



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:50 PM UTC

PDB ID : 6X08 / pdb_00006x08
Title : Nup85-Seh1 from *S. cerevisiae* bound by VHH-SAN2
Authors : Nordeen, S.A.; Schwartz, T.U.
Deposited on : 2020-05-15
Resolution : 4.19 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 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

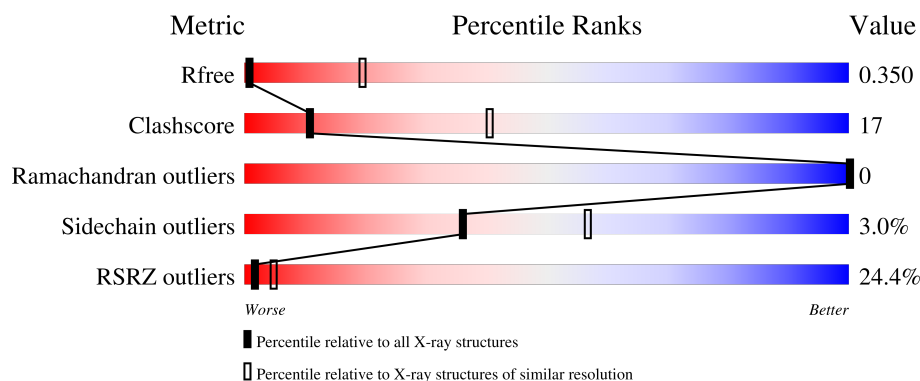
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.19 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}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	353	24% 63% 24% 12%
2	B	568	14% 64% 18% 16%
3	K	125	35% 79% 18% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6827 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 SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2384	1505	408	460	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P53011
A	-2	PRO	-	expression tag	UNP P53011
A	-1	GLY	-	expression tag	UNP P53011
A	0	SER	-	expression tag	UNP P53011

- Molecule 2 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	475	Total	C	N	O	S	0	0	0
			3557	2276	571	694	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	MET	-	expression tag	UNP P46673
B	-2	ALA	-	expression tag	UNP P46673
B	-1	ASP	-	expression tag	UNP P46673
B	0	PRO	-	expression tag	UNP P46673

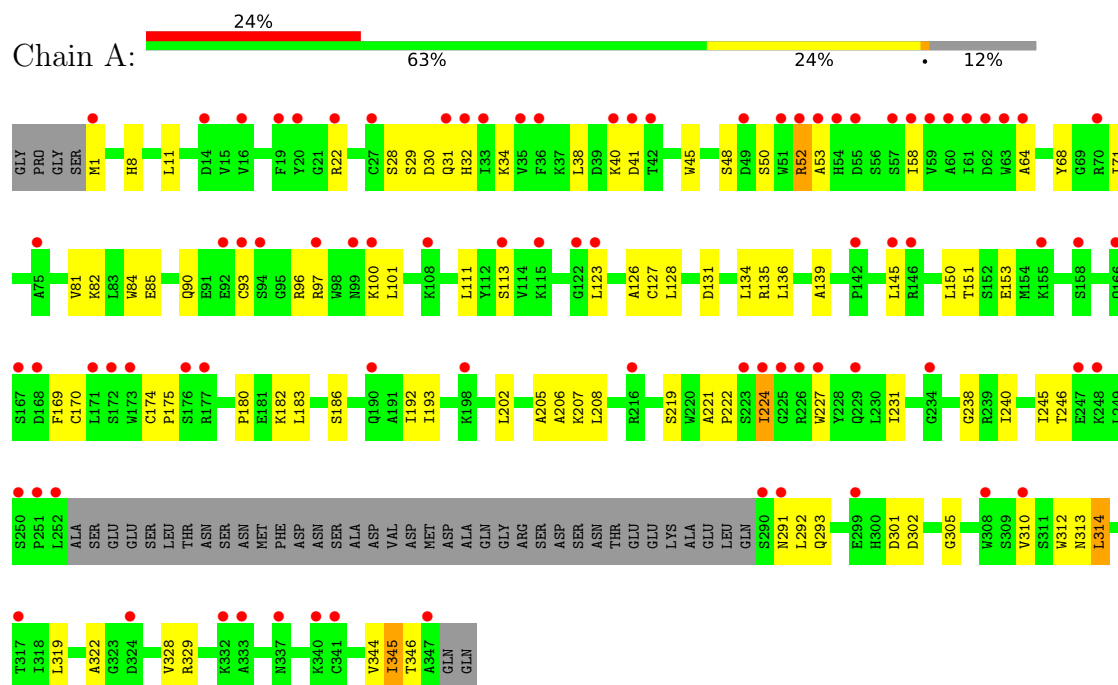
- Molecule 3 is a protein called VHH-SAN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	125	Total	C	N	O	S	465	0	0
			886	546	151	183	6			

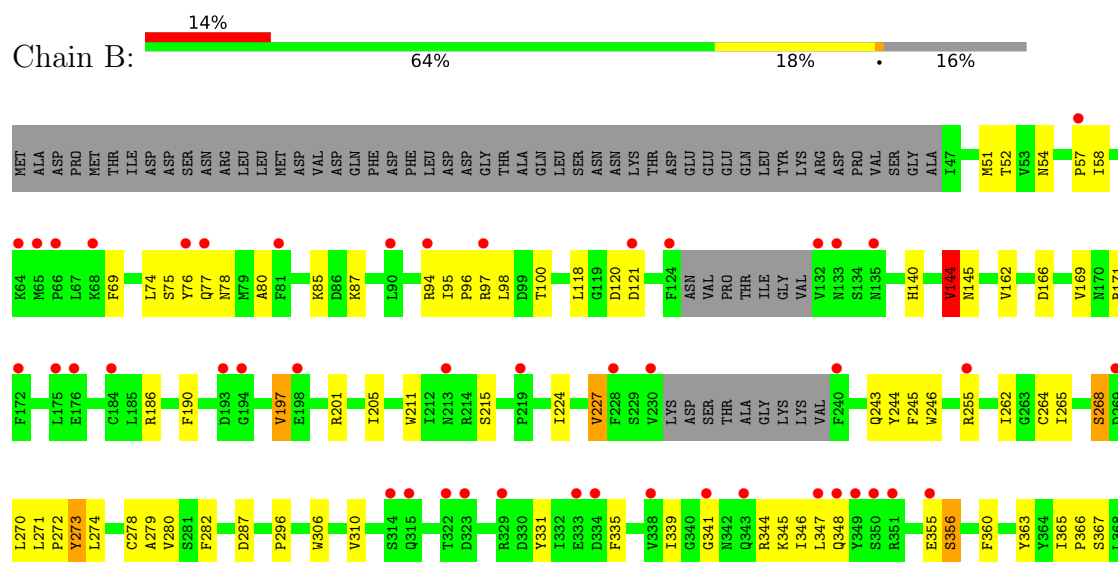
3 Residue-property plots [i](#)

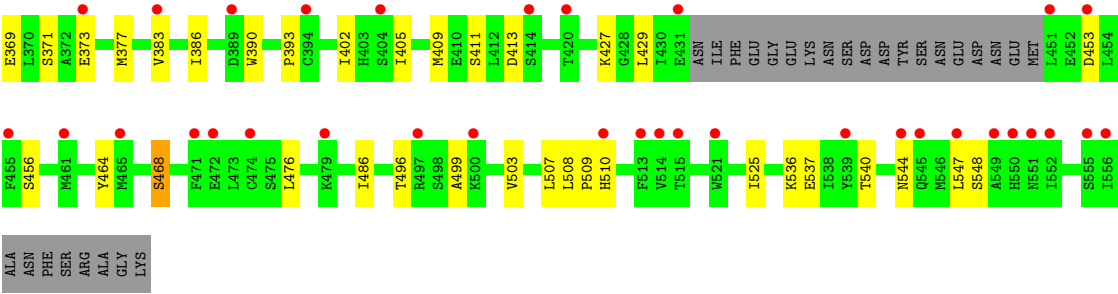
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 SEH1

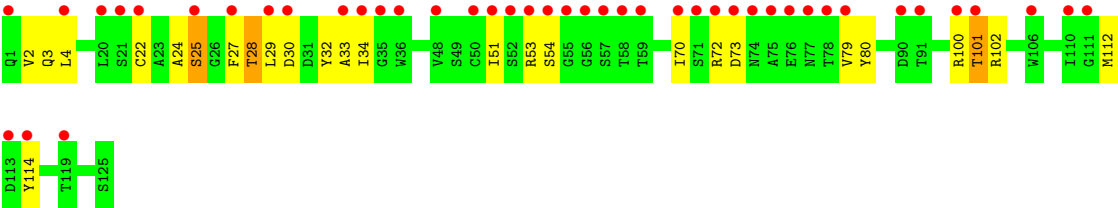
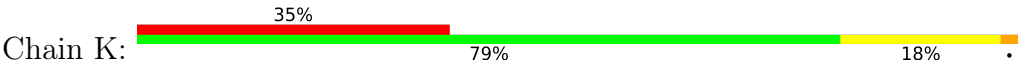


• Molecule 2: Nucleoporin NUP85





• Molecule 3: VHH-SAN2



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	233.99Å 233.99Å 139.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	117.00 – 4.19 117.00 – 4.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (117.00-4.19) 99.9 (117.00-4.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 4.15Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.311 , 0.346 0.316 , 0.350	Depositor DCC
R_{free} test set	1701 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	176.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 504.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6827	wwPDB-VP
Average B, all atoms (Å ²)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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	0.36	0/2442	0.53	2/3323 (0.1%)
2	B	0.48	4/3627 (0.1%)	0.62	4/4940 (0.1%)
3	K	0.41	0/900	0.94	8/1224 (0.7%)
All	All	0.44	4/6969 (0.1%)	0.64	14/9487 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	144	VAL	N-CA	-5.56	1.39	1.46
2	B	367	SER	CA-C	-5.41	1.46	1.52
2	B	365	ILE	CA-C	-5.17	1.47	1.52
2	B	280	VAL	CA-C	-5.14	1.46	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	LEU	N-CA-C	16.79	129.58	111.28
2	B	363	TYR	N-CA-C	7.87	123.84	113.30
3	K	34	ILE	N-CA-C	7.63	118.91	108.84
3	K	24	ALA	N-CA-C	7.32	118.26	108.38
3	K	33	ALA	N-CA-C	-7.11	101.81	112.54
1	A	52	ARG	N-CA-C	6.82	119.36	110.43
3	K	100	ARG	N-CA-C	6.06	117.88	111.28
3	K	25	SER	N-CA-C	5.47	117.82	108.90
2	B	120	ASP	N-CA-C	5.40	117.72	109.62
1	A	41	ASP	N-CA-C	5.38	117.14	111.28
3	K	28	THR	N-CA-C	5.14	117.31	107.75
2	B	144	VAL	CA-C-O	-5.12	115.62	120.95
3	K	101	THR	CA-C-N	-5.02	115.50	123.23
3	K	101	THR	C-N-CA	-5.02	115.50	123.23

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	2384	0	2261	102	0
2	B	3557	0	3267	95	0
3	K	886	0	816	25	0
All	All	6827	0	6344	203	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 17.

All (203) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:HB2	1:A:312:TRP:CG	1.59	1.37
1:A:221:ALA:HB2	1:A:312:TRP:CD2	1.70	1.24
1:A:224:ILE:HG13	2:B:507:LEU:CD1	1.65	1.24
3:K:2:VAL:CG1	3:K:25:SER:HB3	1.67	1.21
1:A:221:ALA:HB2	1:A:312:TRP:CD1	1.80	1.15
1:A:175:PRO:HB2	1:A:222:PRO:HB3	1.29	1.10
3:K:2:VAL:HG11	3:K:25:SER:HB3	1.13	1.06
1:A:221:ALA:CB	1:A:312:TRP:CD2	2.39	1.05
1:A:221:ALA:CB	1:A:312:TRP:CG	2.46	0.98
1:A:221:ALA:HB2	1:A:312:TRP:CE2	1.98	0.97
3:K:51:ILE:HG13	3:K:72:ARG:HG3	1.52	0.91
2:B:144:VAL:HG11	2:B:427:LYS:HG2	1.53	0.90
1:A:224:ILE:CG1	2:B:507:LEU:CD1	2.50	0.90
2:B:145:ASN:OD1	2:B:190:PHE:CA	2.20	0.90
3:K:2:VAL:CG1	3:K:25:SER:CB	2.51	0.88
1:A:205:ALA:HB1	1:A:292:LEU:HD22	1.56	0.87
1:A:246:THR:O	1:A:293:GLN:HB2	1.73	0.87
2:B:344:ARG:CB	3:K:54:SER:HB3	2.04	0.87
3:K:2:VAL:HG11	3:K:25:SER:CB	2.04	0.85
2:B:145:ASN:OD1	2:B:190:PHE:HA	1.76	0.84
2:B:255:ARG:NH2	2:B:355:GLU:OE2	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HG13	2:B:507:LEU:HD13	1.60	0.82
1:A:175:PRO:CB	1:A:222:PRO:HB3	2.06	0.82
1:A:224:ILE:HG13	2:B:507:LEU:HD11	1.61	0.81
1:A:34:LYS:HG2	1:A:50:SER:HB2	1.63	0.81
1:A:183:LEU:O	1:A:183:LEU:HD12	1.80	0.80
1:A:224:ILE:HG13	2:B:507:LEU:HD12	1.64	0.79
2:B:145:ASN:OD1	2:B:190:PHE:C	2.27	0.78
1:A:221:ALA:CB	1:A:312:TRP:CE2	2.64	0.78
1:A:30:ASP:O	1:A:32:HIS:ND1	2.18	0.77
3:K:2:VAL:HG13	3:K:25:SER:HB3	1.67	0.76
3:K:30:ASP:O	3:K:102:ARG:CB	2.34	0.75
2:B:98:LEU:HD21	2:B:476:LEU:HD11	1.69	0.73
1:A:221:ALA:HB2	1:A:312:TRP:NE1	2.03	0.73
2:B:78:ASN:HD21	2:B:95:ILE:HG13	1.53	0.72
1:A:175:PRO:HB2	1:A:222:PRO:CB	2.16	0.72
1:A:32:HIS:HA	1:A:52:ARG:CB	2.20	0.71
2:B:243:GLN:H	2:B:243:GLN:CD	1.98	0.71
1:A:224:ILE:C	1:A:224:ILE:HD13	2.16	0.70
3:K:112:MET:HE2	3:K:114:TYR:HB3	1.74	0.70
3:K:2:VAL:HG13	3:K:25:SER:CB	2.19	0.69
1:A:169:PHE:HA	1:A:186:SER:O	1.93	0.68
2:B:118:LEU:HD23	2:B:118:LEU:O	1.93	0.68
1:A:180:PRO:O	1:A:182:LYS:HG2	1.94	0.68
2:B:75:SER:O	2:B:95:ILE:HG13	1.95	0.67
1:A:90:GLN:O	1:A:97:ARG:NH1	2.28	0.66
1:A:224:ILE:CD1	2:B:507:LEU:HD13	2.26	0.66
1:A:127:CYS:O	1:A:134:LEU:HD12	1.94	0.66
2:B:186:ARG:HA	2:B:190:PHE:HB2	1.78	0.66
3:K:32:TYR:HE2	3:K:72:ARG:HH22	1.42	0.66
1:A:224:ILE:CG1	2:B:507:LEU:HD13	2.21	0.66
1:A:192:ILE:HG22	1:A:207:LYS:HG2	1.78	0.65
1:A:53:ALA:HB3	1:A:84:TRP:CH2	2.32	0.65
1:A:221:ALA:CB	1:A:312:TRP:CD1	2.71	0.65
2:B:279:ALA:O	2:B:282:PHE:HB3	1.96	0.65
1:A:85:GLU:HB2	1:A:101:LEU:HD11	1.79	0.64
1:A:208:LEU:HD11	1:A:231:ILE:CD1	2.28	0.64
1:A:208:LEU:HD11	1:A:231:ILE:HD12	1.80	0.64
2:B:140:HIS:O	2:B:144:VAL:N	2.25	0.64
1:A:174:CYS:SG	1:A:182:LYS:HG3	2.38	0.64
1:A:29:SER:C	1:A:31:GLN:H	2.06	0.63
2:B:118:LEU:HD23	2:B:118:LEU:C	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ARG:NH2	2:B:413:ASP:OD2	2.31	0.63
2:B:243:GLN:OE1	2:B:243:GLN:N	2.24	0.63
2:B:274:LEU:CB	2:B:282:PHE:HB2	2.29	0.63
3:K:32:TYR:CD2	3:K:72:ARG:NH2	2.67	0.62
1:A:205:ALA:CB	1:A:292:LEU:HD22	2.28	0.62
3:K:73:ASP:OD1	3:K:80:TYR:HE2	1.82	0.62
2:B:52:THR:HG22	2:B:54:ASN:H	1.64	0.62
1:A:34:LYS:HA	1:A:50:SER:HB3	1.81	0.61
2:B:296:PRO:HD3	2:B:306:TRP:CD1	2.34	0.61
1:A:224:ILE:HG23	1:A:224:ILE:O	2.00	0.61
1:A:224:ILE:HD11	2:B:503:VAL:HA	1.82	0.61
1:A:64:ALA:HB3	1:A:71:ILE:HB	1.84	0.60
1:A:30:ASP:O	1:A:32:HIS:CE1	2.54	0.60
1:A:136:LEU:HD11	1:A:202:LEU:HD11	1.82	0.60
1:A:131:ASP:OD2	1:A:135:ARG:NH2	2.36	0.59
2:B:118:LEU:HD21	2:B:121:ASP:HB2	1.84	0.59
1:A:31:GLN:O	1:A:58:ILE:HD11	2.03	0.58
1:A:224:ILE:CD1	2:B:507:LEU:CD1	2.82	0.57
2:B:201:ARG:CZ	2:B:205:ILE:HD11	2.35	0.57
1:A:34:LYS:HA	1:A:50:SER:CB	2.35	0.57
2:B:279:ALA:O	2:B:282:PHE:N	2.37	0.57
2:B:464:TYR:O	2:B:468:SER:OG	2.18	0.57
1:A:208:LEU:HD21	1:A:231:ILE:HD11	1.86	0.57
2:B:245:PHE:HZ	2:B:268:SER:OG	1.87	0.57
2:B:393:PRO:HA	2:B:405:ILE:HG22	1.85	0.57
2:B:273:TYR:HD1	2:B:273:TYR:O	1.88	0.56
1:A:170:CYS:N	1:A:186:SER:OG	2.38	0.56
1:A:8:HIS:CE1	1:A:34:LYS:HG3	2.41	0.56
2:B:197:VAL:HB	2:B:366:PRO:O	2.05	0.56
1:A:53:ALA:HB3	1:A:84:TRP:HH2	1.71	0.55
2:B:496:THR:HB	2:B:499:ALA:H	1.71	0.55
1:A:227:TRP:CD1	1:A:227:TRP:N	2.72	0.55
2:B:273:TYR:C	2:B:273:TYR:CD1	2.84	0.55
1:A:150:LEU:HD21	1:A:153:GLU:HG3	1.87	0.55
3:K:28:THR:OG1	3:K:101:THR:HA	2.08	0.54
2:B:245:PHE:CZ	2:B:268:SER:OG	2.59	0.54
1:A:224:ILE:CG1	2:B:507:LEU:HD11	2.29	0.53
2:B:453:ASP:O	2:B:456:SER:OG	2.24	0.53
2:B:282:PHE:C	2:B:282:PHE:CD1	2.84	0.53
2:B:264:CYS:O	2:B:268:SER:N	2.39	0.53
1:A:224:ILE:HD13	1:A:224:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:VAL:HG13	1:A:319:LEU:HD11	1.91	0.52
2:B:78:ASN:ND2	2:B:95:ILE:HG13	2.21	0.52
3:K:2:VAL:HG12	3:K:3:GLN:N	2.23	0.52
1:A:123:LEU:HB2	1:A:139:ALA:HB3	1.92	0.51
2:B:427:LYS:HB3	2:B:429:LEU:HG	1.92	0.51
1:A:329:ARG:HG2	1:A:344:VAL:HG22	1.92	0.51
2:B:69:PHE:HD2	2:B:80:ALA:HB2	1.75	0.51
2:B:227:VAL:HG21	2:B:244:TYR:HB3	1.92	0.51
1:A:22:ARG:NH1	1:A:40:LYS:HA	2.25	0.51
1:A:224:ILE:HD11	2:B:507:LEU:HD13	1.91	0.51
2:B:341:GLY:HA2	2:B:346:ILE:HD11	1.92	0.50
1:A:113:SER:CB	1:A:170:CYS:HA	2.41	0.50
1:A:346:THR:HB	2:B:51:MET:HB3	1.94	0.50
1:A:175:PRO:CG	1:A:222:PRO:HB3	2.41	0.50
3:K:2:VAL:HG13	3:K:25:SER:HB2	1.92	0.50
1:A:224:ILE:HD11	2:B:503:VAL:HG13	1.93	0.49
1:A:301:ASP:N	1:A:301:ASP:OD1	2.45	0.49
1:A:313:ASN:OD1	1:A:314:LEU:N	2.44	0.49
1:A:224:ILE:C	1:A:224:ILE:CD1	2.86	0.49
3:K:27:PHE:C	3:K:32:TYR:OH	2.55	0.49
2:B:246:TRP:CD2	2:B:331:TYR:HB3	2.47	0.49
1:A:113:SER:HB2	1:A:170:CYS:HA	1.95	0.49
2:B:264:CYS:O	2:B:268:SER:OG	2.31	0.49
1:A:291:ASN:OD1	1:A:291:ASN:N	2.44	0.49
3:K:22:CYS:HB3	3:K:79:VAL:HG12	1.95	0.49
1:A:245:ILE:HA	1:A:293:GLN:O	2.13	0.49
2:B:262:ILE:O	2:B:265:ILE:CB	2.61	0.48
2:B:345:LYS:HA	2:B:348:GLN:HB3	1.94	0.48
1:A:219:SER:OG	1:A:310:VAL:HG12	2.13	0.48
1:A:346:THR:HG21	2:B:51:MET:SD	2.53	0.48
2:B:197:VAL:CB	2:B:366:PRO:O	2.61	0.48
2:B:544:ASN:O	2:B:548:SER:N	2.35	0.48
3:K:32:TYR:HD2	3:K:72:ARG:NH2	2.09	0.48
1:A:345:ILE:O	1:A:346:THR:HG22	2.13	0.48
2:B:75:SER:O	2:B:78:ASN:ND2	2.46	0.48
1:A:1:MET:SD	2:B:94:ARG:HB3	2.53	0.48
1:A:38:LEU:HB2	1:A:45:TRP:CZ3	2.49	0.48
2:B:57:PRO:HG2	2:B:58:ILE:HD12	1.95	0.48
1:A:101:LEU:HD13	1:A:145:LEU:HB3	1.95	0.47
2:B:145:ASN:OD1	2:B:190:PHE:O	2.31	0.47
1:A:81:VAL:HG23	1:A:111:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:32:TYR:CE2	3:K:72:ARG:NH2	2.74	0.47
2:B:347:LEU:HD23	2:B:356:SER:HB3	1.96	0.47
1:A:224:ILE:CD1	2:B:503:VAL:HG13	2.44	0.47
1:A:322:ALA:HB2	1:A:328:VAL:HG22	1.97	0.47
2:B:97:ARG:NH2	2:B:411:SER:O	2.47	0.47
2:B:335:PHE:O	2:B:339:ILE:HG13	2.15	0.46
1:A:302:ASP:O	1:A:329:ARG:NH2	2.49	0.46
2:B:145:ASN:OD1	2:B:190:PHE:CB	2.64	0.46
2:B:453:ASP:C	2:B:456:SER:HG	2.22	0.46
2:B:544:ASN:HB3	2:B:547:LEU:HA	1.97	0.46
1:A:314:LEU:HD13	2:B:510:HIS:ND1	2.31	0.45
2:B:245:PHE:CZ	2:B:268:SER:HB3	2.51	0.45
2:B:373:GLU:O	2:B:377:MET:HG3	2.17	0.45
2:B:162:VAL:O	2:B:166:ASP:HB3	2.16	0.45
1:A:128:LEU:HD23	1:A:169:PHE:HB3	1.99	0.45
1:A:312:TRP:CE2	1:A:319:LEU:HD13	2.52	0.44
2:B:74:LEU:HD21	2:B:76:TYR:CE2	2.53	0.44
2:B:486:ILE:HG21	2:B:525:ILE:HD13	2.00	0.44
2:B:369:GLU:C	2:B:371:SER:H	2.26	0.44
2:B:508:LEU:N	2:B:509:PRO:HD2	2.32	0.44
1:A:8:HIS:CG	1:A:28:SER:HG	2.31	0.44
3:K:51:ILE:HD11	3:K:70:ILE:HG12	2.00	0.44
1:A:193:ILE:HD12	1:A:206:ALA:HB3	2.00	0.44
2:B:310:VAL:HG11	2:B:339:ILE:HG22	2.00	0.43
1:A:126:ALA:HB1	1:A:134:LEU:HD11	1.99	0.43
1:A:208:LEU:HD11	1:A:231:ILE:HD11	1.99	0.43
3:K:2:VAL:CG1	3:K:3:GLN:N	2.81	0.43
1:A:29:SER:C	1:A:31:GLN:N	2.76	0.43
1:A:246:THR:O	1:A:246:THR:HG22	2.19	0.43
1:A:246:THR:O	1:A:293:GLN:CB	2.57	0.43
2:B:245:PHE:CZ	2:B:268:SER:CB	3.01	0.43
2:B:390:TRP:C	2:B:393:PRO:HD2	2.43	0.43
2:B:243:GLN:CD	2:B:243:GLN:N	2.73	0.43
1:A:48:SER:O	1:A:93:CYS:N	2.52	0.43
1:A:183:LEU:HD12	1:A:183:LEU:C	2.42	0.43
1:A:82:LYS:HD3	1:A:100:LYS:HE2	2.01	0.42
2:B:87:LYS:HD3	2:B:87:LYS:HA	1.87	0.42
1:A:292:LEU:HD12	1:A:292:LEU:N	2.34	0.42
2:B:211:TRP:O	2:B:215:SER:HB3	2.18	0.42
1:A:11:LEU:HD11	2:B:85:LYS:HG2	2.02	0.42
2:B:273:TYR:O	2:B:273:TYR:CD1	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:MET:HE2	2:B:409:MET:HB3	1.98	0.42
2:B:356:SER:O	2:B:360:PHE:HD1	2.03	0.41
2:B:145:ASN:HD21	2:B:427:LYS:CE	2.33	0.41
1:A:186:SER:O	1:A:186:SER:OG	2.38	0.41
2:B:95:ILE:HG23	2:B:96:PRO:HD2	2.01	0.41
2:B:271:LEU:N	2:B:272:PRO:HD2	2.36	0.41
2:B:476:LEU:HA	2:B:476:LEU:HD12	1.77	0.41
3:K:27:PHE:HA	3:K:32:TYR:OH	2.20	0.41
1:A:136:LEU:O	1:A:151:THR:N	2.50	0.41
2:B:536:LYS:O	2:B:540:THR:HG23	2.20	0.41
1:A:90:GLN:HG3	1:A:96:ARG:O	2.21	0.41
1:A:328:VAL:HB	1:A:345:ILE:CG2	2.51	0.41
2:B:274:LEU:CB	2:B:282:PHE:HD2	2.33	0.41
1:A:68:TYR:CD2	1:A:123:LEU:HG	2.56	0.40
1:A:238:GLY:HA2	1:A:305:GLY:O	2.21	0.40
3:K:4:LEU:HD12	3:K:4:LEU:HA	1.87	0.40
3:K:51:ILE:HG22	3:K:53:ARG:O	2.21	0.40
2:B:76:TYR:CD1	2:B:77:GLN:HG2	2.55	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	306/353 (87%)	284 (93%)	22 (7%)	0	100	100
2	B	467/568 (82%)	424 (91%)	43 (9%)	0	100	100
3	K	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
All	All	896/1046 (86%)	822 (92%)	74 (8%)	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	255/307 (83%)	251 (98%)	4 (2%)	55	69
2	B	355/507 (70%)	339 (96%)	16 (4%)	24	47
3	K	88/100 (88%)	87 (99%)	1 (1%)	65	73
All	All	698/914 (76%)	677 (97%)	21 (3%)	36	57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	ILE
1	A	240	ILE
1	A	314	LEU
1	A	345	ILE
2	B	100	THR
2	B	144	VAL
2	B	169	VAL
2	B	197	VAL
2	B	224	ILE
2	B	227	VAL
2	B	268	SER
2	B	273	TYR
2	B	278	CYS
2	B	287	ASP
2	B	356	SER
2	B	383	VAL
2	B	386	ILE
2	B	402	ILE
2	B	468	SER
2	B	537	GLU
3	K	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	31	GLN
1	A	44	ASN
2	B	200	ASN
2	B	226	GLN
2	B	315	GLN
2	B	388	ASN
2	B	392	GLN
2	B	467	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	310/353 (87%)	1.42	83 (26%)	1 4	140, 171, 205, 284	0
2	B	475/568 (83%)	1.16	80 (16%)	4 8	143, 191, 243, 276	0
3	K	62/125 (49%)	3.52	44 (70%)	0 1	74, 343, 362, 375	1 (1%)
All	All	847/1046 (80%)	1.43	207 (24%)	2 5	74, 185, 338, 375	1 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	106	TRP	10.7
3	K	50	CYS	7.7
2	B	133	ASN	7.7
3	K	74	ASN	7.5
3	K	36	TRP	7.4
1	A	51	TRP	7.2
3	K	54	SER	7.0
3	K	77	ASN	6.9
2	B	514	VAL	6.9
3	K	51	ILE	6.7
3	K	75	ALA	6.6
3	K	71	SER	6.6
3	K	100	ARG	6.4
1	A	14	ASP	5.8
1	A	53	ALA	5.7
3	K	56	GLY	5.6
3	K	119	THR	5.6
1	A	54	HIS	5.6
2	B	132	VAL	5.6
2	B	431	GLU	5.5
1	A	100	LYS	5.5
1	A	223	SER	5.4
3	K	55	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
3	K	34	ILE	5.3
2	B	544	ASN	5.1
2	B	414	SER	5.0
3	K	22	CYS	4.9
3	K	59	THR	4.9
1	A	347	ALA	4.8
3	K	20	LEU	4.7
1	A	58	ILE	4.7
1	A	55	ASP	4.6
2	B	333	GLU	4.6
3	K	72	ARG	4.6
2	B	124	PHE	4.5
2	B	176	GLU	4.5
3	K	76	GLU	4.5
3	K	53	ARG	4.4
1	A	337	ASN	4.4
1	A	52	ARG	4.3
1	A	248	LYS	4.3
2	B	349	TYR	4.2
2	B	455	PHE	4.2
3	K	91	THR	4.2
2	B	552	ILE	4.1
2	B	65	MET	4.1
3	K	33	ALA	4.0
2	B	184	CYS	4.0
1	A	61	ILE	4.0
1	A	115	LYS	4.0
1	A	290	SER	3.9
2	B	338	VAL	3.9
3	K	78	THR	3.9
1	A	225	GLY	3.9
2	B	515	THR	3.9
1	A	70	ARG	3.8
1	A	308	TRP	3.8
2	B	334	ASP	3.8
2	B	555	SER	3.8
1	A	60	ALA	3.8
1	A	59	VAL	3.7
2	B	549	ALA	3.7
3	K	73	ASP	3.6
3	K	35	GLY	3.6
3	K	101	THR	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	394	CYS	3.5
2	B	510	HIS	3.5
1	A	216	ARG	3.5
3	K	52	SER	3.5
1	A	251	PRO	3.4
1	A	32	HIS	3.4
1	A	172	SER	3.4
3	K	30	ASP	3.3
2	B	451	LEU	3.3
2	B	269	ASP	3.3
1	A	33	ILE	3.3
2	B	479	LYS	3.3
3	K	29	LEU	3.2
1	A	252	LEU	3.2
1	A	317	THR	3.2
3	K	110	ILE	3.1
1	A	49	ASP	3.1
2	B	513	PHE	3.1
1	A	226	ARG	3.1
3	K	111	GLY	3.1
2	B	315	GLN	3.1
1	A	27	CYS	3.1
2	B	389	ASP	3.0
1	A	142	PRO	3.0
2	B	76	TYR	3.0
1	A	22	ARG	3.0
2	B	472	GLU	3.0
2	B	213	ASN	3.0
1	A	166	GLN	3.0
1	A	291	ASN	2.9
2	B	240	PHE	2.9
2	B	351	ARG	2.9
2	B	347	LEU	2.9
2	B	474	CYS	2.9
1	A	31	GLN	2.9
2	B	556	ILE	2.8
1	A	93	CYS	2.8
1	A	229	GLN	2.8
2	B	500	LYS	2.8
1	A	62	ASP	2.8
2	B	350	SER	2.7
3	K	79	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	198	LYS	2.7
1	A	19	PHE	2.7
3	K	1	GLN	2.7
3	K	70	ILE	2.7
2	B	322	THR	2.7
1	A	113	SER	2.7
1	A	75	ALA	2.7
2	B	550	HIS	2.7
2	B	545	GLN	2.7
1	A	94	SER	2.7
1	A	224	ILE	2.6
2	B	551	ASN	2.6
2	B	471	PHE	2.6
3	K	27	PHE	2.6
2	B	198	GLU	2.6
1	A	333	ALA	2.6
1	A	145	LEU	2.6
1	A	250	SER	2.6
2	B	90	LEU	2.6
2	B	94	ARG	2.6
2	B	383	VAL	2.6
3	K	114	TYR	2.6
1	A	158	SER	2.5
2	B	348	GLN	2.5
1	A	42	THR	2.5
1	A	167	SER	2.5
2	B	420	THR	2.5
2	B	97	ARG	2.5
3	K	48	VAL	2.5
1	A	176	SER	2.5
1	A	227	TRP	2.5
2	B	68	LYS	2.5
2	B	135	ASN	2.5
2	B	66	PRO	2.4
1	A	1	MET	2.4
1	A	324	ASP	2.4
2	B	172	PHE	2.4
2	B	228	PHE	2.4
1	A	299	GLU	2.4
2	B	230	VAL	2.4
2	B	329	ARG	2.4
2	B	373	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	121	ASP	2.4
3	K	90	ASP	2.4
2	B	461	MET	2.4
2	B	355	GLU	2.4
3	K	58	THR	2.4
3	K	25	SER	2.4
1	A	20	TYR	2.4
1	A	190	GLN	2.3
1	A	92	GLU	2.3
2	B	77	GLN	2.3
1	A	247	GLU	2.3
1	A	168	ASP	2.3
2	B	193	ASP	2.3
2	B	323	ASP	2.3
1	A	108	LYS	2.3
2	B	547	LEU	2.3
1	A	332	LYS	2.2
2	B	57	PRO	2.2
2	B	314	SER	2.2
2	B	341	GLY	2.2
1	A	41	ASP	2.2
2	B	497	ARG	2.2
2	B	64	LYS	2.2
1	A	146	ARG	2.2
2	B	81	PHE	2.2
1	A	171	LEU	2.2
1	A	173	TRP	2.2
1	A	16	VAL	2.2
1	A	97	ARG	2.2
3	K	57	SER	2.2
3	K	113	ASP	2.2
1	A	35	VAL	2.2
2	B	255	ARG	2.2
2	B	175	LEU	2.2
2	B	521	TRP	2.2
1	A	310	VAL	2.2
1	A	234	GLY	2.1
1	A	123	LEU	2.1
1	A	340	LYS	2.1
3	K	4	LEU	2.1
1	A	177	ARG	2.1
2	B	194	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	219	PRO	2.1
2	B	453	ASP	2.1
1	A	341	CYS	2.1
1	A	99	ASN	2.1
1	A	40	LYS	2.1
1	A	122	GLY	2.1
3	K	21	SER	2.1
1	A	57	SER	2.1
1	A	64	ALA	2.0
2	B	404	SER	2.0
1	A	63	TRP	2.0
2	B	343	GLN	2.0
2	B	465	MET	2.0
1	A	155	LYS	2.0
2	B	539	TYR	2.0
1	A	36	PHE	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.