Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 06:17 PM EST

PDB ID	:	2I4O
Title	:	Rhodopseudomonas palustris prolyl-tRNA synthetase in complex with ATP
Authors	:	Crepin, T.; Yaremchuk, A.; Tukalo, M.; Cusack, S.
Deposited on	:	2006-08-22
Resolution	:	2.40 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:

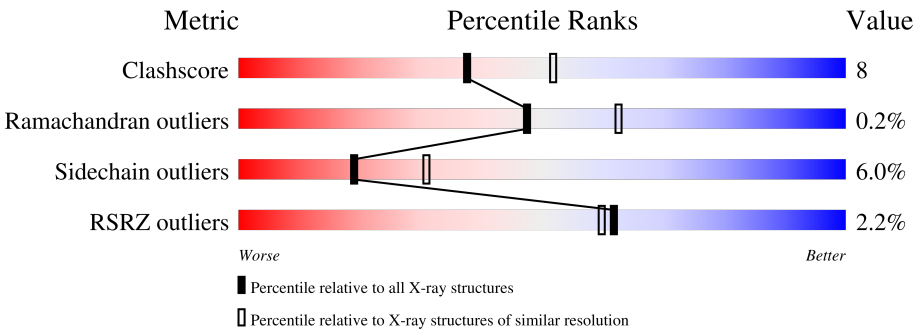
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	458	3% 77% 18%
1	B	458	2% 78% 16%
1	C	458	% 79% 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10865 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 Proline-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	3495	2211	620	650	14	0	0	0
1	B	441	3495	2211	620	650	14	0	0	0
1	C	441	3495	2211	620	650	14	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q6N5P6
A	-18	GLY	-	expression tag	UNP Q6N5P6
A	-17	SER	-	expression tag	UNP Q6N5P6
A	-16	SER	-	expression tag	UNP Q6N5P6
A	-15	HIS	-	expression tag	UNP Q6N5P6
A	-14	HIS	-	expression tag	UNP Q6N5P6
A	-13	HIS	-	expression tag	UNP Q6N5P6
A	-12	HIS	-	expression tag	UNP Q6N5P6
A	-11	HIS	-	expression tag	UNP Q6N5P6
A	-10	HIS	-	expression tag	UNP Q6N5P6
A	-9	SER	-	expression tag	UNP Q6N5P6
A	-8	SER	-	expression tag	UNP Q6N5P6
A	-7	GLY	-	expression tag	UNP Q6N5P6
A	-6	LEU	-	expression tag	UNP Q6N5P6
A	-5	VAL	-	expression tag	UNP Q6N5P6
A	-4	PRO	-	expression tag	UNP Q6N5P6
A	-3	ARG	-	expression tag	UNP Q6N5P6
A	-2	GLY	-	expression tag	UNP Q6N5P6
A	-1	SER	-	expression tag	UNP Q6N5P6
A	0	HIS	-	expression tag	UNP Q6N5P6
B	-19	MET	-	expression tag	UNP Q6N5P6
B	-18	GLY	-	expression tag	UNP Q6N5P6
B	-17	SER	-	expression tag	UNP Q6N5P6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q6N5P6
B	-15	HIS	-	expression tag	UNP Q6N5P6
B	-14	HIS	-	expression tag	UNP Q6N5P6
B	-13	HIS	-	expression tag	UNP Q6N5P6
B	-12	HIS	-	expression tag	UNP Q6N5P6
B	-11	HIS	-	expression tag	UNP Q6N5P6
B	-10	HIS	-	expression tag	UNP Q6N5P6
B	-9	SER	-	expression tag	UNP Q6N5P6
B	-8	SER	-	expression tag	UNP Q6N5P6
B	-7	GLY	-	expression tag	UNP Q6N5P6
B	-6	LEU	-	expression tag	UNP Q6N5P6
B	-5	VAL	-	expression tag	UNP Q6N5P6
B	-4	PRO	-	expression tag	UNP Q6N5P6
B	-3	ARG	-	expression tag	UNP Q6N5P6
B	-2	GLY	-	expression tag	UNP Q6N5P6
B	-1	SER	-	expression tag	UNP Q6N5P6
B	0	HIS	-	expression tag	UNP Q6N5P6
C	-19	MET	-	expression tag	UNP Q6N5P6
C	-18	GLY	-	expression tag	UNP Q6N5P6
C	-17	SER	-	expression tag	UNP Q6N5P6
C	-16	SER	-	expression tag	UNP Q6N5P6
C	-15	HIS	-	expression tag	UNP Q6N5P6
C	-14	HIS	-	expression tag	UNP Q6N5P6
C	-13	HIS	-	expression tag	UNP Q6N5P6
C	-12	HIS	-	expression tag	UNP Q6N5P6
C	-11	HIS	-	expression tag	UNP Q6N5P6
C	-10	HIS	-	expression tag	UNP Q6N5P6
C	-9	SER	-	expression tag	UNP Q6N5P6
C	-8	SER	-	expression tag	UNP Q6N5P6
C	-7	GLY	-	expression tag	UNP Q6N5P6
C	-6	LEU	-	expression tag	UNP Q6N5P6
C	-5	VAL	-	expression tag	UNP Q6N5P6
C	-4	PRO	-	expression tag	UNP Q6N5P6
C	-3	ARG	-	expression tag	UNP Q6N5P6
C	-2	GLY	-	expression tag	UNP Q6N5P6
C	-1	SER	-	expression tag	UNP Q6N5P6
C	0	HIS	-	expression tag	UNP Q6N5P6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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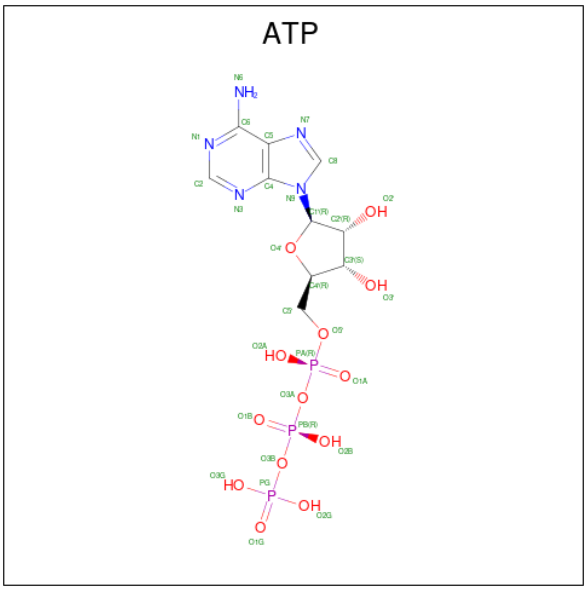
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mg 3 3	0	0
2	B	3	Total Mg 3 3	0	0
2	C	2	Total Mg 2 2	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	86	Total O 86 86	0	0

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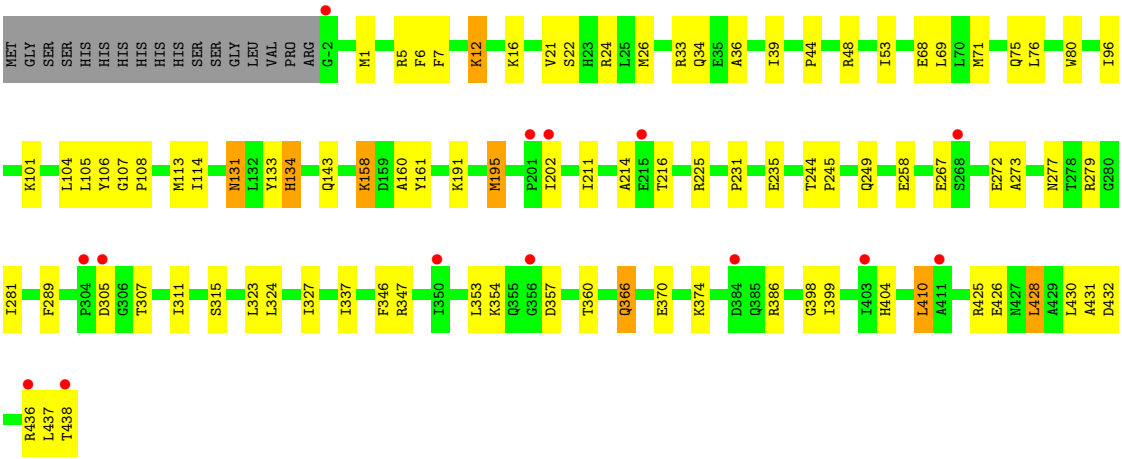
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	117	117	117	0	0

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.

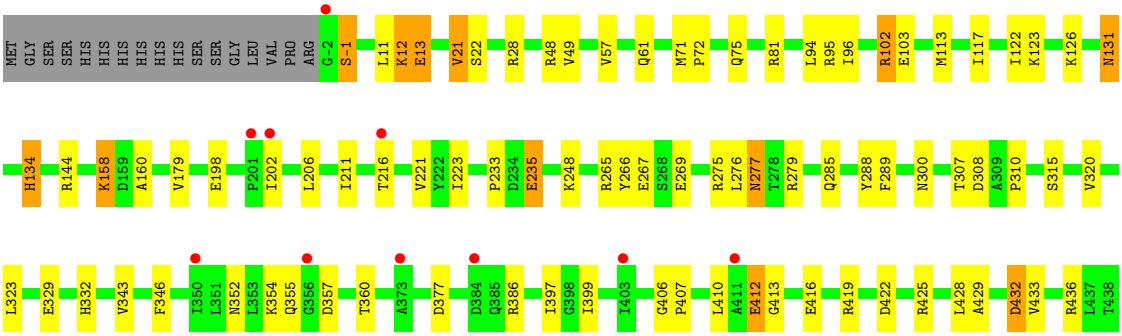
• Molecule 1: Proline-tRNA ligase

Chain A:



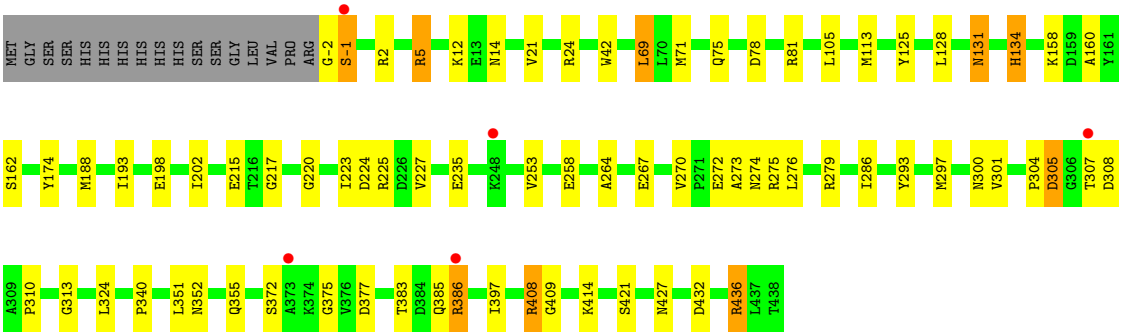
• Molecule 1: Proline-tRNA ligase

Chain B:



• Molecule 1: Proline-tRNA ligase

Chain C:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG G-2 S-1 R2 R5 K12 E13 N14 V21 R24 W42 L69 L70 M71 Q75 D78 R81 L105 M113 Y125 L128 N131 H134 K158 D159 A160 Y161
S162 Y174 M188 I193 E198 I202 E215 T216 G217 G220 I223 D224 R225 D226 V227 E235 K248 V253 E258 A264 E267 V270 P271 E272 A273 N274 R275 L276 R279 I286 Y293 M297 N300 V301 P304 D305 G306 T307 D308
A309 P310 G313 L324 P340 L351 N352 Q355 S372 A373 K374 G375 V376 D377 T383 D384 Q385 R386 I397 R408 G409 K414 S421 M427 D432 R436 L437 T438

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.20Å 211.21Å 148.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.0 ((Not available)-2.40) 96.2 (19.98-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.261 0.196 , (Not available)	Depositor DCC
R_{free} test set	3397 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10865	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: ATP, MG

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	0.62	0/3570	0.72	0/4828
1	B	0.64	0/3570	0.75	0/4828
1	C	0.67	0/3570	0.77	1/4828 (0.0%)
All	All	0.65	0/10710	0.75	1/14484 (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	69	LEU	CA-CB-CG	5.39	127.69	115.30

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	3495	0	3466	56	0
1	B	3495	0	3466	60	0
1	C	3495	0	3466	51	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
3	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	31	0	12	0	0
3	C	31	0	12	0	0
4	A	76	0	0	6	0
4	B	86	0	0	3	0
4	C	117	0	0	2	1
All	All	10865	0	10434	162	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 8.

All (162) 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:386:ARG:HH11	1:C:386:ARG:HG3	1.33	0.92
1:C:131:ASN:HD21	1:C:160:ALA:HB1	1.35	0.92
1:A:21:VAL:HG23	4:A:483:HOH:O	1.72	0.90
1:B:71:MET:H	1:B:134:HIS:HD2	1.25	0.83
1:A:71:MET:H	1:A:134:HIS:CD2	2.02	0.78
1:B:12:LYS:HD3	1:B:12:LYS:H	1.48	0.77
1:B:71:MET:H	1:B:134:HIS:CD2	2.06	0.74
1:C:71:MET:H	1:C:134:HIS:HD2	1.36	0.73
1:B:12:LYS:HD3	1:B:12:LYS:N	2.04	0.73
1:A:131:ASN:HD21	1:A:160:ALA:HB1	1.56	0.70
1:B:12:LYS:H	1:B:12:LYS:CD	2.05	0.69
1:C:21:VAL:HG23	4:C:468:HOH:O	1.91	0.69
1:C:300:ASN:HD22	1:C:310:PRO:HA	1.59	0.68
1:B:300:ASN:HD22	1:B:310:PRO:HA	1.58	0.68
1:B:216:THR:HA	4:B:508:HOH:O	1.95	0.66
1:C:-2:GLY:N	1:C:375:GLY:HA2	2.09	0.66
1:B:102:ARG:HH11	1:B:102:ARG:CG	2.08	0.66
1:C:408:ARG:H	1:C:408:ARG:HH11	1.44	0.65
1:C:71:MET:H	1:C:134:HIS:CD2	2.16	0.64
1:A:71:MET:H	1:A:134:HIS:HD2	1.46	0.64
1:C:383:THR:OG1	1:C:385:GLN:HG2	1.99	0.63
1:A:12:LYS:H	1:A:12:LYS:CD	2.11	0.63
1:A:53:ILE:HD12	1:A:324:LEU:CD1	2.29	0.63
1:A:202:ILE:HG22	1:A:202:ILE:O	1.98	0.63
1:C:414:LYS:HD3	1:C:427:ASN:HB3	1.81	0.63
1:A:289:PHE:HE2	1:A:315:SER:HB3	1.64	0.62
1:A:438:THR:OXT	1:A:438:THR:HG22	1.98	0.62
1:B:102:ARG:HH11	1:B:102:ARG:HG2	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:O	1:A:26:MET:HG3	2.01	0.61
1:B:354:LYS:HG2	1:B:357:ASP:HB2	1.83	0.61
1:B:354:LYS:HG2	1:B:357:ASP:CB	2.31	0.60
1:A:71:MET:SD	1:A:113:MET:HG2	2.41	0.60
1:A:357:ASP:OD2	1:A:360:THR:HG23	2.02	0.60
1:A:360:THR:HG22	1:A:410:LEU:HD22	1.83	0.59
1:A:360:THR:HG22	1:A:410:LEU:CD2	2.33	0.59
1:B:277:ASN:HD22	1:B:277:ASN:N	2.00	0.58
1:A:12:LYS:N	1:A:12:LYS:HD2	2.18	0.58
1:A:7:PHE:HB3	1:A:44:PRO:HG2	1.86	0.58
1:C:408:ARG:HH11	1:C:408:ARG:HB3	1.69	0.58
1:C:408:ARG:HD2	1:C:409:GLY:N	2.19	0.58
1:B:202:ILE:HG22	1:B:202:ILE:O	2.05	0.57
1:C:386:ARG:HG3	1:C:386:ARG:NH1	2.08	0.57
1:B:131:ASN:HD21	1:B:160:ALA:HB1	1.70	0.56
1:B:406:GLY:O	1:B:410:LEU:HB3	2.05	0.56
1:B:346:PHE:HB2	1:B:399:ILE:HD12	1.88	0.56
1:C:408:ARG:H	1:C:408:ARG:NH1	2.04	0.56
1:A:48:ARG:HD3	4:A:452:HOH:O	2.06	0.55
1:B:360:THR:HG22	1:B:410:LEU:HD23	1.89	0.55
1:A:53:ILE:HD12	1:A:324:LEU:HD11	1.88	0.55
1:A:12:LYS:H	1:A:12:LYS:HD2	1.71	0.55
1:A:354:LYS:HG2	1:A:357:ASP:HB2	1.88	0.55
1:A:158:LYS:HD2	1:A:158:LYS:C	2.27	0.54
1:C:131:ASN:C	1:C:131:ASN:HD22	2.11	0.54
1:A:225:ARG:NH1	1:A:273:ALA:O	2.41	0.53
1:A:5:ARG:NH2	4:A:495:HOH:O	2.40	0.53
1:A:96:ILE:HG12	1:B:96:ILE:HG12	1.88	0.53
1:B:75:GLN:HG2	1:B:113:MET:CE	2.39	0.53
1:C:42:TRP:HZ3	1:C:324:LEU:HD22	1.73	0.53
1:A:214:ALA:O	1:A:279:ARG:HB2	2.08	0.53
1:C:-2:GLY:H1	1:C:375:GLY:HA2	1.73	0.52
1:C:300:ASN:HD22	1:C:310:PRO:CA	2.23	0.52
1:B:131:ASN:C	1:B:131:ASN:HD22	2.12	0.52
1:B:397:ILE:HG13	1:B:399:ILE:HG12	1.91	0.52
1:A:195:MET:HG3	1:A:211:ILE:HD12	1.92	0.52
1:C:432:ASP:O	1:C:436:ARG:HG2	2.09	0.52
1:B:266:TYR:OH	1:B:277:ASN:ND2	2.44	0.51
1:A:96:ILE:HG21	1:B:94:LEU:HD21	1.92	0.51
1:C:264:ALA:HB3	4:C:539:HOH:O	2.10	0.51
1:A:370:GLU:O	1:A:374:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:GLN:HG2	1:C:113:MET:CE	2.41	0.50
1:B:410:LEU:C	1:B:412:GLU:H	2.15	0.50
1:B:122:ILE:O	1:B:123:LYS:HD3	2.11	0.50
1:B:360:THR:HA	1:B:410:LEU:CD2	2.42	0.49
1:B:158:LYS:HD2	1:B:158:LYS:C	2.32	0.49
1:C:-2:GLY:H3	1:C:375:GLY:HA2	1.76	0.49
1:B:211:ILE:HG21	1:B:221:VAL:HG11	1.94	0.49
1:A:75:GLN:OE1	1:A:80:TRP:NE1	2.36	0.49
1:B:413:GLY:O	1:B:429:ALA:HA	2.12	0.49
1:A:428:LEU:HD23	1:A:436:ARG:NH2	2.29	0.48
1:C:162:SER:O	1:C:313:GLY:HA2	2.13	0.48
1:B:432:ASP:OD1	1:B:432:ASP:N	2.47	0.48
1:C:224:ASP:OD1	1:C:274:ASN:HB3	2.14	0.48
1:A:311:ILE:HD12	1:A:311:ILE:C	2.34	0.48
1:C:215:GLU:HA	1:C:215:GLU:OE1	2.14	0.48
1:C:408:ARG:HD2	1:C:409:GLY:H	1.78	0.48
1:C:224:ASP:HB3	1:C:253:VAL:HG12	1.96	0.47
1:B:320:VAL:HA	1:B:323:LEU:HD12	1.96	0.47
1:C:188:MET:O	1:C:340:PRO:HG2	2.15	0.47
1:C:223:ILE:HD11	1:C:276:LEU:HD23	1.96	0.47
1:B:13:GLU:HA	4:B:496:HOH:O	2.14	0.47
1:A:33:ARG:HD3	1:B:117:ILE:HG12	1.97	0.47
1:B:419:ARG:NH2	1:B:422:ASP:OD2	2.48	0.47
1:A:337:ILE:O	1:A:398:GLY:HA2	2.14	0.47
1:B:416:GLU:OE1	1:B:425:ARG:HD3	2.15	0.47
1:A:347:ARG:NH1	1:A:437:LEU:O	2.37	0.46
1:B:223:ILE:HD11	1:B:276:LEU:HD23	1.97	0.46
1:C:193:ILE:HG12	1:C:227:VAL:HG13	1.98	0.46
1:A:428:LEU:HD23	1:A:436:ARG:CZ	2.45	0.46
1:A:114:ILE:HG21	1:A:161:TYR:CG	2.51	0.46
1:A:346:PHE:HB2	1:A:399:ILE:HD12	1.98	0.46
1:C:2:ARG:HD2	1:C:5:ARG:HD3	1.96	0.46
1:B:144:ARG:HD3	1:C:258:GLU:OE2	2.17	0.45
1:B:300:ASN:HD22	1:B:310:PRO:CA	2.29	0.45
1:B:360:THR:HG21	1:B:407:PRO:HD3	1.99	0.45
1:C:386:ARG:NH1	1:C:386:ARG:CG	2.76	0.45
1:A:258:GLU:HB2	4:A:515:HOH:O	2.16	0.45
1:B:277:ASN:N	1:B:277:ASN:ND2	2.65	0.45
1:C:267:GLU:HA	1:C:275:ARG:NH2	2.32	0.45
1:C:128:LEU:HD11	1:C:301:VAL:HG11	1.98	0.45
1:B:-1:SER:O	1:B:377:ASP:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:SER:O	1:C:377:ASP:HA	2.17	0.45
1:A:366:GLN:HG2	1:A:370:GLU:OE2	2.17	0.45
1:B:354:LYS:HD2	1:B:407:PRO:HG3	1.98	0.45
1:B:267:GLU:HA	1:B:275:ARG:NH2	2.32	0.45
1:A:353:LEU:HD11	1:A:404:HIS:HB3	1.98	0.44
1:B:95:ARG:HD2	4:B:468:HOH:O	2.17	0.44
1:B:265:ARG:O	1:B:269:GLU:HB2	2.18	0.44
1:B:289:PHE:HE2	1:B:315:SER:HB3	1.82	0.44
1:C:408:ARG:HH11	1:C:408:ARG:CB	2.29	0.44
1:A:101:LYS:NZ	4:A:499:HOH:O	2.50	0.44
1:B:11:LEU:HB2	1:B:28:ARG:HG2	2.00	0.44
1:B:49:VAL:HG13	1:B:343:VAL:O	2.18	0.44
1:B:235:GLU:H	1:B:235:GLU:HG3	1.47	0.44
1:B:428:LEU:HD13	1:B:433:VAL:HG23	2.00	0.44
1:A:24:ARG:HD2	4:A:480:HOH:O	2.18	0.44
1:B:57:VAL:O	1:B:61:GLN:HG2	2.18	0.44
1:A:1:MET:HG2	1:A:6:PHE:CD1	2.53	0.43
1:C:14:ASN:OD1	1:C:24:ARG:HD3	2.17	0.43
1:A:244:THR:N	1:A:245:PRO:HD2	2.33	0.43
1:A:68:GLU:HG3	1:A:133:TYR:CE1	2.54	0.43
1:C:202:ILE:O	1:C:202:ILE:CG2	2.66	0.43
1:B:102:ARG:CG	1:B:102:ARG:NH1	2.76	0.43
1:C:217:GLY:O	1:C:279:ARG:HB3	2.17	0.43
1:B:21:VAL:HG11	1:B:332:HIS:CD2	2.54	0.43
1:B:81:ARG:HH22	1:B:103:GLU:CD	2.22	0.43
1:A:34:GLN:HG3	1:A:36:ALA:O	2.19	0.43
1:C:293:TYR:O	1:C:297:MET:HB2	2.19	0.43
1:B:179:VAL:HG13	1:B:233:PRO:HG2	2.01	0.42
1:C:202:ILE:O	1:C:202:ILE:HG22	2.19	0.42
1:B:206:LEU:HB2	1:B:288:TYR:HB3	2.01	0.42
1:B:75:GLN:HG2	1:B:113:MET:HE3	2.00	0.42
1:B:22:SER:OG	1:B:329:GLU:OE2	2.32	0.42
1:C:305:ASP:OD2	1:C:305:ASP:N	2.50	0.42
1:A:131:ASN:HD22	1:A:131:ASN:C	2.23	0.42
1:A:323:LEU:O	1:A:327:ILE:HG13	2.20	0.42
1:C:225:ARG:NH1	1:C:273:ALA:O	2.53	0.42
1:A:305:ASP:OD2	1:A:307:THR:HG22	2.19	0.42
1:C:125:TYR:CD1	1:C:304:PRO:HG3	2.55	0.42
1:C:174:TYR:CZ	1:C:286:ILE:HG13	2.55	0.42
1:A:76:LEU:HD23	1:A:104:LEU:HD23	2.02	0.41
1:B:352:ASN:HB3	1:B:355:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HG22	1:B:72:PRO:HG3	2.03	0.41
1:C:220:GLY:O	1:C:258:GLU:N	2.50	0.41
1:C:436:ARG:HH11	1:C:436:ARG:HB3	1.85	0.41
1:A:231:PRO:HD2	1:A:249:GLN:NE2	2.36	0.41
1:A:430:LEU:C	1:A:432:ASP:H	2.24	0.41
1:C:352:ASN:HB3	1:C:355:GLN:OE1	2.19	0.41
1:A:107:GLY:HA2	1:A:108:PRO:HD3	1.78	0.41
1:A:202:ILE:O	1:A:202:ILE:CG2	2.66	0.41
1:A:430:LEU:O	1:A:432:ASP:N	2.55	0.40
1:C:78:ASP:OD1	1:C:81:ARG:NH1	2.51	0.40
1:C:270:VAL:HG12	1:C:275:ARG:HG3	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)
4:C:490:HOH:O	4:C:556:HOH:O[3_454]	1.84	0.36

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	439/458 (96%)	409 (93%)	29 (7%)	1 (0%)	47	62
1	B	439/458 (96%)	408 (93%)	30 (7%)	1 (0%)	47	62
1	C	439/458 (96%)	415 (94%)	24 (6%)	0	100	100
All	All	1317/1374 (96%)	1232 (94%)	83 (6%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	431	ALA

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Mol	Chain	Res	Type
1	B	412	GLU

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	361/376 (96%)	338 (94%)	23 (6%)	17	28
1	B	361/376 (96%)	340 (94%)	21 (6%)	20	32
1	C	361/376 (96%)	340 (94%)	21 (6%)	20	32
All	All	1083/1128 (96%)	1018 (94%)	65 (6%)	19	31

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	16	LYS
1	A	69	LEU
1	A	105	LEU
1	A	106	TYR
1	A	131	ASN
1	A	134	HIS
1	A	143	GLN
1	A	158	LYS
1	A	191	LYS
1	A	195	MET
1	A	216	THR
1	A	235	GLU
1	A	267	GLU
1	A	272	GLU
1	A	277	ASN
1	A	281	ILE
1	A	366	GLN
1	A	386	ARG
1	A	410	LEU
1	A	425	ARG

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Mol	Chain	Res	Type
1	A	426	GLU
1	A	428	LEU
1	B	-1	SER
1	B	12	LYS
1	B	13	GLU
1	B	21	VAL
1	B	48	ARG
1	B	102	ARG
1	B	126	LYS
1	B	131	ASN
1	B	134	HIS
1	B	158	LYS
1	B	198	GLU
1	B	235	GLU
1	B	248	LYS
1	B	277	ASN
1	B	279	ARG
1	B	285	GLN
1	B	307	THR
1	B	308	ASP
1	B	386	ARG
1	B	432	ASP
1	B	436	ARG
1	C	-1	SER
1	C	5	ARG
1	C	12	LYS
1	C	69	LEU
1	C	105	LEU
1	C	131	ASN
1	C	134	HIS
1	C	158	LYS
1	C	198	GLU
1	C	235	GLU
1	C	272	GLU
1	C	305	ASP
1	C	307	THR
1	C	308	ASP
1	C	351	LEU
1	C	372	SER
1	C	386	ARG
1	C	397	ILE
1	C	408	ARG

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Mol	Chain	Res	Type
1	C	421	SER
1	C	436	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	134	HIS
1	A	249	GLN
1	A	277	ASN
1	A	300	ASN
1	A	335	ASN
1	A	366	GLN
1	B	0	HIS
1	B	131	ASN
1	B	134	HIS
1	B	277	ASN
1	B	300	ASN
1	C	131	ASN
1	C	134	HIS
1	C	300	ASN
1	C	402	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)

Of 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	ATP	C	441	2	26,33,33	1.07	1 (3%)	31,52,52	1.41	5 (16%)
3	ATP	A	442	2	26,33,33	1.24	3 (11%)	31,52,52	1.41	7 (22%)
3	ATP	B	442	2	26,33,33	1.19	3 (11%)	31,52,52	1.36	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
3	ATP	C	441	2	-	4/18/38/38	0/3/3/3
3	ATP	A	442	2	-	6/18/38/38	0/3/3/3
3	ATP	B	442	2	-	5/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	442	ATP	O4'-C1'	3.38	1.45	1.41
3	B	442	ATP	C5-C4	3.14	1.49	1.40
3	C	441	ATP	C5-C4	2.66	1.48	1.40
3	A	442	ATP	C2-N3	2.61	1.36	1.32
3	B	442	ATP	O4'-C1'	2.60	1.44	1.41
3	A	442	ATP	C5-C4	2.44	1.47	1.40
3	B	442	ATP	C2-N3	2.03	1.35	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	441	ATP	N3-C2-N1	-3.47	123.26	128.68
3	A	442	ATP	N3-C2-N1	-3.26	123.59	128.68
3	B	442	ATP	C3'-C2'-C1'	2.68	105.01	100.98
3	A	442	ATP	C4-C5-N7	-2.53	106.76	109.40
3	C	441	ATP	PB-O3B-PG	-2.42	124.51	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	442	ATP	C4-C5-N7	-2.31	106.99	109.40
3	A	442	ATP	O3B-PG-O1G	-2.30	98.44	111.19
3	B	442	ATP	N3-C2-N1	-2.25	125.17	128.68
3	B	442	ATP	O3G-PG-O1G	2.17	119.19	110.68
3	C	441	ATP	C3'-C2'-C1'	2.15	104.21	100.98
3	A	442	ATP	O3G-PG-O1G	2.13	119.02	110.68
3	A	442	ATP	C3'-C2'-C1'	2.08	104.11	100.98
3	A	442	ATP	PA-O3A-PB	-2.06	125.75	132.83
3	C	441	ATP	PA-O3A-PB	-2.05	125.80	132.83
3	B	442	ATP	PB-O3B-PG	-2.03	125.86	132.83
3	C	441	ATP	O3B-PG-O1G	-2.01	100.04	111.19
3	A	442	ATP	PB-O3B-PG	-2.00	125.96	132.83

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	442	ATP	C5'-O5'-PA-O2A
3	C	441	ATP	C5'-O5'-PA-O2A
3	B	442	ATP	O4'-C4'-C5'-O5'
3	A	442	ATP	C5'-O5'-PA-O3A
3	B	442	ATP	C5'-O5'-PA-O3A
3	C	441	ATP	C5'-O5'-PA-O3A
3	A	442	ATP	O4'-C4'-C5'-O5'
3	A	442	ATP	C5'-O5'-PA-O2A
3	C	441	ATP	C5'-O5'-PA-O1A
3	A	442	ATP	PB-O3B-PG-O1G
3	B	442	ATP	C4'-C5'-O5'-PA
3	A	442	ATP	C3'-C4'-C5'-O5'
3	C	441	ATP	C4'-C5'-O5'-PA
3	A	442	ATP	C5'-O5'-PA-O1A
3	B	442	ATP	C5'-O5'-PA-O1A

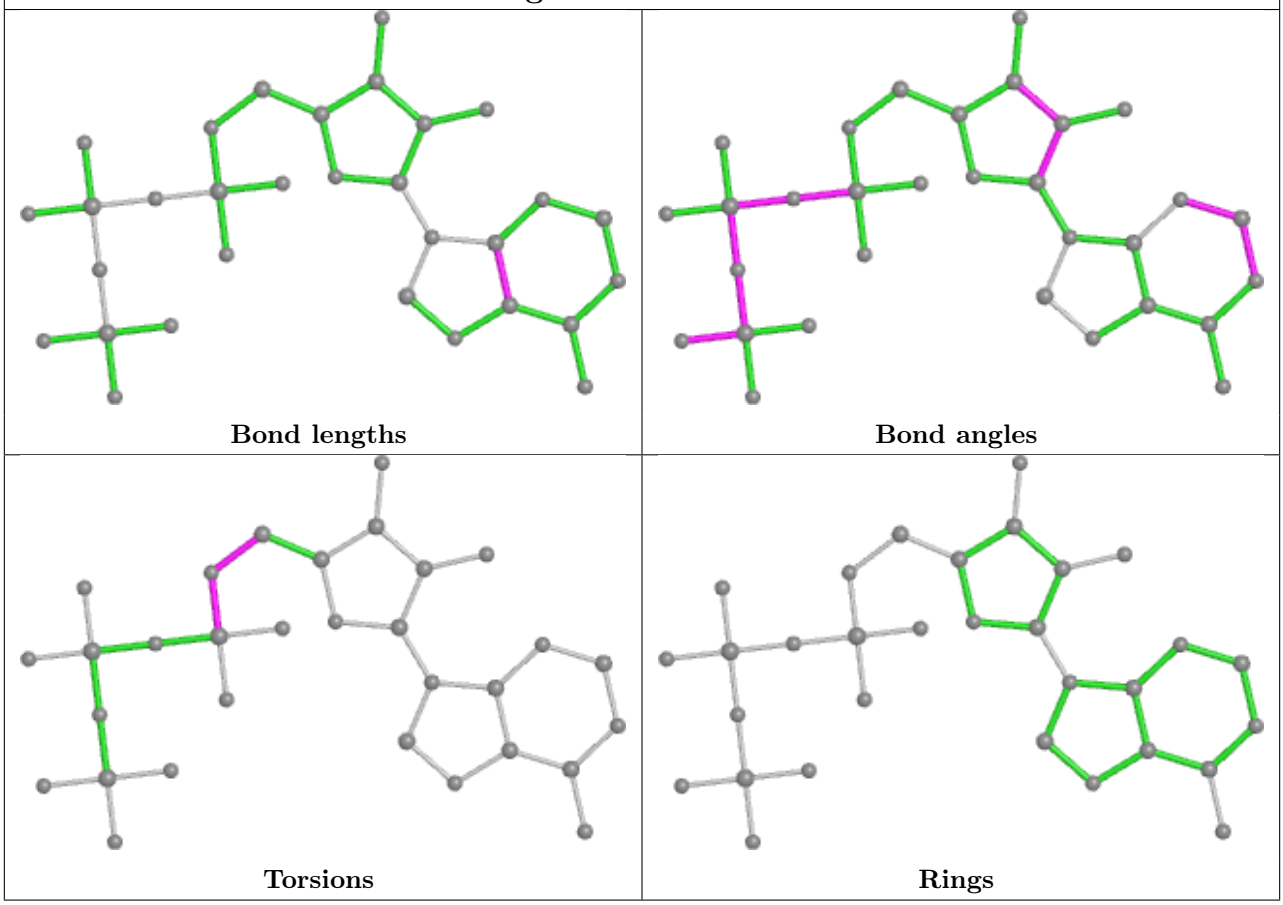
There are no ring outliers.

No monomer is involved in short contacts.

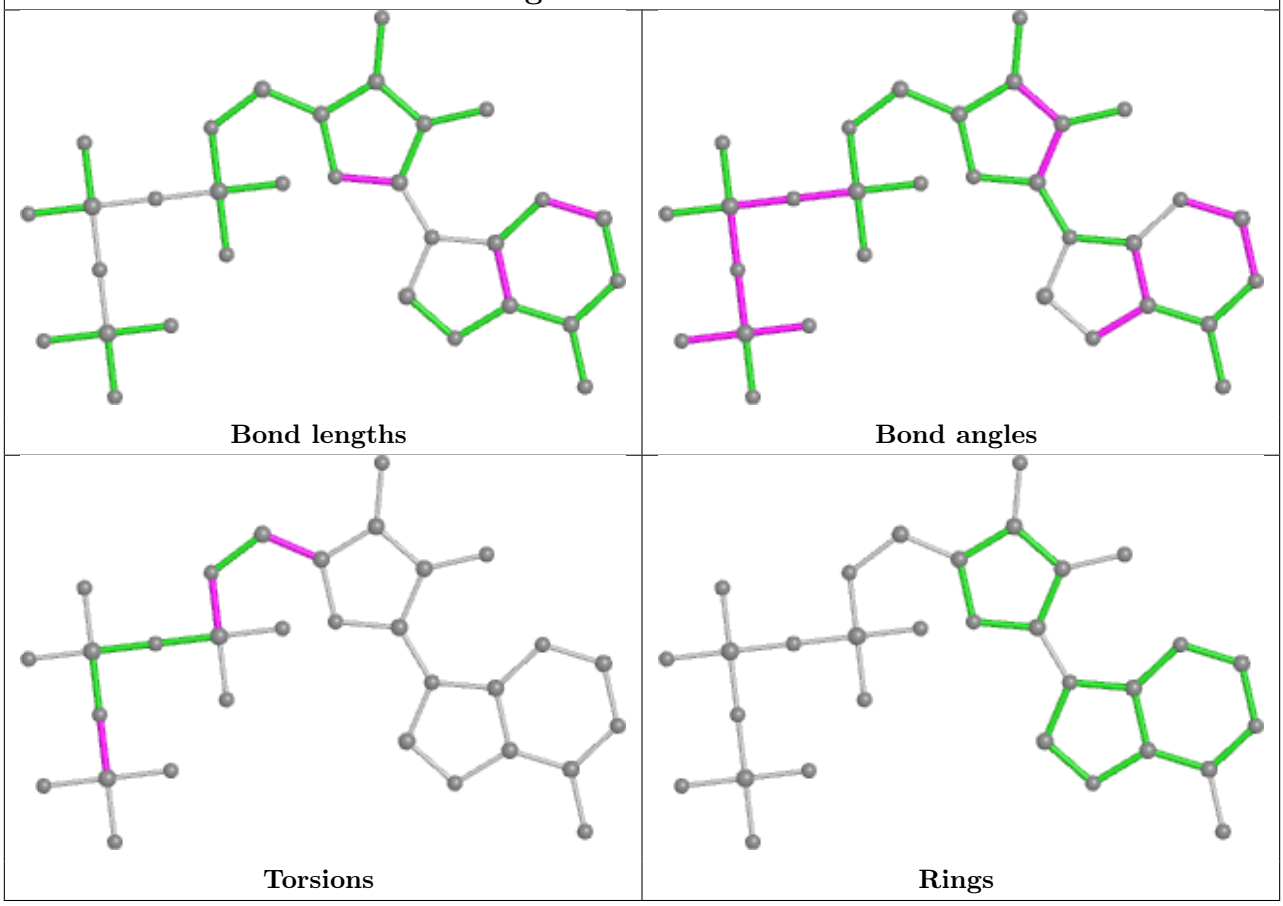
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

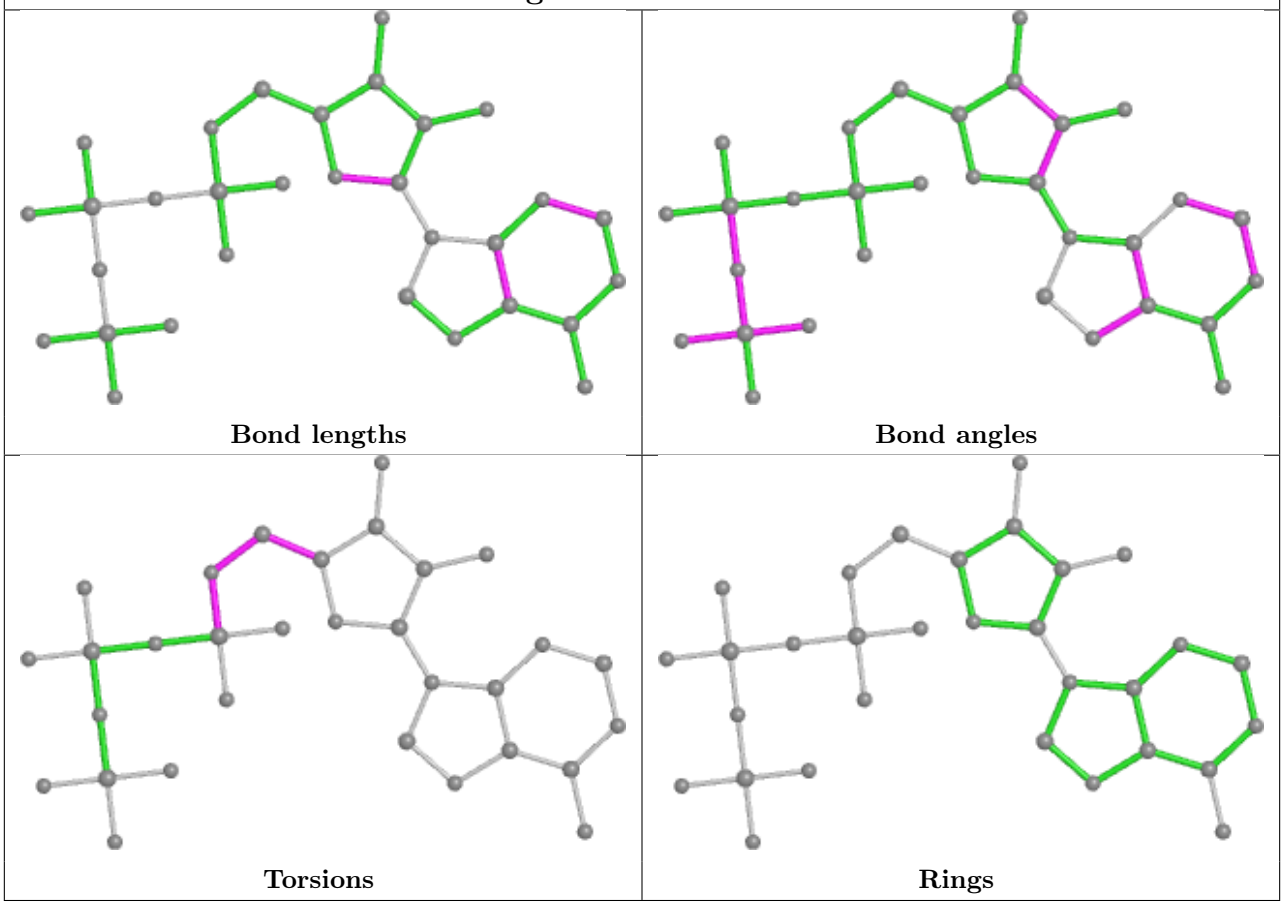
Ligand ATP C 441



Ligand ATP A 442



Ligand ATP B 442



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	441/458 (96%)	-0.13	14 (3%)	47	46	22, 37, 56, 70	0
1	B	441/458 (96%)	-0.21	10 (2%)	60	58	22, 35, 60, 73	0
1	C	441/458 (96%)	-0.39	5 (1%)	80	79	18, 32, 57, 66	0
All	All	1323/1374 (96%)	-0.25	29 (2%)	62	60	18, 35, 58, 73	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	ILE	4.1
1	B	-2	GLY	3.9
1	B	411	ALA	3.9
1	A	350	ILE	3.8
1	A	411	ALA	3.7
1	B	403	ILE	3.6
1	B	202	ILE	3.3
1	A	304	PRO	3.2
1	B	384	ASP	3.0
1	B	350	ILE	3.0
1	B	216	THR	2.9
1	A	201	PRO	2.8
1	A	356	GLY	2.7
1	A	384	ASP	2.6
1	A	403	ILE	2.6
1	B	201	PRO	2.5
1	B	356	GLY	2.5
1	C	386	ARG	2.4
1	B	373	ALA	2.3
1	A	-2	GLY	2.3
1	C	307	THR	2.3
1	C	373	ALA	2.2
1	C	-1	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLU	2.2
1	A	438	THR	2.1
1	A	268	SER	2.1
1	A	305	ASP	2.1
1	A	436	ARG	2.0
1	C	248	LYS	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)

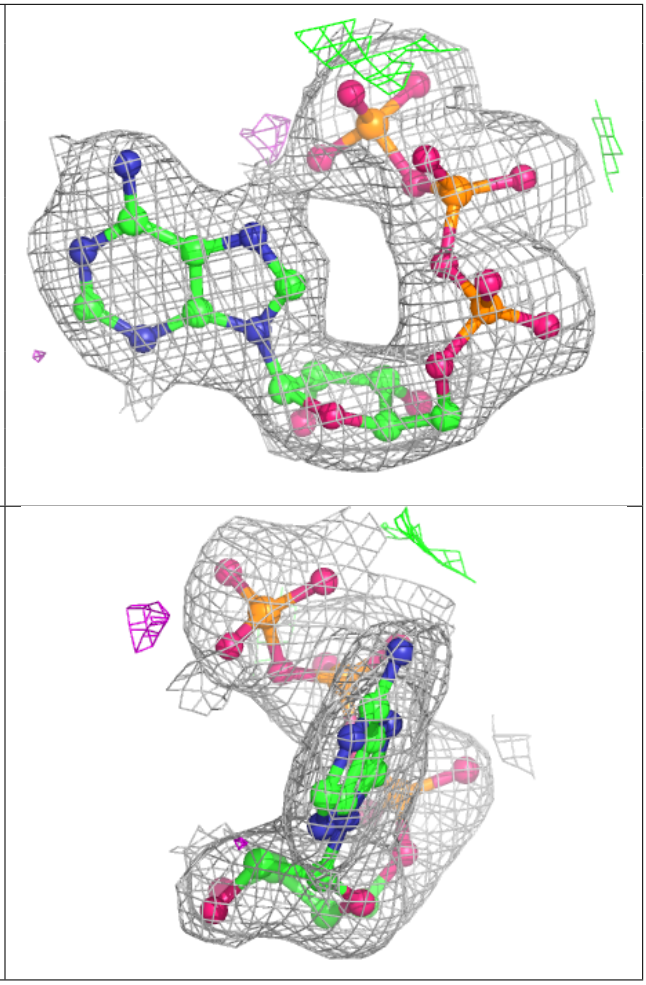
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	A	441	1/1	0.82	0.10	48,48,48,48	0
2	MG	A	439	1/1	0.86	0.19	38,38,38,38	0
2	MG	B	441	1/1	0.86	0.11	39,39,39,39	0
2	MG	B	440	1/1	0.87	0.12	45,45,45,45	0
2	MG	C	440	1/1	0.88	0.10	36,36,36,36	0
2	MG	A	440	1/1	0.90	0.11	48,48,48,48	0
2	MG	C	439	1/1	0.97	0.20	38,38,38,38	0
2	MG	B	439	1/1	0.97	0.07	38,38,38,38	0
3	ATP	A	442	31/31	0.97	0.10	22,29,40,42	0
3	ATP	B	442	31/31	0.98	0.09	21,25,33,35	0
3	ATP	C	441	31/31	0.98	0.09	24,27,34,36	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.

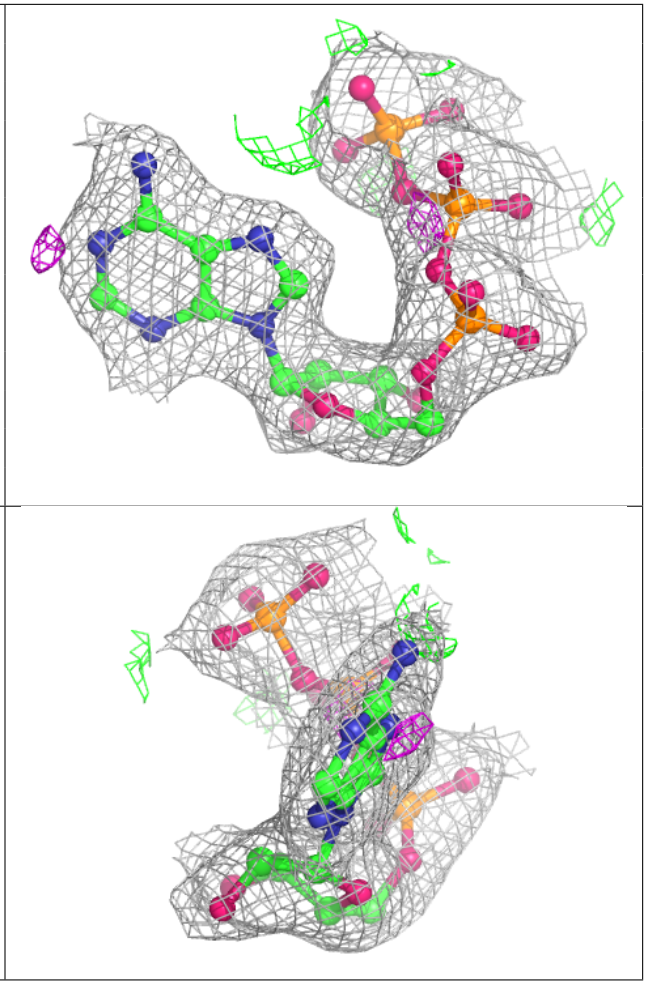
Electron density around ATP A 442:

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



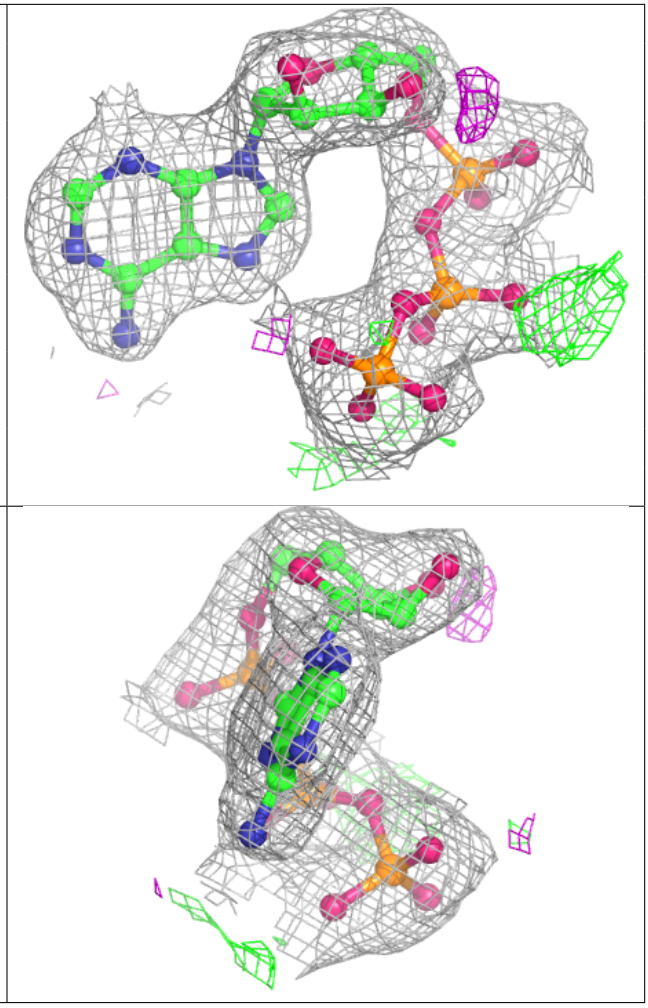
Electron density around ATP B 442:

$2mF_o$-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 C 441:

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.