



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:59 AM UTC

PDB ID : 5YVH / pdb_00005yvh
Title : Crystal structure of Karyopherin beta2 in complex with FUS(371-526)
Authors : Yoshizawa, T.; Fung, H.Y.J.; Chook, Y.M.
Deposited on : 2017-11-25
Resolution : 3.15 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

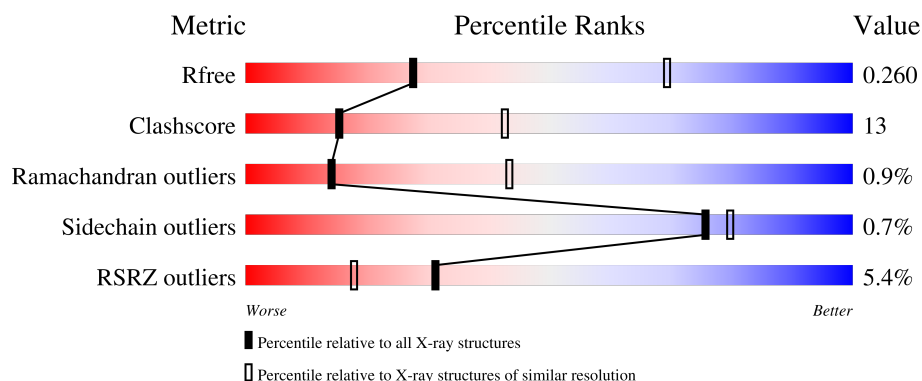
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	868	
2	B	158	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6621 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 Transportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	0	0
			6455	4143	1078	1184	50			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q92973
A	0	SER	-	expression tag	UNP Q92973
A	361	GLY	-	linker	UNP Q92973
A	362	GLY	-	linker	UNP Q92973
A	363	SER	-	linker	UNP Q92973
A	364	GLY	-	linker	UNP Q92973
A	365	GLY	-	linker	UNP Q92973
A	366	SER	-	linker	UNP Q92973
A	367	GLY	-	linker	UNP Q92973

- Molecule 2 is a protein called RNA-binding protein FUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	19	Total	C	N	O	S	0	0	0
			166	96	38	31	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	369	GLY	-	expression tag	UNP P35637
B	370	SER	-	expression tag	UNP P35637

GLY	ASP	ARG	GLY	GLY	PHE	ARG	GLY	GLY	ARG	GLY	GLY	GLY	GLY	ASP	ARG	GLY	GLY	PHE	GLY	P508	G509	K510	R514	R518	R521	R522	P525	Y526
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.43Å 156.53Å 67.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.35 – 3.15 41.35 – 3.15	Depositor EDS
% Data completeness (in resolution range)	87.3 (41.35-3.15) 87.2 (41.35-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.213 , 0.262 0.215 , 0.260	Depositor DCC
R_{free} test set	1075 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6621	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	0.46	1/6591 (0.0%)	0.71	10/8945 (0.1%)
2	B	0.34	0/169	0.59	0/220
All	All	0.46	1/6760 (0.0%)	0.71	10/9165 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	VAL	CA-CB	-17.71	1.45	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	PHE	CA-C-N	10.30	141.22	121.54
1	A	834	PHE	C-N-CA	10.30	141.22	121.54
1	A	160	ALA	N-CA-C	7.92	121.88	111.75
1	A	121	GLY	N-CA-C	-6.16	98.58	113.18
1	A	123	LEU	CA-C-N	-5.75	111.97	121.92
1	A	123	LEU	C-N-CA	-5.75	111.97	121.92
1	A	841	SER	CA-C-N	5.50	129.16	121.24
1	A	841	SER	C-N-CA	5.50	129.16	121.24
1	A	843	ILE	CA-C-N	5.47	135.15	121.80
1	A	843	ILE	C-N-CA	5.47	135.15	121.80

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	6455	0	6518	179	0
2	B	166	0	156	9	0
All	All	6621	0	6674	179	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 13.

All (179) 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:162:ILE:CG2	1:A:171:PRO:HG2	1.61	1.30
1:A:781:VAL:O	1:A:783:PRO:HD3	1.53	1.09
1:A:162:ILE:HG22	1:A:171:PRO:HG2	1.14	1.08
1:A:162:ILE:CG2	1:A:171:PRO:CG	2.32	1.05
1:A:884:LEU:O	1:A:889:GLY:HA2	1.57	1.03
1:A:162:ILE:HG23	1:A:171:PRO:CG	1.88	1.02
1:A:124:GLN:HA	1:A:168:LEU:HD21	1.42	1.01
1:A:854:CYS:HB3	1:A:888:TYR:HB3	1.43	0.99
1:A:781:VAL:O	1:A:783:PRO:CD	2.10	0.97
1:A:163:LEU:HB2	1:A:172:LEU:HD22	1.50	0.92
1:A:600:GLY:O	1:A:603:PRO:HD2	1.69	0.91
1:A:171:PRO:O	1:A:175:MET:SD	2.33	0.87
1:A:162:ILE:HG22	1:A:172:LEU:CD1	2.05	0.86
1:A:588:GLU:OE1	2:B:521:ARG:NH2	2.09	0.86
1:A:763:THR:O	1:A:765:LYS:N	2.11	0.83
1:A:163:LEU:HG	1:A:206:THR:HG23	1.62	0.82
1:A:781:VAL:HG12	1:A:782:CYS:N	1.96	0.80
1:A:124:GLN:CA	1:A:168:LEU:HD21	2.14	0.78
1:A:781:VAL:C	1:A:783:PRO:HD3	2.09	0.77
1:A:794:ILE:CD1	1:A:817:ILE:HD11	2.15	0.77
1:A:747:ILE:CD1	1:A:781:VAL:HG21	2.16	0.76
1:A:802:ARG:HB2	1:A:839:VAL:HG22	1.69	0.75
1:A:847:ASP:HA	1:A:850:ARG:HD3	1.66	0.75
1:A:798:CYS:HB3	1:A:839:VAL:HG21	1.70	0.74
1:A:845:PRO:HG2	1:A:850:ARG:HG2	1.69	0.74
1:A:154:LYS:O	1:A:158:ASP:OD1	2.06	0.74
1:A:600:GLY:O	1:A:603:PRO:CD	2.35	0.73
1:A:158:ASP:OD1	1:A:158:ASP:N	2.22	0.73
1:A:488:ARG:NH1	1:A:491:ASP:OD1	2.21	0.72
1:A:162:ILE:HG23	1:A:171:PRO:HG3	1.70	0.71
1:A:123:LEU:HB3	1:A:168:LEU:HD11	1.74	0.69
1:A:764:PRO:HA	1:A:768:LEU:HD12	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:NH1	1:A:226:ASP:OD2	2.25	0.68
1:A:747:ILE:HD11	1:A:781:VAL:HG21	1.74	0.68
1:A:162:ILE:CG2	1:A:172:LEU:CD1	2.72	0.68
1:A:781:VAL:O	1:A:783:PRO:HD2	1.93	0.67
1:A:171:PRO:C	1:A:172:LEU:HD12	2.20	0.67
1:A:777:ARG:C	1:A:779:GLY:H	2.03	0.67
1:A:841:SER:HB2	1:A:883:ARG:HD2	1.77	0.66
1:A:689:ALA:HB1	2:B:510:LYS:HD2	1.78	0.66
1:A:550:ASP:OD2	2:B:518:ARG:NH2	2.29	0.66
1:A:163:LEU:C	1:A:163:LEU:HD13	2.20	0.66
1:A:597:LEU:O	1:A:598:GLN:C	2.39	0.65
1:A:781:VAL:CG1	1:A:782:CYS:N	2.59	0.65
1:A:781:VAL:HG12	1:A:782:CYS:H	1.63	0.64
1:A:854:CYS:CB	1:A:888:TYR:HB3	2.25	0.63
1:A:884:LEU:O	1:A:889:GLY:CA	2.39	0.63
1:A:384:ASP:OD2	2:B:526:TYR:OH	2.15	0.63
1:A:502:SER:HB3	2:B:522:ARG:HG2	1.82	0.62
1:A:584:PHE:HB2	1:A:585:PRO:HD3	1.82	0.62
1:A:22:SER:HB3	1:A:33:VAL:HG11	1.81	0.61
1:A:781:VAL:CG1	1:A:782:CYS:H	2.12	0.60
1:A:794:ILE:HD12	1:A:817:ILE:HD11	1.85	0.59
1:A:92:LYS:HD3	1:A:126:TRP:CD2	2.37	0.59
1:A:543:ASP:OD1	2:B:521:ARG:NH1	2.35	0.59
1:A:268:GLN:H	1:A:268:GLN:CD	2.05	0.59
1:A:804:ILE:HG13	1:A:810:LYS:HD2	1.85	0.59
1:A:162:ILE:CG2	1:A:172:LEU:HD11	2.33	0.58
1:A:155:ILE:O	1:A:159:SER:HB2	2.04	0.58
1:A:859:GLY:O	1:A:863:GLN:HG3	2.03	0.57
1:A:248:ASP:OD1	1:A:249:ARG:N	2.38	0.57
1:A:844:ASN:O	1:A:844:ASN:ND2	2.37	0.57
1:A:124:GLN:N	1:A:124:GLN:OE1	2.35	0.57
1:A:793:PHE:CD1	1:A:793:PHE:C	2.82	0.57
1:A:703:LYS:HD3	1:A:739:MET:HE1	1.87	0.57
1:A:728:ALA:O	1:A:732:ILE:HG13	2.05	0.56
1:A:108:ALA:O	1:A:112:ILE:HG12	2.06	0.55
1:A:845:PRO:HG2	1:A:850:ARG:CG	2.34	0.55
1:A:672:MET:HE1	1:A:694:LEU:HD12	1.89	0.55
1:A:162:ILE:HB	1:A:172:LEU:HD11	1.89	0.55
1:A:591:SER:OG	2:B:514:ARG:NH2	2.40	0.55
1:A:447:LEU:O	1:A:455:ARG:HG2	2.06	0.54
1:A:601:PHE:O	1:A:602:LEU:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:CG2	1:A:171:PRO:CB	2.85	0.54
1:A:535:HIS:NE2	1:A:582:ASP:OD2	2.39	0.54
1:A:780:TYR:CD1	1:A:780:TYR:N	2.76	0.54
1:A:80:PHE:HB3	1:A:120:LYS:HD2	1.90	0.53
1:A:159:SER:O	1:A:162:ILE:HG13	2.08	0.53
1:A:12:LEU:HD21	1:A:57:LEU:HD11	1.89	0.53
1:A:798:CYS:CB	1:A:839:VAL:HG21	2.39	0.53
1:A:165:SER:HB2	1:A:167:VAL:HG23	1.91	0.53
1:A:171:PRO:O	1:A:172:LEU:HD12	2.09	0.52
1:A:888:TYR:CD1	1:A:888:TYR:N	2.78	0.52
1:A:846:LYS:HD2	1:A:847:ASP:H	1.75	0.52
1:A:806:ASP:OD1	1:A:810:LYS:NZ	2.36	0.52
1:A:577:LYS:HD2	1:A:578:ASP:H	1.74	0.51
1:A:395:LEU:HA	1:A:398:ILE:HG22	1.93	0.51
1:A:162:ILE:O	1:A:171:PRO:HG2	2.10	0.51
1:A:183:PHE:HD2	1:A:219:ASN:HB3	1.76	0.50
1:A:699:PHE:HZ	1:A:739:MET:HE3	1.76	0.50
1:A:817:ILE:HD12	1:A:820:MET:HE3	1.93	0.50
1:A:311:SER:O	1:A:315:ILE:HD12	2.12	0.50
1:A:851:ASP:O	1:A:855:LYS:HB2	2.12	0.50
1:A:460:TRP:CD2	2:B:525:PRO:HG3	2.47	0.49
1:A:210:MET:HE1	1:A:246:ARG:CG	2.43	0.49
1:A:854:CYS:O	1:A:858:HIS:HB2	2.13	0.49
1:A:251:LEU:HD21	1:A:288:ILE:HD13	1.94	0.49
1:A:780:TYR:N	1:A:780:TYR:HD1	2.09	0.49
1:A:818:CYS:O	1:A:821:ILE:HG22	2.13	0.49
1:A:19:LEU:O	1:A:22:SER:OG	2.30	0.48
1:A:395:LEU:HD11	1:A:431:GLY:HA3	1.94	0.48
1:A:746:TYR:HB3	1:A:749:MET:HE2	1.96	0.48
1:A:699:PHE:CZ	1:A:739:MET:HE3	2.48	0.48
1:A:853:PHE:HB2	1:A:888:TYR:HE2	1.77	0.48
1:A:817:ILE:HA	1:A:820:MET:HE3	1.95	0.48
1:A:739:MET:HA	1:A:739:MET:HE2	1.97	0.47
1:A:78:ALA:O	1:A:79:HIS:ND1	2.47	0.47
1:A:460:TRP:CE3	2:B:525:PRO:HG3	2.49	0.47
1:A:763:THR:O	1:A:763:THR:HG22	2.13	0.47
1:A:479:LYS:HE3	1:A:518:TYR:HE1	1.80	0.47
1:A:53:VAL:O	1:A:65:ARG:HG2	2.14	0.47
1:A:381:ALA:O	1:A:385:VAL:HG23	2.15	0.47
1:A:62:GLU:N	1:A:62:GLU:OE1	2.48	0.46
1:A:76:VAL:HG13	1:A:80:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TYR:O	1:A:53:VAL:HG23	2.15	0.46
1:A:848:ASP:OD1	1:A:848:ASP:N	2.49	0.46
1:A:853:PHE:CB	1:A:888:TYR:CE2	2.99	0.46
1:A:313:ILE:O	1:A:313:ILE:HG22	2.15	0.46
1:A:162:ILE:HG22	1:A:172:LEU:HD12	1.92	0.46
1:A:301:ILE:HB	1:A:302:PRO:HD3	1.98	0.46
1:A:676:MET:HE2	1:A:691:LEU:HD22	1.97	0.46
1:A:781:VAL:C	1:A:783:PRO:CD	2.78	0.45
1:A:315:ILE:O	1:A:315:ILE:HG22	2.15	0.45
1:A:871:ARG:O	1:A:874:ASP:HB2	2.16	0.45
1:A:15:ILE:HD11	1:A:50:LEU:HD23	1.97	0.45
1:A:162:ILE:CB	1:A:172:LEU:HD11	2.47	0.45
1:A:508:GLU:HA	1:A:515:LEU:HD11	1.97	0.45
1:A:162:ILE:CG2	1:A:171:PRO:HB2	2.46	0.45
1:A:853:PHE:HB2	1:A:888:TYR:CE2	2.51	0.45
1:A:860:PHE:HA	1:A:863:GLN:OE1	2.16	0.45
1:A:831:ASP:O	1:A:833:ILE:N	2.42	0.45
1:A:541:LEU:O	1:A:545:ILE:HG12	2.17	0.45
1:A:793:PHE:CD1	1:A:793:PHE:O	2.70	0.45
1:A:755:VAL:O	1:A:758:ILE:HG22	2.16	0.45
1:A:777:ARG:C	1:A:779:GLY:N	2.71	0.44
1:A:793:PHE:O	1:A:793:PHE:HD1	2.01	0.44
1:A:31:ARG:O	1:A:34:GLN:HB3	2.18	0.44
1:A:845:PRO:O	1:A:850:ARG:HD2	2.18	0.44
1:A:854:CYS:HB3	1:A:888:TYR:CB	2.30	0.44
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.86	0.43
1:A:181:GLN:O	1:A:184:LYS:HG2	2.18	0.43
1:A:264:ARG:O	1:A:267:ASP:HB2	2.18	0.43
1:A:48:ASN:CG	1:A:87:VAL:HG13	2.43	0.43
1:A:797:TRP:CZ2	1:A:801:LEU:HD12	2.54	0.43
1:A:28:THR:HG23	1:A:31:ARG:HH21	1.82	0.43
1:A:851:ASP:HA	1:A:854:CYS:SG	2.59	0.43
1:A:254:MET:O	1:A:258:VAL:HG23	2.19	0.43
1:A:130:LEU:HB2	1:A:131:PRO:HD3	2.01	0.43
1:A:776:GLY:O	1:A:816:GLY:HA3	2.18	0.43
1:A:243:LEU:HD13	1:A:279:PHE:CE1	2.53	0.43
1:A:16:LEU:HD11	1:A:57:LEU:HD21	2.00	0.43
1:A:612:CYS:SG	1:A:647:LEU:HD23	2.58	0.43
1:A:124:GLN:HA	1:A:168:LEU:CD2	2.31	0.42
1:A:792:GLN:HB3	1:A:793:PHE:H	1.48	0.42
1:A:271:ASN:O	1:A:275:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:GLU:HB3	1:A:537:ASN:OD1	2.19	0.42
1:A:763:THR:C	1:A:765:LYS:N	2.77	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.90	0.42
1:A:162:ILE:O	1:A:171:PRO:CG	2.68	0.42
1:A:111:GLY:O	1:A:115:THR:HG23	2.20	0.42
1:A:137:LEU:HG	1:A:149:PHE:CE2	2.54	0.42
1:A:736:SER:HA	1:A:743:MET:SD	2.60	0.42
1:A:692:GLY:HA3	1:A:730:TRP:CZ3	2.54	0.42
1:A:744:GLN:N	1:A:745:PRO:HD2	2.35	0.42
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.92	0.42
1:A:597:LEU:HA	1:A:597:LEU:HD23	1.69	0.41
1:A:676:MET:HE1	1:A:709:PHE:CD2	2.55	0.41
1:A:11:GLY:O	1:A:15:ILE:HG22	2.21	0.41
1:A:58:LYS:H	1:A:58:LYS:HG2	1.69	0.41
1:A:177:PRO:O	1:A:181:GLN:HG3	2.20	0.41
1:A:6:LYS:HE2	1:A:6:LYS:HB3	1.85	0.41
1:A:297:LEU:HD11	1:A:301:ILE:HD11	2.03	0.41
1:A:246:ARG:NH1	1:A:248:ASP:OD2	2.54	0.40
1:A:48:ASN:OD1	1:A:87:VAL:HG13	2.21	0.40
1:A:162:ILE:HG21	1:A:171:PRO:HB2	2.04	0.40
1:A:282:THR:O	1:A:285:GLU:HG2	2.20	0.40
1:A:854:CYS:HB3	1:A:888:TYR:CD2	2.57	0.40
1:A:123:LEU:O	1:A:168:LEU:HD11	2.22	0.40
1:A:313:ILE:O	1:A:313:ILE:CG2	2.68	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	797/868 (92%)	743 (93%)	47 (6%)	7 (1%)	14 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	17/158 (11%)	17 (100%)	0	0	100	100
All	All	814/1026 (79%)	760 (93%)	47 (6%)	7 (1%)	14	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	GLN
1	A	782	CYS
1	A	833	ILE
1	A	764	PRO
1	A	778	LEU
1	A	123	LEU
1	A	832	PHE

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	728/776 (94%)	723 (99%)	5 (1%)	76	80
2	B	17/94 (18%)	17 (100%)	0	100	100
All	All	745/870 (86%)	740 (99%)	5 (1%)	76	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLU
1	A	158	ASP
1	A	315	ILE
1	A	792	GLN
1	A	888	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	125	ASN
1	A	442	HIS
1	A	598	GLN
1	A	614	ASN
1	A	753	GLN
1	A	759	ASN
1	A	792	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	809/868 (93%)	0.19	44 (5%) 31 18	15, 54, 111, 182	0
2	B	19/158 (12%)	0.00	1 (5%) 32 18	14, 43, 85, 96	0
All	All	828/1026 (80%)	0.19	45 (5%) 31 18	14, 54, 111, 182	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	888	TYR	4.9
1	A	764	PRO	4.8
1	A	833	ILE	4.5
1	A	171	PRO	4.4
1	A	837	ASP	4.2
1	A	763	THR	4.2
1	A	783	PRO	4.1
1	A	889	GLY	3.8
1	A	886	ALA	3.8
1	A	599	SER	3.6
1	A	887	PHE	3.5
1	A	808	GLU	3.5
1	A	784	GLN	3.4
1	A	780	TYR	3.2
1	A	872	PHE	3.2
1	A	792	GLN	3.1
1	A	832	PHE	3.1
1	A	841	SER	2.9
1	A	600	GLY	2.9
1	A	140	GLU	2.9
1	A	822	SER	2.7
1	A	765	LYS	2.7
1	A	781	VAL	2.7
1	A	170	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	743	MET	2.5
1	A	834	PHE	2.5
1	A	163	LEU	2.3
1	A	882	GLU	2.3
1	A	598	GLN	2.3
1	A	836	CYS	2.3
1	A	863	GLN	2.3
1	A	831	ASP	2.3
1	A	166	ASP	2.2
1	A	531	SER	2.2
1	A	778	LEU	2.2
1	A	495	ARG	2.1
2	B	508	PRO	2.1
1	A	28	THR	2.1
1	A	739	MET	2.1
1	A	5	TRP	2.1
1	A	316	ILE	2.1
1	A	885	ALA	2.1
1	A	840	ALA	2.0
1	A	169	ASP	2.0
1	A	825	PRO	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.