Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:25 AM GMT

PDB ID	:	3AQN
Title	:	Complex structure of bacterial protein (apo form II)
Authors	:	Toh, Y.; Takeshita, D.; Tomita , K.
Deposited on	:	2010-11-09
Resolution	:	3.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

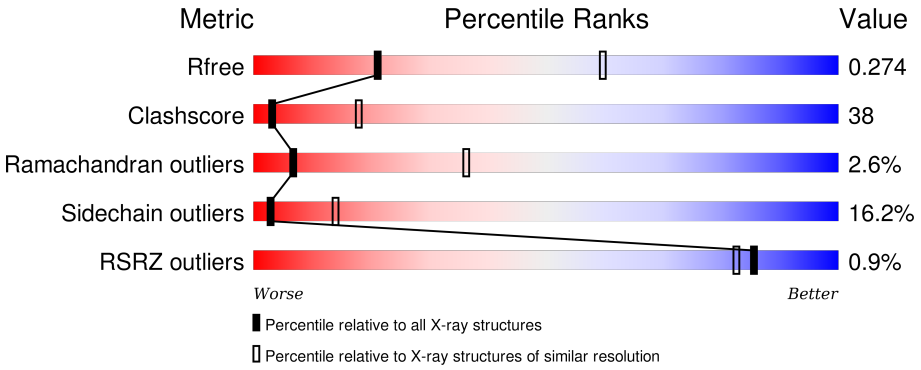
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	415	% 40% 44% 9% • 7%
1	B	415	39% 42% 12% 7%

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
2	ATP	A	501	-	-	-	X
2	ATP	B	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6398 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.

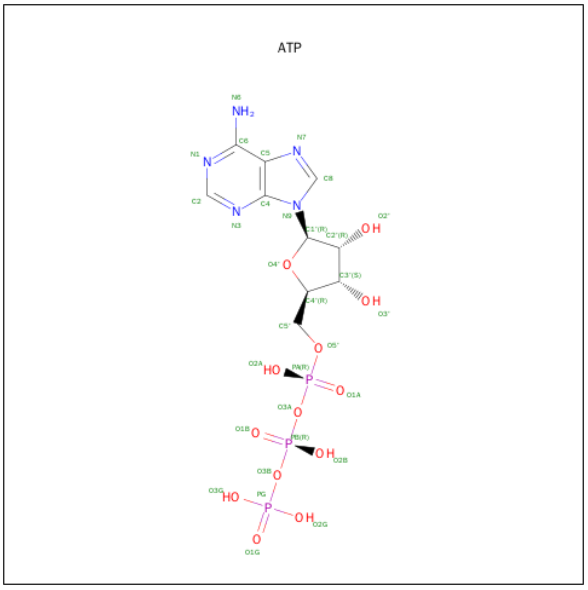
- Molecule 1 is a protein called Poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3164	2022	568	560	14			
1	B	388	Total	C	N	O	S	0	0	0
			3164	2022	568	560	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	HIS	ARG	ENGINEERED MUTATION	UNP C9QS13
B	234	HIS	ARG	ENGINEERED MUTATION	UNP C9QS13

- 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
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

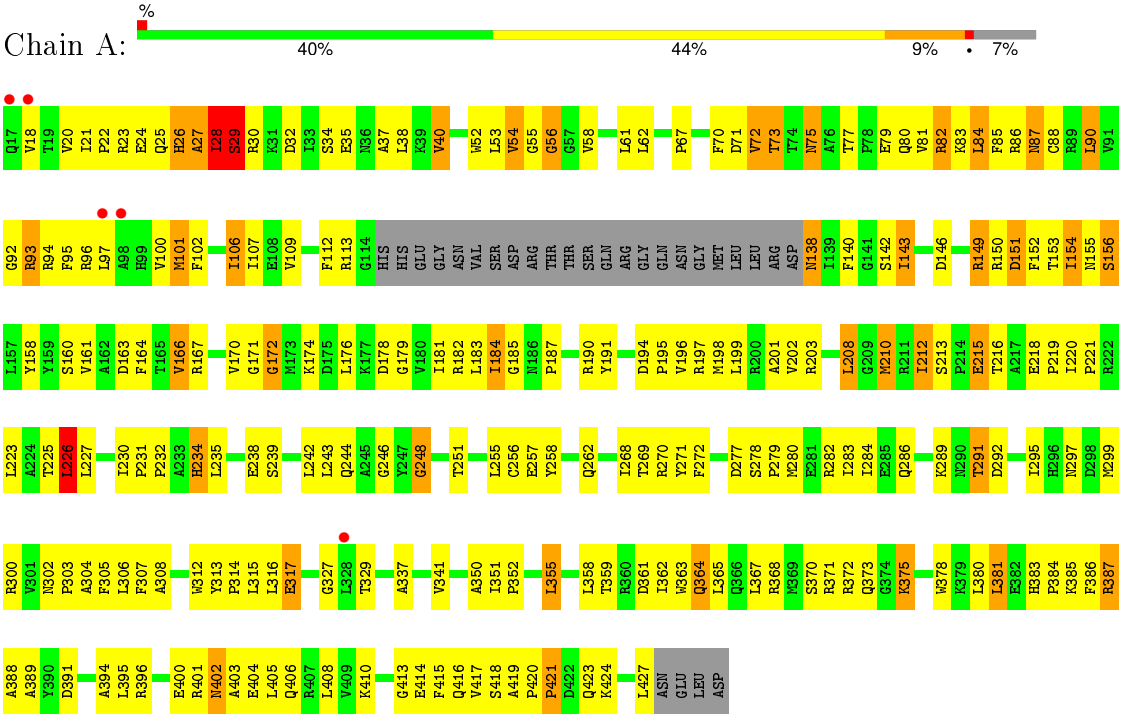
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		
4	B	3	Total	O	0	0
			3	3		

3 Residue-property plots (i)

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.

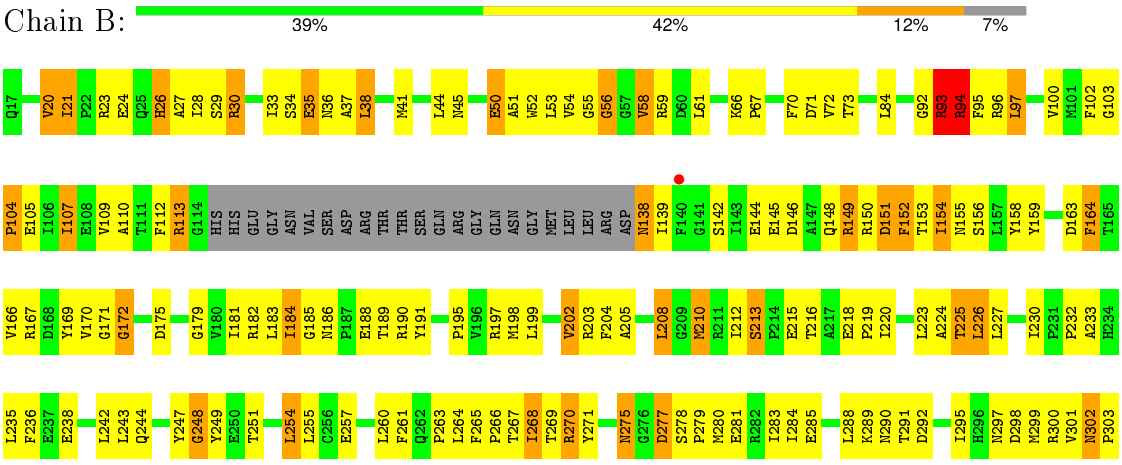
- Molecule 1: Poly(A) polymerase

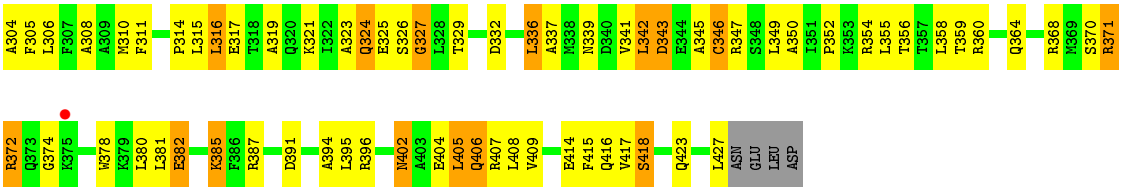
Chain A:



- Molecule 1: Poly(A) polymerase

Chain B:




A304 F305 L306 F307 A308 A309 M310 F311 P314 L315 L316 E317 T318 A319 Q320 K321 I322 A323 Q324 E325 S326 G327 L328 T329 D332 L336 A337 H338 N339 D340 V341 L342 D343 E344 A345 G346 R347 S348 L349 A350 I351 P352 R353 R354 L355 T356 T357 L358 T359 R360 Q364 R368 H369 S370 R371
R372 Q373 G374 R375 W378 R379 L380 L381 E382 K385 P386 R387 D391 A394 L395 R396 N402 A403 E404 L405 Q406 R407 L408 V409 E414 F415 Q416 V417 S418 Q423 L427 ASN GLU LEU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	132.40Å 132.40Å 176.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 3.30 45.24 – 3.16	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.61-3.30) 98.6 (45.24-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 3.19Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.251 , 0.275 0.251 , 0.274	Depositor DCC
R_{free} test set	1188 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	90.5	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	1 of 27191 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6398	wwPDB-VP
Average B, all atoms (Å^2)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/3234	0.59	1/4371 (0.0%)
1	B	0.38	0/3234	0.60	1/4371 (0.0%)
All	All	0.38	0/6468	0.59	2/8742 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	94	ARG	CB-CA-C	6.53	123.46	110.40
1	A	27	ALA	N-CA-C	-6.27	94.07	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3164	0	3197	265	0
1	B	3164	0	3197	228	0
2	A	31	0	12	4	0
2	B	31	0	12	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
All	All	6398	0	6418	484	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 38.

All (484) 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:28:ILE:O	1:A:29:SER:C	1.85	1.15
1:A:191:TYR:CD1	1:A:198:MET:HG3	1.88	1.08
1:B:374:GLY:HA2	1:B:427:LEU:HD22	1.37	1.06
1:B:93:ARG:HD3	1:B:93:ARG:H	1.15	1.06
1:A:184:ILE:HG22	1:A:190:ARG:HH12	1.18	1.05
1:A:26:HIS:HD2	1:A:27:ALA:O	1.38	1.04
1:A:28:ILE:CG2	1:A:30:ARG:HG2	1.87	1.03
1:A:96:ARG:HH12	1:A:113:ARG:HD3	1.11	1.03
1:A:95:PHE:O	1:A:96:ARG:CG	2.08	1.02
1:A:28:ILE:HG23	1:A:30:ARG:HG2	1.03	1.01
1:B:183:LEU:HD23	1:B:184:ILE:H	1.24	1.01
1:A:28:ILE:HG23	1:A:30:ARG:CG	1.93	0.99
1:A:191:TYR:HD1	1:A:198:MET:HG3	1.26	0.95
1:A:95:PHE:O	1:A:96:ARG:HG2	1.66	0.95
1:A:21:ILE:HG23	1:A:166:VAL:HG13	1.46	0.94
1:A:153:THR:HG22	1:A:170:VAL:CG1	1.97	0.94
1:A:28:ILE:HD13	1:A:28:ILE:O	1.66	0.93
1:A:154:ILE:HG13	1:A:155:ASN:ND2	1.84	0.93
1:A:96:ARG:NH1	1:A:113:ARG:HD3	1.83	0.92
1:A:184:ILE:HG22	1:A:190:ARG:NH1	1.85	0.92
1:A:79:GLU:HA	1:A:82:ARG:HE	1.31	0.92
1:A:183:LEU:HD23	1:A:184:ILE:H	1.34	0.92
1:B:202:VAL:HG12	1:B:254:LEU:HB3	1.52	0.91
1:A:77:THR:H	1:A:80:GLN:HE21	1.14	0.91
1:A:153:THR:HG22	1:A:170:VAL:HG11	1.54	0.90
1:B:280:MET:HE2	1:B:314:PRO:HD3	1.54	0.89
1:A:308:ALA:HB2	1:A:359:THR:HG23	1.55	0.88
1:A:212:ILE:HD12	1:A:212:ILE:H	1.35	0.87
1:A:244:GLN:HE22	1:A:303:PRO:HA	1.41	0.86
1:A:34:SER:HB3	1:A:38:LEU:HD21	1.57	0.86
1:B:183:LEU:HB2	1:B:216:THR:HG23	1.57	0.86
1:B:35:GLU:HA	1:B:35:GLU:OE1	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:HIS:CD2	1:A:27:ALA:O	2.28	0.86
1:A:94:ARG:HB3	1:A:97:LEU:HD23	1.58	0.86
1:A:154:ILE:HG13	1:A:155:ASN:HD22	1.40	0.84
1:A:96:ARG:HH22	1:A:113:ARG:HB3	1.42	0.83
1:B:170:VAL:HG12	1:B:171:GLY:H	1.45	0.82
1:A:304:ALA:HB2	1:A:355:LEU:HD12	1.61	0.81
1:B:308:ALA:HB2	1:B:359:THR:HG23	1.63	0.81
1:B:352:PRO:HG2	1:B:355:LEU:HD23	1.63	0.80
1:B:93:ARG:N	1:B:93:ARG:HD3	1.93	0.80
1:A:95:PHE:O	1:A:96:ARG:HG3	1.81	0.80
1:A:28:ILE:CG2	1:A:30:ARG:HE	1.95	0.79
1:A:191:TYR:CE1	1:A:198:MET:HG3	2.19	0.77
1:A:86:ARG:HG3	1:A:87:ASN:HD22	1.48	0.77
1:B:203:ARG:HB2	1:B:242:LEU:HD23	1.66	0.77
1:A:183:LEU:HD23	1:A:184:ILE:N	1.99	0.77
1:B:270:ARG:HD2	1:B:271:TYR:CE2	2.20	0.77
1:B:232:PRO:HB2	1:B:350:ALA:HB2	1.67	0.76
1:A:28:ILE:O	1:A:29:SER:O	2.03	0.76
1:A:402:ASN:HD22	1:A:403:ALA:N	1.83	0.76
1:A:270:ARG:HD2	1:A:271:TYR:CE2	2.21	0.76
1:B:302:ASN:HD22	1:B:303:PRO:HD2	1.51	0.76
1:A:26:HIS:O	1:A:27:ALA:C	2.25	0.75
1:B:202:VAL:CG1	1:B:254:LEU:HB3	2.16	0.74
1:A:170:VAL:HG12	1:A:171:GLY:H	1.53	0.74
1:A:92:GLY:C	1:A:93:ARG:HD2	2.08	0.74
1:A:94:ARG:CZ	1:A:97:LEU:CD2	2.66	0.73
1:A:153:THR:HG22	1:A:170:VAL:HG12	1.69	0.73
1:A:95:PHE:C	1:A:96:ARG:HG2	2.09	0.72
1:A:257:GLU:HG2	1:A:257:GLU:O	1.89	0.72
1:A:218:GLU:HB3	1:A:219:PRO:HD3	1.71	0.72
1:A:151:ASP:OD1	2:A:501:ATP:N3	2.22	0.72
1:B:142:SER:HB3	1:B:145:GLU:HG3	1.72	0.71
1:A:28:ILE:O	1:A:30:ARG:N	2.22	0.71
1:B:170:VAL:HG12	1:B:171:GLY:N	2.05	0.71
1:B:244:GLN:HE22	1:B:303:PRO:HA	1.56	0.71
1:B:151:ASP:OD1	2:B:502:ATP:C2	2.44	0.71
1:A:151:ASP:OD1	2:A:501:ATP:C2	2.44	0.71
1:A:270:ARG:HD2	1:A:271:TYR:HE2	1.56	0.70
1:A:72:VAL:HG22	1:A:109:VAL:HG22	1.72	0.70
1:B:34:SER:HB3	1:B:38:LEU:HD21	1.75	0.69
1:B:342:LEU:O	1:B:346:CYS:HB2	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:O	1:A:29:SER:N	2.22	0.69
1:B:204:PHE:O	1:B:208:LEU:HD12	1.92	0.69
1:B:93:ARG:HG2	1:B:94:ARG:H	1.56	0.69
1:A:378:TRP:HB3	1:B:299:MET:SD	2.32	0.69
1:B:95:PHE:O	1:B:96:ARG:HG2	1.92	0.69
1:B:27:ALA:O	1:B:29:SER:N	2.26	0.69
1:B:151:ASP:OD1	2:B:502:ATP:N3	2.26	0.68
1:A:96:ARG:NH2	1:A:113:ARG:HB3	2.06	0.68
1:A:94:ARG:CB	1:A:97:LEU:HD23	2.22	0.68
1:B:324:GLN:HG2	1:B:325:GLU:N	2.07	0.68
1:A:154:ILE:CG1	1:A:155:ASN:ND2	2.56	0.68
1:A:154:ILE:CG1	1:A:155:ASN:N	2.54	0.68
1:A:113:ARG:HG2	1:A:146:ASP:OD1	1.92	0.68
1:B:218:GLU:HB3	1:B:219:PRO:HD3	1.76	0.68
1:B:95:PHE:O	1:B:96:ARG:CG	2.42	0.68
1:A:149:ARG:HH11	1:A:149:ARG:HB3	1.59	0.67
1:B:35:GLU:CA	1:B:35:GLU:OE1	2.41	0.67
1:B:271:TYR:HE1	1:B:317:GLU:HG2	1.58	0.67
1:A:154:ILE:HG12	1:A:155:ASN:H	1.59	0.67
1:A:28:ILE:HG21	1:A:30:ARG:NE	2.10	0.67
1:A:154:ILE:HG12	1:A:155:ASN:N	2.10	0.67
1:A:28:ILE:HG21	1:A:30:ARG:HE	1.59	0.67
1:A:94:ARG:NE	1:A:97:LEU:HD23	2.10	0.66
1:A:94:ARG:CG	1:A:97:LEU:HD23	2.26	0.66
1:B:321:LYS:HE2	1:B:325:GLU:OE1	1.95	0.66
1:B:93:ARG:CD	1:B:93:ARG:H	1.99	0.66
1:B:26:HIS:O	1:B:27:ALA:C	2.34	0.65
1:A:199:LEU:O	1:A:202:VAL:HG12	1.97	0.65
1:A:420:PRO:O	1:A:424:LYS:HB2	1.96	0.64
1:A:184:ILE:CG2	1:A:185:GLY:N	2.60	0.64
1:A:358:LEU:HD23	1:A:385:LYS:HE2	1.79	0.64
1:B:191:TYR:CD1	1:B:198:MET:HG3	2.33	0.64
1:A:187:PRO:O	1:A:191:TYR:HD2	1.80	0.64
1:B:183:LEU:HB2	1:B:216:THR:CG2	2.28	0.64
1:B:195:PRO:HD2	1:B:230:ILE:HD11	1.80	0.64
1:B:153:THR:HG22	1:B:170:VAL:CG1	2.27	0.63
1:B:28:ILE:O	1:B:29:SER:C	2.36	0.63
1:A:391:ASP:O	1:A:395:LEU:HD13	1.97	0.63
1:A:219:PRO:O	1:A:223:LEU:HD12	1.99	0.63
1:A:232:PRO:HB2	1:A:350:ALA:HB2	1.79	0.63
1:A:151:ASP:N	2:A:501:ATP:O2'	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:HG2	1:B:382:GLU:OE2	1.97	0.63
1:A:271:TYR:HE1	1:A:317:GLU:HG2	1.63	0.63
1:B:144:GLU:HA	1:B:169:TYR:CD2	2.34	0.63
1:B:26:HIS:NE2	1:B:29:SER:HB3	2.14	0.63
1:A:160:SER:HB3	1:A:163:ASP:OD1	1.98	0.63
1:B:243:LEU:HA	1:B:248:GLY:HA2	1.81	0.63
2:A:501:ATP:O1B	2:A:501:ATP:H5'1	1.99	0.63
2:B:502:ATP:O1B	2:B:502:ATP:H5'1	1.99	0.62
1:B:44:LEU:HD23	1:B:84:LEU:HD23	1.81	0.62
1:A:37:ALA:O	1:A:40:VAL:HG13	1.99	0.62
1:A:24:GLU:HG2	1:A:25:GLN:N	2.14	0.62
1:A:299:MET:SD	1:B:378:TRP:HE3	2.22	0.62
1:B:93:ARG:CG	1:B:94:ARG:H	2.11	0.62
1:B:183:LEU:HD23	1:B:184:ILE:N	2.06	0.62
1:A:34:SER:CB	1:A:38:LEU:HD21	2.28	0.62
1:B:33:ILE:HG22	1:B:33:ILE:O	1.99	0.62
1:A:84:LEU:C	1:A:85:PHE:CD1	2.73	0.62
1:A:299:MET:SD	1:B:378:TRP:CE3	2.93	0.62
1:A:153:THR:HB	1:A:172:GLY:H	1.65	0.62
1:B:72:VAL:CG2	1:B:109:VAL:HG22	2.30	0.62
1:B:203:ARG:HB2	1:B:242:LEU:CD2	2.29	0.61
1:B:102:PHE:HB2	1:B:105:GLU:O	1.99	0.61
1:A:28:ILE:CG2	1:A:30:ARG:NE	2.64	0.61
1:A:28:ILE:O	1:A:28:ILE:CD1	2.44	0.61
1:B:153:THR:HG21	1:B:175:ASP:OD2	1.99	0.61
1:A:183:LEU:HB2	1:A:216:THR:HG23	1.82	0.61
1:B:244:GLN:NE2	1:B:303:PRO:HA	2.17	0.60
1:B:358:LEU:HD23	1:B:385:LYS:HE3	1.83	0.60
1:B:290:ASN:O	1:B:291:THR:C	2.40	0.60
1:B:372:ARG:HE	1:B:407:ARG:HH21	1.49	0.60
1:B:381:LEU:HD22	1:B:415:PHE:CE2	2.37	0.60
1:B:352:PRO:CG	1:B:355:LEU:HD23	2.32	0.60
1:B:30:ARG:HE	1:B:33:ILE:HG13	1.67	0.60
1:A:291:THR:O	1:A:295:ILE:HG12	2.02	0.60
1:A:101:MET:HG2	1:A:102:PHE:N	2.17	0.60
1:B:257:GLU:O	1:B:257:GLU:HG2	1.99	0.60
1:B:164:PHE:CD1	1:B:164:PHE:N	2.70	0.59
1:A:84:LEU:C	1:A:85:PHE:HD1	2.05	0.59
1:B:37:ALA:CB	1:B:107:ILE:HG12	2.32	0.59
1:A:195:PRO:HB2	1:A:230:ILE:HD11	1.84	0.59
1:A:67:PRO:HG2	1:A:70:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:O	1:A:81:VAL:HG23	2.03	0.59
1:A:77:THR:HB	1:A:80:GLN:H	1.68	0.59
1:A:213:SER:OG	1:A:215:GLU:HG3	2.03	0.59
1:B:55:GLY:O	1:B:58:VAL:HG13	2.03	0.59
1:A:52:TRP:CZ3	1:A:160:SER:HB2	2.38	0.58
1:B:360:ARG:O	1:B:364:GLN:HG2	2.03	0.58
1:B:53:LEU:HD12	1:B:71:ASP:O	2.03	0.58
1:B:332:ASP:O	1:B:336:LEU:HD22	2.03	0.58
1:A:138:ASN:HD22	1:A:138:ASN:N	2.02	0.58
1:A:381:LEU:HD23	1:A:415:PHE:CE2	2.39	0.58
1:B:151:ASP:N	2:B:502:ATP:O2'	2.32	0.58
1:B:96:ARG:HG3	1:B:97:LEU:N	2.18	0.58
1:B:164:PHE:N	1:B:164:PHE:HD1	2.02	0.58
1:B:20:VAL:HG23	1:B:167:ARG:HD3	1.86	0.58
1:A:87:ASN:HD22	1:A:87:ASN:N	2.01	0.58
1:B:414:GLU:O	1:B:418:SER:HB3	2.04	0.58
1:A:337:ALA:O	1:A:341:VAL:HG23	2.04	0.57
1:A:26:HIS:O	1:A:28:ILE:N	2.37	0.57
1:A:225:THR:O	1:A:227:LEU:N	2.37	0.57
1:B:21:ILE:HB	1:B:166:VAL:HG12	1.85	0.57
1:A:299:MET:SD	1:B:378:TRP:HB3	2.45	0.57
1:B:223:LEU:O	1:B:226:LEU:HB2	2.05	0.57
1:A:269:THR:HA	1:A:272:PHE:CE2	2.39	0.57
1:A:220:ILE:HB	1:A:221:PRO:HD3	1.87	0.57
1:B:153:THR:HG22	1:B:170:VAL:HG12	1.87	0.56
1:B:37:ALA:HB2	1:B:107:ILE:HG12	1.86	0.56
1:A:203:ARG:HB2	1:A:242:LEU:HD23	1.85	0.56
1:A:22:PRO:HD2	1:A:25:GLN:CG	2.35	0.56
1:A:358:LEU:O	1:A:362:ILE:HG13	2.05	0.56
1:B:378:TRP:HZ3	1:B:423:GLN:OE1	1.88	0.56
1:B:270:ARG:HD2	1:B:271:TYR:HE2	1.68	0.56
1:B:152:PHE:CD2	1:B:152:PHE:N	2.73	0.56
1:A:92:GLY:C	1:A:93:ARG:CD	2.75	0.56
1:B:302:ASN:ND2	1:B:303:PRO:HD2	2.20	0.56
1:B:34:SER:CB	1:B:38:LEU:HD21	2.36	0.56
1:A:95:PHE:C	1:A:96:ARG:CG	2.68	0.55
1:A:75:ASN:C	1:A:75:ASN:HD22	2.09	0.55
1:B:280:MET:HE1	1:B:314:PRO:HG3	1.88	0.55
1:A:196:VAL:HG23	1:A:230:ILE:HD13	1.89	0.55
1:A:212:ILE:HD13	1:A:258:TYR:OH	2.05	0.55
1:B:291:THR:O	1:B:295:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LEU:O	1:B:230:ILE:HB	2.07	0.55
1:B:152:PHE:CD1	1:B:181:ILE:HG22	2.41	0.55
1:A:96:ARG:HH12	1:A:113:ARG:CD	2.02	0.55
1:A:93:ARG:O	1:A:94:ARG:HB2	2.07	0.55
1:A:170:VAL:HG12	1:A:171:GLY:N	2.20	0.54
1:A:402:ASN:ND2	1:A:404:GLU:H	2.05	0.54
1:A:238:GLU:O	1:A:242:LEU:HG	2.07	0.54
1:B:387:ARG:NH1	1:B:416:GLN:HE22	2.04	0.54
1:A:170:VAL:HG21	1:A:184:ILE:HD11	1.90	0.54
1:B:38:LEU:N	1:B:38:LEU:HD23	2.22	0.54
1:A:84:LEU:O	1:A:85:PHE:CD1	2.60	0.54
1:A:184:ILE:CG2	1:A:190:ARG:HH12	2.06	0.54
1:A:244:GLN:HE22	1:A:303:PRO:CA	2.15	0.54
1:B:93:ARG:HG2	1:B:94:ARG:N	2.21	0.54
1:A:28:ILE:HG23	1:A:28:ILE:O	2.07	0.54
1:B:295:ILE:HD11	1:B:301:VAL:HG11	1.90	0.54
1:B:198:MET:HG2	1:B:220:ILE:HG12	1.91	0.53
1:B:370:SER:HA	1:B:408:LEU:HD11	1.91	0.53
1:A:198:MET:HG2	1:A:220:ILE:HG12	1.90	0.53
1:A:183:LEU:HB2	1:A:216:THR:CG2	2.38	0.53
1:B:356:THR:O	1:B:360:ARG:HG2	2.08	0.53
1:A:23:ARG:HB2	1:A:164:PHE:HB3	1.90	0.53
1:A:181:ILE:CD1	1:A:210:MET:HG3	2.38	0.53
1:A:86:ARG:HG3	1:A:87:ASN:ND2	2.18	0.53
1:B:170:VAL:CG1	1:B:171:GLY:H	2.20	0.53
1:B:368:ARG:HA	1:B:371:ARG:HD2	1.91	0.53
1:B:244:GLN:OE1	1:B:306:LEU:HD22	2.08	0.53
1:A:109:VAL:HG12	1:A:109:VAL:O	2.08	0.53
1:B:281:GLU:O	1:B:285:GLU:HG3	2.09	0.53
1:B:418:SER:O	1:B:423:GLN:NE2	2.31	0.53
1:A:367:LEU:O	1:A:370:SER:HB3	2.09	0.53
1:A:203:ARG:HB2	1:A:242:LEU:CD2	2.39	0.53
1:A:184:ILE:HG23	1:A:185:GLY:N	2.24	0.52
1:B:59:ARG:NH1	2:B:502:ATP:O1G	2.41	0.52
1:A:40:VAL:HG11	1:A:107:ILE:HG21	1.90	0.52
1:A:18:VAL:O	1:A:18:VAL:HG22	2.08	0.52
1:B:150:ARG:HH21	1:B:150:ARG:HG3	1.74	0.52
1:B:73:THR:HB	1:B:112:PHE:CE2	2.44	0.52
1:B:323:ALA:O	1:B:327:GLY:HA2	2.10	0.52
1:A:223:LEU:O	1:A:226:LEU:HB2	2.09	0.52
1:B:154:ILE:HG12	1:B:155:ASN:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:TRP:CZ3	1:B:423:GLN:OE1	2.62	0.52
1:A:280:MET:HE2	1:A:314:PRO:CG	2.39	0.52
1:B:23:ARG:HD2	1:B:164:PHE:HD2	1.75	0.52
1:A:94:ARG:HB3	1:A:97:LEU:HB3	1.91	0.52
1:A:280:MET:HE2	1:A:314:PRO:HG3	1.91	0.52
1:B:93:ARG:O	1:B:94:ARG:CB	2.56	0.52
1:A:94:ARG:NE	1:A:97:LEU:CD2	2.72	0.52
1:B:303:PRO:HG2	1:B:355:LEU:HD11	1.92	0.52
1:A:385:LYS:O	1:A:386:PHE:C	2.47	0.52
1:A:234:HIS:ND1	1:A:234:HIS:N	2.55	0.52
1:B:395:LEU:O	1:B:396:ARG:C	2.48	0.52
1:A:396:ARG:O	1:A:400:GLU:HG3	2.09	0.52
1:B:153:THR:HB	1:B:172:GLY:H	1.75	0.51
1:A:396:ARG:NH2	1:A:405:LEU:HD11	2.24	0.51
1:B:41:MET:HB3	1:B:51:ALA:HB1	1.91	0.51
1:B:402:ASN:C	1:B:402:ASN:HD22	2.14	0.51
1:A:150:ARG:HG3	1:A:150:ARG:HH21	1.76	0.51
1:B:199:LEU:O	1:B:202:VAL:HG23	2.10	0.51
1:A:365:LEU:HD12	1:A:389:ALA:HB2	1.92	0.51
1:A:383:HIS:CG	1:A:384:PRO:HD2	2.45	0.51
1:A:278:SER:O	1:A:282:ARG:HD3	2.10	0.51
1:B:27:ALA:O	1:B:28:ILE:C	2.49	0.51
1:B:23:ARG:HA	1:B:26:HIS:CE1	2.45	0.51
1:B:402:ASN:C	1:B:402:ASN:ND2	2.63	0.51
1:A:297:ASN:ND2	1:B:378:TRP:NE1	2.57	0.51
1:B:113:ARG:HD3	1:B:146:ASP:OD1	2.11	0.51
1:B:261:PHE:CE2	1:B:265:PHE:HB2	2.45	0.51
1:B:291:THR:HG23	1:B:301:VAL:HG21	1.93	0.50
1:A:417:VAL:HG12	1:B:416:GLN:NE2	2.26	0.50
1:B:158:TYR:O	1:B:166:VAL:HG23	2.11	0.50
1:B:183:LEU:CD2	1:B:184:ILE:H	2.10	0.50
1:B:415:PHE:CD2	1:B:415:PHE:O	2.64	0.50
1:B:304:ALA:HB2	1:B:355:LEU:HD12	1.92	0.50
1:B:271:TYR:CE1	1:B:317:GLU:HG2	2.44	0.50
1:B:325:GLU:HG2	1:B:326:SER:N	2.26	0.50
1:A:150:ARG:HD2	1:A:156:SER:OG	2.12	0.50
1:B:233:ALA:HA	1:B:350:ALA:HB3	1.94	0.50
1:A:402:ASN:HD21	1:A:404:GLU:HB3	1.76	0.50
1:A:143:ILE:HD13	1:A:143:ILE:O	2.11	0.50
1:B:302:ASN:O	1:B:305:PHE:HB3	2.12	0.50
1:A:358:LEU:HD23	1:A:385:LYS:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLU:O	1:A:37:ALA:N	2.41	0.50
1:A:181:ILE:HD11	1:A:210:MET:HG3	1.92	0.50
1:B:381:LEU:HD22	1:B:415:PHE:HE2	1.77	0.50
1:A:55:GLY:O	1:A:56:GLY:C	2.50	0.50
1:A:413:GLY:O	1:B:417:VAL:HG11	2.11	0.50
1:A:410:LYS:O	1:A:414:GLU:HG3	2.11	0.49
1:A:113:ARG:HG3	1:A:149:ARG:HG3	1.94	0.49
1:A:218:GLU:O	1:A:221:PRO:HD2	2.11	0.49
1:B:280:MET:O	1:B:284:ILE:HG13	2.13	0.49
1:B:219:PRO:CB	1:B:223:LEU:HD12	2.43	0.49
1:B:244:GLN:NE2	1:B:303:PRO:CA	2.76	0.49
1:A:271:TYR:HB2	1:A:280:MET:HE1	1.93	0.49
1:B:197:ARG:NH1	2:B:502:ATP:N1	2.60	0.49
1:B:213:SER:HB3	1:B:216:THR:OG1	2.11	0.49
1:A:61:LEU:HG	1:A:67:PRO:HG3	1.95	0.49
1:B:23:ARG:HB3	1:B:164:PHE:HB3	1.94	0.49
1:A:202:VAL:HG11	1:A:255:LEU:HD21	1.95	0.49
1:B:30:ARG:HE	1:B:33:ILE:CG1	2.26	0.49
1:A:28:ILE:HD12	1:A:30:ARG:HG2	1.95	0.48
1:B:73:THR:HA	1:B:110:ALA:O	2.13	0.48
1:A:402:ASN:HD22	1:A:402:ASN:C	2.12	0.48
1:A:202:VAL:HG11	1:A:255:LEU:CD2	2.43	0.48
1:A:26:HIS:C	1:A:26:HIS:CD2	2.86	0.48
1:B:405:LEU:C	1:B:407:ARG:N	2.64	0.48
1:B:405:LEU:O	1:B:406:GLN:C	2.51	0.48
1:B:179:GLY:C	1:B:210:MET:HG2	2.34	0.48
1:A:22:PRO:HD2	1:A:25:GLN:CD	2.33	0.48
1:B:283:ILE:CG2	1:B:284:ILE:N	2.76	0.48
1:A:385:LYS:O	1:A:387:ARG:N	2.47	0.48
1:B:184:ILE:HG22	1:B:185:GLY:N	2.28	0.48
1:B:311:PHE:C	1:B:314:PRO:HD2	2.34	0.48
1:B:26:HIS:O	1:B:26:HIS:CD2	2.67	0.48
1:A:174:LYS:HE2	1:A:178:ASP:OD2	2.12	0.48
1:A:85:PHE:O	1:A:88:CYS:HB2	2.14	0.48
1:A:251:THR:HG22	1:A:251:THR:O	2.14	0.48
1:A:20:VAL:HG23	1:A:167:ARG:HD3	1.96	0.48
1:A:187:PRO:HB3	1:A:191:TYR:HE2	1.79	0.48
1:B:325:GLU:O	1:B:326:SER:C	2.51	0.47
1:A:184:ILE:HG22	1:A:185:GLY:H	1.79	0.47
1:B:50:GLU:HG2	1:B:52:TRP:HE1	1.79	0.47
1:B:66:LYS:HA	1:B:67:PRO:HD2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:O	1:B:292:ASP:HB2	2.14	0.47
1:A:94:ARG:CZ	1:A:97:LEU:HD21	2.43	0.47
1:A:72:VAL:CG2	1:A:109:VAL:HG22	2.43	0.47
1:A:280:MET:HG3	1:A:313:TYR:HB2	1.95	0.47
1:A:419:ALA:HB1	1:A:421:PRO:HD2	1.97	0.47
1:A:152:PHE:CD2	1:A:152:PHE:N	2.83	0.47
1:A:208:LEU:HD13	1:A:210:MET:CE	2.44	0.47
1:A:58:VAL:O	1:A:62:LEU:HD12	2.15	0.47
1:A:391:ASP:O	1:A:394:ALA:HB3	2.15	0.47
1:A:246:GLY:HA2	1:A:292:ASP:HA	1.96	0.47
1:A:312:TRP:CE2	1:A:316:LEU:HD22	2.50	0.47
1:A:195:PRO:O	1:A:198:MET:HB2	2.15	0.47
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.48	0.47
1:A:94:ARG:HG3	1:A:97:LEU:HD23	1.97	0.47
1:B:149:ARG:O	2:B:502:ATP:C2	2.68	0.47
1:B:52:TRP:HA	1:B:159:TYR:O	2.15	0.46
1:B:158:TYR:O	1:B:166:VAL:HA	2.15	0.46
1:A:268:ILE:O	1:A:269:THR:C	2.53	0.46
1:A:371:ARG:O	1:A:373:GLN:N	2.49	0.46
1:A:243:LEU:HA	1:A:248:GLY:HA2	1.98	0.46
1:A:97:LEU:HG	1:A:97:LEU:O	2.16	0.46
1:B:224:ALA:O	1:B:226:LEU:N	2.48	0.46
1:B:182:ARG:HG2	1:B:183:LEU:O	2.15	0.46
1:A:278:SER:HB2	1:A:279:PRO:HD2	1.98	0.46
1:B:268:ILE:HD11	1:B:310:MET:HB3	1.97	0.46
1:B:72:VAL:HG23	1:B:109:VAL:HG22	1.98	0.46
1:B:305:PHE:O	1:B:306:LEU:C	2.53	0.46
1:A:387:ARG:HA	1:A:387:ARG:HD3	1.59	0.46
1:B:387:ARG:HH12	1:B:416:GLN:HE22	1.63	0.46
1:A:195:PRO:HB2	1:A:227:LEU:HD23	1.97	0.45
1:A:27:ALA:C	1:A:29:SER:H	2.19	0.45
1:B:212:ILE:HG22	1:B:213:SER:O	2.17	0.45
1:B:56:GLY:O	1:B:59:ARG:HB3	2.17	0.45
1:B:30:ARG:NE	1:B:33:ILE:HD11	2.31	0.45
1:A:52:TRP:CE3	1:A:160:SER:HB2	2.51	0.45
1:A:158:TYR:O	1:A:166:VAL:HA	2.17	0.45
1:B:26:HIS:C	1:B:26:HIS:CD2	2.90	0.45
1:B:278:SER:HB2	1:B:279:PRO:CD	2.46	0.45
1:B:260:LEU:O	1:B:263:PRO:HD2	2.17	0.45
1:A:280:MET:O	1:A:284:ILE:HG13	2.17	0.45
1:B:236:PHE:HA	1:B:349:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:HD23	1:A:226:LEU:CD1	2.47	0.44
1:A:381:LEU:HD23	1:A:415:PHE:CD2	2.51	0.44
1:B:247:TYR:O	1:B:249:TYR:N	2.50	0.44
1:A:219:PRO:HB3	1:A:223:LEU:CD1	2.48	0.44
1:A:152:PHE:CD1	1:A:181:ILE:HG23	2.53	0.44
1:A:312:TRP:NE1	1:A:316:LEU:HD22	2.32	0.44
1:B:266:PRO:O	1:B:268:ILE:N	2.50	0.44
1:A:84:LEU:HD23	1:A:85:PHE:CE1	2.52	0.44
1:B:21:ILE:HG13	1:B:166:VAL:HG13	1.99	0.44
1:B:232:PRO:CB	1:B:350:ALA:HB2	2.44	0.44
1:A:427:LEU:HA	1:A:427:LEU:HD23	1.77	0.44
1:A:408:LEU:N	1:A:408:LEU:HD23	2.31	0.44
1:B:244:GLN:HE22	1:B:303:PRO:CA	2.27	0.44
1:A:402:ASN:O	1:A:406:GLN:HB2	2.17	0.44
1:A:83:LYS:HG2	1:A:86:ARG:HH21	1.83	0.44
1:B:36:ASN:O	1:B:102:PHE:CZ	2.71	0.44
1:B:261:PHE:CD2	1:B:261:PHE:C	2.91	0.44
1:A:289:LYS:O	1:A:292:ASP:HB2	2.18	0.44
1:B:280:MET:O	1:B:280:MET:HG2	2.16	0.43
1:B:153:THR:HG22	1:B:170:VAL:HG11	1.99	0.43
1:B:364:GLN:HA	1:B:364:GLN:HE21	1.83	0.43
1:A:85:PHE:N	1:A:85:PHE:CD1	2.86	0.43
1:A:152:PHE:CZ	1:A:201:ALA:HA	2.53	0.43
1:B:41:MET:HB3	1:B:51:ALA:CB	2.48	0.43
1:B:290:ASN:C	1:B:292:ASP:N	2.68	0.43
1:A:368:ARG:NH1	1:A:380:LEU:HD11	2.33	0.43
1:B:59:ARG:NE	1:B:208:LEU:HD21	2.33	0.43
1:A:20:VAL:O	1:A:20:VAL:HG13	2.17	0.43
1:A:235:LEU:O	1:A:239:SER:HB3	2.18	0.43
1:A:106:ILE:O	1:A:107:ILE:HD13	2.18	0.43
1:A:361:ASP:O	1:A:365:LEU:HG	2.19	0.43
1:A:79:GLU:HG3	1:A:82:ARG:HH21	1.83	0.43
1:B:268:ILE:HD13	1:B:284:ILE:HD11	2.01	0.43
1:B:144:GLU:HA	1:B:169:TYR:CE2	2.53	0.43
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.61	0.43
1:A:418:SER:O	1:A:423:GLN:NE2	2.45	0.43
1:A:37:ALA:O	1:A:40:VAL:CG1	2.65	0.43
1:B:185:GLY:H	1:B:190:ARG:NH1	2.17	0.43
1:B:339:ASN:O	1:B:343:ASP:HB2	2.18	0.43
1:A:28:ILE:CG2	1:A:30:ARG:CG	2.72	0.43
1:A:94:ARG:HB3	1:A:97:LEU:CD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLY:C	1:B:288:LEU:HD13	2.39	0.43
1:A:151:ASP:N	1:A:151:ASP:OD1	2.51	0.43
1:A:416:GLN:NE2	1:B:417:VAL:HG12	2.34	0.43
1:A:368:ARG:CZ	1:A:380:LEU:HD11	2.49	0.43
1:B:264:LEU:O	1:B:266:PRO:HD2	2.18	0.43
1:A:415:PHE:CD2	1:A:415:PHE:O	2.72	0.43
1:B:268:ILE:CD1	1:B:310:MET:HB3	2.49	0.42
1:A:230:ILE:HG23	1:A:231:PRO:HD2	2.02	0.42
1:A:86:ARG:CG	1:A:87:ASN:HD22	2.25	0.42
1:A:421:PRO:HD3	1:B:290:ASN:ND2	2.34	0.42
1:B:406:GLN:O	1:B:409:VAL:HB	2.18	0.42
1:B:315:LEU:HA	1:B:341:VAL:HG21	2.00	0.42
1:B:251:THR:O	1:B:255:LEU:HG	2.19	0.42
1:B:238:GLU:O	1:B:242:LEU:HD12	2.19	0.42
1:B:295:ILE:HD11	1:B:301:VAL:CG1	2.48	0.42
1:B:219:PRO:O	1:B:223:LEU:HD12	2.19	0.42
1:A:182:ARG:HG3	1:A:182:ARG:HH11	1.85	0.42
1:A:154:ILE:HG13	1:A:155:ASN:N	2.34	0.42
1:B:364:GLN:HA	1:B:364:GLN:NE2	2.34	0.42
1:B:208:LEU:H	1:B:208:LEU:HD12	1.84	0.42
1:A:179:GLY:C	1:A:210:MET:HB2	2.39	0.42
1:B:402:ASN:ND2	1:B:404:GLU:H	2.18	0.42
1:A:383:HIS:ND1	1:A:384:PRO:HD2	2.34	0.42
1:B:170:VAL:CG1	1:B:171:GLY:N	2.75	0.42
1:B:304:ALA:HB2	1:B:355:LEU:CD1	2.50	0.42
1:A:280:MET:HA	1:A:313:TYR:CD2	2.53	0.42
1:B:138:ASN:OD1	1:B:138:ASN:N	2.52	0.42
1:A:305:PHE:O	1:A:306:LEU:C	2.57	0.42
1:B:93:ARG:CG	1:B:94:ARG:N	2.79	0.42
1:B:224:ALA:O	1:B:225:THR:C	2.58	0.42
1:B:103:GLY:O	1:B:105:GLU:N	2.53	0.42
1:A:269:THR:HA	1:A:272:PHE:CD2	2.54	0.42
1:A:150:ARG:NH2	1:A:150:ARG:HG3	2.34	0.42
1:B:316:LEU:O	1:B:319:ALA:HB3	2.20	0.42
1:B:94:ARG:HA	1:B:94:ARG:HD2	2.00	0.42
1:B:283:ILE:HG23	1:B:284:ILE:N	2.35	0.42
1:B:354:ARG:NH1	1:B:355:LEU:HD21	2.35	0.42
1:A:54:VAL:HG22	1:A:73:THR:HG22	2.01	0.42
1:A:375:LYS:H	1:A:375:LYS:HD2	1.85	0.42
1:B:275:ASN:ND2	1:B:277:ASP:H	2.18	0.42
1:A:402:ASN:ND2	1:A:404:GLU:N	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:HA	1:B:405:LEU:HD23	1.75	0.42
1:B:402:ASN:HD21	1:B:404:GLU:HB3	1.85	0.42
1:A:280:MET:CE	1:A:314:PRO:HG3	2.50	0.41
1:B:186:ASN:ND2	1:B:188:GLU:HB3	2.35	0.41
1:A:184:ILE:HG22	1:A:185:GLY:N	2.35	0.41
1:B:152:PHE:H	1:B:152:PHE:HD2	1.67	0.41
1:B:359:THR:O	1:B:360:ARG:C	2.56	0.41
1:B:391:ASP:O	1:B:394:ALA:HB3	2.20	0.41
1:B:45:ASN:HA	1:B:45:ASN:HD22	1.66	0.41
1:A:307:PHE:O	1:A:308:ALA:C	2.55	0.41
1:A:37:ALA:CB	1:A:107:ILE:HG13	2.50	0.41
1:B:260:LEU:C	1:B:263:PRO:HD2	2.41	0.41
1:A:171:GLY:O	1:A:172:GLY:C	2.59	0.41
1:A:152:PHE:CZ	1:A:201:ALA:HB2	2.56	0.41
1:B:61:LEU:HD23	1:B:67:PRO:HD3	2.03	0.41
1:A:364:GLN:HA	1:A:364:GLN:HE21	1.85	0.41
1:A:286:GLN:HA	1:A:286:GLN:NE2	2.35	0.41
1:A:315:LEU:HD22	1:A:363:TRP:CE3	2.56	0.41
1:A:191:TYR:CE1	1:A:198:MET:CG	2.99	0.41
1:A:385:LYS:O	1:A:388:ALA:N	2.54	0.41
1:B:37:ALA:HB2	1:B:107:ILE:CG1	2.49	0.41
1:B:202:VAL:O	1:B:205:ALA:HB3	2.20	0.41
1:A:372:ARG:NH1	1:A:408:LEU:CD2	2.84	0.41
1:A:351:ILE:HA	1:A:352:PRO:HD3	1.87	0.41
1:B:345:ALA:C	1:B:347:ARG:H	2.23	0.41
1:A:372:ARG:HA	1:A:372:ARG:HD2	1.80	0.41
1:A:378:TRP:CE2	1:B:297:ASN:ND2	2.89	0.40
1:B:67:PRO:HG3	1:B:70:PHE:CZ	2.55	0.40
1:A:194:ASP:HB3	1:A:197:ARG:HG3	2.03	0.40
1:B:184:ILE:HG22	1:B:190:ARG:HH12	1.84	0.40
1:B:235:LEU:HD13	1:B:264:LEU:HD22	2.02	0.40
1:B:96:ARG:CG	1:B:97:LEU:N	2.82	0.40
1:A:365:LEU:HD12	1:A:389:ALA:CB	2.51	0.40
1:A:413:GLY:O	1:A:416:GLN:HG2	2.22	0.40
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.76	0.40
1:A:196:VAL:CG2	1:A:230:ILE:HD13	2.49	0.40
1:A:400:GLU:O	1:A:401:ARG:C	2.57	0.40
1:A:302:ASN:HD21	1:A:385:LYS:HE3	1.87	0.40
1:A:203:ARG:HD3	1:A:242:LEU:HD23	2.02	0.40
1:A:90:LEU:H	1:A:90:LEU:CD2	2.35	0.40
1:B:218:GLU:N	1:B:219:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ALA:O	1:B:341:VAL:HG23	2.22	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	384/415 (92%)	334 (87%)	41 (11%)	9 (2%)	8	39
1	B	384/415 (92%)	333 (87%)	40 (10%)	11 (3%)	6	34
All	All	768/830 (92%)	667 (87%)	81 (10%)	20 (3%)	7	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ILE
1	A	248	GLY
1	B	93	ARG
1	B	94	ARG
1	B	97	LEU
1	B	104	PRO
1	B	248	GLY
1	A	172	GLY
1	A	226	LEU
1	B	151	ASP
1	A	29	SER
1	B	172	GLY
1	B	327	GLY
1	B	267	THR
1	A	112	PHE
1	A	421	PRO
1	B	56	GLY

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Mol	Chain	Res	Type
1	B	92	GLY
1	A	56	GLY
1	A	327	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	334/358 (93%)	284 (85%)	50 (15%)	3 17
1	B	334/358 (93%)	276 (83%)	58 (17%)	2 11
All	All	668/716 (93%)	560 (84%)	108 (16%)	3 14

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	28	ILE
1	A	29	SER
1	A	32	ASP
1	A	40	VAL
1	A	53	LEU
1	A	54	VAL
1	A	71	ASP
1	A	72	VAL
1	A	73	THR
1	A	75	ASN
1	A	82	ARG
1	A	84	LEU
1	A	87	ASN
1	A	90	LEU
1	A	93	ARG
1	A	100	VAL
1	A	101	MET
1	A	106	ILE
1	A	138	ASN

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Mol	Chain	Res	Type
1	A	140	PHE
1	A	142	SER
1	A	143	ILE
1	A	149	ARG
1	A	151	ASP
1	A	154	ILE
1	A	156	SER
1	A	161	VAL
1	A	166	VAL
1	A	176	LEU
1	A	184	ILE
1	A	208	LEU
1	A	210	MET
1	A	212	ILE
1	A	215	GLU
1	A	226	LEU
1	A	234	HIS
1	A	256	CYS
1	A	262	GLN
1	A	277	ASP
1	A	283	ILE
1	A	291	THR
1	A	317	GLU
1	A	329	THR
1	A	355	LEU
1	A	364	GLN
1	A	375	LYS
1	A	381	LEU
1	A	387	ARG
1	A	402	ASN
1	B	20	VAL
1	B	21	ILE
1	B	24	GLU
1	B	26	HIS
1	B	30	ARG
1	B	35	GLU
1	B	38	LEU
1	B	50	GLU
1	B	54	VAL
1	B	58	VAL
1	B	93	ARG
1	B	100	VAL

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Mol	Chain	Res	Type
1	B	104	PRO
1	B	107	ILE
1	B	113	ARG
1	B	138	ASN
1	B	139	ILE
1	B	148	GLN
1	B	149	ARG
1	B	152	PHE
1	B	154	ILE
1	B	156	SER
1	B	163	ASP
1	B	164	PHE
1	B	184	ILE
1	B	189	THR
1	B	202	VAL
1	B	208	LEU
1	B	210	MET
1	B	213	SER
1	B	215	GLU
1	B	225	THR
1	B	226	LEU
1	B	254	LEU
1	B	268	ILE
1	B	269	THR
1	B	270	ARG
1	B	275	ASN
1	B	277	ASP
1	B	298	ASP
1	B	300	ARG
1	B	302	ASN
1	B	316	LEU
1	B	324	GLN
1	B	329	THR
1	B	336	LEU
1	B	342	LEU
1	B	343	ASP
1	B	346	CYS
1	B	371	ARG
1	B	372	ARG
1	B	380	LEU
1	B	382	GLU
1	B	385	LYS

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Mol	Chain	Res	Type
1	B	402	ASN
1	B	405	LEU
1	B	406	GLN
1	B	418	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	45	ASN
1	A	75	ASN
1	A	80	GLN
1	A	87	ASN
1	A	155	ASN
1	A	244	GLN
1	A	275	ASN
1	A	286	GLN
1	A	290	ASN
1	A	302	ASN
1	A	364	GLN
1	A	402	ASN
1	A	406	GLN
1	A	416	GLN
1	B	17	GLN
1	B	26	HIS
1	B	45	ASN
1	B	87	ASN
1	B	155	ASN
1	B	244	GLN
1	B	275	ASN
1	B	290	ASN
1	B	302	ASN
1	B	364	GLN
1	B	373	GLN
1	B	402	ASN
1	B	416	GLN

5.3.3 RNA

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 4 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
2	ATP	A	501	3	24,33,33	1.10	2 (8%)	31,52,52	1.72	2 (6%)
2	ATP	B	502	3	24,33,33	1.09	2 (8%)	31,52,52	1.72	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	501	3	-	0/18/38/38	0/3/3/3
2	ATP	B	502	3	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	ATP	O4'-C1'	2.24	1.44	1.41
2	A	501	ATP	O4'-C1'	2.28	1.44	1.41
2	B	502	ATP	C5-C4	3.55	1.48	1.40
2	A	501	ATP	C5-C4	3.58	1.48	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	ATP	N3-C2-N1	-6.82	123.68	128.89
2	B	502	ATP	N3-C2-N1	-6.81	123.68	128.89
2	A	501	ATP	C4-C5-N7	-3.45	106.31	109.48
2	B	502	ATP	C4-C5-N7	-3.39	106.36	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ATP	4	0
2	B	502	ATP	7	0

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

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, 95^{th} 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	388/415 (93%)	0.10	5 (1%)	79	74	75, 122, 169, 219	0
1	B	388/415 (93%)	0.04	2 (0%)	91	90	90, 123, 170, 205	0
All	All	776/830 (93%)	0.07	7 (0%)	85	82	75, 123, 170, 219	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17	GLN	8.5
1	A	18	VAL	2.9
1	A	97	LEU	2.6
1	B	375	LYS	2.5
1	A	328	LEU	2.4
1	B	140	PHE	2.3
1	A	98	ALA	2.3

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, 95^{th} 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
2	ATP	B	502	31/31	0.55	0.86	9.07	240,245,246,248	0
2	ATP	A	501	31/31	0.64	0.64	8.61	234,236,242,242	0
3	MG	B	601	1/1	0.24	0.48	-	93,93,93,93	0
3	MG	A	600	1/1	0.67	0.13	-	117,117,117,117	0

6.5 Other polymers (i)

There are no such residues in this entry.