Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 10:34 PM EDT

PDB ID	:	5JHQ
Title	:	ARCs 1-3 of human Tankyrase-1 bound to a peptide derived from IRAP
Authors	:	Eisemann, T.; Pascal, J.M.
Deposited on	:	2016-04-21
Resolution	:	3.20 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:

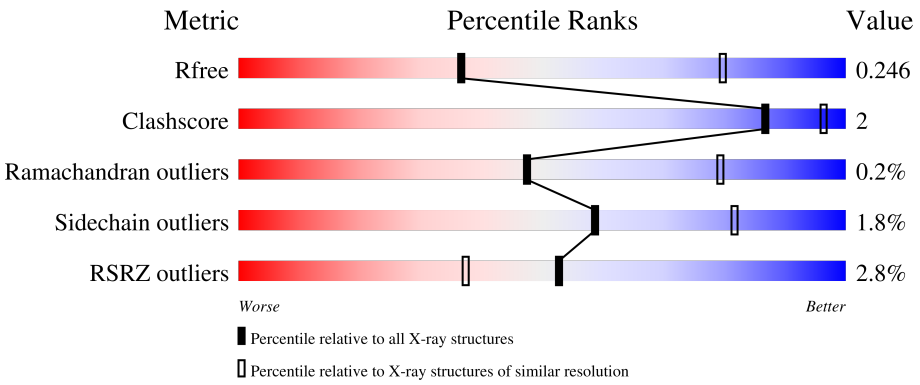
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	482	90% 5% ·
1	B	482	3% 90% 6% ·
1	C	482	3% 89% 7% ·
1	D	482	3% 90% 6% ·
2	E	16	6% 69% 6% 25%

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Mol	Chain	Length	Quality of chain
2	F	16	6% 44% 25% 31%
2	G	16	62% 6% 31%
2	H	16	56% 6% 38%
2	I	16	12% 69% 31%
2	J	16	25% 56% 6% 38%
2	K	16	6% 62% 38%
2	L	16	12% 50% 6% 44%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14657 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 Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3513	2185	654	654	20	0	0	0
1	B	461	3509	2183	653	653	20	0	0	0
1	C	461	3509	2183	653	653	20	0	0	0
1	D	463	3519	2188	655	656	20	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	expression tag	UNP O95271
A	169	SER	-	expression tag	UNP O95271
A	170	HIS	-	expression tag	UNP O95271
A	171	MET	-	expression tag	UNP O95271
A	172	ALA	-	expression tag	UNP O95271
A	173	SER	-	expression tag	UNP O95271
B	168	GLY	-	expression tag	UNP O95271
B	169	SER	-	expression tag	UNP O95271
B	170	HIS	-	expression tag	UNP O95271
B	171	MET	-	expression tag	UNP O95271
B	172	ALA	-	expression tag	UNP O95271
B	173	SER	-	expression tag	UNP O95271
C	168	GLY	-	expression tag	UNP O95271
C	169	SER	-	expression tag	UNP O95271
C	170	HIS	-	expression tag	UNP O95271
C	171	MET	-	expression tag	UNP O95271
C	172	ALA	-	expression tag	UNP O95271
C	173	SER	-	expression tag	UNP O95271
D	168	GLY	-	expression tag	UNP O95271
D	169	SER	-	expression tag	UNP O95271
D	170	HIS	-	expression tag	UNP O95271

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Chain	Residue	Modelled	Actual	Comment	Reference
D	171	MET	-	expression tag	UNP O95271
D	172	ALA	-	expression tag	UNP O95271
D	173	SER	-	expression tag	UNP O95271

- Molecule 2 is a protein called Peptide derived from insulin-responsive aminopeptidase (IRAP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	12	85	50	16	18	1	0	0	0
2	F	11	78	45	15	17	1	0	0	0
2	G	11	74	42	15	16	1	0	0	0
2	H	10	67	37	14	15	1	0	0	0
2	I	11	74	42	15	16	1	0	0	0
2	J	10	67	37	14	15	1	0	0	0
2	K	10	67	37	14	15	1	0	0	0
2	L	9	61	34	13	13	1	0	0	0

- Molecule 3 is water.

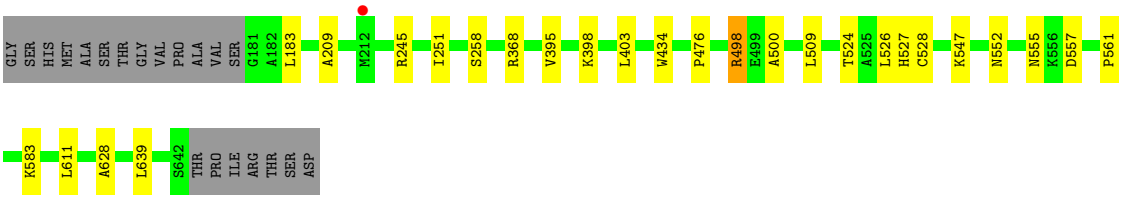
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	12	12	12	0	0
3	B	5	5	5	0	0
3	C	8	8	8	0	0
3	D	9	9	9	0	0

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.

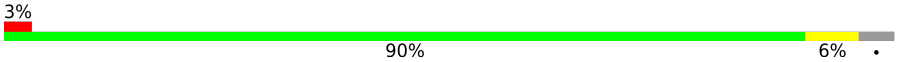
• Molecule 1: Tankyrase-1

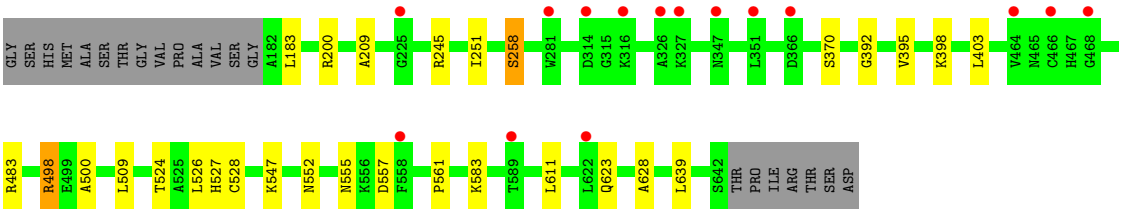
Chain A:



• Molecule 1: Tankyrase-1

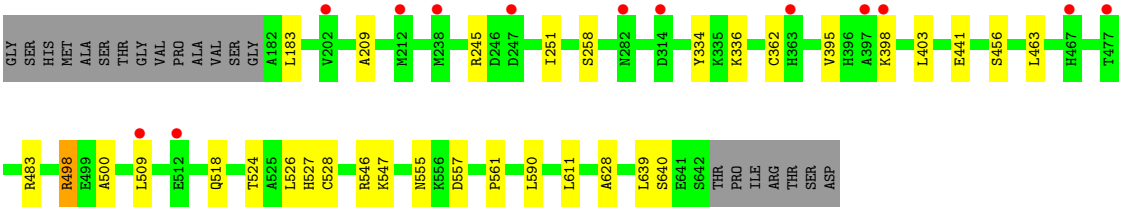
Chain B:





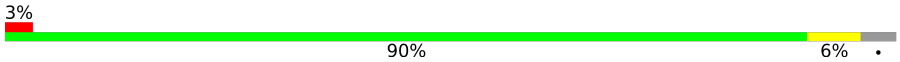
• Molecule 1: Tankyrase-1

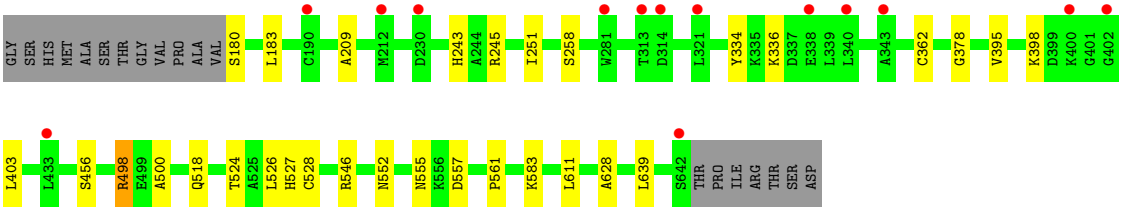
Chain C:



• Molecule 1: Tankyrase-1

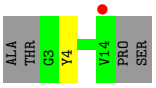
Chain D:





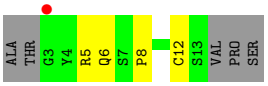
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain E:



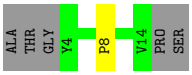
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain F:



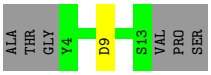
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain G:



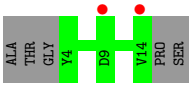
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain H:



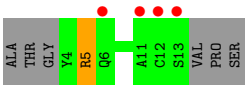
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain I:



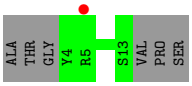
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain J:



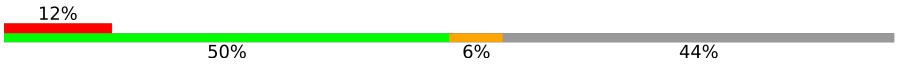
• Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

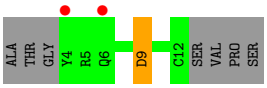
Chain K:



• Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.51Å 129.83Å 123.95Å 90.00° 92.31° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 29.08 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-3.20) 97.0 (29.08-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.214 , 0.239 0.220 , 0.246	Depositor DCC
R_{free} test set	2419 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	114.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 95.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14657	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.41	0/3575	0.65	0/4838
1	B	0.40	0/3571	0.66	1/4833 (0.0%)
1	C	0.42	0/3571	0.66	2/4833 (0.0%)
1	D	0.41	0/3581	0.66	2/4846 (0.0%)
2	E	0.60	0/86	0.72	0/115
2	F	0.60	0/79	0.85	0/105
2	G	0.43	0/74	0.66	0/99
2	H	0.46	0/67	0.69	0/89
2	I	0.41	0/74	0.63	0/99
2	J	0.74	0/67	1.00	0/89
2	K	0.48	0/67	0.65	0/89
2	L	0.53	0/61	0.80	0/81
All	All	0.42	0/14873	0.66	5/20116 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	546	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	546	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	334	TYR	N-CA-C	-5.33	96.60	111.00
1	B	200	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	334	TYR	N-CA-C	-5.05	97.37	111.00

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	3513	0	3531	18	0
1	B	3509	0	3528	17	0
1	C	3509	0	3527	17	0
1	D	3519	0	3535	15	0
2	E	85	0	75	0	0
2	F	78	0	65	5	0
2	G	74	0	65	1	0
2	H	67	0	55	1	0
2	I	74	0	65	0	0
2	J	67	0	56	1	0
2	K	67	0	56	0	0
2	L	61	0	51	1	0
3	A	12	0	0	0	0
3	B	5	0	0	0	0
3	C	8	0	0	0	0
3	D	9	0	0	0	0
All	All	14657	0	14609	61	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 2.

All (61) 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:B:623:GLN:OE1	1:C:463:LEU:HA	1.97	0.64
1:D:524:THR:HG22	1:D:527:HIS:CD2	2.35	0.62
1:C:524:THR:HG22	1:C:527:HIS:CD2	2.36	0.60
1:A:434:TRP:CE3	2:F:5:ARG:HD2	2.37	0.59
1:B:623:GLN:CD	1:C:463:LEU:HD23	2.25	0.57
1:B:392:GLY:HA3	1:C:590:LEU:HD21	1.87	0.55
1:C:498:ARG:NH1	1:C:528:CYS:SG	2.81	0.54
1:A:434:TRP:CD2	2:F:5:ARG:HD2	2.44	0.53
1:A:498:ARG:NH1	1:A:528:CYS:SG	2.82	0.53
1:B:498:ARG:NH1	1:B:528:CYS:SG	2.82	0.53
1:A:368:ARG:NE	2:F:6:GLN:HB2	2.25	0.52
1:D:498:ARG:NH1	1:D:528:CYS:SG	2.82	0.52
1:A:403:LEU:CD1	2:F:8:PRO:HB3	2.41	0.51
1:B:392:GLY:CA	1:C:590:LEU:HD21	2.43	0.49
1:A:398:LYS:HA	1:A:403:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PRO:HB3	1:D:243:HIS:NE2	2.28	0.48
1:C:183:LEU:HD11	1:C:209:ALA:HB1	1.96	0.48
1:D:398:LYS:HA	1:D:403:LEU:O	2.14	0.48
1:A:524:THR:HG22	1:A:527:HIS:ND1	2.29	0.48
1:B:398:LYS:HA	1:B:403:LEU:O	2.14	0.47
1:D:378:GLY:HA3	2:L:9:ASP:O	2.14	0.47
1:C:628:ALA:HA	1:C:639:LEU:HD12	1.96	0.47
1:D:183:LEU:HD11	1:D:209:ALA:HB1	1.96	0.47
1:B:183:LEU:HD11	1:B:209:ALA:HB1	1.96	0.46
1:A:476:PRO:HB3	1:D:243:HIS:CE1	2.50	0.46
1:B:370:SER:OG	2:H:9:ASP:OD2	2.23	0.46
1:C:398:LYS:HA	1:C:403:LEU:O	2.14	0.46
1:D:336:LYS:HE2	1:D:362:CYS:HB2	1.98	0.46
1:A:628:ALA:HA	1:A:639:LEU:HD12	1.98	0.46
1:A:183:LEU:HD11	1:A:209:ALA:HB1	1.97	0.45
1:B:628:ALA:HA	1:B:639:LEU:HD12	1.97	0.45
1:C:441:GLU:OE2	2:J:5:ARG:NH2	2.45	0.45
1:B:524:THR:HG22	1:B:527:HIS:ND1	2.31	0.45
1:B:611:LEU:HD11	1:B:639:LEU:HD23	1.99	0.45
1:C:611:LEU:HD11	1:C:639:LEU:HD23	1.99	0.44
1:D:611:LEU:HD11	1:D:639:LEU:HD23	1.99	0.44
1:D:628:ALA:HA	1:D:639:LEU:HD12	1.99	0.44
1:A:611:LEU:HD11	1:A:639:LEU:HD23	1.99	0.44
1:C:336:LYS:HE2	1:C:362:CYS:HB2	1.99	0.44
1:B:258:SER:OG	2:G:8:PRO:HG2	2.17	0.44
1:A:403:LEU:HD13	2:F:8:PRO:HB3	2.00	0.43
1:B:509:LEU:HD21	1:B:547:LYS:HG3	2.02	0.42
1:B:526:LEU:HD23	1:B:561:PRO:HG2	2.01	0.42
1:A:509:LEU:HD21	1:A:547:LYS:HG3	2.02	0.42
1:D:498:ARG:HB3	1:D:528:CYS:HB3	2.02	0.42
1:D:526:LEU:HD23	1:D:561:PRO:HG2	2.01	0.42
1:A:552:ASN:HD21	1:A:583:LYS:H	1.68	0.41
1:C:456:SER:HB2	1:C:518:GLN:NE2	2.35	0.41
1:C:498:ARG:HB3	1:C:528:CYS:HB3	2.02	0.41
1:C:526:LEU:HD23	1:C:561:PRO:HG2	2.01	0.41
1:A:245:ARG:CZ	1:A:251:ILE:HD11	2.49	0.41
1:D:456:SER:HB2	1:D:518:GLN:NE2	2.35	0.41
1:B:498:ARG:HB3	1:B:528:CYS:HB3	2.02	0.41
1:B:552:ASN:HD21	1:B:583:LYS:H	1.68	0.41
1:A:526:LEU:HD23	1:A:561:PRO:HG2	2.02	0.41
1:B:245:ARG:CZ	1:B:251:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ARG:CZ	1:C:251:ILE:HD11	2.51	0.41
1:C:509:LEU:HD21	1:C:547:LYS:HG3	2.03	0.41
1:A:498:ARG:HB3	1:A:528:CYS:HB3	2.03	0.40
1:D:552:ASN:HD21	1:D:583:LYS:H	1.68	0.40
1:D:245:ARG:CZ	1:D:251:ILE:HD11	2.51	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	460/482 (95%)	441 (96%)	18 (4%)	1 (0%)	47	79
1	B	459/482 (95%)	440 (96%)	18 (4%)	1 (0%)	47	79
1	C	459/482 (95%)	439 (96%)	19 (4%)	1 (0%)	47	79
1	D	461/482 (96%)	441 (96%)	19 (4%)	1 (0%)	47	79
2	E	10/16 (62%)	10 (100%)	0	0	100	100
2	F	9/16 (56%)	9 (100%)	0	0	100	100
2	G	9/16 (56%)	9 (100%)	0	0	100	100
2	H	8/16 (50%)	8 (100%)	0	0	100	100
2	I	9/16 (56%)	9 (100%)	0	0	100	100
2	J	8/16 (50%)	7 (88%)	1 (12%)	0	100	100
2	K	8/16 (50%)	8 (100%)	0	0	100	100
2	L	7/16 (44%)	7 (100%)	0	0	100	100
All	All	1907/2056 (93%)	1828 (96%)	75 (4%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	ALA
1	B	500	ALA
1	C	500	ALA
1	D	500	ALA

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	372/388 (96%)	367 (99%)	5 (1%)	69	87
1	B	372/388 (96%)	366 (98%)	6 (2%)	62	84
1	C	372/388 (96%)	365 (98%)	7 (2%)	57	81
1	D	373/388 (96%)	367 (98%)	6 (2%)	62	84
2	E	9/12 (75%)	8 (89%)	1 (11%)	6	25
2	F	8/12 (67%)	7 (88%)	1 (12%)	4	21
2	G	8/12 (67%)	8 (100%)	0	100	100
2	H	7/12 (58%)	7 (100%)	0	100	100
2	I	8/12 (67%)	8 (100%)	0	100	100
2	J	7/12 (58%)	6 (86%)	1 (14%)	3	15
2	K	7/12 (58%)	7 (100%)	0	100	100
2	L	6/12 (50%)	5 (83%)	1 (17%)	2	10
All	All	1549/1648 (94%)	1521 (98%)	28 (2%)	59	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	SER
1	A	395	VAL
1	A	498	ARG
1	A	555	ASN
1	A	557	ASP
1	B	258	SER
1	B	395	VAL

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Mol	Chain	Res	Type
1	B	483	ARG
1	B	498	ARG
1	B	555	ASN
1	B	557	ASP
1	C	258	SER
1	C	395	VAL
1	C	483	ARG
1	C	498	ARG
1	C	555	ASN
1	C	557	ASP
1	C	640	SER
1	D	180	SER
1	D	258	SER
1	D	395	VAL
1	D	498	ARG
1	D	555	ASN
1	D	557	ASP
2	E	4	TYR
2	F	12	CYS
2	J	5	ARG
2	L	9	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	280	ASN
1	A	552	ASN
1	A	637	GLN
1	B	280	ASN
1	B	552	ASN
1	B	637	GLN
1	C	280	ASN
1	C	303	GLN
1	C	527	HIS
1	C	552	ASN
1	D	280	ASN
1	D	303	GLN
1	D	527	HIS
1	D	552	ASN
1	D	637	GLN

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	462/482 (95%)	-0.09	1 (0%)	95	94	85, 119, 152, 170	0
1	B	461/482 (95%)	0.22	15 (3%)	46	30	92, 140, 176, 197	0
1	C	461/482 (95%)	0.15	13 (2%)	53	37	99, 153, 182, 196	0
1	D	463/482 (96%)	0.14	14 (3%)	50	34	90, 144, 182, 202	0
2	E	12/16 (75%)	0.14	1 (8%)	11	6	115, 125, 156, 164	0
2	F	11/16 (68%)	0.15	1 (9%)	9	5	129, 143, 158, 159	0
2	G	11/16 (68%)	0.52	0	100	100	140, 148, 169, 180	0
2	H	10/16 (62%)	0.31	0	100	100	145, 161, 165, 171	0
2	I	11/16 (68%)	0.69	2 (18%)	1	1	129, 143, 163, 164	0
2	J	10/16 (62%)	1.50	4 (40%)	0	0	188, 202, 206, 210	0
2	K	10/16 (62%)	0.82	1 (10%)	7	4	157, 164, 176, 177	0
2	L	9/16 (56%)	1.13	2 (22%)	0	0	179, 181, 189, 195	0
All	All	1931/2056 (93%)	0.13	54 (2%)	53	37	85, 140, 180, 210	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	642	SER	4.8
2	L	6	GLN	3.9
1	D	338	GLU	3.8
1	D	433	LEU	3.6
1	C	247	ASP	3.3
1	C	212	MET	3.0
1	D	400	LYS	3.0
1	D	313	THR	3.0
1	B	366	ASP	3.0
2	J	12	CYS	2.9
1	B	468	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	282	ASN	2.7
1	C	314	ASP	2.7
2	I	9	ASP	2.7
2	L	4	TYR	2.7
1	D	314	ASP	2.6
1	C	397	ALA	2.6
1	D	321	LEU	2.6
1	B	464	VAL	2.6
1	B	281	TRP	2.6
1	B	326	ALA	2.5
2	I	14	VAL	2.5
1	C	202	VAL	2.5
2	E	14	VAL	2.5
1	D	281	TRP	2.4
1	C	398	LYS	2.4
1	D	340	LEU	2.4
1	B	622	LEU	2.4
1	C	238	MET	2.4
1	B	589	THR	2.4
1	D	343	ALA	2.3
1	C	509	LEU	2.3
1	C	467	HIS	2.3
1	B	314	ASP	2.3
1	C	363	HIS	2.3
1	D	190	CYS	2.2
1	D	230	ASP	2.2
1	A	212	MET	2.2
1	B	558	PHE	2.2
1	C	512	GLU	2.2
1	B	351	LEU	2.2
2	K	5	ARG	2.2
1	B	225	GLY	2.1
1	B	466	CYS	2.1
1	D	402	GLY	2.1
2	J	11	ALA	2.1
2	J	6	GLN	2.1
1	B	327	LYS	2.1
1	C	477	THR	2.1
2	J	13	SER	2.1
1	D	212	MET	2.0
1	B	347	ASN	2.0
1	B	316	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	3	GLY	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.