Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:42 AM GMT

PDB ID	:	3BUZ
Title	:	Crystal structure of ia-bTAD-actin complex
Authors	:	Tsuge, H.; Nagahama, M.; Oda, M.; Iwamoto, S.; Utsunomiya, H.; Marquez, V.E.; Katunuma, N.; Nishizawa, M.; Sakurai, J.
Deposited on	:	2008-01-04
Resolution	:	2.81 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 ⓘ symbol.

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

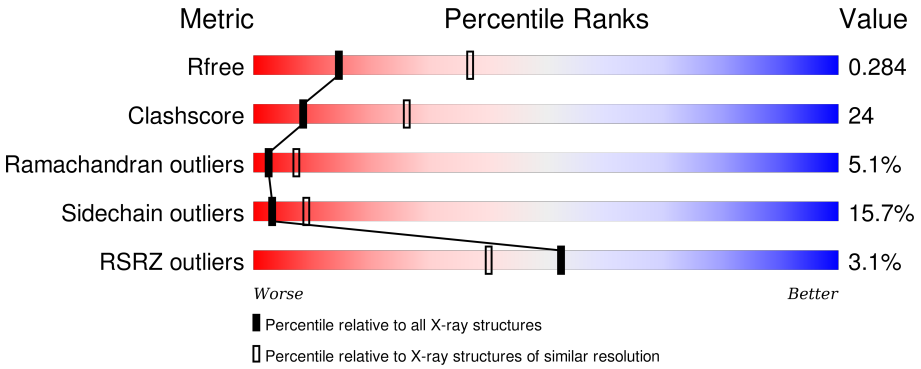
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	413	3%, 50%, 38%, 11%
2	B	375	3%, 48%, 36%, 12%

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
6	LAR	B	901	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6364 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 Iota toxin component Ia.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3364	2146	553	662	3			

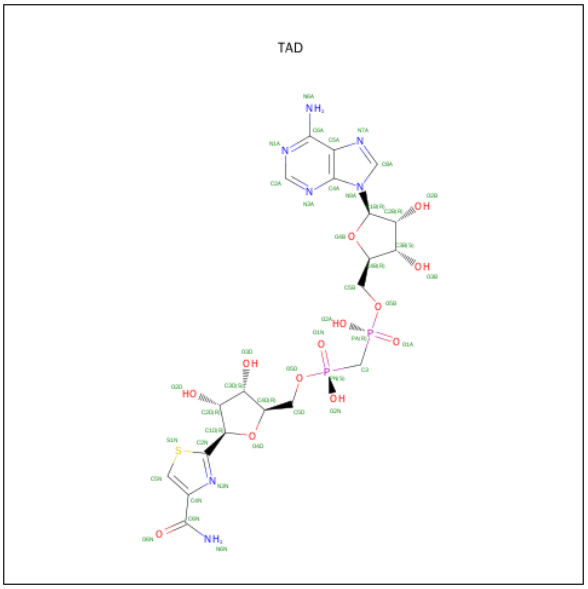
- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	360	Total	C	N	O	S	0	0	0
			2817	1785	474	539	19			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

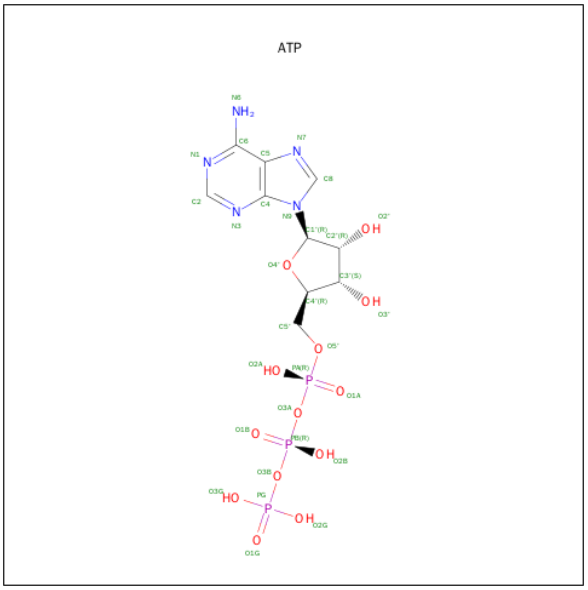
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: TAD) (formula: $C_{20}H_{27}N_7O_{13}P_2S$).



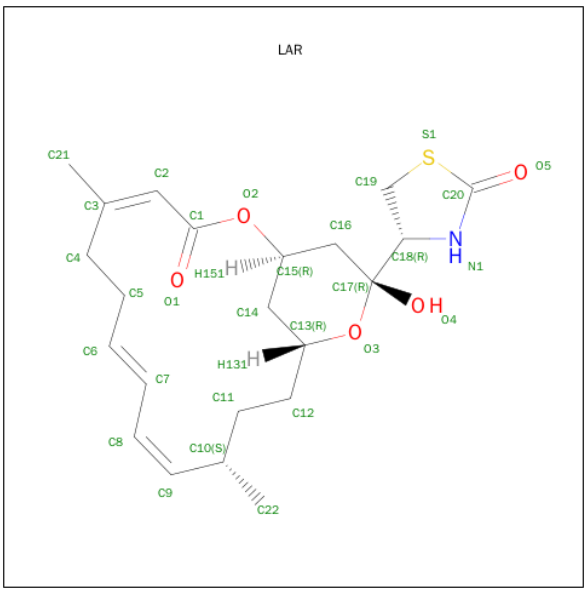
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			43	20	7	13	2	1		

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



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

- Molecule 6 is LATRUNCULIN A (three-letter code: LAR) (formula: $C_{22}H_{31}NO_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			29	22	1	5	1		

- Molecule 7 is water.

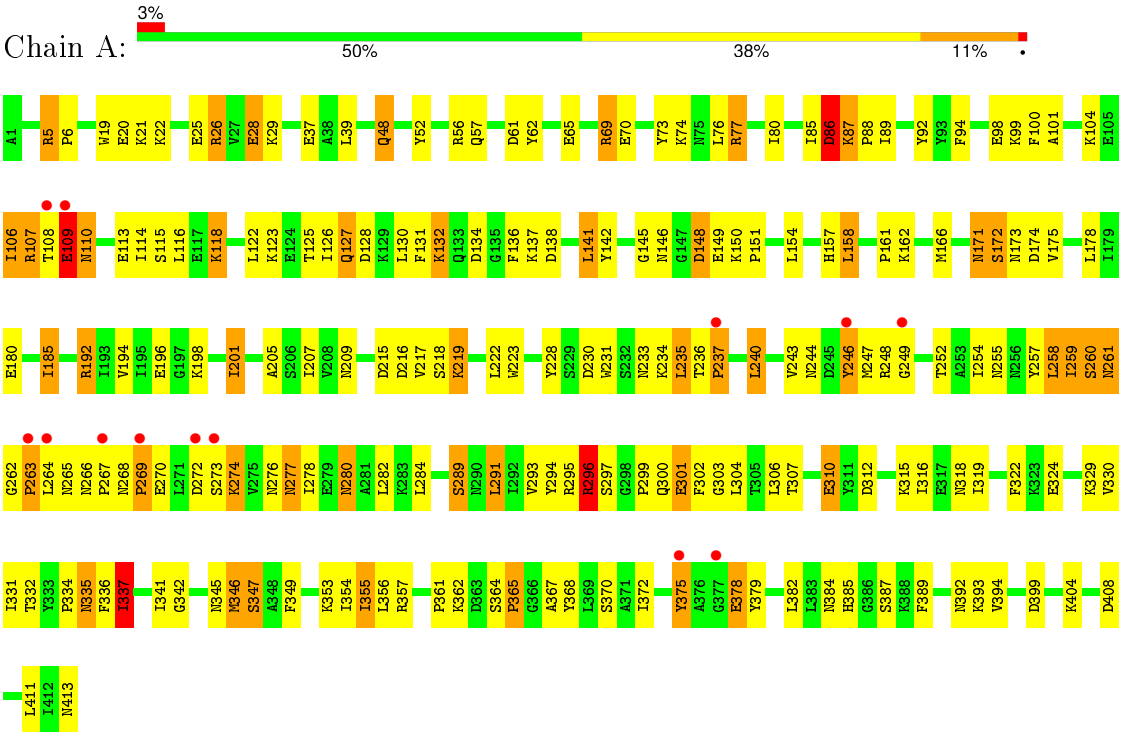
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	38	Total	O	0	0
			38	38		

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.

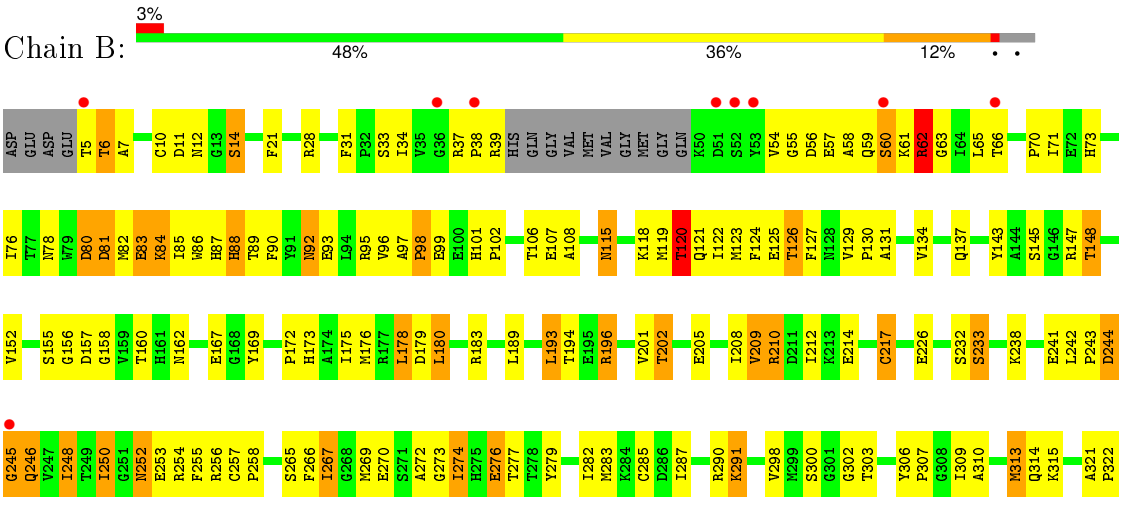
- Molecule 1: Iota toxin component Ia

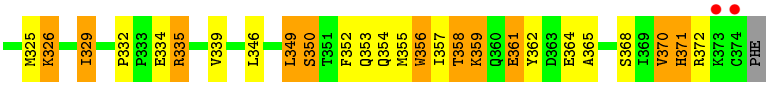
Chain A:



- Molecule 2: Actin, alpha skeletal muscle

Chain B:




M325
K326
I329
P332
P333
E334
R335
V339
L346
L349
S350
T351
F352
Q353
Q354
M355
W356
I357
T358
K359
Q360
E361
Y362
D363
E364
A365
S368
I369
V370
H371
R372
K373
C374
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.01Å 126.34Å 147.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.69 – 2.81 36.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.69-2.81) 99.1 (36.69-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.02 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.298 0.218 , 0.284	Depositor DCC
R_{free} test set	1333 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 26386 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: TAD, CA, ATP, LAR

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	1.08	6/3433 (0.2%)	1.06	9/4637 (0.2%)
2	B	1.03	2/2877 (0.1%)	1.02	8/3899 (0.2%)
All	All	1.06	8/6310 (0.1%)	1.04	17/8536 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	GLU	CG-CD	6.19	1.61	1.51
1	A	215	ASP	C-N	6.00	1.47	1.34
1	A	86	ASP	CB-CG	5.68	1.63	1.51
1	A	86	ASP	CA-CB	5.30	1.65	1.53
1	A	98	GLU	CG-CD	5.25	1.59	1.51
2	B	217	CYS	CB-SG	-5.22	1.73	1.81
1	A	138	ASP	CB-CG	5.11	1.62	1.51
2	B	276	GLU	CD-OE2	5.06	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	296	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	5	ARG	NE-CZ-NH2	-7.13	116.74	120.30
2	B	60	SER	C-N-CA	7.04	139.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ASP	CB-CG-OD2	7.04	124.64	118.30
2	B	62	ARG	O-C-N	-7.00	111.29	123.20
2	B	178	LEU	CA-CB-CG	6.75	130.82	115.30
1	A	77	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	5	ARG	CG-CD-NE	-5.95	99.31	111.80
2	B	62	ARG	CA-C-N	5.75	127.69	116.20
2	B	147	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	116	LEU	CA-CB-CG	5.67	128.33	115.30
2	B	349	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	291	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	162	LYS	C-N-CA	-5.26	108.55	121.70
2	B	335	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	337	ILE	CB-CA-C	5.16	121.92	111.60
2	B	245	GLY	N-CA-C	5.08	125.81	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	337	ILE	Peptide
1	A	85	ILE	Peptide

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	3364	0	3346	164	0
2	B	2817	0	2793	141	0
3	B	1	0	0	0	0
4	A	43	0	25	3	0
5	B	31	0	12	3	0
6	B	29	0	31	5	0
7	A	41	0	0	4	0
7	B	38	0	0	2	0
All	All	6364	0	6207	300	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 24.

All (300) 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:296:ARG:HH11	1:A:296:ARG:CG	1.64	1.09
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.10	1.07
2:B:59:GLN:HB2	6:B:901:LAR:H223	1.33	1.05
2:B:209:VAL:HA	2:B:212:ILE:HD12	1.43	0.97
1:A:107:ARG:HG2	1:A:114:ILE:HG12	1.47	0.96
2:B:193:LEU:O	2:B:196:ARG:HB3	1.66	0.95
1:A:146:ASN:HA	1:A:196:GLU:OE2	1.68	0.92
2:B:314:GLN:HB2	2:B:329:ILE:HG12	1.51	0.92
1:A:132:LYS:NZ	1:A:357:ARG:HH11	1.69	0.89
2:B:88:HIS:CE1	2:B:93:GLU:HG2	2.09	0.87
1:A:240:LEU:O	1:A:243:VAL:HG12	1.73	0.87
1:A:132:LYS:HZ3	1:A:357:ARG:HH11	0.87	0.86
1:A:146:ASN:HD22	1:A:196:GLU:HG2	1.39	0.85
1:A:132:LYS:HZ3	1:A:357:ARG:NH1	1.73	0.83
2:B:267:ILE:HG23	2:B:267:ILE:O	1.78	0.82
2:B:242:LEU:CD2	2:B:248:ILE:HG23	2.09	0.82
1:A:296:ARG:HD2	1:A:349:PHE:CD1	2.16	0.81
2:B:332:PRO:O	2:B:335:ARG:HB2	1.81	0.80
1:A:86:ASP:O	1:A:87:LYS:HD3	1.82	0.80
1:A:254:ILE:O	1:A:258:LEU:HD23	1.82	0.79
2:B:37:ARG:O	2:B:65:LEU:HB2	1.83	0.79
1:A:296:ARG:HD2	1:A:349:PHE:HD1	1.48	0.79
2:B:59:GLN:HB2	6:B:901:LAR:C22	2.11	0.79
2:B:267:ILE:CG2	2:B:267:ILE:O	2.30	0.79
1:A:185:ILE:HD12	1:A:205:ALA:HB1	1.65	0.78
2:B:5:THR:HG23	2:B:6:THR:H	1.48	0.78
1:A:100:PHE:O	1:A:101:ALA:HB3	1.82	0.77
1:A:5:ARG:NH2	1:A:88:PRO:O	2.18	0.77
1:A:274:LYS:O	1:A:278:ILE:HG13	1.85	0.76
1:A:268:ASN:O	1:A:270:GLU:N	2.19	0.75
2:B:115:ASN:H	2:B:115:ASN:HD22	1.35	0.74
1:A:346:MET:HG3	1:A:349:PHE:CZ	2.23	0.74
1:A:240:LEU:O	1:A:244:ASN:ND2	2.21	0.72
1:A:171:ASN:HD22	1:A:172:SER:H	1.35	0.72
1:A:296:ARG:NH1	1:A:296:ARG:CG	2.39	0.72
1:A:145:GLY:O	1:A:150:LYS:NZ	2.23	0.72
2:B:82:MET:O	2:B:85:ILE:HB	1.90	0.71
1:A:331:ILE:HD12	1:A:332:THR:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:SER:O	2:B:233:SER:HB3	1.92	0.70
2:B:98:PRO:O	2:B:129:VAL:HG12	1.92	0.69
2:B:61:LYS:O	2:B:63:GLY:N	2.26	0.68
2:B:59:GLN:CB	6:B:901:LAR:H223	2.17	0.68
2:B:12:ASN:HD21	2:B:86:TRP:HE1	1.41	0.68
1:A:247:MET:HB2	1:A:375:TYR:CE2	2.28	0.68
1:A:248:ARG:NH1	2:B:76:ILE:O	2.26	0.68
1:A:296:ARG:HG3	1:A:296:ARG:NH1	1.96	0.68
2:B:56:ASP:C	2:B:58:ALA:H	1.96	0.67
2:B:96:VAL:HB	2:B:101:HIS:CE1	2.30	0.67
1:A:80:ILE:HD11	1:A:178:LEU:HG	1.77	0.66
2:B:97:ALA:O	2:B:99:GLU:N	2.29	0.66
2:B:244:ASP:O	2:B:246:GLN:NE2	2.30	0.65
1:A:171:ASN:O	1:A:172:SER:C	2.35	0.64
1:A:132:LYS:HE2	1:A:408:ASP:HB2	1.78	0.64
1:A:99:LYS:HE3	7:A:532:HOH:O	1.99	0.63
1:A:300:GLN:HB3	4:A:500:TAD:N3A	2.14	0.63
2:B:115:ASN:N	2:B:115:ASN:HD22	1.95	0.63
2:B:156:GLY:HA3	5:B:380:ATP:O3G	1.97	0.63
2:B:242:LEU:HD12	2:B:243:PRO:HD2	1.81	0.63
1:A:146:ASN:ND2	1:A:196:GLU:HG2	2.13	0.62
1:A:106:ILE:HG22	1:A:107:ARG:HG3	1.82	0.62
1:A:295:ARG:HD2	1:A:337:ILE:HD11	1.82	0.62
1:A:89:ILE:HG21	1:A:166:MET:CE	2.30	0.62
1:A:243:VAL:HG22	1:A:247:MET:SD	2.39	0.62
1:A:228:TYR:CE2	1:A:367:ALA:HA	2.35	0.62
1:A:296:ARG:NH1	7:A:531:HOH:O	2.33	0.61
2:B:131:ALA:HB1	2:B:356:TRP:HB3	1.83	0.61
2:B:78:ASN:ND2	2:B:81:ASP:OD1	2.34	0.60
2:B:102:PRO:HB3	2:B:131:ALA:HB3	1.82	0.60
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.67	0.60
1:A:300:GLN:O	1:A:302:PHE:N	2.35	0.60
2:B:242:LEU:HD21	2:B:248:ILE:CG2	2.31	0.60
2:B:88:HIS:HE1	2:B:93:GLU:HG2	1.61	0.60
1:A:341:ILE:HD11	1:A:379:TYR:HB3	1.83	0.60
1:A:106:ILE:HG22	1:A:107:ARG:CG	2.31	0.60
1:A:171:ASN:HD22	1:A:172:SER:N	1.99	0.60
2:B:56:ASP:O	2:B:58:ALA:N	2.35	0.60
2:B:371:HIS:O	2:B:372:ARG:NH2	2.35	0.59
2:B:157:ASP:O	2:B:183:ARG:HB2	2.01	0.59
1:A:126:ILE:HG22	1:A:131:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:HD21	2:B:248:ILE:HG23	1.83	0.59
1:A:346:MET:CG	1:A:349:PHE:CZ	2.84	0.59
2:B:291:LYS:HG3	2:B:325:MET:HE1	1.83	0.59
2:B:33:SER:O	2:B:70:PRO:HD2	2.03	0.59
1:A:127:GLN:H	1:A:127:GLN:HE21	1.50	0.58
2:B:54:VAL:HG12	2:B:55:GLY:N	2.18	0.58
1:A:277:ASN:O	1:A:280:ASN:N	2.37	0.57
1:A:5:ARG:HG3	1:A:6:PRO:O	2.04	0.57
7:A:525:HOH:O	2:B:176:MET:HE1	2.04	0.57
1:A:107:ARG:HD3	1:A:113:GLU:O	2.04	0.57
1:A:295:ARG:HD2	1:A:337:ILE:CD1	2.35	0.57
2:B:196:ARG:HG3	2:B:196:ARG:O	2.05	0.57
1:A:282:LEU:HD11	1:A:382:LEU:HD23	1.86	0.57
1:A:126:ILE:O	1:A:126:ILE:HG13	2.05	0.57
2:B:155:SER:OG	2:B:160:THR:CG2	2.52	0.57
1:A:393:LYS:HD3	1:A:394:VAL:N	2.21	0.56
2:B:205:GLU:HA	2:B:208:ILE:HD13	1.86	0.56
2:B:37:ARG:O	2:B:65:LEU:CB	2.54	0.56
1:A:127:GLN:HE21	1:A:128:ASP:H	1.51	0.56
2:B:90:PHE:HZ	2:B:123:MET:CE	2.18	0.56
2:B:250:ILE:HD11	2:B:254:ARG:HA	1.88	0.56
2:B:300:SER:HA	2:B:335:ARG:HG2	1.88	0.55
2:B:12:ASN:ND2	2:B:86:TRP:HE1	2.02	0.55
1:A:255:ASN:O	1:A:259:ILE:HG12	2.06	0.55
2:B:252:ASN:ND2	2:B:256:ARG:HH21	2.04	0.55
1:A:130:LEU:HD12	1:A:130:LEU:N	2.22	0.55
1:A:26:ARG:NH1	1:A:26:ARG:HG2	2.20	0.55
2:B:321:ALA:HB1	2:B:322:PRO:HD2	1.89	0.55
2:B:306:TYR:CZ	5:B:380:ATP:H2	2.25	0.54
1:A:277:ASN:HD22	1:A:277:ASN:N	2.05	0.54
1:A:274:LYS:HB3	1:A:278:ILE:HD11	1.89	0.54
1:A:132:LYS:HG3	1:A:408:ASP:CG	2.28	0.54
2:B:61:LYS:O	2:B:62:ARG:C	2.47	0.54
1:A:231:TRP:O	1:A:235:LEU:HG	2.07	0.53
1:A:28:GLU:HG3	1:A:29:LYS:N	2.23	0.53
2:B:252:ASN:HD22	2:B:253:GLU:N	2.06	0.53
2:B:352:PHE:O	2:B:355:MET:HB2	2.08	0.53
1:A:335:ASN:ND2	4:A:500:TAD:N7A	2.57	0.53
1:A:136:PHE:CE2	1:A:180:GLU:HG3	2.44	0.53
1:A:150:LYS:HE3	1:A:196:GLU:HG3	1.89	0.53
1:A:310:GLU:HA	1:A:318:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:THR:O	2:B:361:GLU:HB2	2.09	0.53
1:A:243:VAL:HG13	1:A:244:ASN:N	2.24	0.53
2:B:205:GLU:O	2:B:208:ILE:HB	2.09	0.53
1:A:161:PRO:HD3	1:A:207:ILE:HD12	1.91	0.53
1:A:100:PHE:O	1:A:101:ALA:CB	2.50	0.53
2:B:148:THR:HG23	2:B:167:GLU:HA	1.90	0.53
2:B:97:ALA:HB1	2:B:99:GLU:OE1	2.08	0.52
2:B:325:MET:HE2	2:B:326:LYS:H	1.73	0.52
1:A:61:ASP:OD2	1:A:62:TYR:N	2.42	0.52
2:B:202:THR:OG1	2:B:205:GLU:N	2.43	0.52
1:A:115:SER:HB2	1:A:118:LYS:HG3	1.90	0.52
1:A:194:VAL:HA	1:A:198:LYS:O	2.08	0.52
2:B:362:TYR:O	2:B:365:ALA:O	2.28	0.52
2:B:14:SER:HB3	2:B:71:ILE:HG22	1.92	0.52
1:A:20:GLU:CD	1:A:141:LEU:HD22	2.30	0.52
1:A:254:ILE:HD12	1:A:254:ILE:H	1.74	0.52
2:B:370:VAL:O	2:B:372:ARG:N	2.43	0.52
1:A:291:LEU:CD1	1:A:293:VAL:HG13	2.39	0.52
1:A:257:TYR:HD1	1:A:258:LEU:HD22	1.75	0.51
1:A:243:VAL:HG13	1:A:244:ASN:OD1	2.10	0.51
2:B:130:PRO:O	2:B:359:LYS:N	2.42	0.51
1:A:122:LEU:HD23	1:A:201:ILE:HD12	1.93	0.51
2:B:98:PRO:HB2	2:B:127:PHE:O	2.10	0.51
1:A:136:PHE:CD2	1:A:180:GLU:HG3	2.46	0.51
1:A:266:ASN:N	1:A:267:PRO:HD3	2.26	0.51
1:A:246:TYR:CE2	1:A:336:PHE:HB2	2.46	0.51
2:B:217:CYS:HA	2:B:254:ARG:O	2.11	0.50
2:B:34:ILE:O	2:B:34:ILE:HD12	2.12	0.50
1:A:399:ASP:C	1:A:399:ASP:OD2	2.48	0.50
1:A:233:ASN:O	1:A:235:LEU:N	2.45	0.50
1:A:345:ASN:C	1:A:346:MET:HG2	2.32	0.50
1:A:171:ASN:ND2	1:A:172:SER:H	2.07	0.50
1:A:56:ARG:NH1	1:A:70:GLU:OE2	2.45	0.50
1:A:246:TYR:HE2	1:A:336:PHE:HB2	1.76	0.49
2:B:90:PHE:CZ	2:B:123:MET:CE	2.95	0.49
2:B:124:PHE:CE1	2:B:362:TYR:HB2	2.47	0.49
2:B:372:ARG:HA	2:B:372:ARG:NE	2.28	0.49
2:B:115:ASN:N	2:B:115:ASN:ND2	2.60	0.49
1:A:106:ILE:HD11	1:A:122:LEU:HD22	1.94	0.49
1:A:235:LEU:HD12	1:A:235:LEU:O	2.13	0.49
2:B:80:ASP:O	2:B:83:GLU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:LEU:CD2	2:B:248:ILE:CG2	2.85	0.49
2:B:73:HIS:HD2	2:B:158:GLY:O	1.96	0.48
2:B:21:PHE:CD1	2:B:28:ARG:NH1	2.81	0.48
1:A:5:ARG:HB3	1:A:19:TRP:CE2	2.48	0.48
1:A:248:ARG:NH2	2:B:115:ASN:HD21	2.12	0.48
1:A:315:LYS:HB2	1:A:318:ASN:HD22	1.77	0.48
2:B:122:ILE:O	2:B:126:THR:HB	2.12	0.48
1:A:262:GLY:N	1:A:263:PRO:HD2	2.28	0.48
1:A:185:ILE:HA	1:A:185:ILE:HD13	1.62	0.48
1:A:378:GLU:C	1:A:379:TYR:CD2	2.87	0.48
2:B:274:ILE:HG23	2:B:313:MET:CE	2.43	0.48
2:B:131:ALA:HA	2:B:357:ILE:O	2.12	0.48
2:B:287:ILE:HA	2:B:290:ARG:HG3	1.95	0.48
1:A:21:LYS:HG3	1:A:175:VAL:HG21	1.94	0.48
2:B:257:CYS:HB3	2:B:258:PRO:CD	2.44	0.48
2:B:88:HIS:ND1	2:B:93:GLU:HG2	2.27	0.48
1:A:289:SER:HA	1:A:362:LYS:HD3	1.95	0.48
1:A:257:TYR:CD1	1:A:258:LEU:HD22	2.49	0.48
1:A:158:LEU:HD21	1:A:185:ILE:HD11	1.96	0.48
2:B:155:SER:OG	2:B:160:THR:HG22	2.13	0.48
1:A:243:VAL:O	1:A:247:MET:HG2	2.13	0.47
1:A:334:PRO:O	1:A:385:HIS:HB2	2.13	0.47
2:B:189:LEU:O	2:B:193:LEU:HB2	2.14	0.47
1:A:123:LYS:O	1:A:127:GLN:HG3	2.13	0.47
2:B:31:PHE:CE2	2:B:93:GLU:HG3	2.50	0.47
1:A:217:VAL:HG12	1:A:342:GLY:HA3	1.97	0.47
1:A:355:ILE:N	1:A:355:ILE:HD13	2.29	0.47
2:B:272:ALA:HB1	2:B:276:GLU:HB3	1.96	0.47
2:B:95:ARG:HB2	2:B:95:ARG:HH21	1.80	0.46
1:A:149:GLU:HG2	1:A:151:PRO:HD3	1.98	0.46
1:A:393:LYS:HD3	1:A:394:VAL:H	1.78	0.46
2:B:92:ASN:N	2:B:92:ASN:ND2	2.63	0.46
2:B:56:ASP:C	2:B:58:ALA:N	2.64	0.46
2:B:120:THR:O	2:B:121:GLN:C	2.52	0.46
1:A:295:ARG:HB3	1:A:356:LEU:HB3	1.97	0.46
1:A:126:ILE:HG22	1:A:131:PHE:HZ	1.80	0.46
2:B:202:THR:HG23	2:B:205:GLU:OE2	2.15	0.46
2:B:107:GLU:HA	7:B:935:HOH:O	2.13	0.46
1:A:303:GLY:O	1:A:304:LEU:HD23	2.16	0.46
2:B:194:THR:O	2:B:196:ARG:N	2.48	0.46
2:B:306:TYR:O	2:B:307:PRO:C	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.77	0.46
2:B:83:GLU:O	2:B:84:LYS:C	2.54	0.45
2:B:273:GLY:O	2:B:277:THR:HG23	2.16	0.45
1:A:294:TYR:CE2	1:A:357:ARG:HG3	2.51	0.45
1:A:387:SER:HA	1:A:413:ASN:HD21	1.81	0.45
2:B:279:TYR:CE1	2:B:283:MET:HE2	2.52	0.45
1:A:243:VAL:CG1	1:A:244:ASN:N	2.79	0.45
2:B:267:ILE:HG22	2:B:269:MET:HG3	1.98	0.45
1:A:222:LEU:O	1:A:223:TRP:C	2.55	0.45
2:B:242:LEU:HD22	2:B:248:ILE:HG23	1.94	0.45
1:A:368:TYR:OH	1:A:379:TYR:HA	2.16	0.45
1:A:86:ASP:O	1:A:87:LYS:CD	2.58	0.45
2:B:155:SER:OG	2:B:160:THR:HG21	2.16	0.45
2:B:54:VAL:HB	2:B:88:HIS:CD2	2.52	0.45
1:A:5:ARG:NH1	1:A:86:ASP:OD2	2.50	0.45
2:B:95:ARG:CB	2:B:95:ARG:NH2	2.80	0.45
1:A:142:TYR:N	1:A:142:TYR:CD1	2.84	0.45
1:A:353:LYS:HA	1:A:404:LYS:HD3	1.98	0.45
2:B:209:VAL:O	2:B:210:ARG:C	2.55	0.45
6:B:901:LAR:H42	6:B:901:LAR:O1	2.17	0.45
2:B:7:ALA:HA	2:B:102:PRO:HD2	1.99	0.45
1:A:48:GLN:O	1:A:48:GLN:HG2	2.17	0.45
2:B:21:PHE:HD1	2:B:28:ARG:NH1	2.16	0.44
1:A:132:LYS:HG3	1:A:408:ASP:OD1	2.18	0.44
1:A:52:TYR:CZ	1:A:56:ARG:HG3	2.53	0.44
2:B:54:VAL:CG1	2:B:55:GLY:N	2.80	0.44
1:A:278:ILE:H	1:A:278:ILE:HG13	1.70	0.44
1:A:248:ARG:HH22	2:B:115:ASN:HD21	1.65	0.44
1:A:172:SER:OG	1:A:173:ASN:N	2.50	0.44
1:A:87:LYS:HD2	1:A:87:LYS:HA	1.65	0.44
1:A:297:SER:HB2	1:A:301:GLU:CD	2.38	0.44
1:A:306:LEU:HD21	2:B:265:SER:HB2	2.00	0.44
2:B:210:ARG:HD2	2:B:214:GLU:OE1	2.17	0.44
2:B:325:MET:HA	2:B:325:MET:HE3	2.00	0.43
1:A:384:ASN:OD1	1:A:385:HIS:N	2.51	0.43
1:A:216:ASP:CG	1:A:219:LYS:HB2	2.38	0.43
2:B:119:MET:O	2:B:123:MET:HB2	2.18	0.43
1:A:134:ASP:CG	1:A:357:ARG:HH12	2.17	0.43
2:B:143:TYR:C	2:B:145:SER:H	2.22	0.43
1:A:295:ARG:CD	1:A:337:ILE:HD11	2.47	0.43
1:A:347:SER:OG	2:B:176:MET:CE	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:PHE:CD2	1:A:354:ILE:HD13	2.53	0.43
1:A:134:ASP:OD2	1:A:357:ARG:NH1	2.38	0.43
2:B:118:LYS:O	2:B:122:ILE:HG13	2.19	0.43
2:B:92:ASN:N	2:B:92:ASN:HD22	2.16	0.43
1:A:125:THR:HG22	1:A:125:THR:O	2.19	0.43
2:B:302:GLY:HA3	5:B:380:ATP:O4'	2.18	0.43
2:B:130:PRO:HA	2:B:359:LYS:HD2	2.01	0.43
2:B:108:ALA:HB2	7:B:934:HOH:O	2.18	0.43
2:B:210:ARG:HH11	6:B:901:LAR:H161	1.84	0.43
1:A:361:PRO:HA	7:A:516:HOH:O	2.19	0.43
2:B:21:PHE:HD1	2:B:28:ARG:HH11	1.67	0.42
1:A:335:ASN:OD1	1:A:335:ASN:N	2.48	0.42
1:A:235:LEU:CD1	1:A:240:LEU:HG	2.49	0.42
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.72	0.42
2:B:172:PRO:HA	2:B:175:ILE:HD12	2.01	0.42
1:A:94:PHE:CD2	1:A:151:PRO:HD2	2.54	0.42
2:B:226:GLU:HG3	2:B:255:PHE:CE2	2.54	0.42
1:A:109:GLU:HG3	1:A:110:ASN:N	2.35	0.42
2:B:87:HIS:O	2:B:88:HIS:C	2.57	0.42
1:A:158:LEU:CD2	1:A:185:ILE:HD11	2.50	0.42
1:A:70:GLU:O	1:A:70:GLU:HG3	2.18	0.42
2:B:152:VAL:HA	2:B:298:VAL:O	2.19	0.42
1:A:408:ASP:C	1:A:408:ASP:OD2	2.57	0.42
2:B:137:GLN:HG2	2:B:339:VAL:HG11	2.02	0.42
1:A:236:THR:HB	1:A:237:PRO:HD2	2.01	0.42
1:A:291:LEU:HD13	1:A:293:VAL:HG13	2.01	0.41
1:A:108:THR:O	1:A:110:ASN:N	2.53	0.41
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.67	0.41
1:A:127:GLN:NE2	1:A:128:ASP:H	2.17	0.41
1:A:389:PHE:CE2	1:A:411:LEU:HD13	2.55	0.41
1:A:69:ARG:HB2	1:A:69:ARG:HE	1.79	0.41
2:B:5:THR:HG23	2:B:6:THR:N	2.26	0.41
2:B:11:ASP:OD2	2:B:106:THR:OG1	2.28	0.41
2:B:303:THR:O	2:B:303:THR:HG22	2.20	0.41
1:A:319:ILE:O	1:A:322:PHE:N	2.54	0.41
1:A:299:PRO:HD3	2:B:270:GLU:OE1	2.19	0.41
1:A:300:GLN:C	1:A:302:PHE:N	2.74	0.41
2:B:162:ASN:ND2	2:B:277:THR:OG1	2.54	0.41
1:A:194:VAL:HG23	1:A:198:LYS:O	2.21	0.41
1:A:335:ASN:OD1	4:A:500:TAD:N6A	2.52	0.41
1:A:297:SER:HB2	1:A:301:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:THR:HB	2:B:137:GLN:HG3	2.03	0.41
1:A:192:ARG:HG2	1:A:192:ARG:H	1.62	0.41
2:B:282:ILE:O	2:B:285:CYS:HB2	2.21	0.41
2:B:252:ASN:HD22	2:B:252:ASN:C	2.23	0.41
2:B:274:ILE:O	2:B:313:MET:HE1	2.21	0.41
2:B:349:LEU:O	2:B:350:SER:C	2.59	0.41
1:A:73:TYR:OH	1:A:77:ARG:HD2	2.21	0.40
1:A:269:PRO:HA	1:A:272:ASP:HB2	2.02	0.40
1:A:132:LYS:HD3	1:A:134:ASP:OD2	2.20	0.40
2:B:130:PRO:O	2:B:358:THR:HA	2.20	0.40
1:A:92:TYR:OH	1:A:157:HIS:CE1	2.74	0.40
1:A:145:GLY:O	1:A:148:ASP:OD2	2.39	0.40
2:B:173:HIS:N	2:B:173:HIS:ND1	2.69	0.40
2:B:309:ILE:HG23	2:B:310:ALA:N	2.36	0.40
2:B:329:ILE:O	2:B:329:ILE:HD12	2.21	0.40
2:B:87:HIS:O	2:B:89:THR:N	2.55	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	411/413 (100%)	346 (84%)	45 (11%)	20 (5%)	3 8
2	B	356/375 (95%)	296 (83%)	41 (12%)	19 (5%)	2 7
All	All	767/788 (97%)	642 (84%)	86 (11%)	39 (5%)	2 7

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	104	LYS

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Mol	Chain	Res	Type
1	A	109	GLU
1	A	172	SER
1	A	234	LYS
1	A	237	PRO
1	A	249	GLY
1	A	259	ILE
1	A	261	ASN
1	A	269	PRO
2	B	62	ARG
2	B	364	GLU
2	B	371	HIS
1	A	370	SER
1	A	375	TYR
2	B	98	PRO
2	B	196	ARG
2	B	233	SER
2	B	245	GLY
2	B	266	PHE
2	B	356	TRP
1	A	106	ILE
1	A	263	PRO
1	A	276	ASN
1	A	301	GLU
1	A	312	ASP
2	B	57	GLU
2	B	120	THR
2	B	125	GLU
2	B	126	THR
1	A	260	SER
1	A	365	PRO
2	B	83	GLU
2	B	350	SER
1	A	26	ARG
2	B	60	SER
2	B	88	HIS
2	B	38	PRO
2	B	180	LEU

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	376/376 (100%)	314 (84%)	62 (16%)	3 8
2	B	306/318 (96%)	261 (85%)	45 (15%)	4 11
All	All	682/694 (98%)	575 (84%)	107 (16%)	3 9

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	28	GLU
1	A	37	GLU
1	A	39	LEU
1	A	48	GLN
1	A	57	GLN
1	A	65	GLU
1	A	69	ARG
1	A	74	LYS
1	A	87	LYS
1	A	107	ARG
1	A	109	GLU
1	A	110	ASN
1	A	118	LYS
1	A	127	GLN
1	A	132	LYS
1	A	137	LYS
1	A	141	LEU
1	A	148	ASP
1	A	154	LEU
1	A	158	LEU
1	A	171	ASN
1	A	174	ASP
1	A	185	ILE
1	A	192	ARG
1	A	201	ILE
1	A	209	ASN
1	A	218	SER
1	A	219	LYS
1	A	230	ASP
1	A	235	LEU

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	246	TYR
1	A	252	THR
1	A	258	LEU
1	A	260	SER
1	A	261	ASN
1	A	264	LEU
1	A	265	ASN
1	A	273	SER
1	A	274	LYS
1	A	277	ASN
1	A	280	ASN
1	A	284	LEU
1	A	289	SER
1	A	296	ARG
1	A	307	THR
1	A	310	GLU
1	A	316	ILE
1	A	324	GLU
1	A	329	LYS
1	A	330	VAL
1	A	335	ASN
1	A	337	ILE
1	A	346	MET
1	A	347	SER
1	A	355	ILE
1	A	364	SER
1	A	365	PRO
1	A	372	ILE
1	A	378	GLU
1	A	392	ASN
2	B	6	THR
2	B	10	CYS
2	B	14	SER
2	B	39	ARG
2	B	66	THR
2	B	80	ASP
2	B	81	ASP
2	B	84	LYS
2	B	92	ASN
2	B	115	ASN
2	B	120	THR

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Mol	Chain	Res	Type
2	B	134	VAL
2	B	148	THR
2	B	169	TYR
2	B	178	LEU
2	B	179	ASP
2	B	180	LEU
2	B	193	LEU
2	B	201	VAL
2	B	202	THR
2	B	209	VAL
2	B	210	ARG
2	B	238	LYS
2	B	241	GLU
2	B	244	ASP
2	B	246	GLN
2	B	248	ILE
2	B	250	ILE
2	B	252	ASN
2	B	267	ILE
2	B	274	ILE
2	B	291	LYS
2	B	313	MET
2	B	315	LYS
2	B	326	LYS
2	B	329	ILE
2	B	334	GLU
2	B	346	LEU
2	B	353	GLN
2	B	354	GLN
2	B	358	THR
2	B	359	LYS
2	B	361	GLU
2	B	368	SER
2	B	370	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	51	ASN
1	A	78	ASN
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	127	GLN
1	A	146	ASN
1	A	157	HIS
1	A	171	ASN
1	A	209	ASN
1	A	227	ASN
1	A	261	ASN
1	A	277	ASN
1	A	392	ASN
1	A	413	ASN
2	B	12	ASN
2	B	73	HIS
2	B	78	ASN
2	B	88	HIS
2	B	92	ASN
2	B	101	HIS
2	B	115	ASN
2	B	128	ASN
2	B	162	ASN
2	B	246	GLN
2	B	252	ASN
2	B	353	GLN

5.3.3 RNA

There are no RNA molecules 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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	TAD	A	500	-	37,47,47	1.56	5 (13%)	42,72,72	2.27	13 (30%)
5	ATP	B	380	3	24,33,33	1.02	1 (4%)	31,52,52	2.51	8 (25%)
6	LAR	B	901	-	29,31,31	1.70	5 (17%)	29,43,43	2.15	6 (20%)

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	TAD	A	500	-	-	0/18/62/62	0/5/5/5
5	ATP	B	380	3	-	0/18/38/38	0/3/3/3
6	LAR	B	901	-	-	0/23/51/51	0/1/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	TAD	PA-O2A	-2.30	1.50	1.56
6	B	901	LAR	C20-N1	-2.17	1.33	1.36
6	B	901	LAR	C19-S1	-2.09	1.77	1.81
6	B	901	LAR	O4-C17	2.09	1.44	1.41
6	B	901	LAR	C2-C3	2.17	1.38	1.33
5	B	380	ATP	C5-C4	2.88	1.47	1.40
4	A	500	TAD	C5N-S1N	3.47	1.76	1.70
4	A	500	TAD	C5A-C4A	3.67	1.48	1.40
4	A	500	TAD	PN-O5D	4.07	1.62	1.57
4	A	500	TAD	PA-O5B	5.03	1.63	1.57
6	B	901	LAR	O2-C1	6.87	1.49	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	380	ATP	N3-C2-N1	-8.61	122.30	128.89
4	A	500	TAD	N3A-C2A-N1A	-6.59	123.85	128.89
5	B	380	ATP	PA-O3A-PB	-5.06	118.52	132.73
5	B	380	ATP	C4-C5-N7	-5.05	104.83	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	500	TAD	C2B-C1B-N9A	-4.79	106.98	114.29
5	B	380	ATP	PB-O3B-PG	-4.66	117.03	132.67
6	B	901	LAR	O2-C1-O1	-4.49	116.31	123.30
4	A	500	TAD	O1A-PA-C3	-3.57	100.04	109.02
6	B	901	LAR	O1-C1-C2	-3.33	117.42	126.20
5	B	380	ATP	C2'-C1'-N9	-3.02	109.68	114.29
4	A	500	TAD	O5B-PA-O1A	-3.01	105.97	113.98
5	B	380	ATP	C1'-N9-C4	-2.79	122.73	126.94
4	A	500	TAD	C4A-C5A-N7A	-2.64	107.06	109.48
4	A	500	TAD	O5D-PN-O1N	-2.33	107.77	113.98
5	B	380	ATP	O2'-C2'-C3'	2.13	118.75	111.83
4	A	500	TAD	O4D-C1D-C2D	2.15	106.92	104.73
4	A	500	TAD	O2N-PN-O1N	2.40	117.68	110.12
4	A	500	TAD	C3D-C2D-C1D	2.45	104.63	101.79
4	A	500	TAD	O5B-C5B-C4B	2.47	118.23	109.12
6	B	901	LAR	C21-C3-C4	2.68	119.50	115.41
4	A	500	TAD	O6N-C6N-C4N	2.76	122.22	119.67
5	B	380	ATP	C2-N1-C6	2.87	123.89	118.77
6	B	901	LAR	O2-C15-C14	3.79	117.24	107.80
4	A	500	TAD	O2A-PA-O1A	4.50	124.28	110.12
6	B	901	LAR	C18-N1-C20	4.91	119.47	113.04
6	B	901	LAR	O2-C1-C2	5.88	126.00	111.51
4	A	500	TAD	O5B-PA-C3	6.08	121.43	104.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	500	TAD	3	0
5	B	380	ATP	3	0
6	B	901	LAR	5	0

5.7 Other polymers (i)

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, 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	413/413 (100%)	-0.37	13 (3%)	52	40	24, 43, 90, 108	0
2	B	360/375 (96%)	-0.22	11 (3%)	52	40	20, 46, 95, 117	0
All	All	773/788 (98%)	-0.30	24 (3%)	52	40	20, 44, 92, 117	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	374	CYS	6.0
2	B	66	THR	4.7
2	B	52	SER	4.6
2	B	51	ASP	4.5
1	A	273	SER	3.4
1	A	108	THR	3.2
1	A	237	PRO	3.0
2	B	36	GLY	3.0
1	A	264	LEU	2.9
1	A	249	GLY	2.9
2	B	60	SER	2.8
2	B	5	THR	2.7
1	A	267	PRO	2.7
1	A	272	ASP	2.6
2	B	38	PRO	2.4
1	A	263	PRO	2.3
1	A	269	PRO	2.3
2	B	245	GLY	2.3
2	B	373	LYS	2.3
1	A	246	TYR	2.2
2	B	53	TYR	2.2
1	A	375	TYR	2.2
1	A	377	GLY	2.1
1	A	109	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, 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
6	LAR	B	901	29/29	0.76	0.36	3.42	102,108,112,113	0
3	CA	B	500	1/1	0.99	0.15	-0.11	46,46,46,46	0
4	TAD	A	500	43/43	0.93	0.17	-0.31	60,65,70,73	0
5	ATP	B	380	31/31	0.99	0.13	-0.99	25,29,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.