



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 5JHQ / pdb_00005jhg
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

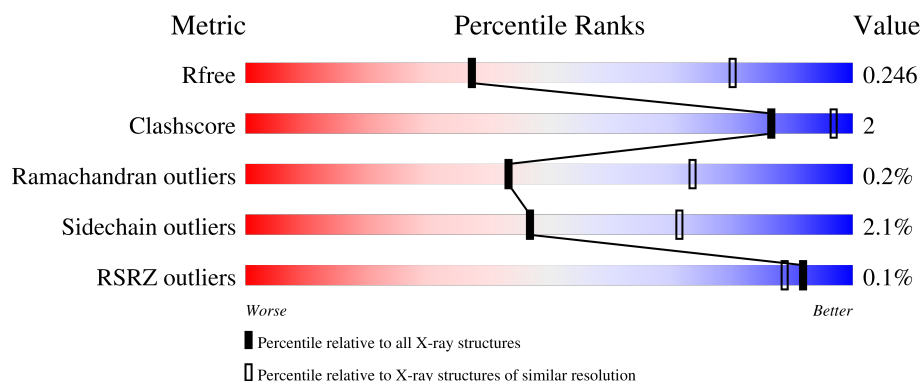
1 Overall quality at a glance

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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 $\leq 5\%$. 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	
1	B	482	
1	C	482	
1	D	482	
2	E	16	

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Mol	Chain	Length	Quality of chain
2	F	16	
2	G	16	
2	H	16	
2	I	16	
2	J	16	
2	K	16	
2	L	16	

2 Entry composition

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
1	A	462	Total	C	N	O	S	0	0	0
			3513	2185	654	654	20			
1	B	461	Total	C	N	O	S	0	0	0
			3509	2183	653	653	20			
1	C	461	Total	C	N	O	S	0	0	0
			3509	2183	653	653	20			
1	D	463	Total	C	N	O	S	0	0	0
			3519	2188	655	656	20			

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

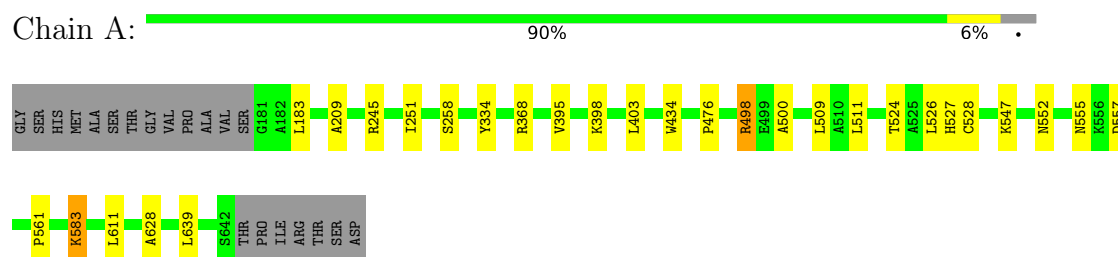
- Molecule 3 is water.

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

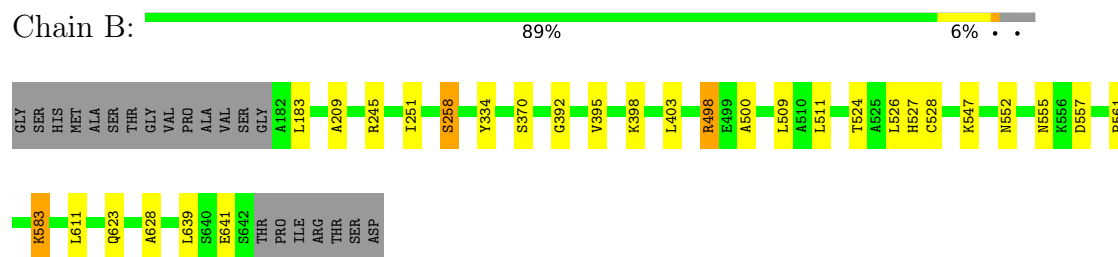
3 Residue-property plots

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.

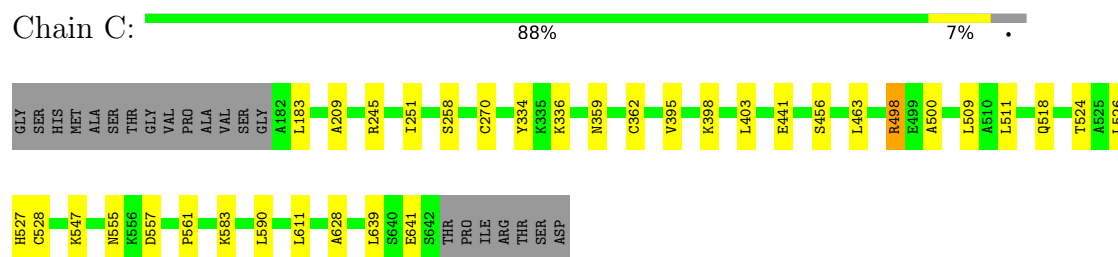
• Molecule 1: Tankyrase-1



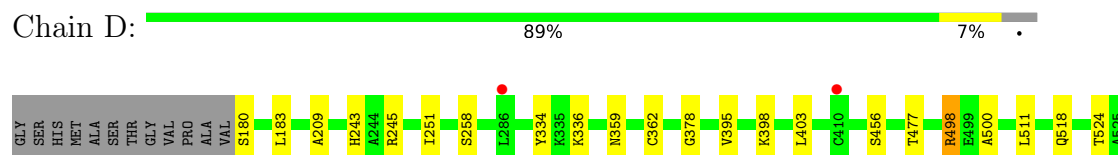
• Molecule 1: Tankyrase-1



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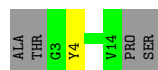


• Molecule 1: Tankyrase-1





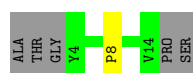
- Molecule 2: Peptide derived from insulin-responsive aminopeptidase (IRAP)



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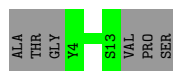


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Chain L:  50% 6% 44%



4 Data and refinement statistics

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 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-3.20) 96.6 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	2447 reflections (4.95%)	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)	0.30 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.61	0/3575	0.89	1/4838 (0.0%)
1	B	0.59	0/3571	0.88	2/4833 (0.0%)
1	C	0.62	1/3571 (0.0%)	0.91	5/4833 (0.1%)
1	D	0.62	0/3581	0.90	3/4846 (0.1%)
2	E	0.77	0/86	0.87	0/115
2	F	0.72	0/79	0.99	0/105
2	G	0.69	0/74	0.81	0/99
2	H	0.64	0/67	0.81	0/89
2	I	0.62	0/74	0.77	0/99
2	J	1.10	0/67	1.24	1/89 (1.1%)
2	K	0.71	0/67	0.78	0/89
2	L	0.81	0/61	0.96	0/81
All	All	0.62	1/14873 (0.0%)	0.89	12/20116 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	641	GLU	N-CA	5.15	1.52	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	334	TYR	N-CA-C	-8.18	97.37	109.15
1	C	641	GLU	N-CA-C	7.86	121.71	108.90
1	A	334	TYR	N-CA-C	7.66	122.18	109.46
1	C	334	TYR	N-CA-C	-7.52	96.60	108.63
1	B	334	TYR	N-CA-C	6.98	121.05	109.46
1	D	359	ASN	N-CA-C	6.44	122.02	112.94
1	D	334	TYR	CB-CA-C	6.14	120.00	110.67
1	C	359	ASN	N-CA-C	5.96	121.35	112.94
1	C	334	TYR	CB-CA-C	5.83	120.20	110.88
1	B	641	GLU	N-CA-C	-5.41	101.43	109.11
1	C	270	CYS	N-CA-C	5.38	117.90	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	12	CYS	N-CA-C	5.18	121.84	110.80

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	3513	0	3531	18	0
1	B	3509	0	3528	17	0
1	C	3509	0	3527	17	0
1	D	3519	0	3535	16	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	62	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 (62) 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:B:623:GLN:CD	1:C:463:LEU:HD23	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:370:SER:OG	2:H:9:ASP:OD2	2.23	0.51
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:625:PHE:HB2	1:D:630:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	43	73
1	B	459/482 (95%)	440 (96%)	18 (4%)	1 (0%)	43	73
1	C	459/482 (95%)	439 (96%)	19 (4%)	1 (0%)	43	73
1	D	461/482 (96%)	441 (96%)	19 (4%)	1 (0%)	43	73
2	E	10/16 (62%)	10 (100%)	0	0	100	100
2	F	9/16 (56%)	9 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	73

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 ⓘ

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%)	365 (98%)	7 (2%)	50	73
1	B	372/388 (96%)	365 (98%)	7 (2%)	50	73
1	C	372/388 (96%)	365 (98%)	7 (2%)	50	73
1	D	373/388 (96%)	364 (98%)	9 (2%)	43	70
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%)	7 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	7/12 (58%)	7 (100%)	0	100	100
2	L	6/12 (50%)	6 (100%)	0	100	100
All	All	1549/1648 (94%)	1517 (98%)	32 (2%)	47	71

All (32) 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	511	LEU
1	A	555	ASN
1	A	557	ASP
1	A	583	LYS
1	B	258	SER
1	B	395	VAL
1	B	498	ARG
1	B	511	LEU
1	B	555	ASN
1	B	557	ASP
1	B	583	LYS
1	C	258	SER
1	C	395	VAL
1	C	498	ARG
1	C	511	LEU
1	C	555	ASN
1	C	557	ASP
1	C	583	LYS
1	D	180	SER
1	D	258	SER
1	D	395	VAL
1	D	477	THR
1	D	498	ARG
1	D	511	LEU
1	D	555	ASN
1	D	557	ASP
1	D	583	LYS
2	E	4	TYR
2	F	12	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	HIS
1	A	280	ASN
1	A	435	GLN
1	A	552	ASN
1	A	571	ASN
1	A	580	HIS
1	A	623	GLN
1	A	637	GLN
1	B	280	ASN
1	B	435	GLN
1	B	534	HIS
1	B	552	ASN
1	B	571	ASN
1	B	580	HIS
1	B	637	GLN
1	C	243	HIS
1	C	280	ASN
1	C	282	ASN
1	C	303	GLN
1	C	435	GLN
1	C	520	GLN
1	C	527	HIS
1	C	534	HIS
1	C	552	ASN
1	C	571	ASN
1	C	580	HIS
1	D	255	ASN
1	D	280	ASN
1	D	303	GLN
1	D	435	GLN
1	D	520	GLN
1	D	527	HIS
1	D	552	ASN
1	D	571	ASN
1	D	580	HIS
1	D	629	GLN
1	D	637	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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%)	-0.53	0	100	100	85, 119, 152, 170	0
1	B	461/482 (95%)	-0.40	0	100	100	92, 140, 176, 197	0
1	C	461/482 (95%)	-0.41	0	100	100	99, 153, 182, 196	0
1	D	463/482 (96%)	-0.30	2 (0%)	88	79	90, 144, 182, 202	0
2	E	12/16 (75%)	-0.53	0	100	100	115, 125, 156, 164	0
2	F	11/16 (68%)	-0.44	0	100	100	129, 143, 158, 159	0
2	G	11/16 (68%)	-0.24	0	100	100	140, 148, 169, 180	0
2	H	10/16 (62%)	-0.08	0	100	100	145, 161, 165, 171	0
2	I	11/16 (68%)	-0.18	0	100	100	129, 143, 163, 164	0
2	J	10/16 (62%)	0.00	0	100	100	188, 202, 206, 210	0
2	K	10/16 (62%)	-0.33	0	100	100	157, 164, 176, 177	0
2	L	9/16 (56%)	-0.23	0	100	100	179, 181, 189, 195	0
All	All	1931/2056 (93%)	-0.40	2 (0%)	92	89	85, 140, 180, 210	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	410	CYS	2.6
1	D	286	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 oligosaccharides 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.