:C:25:LEU:HD13	2.00	0.42
1:A:92:GLN:O	1:A:96:GLU:HG2	2.19	0.42
1:A:97:LEU:HB3	1:B:65:PHE:CE1	2.55	0.42
1:B:24:VAL:HG13	1:B:310:LEU:CD2	2.48	0.42
1:B:148:PRO:CB	1:B:149:PRO:HA	2.50	0.42
1:B:56:LYS:O	1:B:57:ALA:HB2	2.20	0.42
1:B:14:HIS:HE1	1:B:57:ALA:HA	1.85	0.42
1:B:69:LEU:HD22	1:B:71:TRP:CD2	2.55	0.42
1:B:102:TYR:OH	1:B:106:GLY:HA2	2.20	0.42
1:B:266:MET:SD	1:B:289:PHE:HE2	2.43	0.42
1:B:44:LEU:HD21	1:B:61:GLY:HA2	2.01	0.42
1:A:145:PRO:HG2	1:A:146:PHE:HD1	1.85	0.42
1:A:146:PHE:CD1	1:A:146:PHE:N	2.88	0.42
1:A:5:LEU:HD12	1:A:78:PHE:HB3	2.02	0.41
1:A:202:VAL:HG11	1:A:258:TYR:CG	2.55	0.41
1:A:280:LEU:HD23	1:A:280:LEU:C	2.40	0.41
1:C:119:SER:O	1:C:123:LEU:HG	2.20	0.41
1:C:45:LEU:HD22	1:C:69:LEU:CD1	2.50	0.41
1:C:163:ILE:HG22	1:C:164:SER:N	2.35	0.41
1:B:148:PRO:HD3	1:B:169:PHE:HD2	1.84	0.41
1:C:248:GLU:O	1:C:252:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LYS:HA	1:C:101:PRO:HD3	1.96	0.41
1:B:168:ARG:HB3	1:B:170:GLN:HG2	2.03	0.41
1:A:290:THR:C	1:A:292:THR:H	2.24	0.41
1:C:267:ALA:HA	1:C:284:ASN:O	2.21	0.41
1:B:115:ASP:OD2	1:B:115:ASP:C	2.59	0.41
1:B:138:LYS:HA	1:B:180:PHE:CZ	2.56	0.41
1:B:306:TYR:N	1:B:307:PRO:CD	2.84	0.41
1:A:43:TRP:CD1	1:A:43:TRP:N	2.87	0.41
1:A:45:LEU:HD13	1:A:69:LEU:HD23	2.03	0.41
1:A:295:TYR:CE1	1:A:309:LEU:HD21	2.56	0.41
1:B:39:GLN:NE2	1:B:59:PRO:HA	2.36	0.41
1:B:140:GLU:HA	1:B:141:PRO:HD3	1.91	0.41
1:B:222:PHE:HE1	1:B:232:GLY:HA2	1.84	0.41
1:C:34:LEU:HD12	1:C:35:ALA:H	1.85	0.41
1:A:131:VAL:O	1:A:132:PRO:C	2.60	0.41
1:A:9:GLY:O	1:A:14:HIS:CD2	2.70	0.40
1:A:150:PHE:CB	1:A:189:GLU:O	2.67	0.40
1:A:201:GLY:N	1:A:298:LEU:HD23	2.36	0.40
1:A:57:ALA:O	1:A:59:PRO:HD3	2.21	0.40
1:A:66:PRO:HD3	1:B:98:LEU:HD21	2.03	0.40
1:A:72:GLU:CD	1:A:72:GLU:H	2.24	0.40
1:B:43:TRP:CE3	1:B:67:PRO:HG3	2.57	0.40
1:C:168:ARG:NH2	1:C:170:GLN:CG	2.85	0.40
1:B:308:GLU:OE2	1:B:308:GLU:HA	2.22	0.40
1:B:87:GLU:O	1:B:114:MET:HE3	2.22	0.40
1:C:168:ARG:HH21	1:C:168:ARG:CB	2.34	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	313/319 (98%)	289 (92%)	20 (6%)	4 (1%)	12	24
1	B	309/319 (97%)	287 (93%)	19 (6%)	3 (1%)	15	32
1	C	305/319 (96%)	278 (91%)	23 (8%)	4 (1%)	12	24
All	All	927/957 (97%)	854 (92%)	62 (7%)	11 (1%)	13	27

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ALA
1	A	228	LYS
1	C	56	LYS
1	A	86	GLY
1	C	46	GLY
1	B	159	SER
1	C	143	VAL
1	C	86	GLY
1	A	244	PRO
1	B	86	GLY
1	B	193	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/256 (100%)	242 (95%)	13 (5%)	24	46
1	B	250/256 (98%)	227 (91%)	23 (9%)	9	17
1	C	246/256 (96%)	226 (92%)	20 (8%)	11	23
All	All	751/768 (98%)	695 (92%)	56 (8%)	13	27

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

Mol	Chain	Res	Type
1	A	11	SER
1	A	15	GLU

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Mol	Chain	Res	Type
1	A	76	VAL
1	A	78	PHE
1	A	92	GLN
1	A	97	LEU
1	A	223	TYR
1	A	226	GLU
1	A	247	GLN
1	A	253	LEU
1	A	255	LEU
1	A	261	LEU
1	A	294	MET
1	B	19	LEU
1	B	56	LYS
1	B	78	PHE
1	B	80	LEU
1	B	81	LEU
1	B	84	ARG
1	B	92	GLN
1	B	97	LEU
1	B	112	LEU
1	B	138	LYS
1	B	150	PHE
1	B	156	ASN
1	B	169	PHE
1	B	217	ARG
1	B	222	PHE
1	B	229	TYR
1	B	236	LEU
1	B	243	ASP
1	B	255	LEU
1	B	268	ARG
1	B	275	GLU
1	B	289	PHE
1	B	298	LEU
1	C	18	LEU
1	C	54	GLU
1	C	56	LYS
1	C	78	PHE
1	C	81	LEU
1	C	92	GLN
1	C	100	LYS
1	C	112	LEU

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Mol	Chain	Res	Type
1	C	114	MET
1	C	125	GLN
1	C	150	PHE
1	C	156	ASN
1	C	235	GLU
1	C	255	LEU
1	C	261	LEU
1	C	289	PHE
1	C	292	THR
1	C	298	LEU
1	C	308	GLU
1	C	311	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	27	HIS
1	A	92	GLN
1	A	156	ASN
1	A	251	GLN
1	B	14	HIS
1	B	39	GLN
1	B	82	HIS
1	B	92	GLN
1	B	156	ASN
1	B	251	GLN
1	B	281	ASN
1	C	39	GLN
1	C	92	GLN
1	C	156	ASN
1	C	205	ASN
1	C	247	GLN
1	C	251	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)

3 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	ANP	C	403	-	29,33,33	1.67	5 (17%)	31,52,52	1.75	5 (16%)
2	ANP	A	401	-	29,33,33	1.72	5 (17%)	31,52,52	1.77	5 (16%)
2	ANP	B	402	-	29,33,33	1.69	6 (20%)	31,52,52	1.72	5 (16%)

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	ANP	C	403	-	-	5/14/38/38	0/3/3/3
2	ANP	A	401	-	-	1/14/38/38	0/3/3/3
2	ANP	B	402	-	-	2/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	ANP	O4'-C1'	4.72	1.47	1.41
2	A	401	ANP	O4'-C1'	4.31	1.47	1.41
2	C	403	ANP	O4'-C1'	4.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	ANP	PB-O3A	4.09	1.64	1.59
2	B	402	ANP	PB-O3A	3.38	1.63	1.59
2	C	403	ANP	PB-O3A	3.29	1.63	1.59
2	C	403	ANP	PB-N3B	3.29	1.71	1.63
2	C	403	ANP	PG-N3B	3.16	1.71	1.63
2	A	401	ANP	PG-N3B	3.14	1.71	1.63
2	B	402	ANP	PG-N3B	3.09	1.71	1.63
2	A	401	ANP	PB-N3B	2.96	1.71	1.63
2	B	402	ANP	PB-N3B	2.88	1.70	1.63
2	A	401	ANP	C8-N7	-2.31	1.30	1.34
2	B	402	ANP	C8-N7	-2.12	1.30	1.34
2	C	403	ANP	C8-N7	-2.04	1.31	1.34
2	B	402	ANP	PG-O2G	2.00	1.62	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	402	ANP	PB-O3A-PA	-6.22	110.71	132.62
2	C	403	ANP	PB-O3A-PA	-6.11	111.09	132.62
2	A	401	ANP	PB-O3A-PA	-5.97	111.60	132.62
2	A	401	ANP	N3-C2-N1	-4.69	121.35	128.68
2	B	402	ANP	N3-C2-N1	-4.60	121.49	128.68
2	C	403	ANP	N3-C2-N1	-4.51	121.63	128.68
2	C	403	ANP	C3'-C2'-C1'	2.68	105.01	100.98
2	A	401	ANP	PA-O5'-C5'	-2.37	107.78	121.68
2	B	402	ANP	PA-O5'-C5'	-2.30	108.18	121.68
2	B	402	ANP	C3'-C2'-C1'	2.22	104.31	100.98
2	C	403	ANP	PA-O5'-C5'	-2.21	108.73	121.68
2	A	401	ANP	C3'-C2'-C1'	2.18	104.26	100.98
2	C	403	ANP	C4-C5-N7	-2.08	107.23	109.40
2	B	402	ANP	C4-C5-N7	-2.03	107.28	109.40
2	A	401	ANP	O1G-PG-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ANP	PB-N3B-PG-O1G
2	B	402	ANP	PB-N3B-PG-O1G
2	B	402	ANP	PG-N3B-PB-O1B
2	C	403	ANP	PB-N3B-PG-O1G
2	C	403	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	C	403	ANP	PG-N3B-PB-O3A
2	C	403	ANP	PB-O3A-PA-O2A
2	C	403	ANP	PB-O3A-PA-O1A

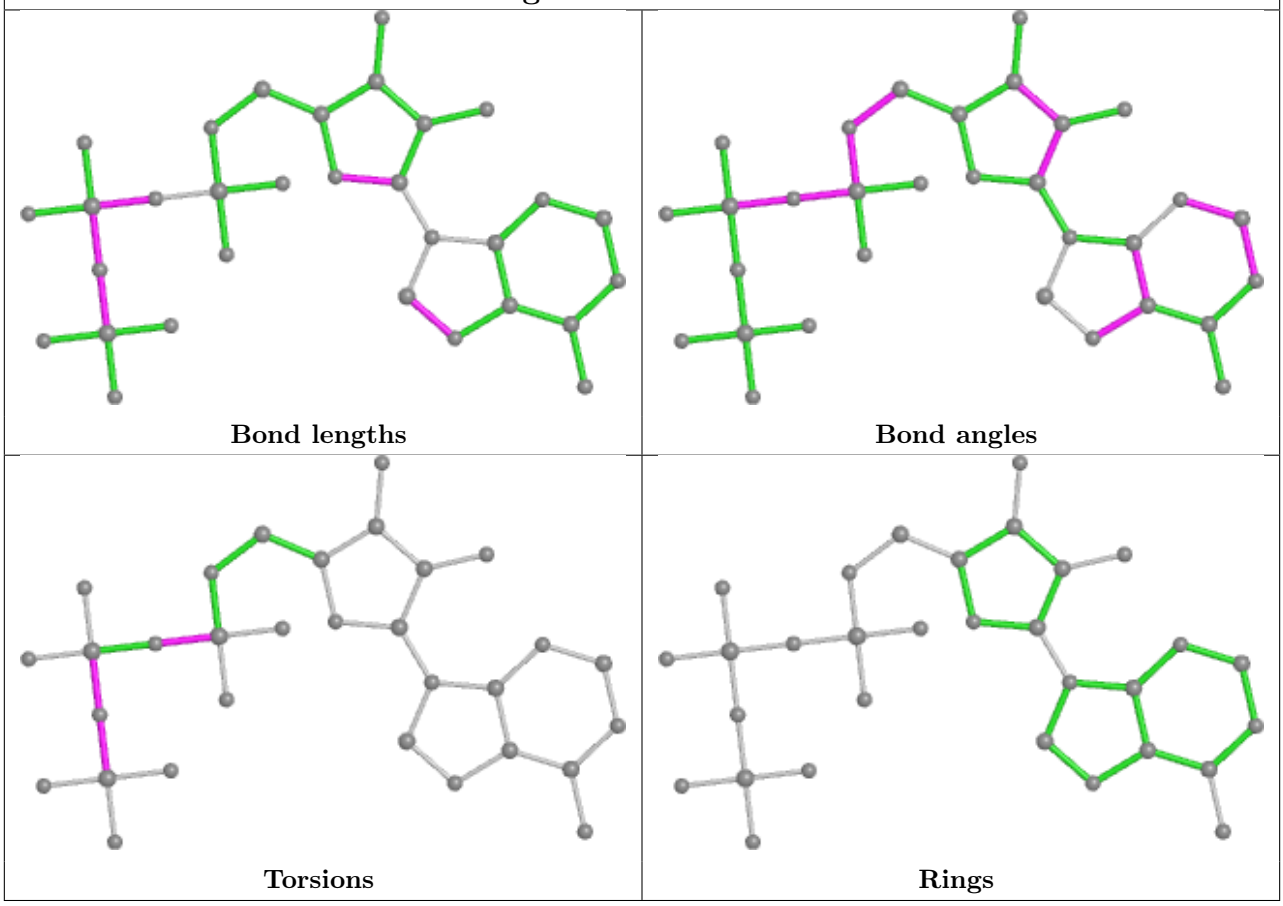
There are no ring outliers.

1 monomer is involved in 1 short contact:

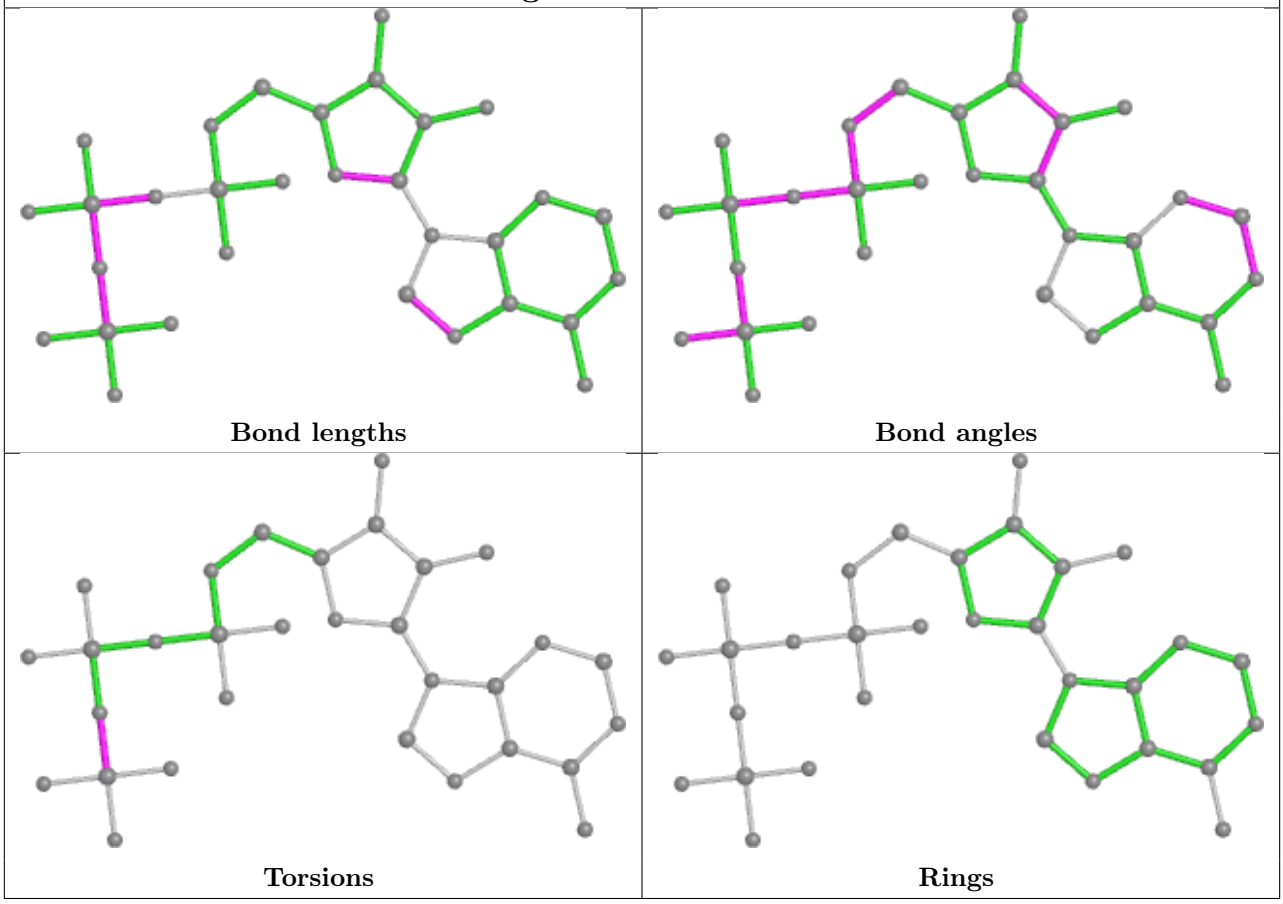
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	ANP	1	0

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.

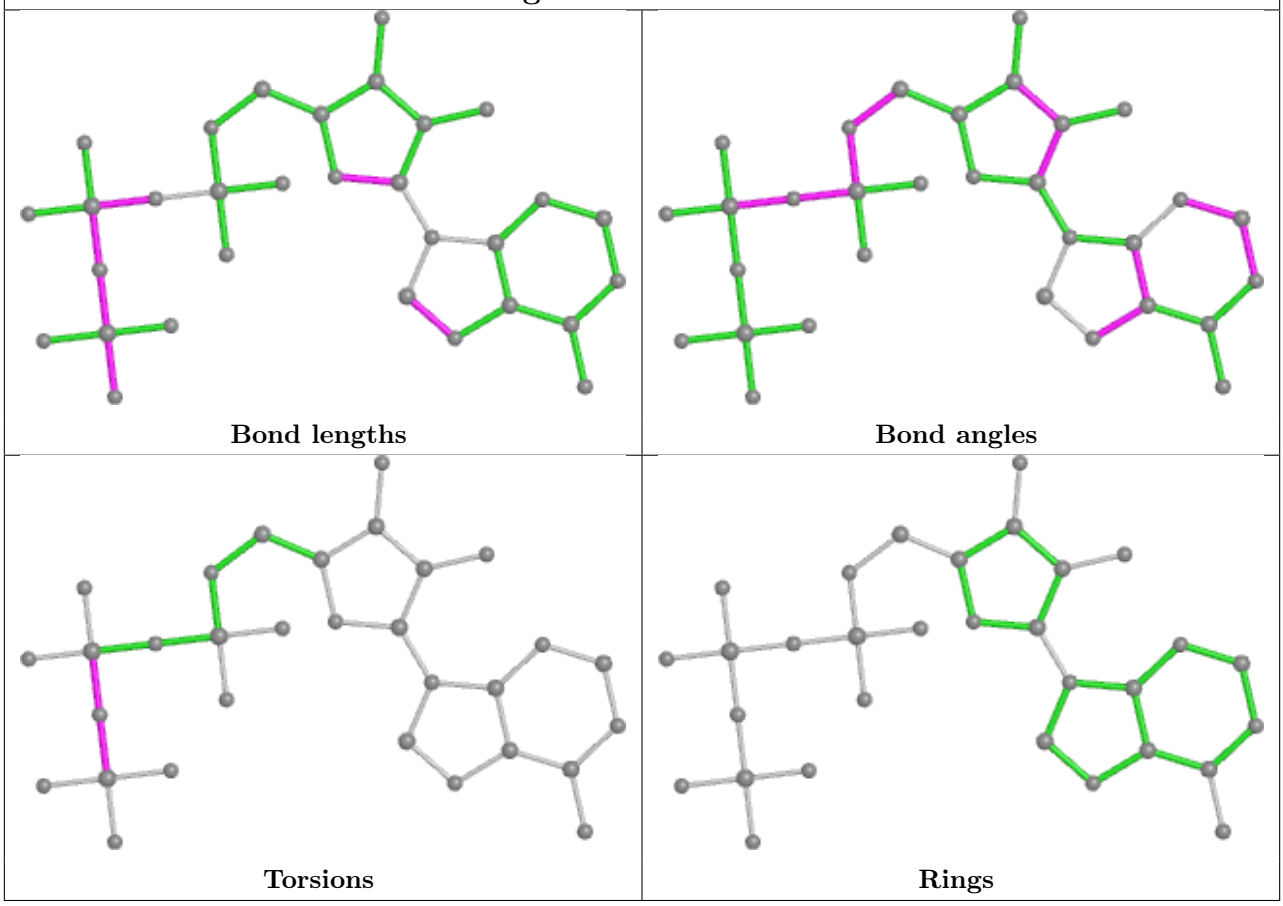
Ligand ANP C 403



Ligand ANP A 401



Ligand ANP B 402



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	317/319 (99%)	-0.02	1 (0%)	94	93	23, 43, 68, 77	0
1	B	313/319 (98%)	0.11	9 (2%)	51	45	27, 50, 78, 86	0
1	C	309/319 (96%)	0.08	9 (2%)	51	45	22, 42, 74, 89	0
All	All	939/957 (98%)	0.06	19 (2%)	65	60	22, 45, 73, 89	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	PHE	3.2
1	B	236	LEU	3.2
1	C	170	GLN	3.1
1	C	182	TYR	3.1
1	A	26	ARG	2.8
1	C	166	VAL	2.8
1	C	159	SER	2.7
1	B	144	VAL	2.7
1	B	176	LEU	2.6
1	B	27	HIS	2.5
1	C	171	ASP	2.4
1	B	167	GLU	2.4
1	C	172	LEU	2.4
1	C	168	ARG	2.3
1	B	56	LYS	2.3
1	C	150	PHE	2.3
1	B	230	THR	2.3
1	C	176	LEU	2.0
1	B	165	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

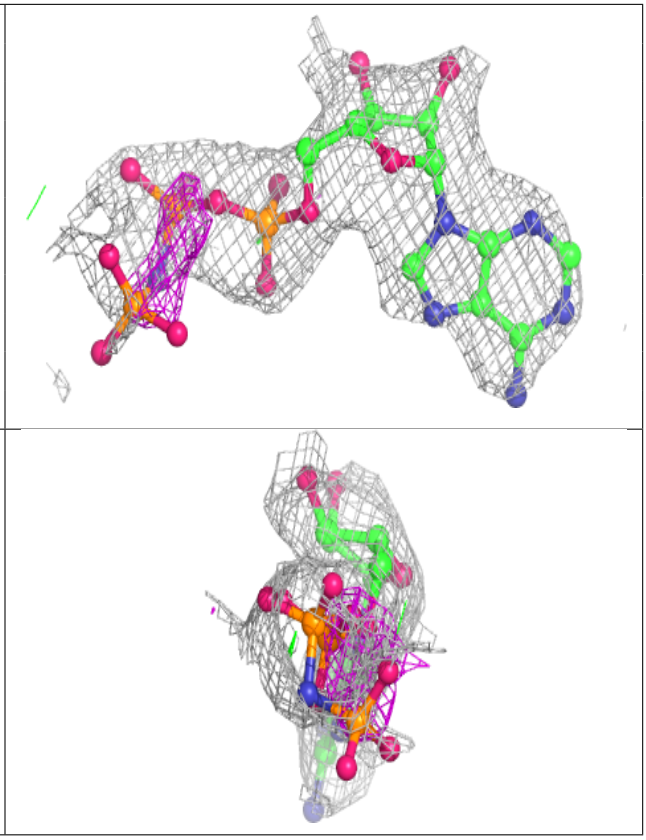
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ANP	A	401	31/31	0.76	0.28	105,109,130,130	0
2	ANP	B	402	31/31	0.83	0.25	84,93,118,118	0
2	ANP	C	403	31/31	0.84	0.23	76,84,102,104	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.

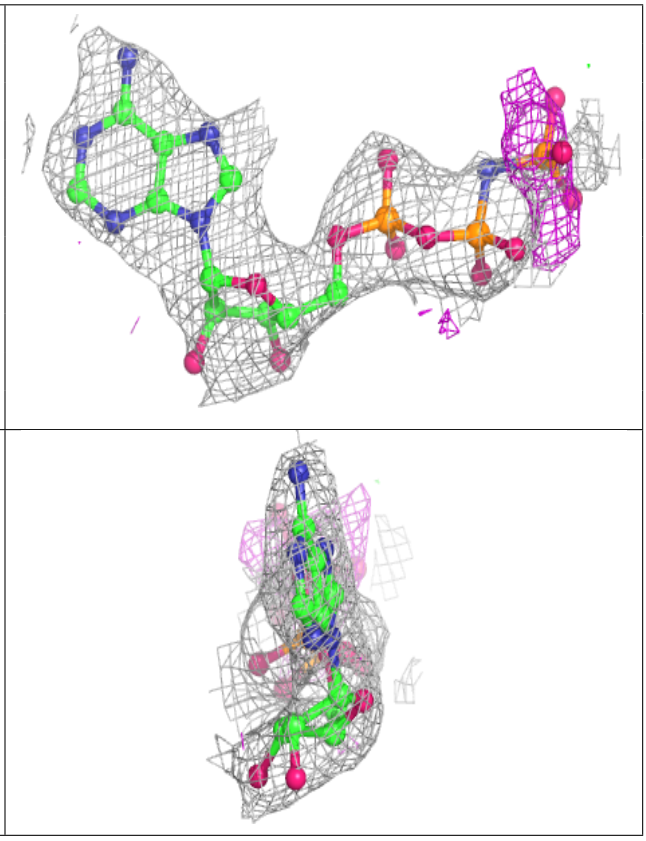
Electron density around ANP A 401:

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



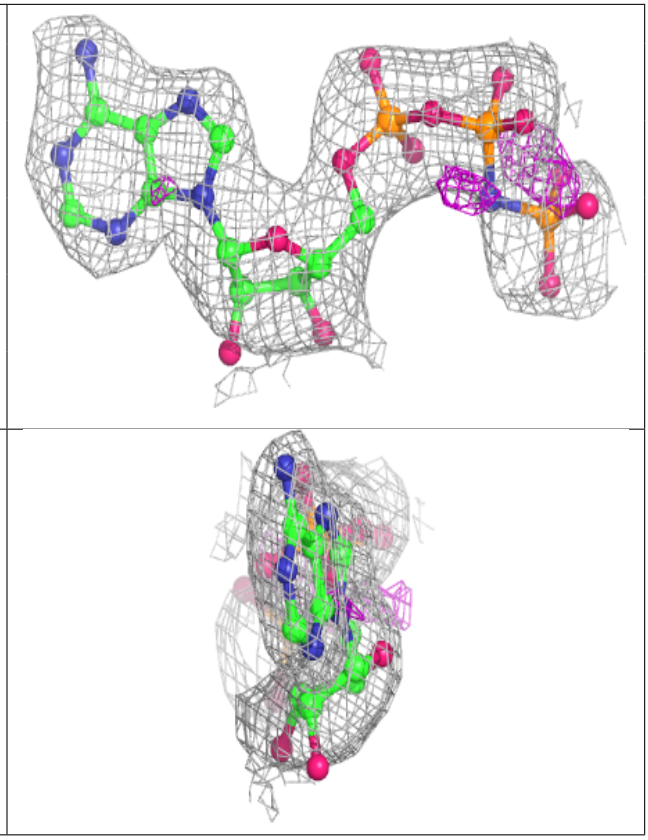
Electron density around ANP B 402:

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



Electron density around ANP C 403:

$2mF_o$-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.