



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 AM UTC

PDB ID : 8JJ9 / pdb_00008jj9
Title : Human FAM91A1 N terminal domain in complex with TBC1D23
Authors : Deng, H.Q.; Zhang, S.T.; Jia, D.
Deposited on : 2023-05-29
Resolution : 2.51 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

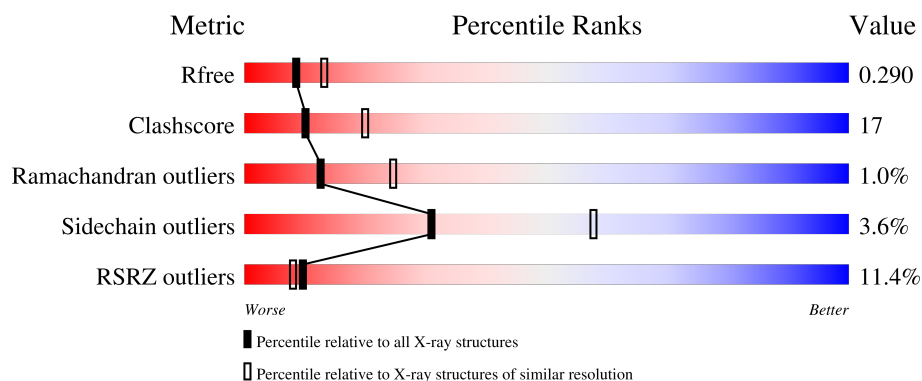
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	312	12% 61% 31% • •
1	B	312	6% 61% 32% • •
2	C	21	52% 57% 43%
2	D	21	24% 52% 43% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5398 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 Protein FAM91A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2443	1564	419	447	13			
1	B	299	Total	C	N	O	S	0	0	0
			2460	1577	421	449	13			

- Molecule 2 is a protein called TBC1 domain family member 23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	0	0	0
			166	104	34	28			
2	D	20	Total	C	N	O	0	0	0
			160	101	33	26			

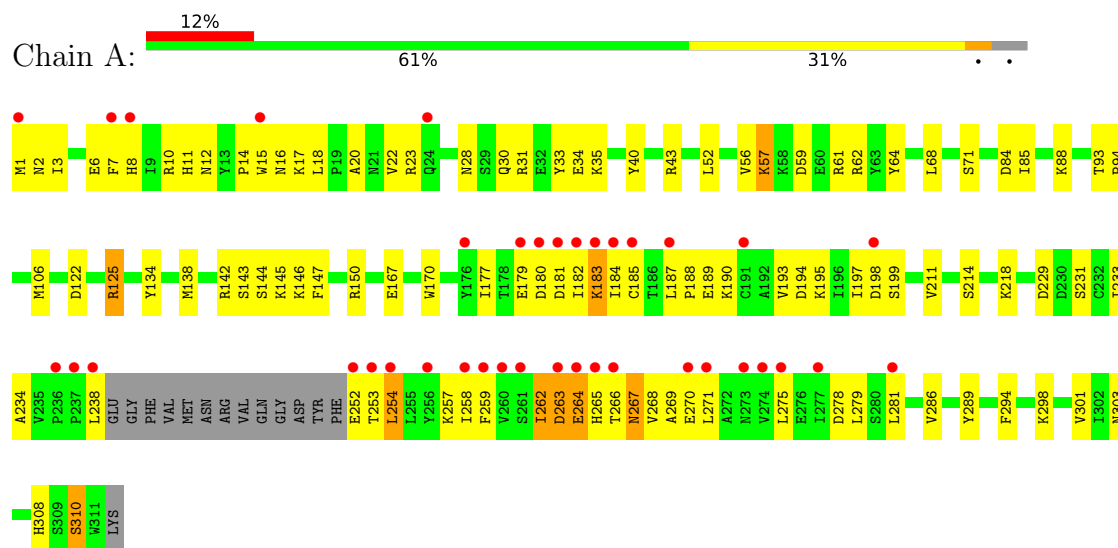
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	81	Total	O	0	0
			81	81		
3	B	84	Total	O	0	0
			84	84		
3	C	1	Total	O	0	0
			1	1		
3	D	3	Total	O	0	0
			3	3		

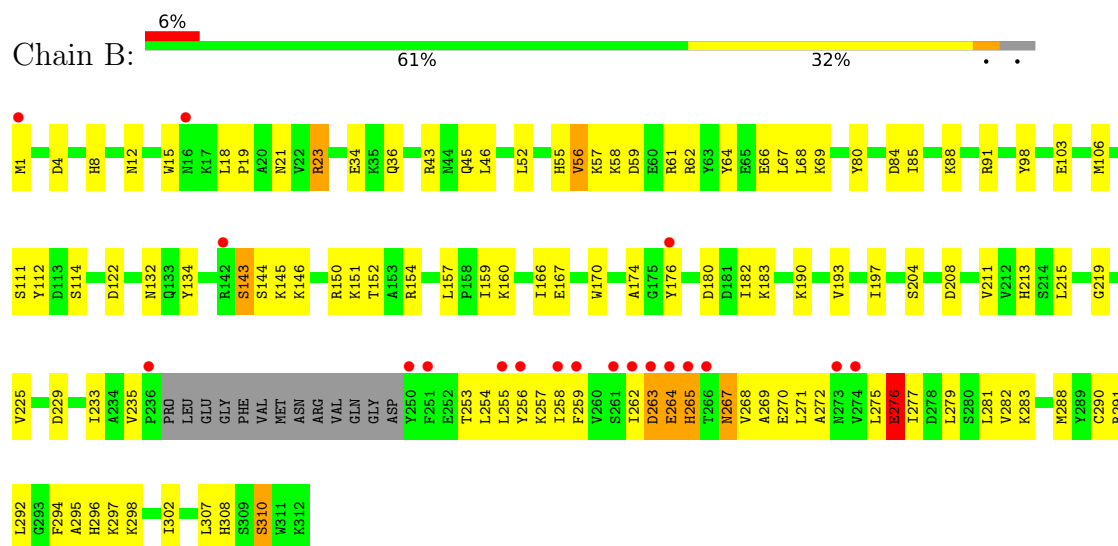
3 Residue-property plots [i](#)

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: Protein FAM91A1

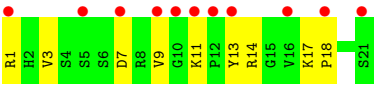


• Molecule 1: Protein FAM91A1

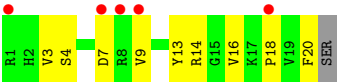


• Molecule 2: TBC1 domain family member 23





● Molecule 2: TBC1 domain family member 23



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.21Å 93.56Å 111.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.01 – 2.51 41.01 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.01-2.51) 99.9 (41.01-2.51)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.225 , 0.277 (Not available) , 0.290	Depositor DCC
R_{free} test set	1598 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5398	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.9866e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.48	0/2497	0.65	2/3380 (0.1%)
1	B	0.50	0/2515	0.67	0/3402
2	C	0.41	0/170	0.52	0/227
2	D	0.35	0/164	0.70	0/219
All	All	0.48	0/5346	0.66	2/7228 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	262	ILE	CA-C-N	5.25	131.56	121.54
1	A	262	ILE	C-N-CA	5.25	131.56	121.54

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	B	264	GLU	Peptide
1	B	276	GLU	Peptide

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	2443	0	2449	86	0
1	B	2460	0	2462	81	0
2	C	166	0	172	11	0
2	D	160	0	167	12	0
3	A	81	0	0	5	0
3	B	84	0	0	3	0
3	C	1	0	0	0	0
3	D	3	0	0	4	0
All	All	5398	0	5250	181	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 (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:LYS:NZ	3:B:401:HOH:O	1.92	1.03
1:A:190:LYS:NZ	2:C:13:TYR:OH	1.94	1.00
1:A:198:ASP:OD2	2:C:14:ARG:NH2	1.95	0.99
2:D:20:PHE:HB2	3:D:101:HOH:O	1.74	0.87
1:A:15:TRP:CG	1:A:30:GLN:HG3	2.16	0.80
1:B:190:LYS:NZ	2:D:13:TYR:OH	2.15	0.79
1:B:57:LYS:NZ	1:B:66:GLU:OE1	2.15	0.79
1:A:106:MET:HG2	1:A:138:MET:HE1	1.63	0.77
1:B:34:GLU:HG2	1:B:56:VAL:HB	1.66	0.77
1:B:1:MET:SD	1:B:43:ARG:NH2	2.58	0.76
1:B:233:ILE:HD11	1:B:262:ILE:HD11	1.69	0.74
1:A:278:ASP:HB3	1:A:281:LEU:HD12	1.71	0.71
1:A:267:ASN:HB3	1:A:270:GLU:HB2	1.74	0.70
2:C:17:LYS:HE2	2:C:18:PRO:HD2	1.74	0.69
1:A:259:PHE:CZ	1:A:294:PHE:HB3	2.27	0.69
1:A:181:ASP:O	1:A:184:ILE:HG22	1.94	0.66
2:C:1:ARG:NH2	2:C:7:ASP:OD2	2.25	0.66
1:A:20:ALA:HA	1:A:23:ARG:HB2	1.77	0.66
2:C:13:TYR:HD1	2:C:14:ARG:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE3	1:A:43:ARG:HH12	1.62	0.65
1:A:30:GLN:HB3	1:A:31:ARG:NH1	2.13	0.64
1:A:234:ALA:HB2	1:A:298:LYS:HD2	1.79	0.64
1:A:15:TRP:CD1	1:A:30:GLN:HG3	2.35	0.62
1:A:34:GLU:HG2	1:A:56:VAL:HG22	1.82	0.62
1:B:254:LEU:HD21	1:B:281:LEU:HD11	1.81	0.62
1:A:122:ASP:OD1	1:A:125:ARG:HD3	2.01	0.61
1:A:254:LEU:O	1:A:258:ILE:HG13	2.01	0.60
1:B:45:GLN:HA	1:B:67:LEU:HD11	1.84	0.60
1:A:2:ASN:ND2	3:A:407:HOH:O	2.35	0.60
1:A:15:TRP:CH2	1:A:23:ARG:HG2	2.38	0.59
1:A:198:ASP:CG	2:C:14:ARG:HH22	2.08	0.59
1:B:103:GLU:OE1	1:B:154:ARG:NH1	2.36	0.59
1:B:256:TYR:CE2	1:B:257:LYS:HD3	2.37	0.59
1:B:263:ASP:OD2	1:B:265:HIS:HA	2.03	0.59
1:A:264:GLU:O	1:A:266:THR:OG1	2.22	0.58
1:A:84:ASP:O	1:A:88:LYS:HB2	2.04	0.57
1:A:182:ILE:HA	1:A:185:CYS:SG	2.44	0.57
1:B:59:ASP:OD2	1:B:62:ARG:HB2	2.05	0.57
1:B:279:LEU:O	1:B:282:VAL:HG12	2.04	0.57
1:B:1:MET:HE2	1:B:36:GLN:HB3	1.87	0.56
1:B:167:GLU:HB2	1:B:170:TRP:CD1	2.40	0.56
1:B:106:MET:HE1	1:B:157:LEU:HD21	1.87	0.55
1:A:182:ILE:HD12	2:C:13:TYR:HE2	1.72	0.55
1:B:18:LEU:HB2	1:B:23:ARG:HD3	1.88	0.55
1:A:194:ASP:OD1	2:C:14:ARG:NH1	2.38	0.55
1:B:193:VAL:O	1:B:197:ILE:HG13	2.06	0.54
2:D:20:PHE:N	3:D:101:HOH:O	2.35	0.54
1:A:18:LEU:HD11	1:A:33:TYR:CE1	2.43	0.53
1:B:233:ILE:HG22	1:B:297:LYS:HA	1.90	0.53
2:D:4:SER:O	2:D:7:ASP:HB2	2.08	0.53
1:A:144:SER:HA	1:A:147:PHE:HD2	1.73	0.53
1:A:144:SER:HA	1:A:147:PHE:CD2	2.44	0.53
1:B:80:TYR:OH	1:B:122:ASP:OD2	2.21	0.53
1:A:64:TYR:CD2	1:A:85:ILE:HG21	2.44	0.52
1:A:143:SER:O	1:A:146:LYS:HG3	2.10	0.52
1:A:6:GLU:HG2	1:A:40:TYR:CD1	2.45	0.51
1:A:229:ASP:OD1	1:A:279:LEU:HD21	2.09	0.51
1:B:267:ASN:OD1	1:B:268:VAL:N	2.43	0.51
2:D:16:VAL:O	2:D:18:PRO:HD3	2.11	0.51
1:B:15:TRP:CH2	1:B:23:ARG:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:THR:HG23	1:B:154:ARG:H	1.75	0.51
1:B:259:PHE:CZ	1:B:294:PHE:HB3	2.46	0.51
1:B:208:ASP:OD2	1:B:211:VAL:HG23	2.10	0.51
1:B:229:ASP:OD1	1:B:283:LYS:HE3	2.10	0.51
1:A:167:GLU:HB2	1:A:170:TRP:CD1	2.46	0.50
1:B:19:PRO:HB2	1:B:21:ASN:OD1	2.12	0.50
1:A:286:VAL:HA	1:A:289:TYR:CD2	2.47	0.50
1:A:10:ARG:NH1	1:A:40:TYR:OH	2.44	0.50
1:B:103:GLU:OE2	1:B:154:ARG:HG3	2.12	0.50
1:A:8:HIS:CD2	1:A:22:VAL:HG21	2.47	0.50
1:B:64:TYR:CD2	1:B:85:ILE:HG21	2.47	0.50
1:A:187:LEU:N	1:A:188:PRO:HD2	2.28	0.49
1:A:8:HIS:HB3	1:A:18:LEU:HD21	1.93	0.49
2:D:20:PHE:CB	3:D:101:HOH:O	2.47	0.49
1:A:142:ARG:NH2	3:A:402:HOH:O	2.45	0.49
1:A:12:ASN:OD1	1:A:52:LEU:N	2.43	0.48
2:D:13:TYR:CE1	2:D:14:ARG:HG3	2.48	0.48
1:A:14:PRO:HG2	1:A:17:LYS:HG2	1.95	0.48
1:B:112:TYR:HB2	1:B:134:TYR:CD2	2.49	0.48
1:B:229:ASP:OD1	1:B:279:LEU:HD21	2.14	0.48
1:B:254:LEU:O	1:B:258:ILE:HG13	2.14	0.48
1:A:59:ASP:C	1:A:59:ASP:OD2	2.57	0.48
1:A:179:GLU:H	1:A:179:GLU:CD	2.20	0.48
1:A:193:VAL:O	1:A:197:ILE:HG13	2.14	0.48
1:B:64:TYR:CG	1:B:85:ILE:HG21	2.49	0.48
1:B:277:ILE:HG21	1:B:281:LEU:HD12	1.96	0.48
1:B:91:ARG:HH11	1:B:176:TYR:HD2	1.61	0.48
2:C:13:TYR:HD1	2:C:13:TYR:C	2.22	0.48
1:B:267:ASN:OD1	1:B:269:ALA:N	2.47	0.47
1:A:252:GLU:OE2	1:A:253:THR:HG23	2.14	0.47
1:B:1:MET:HG3	1:B:36:GLN:OE1	2.15	0.47
1:B:150:ARG:NH1	3:B:405:HOH:O	2.31	0.47
1:B:271:LEU:O	1:B:275:LEU:HD12	2.14	0.47
1:A:16:ASN:OD1	1:A:17:LYS:N	2.47	0.47
1:A:189:GLU:OE2	1:A:218:LYS:HE2	2.15	0.47
1:B:144:SER:HB3	1:B:151:LYS:H	1.80	0.47
1:A:263:ASP:O	1:A:265:HIS:N	2.47	0.47
1:B:21:ASN:OD1	1:B:21:ASN:N	2.48	0.47
1:A:265:HIS:CG	1:A:265:HIS:O	2.68	0.47
1:A:134:TYR:CZ	1:A:138:MET:HE3	2.49	0.46
1:A:264:GLU:N	1:A:264:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:VAL:O	2:D:9:VAL:HG13	2.14	0.46
1:A:35:LYS:NZ	3:A:401:HOH:O	2.25	0.46
1:B:132:ASN:ND2	3:B:411:HOH:O	2.48	0.46
1:B:167:GLU:O	1:B:204:SER:OG	2.30	0.46
1:A:218:LYS:O	2:C:3:VAL:HG13	2.14	0.46
1:A:57:LYS:HE3	1:A:62:ARG:HB3	1.98	0.46
1:A:265:HIS:O	1:A:265:HIS:ND1	2.49	0.46
1:A:134:TYR:CE1	1:A:138:MET:HE3	2.51	0.45
1:A:269:ALA:HA	1:A:279:LEU:HD13	1.99	0.45
1:A:303:ASN:ND2	3:A:415:HOH:O	2.49	0.45
1:A:189:GLU:HA	1:A:211:VAL:HG13	1.97	0.45
1:B:12:ASN:OD1	1:B:52:LEU:N	2.45	0.45
1:B:308:HIS:ND1	1:B:310:SER:OG	2.41	0.45
1:A:15:TRP:O	1:A:18:LEU:HB2	2.16	0.45
1:A:195:LYS:HE2	1:A:199:SER:HB2	1.98	0.45
1:B:296:HIS:ND1	1:B:298:LYS:HE2	2.31	0.45
1:A:310:SER:H	1:A:310:SER:HG	1.39	0.45
1:B:225:VAL:HG21	1:B:291:ARG:HB2	1.98	0.45
1:A:7:PHE:CE2	1:A:11:HIS:CD2	3.05	0.44
1:A:189:GLU:O	1:A:193:VAL:HG23	2.17	0.44
1:B:166:ILE:HD12	1:B:213:HIS:CE1	2.52	0.44
1:A:271:LEU:HD12	1:A:275:LEU:HD23	1.99	0.44
1:B:263:ASP:CG	1:B:265:HIS:HA	2.42	0.44
1:B:272:ALA:HB2	1:B:282:VAL:HG11	2.00	0.44
1:B:277:ILE:CG2	1:B:281:LEU:HD12	2.48	0.44
2:D:20:PHE:CA	3:D:101:HOH:O	2.65	0.44
1:B:308:HIS:CE1	1:B:310:SER:HG	2.32	0.44
2:C:13:TYR:C	2:C:13:TYR:CD1	2.94	0.44
1:B:159:ILE:HG13	1:B:160:LYS:HD3	2.00	0.43
1:B:267:ASN:OD1	1:B:267:ASN:C	2.61	0.43
1:A:278:ASP:OD1	1:A:279:LEU:N	2.51	0.43
1:A:286:VAL:HA	1:A:289:TYR:HD2	1.83	0.43
1:B:68:LEU:HD12	1:B:68:LEU:HA	1.80	0.43
1:B:143:SER:O	1:B:146:LYS:HG2	2.18	0.43
1:A:253:THR:O	1:A:257:LYS:HG2	2.19	0.43
1:B:111:SER:O	1:B:114:SER:OG	2.36	0.43
1:B:263:ASP:OD2	1:B:265:HIS:CG	2.71	0.43
1:A:189:GLU:OE2	1:A:214:SER:OG	2.29	0.43
1:B:276:GLU:HG3	1:B:277:ILE:HG12	2.00	0.43
1:B:55:HIS:O	1:B:58:LYS:NZ	2.51	0.43
1:B:263:ASP:O	1:B:264:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:O	1:A:145:LYS:HG2	2.19	0.43
2:D:13:TYR:CZ	2:D:14:ARG:HG3	2.53	0.43
1:A:61:ARG:NH2	3:A:412:HOH:O	2.45	0.43
1:A:257:LYS:HD3	1:A:257:LYS:HA	1.81	0.43
1:B:288:MET:HB3	1:B:288:MET:HE3	1.73	0.43
1:A:262:ILE:CG2	1:A:271:LEU:HD11	2.49	0.42
1:A:308:HIS:ND1	1:A:310:SER:OG	2.47	0.42
1:B:302:ILE:HD13	1:B:307:LEU:HD22	2.00	0.42
1:A:231:SER:O	1:A:268:VAL:HG23	2.20	0.42
1:B:58:LYS:HD2	1:B:58:LYS:HA	1.82	0.42
1:A:93:THR:O	1:A:94:PRO:C	2.63	0.42
1:B:84:ASP:OD1	1:B:84:ASP:N	2.52	0.42
1:B:180:ASP:HA	1:B:183:LYS:HD2	2.00	0.42
1:A:258:ILE:O	1:A:262:ILE:HG23	2.19	0.42
1:B:253:THR:O	1:B:257:LYS:HG2	2.20	0.42
1:B:88:LYS:NZ	1:B:174:ALA:O	2.48	0.41
1:B:98:TYR:CZ	1:B:122:ASP:HB3	2.55	0.41
1:B:255:LEU:HD22	1:B:288:MET:HE1	2.02	0.41
1:B:4:ASP:O	1:B:8:HIS:ND1	2.47	0.41
1:B:219:GLY:HA3	2:D:3:VAL:HG22	2.01	0.41
1:A:31:ARG:HA	1:A:31:ARG:HD3	1.68	0.41
1:A:145:LYS:HA	1:A:150:ARG:HG2	2.02	0.41
1:A:195:LYS:HE2	1:A:199:SER:CB	2.50	0.41
1:B:145:LYS:HB3	1:B:145:LYS:HE2	1.63	0.41
1:B:208:ASP:HB3	1:B:211:VAL:HB	2.01	0.41
1:B:235:VAL:HG21	1:B:262:ILE:CG1	2.50	0.41
1:A:30:GLN:HB3	1:A:31:ARG:HH11	1.81	0.41
1:B:61:ARG:HG3	2:D:20:PHE:CE2	2.56	0.41
1:A:262:ILE:HG22	1:A:271:LEU:HD11	2.02	0.41
1:A:7:PHE:HA	1:A:10:ARG:HH21	1.86	0.41
1:B:46:LEU:HD23	1:B:46:LEU:HA	1.88	0.41
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.83	0.41
1:A:182:ILE:HD11	1:A:190:LYS:HD2	2.03	0.41
1:A:263:ASP:N	1:A:264:GLU:OE1	2.54	0.41
1:B:84:ASP:O	1:B:88:LYS:HB2	2.21	0.41
1:A:233:ILE:HD11	1:A:262:ILE:HD13	2.03	0.40
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.86	0.40
1:B:290:CYS:HA	1:B:295:ALA:O	2.21	0.40
1:B:182:ILE:HD12	1:B:182:ILE:HA	1.91	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	294/312 (94%)	279 (95%)	11 (4%)	4 (1%)	9	17
1	B	295/312 (95%)	284 (96%)	9 (3%)	2 (1%)	18	34
2	C	19/21 (90%)	19 (100%)	0	0	100	100
2	D	18/21 (86%)	15 (83%)	3 (17%)	0	100	100
All	All	626/666 (94%)	597 (95%)	23 (4%)	6 (1%)	12	24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASP
1	A	267	ASN
1	B	263	ASP
1	A	264	GLU
1	B	265	HIS
1	A	183	LYS

5.3.2 Protein sidechains [i](#)

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	274/286 (96%)	263 (96%)	11 (4%)	28	54
1	B	275/286 (96%)	267 (97%)	8 (3%)	37	65
2	C	19/19 (100%)	17 (90%)	2 (10%)	6	14
2	D	18/19 (95%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	586/610 (96%)	565 (96%)	21 (4%)	31 58

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

Mol	Chain	Res	Type
1	A	3	ILE
1	A	28	ASN
1	A	57	LYS
1	A	71	SER
1	A	177	ILE
1	A	180	ASP
1	A	183	LYS
1	A	238	LEU
1	A	254	LEU
1	A	301	VAL
1	A	310	SER
1	B	23	ARG
1	B	56	VAL
1	B	143	SER
1	B	267	ASN
1	B	270	GLU
1	B	276	GLU
1	B	292	LEU
1	B	310	SER
2	C	9	VAL
2	C	11	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	11	HIS
1	A	45	GLN
1	A	303	ASN
1	B	44	ASN
1	B	45	GLN
1	B	74	HIS
1	B	132	ASN
1	B	210	ASN
1	B	213	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 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	298/312 (95%)	0.68	38 (12%) 7 6	11, 34, 66, 84	0
1	B	299/312 (95%)	0.40	19 (6%) 25 22	9, 29, 58, 75	0
2	C	21/21 (100%)	2.05	11 (52%) 0 0	34, 57, 71, 77	0
2	D	20/21 (95%)	1.45	5 (25%) 2 1	33, 48, 68, 88	0
All	All	638/666 (95%)	0.62	73 (11%) 10 8	9, 32, 65, 88	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	7.5
1	B	251	PHE	5.4
2	C	9	VAL	5.4
1	A	237	PRO	5.1
1	B	176	TYR	5.1
1	B	262	ILE	4.7
1	B	250	TYR	4.5
1	B	256	TYR	4.3
1	A	256	TYR	4.3
2	C	16	VAL	4.2
1	A	259	PHE	4.2
1	B	261	SER	3.9
1	A	179	GLU	3.9
1	A	185	CYS	3.9
1	A	260	VAL	3.8
1	B	263	ASP	3.8
1	A	274	VAL	3.7
1	B	265	HIS	3.7
1	A	176	TYR	3.5
1	A	1	MET	3.5
1	B	266	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	1	ARG	3.4
2	D	9	VAL	3.4
1	B	1	MET	3.3
1	A	236	PRO	3.3
1	A	253	THR	3.2
2	C	21	SER	3.2
1	A	263	ASP	3.2
1	A	252	GLU	3.1
1	A	7	PHE	3.1
2	D	7	ASP	3.1
1	A	24	GLN	3.0
1	A	8	HIS	2.9
1	A	181	ASP	2.8
1	A	275	LEU	2.8
1	A	182	ILE	2.7
1	B	259	PHE	2.7
1	B	274	VAL	2.7
2	C	5	SER	2.7
1	A	273	ASN	2.6
1	A	265	HIS	2.6
2	C	13	TYR	2.6
1	A	183	LYS	2.6
1	B	236	PRO	2.6
1	A	270	GLU	2.6
1	A	180	ASP	2.5
1	A	187	LEU	2.5
1	B	255	LEU	2.5
2	D	8	ARG	2.4
1	A	277	ILE	2.4
1	A	266	THR	2.3
1	A	184	ILE	2.3
1	B	142	ARG	2.3
2	C	1	ARG	2.3
1	A	254	LEU	2.3
1	B	264	GLU	2.3
1	A	258	ILE	2.3
2	C	11	LYS	2.3
2	C	18	PRO	2.3
2	C	10	GLY	2.2
1	A	281	LEU	2.2
1	A	264	GLU	2.2
1	B	258	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	15	TRP	2.2
1	A	191	CYS	2.2
2	C	12	PRO	2.1
2	C	7	ASP	2.1
2	D	18	PRO	2.1
1	A	198	ASP	2.1
1	B	273	ASN	2.1
1	A	271	LEU	2.0
1	B	16	ASN	2.0
1	A	261	SER	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.