



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:53 PM GMT

PDB ID : 1XTJ
Title : structure of human UAP56 in complex with ADP
Authors : Shi, H.; Cordin, O.; Minder, C.M.; Linder, P.; Xu, R.-M.
Deposited on : 2004-10-22
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

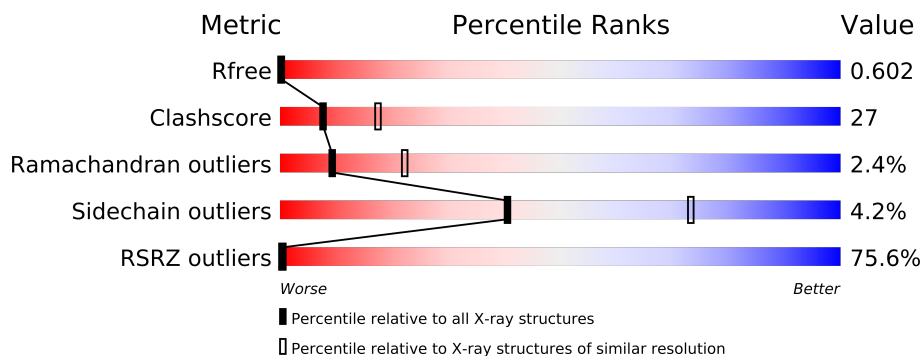
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	386	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3139 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Probable ATP-dependent RNA helicase p47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	3022	1923	525	553	21	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLY	-	CLONING ARTIFACT	UNP Q13838
A	39	SER	-	CLONING ARTIFACT	UNP Q13838
A	40	PRO	-	CLONING ARTIFACT	UNP Q13838
A	41	GLY	-	CLONING ARTIFACT	UNP Q13838
A	42	HIS	-	CLONING ARTIFACT	UNP Q13838
A	43	MET	-	CLONING ARTIFACT	UNP Q13838

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

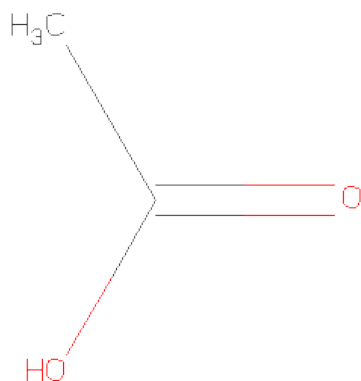
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total 85	O 85	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.99Å 78.20Å 63.19Å 90.00° 103.42° 90.00°	Depositor
Resolution (Å)	32.70 – 2.70 78.20 – 2.26	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.70-2.70) 59.4 (78.20-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.300 0.574 , 0.602	Depositor DCC
R_{free} test set	357 reflections (3.64%)	DCC
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	1.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 410.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 15975 reflections	Xtriage
F_o, F_c correlation	0.41	EDS
Total number of atoms	3139	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/3075	0.65	0/4137

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3022	0	3054	168	0
2	A	1	0	0	0	0
3	A	27	0	12	0	0
4	A	4	0	3	0	0
5	A	85	0	0	8	0
All	All	3139	0	3069	168	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (168) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:364:MET:HE1	1:A:400:LEU:HD13	1.48	0.95
1:A:262:LEU:HD21	1:A:375:VAL:HG12	1.52	0.90
1:A:106:GLN:HE22	1:A:223:GLN:HE22	1.23	0.83
1:A:417:GLU:HG2	1:A:418:ILE:HG13	1.61	0.82
1:A:53:LYS:HG3	1:A:105:GLN:HE22	1.45	0.81
1:A:120:CYS:SG	1:A:129:ILE:HD12	2.25	0.77
1:A:192:HIS:HD2	1:A:223:GLN:HE21	1.32	0.76
1:A:391:VAL:HG13	1:A:396:ASP:HB2	1.69	0.73
1:A:319:ARG:H	1:A:344:THR:HG21	1.51	0.73
1:A:313:PRO:HG2	1:A:339:ARG:HB2	1.72	0.71
1:A:179:LEU:HA	1:A:182:ASN:HD22	1.55	0.71
1:A:267:VAL:HG13	5:A:584:HOH:O	1.90	0.70
1:A:269:LEU:HD22	1:A:273:GLU:HB3	1.76	0.68
1:A:130:SER:HB2	1:A:147:VAL:HG13	1.75	0.68
1:A:198:CYS:SG	1:A:226:MET:HB3	2.34	0.67
1:A:195:LEU:HB3	1:A:201:MET:HE1	1.75	0.66
1:A:53:LYS:HG3	1:A:105:GLN:NE2	2.10	0.66
1:A:262:LEU:HD21	1:A:375:VAL:CG1	2.24	0.66
1:A:284:VAL:HG21	5:A:611:HOH:O	1.96	0.65
1:A:319:ARG:HG3	1:A:345:ASN:HD21	1.61	0.64
1:A:406:ARG:HH11	1:A:406:ARG:HB3	1.62	0.63
1:A:214:ILE:HA	1:A:217:MET:CE	2.29	0.63
1:A:190:ILE:HB	1:A:218:THR:HG23	1.80	0.63
1:A:145:VAL:HG12	1:A:146:ALA:N	2.14	0.63
1:A:269:LEU:HD11	1:A:277:LYS:HG3	1.80	0.63
1:A:319:ARG:N	1:A:344:THR:HG21	2.13	0.63
1:A:106:GLN:NE2	1:A:223:GLN:HE22	1.97	0.62
1:A:236:ARG:N	1:A:237:PRO:HD2	2.14	0.62
1:A:258:THR:HG22	1:A:260:HIS:H	1.63	0.62
1:A:110:VAL:HG11	1:A:113:GLN:NE2	2.15	0.62
1:A:232:SER:HB3	1:A:235:ILE:HB	1.81	0.61
1:A:259:LEU:HD21	1:A:264:GLN:HE22	1.64	0.61
1:A:47:PHE:O	1:A:50:PHE:HB2	2.01	0.61
1:A:420:ILE:N	1:A:420:ILE:HD13	2.16	0.60
1:A:90:LYS:O	1:A:93:MET:HB2	2.00	0.60
1:A:420:ILE:HG12	1:A:421:SER:H	1.67	0.60
1:A:155:LYS:O	1:A:159:GLU:HG3	2.02	0.60
1:A:297:VAL:HG22	1:A:318:HIS:HB2	1.84	0.59
1:A:159:GLU:HB3	1:A:163:LYS:NZ	2.16	0.59
1:A:294:VAL:HG21	1:A:300:CYS:HA	1.83	0.59
1:A:319:ARG:NE	1:A:345:ASN:OD1	2.36	0.59
1:A:54:PRO:HG2	1:A:55:GLU:OE2	2.02	0.59
1:A:333:PHE:CE1	1:A:341:LEU:HB2	2.37	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:MET:HE1	1:A:254:GLU:H	1.68	0.57
1:A:195:LEU:HB3	1:A:201:MET:CE	2.34	0.57
1:A:192:HIS:HD2	1:A:223:GLN:NE2	2.02	0.57
1:A:384:LYS:HB3	5:A:632:HOH:O	2.04	0.56
1:A:182:ASN:O	1:A:183:LYS:HB2	2.06	0.56
1:A:288:ASN:H	1:A:357:ASN:HD22	1.54	0.56
1:A:377:ARG:HD3	1:A:384:LYS:O	2.06	0.55
1:A:294:VAL:HG12	1:A:362:TYR:CD2	2.41	0.55
1:A:380:ARG:HA	1:A:380:ARG:NE	2.22	0.55
1:A:214:ILE:HA	1:A:217:MET:HE2	1.89	0.55
1:A:218:THR:HG23	1:A:219:PRO:HD2	1.89	0.54
1:A:288:ASN:HB2	1:A:357:ASN:HD21	1.72	0.54
1:A:86:LEU:HD12	1:A:226:MET:HB2	1.90	0.54
1:A:285:LEU:HD13	1:A:358:ILE:HD13	1.90	0.54
1:A:243:MET:HB3	1:A:246:PRO:HB3	1.90	0.54
1:A:391:VAL:HG13	1:A:396:ASP:CB	2.38	0.54
1:A:305:GLN:HA	5:A:624:HOH:O	2.08	0.54
1:A:294:VAL:HA	1:A:363:ASP:OD1	2.07	0.54
1:A:93:MET:HE1	1:A:254:GLU:N	2.23	0.54
1:A:93:MET:HE2	1:A:253:ASP:HA	1.91	0.53
1:A:415:PRO:O	1:A:416:ASP:HB3	2.09	0.53
1:A:179:LEU:HA	1:A:182:ASN:ND2	2.23	0.53
1:A:409:VAL:HG12	1:A:410:ASN:H	1.73	0.53
1:A:335:ASP:OD2	1:A:337:GLN:HB2	2.07	0.52
1:A:53:LYS:H	1:A:105:GLN:HE22	1.57	0.52
1:A:289:GLN:HG3	1:A:336:PHE:HE1	1.74	0.52
1:A:409:VAL:HG12	1:A:410:ASN:N	2.25	0.52
1:A:123:ARG:HG2	1:A:124:GLU:OE2	2.10	0.52
1:A:154:ILE:HD11	1:A:182:ASN:HD21	1.75	0.51
1:A:131:LYS:HD2	1:A:134:GLU:OE2	2.11	0.51
1:A:294:VAL:HG21	1:A:300:CYS:CA	2.40	0.51
1:A:208:ARG:HH21	1:A:238:VAL:HG22	1.75	0.51
1:A:240:ARG:HH11	1:A:240:ARG:HB2	1.76	0.51
1:A:406:ARG:NH1	1:A:406:ARG:HB3	2.25	0.51
1:A:195:LEU:HD22	1:A:201:MET:CE	2.41	0.50
1:A:193:PHE:O	1:A:224:VAL:HA	2.12	0.50
1:A:258:THR:HG22	1:A:260:HIS:N	2.26	0.50
1:A:238:VAL:HG12	1:A:242:PHE:HE1	1.77	0.50
1:A:399:ILE:O	1:A:403:VAL:HG23	2.12	0.49
1:A:417:GLU:HG2	1:A:418:ILE:N	2.26	0.49
1:A:323:GLN:O	1:A:327:LEU:HG	2.12	0.49
1:A:234:GLU:HA	1:A:234:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:333:PHE:CD1	1:A:341:LEU:HB2	2.48	0.49
1:A:218:THR:HG22	1:A:222:LYS:HD3	1.94	0.49
1:A:293:PHE:O	1:A:362:TYR:HB3	2.12	0.49
1:A:326:ARG:HH11	1:A:326:ARG:HB2	1.77	0.49
1:A:195:LEU:HB2	1:A:198:CYS:SG	2.52	0.49
1:A:55:GLU:CD	1:A:55:GLU:H	2.16	0.48
1:A:72:GLN:O	1:A:76:ILE:HB	2.12	0.48
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.78	0.48
1:A:130:SER:HB2	1:A:147:VAL:CG1	2.43	0.48
1:A:232:SER:CB	1:A:235:ILE:HB	2.44	0.48
1:A:419:ASP:C	1:A:420:ILE:HD13	2.34	0.48
1:A:238:VAL:HG12	1:A:242:PHE:CE1	2.49	0.47
1:A:100:VAL:HG11	1:A:136:PHE:HD2	1.79	0.47
1:A:313:PRO:CG	1:A:339:ARG:HB2	2.42	0.47
1:A:269:LEU:HD22	1:A:273:GLU:CB	2.43	0.47
1:A:420:ILE:CG1	1:A:421:SER:H	2.25	0.47
1:A:358:ILE:HG12	1:A:386:LEU:HD23	1.97	0.47
1:A:164:ASN:HB2	5:A:596:HOH:O	2.14	0.47
1:A:218:THR:CG2	1:A:219:PRO:HD2	2.43	0.47
1:A:145:VAL:HG12	1:A:146:ALA:H	1.79	0.47
1:A:48:ARG:C	1:A:50:PHE:H	2.15	0.47
1:A:186:ASN:HD21	1:A:189:HIS:CE1	2.32	0.47
1:A:214:ILE:HA	1:A:217:MET:HE3	1.96	0.47
1:A:393:ASP:OD1	1:A:395:ASN:HB2	2.14	0.47
1:A:364:MET:SD	1:A:365:PRO:HD2	2.55	0.47
1:A:353:ILE:O	1:A:354:GLU:HB2	2.15	0.47
1:A:326:ARG:HH11	1:A:326:ARG:CB	2.27	0.46
1:A:186:ASN:HD21	1:A:189:HIS:HE1	1.62	0.46
1:A:365:PRO:HB3	1:A:374:ARG:NH1	2.31	0.46
1:A:215:PHE:CD1	1:A:242:PHE:HD2	2.33	0.46
1:A:147:VAL:HA	1:A:170:VAL:O	2.16	0.46
1:A:240:ARG:NH1	1:A:240:ARG:HB2	2.31	0.46
1:A:154:ILE:O	1:A:158:GLU:HG3	2.16	0.45
1:A:420:ILE:HG12	1:A:421:SER:N	2.29	0.45
1:A:182:ASN:O	1:A:183:LYS:CB	2.64	0.45
1:A:305:GLN:O	1:A:309:GLU:HG3	2.17	0.45
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.81	0.45
1:A:236:ARG:N	1:A:237:PRO:CD	2.79	0.45
1:A:420:ILE:O	1:A:421:SER:HB3	2.16	0.45
1:A:322:PRO:HD2	1:A:325:GLU:OE2	2.17	0.45
1:A:117:LEU:HB2	1:A:190:ILE:HD12	1.99	0.45
1:A:292:ILE:HA	1:A:360:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:286:GLU:OE2	1:A:422:SER:OG	2.31	0.44
1:A:232:SER:OG	1:A:235:ILE:HD13	2.17	0.44
1:A:159:GLU:HB3	1:A:163:LYS:HZ2	1.80	0.44
1:A:139:TYR:C	1:A:141:PRO:HD3	2.37	0.44
1:A:289:GLN:HA	1:A:339:ARG:O	2.17	0.44
1:A:100:VAL:O	1:A:104:LEU:HB2	2.17	0.44
1:A:60:ILE:HD13	1:A:136:PHE:CE1	2.52	0.44
1:A:226:MET:HE3	1:A:239:CYS:SG	2.58	0.44
1:A:113:GLN:HA	5:A:561:HOH:O	2.16	0.44
1:A:407:PHE:O	1:A:409:VAL:N	2.50	0.44
1:A:297:VAL:HG13	1:A:318:HIS:CD2	2.53	0.44
1:A:53:LYS:NZ	5:A:587:HOH:O	2.50	0.44
1:A:319:ARG:HB2	1:A:344:THR:HG21	1.99	0.44
1:A:358:ILE:CD1	1:A:386:LEU:HD23	2.48	0.43
1:A:415:PRO:O	1:A:416:ASP:CB	2.66	0.43
1:A:140:MET:N	1:A:141:PRO:HD3	2.34	0.43
1:A:304:ALA:O	1:A:308:VAL:HG23	2.18	0.43
1:A:192:HIS:CD2	1:A:223:GLN:HE21	2.23	0.43
1:A:78:GLN:HG2	1:A:247:MET:SD	2.59	0.43
1:A:121:HIS:CD2	1:A:122:THR:HG23	2.54	0.43
1:A:106:GLN:HE22	1:A:223:GLN:NE2	2.04	0.42
1:A:145:VAL:CG1	1:A:146:ALA:N	2.80	0.42
1:A:239:CYS:C	1:A:241:LYS:H	2.23	0.42
1:A:318:HIS:HA	1:A:344:THR:HB	2.02	0.42
1:A:85:VAL:HG12	1:A:86:LEU:N	2.35	0.42
1:A:414:LEU:HD12	1:A:415:PRO:HD2	2.01	0.42
1:A:235:ILE:O	1:A:235:ILE:CG2	2.68	0.42
1:A:208:ARG:NH2	1:A:238:VAL:CG2	2.83	0.42
1:A:87:CYS:O	1:A:227:PHE:HA	2.20	0.42
1:A:195:LEU:CB	1:A:201:MET:HE1	2.49	0.42
1:A:379:GLY:O	1:A:380:ARG:NE	2.50	0.41
1:A:189:HIS:HB2	5:A:634:HOH:O	2.20	0.41
1:A:231:LEU:HD23	1:A:231:LEU:N	2.36	0.41
1:A:177:LEU:HD13	1:A:214:ILE:HG13	2.01	0.41
1:A:382:GLY:O	1:A:383:THR:HG23	2.21	0.41
1:A:375:VAL:CG1	1:A:387:ALA:HB2	2.51	0.41
1:A:353:ILE:HG12	1:A:381:PHE:HE1	1.86	0.41
1:A:195:LEU:HD22	1:A:201:MET:HE3	2.02	0.41
1:A:358:ILE:HG12	1:A:386:LEU:HB3	2.03	0.41
1:A:276:ARG:HG2	1:A:280:ASP:OD2	2.21	0.40
1:A:106:GLN:O	1:A:108:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	370/386 (96%)	333 (90%)	28 (8%)	9 (2%)	9	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	PRO
1	A	416	ASP
1	A	420	ILE
1	A	421	SER
1	A	183	LYS
1	A	295	LYS
1	A	417	GLU
1	A	378	ALA
1	A	232	SER

5.3.2 Protein sidechains ⓘ

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	337/347 (97%)	323 (96%)	14 (4%)	40	73

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	93	MET
1	A	104	LEU
1	A	147	VAL
1	A	199	ASP

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Mol	Chain	Res	Type
1	A	228	SER
1	A	239	CYS
1	A	253	ASP
1	A	326	ARG
1	A	344	THR
1	A	363	ASP
1	A	406	ARG
1	A	407	PHE
1	A	420	ILE

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

Mol	Chain	Res	Type
1	A	67	HIS
1	A	78	GLN
1	A	88	GLN
1	A	105	GLN
1	A	113	GLN
1	A	182	ASN
1	A	189	HIS
1	A	192	HIS
1	A	212	GLN
1	A	220	HIS
1	A	223	GLN
1	A	264	GLN
1	A	305	GLN
1	A	323	GLN
1	A	331	GLN
1	A	332	GLN
1	A	357	ASN
1	A	395	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACY	A	500	-	3,3,3	1.35	0	3,3,3	1.15	0
3	ADP	A	550	2	29,29,29	0.94	2 (6%)	45,45,45	1.54	5 (11%)

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
4	ACY	A	500	-	-	0/0/0/0	0/0/0/0
3	ADP	A	550	2	-	0/16/32/32	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	ADP	C2-N1	2.63	1.39	1.33
3	A	550	ADP	C6-N6	-2.14	1.28	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	550	ADP	N3-C2-N1	-6.85	122.98	128.71
3	A	550	ADP	C4'-O4'-C1'	3.28	113.31	109.75
3	A	550	ADP	C2-N1-C6	2.75	123.73	118.77
3	A	550	ADP	C3'-C2'-C1'	2.63	105.02	100.91
3	A	550	ADP	C5-C6-N6	2.48	126.33	120.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	374/386 (96%)	3.74	284 (75%) 0 0	14, 42, 79, 101	0

All (284) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	18.5
1	A	292	ILE	14.9
1	A	154	ILE	13.2
1	A	322	PRO	11.9
1	A	342	VAL	11.4
1	A	88	GLN	11.1
1	A	171	GLY	10.5
1	A	54	PRO	10.1
1	A	46	GLY	10.0
1	A	100	VAL	9.6
1	A	114	VAL	9.6
1	A	137	SER	9.5
1	A	372	LEU	9.4
1	A	403	VAL	9.0
1	A	362	TYR	9.0
1	A	361	ASN	8.6
1	A	201	MET	8.6
1	A	98	VAL	8.5
1	A	274	LYS	8.4
1	A	247	MET	8.2
1	A	290	VAL	8.1
1	A	278	LEU	8.1
1	A	279	PHE	8.0
1	A	388	ILE	8.0
1	A	343	ALA	7.9
1	A	243	MET	7.9
1	A	105	GLN	7.9

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Mol	Chain	Res	Type	RSRZ
1	A	190	ILE	7.9
1	A	356	VAL	7.7
1	A	213	GLU	7.7
1	A	323	GLN	7.5
1	A	72	GLN	7.5
1	A	198	CYS	7.5
1	A	62	ASP	7.5
1	A	262	LEU	7.4
1	A	126	ALA	7.3
1	A	218	THR	7.3
1	A	387	ALA	7.2
1	A	266	TYR	7.1
1	A	237	PRO	6.9
1	A	354	GLU	6.9
1	A	402	ASP	6.7
1	A	170	VAL	6.7
1	A	90	LYS	6.7
1	A	238	VAL	6.6
1	A	81	LEU	6.6
1	A	374	ARG	6.6
1	A	281	LEU	6.5
1	A	358	ILE	6.4
1	A	73	HIS	6.4
1	A	99	PHE	6.3
1	A	116	VAL	6.3
1	A	399	ILE	6.2
1	A	321	MET	6.2
1	A	291	VAL	6.2
1	A	65	PHE	6.2
1	A	365	PRO	6.1
1	A	50	PHE	6.0
1	A	390	PHE	6.0
1	A	152	LEU	6.0
1	A	289	GLN	5.8
1	A	145	VAL	5.8
1	A	263	GLN	5.8
1	A	138	LYS	5.8
1	A	174	GLY	5.7
1	A	379	GLY	5.7
1	A	147	VAL	5.7
1	A	151	GLY	5.7
1	A	146	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	193	PHE	5.6
1	A	70	GLU	5.6
1	A	210	ASP	5.6
1	A	419	ASP	5.6
1	A	53	LYS	5.6
1	A	265	TYR	5.6
1	A	267	VAL	5.5
1	A	308	VAL	5.5
1	A	248	GLU	5.5
1	A	357	ASN	5.4
1	A	389	THR	5.3
1	A	231	LEU	5.3
1	A	311	ASN	5.3
1	A	157	ASP	5.3
1	A	418	ILE	5.2
1	A	338	ARG	5.2
1	A	59	ALA	5.2
1	A	375	VAL	5.2
1	A	167	HIS	5.1
1	A	194	ILE	5.0
1	A	132	GLU	5.0
1	A	104	LEU	5.0
1	A	299	ARG	4.9
1	A	185	LEU	4.9
1	A	225	MET	4.9
1	A	400	LEU	4.9
1	A	180	ALA	4.9
1	A	297	VAL	4.9
1	A	393	ASP	4.9
1	A	228	SER	4.9
1	A	352	ASP	4.9
1	A	270	LYS	4.8
1	A	217	MET	4.8
1	A	153	SER	4.7
1	A	259	LEU	4.7
1	A	235	ILE	4.7
1	A	368	SER	4.6
1	A	177	LEU	4.6
1	A	339	ARG	4.6
1	A	169	VAL	4.6
1	A	232	SER	4.6
1	A	392	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	319	ARG	4.5
1	A	316	ALA	4.5
1	A	373	HIS	4.5
1	A	249	ILE	4.5
1	A	364	MET	4.5
1	A	386	LEU	4.4
1	A	287	PHE	4.4
1	A	55	GLU	4.3
1	A	64	GLY	4.3
1	A	159	GLU	4.3
1	A	75	CYS	4.3
1	A	196	ASP	4.2
1	A	396	ASP	4.2
1	A	130	SER	4.2
1	A	408	GLU	4.2
1	A	121	HIS	4.1
1	A	205	LEU	4.1
1	A	223	GLN	4.1
1	A	125	LEU	4.1
1	A	344	THR	4.1
1	A	123	ARG	4.0
1	A	336	PHE	4.0
1	A	300	CYS	4.0
1	A	330	TYR	4.0
1	A	178	ALA	4.0
1	A	239	CYS	3.9
1	A	97	ALA	3.9
1	A	253	ASP	3.9
1	A	212	GLN	3.8
1	A	229	ALA	3.8
1	A	103	THR	3.8
1	A	191	LYS	3.8
1	A	189	HIS	3.8
1	A	391	VAL	3.7
1	A	82	GLY	3.7
1	A	302	ALA	3.7
1	A	119	MET	3.7
1	A	269	LEU	3.7
1	A	355	ARG	3.6
1	A	84	ASP	3.6
1	A	264	GLN	3.5
1	A	89	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	141	PRO	3.5
1	A	309	GLU	3.5
1	A	407	PHE	3.5
1	A	421	SER	3.4
1	A	298	GLN	3.4
1	A	250	PHE	3.4
1	A	410	ASN	3.4
1	A	420	ILE	3.3
1	A	329	ARG	3.3
1	A	102	ALA	3.3
1	A	165	CYS	3.3
1	A	317	ILE	3.3
1	A	380	ARG	3.3
1	A	333	PHE	3.3
1	A	254	GLU	3.3
1	A	76	ILE	3.3
1	A	69	SER	3.3
1	A	95	LYS	3.3
1	A	268	LYS	3.3
1	A	303	LEU	3.2
1	A	227	PHE	3.2
1	A	414	LEU	3.2
1	A	246	PRO	3.2
1	A	423	TYR	3.2
1	A	242	PHE	3.1
1	A	51	LEU	3.1
1	A	184	SER	3.1
1	A	60	ILE	3.1
1	A	107	LEU	3.1
1	A	214	ILE	3.1
1	A	221	GLU	3.1
1	A	49	ASP	3.1
1	A	129	ILE	3.1
1	A	142	ASN	3.0
1	A	328	SER	3.0
1	A	160	VAL	3.0
1	A	310	GLN	3.0
1	A	83	MET	3.0
1	A	422	SER	3.0
1	A	294	VAL	3.0
1	A	57	LEU	3.0
1	A	122	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	78	GLN	3.0
1	A	109	PRO	3.0
1	A	120	CYS	3.0
1	A	395	ASN	2.9
1	A	127	PHE	2.9
1	A	52	LEU	2.9
1	A	230	THR	2.9
1	A	203	GLU	2.9
1	A	313	PRO	2.9
1	A	124	GLU	2.9
1	A	284	VAL	2.9
1	A	398	LYS	2.9
1	A	307	LEU	2.9
1	A	71	VAL	2.8
1	A	110	VAL	2.8
1	A	168	ILE	2.8
1	A	332	GLN	2.8
1	A	96	THR	2.8
1	A	416	ASP	2.8
1	A	162	LYS	2.8
1	A	111	THR	2.7
1	A	275	ASN	2.7
1	A	87	CYS	2.7
1	A	381	PHE	2.7
1	A	45	SER	2.7
1	A	187	LEU	2.6
1	A	166	PRO	2.6
1	A	48	ARG	2.6
1	A	256	LYS	2.6
1	A	80	ILE	2.6
1	A	276	ARG	2.6
1	A	312	PHE	2.5
1	A	241	LYS	2.5
1	A	101	LEU	2.5
1	A	280	ASP	2.5
1	A	376	ALA	2.5
1	A	261	GLY	2.5
1	A	202	LEU	2.5
1	A	314	ALA	2.5
1	A	334	LYS	2.4
1	A	383	THR	2.4
1	A	158	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	236	ARG	2.4
1	A	285	LEU	2.4
1	A	417	GLU	2.4
1	A	353	ILE	2.4
1	A	58	ARG	2.3
1	A	86	LEU	2.3
1	A	195	LEU	2.3
1	A	128	GLN	2.3
1	A	346	LEU	2.3
1	A	413	GLU	2.3
1	A	315	ILE	2.3
1	A	345	ASN	2.3
1	A	378	ALA	2.3
1	A	204	GLN	2.3
1	A	112	GLY	2.3
1	A	272	ASN	2.3
1	A	61	VAL	2.3
1	A	143	VAL	2.3
1	A	67	HIS	2.3
1	A	197	GLU	2.3
1	A	139	TYR	2.3
1	A	326	ARG	2.3
1	A	244	GLN	2.2
1	A	133	TYR	2.2
1	A	79	ALA	2.2
1	A	118	VAL	2.2
1	A	271	ASP	2.2
1	A	234	GLU	2.2
1	A	173	PRO	2.2
1	A	304	ALA	2.2
1	A	409	VAL	2.2
1	A	233	LYS	2.2
1	A	149	PHE	2.1
1	A	288	ASN	2.1
1	A	325	GLU	2.1
1	A	150	GLY	2.1
1	A	179	LEU	2.1
1	A	382	GLY	2.1
1	A	163	LYS	2.1
1	A	331	GLN	2.1
1	A	211	VAL	2.0
1	A	340	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	245	ASP	2.0
1	A	296	SER	2.0
1	A	359	ALA	2.0
1	A	85	VAL	2.0
1	A	144	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ACY	A	500	4/4	0.44	1.32	66,66,66,66	0
3	ADP	A	550	27/27	0.30	-0.77	32,41,44,47	0
2	MG	A	501	1/1	0.21	-3.59	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.