Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 10:25 am GMT

PDB ID	:	2J3M
Title	:	PROLYL-TRNA SYNTHETASE FROM ENTEROCOCCUS FAECALIS COMPLEXED WITH ATP, manganese and prolinol
Authors	:	Crepin, T.; Yaremchuk, A.; Tukalo, M.; Cusack, S.
Deposited on	:	2006-08-22
Resolution	:	2.30 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:

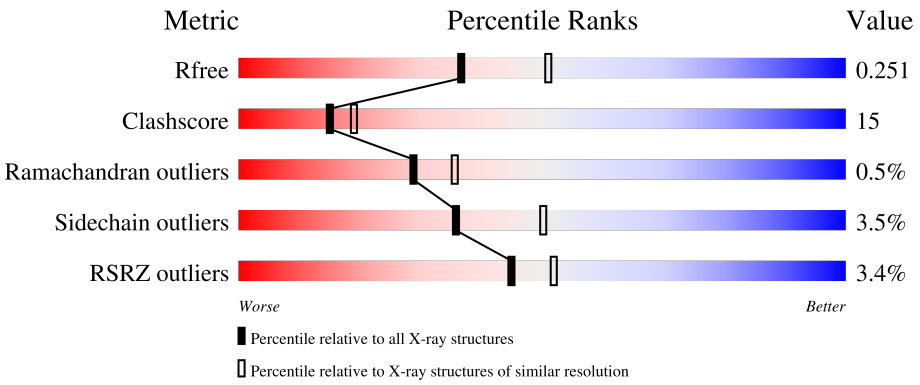
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	572	2% 65% 29%
1	B	572	5% 66% 30%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PRI	B	1566	-	-	X	-

2 Entry composition (i)

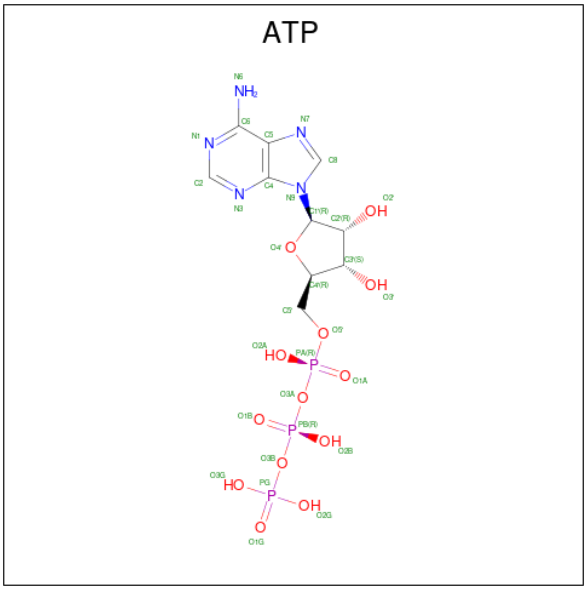
There are 5 unique types of molecules in this entry. The entry contains 9247 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROLYL-TRNA SYNTHETASE.

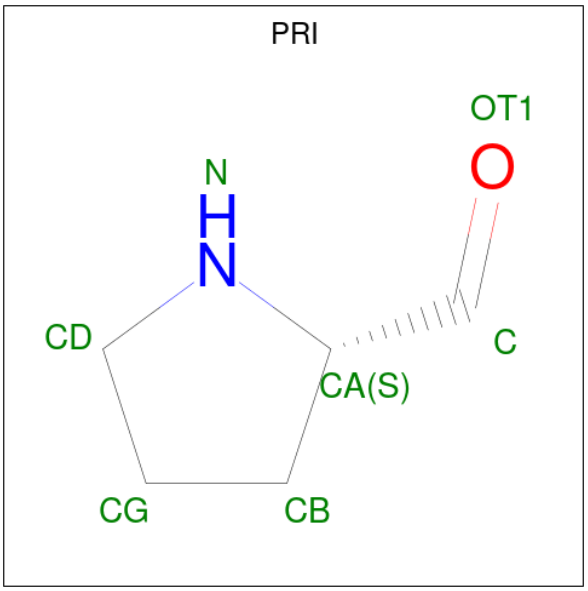
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	554	4396	2772	742	862	20	0	1	0
1	B	558	4406	2775	745	865	21	0	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 3 is PYRROLIDINE-2-CARBALDEHYDE (three-letter code: PRI) (formula: C_5H_9NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	7	5	1	1	0	0
3	B	1	7	5	1	1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	2	2	2	0	0
4	B	4	4	4	0	0

- Molecule 5 is water.

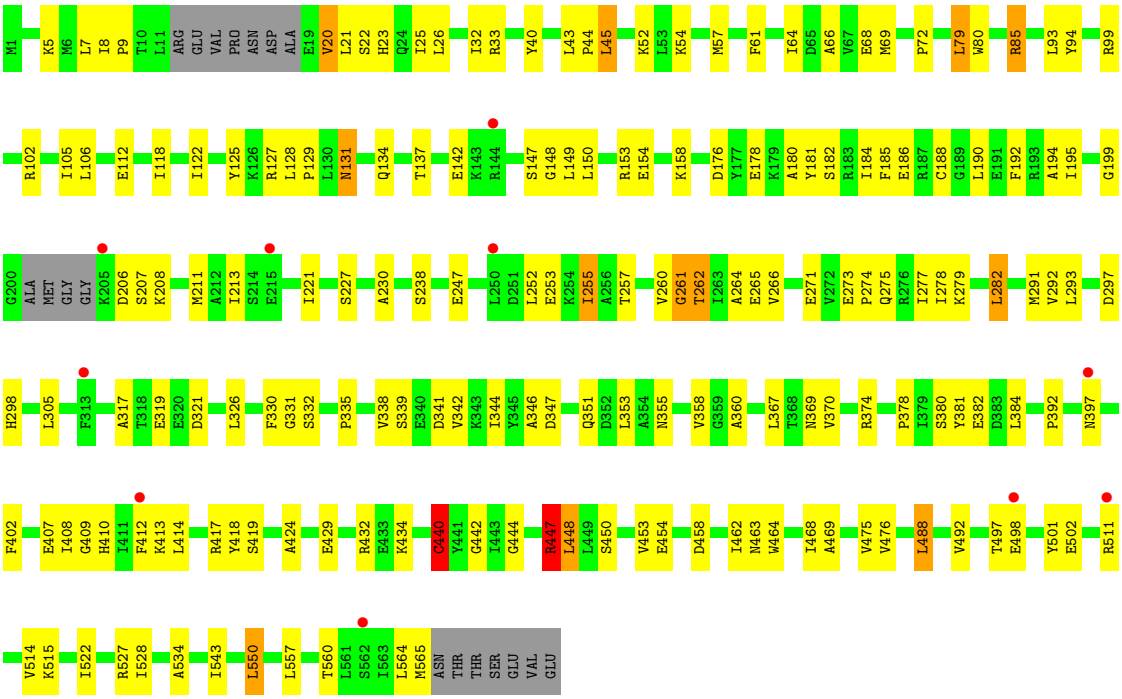
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	201	201	201	0	0
5	B	162	162	162	0	0

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.

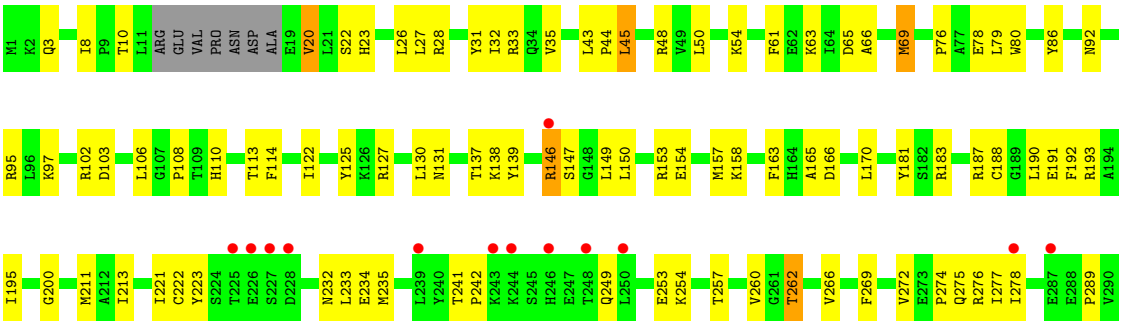
• Molecule 1: PROLYL-TRNA SYNTHETASE

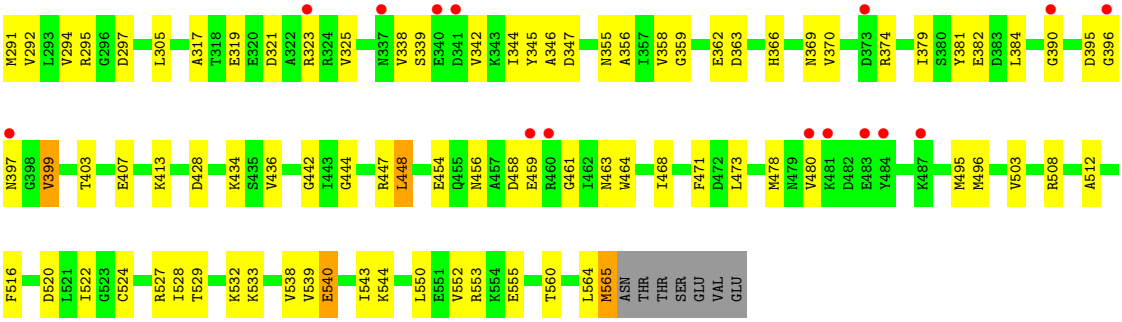
Chain A: 2% 65% 29%



• Molecule 1: PROLYL-TRNA SYNTHETASE

Chain B: 5% 66% 30%




M291 V292 L293 V294 R295 G296 D297 L305 A317 T318 E319 E320 D321 A322 R323 R324 V325 N337 V338 S339 E340 D341 V342 K343 I344 Y345 A346 D347 N355 A356 I357 V358 G359 E362 D363 H366 N369 V370 D373 R374 I379 S380 Y381 E382 D383 L384 G390 D395 G396
N397 G398 V399 T403 E407 K413 D428 K434 S435 V436 G442 I443 G444 R447 L448 E454 Q455 N456 A457 D458 E459 R460 G461 I462 N463 W464 I468 F471 D472 L473 M478 N479 V480 K481 D482 E483 Y484 K487 M495 M496 V503 R508 A512
F516 D520 L521 I522 G523 C524 R527 I528 T529 K532 K533 V538 V539 E540 I543 K544 L550 E551 V552 R553 K554 E555 T560 L564 M565 ASN THR THR SER GLU VAL GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.58Å 92.68Å 101.22Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	29.49 – 2.30 29.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.49-2.30) 100.0 (29.44-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.260 0.190 , 0.251	Depositor DCC
R_{free} test set	1894 reflections (3.50%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 34.9	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	0.94	EDS
Total number of atoms	9247	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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, PRI, MN

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	0.81	2/4468 (0.0%)	0.84	3/6027 (0.0%)
1	B	0.77	2/4478 (0.0%)	0.81	1/6041 (0.0%)
All	All	0.79	4/8946 (0.0%)	0.83	4/12068 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	CYS	CB-SG	-5.64	1.72	1.81
1	B	407	GLU	CG-CD	-5.39	1.43	1.51
1	B	540	GLU	CG-CD	5.13	1.59	1.51
1	A	271	GLU	CG-CD	5.05	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	447	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	85	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	130	LEU	CB-CG-CD1	-5.07	102.38	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	4396	0	4350	136	2
1	B	4406	0	4363	135	1
2	A	31	0	12	2	0
2	B	31	0	12	5	0
3	A	7	0	9	2	0
3	B	7	0	9	7	0
4	A	2	0	0	0	0
4	B	4	0	0	0	0
5	A	201	0	0	7	0
5	B	162	0	0	4	0
All	All	9247	0	8755	267	2

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 15.

All (267) 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:146:ARG:H	1:B:146:ARG:HD2	1.05	1.12
1:A:543:ILE:HD12	1:A:565:MET:HE1	1.44	0.95
1:A:25:ILE:HD13	1:A:462:ILE:HG12	1.50	0.93
1:B:146:ARG:HD2	1:B:146:ARG:N	1.84	0.92
1:A:255:ILE:HB	5:A:2101:HOH:O	1.74	0.85
1:B:165:ALA:O	1:B:434:LYS:HE2	1.80	0.81
1:A:44:PRO:HD3	1:B:69:MET:HG3	1.64	0.80
1:B:193:ARG:HG3	1:B:213:ILE:HD11	1.66	0.78
1:B:235:MET:HE2	5:B:2077:HOH:O	1.85	0.77
1:A:85:ARG:HD3	1:A:112:GLU:OE2	1.86	0.76
1:B:235:MET:CE	5:B:2077:HOH:O	2.34	0.75
1:B:442:GLY:CA	3:B:1566:PRI:HCG1	2.16	0.75
1:A:25:ILE:HD13	1:A:462:ILE:CG1	2.17	0.75
1:B:61:PHE:CE2	1:B:158:LYS:HD2	2.22	0.75
1:B:78:GLU:OE1	1:B:102:ARG:NH2	2.19	0.74
1:B:20:VAL:HG13	1:B:454:GLU:OE1	1.87	0.74
1:A:206:ASP:HB2	1:A:413:LYS:HD2	1.70	0.73
1:A:5:LYS:HG2	1:B:65:ASP:HB3	1.71	0.72
1:B:550:LEU:HD21	1:B:564:LEU:HD11	1.71	0.71
1:B:275:GLN:HG3	1:B:295:ARG:HH11	1.55	0.70
1:A:85:ARG:HD2	1:A:418:TYR:HE1	1.55	0.70
1:A:412[B]:PHE:CD2	1:A:414:LEU:HD23	2.26	0.70
1:A:207:SER:HG	1:A:410:HIS:HE2	1.38	0.68
1:A:458:ASP:HB2	1:A:463:ASN:ND2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ARG:O	1:B:187:ARG:HG3	1.94	0.67
1:A:488:LEU:HD12	1:A:534:ALA:HA	1.77	0.67
1:B:442:GLY:HA3	3:B:1566:PRI:HCG1	1.78	0.65
1:A:61:PHE:HB3	1:A:66:ALA:HB3	1.77	0.65
1:B:26:LEU:HB3	1:B:32:ILE:HG12	1.77	0.65
1:B:295:ARG:HD2	1:B:297:ASP:OD1	1.96	0.65
1:B:257:THR:HB	1:B:260:VAL:HB	1.78	0.65
1:B:540:GLU:HG3	5:B:2151:HOH:O	1.98	0.63
1:B:565:MET:HA	1:B:565:MET:HE2	1.80	0.63
1:B:323:ARG:NH1	1:B:363:ASP:OD2	2.24	0.63
1:A:238:SER:HB2	1:A:392:PRO:O	2.00	0.62
1:A:412[A]:PHE:CE1	3:A:1566:PRI:HCA	2.36	0.61
1:B:163:PHE:HB3	1:B:436:VAL:HG11	1.81	0.61
1:A:414:LEU:HD11	1:A:440:CYS:HB3	1.81	0.61
1:A:199:GLY:HA3	1:A:412[B]:PHE:CE1	2.36	0.61
1:A:292:VAL:HG21	1:A:305:LEU:HD22	1.83	0.61
1:B:222:CYS:SG	1:B:233:LEU:HA	2.41	0.61
1:A:25:ILE:HD11	1:A:453:VAL:HG11	1.83	0.60
1:A:85:ARG:NH2	5:A:2030:HOH:O	2.34	0.60
1:A:247:GLU:OE2	1:A:355:ASN:ND2	2.24	0.60
1:B:63:LYS:HZ3	1:B:183:ARG:NH2	1.99	0.60
1:B:157:MET:SD	3:B:1566:PRI:HCG2	2.42	0.60
1:A:262:THR:O	1:A:266:VAL:HG23	2.02	0.59
1:B:317:ALA:HB1	1:B:321:ASP:HB2	1.83	0.59
1:A:44:PRO:CD	1:B:69:MET:HG3	2.32	0.59
1:B:291:MET:HB3	1:B:344:ILE:HG12	1.83	0.59
1:A:511:ARG:HE	1:A:514:VAL:HG23	1.66	0.59
1:A:25:ILE:CG1	1:A:453:VAL:HG11	2.32	0.59
1:A:458:ASP:HB2	1:A:463:ASN:HD21	1.66	0.59
1:A:54:LYS:HA	1:A:57:MET:HE3	1.85	0.59
1:B:565:MET:HA	1:B:565:MET:CE	2.33	0.59
1:A:279:LYS:NZ	1:A:298:HIS:O	2.26	0.58
1:A:192:PHE:HA	1:A:211:MET:O	2.03	0.58
1:A:32:ILE:HD13	1:A:149:LEU:HD13	1.86	0.58
1:B:442:GLY:HA3	3:B:1566:PRI:CG	2.33	0.58
1:A:118:ILE:HD12	1:A:122:ILE:HD13	1.85	0.58
1:A:252:LEU:HD21	1:A:367:LEU:HD22	1.84	0.58
1:B:232:ASN:OD1	1:B:234:GLU:HG3	2.04	0.58
1:A:194:ALA:HB1	1:A:208:LYS:HE3	1.84	0.58
1:B:61:PHE:HB3	1:B:66:ALA:HB3	1.86	0.57
1:B:294:VAL:HG12	1:B:347:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:NH2	2:A:701:ATP:O3G	2.30	0.56
1:B:44:PRO:O	1:B:48:ARG:HG3	2.05	0.56
1:A:262:THR:HG22	1:A:265:GLU:H	1.69	0.56
1:A:227:SER:HB3	1:A:397:ASN:HB2	1.87	0.56
1:A:262:THR:HG23	5:A:2105:HOH:O	2.05	0.56
1:B:211:MET:CB	1:B:221:ILE:HD11	2.35	0.56
1:A:358:VAL:HG22	1:A:370:VAL:HG21	1.88	0.56
1:B:146:ARG:H	1:B:146:ARG:CD	1.93	0.56
1:B:278:ILE:HB	1:B:358:VAL:HG12	1.88	0.56
1:B:358:VAL:HG22	1:B:370:VAL:HG21	1.88	0.55
1:B:456:ASN:HB3	1:B:463:ASN:O	2.07	0.55
1:B:442:GLY:N	3:B:1566:PRI:HCG1	2.21	0.55
1:B:464:TRP:CE3	1:B:468:ILE:HG22	2.41	0.55
1:A:195:ILE:HG22	1:A:230:ALA:HB1	1.88	0.55
1:B:471:PHE:HB2	1:B:524:CYS:SG	2.47	0.55
1:A:106:LEU:HD11	1:B:106:LEU:HD21	1.88	0.54
1:A:158:LYS:NZ	1:A:181:TYR:OH	2.40	0.54
1:A:543:ILE:HD12	1:A:565:MET:CE	2.28	0.54
1:A:25:ILE:HG12	1:A:453:VAL:CG1	2.38	0.54
1:A:85:ARG:HD2	1:A:418:TYR:CE1	2.39	0.54
1:A:23:HIS:CD2	1:A:32:ILE:HD11	2.43	0.54
1:B:22:SER:HB3	1:B:454:GLU:HG2	1.90	0.54
1:B:158:LYS:O	1:B:442:GLY:HA2	2.07	0.54
1:B:195:ILE:HD12	1:B:232:ASN:N	2.23	0.54
1:B:319:GLU:O	1:B:323:ARG:HG2	2.08	0.53
1:A:43:LEU:HB3	1:A:44:PRO:HD2	1.90	0.53
1:B:63:LYS:NZ	1:B:183:ARG:NH2	2.56	0.53
1:A:125:TYR:CE1	1:A:429:GLU:HG3	2.44	0.53
1:B:63:LYS:HZ3	1:B:183:ARG:HH21	1.57	0.53
1:B:86:TYR:O	1:B:95:ARG:NH2	2.42	0.53
1:B:338:VAL:CG1	1:B:342:VAL:HB	2.40	0.52
1:A:475:VAL:HA	1:A:528:ILE:O	2.10	0.52
1:B:33:ARG:HG2	1:B:43:LEU:HD11	1.91	0.52
1:B:395:ASP:C	1:B:397:ASN:H	2.13	0.52
1:A:412[B]:PHE:CE2	1:A:414:LEU:HD23	2.45	0.52
1:B:254:LYS:NZ	1:B:362:GLU:OE1	2.39	0.52
1:A:23:HIS:HD2	5:A:2060:HOH:O	1.93	0.52
1:A:407:GLU:HB3	1:A:447:ARG:HH21	1.76	0.51
1:B:260:VAL:HG21	1:B:269:PHE:CD1	2.46	0.51
1:B:276:ARG:O	1:B:356:ALA:HA	2.11	0.51
1:B:552:VAL:HG12	1:B:553:ARG:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:NZ	1:B:181:TYR:OH	2.44	0.51
1:A:178:GLU:OE1	1:A:208:LYS:HE2	2.11	0.50
1:A:5:LYS:HG2	1:B:65:ASP:CB	2.41	0.50
1:A:25:ILE:CD1	1:A:453:VAL:HG11	2.41	0.50
1:B:262:THR:O	1:B:266:VAL:HG23	2.11	0.50
1:B:358:VAL:HG23	1:B:359:GLY:O	2.11	0.50
1:A:282:LEU:HG	1:A:326:LEU:HD11	1.93	0.50
1:B:43:LEU:HB3	1:B:44:PRO:HD2	1.92	0.50
1:B:97:LYS:HE3	1:B:103:ASP:OD1	2.11	0.50
1:B:272:VAL:HG11	1:B:276:ARG:HD2	1.93	0.50
1:A:137:THR:CG2	1:A:154:GLU:HG3	2.42	0.50
1:B:76:PRO:HB2	1:B:78:GLU:OE2	2.11	0.50
1:A:282:LEU:HD13	1:A:317:ALA:CB	2.42	0.50
1:A:25:ILE:HD11	1:A:453:VAL:CG1	2.42	0.49
1:B:114:PHE:HB3	1:B:163:PHE:HZ	1.77	0.49
1:A:25:ILE:CD1	1:A:462:ILE:HG12	2.34	0.49
1:A:378:PRO:HG2	1:A:381:TYR:CZ	2.48	0.49
1:B:63:LYS:NZ	1:B:183:ARG:HH21	2.11	0.49
1:B:292:VAL:HG21	1:B:305:LEU:HD22	1.94	0.49
1:A:43:LEU:HB3	1:A:44:PRO:CD	2.42	0.49
1:B:289:PRO:HG3	1:B:325:VAL:HG21	1.95	0.49
1:A:21:LEU:O	1:A:25:ILE:HG23	2.13	0.49
1:A:560:THR:O	1:A:564:LEU:HG	2.13	0.49
1:B:529:THR:HB	1:B:540:GLU:HB3	1.95	0.49
1:B:188:CYS:HA	1:B:468:ILE:CD1	2.43	0.48
1:A:69:MET:CG	1:B:44:PRO:HD3	2.43	0.48
1:A:347:ASP:HA	1:A:382:GLU:O	2.13	0.48
1:B:339:SER:HB2	1:B:342:VAL:HG23	1.95	0.48
1:A:122:ILE:HG23	1:A:127:ARG:HB2	1.94	0.48
1:A:207:SER:OG	1:A:410:HIS:NE2	2.33	0.48
2:B:701:ATP:C5'	3:B:1566:PRI:HCB1	2.42	0.48
1:B:195:ILE:HD13	1:B:221:ILE:HG12	1.96	0.48
1:A:261:GLY:HA2	1:A:331:GLY:O	2.13	0.48
1:A:412[B]:PHE:CD2	1:A:414:LEU:CD2	2.96	0.48
1:B:382:GLU:HB2	1:B:384:LEU:HG	1.96	0.48
1:A:147:SER:HB2	1:A:150:LEU:HB2	1.95	0.48
1:B:10:THR:HA	1:B:28:ARG:O	2.14	0.48
1:B:8:ILE:HG22	1:B:10:THR:HG23	1.95	0.48
1:B:190:LEU:HD11	1:B:448:LEU:CD2	2.44	0.48
1:A:64:ILE:HB	1:A:176:ASP:HB3	1.96	0.47
1:A:182:SER:O	1:A:186:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PHE:HA	1:B:211:MET:O	2.14	0.47
1:A:274:PRO:HA	1:A:277:ILE:HD12	1.97	0.47
1:A:94:TYR:HB2	1:A:106:LEU:HB2	1.97	0.47
1:A:297:ASP:OD1	1:A:297:ASP:N	2.43	0.47
2:B:701:ATP:H5'1	3:B:1566:PRI:HCB1	1.96	0.47
1:A:257:THR:HB	1:A:260:VAL:HB	1.97	0.47
1:A:278:ILE:HB	1:A:358:VAL:HG12	1.96	0.47
1:A:440:CYS:SG	3:A:1566:PRI:N	2.88	0.47
1:B:170:LEU:HD21	1:B:413:LYS:HB3	1.97	0.47
1:B:50:LEU:O	1:B:54:LYS:HG3	2.15	0.47
1:B:80:TRP:CH2	1:B:108:PRO:HG2	2.50	0.47
1:B:122:ILE:HD12	1:B:127:ARG:HB3	1.97	0.46
1:A:319:GLU:OE2	1:A:330:PHE:N	2.48	0.46
1:A:68:GLU:O	1:B:44:PRO:HA	2.14	0.46
1:A:61:PHE:CE2	1:A:158:LYS:HD2	2.50	0.46
1:A:380:SER:OG	1:A:382:GLU:OE2	2.29	0.46
1:A:25:ILE:HG12	1:A:453:VAL:HG11	1.97	0.46
1:A:351:GLN:HB2	1:A:381:TYR:CD2	2.50	0.46
1:B:45:LEU:HD21	1:B:522:ILE:HG12	1.96	0.46
1:A:79:LEU:HB3	1:A:80:TRP:HD1	1.80	0.46
2:B:701:ATP:H3'	2:B:701:ATP:O3A	2.15	0.46
1:B:249:GLN:OE1	1:B:374:ARG:HD3	2.15	0.46
1:B:495:MET:HG2	1:B:496:MET:CE	2.45	0.46
1:B:260:VAL:O	5:B:2099:HOH:O	2.21	0.46
1:A:8:ILE:HG23	1:A:45:LEU:HD22	1.97	0.46
1:B:317:ALA:HB1	1:B:321:ASP:CB	2.46	0.46
1:A:382:GLU:HB2	1:A:384:LEU:HG	1.98	0.45
1:B:395:ASP:O	1:B:397:ASN:N	2.49	0.45
1:A:476:VAL:HG13	1:A:515:LYS:HB3	1.97	0.45
1:B:61:PHE:HE2	1:B:158:LYS:HD2	1.77	0.45
1:B:223:TYR:HE2	1:B:403:THR:HG23	1.80	0.45
1:A:291:MET:HB3	1:A:344:ILE:HG12	1.98	0.45
1:B:146:ARG:N	1:B:146:ARG:CD	2.63	0.45
1:B:346:ALA:HB3	1:B:381:TYR:CD2	2.52	0.45
1:A:26:LEU:HB3	1:A:32:ILE:HG12	1.99	0.45
1:A:253:GLU:O	1:A:367:LEU:HA	2.16	0.45
1:B:61:PHE:CZ	1:B:158:LYS:HD2	2.50	0.45
1:A:488:LEU:HD22	1:A:492:VAL:HG23	1.98	0.45
1:A:20:VAL:HB	5:A:2057:HOH:O	2.16	0.45
1:B:23:HIS:CD2	1:B:32:ILE:HD11	2.51	0.45
1:A:409:GLY:HA2	1:A:442:GLY:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:NH2	1:B:459:GLU:O	2.30	0.44
1:B:191:GLU:HG2	1:B:213:ILE:HD13	1.99	0.44
1:B:272:VAL:CG1	1:B:276:ARG:HD2	2.47	0.44
1:A:462:ILE:HG21	1:A:464:TRP:CE2	2.52	0.44
1:B:211:MET:HB3	1:B:221:ILE:HD11	1.99	0.44
1:A:221:ILE:O	1:A:402:PHE:HA	2.17	0.44
1:A:528:ILE:HD13	1:A:557:LEU:HD21	2.00	0.44
2:B:701:ATP:O3A	2:B:701:ATP:H8	2.01	0.44
1:B:355:ASN:HA	1:B:369:ASN:HA	1.99	0.44
1:A:464:TRP:CD1	1:A:469:ALA:HA	2.53	0.44
1:B:147:SER:HB2	1:B:150:LEU:HB2	2.00	0.44
1:A:262:THR:HG22	1:A:264:ALA:N	2.33	0.43
1:A:93:LEU:HD21	1:A:105:ILE:HG21	1.99	0.43
1:B:480:VAL:HG11	1:B:508:ARG:O	2.17	0.43
1:A:275:GLN:O	1:A:353:LEU:HD21	2.18	0.43
1:B:345:TYR:CE2	1:B:379:ILE:HB	2.54	0.43
1:A:339:SER:HB3	1:A:341:ASP:OD1	2.19	0.43
1:B:478:MET:HE3	1:B:512:ALA:HB2	2.00	0.43
1:A:22:SER:HB3	1:A:454:GLU:HG2	1.99	0.43
1:A:72:PRO:HG3	1:B:35:VAL:HG21	1.99	0.43
1:A:434:LYS:HE3	5:A:2157:HOH:O	2.19	0.43
1:A:346:ALA:HB3	1:A:381:TYR:CD2	2.53	0.43
1:A:45:LEU:HD21	1:A:522:ILE:HG12	2.01	0.43
1:B:223:TYR:CE2	1:B:403:THR:HG23	2.52	0.43
1:B:552:VAL:HG21	1:B:560:THR:HG21	2.01	0.43
1:B:139:TYR:HA	1:B:153:ARG:O	2.19	0.43
1:B:473:LEU:O	1:B:503:VAL:HA	2.18	0.43
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.85	0.42
1:B:26:LEU:O	1:B:31:TYR:HB2	2.18	0.42
1:A:178:GLU:HG3	1:A:208:LYS:HE2	2.00	0.42
1:A:180:ALA:O	1:A:184:ILE:HG13	2.20	0.42
1:B:289:PRO:HB3	1:B:325:VAL:HG11	2.00	0.42
1:B:516:PHE:CD1	1:B:527:ARG:CZ	3.01	0.42
1:A:131:ASN:C	1:A:131:ASN:HD22	2.22	0.42
1:A:444:GLY:O	1:A:448:LEU:HB2	2.20	0.42
1:A:527:ARG:HE	1:A:527:ARG:HB2	1.69	0.42
1:B:110:HIS:HD2	1:B:138:LYS:HE3	1.85	0.42
1:A:293:LEU:HD11	1:A:335:PRO:HB3	2.01	0.42
1:A:497:THR:HA	1:A:501:TYR:O	2.20	0.42
1:A:550:LEU:HD21	1:A:564:LEU:HD11	2.01	0.42
1:B:292:VAL:HA	1:B:345:TYR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLY:HA3	1:B:520:ASP:O	2.20	0.42
1:B:533:LYS:HB3	1:B:538:VAL:HB	2.01	0.42
1:A:498:GLU:HA	5:A:2167:HOH:O	2.19	0.42
1:A:369:ASN:O	1:A:374:ARG:NH2	2.52	0.41
1:A:444:GLY:HA3	2:A:701:ATP:H1'	2.01	0.41
1:B:137:THR:CG2	1:B:154:GLU:HG3	2.50	0.41
1:B:447:ARG:NH1	2:B:701:ATP:H2'	2.35	0.41
1:B:543:ILE:HD13	1:B:564:LEU:HD13	2.02	0.41
1:A:317:ALA:HB1	1:A:321:ASP:HB2	2.01	0.41
1:A:419:SER:HA	1:A:424:ALA:HB3	2.02	0.41
1:B:338:VAL:HG12	1:B:342:VAL:HB	2.02	0.41
1:B:495:MET:HG2	1:B:496:MET:HE2	2.03	0.41
1:B:274:PRO:HA	1:B:277:ILE:HD12	2.02	0.41
1:A:7:LEU:HG	1:A:9:PRO:HD3	2.01	0.41
1:A:185:PHE:CD1	1:A:408:ILE:HD12	2.56	0.41
1:B:528:ILE:HG23	1:B:539:VAL:HB	2.02	0.41
1:A:128:LEU:HB3	1:A:129:PRO:HA	2.03	0.41
1:B:257:THR:OG1	1:B:366:HIS:HD2	2.01	0.41
1:A:142:GLU:H	1:A:153:ARG:HG2	1.86	0.41
1:A:40:TYR:CZ	1:A:148:GLY:HA2	2.56	0.41
1:A:360:ALA:HA	1:A:367:LEU:HG	2.02	0.41
1:A:134:GLN:O	1:A:158:LYS:HA	2.20	0.41
1:A:511:ARG:NE	1:A:514:VAL:HG23	2.32	0.41
1:B:3:GLN:HG3	1:B:8:ILE:HD12	2.03	0.41
1:B:395:ASP:C	1:B:397:ASN:N	2.74	0.41
1:A:355:ASN:HA	1:A:369:ASN:HA	2.03	0.41
1:B:390:GLY:O	1:B:399:VAL:HG22	2.21	0.41
1:B:444:GLY:O	1:B:448:LEU:HB2	2.21	0.41
1:B:125:TYR:HB3	1:B:428:ASP:HA	2.03	0.40
1:A:52:LYS:HZ1	1:A:502:GLU:CD	2.24	0.40
1:A:188:CYS:HA	1:A:468:ILE:CD1	2.52	0.40
1:A:338:VAL:CG1	1:A:342:VAL:HB	2.52	0.40
1:B:32:ILE:HD13	1:B:149:LEU:HD13	2.03	0.40
1:B:478:MET:CE	1:B:512:ALA:HB2	2.51	0.40
1:A:33:ARG:HD3	1:A:33:ARG:HA	1.84	0.40
1:A:149:LEU:HB2	1:A:450:SER:OG	2.21	0.40
1:B:23:HIS:CE1	1:B:27:LEU:HD11	2.57	0.40
1:B:233:LEU:O	1:B:233:LEU:HD12	2.22	0.40

All (2) 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)
1:A:432:ARG:NH2	1:B:200:GLY:O[1_655]	1.91	0.29
1:A:102:ARG:NH1	1:A:273:GLU:OE2[2_655]	2.16	0.04

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	549/572 (96%)	530 (96%)	18 (3%)	1 (0%)	47	58
1	B	554/572 (97%)	524 (95%)	26 (5%)	4 (1%)	22	26
All	All	1103/1144 (96%)	1054 (96%)	44 (4%)	5 (0%)	29	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLY
1	B	242	PRO
1	B	20	VAL
1	B	262	THR
1	A	261	GLY

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	474/487 (97%)	458 (97%)	16 (3%)	37	51
1	B	474/487 (97%)	457 (96%)	17 (4%)	35	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	948/974 (97%)	915 (96%)	33 (4%)	36 50

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	45	LEU
1	A	79	LEU
1	A	131	ASN
1	A	190	LEU
1	A	213	ILE
1	A	255	ILE
1	A	262	THR
1	A	282	LEU
1	A	332	SER
1	A	417	ARG
1	A	440	CYS
1	A	447	ARG
1	A	448	LEU
1	A	488	LEU
1	A	550	LEU
1	B	45	LEU
1	B	69	MET
1	B	79	LEU
1	B	92	ASN
1	B	113	THR
1	B	131	ASN
1	B	146	ARG
1	B	166	ASP
1	B	241	THR
1	B	253	GLU
1	B	399	VAL
1	B	448	LEU
1	B	458	ASP
1	B	532	LYS
1	B	544	LYS
1	B	555	GLU
1	B	565	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	34	GLN
1	A	131	ASN
1	A	337	ASN
1	A	388	GLN
1	A	456	ASN
1	B	23	HIS
1	B	34	GLN
1	B	92	ASN
1	B	131	ASN
1	B	366	HIS
1	B	456	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	PRI	B	1566	-	5,7,7	0.52	0	7,8,8	1.34	0
2	ATP	B	701	4	26,33,33	0.93	0	31,52,52	1.44	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	A	701	4	26,33,33	0.86	1 (3%)	31,52,52	1.60	5 (16%)
3	PRI	A	1566	-	5,7,7	0.88	0	7,8,8	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PRI	B	1566	-	-	0/0/9/9	0/1/1/1
2	ATP	B	701	4	-	5/18/38/38	0/3/3/3
2	ATP	A	701	4	-	3/18/38/38	0/3/3/3
3	PRI	A	1566	-	-	0/0/9/9	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ATP	C5-C4	2.28	1.46	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	ATP	N3-C2-N1	-4.69	121.35	128.68
2	B	701	ATP	N3-C2-N1	-3.67	122.95	128.68
2	A	701	ATP	C2-N1-C6	3.45	124.65	118.75
2	B	701	ATP	C4-C5-N7	-2.84	106.44	109.40
2	A	701	ATP	PB-O3B-PG	-2.51	124.22	132.83
2	B	701	ATP	PB-O3B-PG	-2.44	124.47	132.83
2	A	701	ATP	O2B-PB-O1B	2.14	122.82	112.24
2	B	701	ATP	PA-O3A-PB	-2.13	125.52	132.83
2	B	701	ATP	C3'-C2'-C1'	2.08	104.10	100.98
2	A	701	ATP	O2A-PA-O1A	2.01	122.17	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O1A
2	B	701	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	A	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	C5'-O5'-PA-O2A
2	B	701	ATP	O4'-C4'-C5'-O5'
2	B	701	ATP	C4'-C5'-O5'-PA
2	A	701	ATP	C5'-O5'-PA-O3A

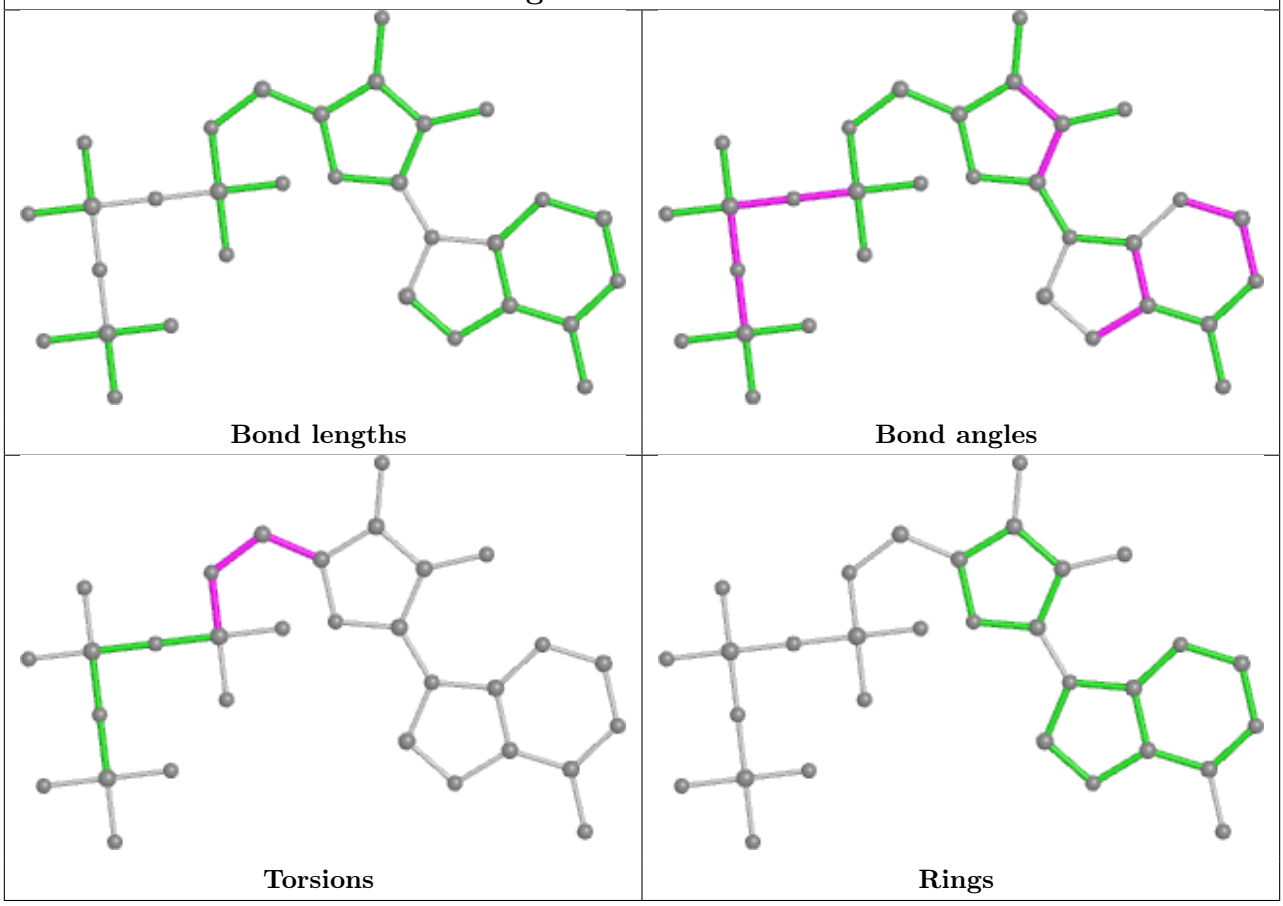
There are no ring outliers.

4 monomers are involved in 14 short contacts:

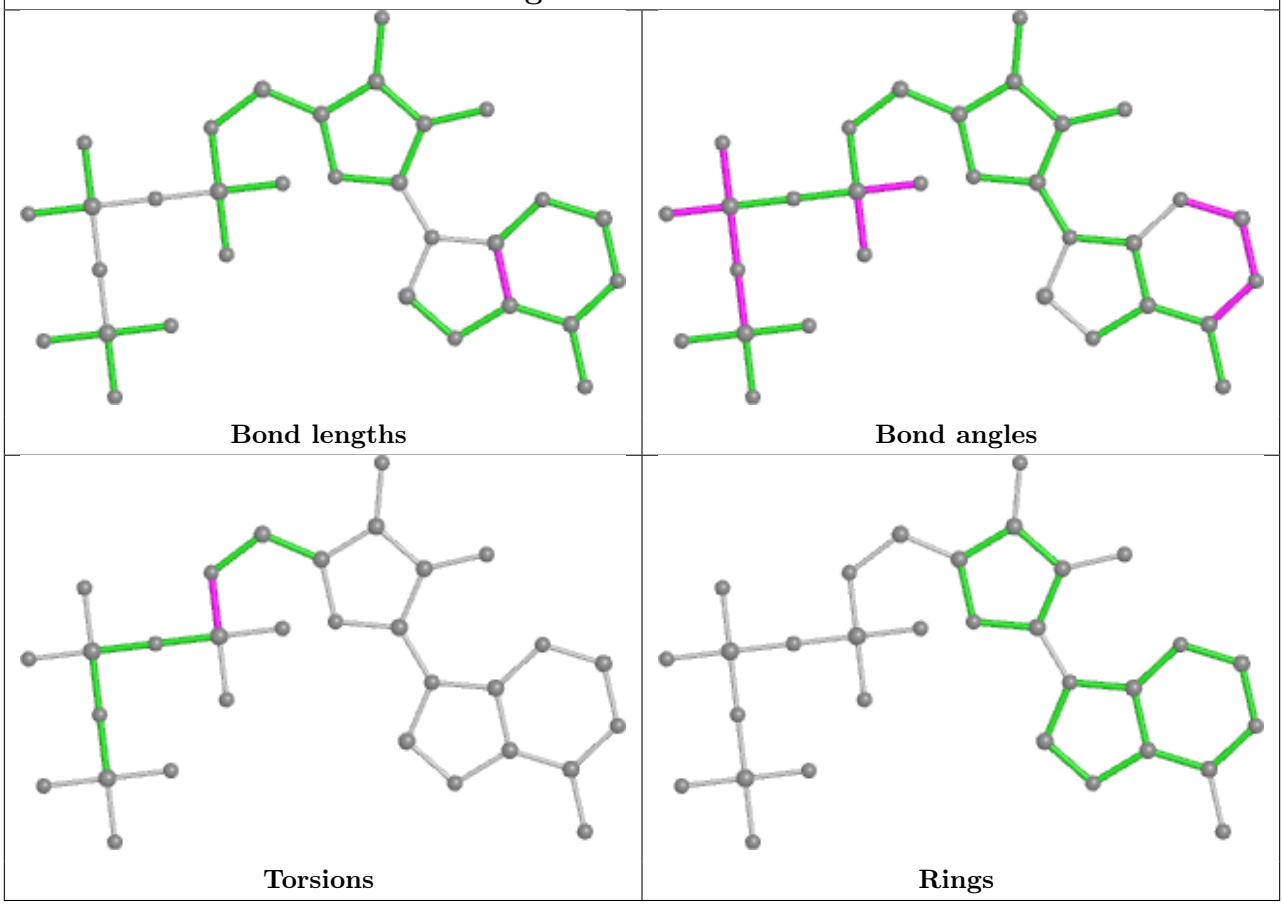
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1566	PRI	7	0
2	B	701	ATP	5	0
2	A	701	ATP	2	0
3	A	1566	PRI	2	0

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 ATP B 701



Ligand ATP A 701



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	554/572 (96%)	0.11	10 (1%)	68	74	7, 19, 30, 40	0
1	B	558/572 (97%)	0.33	28 (5%)	28	35	8, 22, 42, 63	0
All	All	1112/1144 (97%)	0.22	38 (3%)	45	52	7, 21, 37, 63	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	HIS	6.3
1	B	248	THR	4.3
1	B	484	TYR	3.8
1	A	412[A]	PHE	3.5
1	B	244	LYS	3.5
1	B	460	ARG	3.5
1	A	205	LYS	3.3
1	B	243	LYS	3.3
1	A	511	ARG	3.3
1	B	226	GLU	3.2
1	A	313	PHE	3.1
1	B	373	ASP	3.0
1	A	144	ARG	3.0
1	B	459	GLU	2.9
1	B	397	ASN	2.8
1	A	498	GLU	2.8
1	B	340	GLU	2.8
1	B	481	LYS	2.7
1	B	487	LYS	2.7
1	B	250	LEU	2.6
1	B	225	THR	2.6
1	B	480	VAL	2.5
1	B	483	GLU	2.5
1	B	337	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	287	GLU	2.4
1	B	239	LEU	2.4
1	B	227	SER	2.3
1	A	562	SER	2.3
1	B	396	GLY	2.3
1	B	323	ARG	2.3
1	B	390	GLY	2.2
1	B	228	ASP	2.2
1	B	146	ARG	2.2
1	A	250	LEU	2.1
1	A	215	GLU	2.1
1	B	341	ASP	2.0
1	A	397	ASN	2.0
1	B	278	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 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
3	PRI	A	1566	7/7	0.86	0.45	58,58,59,59	0
3	PRI	B	1566	7/7	0.90	0.28	38,38,38,39	0
2	ATP	A	701	31/31	0.98	0.12	7,11,18,20	0
2	ATP	B	701	31/31	0.98	0.10	5,14,19,23	0
4	MN	A	1567	1/1	0.98	0.10	17,17,17,17	0
4	MN	A	1568	1/1	0.98	0.09	22,22,22,22	0
4	MN	B	1568	1/1	0.98	0.07	28,28,28,28	0
4	MN	B	1569	1/1	0.98	0.07	29,29,29,29	0
4	MN	B	1570	1/1	0.98	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MN	B	1567	1/1	0.99	0.06	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.