



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:06 am BST

PDB ID : 4JQ5
Title : Crystal structure of the human Nup49CCS2+3* coiled-coil segment
Authors : Stuwe, T.; Bley, C.J.; Mayo, D.J.; Hoelz, A.
Deposited on : 2013-03-20
Resolution : 2.19 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

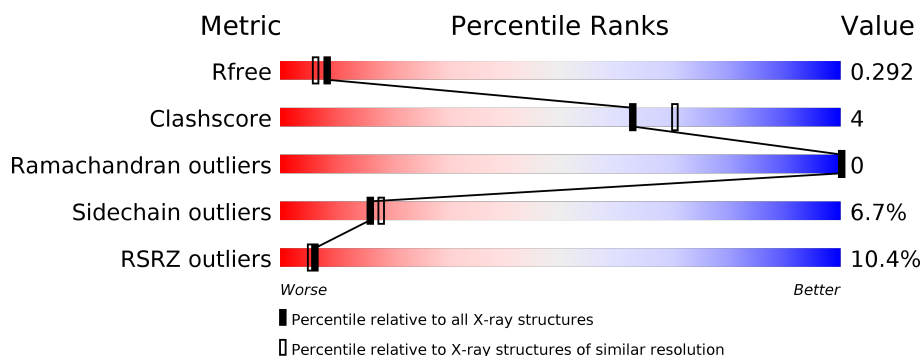
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	86	<div> <div>12%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	B	86	<div> <div>7%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	C	86	<div> <div>14%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	D	86	<div> <div>8%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	E	86	<div> <div>12%</div> <div>79%</div> <div>21%</div> <div></div> </div>
1	F	86	<div> <div>9%</div> <div>83%</div> <div>17%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	86	
1	H	86	
1	I	86	
1	J	86	
1	K	86	
1	L	86	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17026 atoms, of which 8500 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 Nucleoporin p58/p45.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	85	Total	C	H	N	O	S	0	0	0
			1413	452	706	122	130	3			
1	B	85	Total	C	H	N	O	S	0	0	0
			1413	452	706	122	130	3			
1	C	85	Total	C	H	N	O	S	0	0	0
			1413	452	706	122	130	3			
1	D	85	Total	C	H	N	O	S	0	0	0
			1413	452	706	122	130	3			
1	E	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			
1	F	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			
1	G	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			
1	H	85	Total	C	H	N	O	S	0	0	0
			1413	452	706	122	130	3			
1	I	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			
1	J	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			
1	K	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			
1	L	86	Total	C	H	N	O	S	0	0	0
			1423	455	710	123	132	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
B	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
C	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
D	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
E	326	SER	-	EXPRESSION TAG	UNP Q9BVL2

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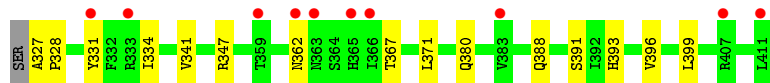
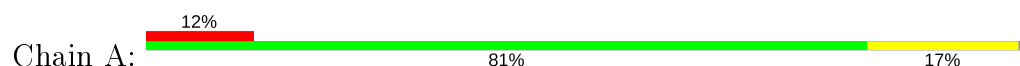
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Chain	Residue	Modelled	Actual	Comment	Reference
F	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
G	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
H	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
I	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
J	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
K	326	SER	-	EXPRESSION TAG	UNP Q9BVL2
L	326	SER	-	EXPRESSION TAG	UNP Q9BVL2

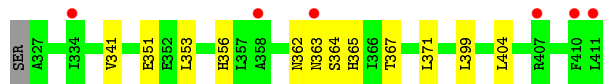
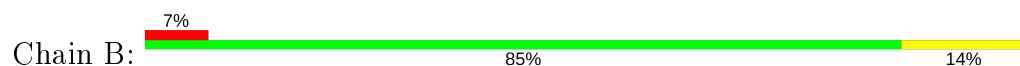
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Nucleoporin p58/p45



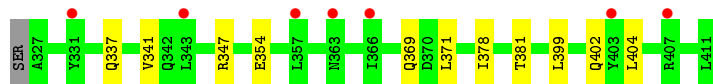
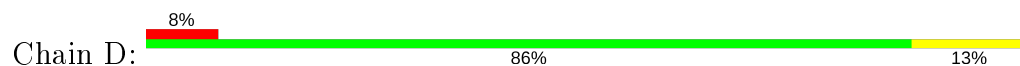
- Molecule 1: Nucleoporin p58/p45



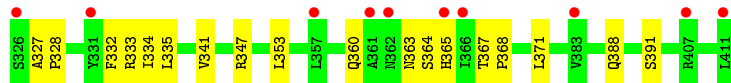
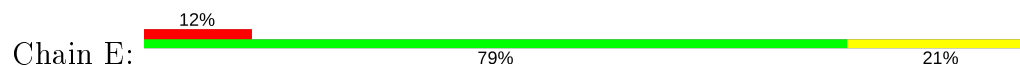
- Molecule 1: Nucleoporin p58/p45



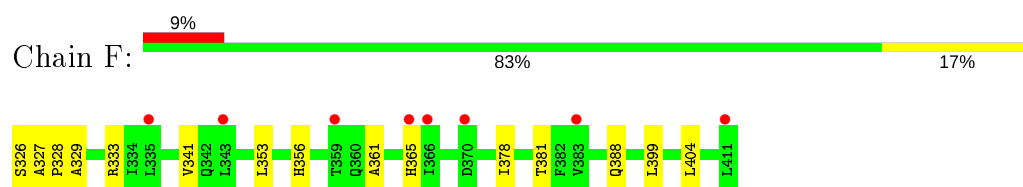
- Molecule 1: Nucleoporin p58/p45



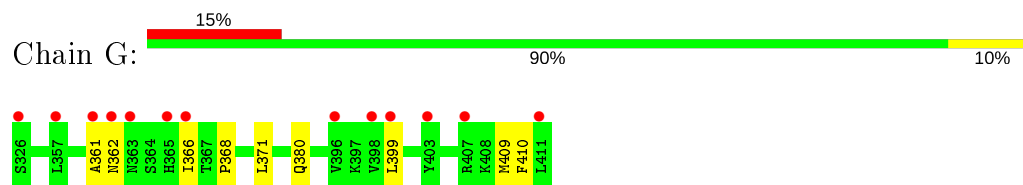
- Molecule 1: Nucleoporin p58/p45



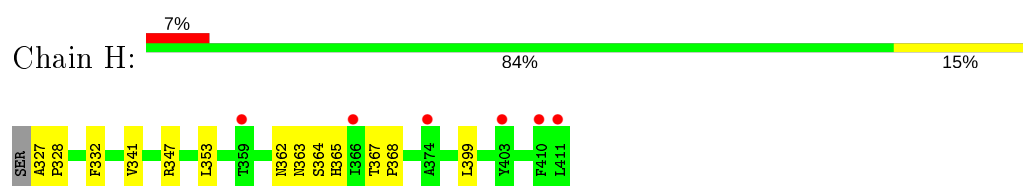
- Molecule 1: Nucleoporin p58/p45



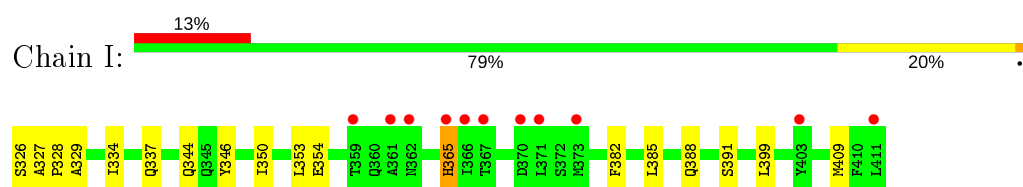
- Molecule 1: Nucleoporin p58/p45



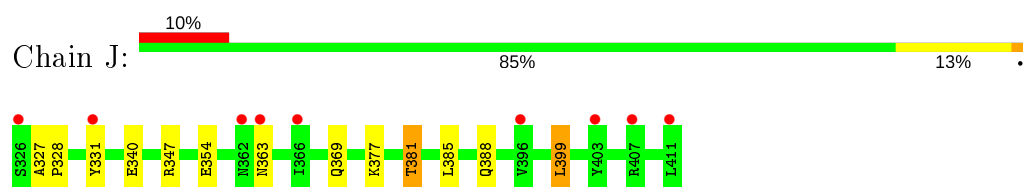
- Molecule 1: Nucleoporin p58/p45



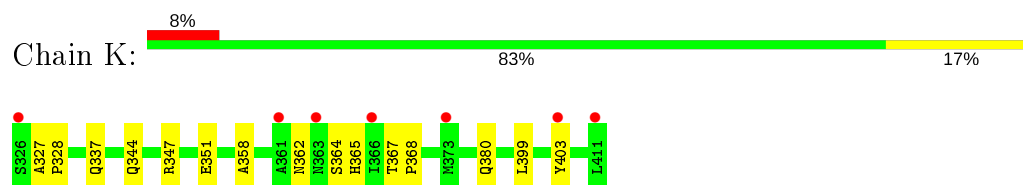
- Molecule 1: Nucleoporin p58/p45



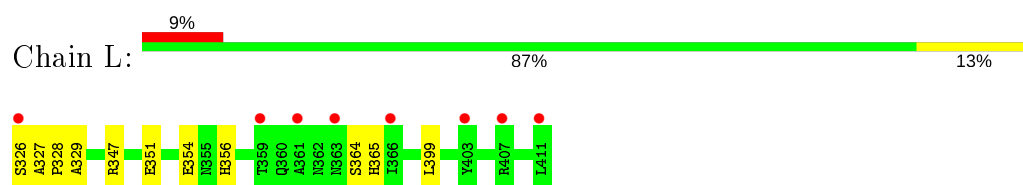
- Molecule 1: Nucleoporin p58/p45



- Molecule 1: Nucleoporin p58/p45



- Molecule 1: Nucleoporin p58/p45



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.82Å 77.10Å 77.20Å 120.04° 90.12° 89.96°	Depositor
Resolution (Å)	19.83 – 2.19 19.83 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.83-2.19) 89.6 (19.83-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.285 , 0.293 0.287 , 0.292	Depositor DCC
R_{free} test set	1990 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.458 for h,-l,k+l 0.458 for h,k+l,-k 0.457 for h,-k-l,k 0.457 for h,l,-k-l 0.487 for h,-k,-l 0.458 for -h,k,-k-l 0.460 for -h,l,k 0.477 for -h,-k-l,l 0.477 for -h,k+l,-l 0.459 for -h,-k,k+l 0.459 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17026	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.06% 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 [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	0.23	0/720	0.36	0/972
1	B	0.23	0/720	0.37	0/972
1	C	0.23	0/720	0.35	0/972
1	D	0.24	0/720	0.38	0/972
1	E	0.22	0/726	0.34	0/980
1	F	0.23	0/726	0.36	0/980
1	G	0.23	0/726	0.35	0/980
1	H	0.23	0/720	0.35	0/972
1	I	0.22	0/726	0.34	0/980
1	J	0.23	0/726	0.37	0/980
1	K	0.23	0/726	0.34	0/980
1	L	0.22	0/726	0.35	0/980
All	All	0.23	0/8682	0.36	0/11720

There are no bond length outliers.

There are no bond angle outliers.

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	707	706	702	8	0
1	B	707	706	702	3	0
1	C	707	706	702	6	0
1	D	707	706	702	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	713	710	707	11	0
1	F	713	710	707	10	0
1	G	713	710	707	5	0
1	H	707	706	702	6	0
1	I	713	710	707	13	0
1	J	713	710	707	9	0
1	K	713	710	707	11	0
1	L	713	710	707	10	0
All	All	8526	8500	8459	73	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 4.

All (73) 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:L:326:SER:OG	1:L:329:ALA:CB	2.34	0.75
1:L:326:SER:OG	1:L:329:ALA:HB3	1.89	0.72
1:B:362:ASN:O	1:C:333:ARG:NE	2.24	0.70
1:E:332:PHE:O	1:E:335:LEU:N	2.26	0.69
1:K:358:ALA:O	1:K:362:ASN:ND2	2.30	0.65
1:I:326:SER:OG	1:I:329:ALA:HB3	1.98	0.64
1:F:326:SER:OG	1:F:329:ALA:HB3	2.00	0.62
1:I:326:SER:OG	1:I:329:ALA:CB	2.48	0.62
1:I:354:GLU:OE1	1:J:347:ARG:NH1	2.33	0.61
1:C:364:SER:OG	1:C:365:HIS:N	2.33	0.61
1:L:326:SER:OG	1:L:329:ALA:HB2	2.02	0.59
1:I:365:HIS:ND1	1:I:365:HIS:O	2.37	0.58
1:L:327:ALA:N	1:L:328:PRO:HD2	2.20	0.56
1:F:327:ALA:N	1:F:328:PRO:HD2	2.20	0.55
1:E:360:GLN:O	1:E:364:SER:N	2.39	0.55
1:I:327:ALA:N	1:I:328:PRO:HD2	2.21	0.54
1:H:327:ALA:N	1:H:328:PRO:HD2	2.21	0.54
1:J:340:GLU:OE1	1:K:362:ASN:ND2	2.42	0.53
1:F:356:HIS:ND1	1:F:356:HIS:O	2.43	0.51
1:F:326:SER:OG	1:F:329:ALA:CB	2.57	0.51
1:C:327:ALA:N	1:C:328:PRO:CD	2.74	0.51
1:K:327:ALA:N	1:K:328:PRO:HD2	2.26	0.51
1:C:351:GLU:HG2	1:D:347:ARG:NE	2.26	0.50
1:L:356:HIS:ND1	1:L:356:HIS:O	2.44	0.50
1:A:327:ALA:N	1:A:328:PRO:CD	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:OE1	1:E:391:SER:OG	2.31	0.49
1:L:364:SER:OG	1:L:365:HIS:N	2.45	0.49
1:F:341:VAL:HG21	1:I:334:ILE:CD1	2.44	0.47
1:J:327:ALA:N	1:J:328:PRO:HD2	2.29	0.47
1:J:377:LYS:O	1:J:381:THR:HB	2.15	0.47
1:G:368:PRO:HG3	1:H:332:PHE:CE1	2.50	0.46
1:A:331:TYR:CD1	1:E:341:VAL:HG11	2.50	0.46
1:G:409:MET:HE3	1:G:410:PHE:CE1	2.50	0.46
1:I:385:LEU:O	1:I:388:GLN:N	2.49	0.46
1:E:327:ALA:N	1:E:328:PRO:HD2	2.31	0.45
1:J:331:TYR:CD2	1:J:399:LEU:HD11	2.51	0.45
1:G:409:MET:CE	1:G:410:PHE:CE1	3.00	0.45
1:F:361:ALA:HB3	1:G:362:ASN:OD1	2.17	0.45
1:H:327:ALA:N	1:H:328:PRO:CD	2.80	0.45
1:K:347:ARG:HD2	1:L:351:GLU:CG	2.47	0.45
1:K:403:TYR:CD1	1:K:403:TYR:C	2.90	0.45
1:H:364:SER:OG	1:H:365:HIS:N	2.50	0.44
1:A:334:ILE:CD1	1:E:341:VAL:HG21	2.47	0.44
1:E:367:THR:CG2	1:E:368:PRO:HD2	2.47	0.44
1:E:332:PHE:O	1:E:333:ARG:C	2.55	0.44
1:K:364:SER:OG	1:K:365:HIS:N	2.48	0.44
1:B:364:SER:O	1:B:365:HIS:C	2.57	0.43
1:H:367:THR:CG2	1:H:368:PRO:HD2	2.49	0.43
1:I:382:PHE:O	1:I:385:LEU:N	2.51	0.43
1:J:385:LEU:O	1:J:388:GLN:N	2.51	0.43
1:A:391:SER:OG	1:E:388:GLN:OE1	2.37	0.43
1:J:363:ASN:OD1	1:K:337:GLN:NE2	2.51	0.43
1:K:347:ARG:HD2	1:L:351:GLU:HG3	2.01	0.43
1:F:341:VAL:HG21	1:I:334:ILE:HD13	2.01	0.43
1:F:388:GLN:OE1	1:I:391:SER:OG	2.37	0.43
1:K:367:THR:CG2	1:K:368:PRO:HD2	2.48	0.43
1:K:344:GLN:HG2	1:L:354:GLU:OE2	2.19	0.43
1:G:361:ALA:HB2	1:G:366:ILE:HB	2.01	0.42
1:D:378:ILE:O	1:D:381:THR:HG22	2.19	0.42
1:A:341:VAL:HG21	1:E:334:ILE:CD1	2.50	0.41
1:C:347:ARG:NH1	1:D:354:GLU:OE1	2.50	0.41
1:I:346:TYR:CZ	1:I:350:ILE:HD11	2.56	0.41
1:E:333:ARG:HG2	1:E:334:ILE:N	2.34	0.41
1:F:327:ALA:N	1:F:328:PRO:CD	2.84	0.41
1:H:362:ASN:OD1	1:H:362:ASN:N	2.53	0.41
1:A:347:ARG:HD2	1:B:351:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:THR:HG22	1:C:370:ASP:OD2	2.20	0.41
1:I:326:SER:OG	1:I:329:ALA:HB2	2.21	0.40
1:J:327:ALA:HB3	1:J:328:PRO:HD3	2.03	0.40
1:K:351:GLU:CG	1:L:347:ARG:HD2	2.52	0.40
1:I:344:GLN:HG2	1:J:354:GLU:OE2	2.22	0.40
1:A:393:HIS:O	1:A:396:VAL:HG22	2.21	0.40
1:F:378:ILE:O	1:F:381:THR:HG22	2.21	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	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
1	B	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
1	C	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
1	D	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
1	E	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
1	F	84/86 (98%)	84 (100%)	0	0	100	100
1	G	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
1	H	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
1	I	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
1	J	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
1	K	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
1	L	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
All	All	1003/1032 (97%)	964 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	76/77 (99%)	71 (93%)	5 (7%)	16	19
1	B	76/77 (99%)	68 (90%)	8 (10%)	7	6
1	C	76/77 (99%)	63 (83%)	13 (17%)	2	1
1	D	76/77 (99%)	69 (91%)	7 (9%)	9	9
1	E	77/77 (100%)	72 (94%)	5 (6%)	17	19
1	F	77/77 (100%)	72 (94%)	5 (6%)	17	19
1	G	77/77 (100%)	74 (96%)	3 (4%)	32	41
1	H	76/77 (99%)	71 (93%)	5 (7%)	16	19
1	I	77/77 (100%)	72 (94%)	5 (6%)	17	19
1	J	77/77 (100%)	74 (96%)	3 (4%)	32	41
1	K	77/77 (100%)	75 (97%)	2 (3%)	46	58
1	L	77/77 (100%)	76 (99%)	1 (1%)	69	81
All	All	919/924 (100%)	857 (93%)	62 (7%)	16	18

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	ASN
1	A	367	THR
1	A	371	LEU
1	A	380	GLN
1	A	399	LEU
1	B	341	VAL
1	B	353	LEU
1	B	356	HIS
1	B	363	ASN
1	B	367	THR
1	B	371	LEU
1	B	399	LEU
1	B	404	LEU
1	C	337	GLN

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Mol	Chain	Res	Type
1	C	347	ARG
1	C	353	LEU
1	C	363	ASN
1	C	365	HIS
1	C	366	ILE
1	C	369	GLN
1	C	371	LEU
1	C	375	MET
1	C	380	GLN
1	C	399	LEU
1	C	404	LEU
1	C	410	PHE
1	D	337	GLN
1	D	341	VAL
1	D	369	GLN
1	D	371	LEU
1	D	399	LEU
1	D	402	GLN
1	D	404	LEU
1	E	347	ARG
1	E	353	LEU
1	E	363	ASN
1	E	365	HIS
1	E	371	LEU
1	F	333	ARG
1	F	353	LEU
1	F	365	HIS
1	F	399	LEU
1	F	404	LEU
1	G	371	LEU
1	G	380	GLN
1	G	399	LEU
1	H	341	VAL
1	H	347	ARG
1	H	353	LEU
1	H	363	ASN
1	H	399	LEU
1	I	337	GLN
1	I	353	LEU
1	I	365	HIS
1	I	399	LEU
1	I	409	MET

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Mol	Chain	Res	Type
1	J	369	GLN
1	J	381	THR
1	J	399	LEU
1	K	380	GLN
1	K	399	LEU
1	L	399	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	342	GLN
1	E	365	HIS

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 carbohydrates 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 ⓘ

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, 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	85/86 (98%)	1.10	10 (11%) 4 4	28, 50, 86, 93	0
1	B	85/86 (98%)	0.95	6 (7%) 16 14	28, 49, 81, 94	0
1	C	85/86 (98%)	1.17	12 (14%) 2 2	28, 49, 87, 93	0
1	D	85/86 (98%)	0.96	7 (8%) 11 10	28, 49, 79, 86	0
1	E	86/86 (100%)	1.14	10 (11%) 4 4	28, 50, 86, 95	0
1	F	86/86 (100%)	0.98	8 (9%) 8 7	29, 50, 83, 95	0
1	G	86/86 (100%)	1.18	13 (15%) 2 2	27, 51, 82, 97	0
1	H	85/86 (98%)	1.03	6 (7%) 16 14	29, 50, 86, 93	0
1	I	86/86 (100%)	1.04	11 (12%) 3 3	29, 49, 84, 93	0
1	J	86/86 (100%)	0.89	9 (10%) 6 5	27, 49, 80, 89	0
1	K	86/86 (100%)	1.04	7 (8%) 12 10	28, 48, 84, 92	0
1	L	86/86 (100%)	1.01	8 (9%) 8 7	27, 48, 81, 93	0
All	All	1027/1032 (99%)	1.04	107 (10%) 6 5	27, 50, 85, 97	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	ILE	7.7
1	E	411	LEU	6.7
1	K	326	SER	6.4
1	C	411	LEU	5.6
1	G	366	ILE	5.5
1	J	326	SER	5.5
1	C	366	ILE	5.3
1	G	411	LEU	5.0
1	I	366	ILE	5.0
1	K	366	ILE	4.7
1	L	363	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	L	411	LEU	4.6
1	A	411	LEU	4.4
1	E	362	ASN	4.3
1	G	362	ASN	4.2
1	C	407	ARG	4.2
1	A	363	ASN	4.2
1	H	366	ILE	3.8
1	B	407	ARG	3.6
1	K	411	LEU	3.6
1	G	326	SER	3.6
1	J	366	ILE	3.5
1	L	366	ILE	3.4
1	I	359	THR	3.4
1	L	361	ALA	3.3
1	E	366	ILE	3.3
1	L	326	SER	3.3
1	J	403	TYR	3.3
1	E	331	TYR	3.2
1	D	331	TYR	3.2
1	F	411	LEU	3.2
1	B	411	LEU	3.2
1	F	359	THR	3.1
1	C	365	HIS	3.1
1	A	365	HIS	3.0
1	A	407	ARG	3.0
1	C	333	ARG	2.9
1	E	361	ALA	2.9
1	K	363	ASN	2.9
1	E	407	ARG	2.8
1	D	357	LEU	2.8
1	D	403	TYR	2.8
1	E	365	HIS	2.7
1	J	331	TYR	2.7
1	D	366	ILE	2.7
1	H	411	LEU	2.7
1	L	359	THR	2.7
1	B	334	ILE	2.7
1	F	366	ILE	2.7
1	A	359	THR	2.7
1	B	358	ALA	2.6
1	F	370	ASP	2.6
1	I	370	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	410	PHE	2.6
1	I	371	LEU	2.6
1	G	361	ALA	2.6
1	B	363	ASN	2.6
1	C	410	PHE	2.6
1	I	403	TYR	2.5
1	J	362	ASN	2.5
1	I	361	ALA	2.5
1	G	365	HIS	2.5
1	G	407	ARG	2.5
1	C	403	TYR	2.5
1	G	363	ASN	2.4
1	E	326	SER	2.4
1	A	331	TYR	2.4
1	K	361	ALA	2.4
1	I	373	MET	2.4
1	H	359	THR	2.4
1	J	407	ARG	2.4
1	H	403	TYR	2.4
1	K	403	TYR	2.3
1	D	363	ASN	2.3
1	F	335	LEU	2.3
1	I	411	LEU	2.3
1	G	357	LEU	2.3
1	E	357	LEU	2.2
1	E	383	VAL	2.2
1	C	409	MET	2.2
1	K	373	MET	2.2
1	C	371	LEU	2.2
1	C	383	VAL	2.2
1	D	407	ARG	2.2
1	I	367	THR	2.2
1	L	407	ARG	2.2
1	D	343	LEU	2.2
1	G	396	VAL	2.2
1	I	365	HIS	2.2
1	C	359	THR	2.2
1	I	362	ASN	2.2
1	F	343	LEU	2.2
1	J	411	LEU	2.2
1	L	403	TYR	2.2
1	A	362	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	383	VAL	2.1
1	F	365	HIS	2.1
1	B	410	PHE	2.1
1	A	333	ARG	2.1
1	G	403	TYR	2.1
1	J	363	ASN	2.1
1	F	383	VAL	2.1
1	C	378	ILE	2.1
1	G	399	LEU	2.1
1	G	398	VAL	2.1
1	J	396	VAL	2.1
1	H	374	ALA	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.