Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:34 PM GMT

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PDB ID	:	1XTJ
Title	:	structure of human UAP56 in complex with ADP
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Deposited on	:	2004-10-22
Resolution	:	2.70 Å(reported)

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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 2.70 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	Percentile Ranks	Value
Rfree		0.602
Clashscore		27
Ramachandran outliers		2.4%
Sidechain outliers		4.2%
RSRZ outliers		91.4%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
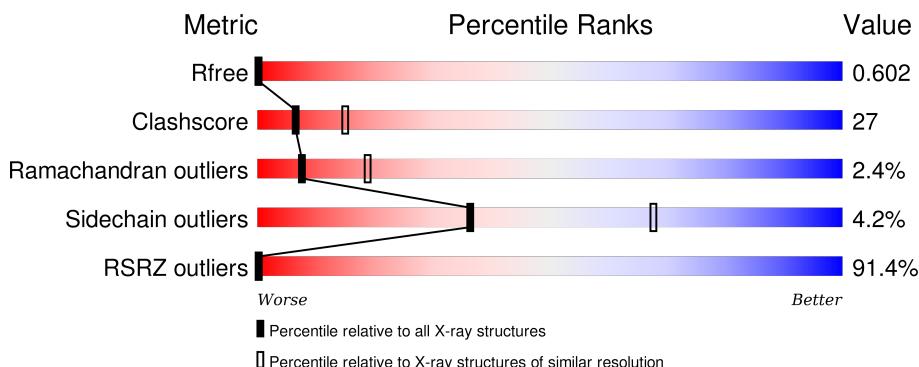
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	386	89% / 53% 40% · ·

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3139 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 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
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
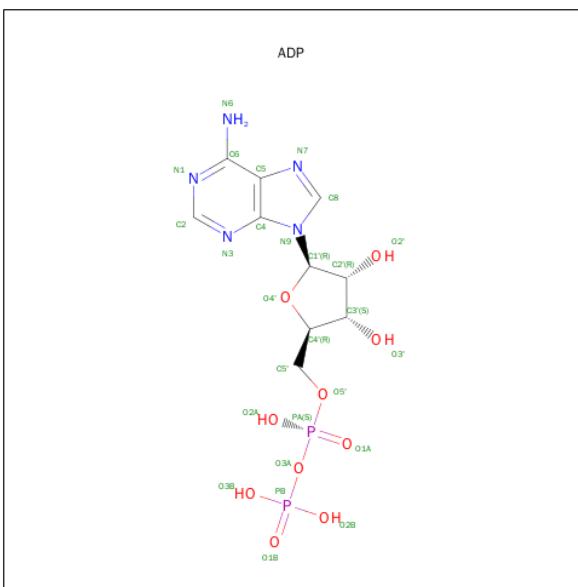
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).
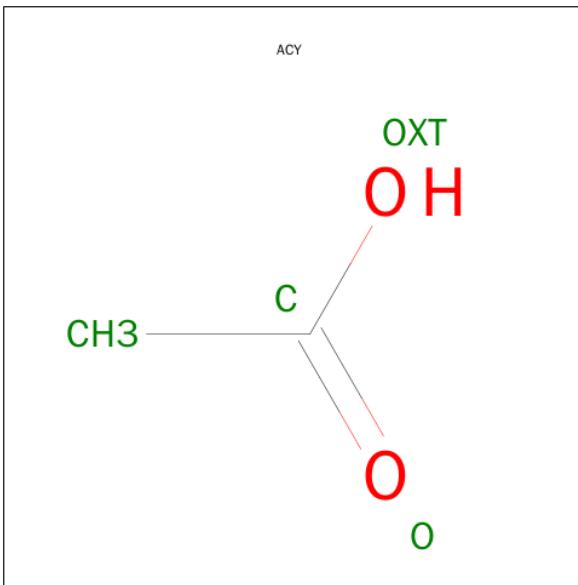
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Probable ATP-dependent RNA helicase p47
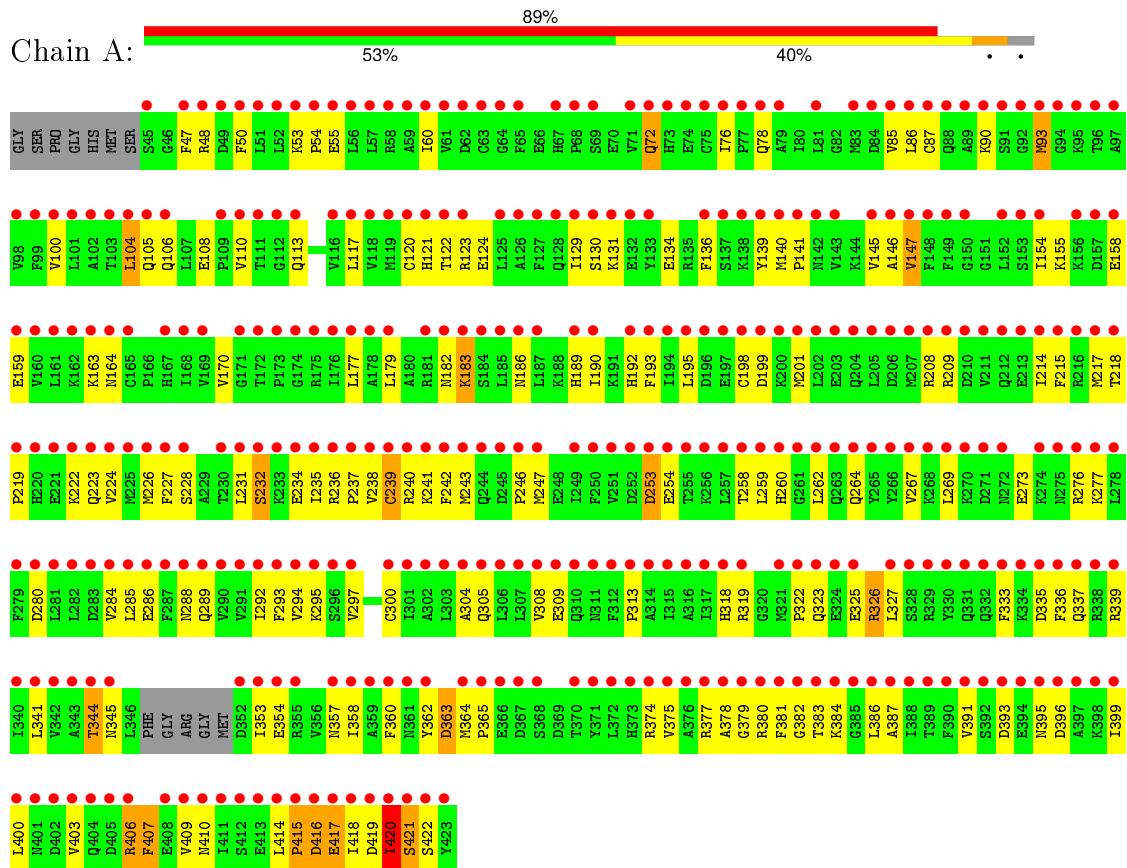
4 Data and refinement statistics (i)

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
$<I/\sigma(I)>$ [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)	0.35 , 3259.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.52, <L^2> = 0.36$	Xtriage
Outliers	0 of 15975 reflections	Xtriage
F_o,F_c correlation	0.40	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.*

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[1]Intensities estimated from amplitudes.

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

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 27.

All (168) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CE1	1:A:341:LEU:HB2	2.37	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	370/386 (96%)	333 (90%)	28 (8%)	9 (2%)	7 19

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 (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	337/347 (97%)	323 (96%)	14 (4%)	36 68

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
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 (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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	-	1,3,3	2.44	1 (100%)	0,3,3	0.00	-
3	ADP	A	550	2	22,29,29	0.98	2 (9%)	27,45,45	1.90	3 (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	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	550	ADP	C6-N6	-2.20	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	ACY	CH3-C	2.44	1.52	1.48
3	A	550	ADP	C2-N1	2.73	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	550	ADP	N3-C2-N1	-7.72	122.98	128.89
3	A	550	ADP	C2-N1-C6	2.78	123.73	118.77
3	A	550	ADP	C4'-O4'-C1'	3.27	113.31	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	374/386 (96%)	4.56	342 (91%)	0	0	14, 42, 79, 101	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	ALA	15.9
1	A	383	THR	14.9
1	A	401	ASN	13.2
1	A	243	MET	12.9
1	A	392	SER	12.9
1	A	54	PRO	12.3
1	A	361	ASN	12.0
1	A	94	GLY	11.7
1	A	339	ARG	11.6
1	A	317	ILE	11.3
1	A	65	PHE	11.1
1	A	75	CYS	10.9
1	A	275	ASN	10.6
1	A	322	PRO	10.3
1	A	88	GLN	10.2
1	A	97	ALA	10.0
1	A	360	PHE	9.9
1	A	69	SER	9.9
1	A	237	PRO	9.6
1	A	333	PHE	9.5
1	A	284	VAL	9.3
1	A	245	ASP	9.3
1	A	102	ALA	9.3
1	A	403	VAL	9.3
1	A	56	LEU	9.3
1	A	386	LEU	9.2
1	A	126	ALA	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	138	LYS	9.0
1	A	314	ALA	8.9
1	A	149	PHE	8.6
1	A	127	PHE	8.5
1	A	373	HIS	8.4
1	A	345	ASN	8.4
1	A	255	THR	8.4
1	A	84	ASP	8.3
1	A	292	ILE	8.3
1	A	291	VAL	8.1
1	A	64	GLY	8.0
1	A	332	GLN	7.8
1	A	242	PHE	7.8
1	A	388	ILE	7.7
1	A	387	ALA	7.6
1	A	378	ALA	7.5
1	A	197	GLU	7.5
1	A	112	GLY	7.4
1	A	254	GLU	7.2
1	A	253	ASP	7.2
1	A	87	CYS	7.2
1	A	342	VAL	7.2
1	A	302	ALA	7.1
1	A	238	VAL	7.1
1	A	150	GLY	7.1
1	A	55	GLU	7.0
1	A	201	MET	7.0
1	A	83	MET	7.0
1	A	372	LEU	6.9
1	A	382	GLY	6.8
1	A	73	HIS	6.8
1	A	330	TYR	6.8
1	A	274	LYS	6.7
1	A	343	ALA	6.7
1	A	96	THR	6.7
1	A	50	PHE	6.5
1	A	168	ILE	6.5
1	A	282	LEU	6.4
1	A	391	VAL	6.3
1	A	359	ALA	6.3
1	A	354	GLU	6.3
1	A	153	SER	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	6.3
1	A	421	SER	6.3
1	A	116	VAL	6.3
1	A	294	VAL	6.2
1	A	189	HIS	6.1
1	A	290	VAL	6.1
1	A	337	GLN	6.1
1	A	171	GLY	6.1
1	A	272	ASN	6.0
1	A	266	TYR	6.0
1	A	327	LEU	6.0
1	A	198	CYS	6.0
1	A	315	ILE	5.9
1	A	231	LEU	5.9
1	A	257	LEU	5.9
1	A	212	GLN	5.9
1	A	223	GLN	5.9
1	A	179	LEU	5.9
1	A	208	ARG	5.8
1	A	416	ASP	5.7
1	A	228	SER	5.7
1	A	104	LEU	5.6
1	A	230	THR	5.6
1	A	235	ILE	5.6
1	A	133	TYR	5.6
1	A	193	PHE	5.5
1	A	300	CYS	5.5
1	A	303	LEU	5.4
1	A	250	PHE	5.4
1	A	224	VAL	5.4
1	A	216	ARG	5.4
1	A	177	LEU	5.3
1	A	411	ILE	5.3
1	A	402	ASP	5.3
1	A	148	PHE	5.3
1	A	199	ASP	5.2
1	A	376	ALA	5.2
1	A	419	ASP	5.2
1	A	313	PRO	5.2
1	A	308	VAL	5.2
1	A	365	PRO	5.2
1	A	362	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	412	SER	5.2
1	A	53	LYS	5.1
1	A	381	PHE	5.1
1	A	92	GLY	5.1
1	A	389	THR	5.1
1	A	90	LYS	5.1
1	A	259	LEU	5.1
1	A	398	LYS	5.1
1	A	62	ASP	5.1
1	A	154	ILE	5.1
1	A	63	CYS	5.0
1	A	128	GLN	5.0
1	A	262	LEU	5.0
1	A	72	GLN	4.9
1	A	241	LYS	4.9
1	A	152	LEU	4.9
1	A	355	ARG	4.9
1	A	68	PRO	4.9
1	A	247	MET	4.9
1	A	99	PHE	4.9
1	A	417	GLU	4.8
1	A	174	GLY	4.8
1	A	353	ILE	4.8
1	A	306	LEU	4.8
1	A	319	ARG	4.8
1	A	207	MET	4.7
1	A	85	VAL	4.7
1	A	185	LEU	4.7
1	A	357	ASN	4.7
1	A	130	SER	4.7
1	A	215	PHE	4.7
1	A	397	ALA	4.7
1	A	165	CYS	4.6
1	A	415	PRO	4.6
1	A	380	ARG	4.6
1	A	367	ASP	4.6
1	A	117	LEU	4.6
1	A	283	ASP	4.6
1	A	321	MET	4.6
1	A	263	GLN	4.6
1	A	227	PHE	4.5
1	A	323	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	49	ASP	4.5
1	A	173	PRO	4.5
1	A	78	GLN	4.5
1	A	296	SER	4.5
1	A	184	SER	4.5
1	A	385	GLY	4.5
1	A	265	TYR	4.4
1	A	269	LEU	4.4
1	A	371	TYR	4.4
1	A	297	VAL	4.4
1	A	267	VAL	4.4
1	A	48	ARG	4.4
1	A	162	LYS	4.4
1	A	145	VAL	4.4
1	A	137	SER	4.4
1	A	420	ILE	4.4
1	A	103	THR	4.3
1	A	236	ARG	4.3
1	A	368	SER	4.3
1	A	328	SER	4.3
1	A	146	ALA	4.3
1	A	285	LEU	4.2
1	A	163	LYS	4.2
1	A	110	VAL	4.2
1	A	276	ARG	4.2
1	A	76	ILE	4.2
1	A	279	PHE	4.2
1	A	404	GLN	4.2
1	A	418	ILE	4.1
1	A	396	ASP	4.1
1	A	74	GLU	4.1
1	A	95	LYS	4.1
1	A	335	ASP	4.1
1	A	213	GLU	4.1
1	A	379	GLY	4.1
1	A	196	ASP	4.0
1	A	47	PHE	4.0
1	A	222	LYS	4.0
1	A	157	ASP	4.0
1	A	260	HIS	4.0
1	A	305	GLN	4.0
1	A	98	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	264	GLN	4.0
1	A	340	ILE	4.0
1	A	293	PHE	3.9
1	A	57	LEU	3.9
1	A	101	LEU	3.9
1	A	91	SER	3.9
1	A	334	LYS	3.9
1	A	246	PRO	3.8
1	A	240	ARG	3.8
1	A	120	CYS	3.8
1	A	318	HIS	3.8
1	A	178	ALA	3.8
1	A	344	THR	3.8
1	A	160	VAL	3.8
1	A	225	MET	3.7
1	A	71	VAL	3.7
1	A	405	ASP	3.7
1	A	125	LEU	3.7
1	A	105	GLN	3.7
1	A	239	CYS	3.7
1	A	393	ASP	3.7
1	A	113	GLN	3.7
1	A	221	GLU	3.7
1	A	408	GLU	3.7
1	A	358	ILE	3.6
1	A	45	SER	3.6
1	A	364	MET	3.6
1	A	129	ILE	3.6
1	A	366	GLU	3.6
1	A	123	ARG	3.6
1	A	277	LYS	3.6
1	A	304	ALA	3.6
1	A	219	PRO	3.6
1	A	206	ASP	3.5
1	A	394	GLU	3.5
1	A	139	TYR	3.5
1	A	377	ARG	3.5
1	A	77	PRO	3.5
1	A	395	ASN	3.5
1	A	281	LEU	3.5
1	A	186	ASN	3.5
1	A	147	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	LYS	3.4
1	A	132	GLU	3.4
1	A	217	MET	3.4
1	A	233	LYS	3.4
1	A	338	ARG	3.3
1	A	52	LEU	3.3
1	A	390	PHE	3.3
1	A	312	PHE	3.3
1	A	141	PRO	3.3
1	A	287	PHE	3.3
1	A	183	LYS	3.3
1	A	249	ILE	3.3
1	A	167	HIS	3.2
1	A	311	ASN	3.2
1	A	289	GLN	3.2
1	A	286	GLU	3.2
1	A	423	TYR	3.2
1	A	67	HIS	3.2
1	A	172	THR	3.2
1	A	268	LYS	3.1
1	A	169	VAL	3.1
1	A	93	MET	3.1
1	A	406	ARG	3.0
1	A	159	GLU	3.0
1	A	295	LYS	3.0
1	A	136	PHE	3.0
1	A	161	LEU	3.0
1	A	352	ASP	3.0
1	A	414	LEU	3.0
1	A	79	ALA	2.9
1	A	310	GLN	2.9
1	A	176	ILE	2.9
1	A	190	ILE	2.9
1	A	156	LYS	2.9
1	A	203	GLU	2.9
1	A	325	GLU	2.9
1	A	81	LEU	2.8
1	A	384	LYS	2.8
1	A	329	ARG	2.8
1	A	121	HIS	2.8
1	A	210	ASP	2.8
1	A	258	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	409	VAL	2.8
1	A	280	ASP	2.8
1	A	58	ARG	2.8
1	A	370	THR	2.8
1	A	422	SER	2.8
1	A	143	VAL	2.7
1	A	309	GLU	2.7
1	A	100	VAL	2.7
1	A	251	VAL	2.7
1	A	375	VAL	2.7
1	A	336	PHE	2.7
1	A	142	ASN	2.7
1	A	131	LYS	2.7
1	A	324	GLU	2.7
1	A	288	ASN	2.7
1	A	214	ILE	2.7
1	A	261	GLY	2.7
1	A	271	ASP	2.7
1	A	122	THR	2.7
1	A	175	ARG	2.6
1	A	106	GLN	2.6
1	A	192	HIS	2.6
1	A	182	ASN	2.6
1	A	195	LEU	2.6
1	A	218	THR	2.6
1	A	399	ILE	2.6
1	A	205	LEU	2.5
1	A	278	LEU	2.5
1	A	301	ILE	2.5
1	A	89	ALA	2.5
1	A	220	HIS	2.5
1	A	413	GLU	2.5
1	A	109	PRO	2.5
1	A	61	VAL	2.5
1	A	204	GLN	2.4
1	A	252	ASP	2.4
1	A	111	THR	2.4
1	A	187	LEU	2.4
1	A	244	GLN	2.4
1	A	400	LEU	2.4
1	A	341	LEU	2.3
1	A	118	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	232	SER	2.3
1	A	119	MET	2.3
1	A	410	ASN	2.3
1	A	194	ILE	2.3
1	A	59	ALA	2.3
1	A	256	LYS	2.3
1	A	140	MET	2.2
1	A	181	ARG	2.2
1	A	200	LYS	2.2
1	A	209	ARG	2.2
1	A	331	GLN	2.1
1	A	164	ASN	2.1
1	A	158	GLU	2.1
1	A	211	VAL	2.1
1	A	307	LEU	2.1
1	A	60	ILE	2.1
1	A	86	LEU	2.1
1	A	51	LEU	2.1
1	A	226	MET	2.0
1	A	374	ARG	2.0
1	A	234	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. 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	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
4	ACY	A	500	4/4	0.86	0.37	-0.73	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ADP	A	550	27/27	0.53	0.30	-1.61	32,41,44,47	0
2	MG	A	501	1/1	0.73	0.74	-	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.