



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:20 PM UTC

PDB ID : 6NFJ / pdb_00006nfj
Title : Structure of Beta-Klotho in Complex with FGF19 C-terminal peptide
Authors : Kuzina, E.; Schlessinger, J.; Lee, S.
Deposited on : 2018-12-20
Resolution : 3.19 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

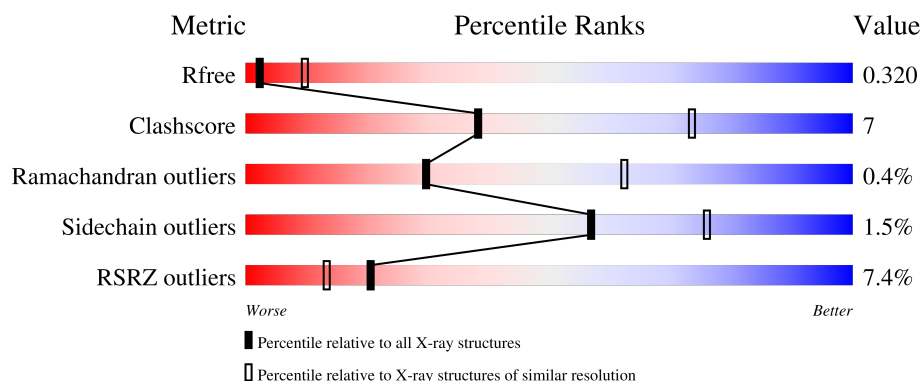
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	960	5% 72% 16% 12%
1	D	960	8% 75% 13% 12%
2	B	133	8% 68% 16% 17%
2	E	133	5% 67% 17% 15%
3	C	50	4% 38% 62%

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Mol	Chain	Length	Quality of chain
3	F	50	4% 38% 62%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14271 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 Beta-klotho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	0	0	0
			6373	4149	1076	1126	22			
1	D	846	Total	C	N	O	S	0	0	0
			6129	3969	1051	1088	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	GLN	ASN	engineered mutation	UNP Q86Z14
A	611	GLN	ASN	engineered mutation	UNP Q86Z14
A	985	ASN	-	expression tag	UNP Q86Z14
A	986	LEU	-	expression tag	UNP Q86Z14
A	987	TYR	-	expression tag	UNP Q86Z14
A	988	PHE	-	expression tag	UNP Q86Z14
A	989	GLN	-	expression tag	UNP Q86Z14
D	308	GLN	ASN	engineered mutation	UNP Q86Z14
D	611	GLN	ASN	engineered mutation	UNP Q86Z14
D	985	ASN	-	expression tag	UNP Q86Z14
D	986	LEU	-	expression tag	UNP Q86Z14
D	987	TYR	-	expression tag	UNP Q86Z14
D	988	PHE	-	expression tag	UNP Q86Z14
D	989	GLN	-	expression tag	UNP Q86Z14

- Molecule 2 is a protein called Nanobody 30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	111	Total	C	N	O	S	0	0	0
			762	490	136	132	4			
2	E	113	Total	C	N	O	S	0	0	0
			763	488	135	136	4			

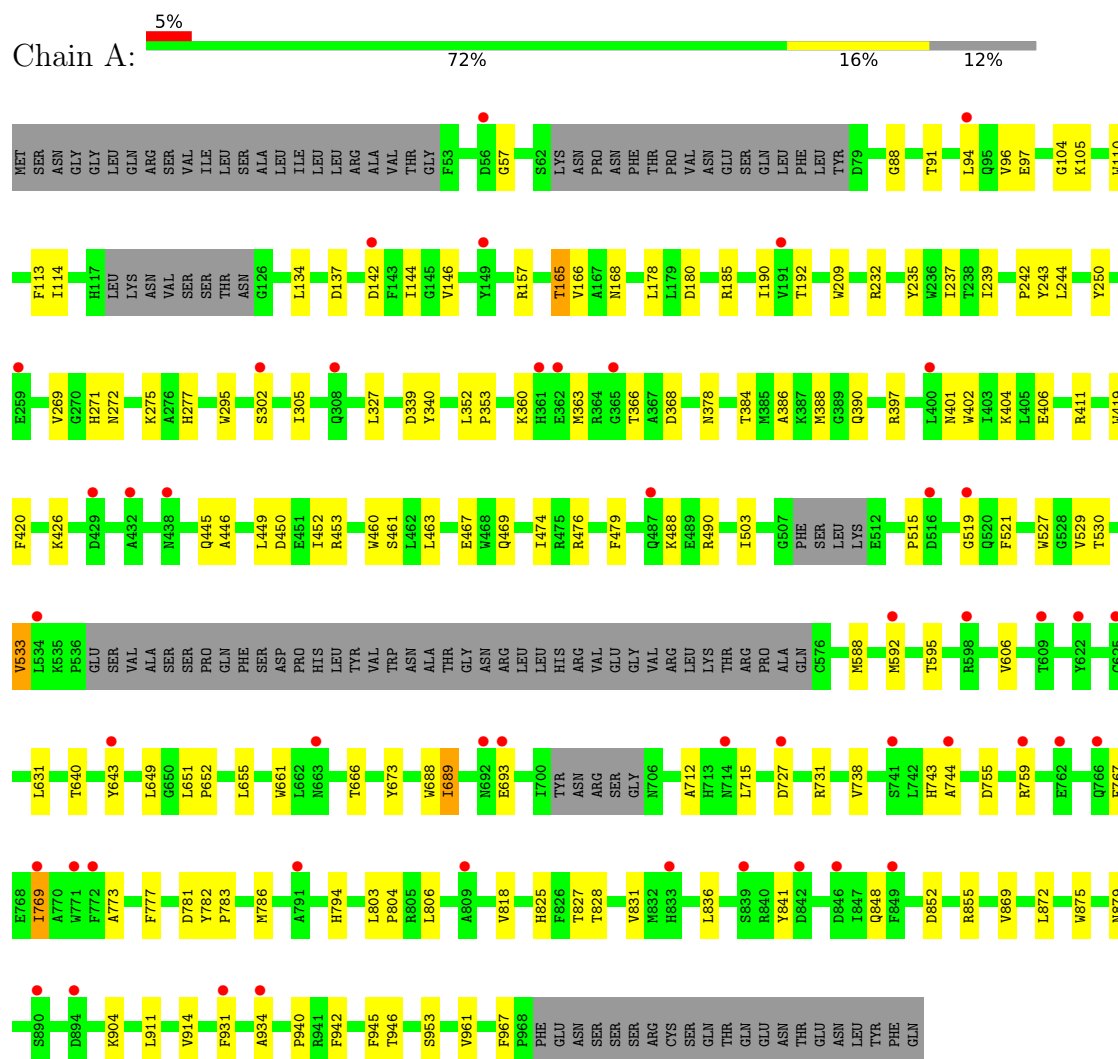
- Molecule 3 is a protein called Fibroblast growth factor 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	19	Total 122	C 77	N 19	O 25	S 1	0	0	0
3	F	19	Total 122	C 77	N 19	O 25	S 1	0	0	0

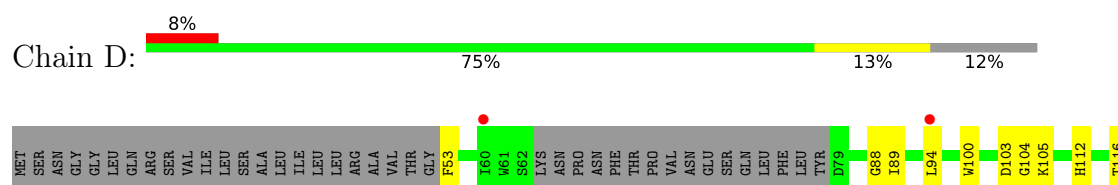
3 Residue-property plots

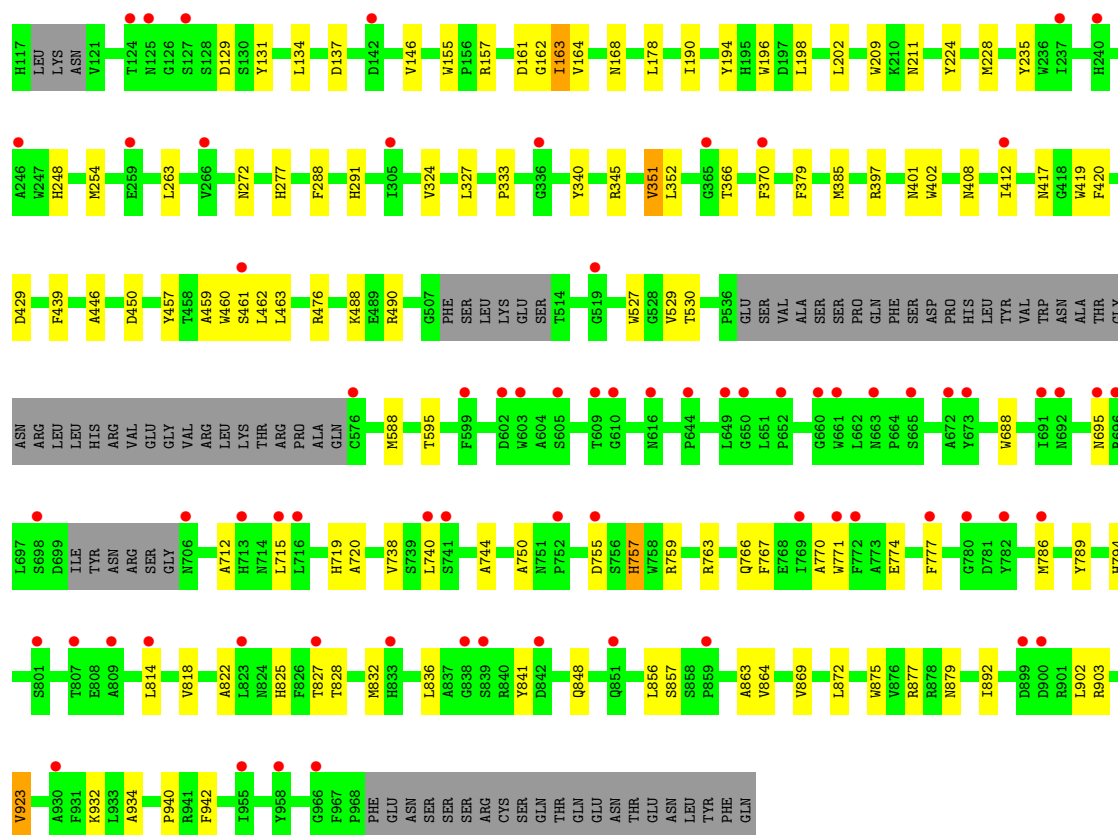
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

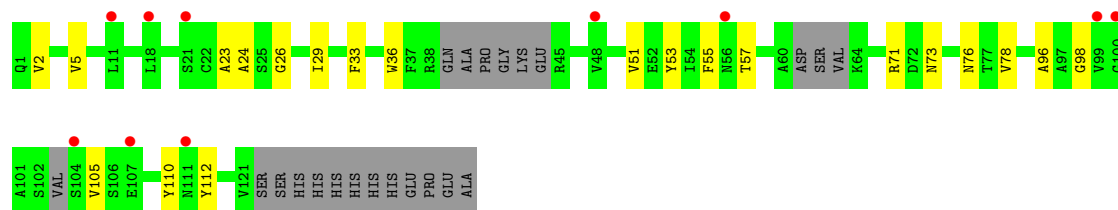


• Molecule 1: Beta-klotho

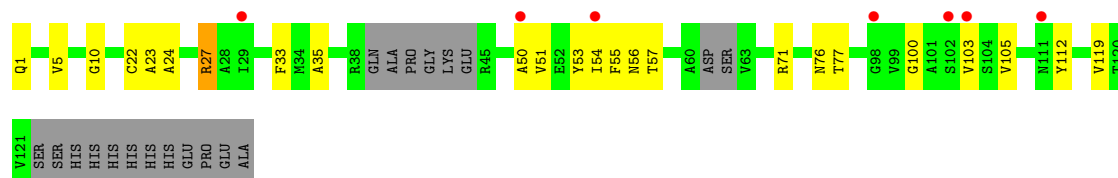




• Molecule 2: Nanobody 30

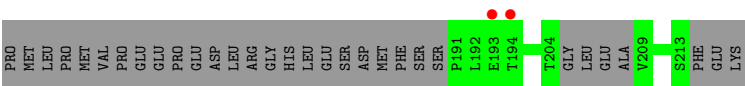


• Molecule 2: Nanobody 30

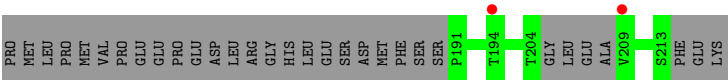


• Molecule 3: Fibroblast growth factor 19





● Molecule 3: Fibroblast growth factor 19



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.09Å 143.90Å 141.05Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	59.42 – 3.19 59.42 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.8 (59.42-3.19) 97.7 (59.42-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.280 , 0.320 0.281 , 0.320	Depositor DCC
R_{free} test set	1989 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	77.8	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 105.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14271	wwPDB-VP
Average B, all atoms (Å ²)	80.0	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 55.18 % 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 3.2847e-05. 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

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	0.09	0/6569	0.25	0/8979
1	D	0.10	0/6319	0.29	0/8666
2	B	0.09	0/778	0.28	0/1059
2	E	0.12	0/780	0.34	0/1064
3	C	0.12	0/124	0.24	0/168
3	F	0.24	0/124	0.38	0/168
All	All	0.10	0/14694	0.28	0/20104

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6373	0	5751	86	0
1	D	6129	0	5196	78	0
2	B	762	0	624	13	0
2	E	763	0	597	13	0
3	C	122	0	99	0	0
3	F	122	0	99	0	0
All	All	14271	0	12366	184	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 7.

All (184) 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)
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.56	0.86
1:D:755:ASP:OD2	2:E:56:ASN:N	2.15	0.80
1:D:759:ARG:NH2	2:E:100:GLY:O	2.19	0.76
1:A:96:VAL:HG13	1:A:463:LEU:HD11	1.70	0.74
2:E:10:GLY:HA3	2:E:119:VAL:HA	1.73	0.69
1:A:339:ASP:HB2	1:A:360:LYS:HD3	1.76	0.68
1:A:404:LYS:HD3	1:A:452:ILE:HD13	1.76	0.68
1:D:488:LYS:O	1:D:490:ARG:NH1	2.26	0.68
1:A:836:LEU:HD11	1:A:848:GLN:HG3	1.77	0.65
1:D:767:PHE:O	1:D:841:TYR:OH	2.14	0.65
1:A:305:ILE:HD11	1:A:390:GLN:HB2	1.79	0.65
1:D:527:TRP:O	1:D:595:THR:N	2.28	0.65
2:B:2:VAL:H	2:B:112:TYR:HE1	1.44	0.65
1:A:134:LEU:HD11	1:A:178:LEU:HD13	1.79	0.64
1:A:446:ALA:HB1	1:A:452:ILE:HG13	1.80	0.64
1:A:688:TRP:HB2	1:A:738:VAL:HG22	1.79	0.64
1:A:209:TRP:O	1:A:272:ASN:ND2	2.30	0.64
2:B:51:VAL:HG12	2:B:57:THR:HG22	1.78	0.64
1:D:688:TRP:HB2	1:D:738:VAL:HG22	1.79	0.64
1:A:767:PHE:O	1:A:841:TYR:OH	2.17	0.63
2:E:1:GLN:N	2:E:112:TYR:OH	2.32	0.63
1:D:767:PHE:HA	1:D:786:MET:HE2	1.81	0.63
2:B:5:VAL:HB	2:B:23:ALA:HB3	1.81	0.62
1:A:744:ALA:HB1	1:A:872:LEU:HD21	1.81	0.62
1:D:417:ASN:HD22	1:D:457:TYR:HE1	1.48	0.61
2:E:51:VAL:HG12	2:E:57:THR:HG22	1.82	0.61
1:A:652:PRO:HD2	1:A:655:LEU:HD12	1.83	0.60
1:D:209:TRP:O	1:D:272:ASN:ND2	2.31	0.60
1:A:104:GLY:O	1:A:168:ASN:ND2	2.31	0.60
1:D:340:TYR:HD2	1:D:352:LEU:HD21	1.67	0.59
1:D:588:MET:HE1	1:D:934:ALA:HB2	1.84	0.59
1:D:864:VAL:HG21	1:D:902:LEU:HD11	1.85	0.58
1:A:275:LYS:HG2	1:A:363:MET:HE1	1.85	0.58
1:D:327:LEU:HD23	1:D:402:TRP:HZ3	1.68	0.58
1:A:180:ASP:OD1	1:A:232:ARG:NH1	2.35	0.58
1:D:104:GLY:O	1:D:168:ASN:ND2	2.36	0.58
1:D:137:ASP:OD1	1:D:490:ARG:NE	2.37	0.57
1:D:397:ARG:O	1:D:401:ASN:ND2	2.31	0.57
1:D:162:GLY:HA3	1:D:202:LEU:HD11	1.87	0.57
1:D:794:HIS:O	1:D:794:HIS:ND1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:PHE:HA	1:D:385:MET:HE1	1.87	0.56
1:A:142:ASP:OD2	1:A:185:ARG:NH1	2.39	0.56
1:A:97:GLU:HB3	1:A:157:ARG:HH12	1.71	0.56
1:A:783:PRO:HG2	1:A:786:MET:HB3	1.88	0.55
1:D:446:ALA:HA	1:D:450:ASP:HB2	1.88	0.55
1:D:836:LEU:HD11	1:D:848:GLN:HG3	1.89	0.55
1:A:533:VAL:HG13	1:A:643:TYR:HD2	1.71	0.55
1:A:592:MET:HE3	1:A:945:PHE:HE1	1.72	0.55
1:A:655:LEU:HD13	1:A:666:THR:HG23	1.89	0.55
1:A:904:LYS:HZ1	1:A:953:SER:HB3	1.71	0.55
1:A:693:GLU:HG3	1:A:743:HIS:HB2	1.88	0.54
1:A:488:LYS:O	1:A:490:ARG:NH1	2.40	0.54
1:A:827:THR:OG1	1:A:828:THR:N	2.40	0.54
1:D:134:LEU:HD11	1:D:178:LEU:HD13	1.90	0.54
1:A:803:LEU:HD12	1:A:804:PRO:HD2	1.88	0.54
1:D:190:ILE:HG12	1:D:235:TYR:HB2	1.90	0.53
1:A:446:ALA:HA	1:A:450:ASP:HB2	1.89	0.53
1:D:462:LEU:HB3	1:D:463:LEU:HD12	1.90	0.53
1:A:88:GLY:HA2	1:A:146:VAL:HB	1.89	0.53
2:E:24:ALA:HB3	2:E:76:ASN:HB3	1.89	0.53
1:A:781:ASP:OD2	1:A:782:TYR:N	2.41	0.53
1:A:94:LEU:HD11	1:A:110:TRP:HB2	1.91	0.53
1:A:165:THR:HG23	1:A:166:VAL:H	1.74	0.53
1:D:129:ASP:OD2	1:D:488:LYS:NZ	2.41	0.52
1:D:224:TYR:CZ	1:D:228:MET:HG3	2.44	0.52
1:A:519:GLY:N	1:A:967:PHE:O	2.43	0.52
1:D:712:ALA:HB3	1:D:771:TRP:HZ2	1.75	0.52
1:A:420:PHE:HB3	1:A:476:ARG:HG2	1.91	0.52
1:D:88:GLY:HA2	1:D:146:VAL:HB	1.93	0.51
1:D:825:HIS:NE2	1:D:827:THR:O	2.42	0.50
1:A:302:SER:HB3	1:A:327:LEU:HD13	1.93	0.50
1:A:588:MET:HE1	1:A:934:ALA:HB2	1.93	0.50
2:E:22:CYS:O	2:E:77:THR:HA	2.11	0.50
2:B:24:ALA:HB1	2:B:29:ILE:HD13	1.93	0.50
1:D:105:LYS:HG3	1:D:157:ARG:HA	1.94	0.50
1:D:333:PRO:HG3	1:D:340:TYR:HD1	1.77	0.49
1:D:370:PHE:HD2	1:D:412:ILE:HG23	1.77	0.49
1:A:386:ALA:HB1	1:A:388:MET:HE3	1.94	0.49
2:B:24:ALA:HB3	2:B:76:ASN:HB3	1.94	0.49
1:D:248:HIS:HD1	1:D:254:MET:HB3	1.77	0.49
1:A:781:ASP:HA	1:A:806:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:HIS:NE2	1:D:366:THR:O	2.45	0.49
1:D:857:SER:HA	1:D:863:ALA:HA	1.95	0.49
1:A:712:ALA:HA	1:A:715:LEU:HD12	1.95	0.49
1:D:763:ARG:HD2	1:D:789:TYR:CD1	2.48	0.49
2:B:98:GLY:HA2	2:B:110:TYR:HA	1.94	0.49
1:D:112:HIS:O	1:D:116:THR:OG1	2.28	0.48
1:D:750:ALA:HB3	1:D:757:HIS:CE1	2.48	0.48
1:D:766:GLN:HA	1:D:770:ALA:HB3	1.95	0.48
1:A:527:TRP:O	1:A:595:THR:N	2.45	0.48
1:A:651:LEU:HD11	1:A:661:TRP:CD1	2.48	0.48
1:A:606:VAL:HB	1:A:673:TYR:HE1	1.78	0.48
1:A:277:HIS:NE2	1:A:366:THR:O	2.43	0.47
1:A:777:PHE:HE1	1:A:818:VAL:HG11	1.79	0.47
1:D:460:TRP:CD1	1:D:461:SER:HB3	2.49	0.47
2:E:35:ALA:HA	2:E:50:ALA:HA	1.96	0.47
1:A:144:ILE:HD11	1:A:479:PHE:HE1	1.79	0.47
1:D:875:TRP:O	1:D:879:ASN:ND2	2.41	0.47
1:A:209:TRP:HB2	1:A:269:VAL:HG22	1.97	0.47
1:A:340:TYR:CG	1:A:352:LEU:HD21	2.50	0.47
1:A:460:TRP:HA	1:A:461:SER:HA	1.56	0.47
2:B:96:ALA:HB1	2:B:110:TYR:HB3	1.96	0.47
1:A:397:ARG:O	1:A:401:ASN:ND2	2.41	0.46
1:D:103:ASP:OD2	1:D:131:TYR:OH	2.30	0.46
1:D:827:THR:OG1	1:D:828:THR:N	2.48	0.46
1:A:192:THR:HG22	1:A:237:ILE:HB	1.96	0.46
1:A:911:LEU:HD13	1:A:961:VAL:HG11	1.97	0.46
1:A:521:PHE:HZ	1:A:914:VAL:HG23	1.80	0.46
1:A:530:THR:HB	1:A:931:PHE:O	2.16	0.46
1:A:110:TRP:HA	1:A:113:PHE:HB3	1.97	0.46
1:A:295:TRP:HD1	1:A:368:ASP:HB3	1.81	0.46
1:D:327:LEU:HD23	1:D:402:TRP:CZ3	2.49	0.45
1:A:105:LYS:HD2	1:A:157:ARG:HE	1.81	0.45
1:A:419:TRP:CD1	1:A:420:PHE:H	2.34	0.45
1:A:875:TRP:O	1:A:879:ASN:ND2	2.41	0.45
1:D:89:ILE:HD13	1:D:462:LEU:HD12	1.98	0.45
1:D:53:PHE:N	1:D:408:ASN:OD1	2.49	0.45
2:E:53:TYR:HD2	2:E:54:ILE:HG22	1.82	0.45
1:D:89:ILE:HG13	1:D:459:ALA:O	2.17	0.45
1:D:161:ASP:O	1:D:163:ILE:N	2.47	0.45
1:A:378:ASN:HA	1:A:384:THR:HG21	1.99	0.45
1:D:755:ASP:CG	2:E:55:PHE:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASP:OD1	1:A:490:ARG:NE	2.42	0.44
2:B:2:VAL:HB	2:B:112:TYR:CD1	2.52	0.44
1:A:755:ASP:CG	2:B:55:PHE:H	2.25	0.44
1:D:877:ARG:HE	1:D:923:VAL:HG23	1.83	0.44
1:A:144:ILE:HG22	1:A:503:ILE:HD12	2.00	0.44
1:A:445:GLN:O	1:A:449:LEU:HB2	2.18	0.44
2:B:36:TRP:HE1	2:B:78:VAL:HG12	1.83	0.44
1:A:243:TYR:HD2	1:A:244:LEU:HD12	1.83	0.44
1:D:740:LEU:O	1:D:822:ALA:HB3	2.18	0.44
1:A:110:TRP:O	1:A:114:ILE:N	2.46	0.43
1:A:759:ARG:HH11	2:B:33:PHE:HB3	1.83	0.43
1:D:419:TRP:CD1	1:D:420:PHE:H	2.37	0.43
1:D:695:ASN:OD1	1:D:695:ASN:N	2.51	0.43
2:E:5:VAL:HB	2:E:23:ALA:HB3	2.00	0.43
1:D:100:TRP:O	1:D:105:LYS:HD3	2.18	0.43
1:A:271:HIS:CE1	1:A:353:PRO:HB2	2.53	0.43
1:D:401:ASN:ND2	1:D:450:ASP:OD2	2.39	0.43
1:A:640:THR:HA	1:A:689:ILE:O	2.19	0.43
1:D:825:HIS:ND1	1:D:869:VAL:HG12	2.33	0.43
1:A:91:THR:HB	1:A:96:VAL:HG21	2.01	0.43
1:A:411:ARG:HH11	1:A:453:ARG:NH2	2.17	0.43
1:A:529:VAL:HG22	1:A:530:THR:H	1.84	0.43
1:D:420:PHE:HB3	1:D:476:ARG:HG2	1.99	0.43
1:D:757:HIS:NE2	1:D:832:MET:HG3	2.34	0.43
1:A:773:ALA:O	1:A:777:PHE:N	2.47	0.42
1:D:263:LEU:HG	1:D:351:VAL:HG11	2.01	0.42
1:A:794:HIS:O	1:A:794:HIS:ND1	2.52	0.42
1:D:529:VAL:HG22	1:D:530:THR:H	1.84	0.42
1:D:777:PHE:CE1	1:D:818:VAL:HG21	2.53	0.42
1:A:744:ALA:HA	1:A:769:ILE:HD11	2.01	0.42
1:A:411:ARG:HH11	1:A:453:ARG:HH21	1.67	0.42
1:D:417:ASN:HD21	1:D:439:PHE:HB3	1.85	0.42
1:A:57:GLY:HA3	1:A:406:GLU:HG2	2.00	0.42
1:A:190:ILE:HG12	1:A:235:TYR:HB2	2.01	0.42
1:A:727:ASP:HA	1:A:731:ARG:HE	1.83	0.42
1:A:852:ASP:OD2	1:A:855:ARG:HG3	2.20	0.42
1:D:460:TRP:HA	1:D:461:SER:HA	1.63	0.42
1:D:774:GLU:OE1	2:E:27:ARG:NH2	2.52	0.42
2:B:53:TYR:O	2:B:71:ARG:HD3	2.19	0.42
1:D:155:TRP:NE1	1:D:162:GLY:HA2	2.35	0.42
1:D:194:TYR:HE1	1:D:198:LEU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:PHE:HD2	1:D:841:TYR:HE1	1.68	0.41
1:D:712:ALA:HA	1:D:715:LEU:HD12	2.01	0.41
1:A:327:LEU:HD23	1:A:402:TRP:CZ3	2.56	0.41
1:A:469:GLN:OE1	1:A:469:GLN:N	2.48	0.41
1:D:771:TRP:HA	1:D:786:MET:HE1	2.01	0.41
1:D:940:PRO:O	1:D:942:PHE:N	2.53	0.41
1:A:239:ILE:HG21	1:A:242:PRO:HB3	2.02	0.41
1:D:892:ILE:HG22	1:D:903:ARG:HD3	2.02	0.41
1:D:744:ALA:HB1	1:D:872:LEU:HD21	2.03	0.41
1:A:467:GLU:HG3	1:A:474:ILE:HG13	2.02	0.41
1:A:940:PRO:O	1:A:942:PHE:N	2.54	0.41
1:D:196:TRP:CD1	1:D:196:TRP:N	2.87	0.41
1:A:825:HIS:CD2	1:A:869:VAL:HB	2.55	0.41
1:D:429:ASP:N	1:D:429:ASP:OD1	2.53	0.41
1:D:340:TYR:O	1:D:345:ARG:NH1	2.54	0.41
1:A:250:TYR:CE1	1:A:269:VAL:HG21	2.57	0.40
1:D:720:ALA:HB2	1:D:814:LEU:HD23	2.02	0.40
1:D:288:PHE:HA	1:D:291:HIS:CE1	2.57	0.40
2:E:33:PHE:HA	2:E:71:ARG:HH12	1.87	0.40
1:A:327:LEU:HD23	1:A:402:TRP:HZ3	1.86	0.40
1:D:719:HIS:CG	1:D:740:LEU:HD23	2.57	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	832/960 (87%)	771 (93%)	59 (7%)	2 (0%)	43	73
1	D	834/960 (87%)	729 (87%)	103 (12%)	2 (0%)	43	73
2	B	103/133 (77%)	85 (82%)	17 (16%)	1 (1%)	12	45
2	E	107/133 (80%)	87 (81%)	18 (17%)	2 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	15/50 (30%)	15 (100%)	0	0	100	100
3	F	15/50 (30%)	14 (93%)	1 (7%)	0	100	100
All	All	1906/2286 (83%)	1701 (89%)	198 (10%)	7 (0%)	30	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	LYS
2	E	103	VAL
2	B	105	VAL
1	D	932	LYS
2	E	27	ARG
1	A	515	PRO
1	D	856	LEU

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	583/827 (70%)	575 (99%)	8 (1%)	59	77
1	D	505/827 (61%)	497 (98%)	8 (2%)	55	75
2	B	52/106 (49%)	51 (98%)	1 (2%)	50	73
2	E	49/106 (46%)	48 (98%)	1 (2%)	48	72
3	C	12/46 (26%)	12 (100%)	0	100	100
3	F	12/46 (26%)	12 (100%)	0	100	100
All	All	1213/1958 (62%)	1195 (98%)	18 (2%)	57	76

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	A	533	VAL
1	A	631	LEU

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Mol	Chain	Res	Type
1	A	649	LEU
1	A	689	ILE
1	A	769	ILE
1	A	831	VAL
1	A	946	THR
2	B	73	ASN
1	D	94	LEU
1	D	163	ILE
1	D	164	VAL
1	D	211	ASN
1	D	324	VAL
1	D	351	VAL
1	D	757	HIS
1	D	923	VAL
2	E	105	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	240	HIS
1	A	241	ASN
1	A	282	HIS
1	A	335	HIS
1	A	501	GLN
1	A	824	ASN
1	A	833	HIS
1	D	203	GLN
1	D	395	ASN
1	D	497	HIS
1	D	743	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	844/960 (87%)	0.54	49 (5%)	29	18	37, 75, 105, 139	0
1	D	846/960 (88%)	0.73	74 (8%)	16	11	28, 83, 147, 182	0
2	B	111/133 (83%)	0.78	10 (9%)	15	10	56, 89, 119, 147	0
2	E	113/133 (84%)	0.72	7 (6%)	26	17	62, 92, 113, 134	0
3	C	19/50 (38%)	0.74	2 (10%)	11	8	66, 77, 110, 114	0
3	F	19/50 (38%)	1.16	2 (10%)	11	8	78, 100, 124, 129	0
All	All	1952/2286 (85%)	0.65	144 (7%)	20	13	28, 80, 133, 182	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	194	THR	6.5
1	D	695	ASN	5.4
1	D	603	TRP	4.5
1	D	124	THR	4.1
1	A	400	LEU	3.9
1	D	660	GLY	3.9
1	A	846	ASP	3.8
1	D	771	TRP	3.7
1	A	429	ASP	3.6
1	A	766	GLN	3.6
1	D	777	PHE	3.5
1	A	714	ASN	3.5
1	D	125	ASN	3.5
1	D	706	ASN	3.5
1	D	769	ILE	3.4
1	A	365	GLY	3.4
1	A	692	ASN	3.3
1	D	809	ALA	3.3
1	D	692	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	966	GLY	3.3
1	A	643	TYR	3.3
1	D	772	PHE	3.3
1	D	842	ASP	3.2
1	A	762	GLU	3.1
1	D	370	PHE	3.1
1	D	644	PRO	3.1
1	D	609	THR	3.1
1	A	259	GLU	3.1
1	D	652	PRO	3.1
1	D	266	VAL	3.0
1	A	438	ASN	3.0
1	D	661	TRP	2.9
1	A	94	LEU	2.9
1	D	259	GLU	2.9
1	D	650	GLY	2.9
1	D	665	SER	2.9
1	D	780	GLY	2.9
1	D	60	ILE	2.9
1	D	740	LEU	2.8
1	A	759	ARG	2.8
1	D	616	ASN	2.8
1	A	849	PHE	2.7
1	D	599	PHE	2.7
1	A	308	GLN	2.7
1	A	516	ASP	2.7
1	A	361	HIS	2.7
1	A	772	PHE	2.7
1	D	246	ALA	2.7
1	A	663	ASN	2.6
1	D	900	ASP	2.6
1	A	622	TYR	2.6
1	D	833	HIS	2.5
1	D	823	LEU	2.5
2	B	48	VAL	2.5
1	A	890	SER	2.5
2	E	111	ASN	2.5
1	D	336	GLY	2.5
1	D	741	SER	2.5
1	A	432	ALA	2.5
1	A	744	ALA	2.5
1	A	791	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	801	SER	2.5
2	E	29	ILE	2.5
1	D	752	PRO	2.5
1	D	461	SER	2.4
2	E	102	SER	2.4
1	A	931	PHE	2.4
1	D	716	LEU	2.4
2	B	99	VAL	2.4
1	A	769	ILE	2.4
1	D	365	GLY	2.4
1	D	237	ILE	2.4
1	D	930	ALA	2.4
2	E	54	ILE	2.4
1	A	609	THR	2.4
1	D	663	ASN	2.4
2	B	104	SER	2.4
1	A	149	TYR	2.3
1	D	94	LEU	2.3
1	A	771	TRP	2.3
1	A	598	ARG	2.3
1	D	576	CYS	2.3
1	A	727	ASP	2.3
1	A	934	ALA	2.3
2	B	18	LEU	2.3
1	D	142	ASP	2.3
1	D	851	GLN	2.3
1	A	693	GLU	2.3
1	D	713	HIS	2.3
1	D	839	SER	2.3
1	D	715	LEU	2.3
1	A	625	CYS	2.3
1	D	602	ASP	2.3
1	D	605	SER	2.3
1	A	487	GLN	2.3
1	D	899	ASP	2.3
2	B	11	LEU	2.2
2	B	111	ASN	2.2
1	D	786	MET	2.2
2	E	98	GLY	2.2
1	D	955	ILE	2.2
1	A	592	MET	2.2
1	D	610	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	142	ASP	2.2
3	C	194	THR	2.2
1	A	839	SER	2.2
1	D	649	LEU	2.2
1	D	305	ILE	2.1
1	A	534	LEU	2.1
1	D	672	ALA	2.1
2	B	107	GLU	2.1
1	A	519	GLY	2.1
2	B	100	GLY	2.1
1	A	56	ASP	2.1
1	D	755	ASP	2.1
3	F	209	VAL	2.1
1	D	807	THR	2.1
1	D	827	THR	2.1
1	D	698	SER	2.1
1	A	191	VAL	2.1
1	A	894	ASP	2.1
1	D	240	HIS	2.1
1	D	412	ILE	2.1
1	D	814	LEU	2.1
2	E	50	ALA	2.1
1	D	838	GLY	2.1
1	A	302	SER	2.1
1	A	741	SER	2.1
2	E	103	VAL	2.1
2	B	56	ASN	2.1
1	D	691	ILE	2.1
3	C	193	GLU	2.1
1	D	127	SER	2.0
1	A	833	HIS	2.0
1	A	842	ASP	2.0
1	D	673	TYR	2.0
1	D	782	TYR	2.0
1	D	859	PRO	2.0
1	D	696	ARG	2.0
2	B	21	SER	2.0
1	A	809	ALA	2.0
1	D	958	TYR	2.0
1	D	519	GLY	2.0
1	A	362	GLU	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.