



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:51 PM UTC

PDB ID : 6X04 / pdb_00006x04
Title : Nup133 (aa55-481) from *S. cerevisiae* bound by VHH-SAN5
Authors : Nordeen, S.A.; Schwartz, T.U.
Deposited on : 2020-05-15
Resolution : 2.68 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

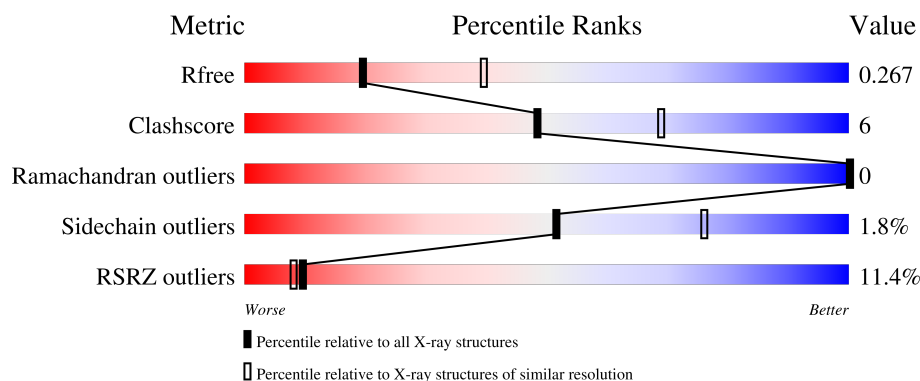
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	428	
1	C	428	
1	E	428	
1	G	428	
1	I	428	

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Mol	Chain	Length	Quality of chain
1	K	428	
2	B	118	
2	D	118	
2	F	118	
2	H	118	
2	J	118	
2	L	118	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20015 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 Nucleoporin NUP133.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2739	1769	435	525	10			
1	C	337	Total	C	N	O	S	0	0	0
			2405	1546	384	466	9			
1	E	315	Total	C	N	O	S	0	0	0
			2305	1491	363	442	9			
1	G	334	Total	C	N	O	S	0	0	0
			2486	1613	391	473	9			
1	I	346	Total	C	N	O	S	0	0	0
			2569	1660	410	488	11			
1	K	328	Total	C	N	O	S	0	0	0
			2414	1564	382	459	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	expression tag	UNP P36161
C	54	GLY	-	expression tag	UNP P36161
E	54	GLY	-	expression tag	UNP P36161
G	54	GLY	-	expression tag	UNP P36161
I	54	GLY	-	expression tag	UNP P36161
K	54	GLY	-	expression tag	UNP P36161

- Molecule 2 is a protein called VHH-SAN5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			853	534	152	162	5			
2	D	116	Total	C	N	O	S	0	0	0
			852	534	150	163	5			
2	F	116	Total	C	N	O	S	0	0	0
			844	528	149	162	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	116	Total	C	N	O	S	0	0	0
			847	531	149	162	5			
2	J	116	Total	C	N	O	S	0	0	0
			844	527	149	163	5			
2	L	116	Total	C	N	O	S	0	0	0
			842	528	146	163	5			

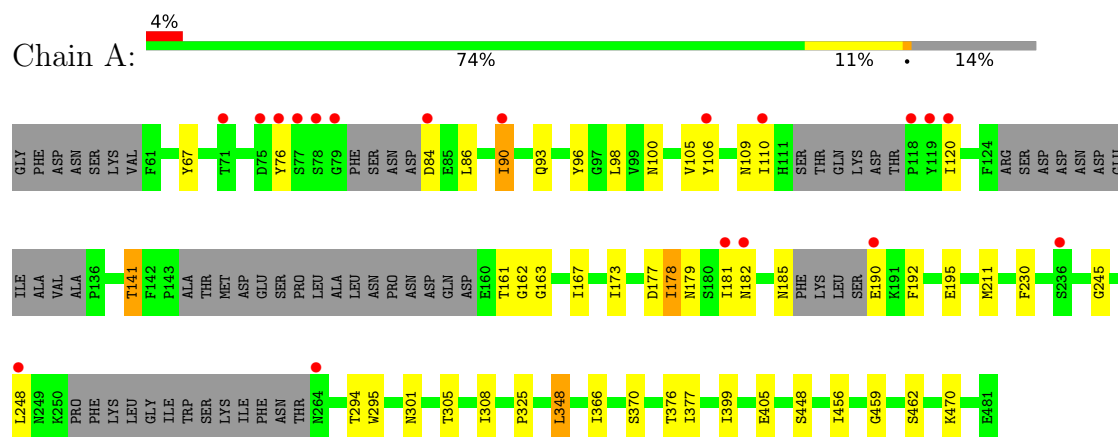
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	1	Total	O	0	0
			1	1		
3	E	1	Total	O	0	0
			1	1		
3	G	3	Total	O	0	0
			3	3		
3	I	3	Total	O	0	0
			3	3		
3	J	1	Total	O	0	0
			1	1		
3	K	2	Total	O	0	0
			2	2		

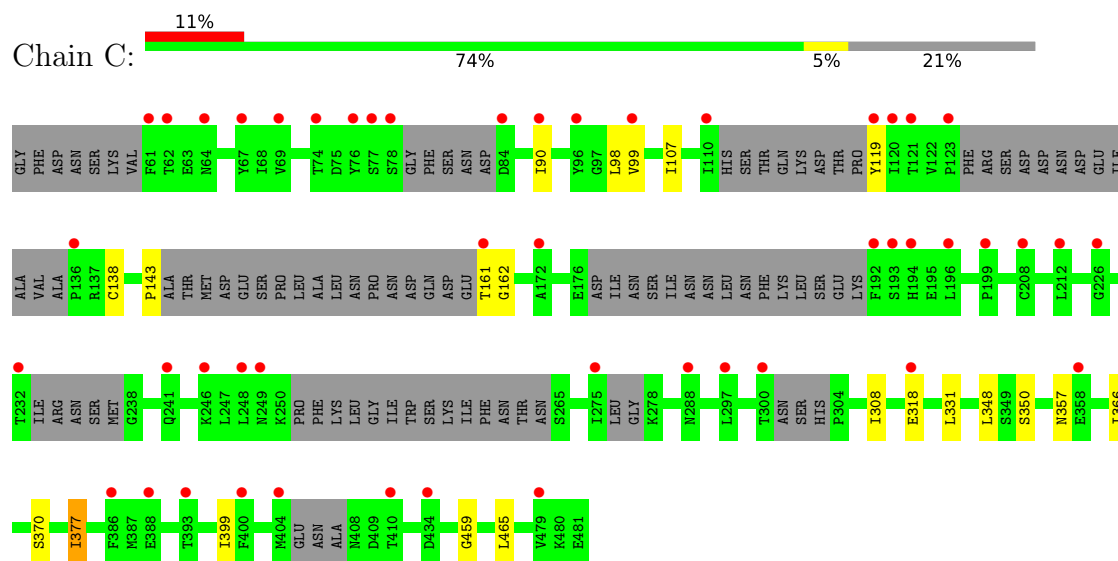
3 Residue-property plots [i](#)

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: Nucleoporin NUP133

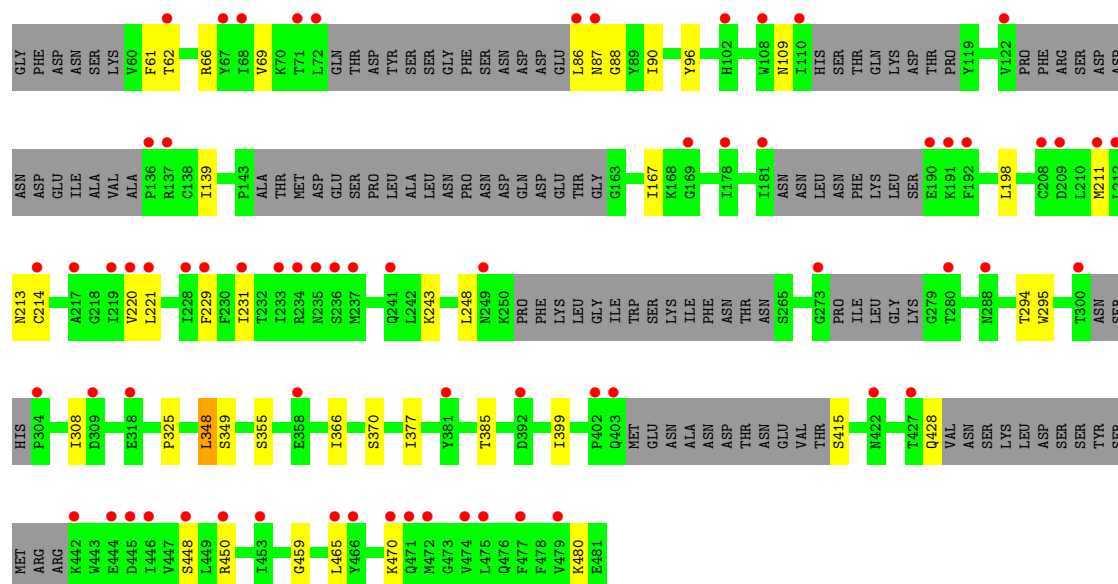


• Molecule 1: Nucleoporin NUP133

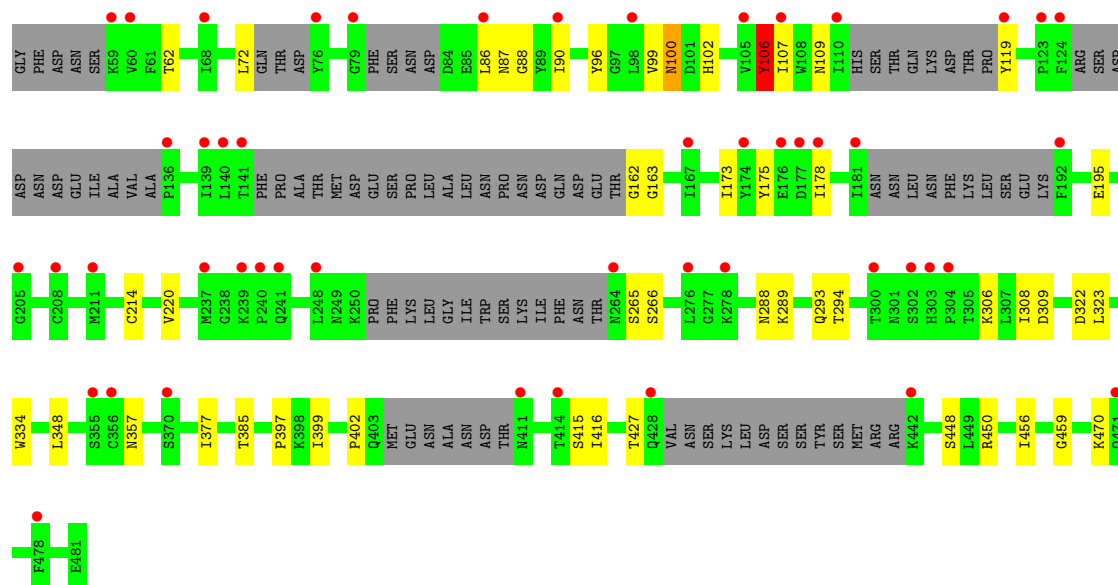


• Molecule 1: Nucleoporin NUP133

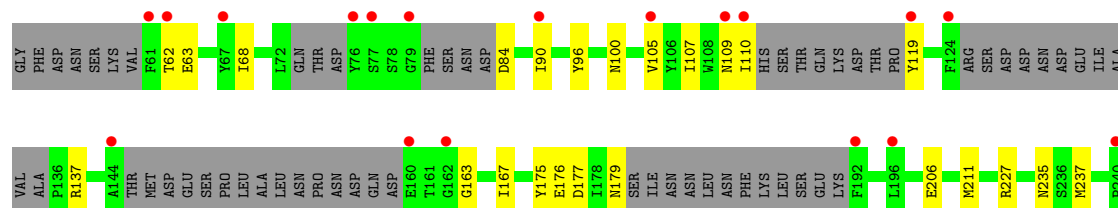


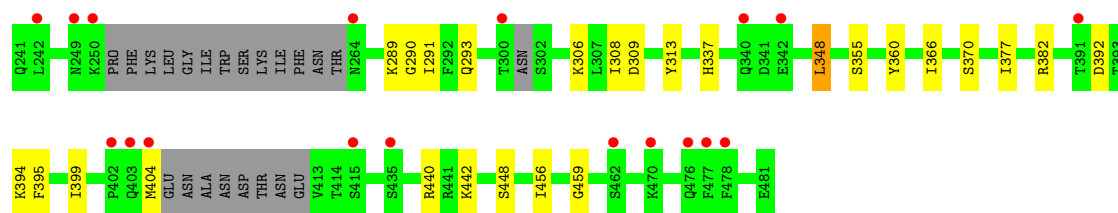


• Molecule 1: Nucleoporin NUP133

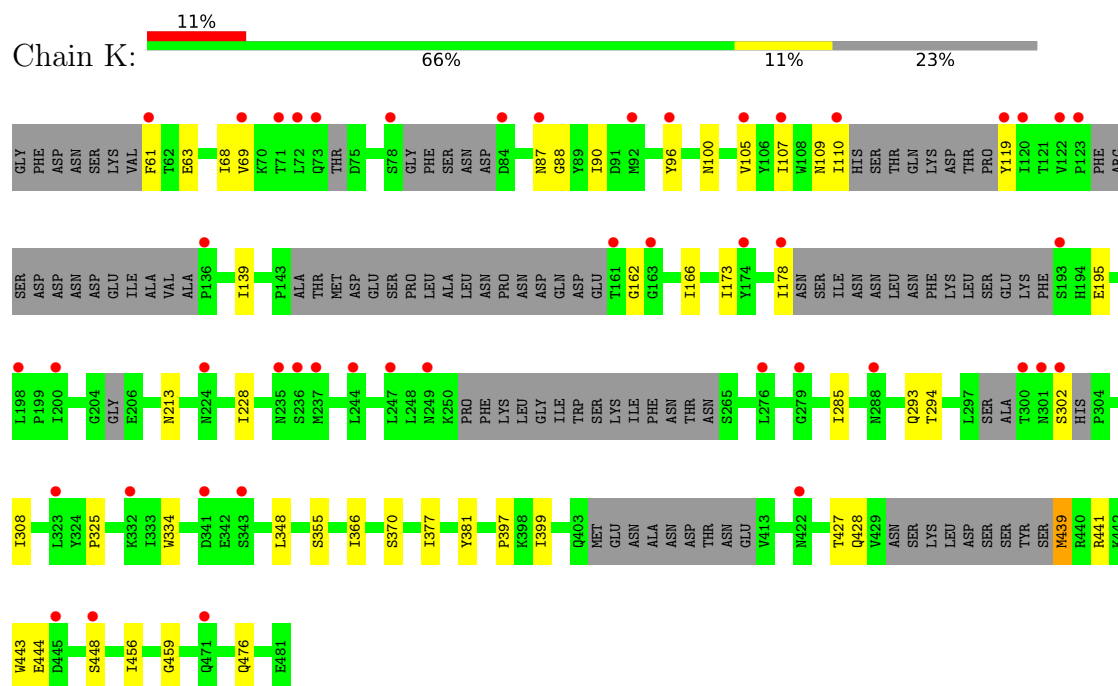


• Molecule 1: Nucleoporin NUP133

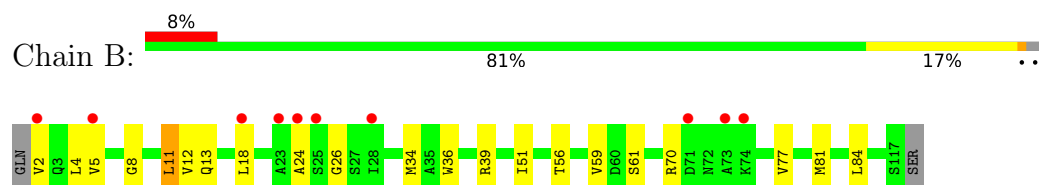




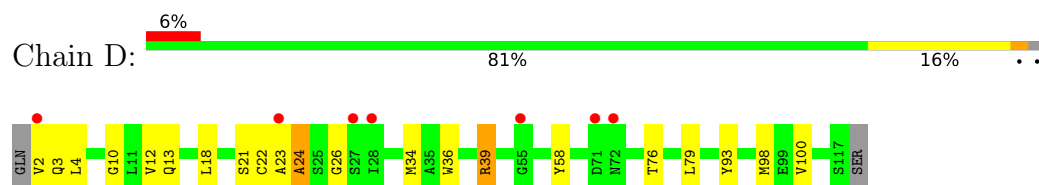
● Molecule 1: Nucleoporin NUP133



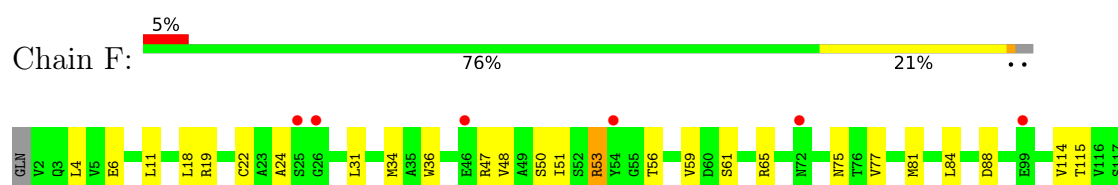
● Molecule 2: VHH-SAN5



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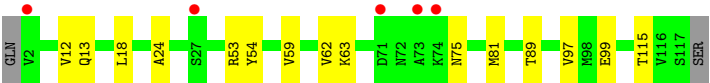
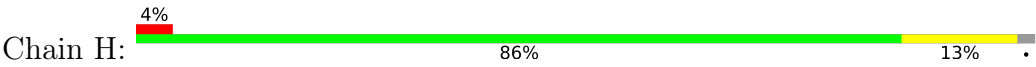


● Molecule 2: VHH-SAN5

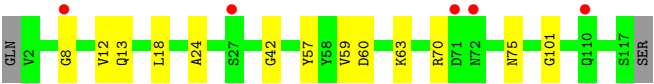
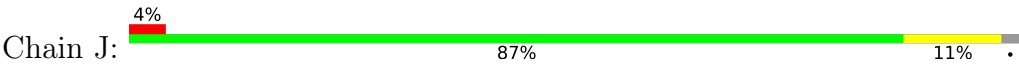


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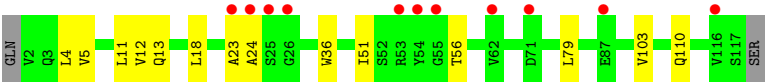
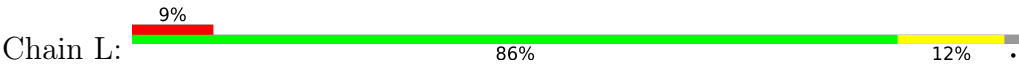
• Molecule 2: VHH-SAN5



• Molecule 2: VHH-SAN5



• Molecule 2: VHH-SAN5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.80Å 204.76Å 205.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.68 49.68 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.1 (49.68-2.68) 98.0 (49.68-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.243 , 0.261 0.247 , 0.267	Depositor DCC
R_{free} test set	2000 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20015	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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	0.39	0/2795	0.49	5/3812 (0.1%)
1	C	0.18	0/2446	0.32	1/3338 (0.0%)
1	E	0.13	0/2345	0.34	0/3193
1	G	0.26	1/2533 (0.0%)	0.41	2/3450 (0.1%)
1	I	0.32	2/2616 (0.1%)	0.40	0/3560
1	K	0.18	0/2455	0.34	0/3339
2	B	0.29	1/867 (0.1%)	0.37	0/1174
2	D	0.73	7/866 (0.8%)	0.46	0/1172
2	F	0.25	0/858	0.36	0/1163
2	H	0.13	0/861	0.37	0/1167
2	J	0.62	2/858 (0.2%)	0.47	0/1164
2	L	0.13	0/856	0.35	0/1161
All	All	0.31	13/20356 (0.1%)	0.39	8/27693 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	291	ILE	C-O	-6.91	1.16	1.24
2	D	22	CYS	CA-C	-6.77	1.44	1.52
2	D	23	ALA	CA-C	-6.18	1.45	1.52
2	D	22	CYS	C-O	-6.17	1.17	1.23
2	D	23	ALA	N-CA	-6.13	1.39	1.46
2	D	21	SER	C-O	-5.85	1.16	1.23
2	D	24	ALA	C-O	-5.81	1.17	1.23
2	J	70	ARG	CA-C	-5.58	1.45	1.52
2	J	70	ARG	N-CA	-5.55	1.39	1.46
1	I	290	GLY	C-O	-5.48	1.16	1.24
2	D	39	ARG	C-O	-5.33	1.18	1.24
1	G	106	TYR	C-O	-5.30	1.17	1.24
2	B	39	ARG	C-O	-5.04	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ASN	N-CA-C	-7.60	101.11	110.61
1	A	181	ILE	N-CA-C	6.73	118.83	107.18
1	G	100	ASN	N-CA-C	6.60	119.11	109.07
1	C	162	GLY	N-CA-C	5.63	119.51	111.12
1	G	106	TYR	N-CA-CB	-5.59	101.77	110.55
1	A	181	ILE	CB-CA-C	-5.50	104.14	110.41
1	A	182	ASN	N-CA-CB	5.16	118.88	111.65
1	A	301	ASN	N-CA-C	-5.15	101.73	109.15

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	2739	0	2518	26	1
1	C	2405	0	2125	12	0
1	E	2305	0	2086	25	0
1	G	2486	0	2289	37	0
1	I	2569	0	2371	27	0
1	K	2414	0	2212	31	0
2	B	853	0	817	14	0
2	D	852	0	820	18	0
2	F	844	0	797	15	0
2	H	847	0	806	12	0
2	J	844	0	792	8	1
2	L	842	0	798	12	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	3	0	0	0	0
3	I	3	0	0	0	0
3	J	1	0	0	0	0
3	K	2	0	0	0	0
All	All	20015	0	18431	213	1

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 6.

All (213) 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:G:265:SER:CA	1:G:288:ASN:HD21	1.31	1.42
1:G:265:SER:HA	1:G:288:ASN:ND2	1.43	1.28
1:C:143:PRO:HB3	1:C:161:THR:O	1.32	1.25
1:G:266:SER:H	1:G:288:ASN:ND2	1.54	1.06
1:C:143:PRO:CB	1:C:161:THR:O	2.03	1.05
1:G:266:SER:N	1:G:288:ASN:ND2	2.06	1.04
2:D:4:LEU:HD22	2:D:24:ALA:HB3	1.41	0.99
2:F:53:ARG:H	2:F:53:ARG:HD2	1.31	0.96
2:D:4:LEU:CD2	2:D:24:ALA:HB3	1.95	0.95
2:D:4:LEU:HA	2:D:24:ALA:CB	1.98	0.92
2:D:3:GLN:O	2:D:24:ALA:HB1	1.78	0.83
1:G:106:TYR:CE1	1:G:119:TYR:HB2	2.15	0.81
1:G:265:SER:HA	1:G:288:ASN:HD21	0.63	0.78
1:G:162:GLY:HA2	1:G:178:ILE:HG22	1.66	0.77
1:G:265:SER:C	1:G:288:ASN:ND2	2.42	0.77
1:G:265:SER:C	1:G:288:ASN:HD21	1.91	0.77
1:I:392:ASP:OD1	1:I:394:LYS:N	2.18	0.76
1:C:143:PRO:CA	1:C:161:THR:O	2.35	0.75
1:K:439:MET:HE2	2:L:103:VAL:HG13	1.71	0.72
1:I:348:LEU:HB2	1:I:399:ILE:HD11	1.72	0.71
1:A:448:SER:HB2	2:D:12:VAL:HG22	1.72	0.70
1:A:173:ILE:HG22	1:A:195:GLU:HG2	1.73	0.70
1:E:86:LEU:HD12	1:E:470:LYS:HG3	1.75	0.69
2:D:4:LEU:HA	2:D:24:ALA:HB2	1.75	0.69
1:E:348:LEU:HB2	1:E:399:ILE:HD11	1.76	0.67
1:G:86:LEU:HD12	1:G:470:LYS:HG3	1.77	0.66
2:D:4:LEU:HD23	2:D:24:ALA:HB3	1.79	0.65
1:A:90:ILE:HG23	1:A:459:GLY:HA3	1.78	0.65
1:I:163:GLY:HA2	1:I:175:TYR:O	1.97	0.65
1:E:355:SER:HA	1:K:325:PRO:HB2	1.78	0.64
1:G:265:SER:CA	1:G:288:ASN:ND2	2.16	0.64
1:G:288:ASN:OD1	1:G:289:LYS:N	2.31	0.64
2:B:5:VAL:HG22	2:B:24:ALA:HB2	1.81	0.63
1:K:173:ILE:HG22	1:K:195:GLU:HG2	1.80	0.63
2:F:53:ARG:H	2:F:53:ARG:CD	1.98	0.63
1:G:173:ILE:HG22	1:G:195:GLU:HG2	1.80	0.62
2:F:53:ARG:HD2	2:F:53:ARG:N	2.11	0.61
1:K:107:ILE:O	1:K:119:TYR:HA	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:ILE:HD13	1:I:211:MET:HE1	1.83	0.60
1:G:266:SER:N	1:G:288:ASN:HD22	1.98	0.60
1:I:177:ASP:OD1	1:I:179:ASN:ND2	2.34	0.60
1:I:306:LYS:HD2	1:I:309:ASP:HB2	1.84	0.59
1:G:90:ILE:HG23	1:G:459:GLY:HA3	1.84	0.59
2:J:12:VAL:HG21	2:J:18:LEU:HG	1.84	0.59
2:L:12:VAL:HG21	2:L:18:LEU:HG	1.85	0.58
2:D:4:LEU:HD23	2:D:24:ALA:CB	2.34	0.58
1:E:90:ILE:HG23	1:E:459:GLY:HA3	1.84	0.58
2:L:51:ILE:HG13	2:L:56:THR:HG22	1.85	0.58
2:L:4:LEU:HA	2:L:24:ALA:HB3	1.86	0.58
2:B:36:TRP:HE1	2:B:77:VAL:HG12	1.68	0.58
2:F:65:ARG:NH2	2:F:88:ASP:OD2	2.37	0.57
1:G:107:ILE:O	1:G:119:TYR:HA	2.04	0.57
2:F:47:ARG:HD2	2:F:50:SER:HB3	1.86	0.57
2:F:81:MET:HE1	2:F:114:VAL:HG11	1.85	0.57
1:C:357:ASN:O	2:H:63:LYS:NZ	2.37	0.57
1:C:90:ILE:HG23	1:C:459:GLY:HA3	1.86	0.57
2:B:51:ILE:HG13	2:B:56:THR:HG22	1.85	0.57
1:I:90:ILE:HG23	1:I:459:GLY:HA3	1.86	0.56
2:B:34:MET:HB3	2:B:77:VAL:HG21	1.87	0.56
2:J:24:ALA:HB3	2:J:75:ASN:HB3	1.87	0.56
1:E:415:SER:HA	1:E:428:GLN:HA	1.86	0.56
1:G:334:TRP:HB3	1:G:397:PRO:HG2	1.87	0.56
1:I:440:ARG:O	1:I:442:LYS:NZ	2.33	0.56
1:A:308:ILE:HD11	1:A:370:SER:HA	1.88	0.55
1:A:178:ILE:HD12	1:A:178:ILE:O	2.06	0.55
2:D:39:ARG:NH1	2:D:93:TYR:OH	2.35	0.55
1:G:448:SER:HB2	2:J:12:VAL:HA	1.88	0.54
1:A:325:PRO:HB2	1:I:355:SER:HA	1.90	0.54
1:G:385:THR:HG22	2:J:8:GLY:HA2	1.90	0.54
2:F:59:VAL:HG12	2:F:61:SER:H	1.73	0.54
1:A:86:LEU:HD12	1:A:470:LYS:HG3	1.90	0.54
1:A:348:LEU:HB2	1:A:399:ILE:HD11	1.90	0.53
1:K:308:ILE:HD11	1:K:370:SER:HA	1.90	0.53
1:A:96:TYR:HH	1:A:161:THR:HG1	1.53	0.53
2:H:13:GLN:NE2	1:K:448:SER:O	2.39	0.53
1:G:102:HIS:C	1:G:102:HIS:CD2	2.87	0.53
1:K:162:GLY:HA2	1:K:178:ILE:HG22	1.91	0.53
2:F:51:ILE:HG13	2:F:56:THR:HG22	1.90	0.53
1:A:167:ILE:HD13	1:A:211:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:TYR:O	1:G:357:ASN:ND2	2.41	0.52
1:G:87:ASN:OD1	1:G:88:GLY:N	2.41	0.52
2:B:8:GLY:HA2	1:E:385:THR:HG22	1.92	0.52
1:E:66:ARG:O	1:E:480:LYS:N	2.43	0.52
2:J:101:GLY:HA2	2:L:23:ALA:HB3	1.92	0.52
2:D:4:LEU:CD2	2:D:24:ALA:CB	2.78	0.52
1:G:416:ILE:HG23	1:G:427:THR:HG23	1.93	0.51
1:C:308:ILE:HD11	1:C:370:SER:HA	1.93	0.51
2:B:4:LEU:HA	2:B:24:ALA:HB3	1.92	0.51
1:K:366:ILE:HG12	1:K:377:ILE:HD13	1.92	0.50
1:C:143:PRO:HA	1:C:161:THR:O	2.09	0.50
1:E:308:ILE:HD11	1:E:370:SER:HA	1.93	0.50
1:A:162:GLY:HA2	1:A:178:ILE:HG22	1.94	0.50
1:E:167:ILE:HD13	1:E:211:MET:HE1	1.94	0.50
2:B:13:GLN:HG3	1:E:450:ARG:HA	1.94	0.49
1:I:392:ASP:OD1	1:I:395:PHE:N	2.45	0.49
1:C:107:ILE:O	1:C:119:TYR:HA	2.12	0.49
1:A:93:GLN:NE2	1:A:405:GLU:OE2	2.45	0.49
1:I:293:GLN:HA	1:I:308:ILE:O	2.13	0.49
2:B:81:MET:HE2	2:B:84:LEU:HD21	1.95	0.48
2:J:60:ASP:HA	2:J:63:LYS:HE3	1.95	0.48
2:H:12:VAL:HG21	2:H:18:LEU:HG	1.95	0.48
1:K:439:MET:CE	2:L:103:VAL:HG13	2.42	0.48
1:K:100:ASN:HB3	1:K:105:VAL:HG23	1.96	0.48
1:G:100:ASN:C	1:G:100:ASN:ND2	2.71	0.48
2:H:12:VAL:HG12	2:H:13:GLN:O	2.14	0.48
1:I:63:GLU:HG3	1:I:68:ILE:HG12	1.95	0.48
1:E:325:PRO:HB2	1:K:355:SER:HA	1.96	0.48
1:G:402:PRO:HD2	1:G:415:SER:O	2.14	0.48
1:C:366:ILE:HG12	1:C:377:ILE:HD13	1.95	0.48
1:I:360:TYR:HD1	1:I:382:ARG:HD2	1.79	0.48
1:I:107:ILE:O	1:I:119:TYR:HA	2.14	0.47
1:I:137:ARG:HH21	1:I:211:MET:HG2	1.78	0.47
1:K:87:ASN:OD1	1:K:88:GLY:N	2.46	0.47
1:K:428:GLN:OE1	1:K:443:TRP:NE1	2.44	0.47
1:I:289:LYS:O	1:I:313:TYR:HB2	2.14	0.47
1:E:220:VAL:HA	1:E:229:PHE:O	2.15	0.47
1:A:185:ASN:HD22	1:A:190:GLU:N	2.12	0.47
2:L:5:VAL:HG23	2:L:110:GLN:HE22	1.79	0.47
1:G:163:GLY:HA2	1:G:175:TYR:O	2.15	0.47
2:H:24:ALA:HB3	2:H:75:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:61:PHE:HA	1:K:69:VAL:O	2.15	0.46
1:K:162:GLY:HA2	1:K:178:ILE:H	1.80	0.46
1:K:348:LEU:HB2	1:K:399:ILE:HD11	1.96	0.46
1:K:427:THR:HG22	1:K:444:GLU:HG3	1.96	0.46
1:E:96:TYR:HA	1:E:109:ASN:HA	1.98	0.46
1:A:405:GLU:HB2	1:A:462:SER:HA	1.98	0.46
1:E:139:ILE:HD11	1:E:213:ASN:HB2	1.98	0.46
1:G:266:SER:H	1:G:288:ASN:CG	2.20	0.46
1:I:90:ILE:HD11	1:I:110:ILE:HG21	1.98	0.46
1:A:366:ILE:HG12	1:A:377:ILE:HD13	1.97	0.46
1:A:177:ASP:OD1	1:A:179:ASN:CB	2.64	0.45
1:E:231:ILE:HG23	1:E:243:LYS:O	2.16	0.45
2:B:2:VAL:HG22	2:B:26:GLY:HA3	1.97	0.45
1:C:348:LEU:HB2	1:C:399:ILE:HD11	1.98	0.45
1:A:90:ILE:HD11	1:A:110:ILE:HG21	1.97	0.45
1:A:98:LEU:HA	1:A:106:TYR:O	2.15	0.45
1:E:214:CYS:SG	1:E:220:VAL:HG23	2.57	0.45
1:I:337:HIS:HE1	1:I:404:MET:HG3	1.81	0.45
1:K:90:ILE:HG23	1:K:459:GLY:HA3	1.98	0.45
1:I:360:TYR:CD1	1:I:382:ARG:HD2	2.51	0.45
1:G:322:ASP:HB2	2:H:97:VAL:HG21	1.98	0.45
1:K:90:ILE:HD11	1:K:110:ILE:HG21	1.98	0.45
1:A:230:PHE:O	1:A:245:GLY:N	2.47	0.44
2:H:18:LEU:HB2	2:H:81:MET:HE2	1.99	0.44
1:G:306:LYS:HE3	1:G:309:ASP:HB2	1.99	0.44
1:E:366:ILE:HG12	1:E:377:ILE:HD13	1.98	0.44
2:B:12:VAL:HG21	2:B:18:LEU:HG	1.99	0.44
1:E:87:ASN:OD1	1:E:88:GLY:N	2.47	0.44
2:F:31:LEU:HD12	2:F:34:MET:HE3	2.00	0.44
1:E:294:THR:HB	1:E:308:ILE:HB	1.99	0.43
1:K:439:MET:CE	2:L:103:VAL:HG22	2.47	0.43
2:B:11:LEU:HD13	1:E:62:THR:OG1	2.18	0.43
1:A:141:THR:OG1	1:A:163:GLY:HA3	2.19	0.43
1:E:61:PHE:HB3	1:E:69:VAL:O	2.18	0.43
1:I:62:THR:HG22	2:L:11:LEU:HD13	2.00	0.43
1:G:294:THR:HB	1:G:308:ILE:HB	2.00	0.43
1:K:139:ILE:HD11	1:K:213:ASN:HB2	2.00	0.43
1:G:214:CYS:SG	1:G:220:VAL:HG23	2.58	0.43
1:G:323:LEU:HB2	2:H:97:VAL:HG11	2.01	0.43
1:E:198:LEU:HD21	1:E:231:ILE:HD11	2.01	0.43
1:K:302:SER:O	1:K:302:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:69:VAL:HA	1:K:476:GLN:O	2.18	0.42
2:J:57:TYR:OH	2:J:59:VAL:HG22	2.19	0.42
2:B:59:VAL:HG12	2:B:61:SER:H	1.83	0.42
2:B:70:ARG:HB2	2:B:77:VAL:HG22	2.01	0.42
2:D:2:VAL:HG13	2:D:26:GLY:HA3	2.01	0.42
2:D:12:VAL:HG21	2:D:18:LEU:HG	2.01	0.42
1:A:294:THR:HB	1:A:308:ILE:HB	2.01	0.42
1:G:323:LEU:HD21	2:H:99:GLU:HB2	2.02	0.42
2:H:59:VAL:HG12	2:H:62:VAL:HG22	2.02	0.42
2:D:12:VAL:HG12	2:D:13:GLN:O	2.19	0.42
1:E:248:LEU:HD22	1:E:295:TRP:CZ3	2.55	0.42
2:F:24:ALA:HB3	2:F:75:ASN:HB3	2.02	0.42
1:K:166:ILE:HB	1:K:173:ILE:HG13	2.01	0.42
2:D:34:MET:HE1	2:D:76:THR:N	2.35	0.42
1:I:206:GLU:OE1	1:I:227:ARG:NH2	2.53	0.42
2:D:36:TRP:CD1	2:D:79:LEU:HB2	2.55	0.41
1:I:366:ILE:HG12	1:I:377:ILE:HD13	2.02	0.41
1:I:448:SER:HB2	2:L:12:VAL:HG22	2.02	0.41
1:K:228:ILE:HD13	1:K:285:ILE:HD13	2.02	0.41
2:L:12:VAL:HG12	2:L:13:GLN:O	2.19	0.41
2:B:12:VAL:HA	1:E:448:SER:HB2	2.02	0.41
1:I:100:ASN:HB3	1:I:105:VAL:HG23	2.02	0.41
1:K:294:THR:HB	1:K:308:ILE:HB	2.02	0.41
2:L:36:TRP:CD1	2:L:79:LEU:HB2	2.55	0.41
2:F:18:LEU:HD23	2:F:19:ARG:N	2.35	0.41
1:I:308:ILE:HD11	1:I:370:SER:HA	2.03	0.41
2:F:11:LEU:HD13	2:F:115:THR:HB	2.02	0.41
2:H:89:THR:HG23	2:H:115:THR:HA	2.02	0.41
1:K:96:TYR:HA	1:K:109:ASN:HA	2.02	0.41
1:E:221:LEU:HB2	1:E:229:PHE:HB2	2.02	0.41
1:K:63:GLU:HG3	1:K:68:ILE:HG23	2.03	0.41
1:A:96:TYR:HA	1:A:109:ASN:HA	2.03	0.41
1:C:331:LEU:HA	1:C:350:SER:O	2.21	0.41
2:F:81:MET:HE3	2:F:84:LEU:HD11	2.02	0.41
1:G:293:GLN:HA	1:G:308:ILE:O	2.20	0.41
1:K:334:TRP:HB3	1:K:397:PRO:HG2	2.03	0.41
1:A:67:TYR:OH	2:D:10:GLY:HA2	2.21	0.41
2:F:4:LEU:HD22	2:F:22:CYS:SG	2.61	0.41
1:A:100:ASN:HB3	1:A:105:VAL:HG23	2.01	0.40
2:F:36:TRP:O	2:F:48:VAL:HG12	2.20	0.40
1:G:348:LEU:HB2	1:G:399:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:TYR:CZ	1:A:109:ASN:HB3	2.56	0.40
1:G:450:ARG:HA	2:J:13:GLN:HG3	2.02	0.40
2:H:53:ARG:NH2	2:H:54:TYR:OH	2.54	0.40
1:K:381:TYR:CE1	1:K:441:ARG:HG3	2.56	0.40
1:G:96:TYR:HA	1:G:109:ASN:HA	2.03	0.40
1:I:96:TYR:CZ	1:I:109:ASN:HB3	2.57	0.40
1:I:235:ASN:C	1:I:237:MET:H	2.30	0.40
1:A:248:LEU:HD22	1:A:295:TRP:CZ3	2.57	0.40
1:C:98:LEU:HD21	1:C:138:CYS:HB2	2.03	0.40
2:D:98:MET:HE3	2:D:98:MET:HB2	1.90	0.40
1:K:293:GLN:HA	1:K:308:ILE:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:ND2	2:J:42:GLY:O[4_456]	1.59	0.61

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	353/428 (82%)	328 (93%)	25 (7%)	0	100	100
1	C	315/428 (74%)	302 (96%)	13 (4%)	0	100	100
1	E	293/428 (68%)	278 (95%)	15 (5%)	0	100	100
1	G	314/428 (73%)	294 (94%)	20 (6%)	0	100	100
1	I	326/428 (76%)	310 (95%)	16 (5%)	0	100	100
1	K	302/428 (71%)	288 (95%)	14 (5%)	0	100	100
2	B	114/118 (97%)	111 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
2	F	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
2	H	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
2	J	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
2	L	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
All	All	2587/3276 (79%)	2461 (95%)	126 (5%)	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	280/394 (71%)	269 (96%)	11 (4%)	28	54
1	C	230/394 (58%)	226 (98%)	4 (2%)	53	77
1	E	228/394 (58%)	225 (99%)	3 (1%)	61	81
1	G	252/394 (64%)	246 (98%)	6 (2%)	43	70
1	I	260/394 (66%)	256 (98%)	4 (2%)	57	79
1	K	242/394 (61%)	240 (99%)	2 (1%)	73	87
2	B	83/94 (88%)	82 (99%)	1 (1%)	63	82
2	D	84/94 (89%)	83 (99%)	1 (1%)	63	82
2	F	81/94 (86%)	78 (96%)	3 (4%)	30	56
2	H	82/94 (87%)	82 (100%)	0	100	100
2	J	81/94 (86%)	81 (100%)	0	100	100
2	L	82/94 (87%)	82 (100%)	0	100	100
All	All	1985/2928 (68%)	1950 (98%)	35 (2%)	51	76

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	84	ASP
1	A	90	ILE
1	A	120	ILE
1	A	141	THR
1	A	178	ILE
1	A	192	PHE
1	A	305	THR
1	A	348	LEU
1	A	376	THR
1	A	456	ILE
2	B	11	LEU
1	C	99	VAL
1	C	318	GLU
1	C	377	ILE
1	C	465	LEU
2	D	100	VAL
1	E	348	LEU
1	E	349	SER
1	E	465	LEU
2	F	6	GLU
2	F	53	ARG
2	F	77	VAL
1	G	62	THR
1	G	72	LEU
1	G	99	VAL
1	G	106	TYR
1	G	377	ILE
1	G	456	ILE
1	I	84	ASP
1	I	176	GLU
1	I	348	LEU
1	I	456	ILE
1	K	439	MET
1	K	456	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	241	GLN
1	C	428	GLN
1	C	476	GLN

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Mol	Chain	Res	Type
2	D	3	GLN
1	E	100	ASN
1	G	102	HIS
1	G	288	ASN
2	H	80	GLN
2	H	82	ASN
1	I	430	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 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

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	367/428 (85%)	0.39	19 (5%) 33 28	36, 70, 112, 161	0
1	C	337/428 (78%)	0.94	48 (14%) 6 5	54, 112, 166, 201	0
1	E	315/428 (73%)	1.31	68 (21%) 2 2	65, 117, 175, 218	0
1	G	334/428 (78%)	0.93	49 (14%) 6 4	43, 96, 164, 228	0
1	I	346/428 (80%)	0.69	36 (10%) 11 10	36, 80, 152, 191	0
1	K	328/428 (76%)	1.01	46 (14%) 6 5	57, 100, 154, 217	0
2	B	116/118 (98%)	0.46	10 (8%) 16 13	43, 65, 132, 176	0
2	D	116/118 (98%)	0.18	7 (6%) 27 24	42, 59, 95, 170	0
2	F	116/118 (98%)	0.62	6 (5%) 33 28	70, 86, 116, 144	0
2	H	116/118 (98%)	0.30	5 (4%) 40 35	48, 65, 102, 152	0
2	J	116/118 (98%)	0.08	5 (4%) 40 35	36, 48, 89, 168	0
2	L	116/118 (98%)	0.63	11 (9%) 14 11	58, 77, 113, 138	0
All	All	2723/3276 (83%)	0.74	310 (11%) 10 8	36, 84, 154, 228	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	ILE	5.4
1	E	444	GLU	5.3
1	A	118	PRO	5.2
1	E	190	GLU	5.2
1	C	96	TYR	5.0
1	E	448	SER	4.9
1	C	172	ALA	4.8
1	A	71	THR	4.8
2	L	23	ALA	4.7
1	C	192	PHE	4.6
1	K	193	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	181	ILE	4.5
2	B	23	ALA	4.4
2	L	54	TYR	4.3
1	E	211	MET	4.3
1	E	229	PHE	4.2
1	A	119	TYR	4.2
1	E	427	THR	4.2
1	E	231	ILE	4.0
1	G	355	SER	4.0
1	G	356	CYS	3.9
2	B	24	ALA	3.9
1	E	300	THR	3.9
1	I	402	PRO	3.8
1	G	110	ILE	3.8
1	G	178	ILE	3.8
1	E	220	VAL	3.8
1	E	471	GLN	3.8
1	E	212	LEU	3.8
1	G	86	LEU	3.8
1	G	192	PHE	3.8
1	I	415	SER	3.8
2	D	27	SER	3.8
1	G	76	TYR	3.7
1	E	86	LEU	3.7
1	G	208	CYS	3.7
1	A	77	SER	3.7
1	G	124	PHE	3.6
2	B	18	LEU	3.6
1	A	181	ILE	3.6
1	G	300	THR	3.5
2	B	71	ASP	3.5
2	J	27	SER	3.5
1	E	217	ALA	3.5
1	K	136	PRO	3.5
1	E	402	PRO	3.5
1	E	221	LEU	3.5
1	G	68	ILE	3.4
1	K	161	THR	3.4
2	D	2	VAL	3.4
1	E	219	ILE	3.4
1	G	278	LYS	3.4
1	E	72	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	73	GLN	3.4
1	E	472	MET	3.4
1	C	400	PHE	3.4
1	E	318	GLU	3.3
2	H	73	ALA	3.3
1	I	192	PHE	3.3
1	I	391	THR	3.3
1	G	176	GLU	3.3
1	K	123	PRO	3.3
1	I	249	ASN	3.3
1	A	106	TYR	3.3
2	F	46	GLU	3.3
1	K	110	ILE	3.3
1	G	211	MET	3.3
2	L	55	GLY	3.3
1	K	105	VAL	3.3
1	K	178	ILE	3.3
1	C	194	HIS	3.2
1	K	61	PHE	3.2
1	C	61	PHE	3.2
2	F	72	ASN	3.2
1	E	233	ILE	3.2
1	G	302	SER	3.2
2	L	24	ALA	3.2
1	C	76	TYR	3.2
1	C	388	GLU	3.1
1	K	343	SER	3.1
1	I	119	TYR	3.1
1	G	139	ILE	3.1
2	B	74	LYS	3.1
1	E	87	ASN	3.1
1	G	264	ASN	3.1
1	K	244	LEU	3.1
1	C	90	ILE	3.1
1	E	381	TYR	3.0
1	A	182	ASN	3.0
1	I	264	ASN	3.0
1	E	110	ILE	3.0
1	I	110	ILE	3.0
1	E	465	LEU	3.0
2	D	72	ASN	3.0
1	K	92	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	403	GLN	3.0
1	G	123	PRO	2.9
1	C	241	GLN	2.9
1	E	181	ILE	2.9
1	K	72	LEU	2.9
1	K	78	SER	2.9
1	A	264	ASN	2.9
2	L	25	SER	2.9
1	G	411	ASN	2.9
1	E	470	LYS	2.9
1	A	190	GLU	2.8
1	E	178	ILE	2.8
1	I	342	GLU	2.8
1	I	162	GLY	2.8
1	C	358	GLU	2.8
1	E	249	ASN	2.8
1	E	288	ASN	2.8
1	K	198	LEU	2.8
1	C	69	VAL	2.8
1	E	192	PHE	2.8
1	I	76	TYR	2.8
1	K	119	TYR	2.8
1	E	235	ASN	2.8
1	E	422	ASN	2.8
1	C	434	ASP	2.8
2	H	71	ASP	2.8
1	C	74	THR	2.8
1	I	144	ALA	2.8
1	K	71	THR	2.8
1	E	234	ARG	2.8
1	C	77	SER	2.7
1	C	136	PRO	2.7
1	K	276	LEU	2.7
1	G	240	PRO	2.7
1	E	273	GLY	2.7
1	I	79	GLY	2.7
1	E	450	ARG	2.7
1	E	122	VAL	2.7
1	I	477	PHE	2.7
1	G	237	MET	2.7
1	K	122	VAL	2.7
1	C	84	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	174	TYR	2.6
1	E	68	ILE	2.6
1	I	404	MET	2.6
1	G	98	LEU	2.6
1	G	303	HIS	2.6
1	K	279	GLY	2.6
1	K	302	SER	2.6
1	C	119	TYR	2.6
1	E	442	LYS	2.6
1	C	288	ASN	2.6
1	E	479	VAL	2.6
1	I	105	VAL	2.6
1	C	121	THR	2.6
1	E	228	ILE	2.6
1	G	59	LYS	2.6
1	E	214	CYS	2.6
1	G	471	GLN	2.6
2	J	72	ASN	2.6
1	I	300	THR	2.5
2	D	71	ASP	2.5
1	C	246	LYS	2.5
1	G	239	LYS	2.5
1	K	69	VAL	2.5
1	K	301	ASN	2.5
1	I	462	SER	2.5
2	B	25	SER	2.5
1	K	445	ASP	2.5
1	C	297	LEU	2.5
2	F	26	GLY	2.5
1	C	479	VAL	2.5
2	B	2	VAL	2.5
1	C	64	ASN	2.5
1	E	71	THR	2.5
1	E	208	CYS	2.5
1	K	224	ASN	2.5
2	H	27	SER	2.5
2	B	28	ILE	2.5
1	G	140	LEU	2.5
1	I	250	LYS	2.5
1	G	167	ILE	2.5
1	I	196	LEU	2.5
2	L	71	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	199	PRO	2.5
1	C	404	MET	2.5
1	E	237	MET	2.5
1	G	304	PRO	2.5
1	E	477	PHE	2.5
1	I	61	PHE	2.5
1	K	249	ASN	2.4
2	F	99	GLU	2.4
1	C	62	THR	2.4
1	C	275	ILE	2.4
1	K	288	ASN	2.4
2	D	28	ILE	2.4
1	E	209	ASP	2.4
1	E	136	PRO	2.4
1	E	241	GLN	2.4
1	K	96	TYR	2.4
2	F	54	TYR	2.4
1	G	478	PHE	2.4
1	E	280	THR	2.4
1	C	318	GLU	2.4
1	G	442	LYS	2.4
1	C	120	ILE	2.4
1	K	422	ASN	2.4
1	E	309	ASP	2.4
1	K	84	ASP	2.4
1	A	79	GLY	2.4
1	A	110	ILE	2.3
1	K	107	ILE	2.3
1	C	161	THR	2.3
1	K	235	ASN	2.3
1	E	169	GLY	2.3
1	K	163	GLY	2.3
1	E	475	LEU	2.3
2	D	23	ALA	2.3
2	H	74	LYS	2.3
2	L	87	GLU	2.3
1	G	136	PRO	2.3
1	E	137	ARG	2.3
1	G	248	LEU	2.3
1	G	414	THR	2.3
1	C	193	SER	2.3
2	J	71	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	53	ARG	2.3
1	G	205	GLY	2.3
1	G	428	GLN	2.3
2	D	55	GLY	2.3
2	J	8	GLY	2.3
1	C	196	LEU	2.3
1	K	247	LEU	2.3
1	K	300	THR	2.3
1	C	67	TYR	2.3
1	I	67	TYR	2.3
1	K	341	ASP	2.3
1	A	248	LEU	2.3
1	C	212	LEU	2.3
1	I	478	PHE	2.3
1	C	232	THR	2.2
1	G	174	TYR	2.2
1	A	236	SER	2.2
1	E	236	SER	2.2
1	E	445	ASP	2.2
1	G	370	SER	2.2
1	K	323	LEU	2.2
2	B	5	VAL	2.2
1	C	393	THR	2.2
1	E	67	TYR	2.2
1	G	119	TYR	2.2
1	K	87	ASN	2.2
1	C	123	PRO	2.2
1	I	242	LEU	2.2
1	G	60	VAL	2.2
1	G	105	VAL	2.2
1	G	90	ILE	2.2
1	C	300	THR	2.2
1	A	76	TYR	2.2
2	L	62	VAL	2.2
1	E	358	GLU	2.2
1	I	476	GLN	2.2
1	I	470	LYS	2.2
1	C	248	LEU	2.2
1	G	79	GLY	2.2
1	A	75	ASP	2.2
1	E	446	ILE	2.2
1	I	90	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	108	TRP	2.1
1	C	410	THR	2.1
1	E	62	THR	2.1
1	C	208	CYS	2.1
1	I	340	GLN	2.1
1	I	403	GLN	2.1
1	A	84	ASP	2.1
1	I	435	SER	2.1
1	G	141	THR	2.1
1	E	191	LYS	2.1
1	G	276	LEU	2.1
1	K	200	ILE	2.1
2	L	116	VAL	2.1
1	I	124	PHE	2.1
1	I	62	THR	2.1
1	E	466	TYR	2.1
2	L	26	GLY	2.1
2	H	2	VAL	2.1
1	E	392	ASP	2.1
1	G	177	ASP	2.1
1	A	78	SER	2.1
1	K	448	SER	2.1
2	B	73	ALA	2.1
1	I	240	PRO	2.1
1	K	471	GLN	2.1
2	J	110	GLN	2.1
1	E	102	HIS	2.1
1	K	120	ILE	2.1
1	E	474	VAL	2.1
1	C	386	PHE	2.1
1	C	78	SER	2.0
1	K	332	LYS	2.0
1	E	304	PRO	2.0
1	A	90	ILE	2.0
1	I	160	GLU	2.0
1	I	77	SER	2.0
1	K	236	SER	2.0
2	F	25	SER	2.0
1	K	237	MET	2.0
1	G	241	GLN	2.0
1	A	120	ILE	2.0
1	C	226	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	249	ASN	2.0
1	E	453	ILE	2.0
1	G	107	ILE	2.0
1	I	109	ASN	2.0
1	C	99	VAL	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.