Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:39 PM GMT

PDB ID	:	1Q1S
Title	:	Mouse Importin alpha- phosphorylated SV40 CN peptide complex
Authors	:	Fontes, M.R.M.; Teh, T.; Toth, G.; John, A.; Pavo, I.; Jans, D.A.; Kobe, B.
Deposited on	:	2003-07-22
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

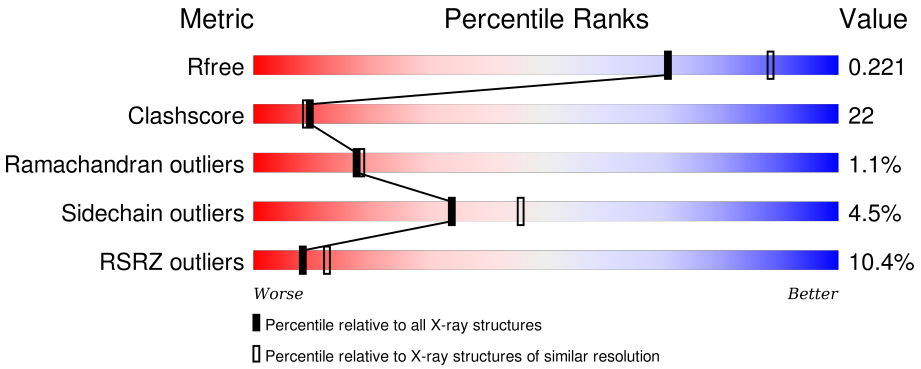
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	24	21%, 8%, 13%, 79%
1	B	24	25%, 29%, 21%, •, 8%, 38%
2	C	466	8%, 67%, 23%, ••, 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3764 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 Large T antigen.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	5	Total	C	N	O	0	0	0
			45	29	11	5			
1	B	15	Total	C	N	O	0	0	0
			115	71	25	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	GLY	SER	ENGINEERED	UNP P03070
A	112	SEP	SER	MODIFIED RESIDUE	UNP P03070
A	117	ALA	THR	ENGINEERED	UNP P03070
A	120	ALA	SER	ENGINEERED	UNP P03070
A	123	ALA	SER	ENGINEERED	UNP P03070
A	124	ALA	THR	ENGINEERED	UNP P03070
B	111	GLY	SER	ENGINEERED	UNP P03070
B	112	SEP	SER	MODIFIED RESIDUE	UNP P03070
B	117	ALA	THR	ENGINEERED	UNP P03070
B	120	ALA	SER	ENGINEERED	UNP P03070
B	123	ALA	SER	ENGINEERED	UNP P03070
B	124	ALA	THR	ENGINEERED	UNP P03070

- Molecule 2 is a protein called Importin alpha-2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	434	Total	C	N	O	S	0	0	0
			3299	2098	560	630	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	64	MET	-	CLONING ARTIFACT	UNP P03070
C	65	ALA	-	CLONING ARTIFACT	UNP P03070

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	ASP	-	CLONING ARTIFACT	UNP P03070
C	67	ILE	-	CLONING ARTIFACT	UNP P03070
C	68	GLY	-	CLONING ARTIFACT	UNP P03070
C	69	SER	-	CLONING ARTIFACT	UNP P03070

- Molecule 3 is water.

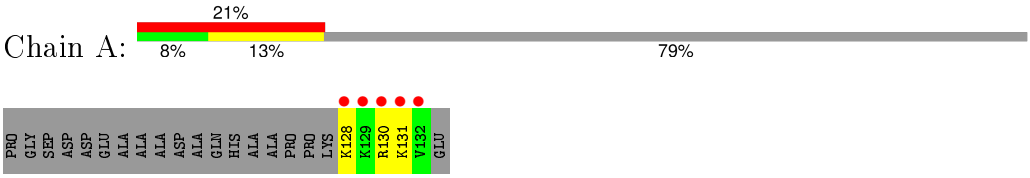
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	16	Total O 16 16	0	0
3	C	287	Total O 287 287	0	0

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.

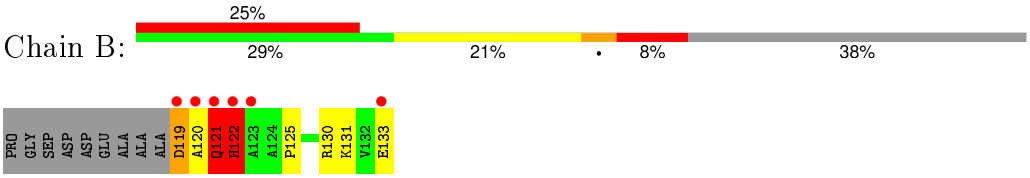
- Molecule 1: Large T antigen

Chain A:



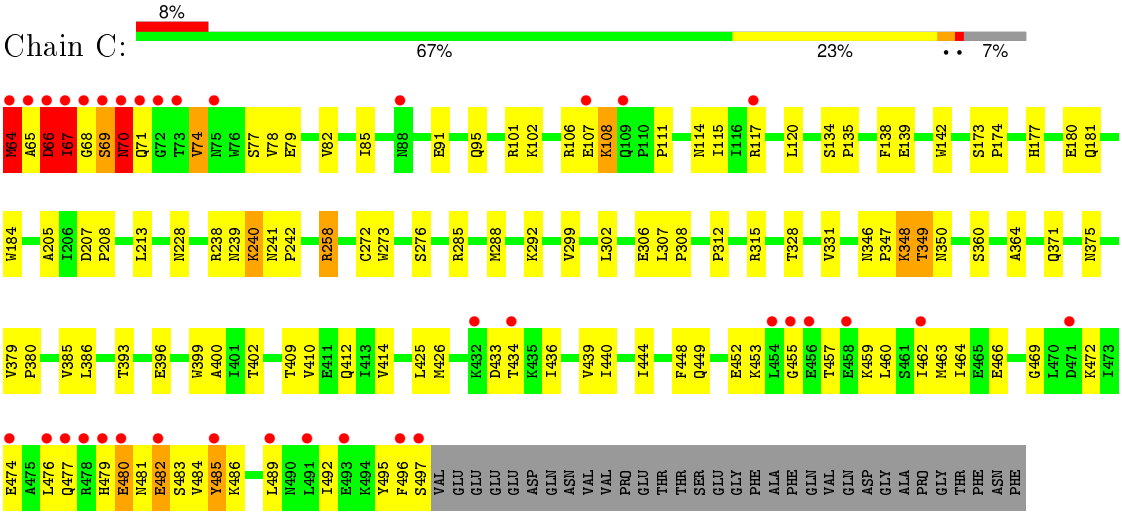
- Molecule 1: Large T antigen

Chain B:



- Molecule 2: Importin alpha-2 subunit

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.83Å 89.75Å 99.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 – 2.30 28.65 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (28.65-2.30) 99.5 (28.65-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.90 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.221 0.198 , 0.221	Depositor DCC
R_{free} test set	2229 reflections (6.99%)	DCC
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.565	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 52.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 31890 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3764	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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

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	0.43	0/44	0.76	0/54
1	B	0.66	0/117	2.11	6/153 (3.9%)
2	C	0.36	0/3357	0.66	6/4574 (0.1%)
All	All	0.38	0/3518	0.75	12/4781 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	GLN	N-CA-CB	-13.70	85.95	110.60
2	C	69	SER	N-CA-C	-9.92	84.22	111.00
1	B	120	ALA	N-CA-C	-9.13	86.34	111.00
1	B	121	GLN	C-N-CA	8.68	143.39	121.70
1	B	121	GLN	N-CA-C	8.61	134.24	111.00
2	C	64	MET	CG-SD-CE	-8.09	87.25	100.20
1	B	119	ASP	N-CA-C	7.96	132.48	111.00
2	C	70	ASN	N-CA-C	7.25	130.59	111.00
2	C	71	GLN	N-CA-C	-6.75	92.78	111.00
2	C	66	ASP	N-CA-C	6.74	129.19	111.00
2	C	240	LYS	N-CA-C	5.38	125.52	111.00
1	B	122	HIS	N-CA-C	5.06	124.67	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	45	0	60	6	0
1	B	115	0	122	28	0
2	C	3299	0	3368	141	0
3	A	2	0	0	1	0
3	B	16	0	0	1	0
3	C	287	0	0	8	0
All	All	3764	0	3550	157	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 22.

All (157) 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)
2:C:64:MET:HE1	2:C:184:TRP:CE3	1.82	1.13
2:C:64:MET:HE1	2:C:184:TRP:HE3	1.05	1.11
1:B:121:GLN:CG	1:B:122:HIS:H	1.53	1.08
2:C:64:MET:CE	2:C:184:TRP:CE3	2.36	1.07
2:C:64:MET:CE	2:C:184:TRP:HE3	1.68	1.06
1:B:121:GLN:HG3	1:B:122:HIS:H	1.19	1.03
1:B:131:LYS:NZ	2:C:64:MET:HG2	1.77	0.99
2:C:68:GLY:HA3	2:C:70:ASN:HB2	1.45	0.96
2:C:70:ASN:HD22	2:C:102:LYS:NZ	1.64	0.96
1:B:131:LYS:NZ	2:C:64:MET:CG	2.31	0.94
1:B:131:LYS:HZ2	2:C:64:MET:CG	1.81	0.92
1:B:121:GLN:CG	1:B:122:HIS:N	2.30	0.90
2:C:68:GLY:HA2	2:C:102:LYS:HZ1	1.35	0.89
2:C:477:GLN:HE21	2:C:489:LEU:HA	1.33	0.89
2:C:101:ARG:HD3	2:C:139:GLU:OE1	1.76	0.85
2:C:67:ILE:HD13	2:C:68:GLY:N	1.92	0.84
2:C:70:ASN:HD22	2:C:102:LYS:HZ3	1.26	0.83
2:C:70:ASN:HB2	2:C:102:LYS:HZ3	1.45	0.80
2:C:70:ASN:HD22	2:C:102:LYS:CE	1.96	0.79
1:B:121:GLN:NE2	3:B:147:HOH:O	2.13	0.79
1:B:131:LYS:HZ2	2:C:64:MET:HG2	1.40	0.79
2:C:371:GLN:HE21	2:C:375:ASN:HD21	1.31	0.78
1:A:131:LYS:NZ	3:A:16:HOH:O	2.20	0.74
1:B:121:GLN:HG3	1:B:122:HIS:CG	2.26	0.71
1:B:131:LYS:NZ	2:C:64:MET:HG3	2.05	0.71
2:C:68:GLY:HA2	2:C:102:LYS:NZ	2.04	0.71
2:C:64:MET:SD	2:C:184:TRP:CE3	2.84	0.70
2:C:70:ASN:ND2	2:C:102:LYS:NZ	2.37	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:402:THR:HG21	2:C:439:VAL:HG13	1.74	0.69
2:C:64:MET:SD	2:C:184:TRP:HE3	2.17	0.68
2:C:328:THR:O	2:C:331:VAL:HG22	1.94	0.68
2:C:70:ASN:HD21	2:C:74:VAL:HG23	1.59	0.67
1:A:128:LYS:HB3	2:C:364:ALA:HB1	1.75	0.67
1:B:133:GLU:O	2:C:65:ALA:HB1	1.94	0.66
2:C:67:ILE:CD1	2:C:68:GLY:N	2.58	0.65
2:C:101:ARG:HD2	2:C:142:TRP:CE3	2.32	0.65
2:C:452:GLU:HG3	2:C:457:THR:HG21	1.77	0.65
2:C:346:ASN:HD22	2:C:348:LYS:H	1.45	0.64
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.61	0.64
2:C:70:ASN:ND2	2:C:102:LYS:HD3	2.12	0.64
2:C:207:ASP:HB2	2:C:208:PRO:HD3	1.79	0.63
2:C:409:THR:H	2:C:412:GLN:NE2	1.95	0.63
1:B:121:GLN:HG2	1:B:122:HIS:N	2.13	0.63
1:B:121:GLN:HG3	1:B:122:HIS:N	2.03	0.62
1:B:131:LYS:NZ	2:C:64:MET:O	2.30	0.61
1:B:131:LYS:HZ3	2:C:64:MET:CG	2.12	0.60
2:C:70:ASN:HB2	2:C:102:LYS:NZ	2.16	0.60
1:B:121:GLN:NE2	1:B:122:HIS:CE1	2.69	0.60
2:C:476:LEU:O	2:C:479:HIS:HB2	2.02	0.59
2:C:70:ASN:ND2	2:C:74:VAL:HG23	2.18	0.59
2:C:386:LEU:HD21	2:C:425:LEU:HD13	1.84	0.59
1:A:130:ARG:NH2	2:C:396:GLU:OE1	2.32	0.59
2:C:64:MET:HE2	2:C:184:TRP:CE3	2.36	0.58
2:C:371:GLN:HE21	2:C:375:ASN:ND2	2.00	0.58
2:C:460:LEU:HA	2:C:463:MET:HE2	1.86	0.58
2:C:70:ASN:ND2	2:C:102:LYS:HZ3	1.96	0.57
2:C:486:LYS:HE3	3:C:778:HOH:O	2.03	0.57
2:C:68:GLY:CA	2:C:102:LYS:NZ	2.67	0.57
2:C:78:VAL:O	2:C:82:VAL:HG23	2.04	0.57
2:C:433:ASP:HB3	2:C:436:ILE:HG22	1.87	0.56
1:B:121:GLN:HE21	1:B:122:HIS:CE1	2.24	0.56
2:C:292:LYS:HE2	3:C:546:HOH:O	2.04	0.56
2:C:240:LYS:HG3	3:C:769:HOH:O	2.04	0.56
2:C:67:ILE:HD12	2:C:67:ILE:H	1.71	0.56
2:C:346:ASN:ND2	2:C:348:LYS:H	2.05	0.55
2:C:474:GLU:O	2:C:477:GLN:HB3	2.07	0.55
2:C:449:GLN:O	2:C:453:LYS:HG3	2.07	0.55
2:C:134:SER:OG	2:C:135:PRO:HD3	2.07	0.55
2:C:399:TRP:HA	2:C:402:THR:HG22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:O	2:C:65:ALA:CB	2.55	0.54
2:C:306:GLU:HB3	2:C:308:PRO:HD2	1.90	0.54
2:C:425:LEU:HG	2:C:440:ILE:HG23	1.89	0.54
2:C:307:LEU:CD2	2:C:348:LYS:HE2	2.39	0.53
2:C:68:GLY:CA	2:C:102:LYS:HZ1	2.16	0.53
2:C:67:ILE:CG1	2:C:68:GLY:H	2.19	0.53
2:C:70:ASN:OD1	2:C:70:ASN:O	2.27	0.53
1:A:130:ARG:NH1	1:A:130:ARG:HG2	2.24	0.52
2:C:307:LEU:N	2:C:308:PRO:CD	2.72	0.52
2:C:477:GLN:O	2:C:485:TYR:HB2	2.09	0.52
2:C:472:LYS:O	2:C:476:LEU:HG	2.09	0.52
2:C:91:GLU:O	2:C:95:GLN:HG2	2.09	0.52
1:B:121:GLN:HG3	1:B:122:HIS:CB	2.39	0.51
2:C:452:GLU:HA	2:C:457:THR:HG23	1.91	0.51
2:C:70:ASN:ND2	2:C:102:LYS:CE	2.72	0.50
2:C:77:SER:OG	2:C:79:GLU:HG2	2.10	0.50
2:C:64:MET:SD	2:C:184:TRP:CZ3	3.05	0.50
1:A:128:LYS:HA	3:C:799:HOH:O	2.12	0.50
2:C:479:HIS:HD2	2:C:481:ASN:H	1.59	0.50
2:C:68:GLY:HA3	2:C:70:ASN:CB	2.31	0.50
2:C:213:LEU:O	2:C:258:ARG:NH2	2.44	0.50
2:C:410:VAL:O	2:C:414:VAL:HG23	2.12	0.50
2:C:379:VAL:HB	2:C:380:PRO:HD3	1.93	0.50
2:C:238:ARG:O	2:C:239:ASN:HB2	2.12	0.50
2:C:479:HIS:CD2	2:C:481:ASN:H	2.31	0.49
2:C:455:GLY:HA2	3:C:798:HOH:O	2.11	0.49
2:C:70:ASN:OD1	2:C:74:VAL:HG23	2.13	0.49
2:C:114:ASN:HA	2:C:117:ARG:NH1	2.27	0.49
2:C:66:ASP:HB2	2:C:138:PHE:HE2	1.78	0.49
2:C:70:ASN:ND2	2:C:102:LYS:CD	2.76	0.49
2:C:272:CYS:HB3	2:C:312:PRO:HB2	1.95	0.48
2:C:276:SER:HB2	2:C:315:ARG:HG3	1.94	0.48
2:C:64:MET:HG3	2:C:181:GLN:OE1	2.13	0.48
1:B:131:LYS:HE3	1:B:133:GLU:OXT	2.13	0.48
2:C:496:PHE:O	2:C:497:SER:C	2.52	0.48
2:C:70:ASN:HD21	2:C:102:LYS:HD3	1.77	0.48
2:C:479:HIS:CD2	2:C:480:GLU:H	2.32	0.48
2:C:64:MET:HA	2:C:177:HIS:HB2	1.96	0.48
2:C:479:HIS:CG	2:C:480:GLU:H	2.31	0.48
1:B:131:LYS:HD2	2:C:64:MET:HE2	1.96	0.48
2:C:70:ASN:CB	2:C:102:LYS:HZ3	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LYS:HZ3	2:C:64:MET:C	2.15	0.47
2:C:64:MET:HB3	2:C:180:GLU:HG2	1.96	0.47
1:B:131:LYS:HZ3	2:C:64:MET:HG3	1.70	0.47
2:C:464:ILE:O	2:C:469:GLY:N	2.47	0.47
1:B:130:ARG:NH2	2:C:106:ARG:O	2.48	0.47
2:C:111:PRO:O	2:C:115:ILE:HG12	2.14	0.47
2:C:107:GLU:C	2:C:108:LYS:HG2	2.36	0.47
2:C:485:TYR:HD2	3:C:758:HOH:O	1.97	0.46
2:C:452:GLU:OE2	2:C:495:TYR:HE1	1.98	0.46
2:C:448:PHE:CD1	2:C:460:LEU:HD23	2.50	0.46
2:C:349:THR:HG21	3:C:713:HOH:O	2.14	0.46
2:C:64:MET:O	2:C:64:MET:CG	2.63	0.46
2:C:386:LEU:HD21	2:C:425:LEU:CD1	2.45	0.46
2:C:460:LEU:HA	2:C:463:MET:CE	2.44	0.46
1:B:121:GLN:CG	1:B:122:HIS:CG	2.99	0.46
2:C:433:ASP:O	2:C:436:ILE:HG22	2.17	0.45
2:C:385:VAL:HG13	2:C:393:THR:HG22	1.99	0.45
2:C:385:VAL:CG1	2:C:393:THR:HG22	2.46	0.45
2:C:70:ASN:OD1	2:C:74:VAL:CG2	2.64	0.45
2:C:409:THR:H	2:C:412:GLN:HE21	1.62	0.44
1:B:125:PRO:HD3	2:C:273:TRP:CD1	2.53	0.44
2:C:67:ILE:N	2:C:67:ILE:HD12	2.29	0.44
2:C:459:LYS:O	2:C:463:MET:HG3	2.17	0.44
2:C:64:MET:HB3	2:C:180:GLU:CG	2.48	0.44
2:C:285:ARG:HD2	3:C:705:HOH:O	2.18	0.44
2:C:85:ILE:HD12	2:C:120:LEU:HD22	2.00	0.44
2:C:66:ASP:HB2	2:C:142:TRP:HZ3	1.82	0.44
1:B:131:LYS:NZ	2:C:64:MET:C	2.71	0.44
2:C:205:ALA:O	2:C:208:PRO:HD2	2.18	0.43
2:C:348:LYS:HD3	2:C:348:LYS:HA	1.87	0.43
2:C:285:ARG:O	2:C:288:MET:HG2	2.18	0.43
2:C:452:GLU:OE2	2:C:495:TYR:CE1	2.71	0.43
2:C:481:ASN:OD1	2:C:483:SER:HB3	2.19	0.42
2:C:299:VAL:O	2:C:302:LEU:HB3	2.19	0.42
2:C:173:SER:HA	2:C:174:PRO:HD3	1.88	0.42
2:C:462:ILE:O	2:C:466:GLU:HG2	2.19	0.42
2:C:307:LEU:HD22	2:C:348:LYS:HE2	2.03	0.41
2:C:67:ILE:CD1	2:C:67:ILE:C	2.88	0.41
2:C:346:ASN:HA	2:C:347:PRO:HD3	1.91	0.41
2:C:241:ASN:HA	2:C:242:PRO:HA	1.88	0.41
2:C:107:GLU:HA	2:C:107:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLN:HB2	2:C:307:LEU:HD21	2.03	0.40
2:C:481:ASN:O	2:C:484:VAL:N	2.54	0.40
2:C:482:GLU:HA	2:C:485:TYR:CE2	2.56	0.40
2:C:360:SER:HA	2:C:400:ALA:HA	2.04	0.40
2:C:426:MET:CE	2:C:444:ILE:HD11	2.51	0.40
2:C:273:TRP:CE2	2:C:312:PRO:HB3	2.57	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	3/24 (12%)	3 (100%)	0	0	100 100
1	B	13/24 (54%)	11 (85%)	1 (8%)	1 (8%)	1 0
2	C	432/466 (93%)	415 (96%)	13 (3%)	4 (1%)	21 24
All	All	448/514 (87%)	429 (96%)	14 (3%)	5 (1%)	17 18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	70	ASN
2	C	67	ILE
2	C	69	SER
1	B	122	HIS
2	C	492	ILE

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	5/16 (31%)	5 (100%)	0	100 100
1	B	11/16 (69%)	8 (73%)	3 (27%)	0 0
2	C	362/390 (93%)	348 (96%)	14 (4%)	39 53
All	All	378/422 (90%)	361 (96%)	17 (4%)	34 46

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	119	ASP
1	B	121	GLN
1	B	122	HIS
2	C	64	MET
2	C	66	ASP
2	C	67	ILE
2	C	74	VAL
2	C	108	LYS
2	C	228	ASN
2	C	258	ARG
2	C	348	LYS
2	C	349	THR
2	C	350	ASN
2	C	434	THR
2	C	480	GLU
2	C	482	GLU
2	C	485	TYR

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

Mol	Chain	Res	Type
1	B	121	GLN
2	C	70	ASN
2	C	86	ASN
2	C	261	HIS
2	C	283	ASN
2	C	346	ASN
2	C	352	GLN
2	C	375	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	412	GLN
2	C	438	GLN
2	C	477	GLN
2	C	479	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	5/24 (20%)	3.42	5 (100%) 0 0	74, 76, 78, 81	0
1	B	15/24 (62%)	2.75	6 (40%) 0 0	24, 36, 74, 77	0
2	C	434/466 (93%)	0.37	36 (8%) 14 20	20, 32, 77, 96	0
All	All	454/514 (88%)	0.49	47 (10%) 8 12	20, 32, 77, 96	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	64	MET	14.7
1	B	120	ALA	13.7
2	C	70	ASN	9.8
2	C	67	ILE	8.6
1	B	119	ASP	7.8
2	C	71	GLN	7.7
1	B	121	GLN	7.7
1	B	122	HIS	7.3
2	C	65	ALA	7.1
2	C	485	TYR	6.8
2	C	497	SER	6.6
2	C	69	SER	6.4
2	C	66	ASP	6.1
2	C	68	GLY	4.1
2	C	455	GLY	4.0
2	C	482	GLU	4.0
2	C	496	PHE	4.0
1	A	130	ARG	3.9
2	C	489	LEU	3.9
1	A	131	LYS	3.8
2	C	73	THR	3.8
2	C	432	LYS	3.7
1	B	123	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	480	GLU	3.7
2	C	478	ARG	3.7
1	A	128	LYS	3.5
2	C	72	GLY	3.3
2	C	88	ASN	3.3
2	C	493	GLU	3.2
2	C	75	ASN	3.1
1	B	133	GLU	3.1
1	A	129	LYS	3.0
1	A	132	VAL	3.0
2	C	479	HIS	2.9
2	C	474	GLU	2.8
2	C	107	GLU	2.6
2	C	476	LEU	2.6
2	C	458	GLU	2.6
2	C	434	THR	2.5
2	C	462	ILE	2.4
2	C	117	ARG	2.4
2	C	109	GLN	2.4
2	C	456	GLU	2.3
2	C	477	GLN	2.2
2	C	454	LEU	2.2
2	C	471	ASP	2.1
2	C	491	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.