Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2023 – 01:32 AM EDT

PDB ID	:	3W3X
Title	:	Crystal structure of Kap121p bound to Pho4p
Authors	:	Kobayashi, J.; Matsuura, Y.
Deposited on	:	2012-12-28
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

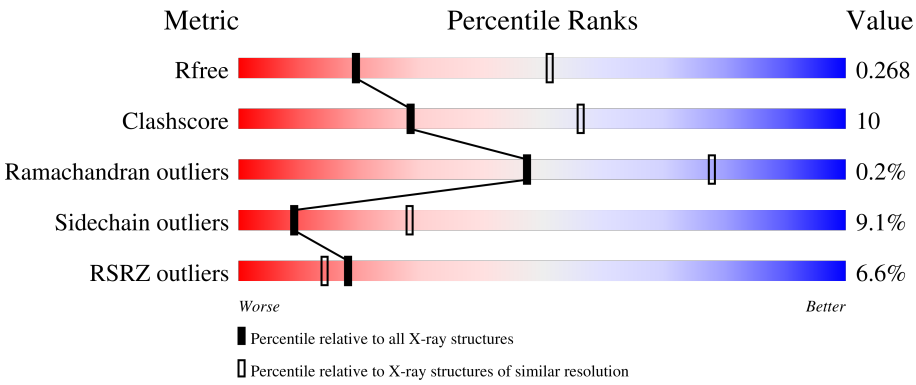
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	1078	6% 75% 16% • 5%
2	B	27	19% 11% 7% 63%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7849 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 Importin subunit beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1021	7773	4994	1246	1498	35	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	LYS	deletion	UNP P32337
A	?	-	LEU	deletion	UNP P32337
A	?	-	MET	deletion	UNP P32337
A	?	-	ILE	deletion	UNP P32337
A	?	-	MET	deletion	UNP P32337
A	?	-	SER	deletion	UNP P32337
A	?	-	LYS	deletion	UNP P32337
A	?	-	ASN	deletion	UNP P32337

- Molecule 2 is a protein called Phosphate system positive regulatory protein PHO4.

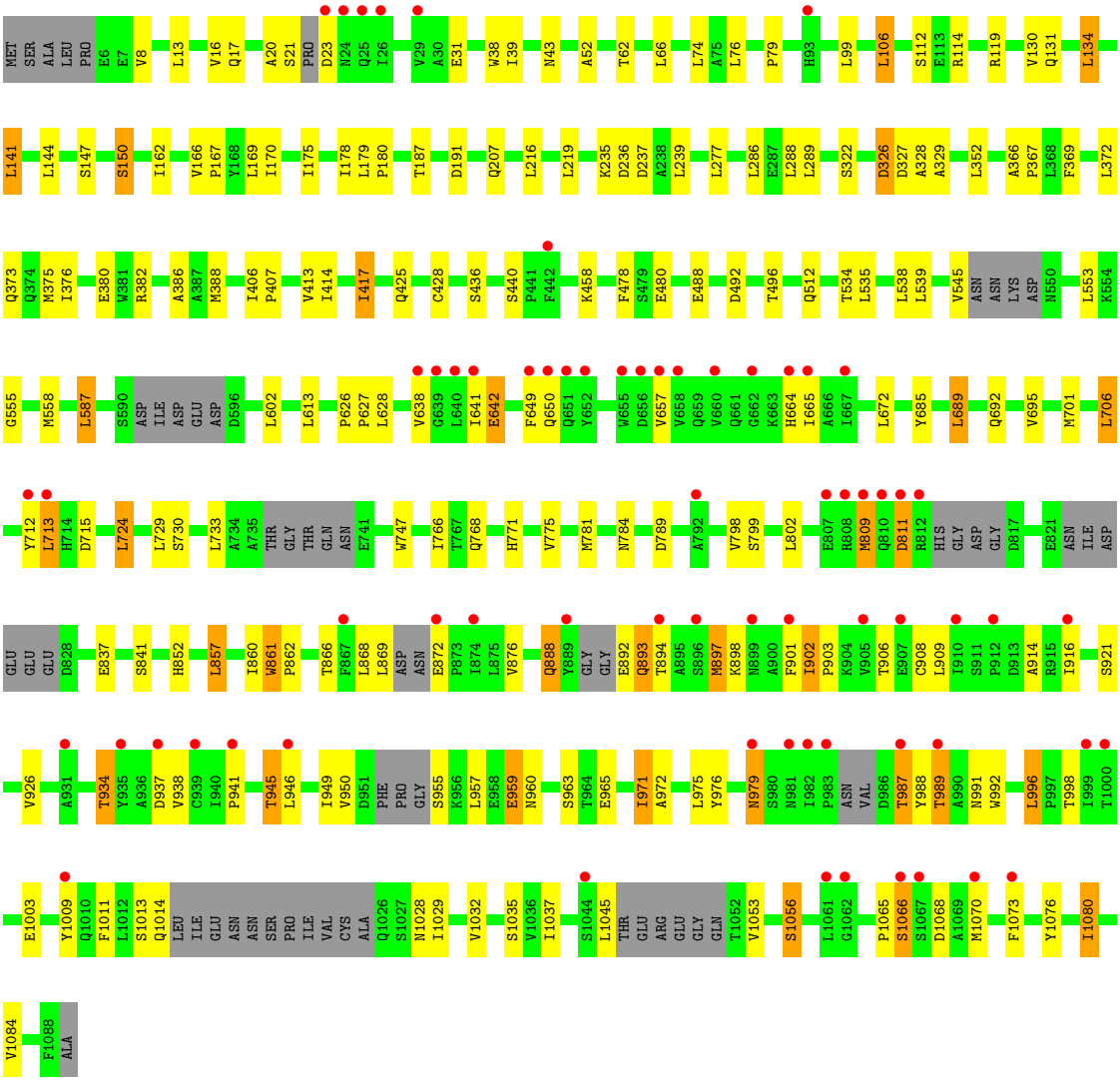
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	10	76	45	16	15	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

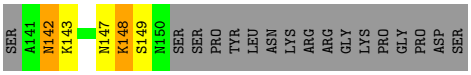
• Molecule 1: Importin subunit beta-3

Chain A: 6% 75% 16% • 5%



• Molecule 2: Phosphate system positive regulatory protein PHO4

Chain B: 19% 11% 7% 63%


SER
A141
N142
K143
N147
K148
S149
N150
SER
SER
PRO
TYR
LEU
ASN
LYS
ARG
ARG
GLY
LYS
PRO
GLY
PRO
ASP
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.09Å 126.31Å 128.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.90 29.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.50-2.90) 98.6 (29.48-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.224 , 0.268 0.224 , 0.268	Depositor DCC
R_{free} test set	1426 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7849	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.55	0/7908	0.74	2/10781 (0.0%)
2	B	0.66	0/75	1.19	0/98
All	All	0.55	0/7983	0.75	2/10879 (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	A	237	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	724	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7773	0	7641	151	0
2	B	76	0	82	4	0
All	All	7849	0	7723	153	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 10.

All (153) 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:558:MET:SD	1:A:602:LEU:HD23	1.72	1.29
1:A:1011:PHE:CE1	1:A:1014:GLN:OE1	1.86	1.28
1:A:1011:PHE:CD1	1:A:1014:GLN:OE1	1.94	1.20
1:A:406:ILE:HG23	1:A:407:PRO:HD3	1.21	1.13
1:A:892:GLU:CB	1:A:934:THR:HG21	1.82	1.09
1:A:1009:TYR:HB3	1:A:1053:VAL:HG21	1.40	1.02
1:A:558:MET:SD	1:A:602:LEU:CD2	2.49	1.00
1:A:902:ILE:N	1:A:903:PRO:HD2	1.81	0.95
1:A:638:VAL:HG23	1:A:665:ILE:CG2	1.96	0.94
1:A:1011:PHE:HE1	1:A:1014:GLN:OE1	1.43	0.92
1:A:1011:PHE:HD1	1:A:1014:GLN:OE1	1.58	0.87
1:A:892:GLU:CB	1:A:934:THR:CG2	2.52	0.87
1:A:987:THR:HG23	1:A:991:ASN:HD21	1.40	0.86
1:A:406:ILE:CG2	1:A:407:PRO:HD3	2.04	0.85
1:A:1011:PHE:O	1:A:1014:GLN:HG2	1.80	0.82
1:A:988:TYR:HA	1:A:991:ASN:HD22	1.49	0.78
1:A:894:THR:O	1:A:897:MET:HG3	1.83	0.78
1:A:965:GLU:HG2	1:A:998:THR:HG23	1.67	0.77
1:A:641:ILE:HG23	1:A:664:HIS:HB3	1.66	0.76
1:A:1013:SER:HG	1:A:1056:SER:HG	1.30	0.76
1:A:534:THR:O	1:A:538:LEU:HD13	1.85	0.75
1:A:406:ILE:HG23	1:A:407:PRO:CD	2.11	0.75
1:A:987:THR:HG23	1:A:991:ASN:ND2	2.01	0.75
1:A:638:VAL:HG23	1:A:665:ILE:HG22	1.69	0.74
1:A:414:ILE:O	1:A:417:ILE:HG22	1.85	0.74
2:B:147:ASN:C	2:B:148:LYS:HG2	2.09	0.73
1:A:638:VAL:CG2	1:A:665:ILE:CG2	2.67	0.72
1:A:1013:SER:OG	1:A:1056:SER:OG	2.00	0.72
1:A:480:GLU:OE2	2:B:143:LYS:NZ	2.21	0.72
1:A:369:PHE:O	1:A:373:GLN:HG2	1.89	0.71
1:A:650:GLN:HG2	1:A:657:VAL:HG22	1.73	0.71
1:A:1011:PHE:HD1	1:A:1014:GLN:CD	1.93	0.71
1:A:937:ASP:O	1:A:941:PRO:HG2	1.91	0.71
1:A:898:LYS:HG3	1:A:902:ILE:HD11	1.72	0.71
1:A:987:THR:HG22	1:A:988:TYR:N	2.06	0.70
1:A:626:PRO:HB2	1:A:627:PRO:HD3	1.73	0.70
1:A:902:ILE:N	1:A:903:PRO:CD	2.56	0.68
1:A:1011:PHE:CD1	1:A:1014:GLN:CD	2.68	0.67
1:A:1066:SER:O	1:A:1070:MET:HG2	1.97	0.65
1:A:492:ASP:O	1:A:496:THR:HG23	1.97	0.64
1:A:558:MET:CE	1:A:587:LEU:HD23	2.28	0.63
1:A:638:VAL:CG2	1:A:665:ILE:HG23	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:THR:CG2	1:A:988:TYR:N	2.62	0.62
1:A:131:GLN:HB3	1:A:134:LEU:HB2	1.81	0.62
1:A:558:MET:HE1	1:A:587:LEU:HD23	1.82	0.62
1:A:987:THR:CG2	1:A:991:ASN:HD21	2.11	0.62
1:A:893:GLN:HG2	1:A:893:GLN:O	2.00	0.62
1:A:20:ALA:O	1:A:21:SER:HB2	1.99	0.61
1:A:641:ILE:HG22	1:A:664:HIS:O	2.01	0.60
1:A:908:CYS:HB3	1:A:916:ILE:HG22	1.82	0.60
1:A:975:LEU:HD22	1:A:989:THR:HG22	1.82	0.60
1:A:388:MET:SD	1:A:413:VAL:HG22	2.42	0.59
1:A:898:LYS:O	1:A:902:ILE:CG1	2.51	0.59
1:A:715:ASP:HB2	1:A:766:ILE:HD11	1.84	0.58
1:A:861:TRP:HE1	1:A:897:MET:HE1	1.68	0.57
1:A:901:PHE:C	1:A:903:PRO:HD2	2.25	0.57
1:A:170:ILE:HG23	1:A:178:ILE:HG12	1.87	0.57
1:A:972:ALA:HB2	1:A:992:TRP:NE1	2.19	0.56
1:A:712:TYR:CD1	1:A:713:LEU:HD13	2.39	0.56
1:A:638:VAL:HG23	1:A:665:ILE:HG23	1.85	0.56
1:A:1009:TYR:O	1:A:1053:VAL:HG22	2.06	0.55
1:A:971:ILE:HD11	1:A:992:TRP:HB2	1.89	0.55
1:A:902:ILE:HG21	1:A:938:VAL:HG11	1.89	0.54
1:A:747:TRP:CG	1:A:781:MET:HG3	2.43	0.54
1:A:898:LYS:O	1:A:902:ILE:HG12	2.08	0.54
1:A:893:GLN:O	1:A:893:GLN:CG	2.56	0.54
1:A:112:SER:O	1:A:119:ARG:NH2	2.42	0.53
1:A:1003:GLU:H	1:A:1003:GLU:CD	2.12	0.53
1:A:1080:ILE:O	1:A:1080:ILE:HD12	2.08	0.53
1:A:20:ALA:O	1:A:21:SER:CB	2.57	0.53
1:A:1037:ILE:HD12	1:A:1084:VAL:HG22	1.90	0.53
1:A:650:GLN:CG	1:A:657:VAL:HG22	2.36	0.52
1:A:191:ASP:OD2	1:A:235:LYS:HG2	2.08	0.52
1:A:898:LYS:HG3	1:A:902:ILE:CD1	2.40	0.52
1:A:366:ALA:HB3	1:A:367:PRO:CD	2.40	0.52
1:A:945:THR:O	1:A:949:ILE:HG13	2.09	0.52
1:A:16:VAL:HG23	1:A:66:LEU:HD12	1.91	0.52
1:A:512:GLN:OE1	2:B:142:ASN:ND2	2.43	0.52
1:A:76:LEU:O	1:A:79:PRO:HB3	2.10	0.51
1:A:861:TRP:HE1	1:A:897:MET:CE	2.22	0.51
1:A:144:LEU:HD21	1:A:162:ILE:HD12	1.92	0.51
1:A:861:TRP:N	1:A:862:PRO:HD2	2.24	0.51
1:A:372:LEU:O	1:A:376:ILE:HG12	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HG13	1:A:428:CYS:SG	2.52	0.50
1:A:898:LYS:O	1:A:902:ILE:HG13	2.11	0.50
1:A:39:ILE:HG22	1:A:39:ILE:O	2.10	0.50
1:A:906:THR:HA	1:A:909:LEU:HD12	1.93	0.50
1:A:99:LEU:HD21	1:A:134:LEU:HG	1.92	0.50
1:A:641:ILE:HG12	1:A:642:GLU:N	2.27	0.50
1:A:934:THR:O	1:A:934:THR:OG1	2.30	0.50
1:A:946:LEU:CD1	1:A:971:ILE:HG22	2.42	0.49
1:A:417:ILE:O	1:A:425:GLN:HG2	2.12	0.49
1:A:861:TRP:NE1	1:A:897:MET:CE	2.75	0.49
1:A:914:ALA:O	1:A:963:SER:OG	2.22	0.49
1:A:1073:PHE:HA	1:A:1076:TYR:CD2	2.48	0.48
1:A:809:MET:C	1:A:811:ASP:H	2.18	0.48
1:A:130:VAL:HG11	1:A:169:LEU:HD21	1.96	0.48
1:A:328:ALA:O	1:A:329:ALA:C	2.51	0.48
1:A:167:PRO:HG3	1:A:207:GLN:CB	2.44	0.47
1:A:641:ILE:CG2	1:A:664:HIS:HB3	2.42	0.47
1:A:366:ALA:HB3	1:A:367:PRO:HD3	1.97	0.47
1:A:976:TYR:HE1	1:A:1014:GLN:HE22	1.62	0.46
1:A:1009:TYR:O	1:A:1053:VAL:CG2	2.63	0.46
1:A:898:LYS:NZ	1:A:937:ASP:OD1	2.41	0.46
1:A:322:SER:O	1:A:382:ARG:NH2	2.46	0.46
1:A:417:ILE:HG13	1:A:458:LYS:HD3	1.97	0.46
1:A:1009:TYR:CB	1:A:1053:VAL:HG21	2.30	0.45
1:A:641:ILE:HG12	1:A:642:GLU:H	1.80	0.45
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.90	0.45
1:A:641:ILE:HG22	1:A:664:HIS:C	2.36	0.45
1:A:375:MET:HE2	1:A:386:ALA:HB3	1.99	0.45
1:A:768:GLN:HG3	1:A:837:GLU:HG3	1.98	0.45
2:B:147:ASN:O	2:B:148:LYS:HG2	2.16	0.45
1:A:13:LEU:HG	1:A:17:GLN:OE1	2.17	0.44
1:A:66:LEU:C	1:A:66:LEU:HD13	2.38	0.44
1:A:327:ASP:O	1:A:328:ALA:HB3	2.17	0.44
1:A:996:LEU:N	1:A:996:LEU:HD23	2.32	0.44
1:A:1028:ASN:O	1:A:1032:VAL:HG23	2.17	0.44
1:A:857:LEU:O	1:A:857:LEU:HD12	2.17	0.44
1:A:175:ILE:HA	1:A:178:ILE:HG22	2.00	0.44
1:A:436:SER:HB3	1:A:478:PHE:HA	2.00	0.44
1:A:987:THR:HG22	1:A:988:TYR:H	1.77	0.44
1:A:988:TYR:O	1:A:991:ASN:HB2	2.18	0.43
1:A:979:ASN:ND2	1:A:979:ASN:H	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:VAL:O	1:A:695:VAL:HG22	2.17	0.43
1:A:417:ILE:CG1	1:A:458:LYS:HD3	2.48	0.43
1:A:1009:TYR:OH	1:A:1035:SER:O	2.23	0.43
1:A:326:ASP:OD1	1:A:382:ARG:NH1	2.52	0.43
1:A:685:TYR:O	1:A:689:LEU:HB2	2.19	0.43
1:A:701:MET:HG3	1:A:706:LEU:HD22	2.00	0.43
1:A:147:SER:O	1:A:150:SER:HB3	2.19	0.43
1:A:406:ILE:CG2	1:A:407:PRO:CD	2.84	0.43
1:A:1076:TYR:CG	1:A:1080:ILE:HD11	2.54	0.43
1:A:52:ALA:HB1	1:A:106:LEU:HD13	2.01	0.42
1:A:775:VAL:HG22	1:A:841:SER:HA	2.01	0.42
1:A:1073:PHE:HA	1:A:1076:TYR:HD2	1.84	0.42
1:A:771:HIS:O	1:A:775:VAL:HG23	2.20	0.42
1:A:959:GLU:N	1:A:959:GLU:OE1	2.52	0.42
1:A:555:GLY:O	1:A:558:MET:HG2	2.20	0.42
1:A:902:ILE:CG2	1:A:938:VAL:HG11	2.49	0.42
1:A:13:LEU:O	1:A:17:GLN:HG3	2.19	0.41
1:A:436:SER:O	1:A:440:SER:HB3	2.20	0.41
1:A:1065:PRO:HG2	1:A:1068:ASP:HB2	2.02	0.41
1:A:38:TRP:CE3	1:A:43:ASN:HB3	2.55	0.41
1:A:798:VAL:O	1:A:802:LEU:HG	2.20	0.41
1:A:628:LEU:HD23	1:A:628:LEU:HA	1.89	0.41
1:A:799:SER:HB2	1:A:860:ILE:CG2	2.51	0.40
1:A:888:GLN:HE21	1:A:888:GLN:HB2	1.68	0.40
1:A:897:MET:O	1:A:898:LYS:C	2.59	0.40
1:A:141:LEU:HD12	1:A:141:LEU:HA	1.81	0.40
1:A:872:GLU:O	1:A:876:VAL:HG23	2.22	0.40
1:A:747:TRP:CD1	1:A:781:MET:HG3	2.57	0.40
1:A:959:GLU:CD	1:A:959:GLU:H	2.23	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	995/1078 (92%)	951 (96%)	42 (4%)	2 (0%)	47	78
2	B	8/27 (30%)	6 (75%)	2 (25%)	0	100	100
All	All	1003/1105 (91%)	957 (95%)	44 (4%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	HIS
1	A	8	VAL

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	833/937 (89%)	759 (91%)	74 (9%)	9	29
2	B	9/24 (38%)	6 (67%)	3 (33%)	0	0
All	All	842/961 (88%)	765 (91%)	77 (9%)	9	28

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	31	GLU
1	A	62	THR
1	A	74	LEU
1	A	106	LEU
1	A	134	LEU
1	A	141	LEU
1	A	150	SER
1	A	166	VAL
1	A	179	LEU
1	A	180	PRO
1	A	187	THR
1	A	216	LEU
1	A	219	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	236	ASP
1	A	239	LEU
1	A	277	LEU
1	A	286	LEU
1	A	288	LEU
1	A	289	LEU
1	A	326	ASP
1	A	352	LEU
1	A	380	GLU
1	A	417	ILE
1	A	488	GLU
1	A	535	LEU
1	A	539	LEU
1	A	545	VAL
1	A	553	LEU
1	A	587	LEU
1	A	613	LEU
1	A	642	GLU
1	A	649	PHE
1	A	672	LEU
1	A	689	LEU
1	A	692	GLN
1	A	706	LEU
1	A	713	LEU
1	A	724	LEU
1	A	729	LEU
1	A	730	SER
1	A	733	LEU
1	A	784	ASN
1	A	789	ASP
1	A	809	MET
1	A	811	ASP
1	A	857	LEU
1	A	861	TRP
1	A	866	THR
1	A	868	LEU
1	A	869	LEU
1	A	888	GLN
1	A	893	GLN
1	A	897	MET
1	A	902	ILE
1	A	921	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	926	VAL
1	A	934	THR
1	A	945	THR
1	A	950	VAL
1	A	955	SER
1	A	957	LEU
1	A	959	GLU
1	A	960	ASN
1	A	971	ILE
1	A	979	ASN
1	A	987	THR
1	A	989	THR
1	A	996	LEU
1	A	1029	ILE
1	A	1045	LEU
1	A	1056	SER
1	A	1066	SER
1	A	1080	ILE
2	B	142	ASN
2	B	148	LYS
2	B	149	SER

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	303	ASN
1	A	430	ASN
1	A	541	ASN
1	A	856	ASN
1	A	888	GLN
1	A	893	GLN
1	A	918	GLN
1	A	979	ASN
1	A	991	ASN
1	A	1014	GLN
2	B	150	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1021/1078 (94%)	0.11	68 (6%) 17 13	30, 68, 147, 212	0
2	B	10/27 (37%)	-0.03	0 100 100	38, 49, 72, 85	0
All	All	1031/1105 (93%)	0.11	68 (6%) 18 14	30, 68, 147, 212	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	649	PHE	6.3
1	A	810	GLN	5.5
1	A	665	ILE	5.4
1	A	638	VAL	5.4
1	A	639	GLY	5.1
1	A	656	ASP	5.1
1	A	25	GLN	4.9
1	A	987	THR	4.9
1	A	667	ILE	4.7
1	A	658	VAL	4.6
1	A	26	ILE	4.5
1	A	899	ASN	4.5
1	A	652	TYR	4.2
1	A	867	PHE	3.7
1	A	874	ILE	3.7
1	A	662	GLY	3.6
1	A	981	ASN	3.6
1	A	1066	SER	3.5
1	A	713	LEU	3.4
1	A	941	PRO	3.3
1	A	93	HIS	3.3
1	A	946	LEU	3.1
1	A	657	VAL	3.1
1	A	1061	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	23	ASP	3.0
1	A	650	GLN	3.0
1	A	660	VAL	3.0
1	A	935	TYR	3.0
1	A	910	ILE	3.0
1	A	894	THR	2.9
1	A	641	ILE	2.9
1	A	1044	SER	2.9
1	A	640	LEU	2.9
1	A	896	SER	2.9
1	A	811	ASP	2.9
1	A	812	ARG	2.8
1	A	664	HIS	2.8
1	A	889	TYR	2.7
1	A	901	PHE	2.6
1	A	939	CYS	2.4
1	A	905	VAL	2.4
1	A	651	GLN	2.4
1	A	982	ILE	2.4
1	A	1067	SER	2.3
1	A	792	ALA	2.3
1	A	931	ALA	2.3
1	A	989	THR	2.3
1	A	655	TRP	2.2
1	A	983	PRO	2.2
1	A	1073	PHE	2.2
1	A	1009	TYR	2.2
1	A	809	MET	2.2
1	A	872	GLU	2.2
1	A	1000	THR	2.2
1	A	807	GLU	2.2
1	A	29	VAL	2.2
1	A	24	ASN	2.1
1	A	808	ARG	2.1
1	A	999	ILE	2.1
1	A	1062	GLY	2.1
1	A	937	ASP	2.1
1	A	1070	MET	2.1
1	A	712	TYR	2.1
1	A	907	GLU	2.1
1	A	442	PHE	2.1
1	A	916	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	912	PRO	2.0
1	A	979	ASN	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 monosaccharides 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.