



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:23 AM UTC

PDB ID : 6JLD / pdb_00006jld
Title : Crystal structure of a human ependymin related protein
Authors : Park, S.Y.
Deposited on : 2019-03-05
Resolution : 2.00 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

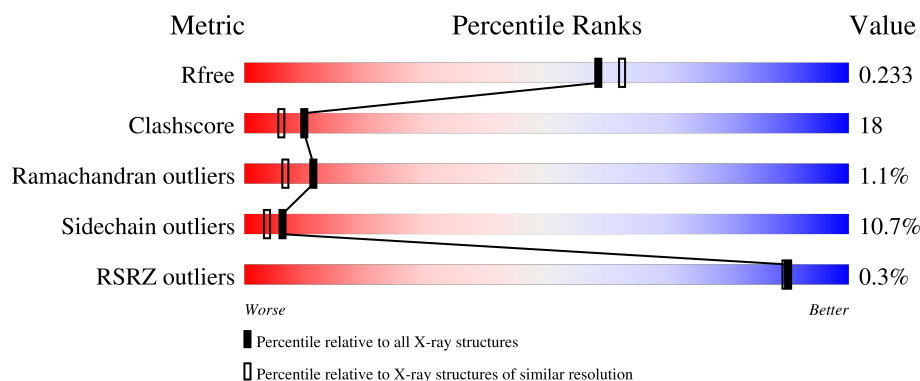
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	198	
1	B	198	
1	C	198	
1	D	198	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6147 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 Mammalian ependymin-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1506	950	255	290	11			
1	B	183	Total	C	N	O	S	0	0	0
			1494	944	253	287	10			
1	C	184	Total	C	N	O	S	0	1	0
			1505	950	254	290	11			
1	D	180	Total	C	N	O	S	0	1	0
			1476	932	250	284	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP Q9UM22
A	28	ASP	-	expression tag	UNP Q9UM22
A	29	PRO	-	expression tag	UNP Q9UM22
A	30	HIS	-	expression tag	UNP Q9UM22
A	31	HIS	-	expression tag	UNP Q9UM22
A	32	HIS	-	expression tag	UNP Q9UM22
A	33	HIS	-	expression tag	UNP Q9UM22
A	34	HIS	-	expression tag	UNP Q9UM22
A	35	HIS	-	expression tag	UNP Q9UM22
A	36	HIS	-	expression tag	UNP Q9UM22
A	37	HIS	-	expression tag	UNP Q9UM22
B	27	ALA	-	expression tag	UNP Q9UM22
B	28	ASP	-	expression tag	UNP Q9UM22
B	29	PRO	-	expression tag	UNP Q9UM22
B	30	HIS	-	expression tag	UNP Q9UM22
B	31	HIS	-	expression tag	UNP Q9UM22
B	32	HIS	-	expression tag	UNP Q9UM22
B	33	HIS	-	expression tag	UNP Q9UM22
B	34	HIS	-	expression tag	UNP Q9UM22
B	35	HIS	-	expression tag	UNP Q9UM22
B	36	HIS	-	expression tag	UNP Q9UM22

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	HIS	-	expression tag	UNP Q9UM22
C	27	ALA	-	expression tag	UNP Q9UM22
C	28	ASP	-	expression tag	UNP Q9UM22
C	29	PRO	-	expression tag	UNP Q9UM22
C	30	HIS	-	expression tag	UNP Q9UM22
C	31	HIS	-	expression tag	UNP Q9UM22
C	32	HIS	-	expression tag	UNP Q9UM22
C	33	HIS	-	expression tag	UNP Q9UM22
C	34	HIS	-	expression tag	UNP Q9UM22
C	35	HIS	-	expression tag	UNP Q9UM22
C	36	HIS	-	expression tag	UNP Q9UM22
C	37	HIS	-	expression tag	UNP Q9UM22
D	27	ALA	-	expression tag	UNP Q9UM22
D	28	ASP	-	expression tag	UNP Q9UM22
D	29	PRO	-	expression tag	UNP Q9UM22
D	30	HIS	-	expression tag	UNP Q9UM22
D	31	HIS	-	expression tag	UNP Q9UM22
D	32	HIS	-	expression tag	UNP Q9UM22
D	33	HIS	-	expression tag	UNP Q9UM22
D	34	HIS	-	expression tag	UNP Q9UM22
D	35	HIS	-	expression tag	UNP Q9UM22
D	36	HIS	-	expression tag	UNP Q9UM22
D	37	HIS	-	expression tag	UNP Q9UM22

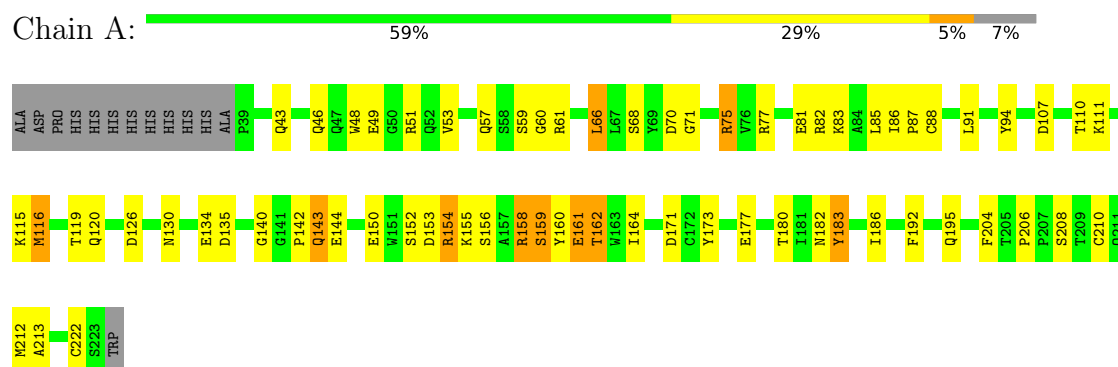
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	33	Total O 33 33	0	0
2	B	40	Total O 40 40	0	0
2	C	53	Total O 53 53	0	0
2	D	40	Total O 40 40	0	0

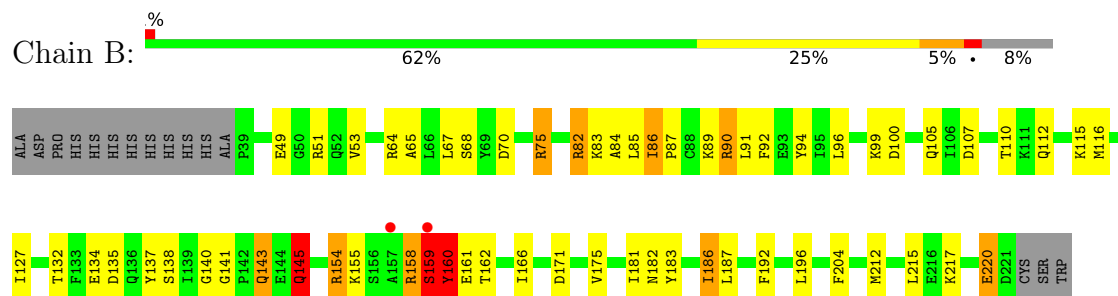
3 Residue-property plots

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.

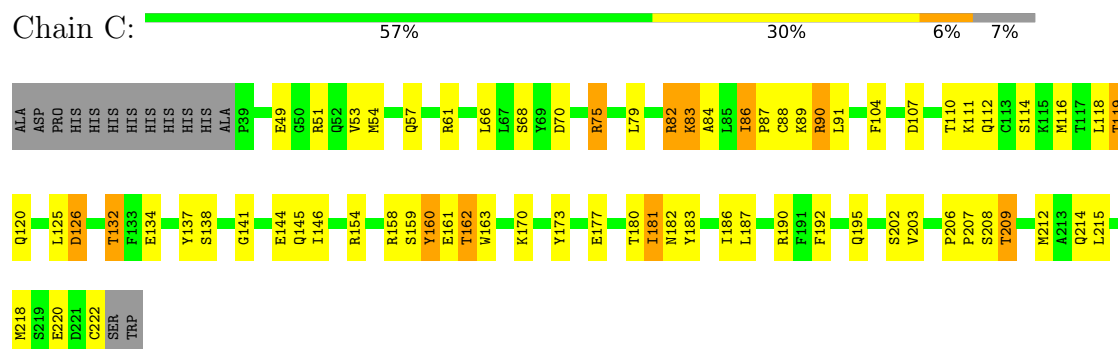
• Molecule 1: Mammalian endymin-related protein 1



• Molecule 1: Mammalian endymin-related protein 1

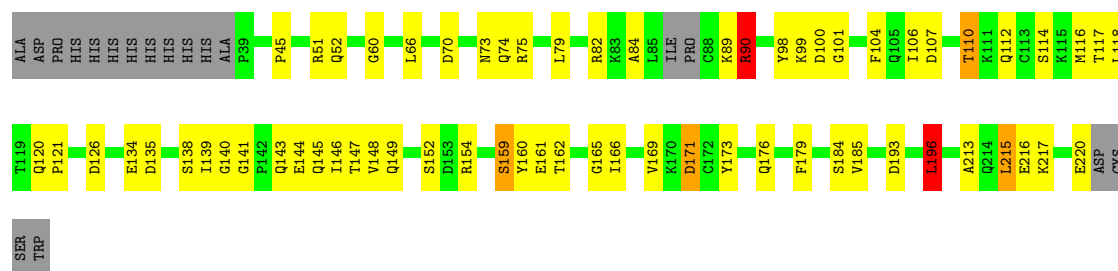


• Molecule 1: Mammalian endymin-related protein 1



• Molecule 1: Mammalian endymin-related protein 1

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	55.86Å 55.86Å 273.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.71 – 2.00 26.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (26.71-2.00) 99.8 (26.71-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.199 , 0.235 0.201 , 0.233	Depositor DCC
R_{free} test set	2848 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.305 for h,-k,-l	Xtriage
Reported twinning fraction	0.688 for H, K, L 0.312 for K, H, -L	Depositor
Outliers	0 of 56208 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6147	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.24	4/1541 (0.3%)	1.18	8/2088 (0.4%)
1	B	1.20	4/1529 (0.3%)	1.21	4/2072 (0.2%)
1	C	1.24	4/1543 (0.3%)	1.17	0/2091
1	D	1.20	6/1512 (0.4%)	1.19	4/2046 (0.2%)
All	All	1.22	18/6125 (0.3%)	1.19	16/8297 (0.2%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	54	MET	N-CA	-7.44	1.37	1.46
1	B	65	ALA	CA-C	-7.28	1.43	1.52
1	D	60	GLY	C-O	-6.86	1.15	1.24
1	C	195	GLN	CA-C	-6.20	1.45	1.52
1	B	145	GLN	CA-C	-5.88	1.45	1.52
1	D	185	VAL	C-O	-5.87	1.17	1.24
1	A	195	GLN	C-O	-5.78	1.17	1.23
1	A	177	GLU	N-CA	5.78	1.53	1.46
1	C	132	THR	CA-C	-5.76	1.45	1.52
1	A	43	GLN	C-O	-5.75	1.17	1.24
1	C	134	GLU	CA-C	-5.69	1.46	1.52
1	D	79	LEU	CA-C	-5.64	1.46	1.52
1	A	48	TRP	CA-C	5.52	1.59	1.52
1	D	165	GLY	CA-C	-5.30	1.47	1.52
1	D	52	GLN	CA-C	-5.25	1.46	1.52
1	D	106	ILE	CA-C	-5.25	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	160	TYR	CA-C	5.19	1.58	1.52
1	B	127	ILE	CA-C	5.15	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	VAL	N-CA-C	-8.38	105.00	111.62
1	A	81	GLU	N-CA-C	-7.23	98.07	109.50
1	B	186	ILE	CB-CA-C	-7.10	102.62	111.92
1	A	159	SER	N-CA-C	6.62	119.06	108.41
1	A	60	GLY	N-CA-C	-6.45	106.42	115.32
1	A	88	CYS	CB-CA-C	6.39	120.26	109.84
1	A	222	CYS	CA-CB-SG	6.15	128.54	114.40
1	A	222	CYS	N-CA-C	-5.99	102.05	110.50
1	D	126	ASP	CA-C-N	-5.72	118.47	122.59
1	D	126	ASP	C-N-CA	-5.72	118.47	122.59
1	B	160	TYR	N-CA-C	5.66	118.33	108.76
1	D	140	GLY	N-CA-C	5.51	122.75	112.77
1	B	154	ARG	N-CA-C	5.38	117.23	110.24
1	A	140	GLY	N-CA-C	5.32	121.47	112.22
1	D	196	LEU	CA-CB-CG	-5.20	98.08	116.30
1	A	130	ASN	N-CA-C	5.15	118.70	112.93

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	THR	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	1506	0	1465	57	0
1	B	1494	0	1455	64	0
1	C	1505	0	1462	63	0
1	D	1476	0	1436	58	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	33	0	0	5	0
2	B	40	0	0	2	0
2	C	53	0	0	5	0
2	D	40	0	0	3	0
All	All	6147	0	5818	207	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 18.

All (207) 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:D:145:GLN:HG2	2:D:313:HOH:O	1.46	1.13
1:D:148:VAL:HG11	1:D:166:ILE:CG2	1.82	1.08
1:B:82:ARG:HG3	1:B:91:LEU:HD11	1.46	0.96
1:A:192:PHE:CD2	2:A:327:HOH:O	2.17	0.95
1:D:148:VAL:HG11	1:D:166:ILE:HG23	1.49	0.94
1:D:148:VAL:CG1	1:D:166:ILE:HG23	2.03	0.88
1:B:138:SER:OG	1:B:145:GLN:HG2	1.74	0.88
1:B:85:LEU:HD23	1:B:86:ILE:HG13	1.56	0.85
1:A:154:ARG:HG3	1:A:159:SER:HB2	1.58	0.84
1:A:192:PHE:HB3	2:A:327:HOH:O	1.77	0.83
1:B:82:ARG:CG	1:B:91:LEU:HD11	2.09	0.82
1:A:158:ARG:HA	1:B:86:ILE:HD11	1.60	0.82
1:C:82:ARG:O	1:C:83:LYS:HG2	1.79	0.81
1:B:132:THR:OG1	1:B:154:ARG:O	1.97	0.81
1:A:182:ASN:C	1:A:183:TYR:HD1	1.90	0.80
1:D:148:VAL:CG1	1:D:166:ILE:CG2	2.59	0.79
1:C:222:CYS:O	2:C:301:HOH:O	2.00	0.78
1:C:163:TRP:NE1	1:C:177:GLU:OE2	2.15	0.78
1:C:146:ILE:HG13	1:D:144:GLU:HG2	1.66	0.77
1:C:112:GLN:HG2	1:C:214:GLN:HE22	1.47	0.77
1:A:150:GLU:OE1	1:B:64:ARG:NH2	2.18	0.77
1:C:90:ARG:NH1	1:C:107:ASP:OD2	2.18	0.76
1:B:116:MET:HE2	1:B:217:LYS:HD3	1.68	0.75
1:D:90:ARG:HB2	1:D:220:GLU:HA	1.70	0.74
1:B:159:SER:O	1:B:183:TYR:OH	2.03	0.74
1:A:182:ASN:C	1:A:183:TYR:CD1	2.65	0.74
1:A:159:SER:N	1:B:86:ILE:CD1	2.51	0.74
1:B:181:ILE:CD1	1:B:186:ILE:HD11	2.17	0.72
1:C:181:ILE:HG12	1:C:186:ILE:HD11	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:NH1	1:D:107:ASP:OD2	2.23	0.71
1:D:116:MET:SD	1:D:215:LEU:O	2.49	0.71
1:C:86:ILE:HD11	1:D:159:SER:OG	1.91	0.71
1:B:181:ILE:HD12	1:B:186:ILE:HD11	1.73	0.70
1:A:158:ARG:C	1:B:86:ILE:HD13	2.17	0.70
1:C:51:ARG:NH2	1:D:135:ASP:OD2	2.24	0.68
1:C:111:LYS:HG2	1:C:209:THR:HG21	1.76	0.68
1:A:183:TYR:OH	1:B:86:ILE:HG22	1.95	0.66
1:D:148:VAL:HG11	1:D:166:ILE:HG22	1.76	0.66
1:C:181:ILE:CG1	1:C:186:ILE:HD11	2.26	0.66
1:D:51:ARG:HG2	1:D:66:LEU:HD12	1.78	0.66
1:C:209:THR:O	1:C:212:MET:O	2.13	0.65
1:C:90:ARG:HH21	1:C:218:MET:HE2	1.61	0.65
1:A:173:TYR:CE2	1:B:141:GLY:HA3	2.31	0.65
1:D:45:PRO:CB	1:D:196:LEU:HD21	2.26	0.65
1:D:45:PRO:HB3	1:D:196:LEU:HD21	1.79	0.65
1:D:171:ASP:HB3	1:D:173:TYR:CD1	2.33	0.63
1:A:51:ARG:HG2	1:A:66:LEU:HD12	1.82	0.62
1:A:158:ARG:C	1:B:86:ILE:CD1	2.72	0.61
1:C:110:THR:HG23	1:C:112:GLN:HB2	1.81	0.61
1:A:192:PHE:CG	2:A:327:HOH:O	2.44	0.61
1:A:126:ASP:HB2	2:A:309:HOH:O	2.00	0.61
1:C:160:TYR:HB2	1:C:183:TYR:OH	2.01	0.60
1:A:57:GLN:HA	1:A:57:GLN:OE1	2.00	0.60
1:A:159:SER:N	1:B:86:ILE:HD13	2.16	0.60
1:C:119:THR:OG1	1:C:120:GLN:N	2.36	0.59
1:A:82:ARG:HD3	1:A:85:LEU:HD23	1.84	0.59
1:C:182:ASN:C	1:C:183:TYR:CD1	2.80	0.59
1:A:83:LYS:HE2	1:B:134:GLU:O	2.03	0.59
1:B:82:ARG:HG3	1:B:91:LEU:CD1	2.28	0.59
1:C:66:LEU:HD22	1:C:79:LEU:HD23	1.85	0.59
1:C:146:ILE:CG1	1:D:144:GLU:HG2	2.33	0.59
1:C:49:GLU:HG2	1:C:68:SER:HA	1.85	0.58
1:A:183:TYR:CE2	1:B:86:ILE:HG22	2.39	0.58
1:B:70:ASP:OD2	1:B:75:ARG:HD2	2.03	0.58
1:C:82:ARG:O	1:C:83:LYS:CG	2.49	0.58
1:C:66:LEU:HB2	1:C:79:LEU:HB3	1.85	0.58
1:C:82:ARG:HD3	1:C:91:LEU:HD11	1.87	0.57
1:C:86:ILE:HA	1:C:87:PRO:C	2.28	0.57
1:C:182:ASN:C	1:C:183:TYR:HD1	2.14	0.56
1:A:173:TYR:CD2	1:B:141:GLY:HA3	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ARG:HD3	1:B:204:PHE:CG	2.40	0.56
1:B:85:LEU:HD23	1:B:86:ILE:CG1	2.32	0.56
1:C:84:ALA:HB1	1:D:159:SER:HB2	1.88	0.55
1:A:192:PHE:CB	2:A:327:HOH:O	2.42	0.55
1:B:107:ASP:CG	1:B:110:THR:HG22	2.31	0.55
1:D:110:THR:HG23	1:D:112:GLN:HG3	1.88	0.55
1:C:170:LYS:HB2	1:D:144:GLU:CD	2.31	0.55
1:D:110:THR:HG21	1:D:112:GLN:OE1	2.07	0.55
1:D:173:TYR:OH	1:D:196:LEU:HD13	2.07	0.55
1:B:94:TYR:CE2	1:B:105:GLN:HG3	2.42	0.55
1:A:183:TYR:CZ	1:B:86:ILE:HG22	2.42	0.54
1:A:46:GLN:O	1:A:71:GLY:N	2.39	0.54
1:B:75:ARG:HD3	1:B:204:PHE:CD2	2.43	0.54
1:C:90:ARG:NH2	1:C:218:MET:HE2	2.23	0.53
1:D:107:ASP:C	1:D:107:ASP:OD1	2.51	0.53
1:A:183:TYR:OH	1:B:86:ILE:CG2	2.56	0.53
1:A:77:ARG:HA	1:A:94:TYR:O	2.09	0.53
1:B:85:LEU:CD2	1:B:86:ILE:HG13	2.33	0.53
1:C:86:ILE:CD1	1:D:159:SER:OG	2.57	0.53
1:C:110:THR:HG23	1:C:112:GLN:H	1.74	0.53
1:C:190:ARG:NH1	2:C:303:HOH:O	2.41	0.53
1:C:90:ARG:NH2	1:C:218:MET:CE	2.73	0.52
1:C:146:ILE:CD1	1:D:144:GLU:HG2	2.38	0.52
1:A:134:GLU:OE2	1:A:152:SER:OG	2.26	0.52
1:C:161:GLU:O	1:C:162:THR:HG23	2.10	0.52
1:B:92:PHE:HE2	1:B:220:GLU:HG3	1.74	0.51
1:D:149:GLN:HG3	1:D:169:VAL:HG22	1.91	0.51
1:A:158:ARG:CA	1:B:86:ILE:HD11	2.36	0.51
1:A:115:LYS:C	1:A:116:MET:HG2	2.36	0.50
1:A:59:SER:OG	1:A:61:ARG:HG2	2.12	0.50
1:D:161:GLU:O	1:D:162:THR:HG23	2.11	0.50
1:D:107:ASP:HB3	1:D:110:THR:HG22	1.94	0.50
1:D:138:SER:OG	1:D:145:GLN:HG3	2.11	0.50
1:A:86:ILE:HD11	1:B:158:ARG:C	2.36	0.50
1:A:182:ASN:O	1:A:183:TYR:HD1	1.95	0.50
1:C:88:CYS:C	1:C:222:CYS:SG	2.95	0.50
1:A:107:ASP:CG	1:A:110:THR:HG22	2.37	0.50
1:A:161:GLU:HG3	1:A:164:ILE:HD11	1.94	0.50
1:C:141:GLY:O	1:C:145:GLN:HB2	2.10	0.50
1:C:181:ILE:HG12	1:C:186:ILE:CD1	2.42	0.49
1:D:139:ILE:O	1:D:145:GLN:HA	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:HG2	1:B:89:LYS:NZ	2.27	0.49
1:B:181:ILE:CG1	1:B:186:ILE:HD11	2.42	0.49
1:C:144:GLU:HG2	1:D:146:ILE:HG13	1.95	0.49
1:A:86:ILE:HD11	1:B:159:SER:N	2.27	0.49
1:C:173:TYR:CE2	1:D:141:GLY:CA	2.95	0.49
1:A:160:TYR:CD1	1:B:86:ILE:HG21	2.48	0.49
1:B:154:ARG:HB2	1:B:161:GLU:HG3	1.95	0.49
1:D:148:VAL:HG12	1:D:149:GLN:N	2.28	0.49
1:B:75:ARG:HA	1:B:96:LEU:O	2.13	0.49
1:A:75:ARG:HD3	1:A:204:PHE:CD1	2.48	0.48
1:A:171:ASP:HB3	1:A:173:TYR:CE1	2.48	0.48
1:C:86:ILE:N	1:C:86:ILE:HD13	2.28	0.48
1:D:101:GLY:C	1:D:118:LEU:HB2	2.39	0.48
1:C:190:ARG:CZ	2:C:303:HOH:O	2.61	0.48
1:D:162:THR:O	1:D:179:PHE:HA	2.14	0.48
1:D:173:TYR:CZ	1:D:196:LEU:HD13	2.49	0.47
1:B:161:GLU:OE2	1:B:183:TYR:CE2	2.67	0.47
1:B:110:THR:O	1:B:110:THR:OG1	2.30	0.47
1:C:88:CYS:O	1:C:89:LYS:HE2	2.14	0.47
1:A:70:ASP:HB3	1:A:75:ARG:HG3	1.96	0.47
1:A:156:SER:HA	1:A:159:SER:HB3	1.97	0.47
1:D:45:PRO:HB2	1:D:196:LEU:HD21	1.97	0.47
1:A:171:ASP:HB3	1:A:173:TYR:CD1	2.50	0.47
1:B:140:GLY:O	2:B:301:HOH:O	2.21	0.47
1:B:181:ILE:HG13	1:B:186:ILE:HD11	1.96	0.47
1:B:116:MET:HG3	1:B:217:LYS:HE2	1.98	0.46
1:D:70:ASP:HB3	1:D:75:ARG:HG3	1.96	0.46
1:D:145:GLN:CG	2:D:313:HOH:O	2.25	0.46
1:D:73:ASN:HB2	1:D:75:ARG:HG2	1.98	0.46
1:B:90:ARG:H	1:B:220:GLU:HB3	1.81	0.46
1:D:148:VAL:CG1	1:D:149:GLN:N	2.78	0.46
1:A:144:GLU:OE1	1:B:171:ASP:OD2	2.34	0.45
1:B:181:ILE:O	1:B:182:ASN:C	2.58	0.45
1:C:112:GLN:HG2	1:C:214:GLN:NE2	2.23	0.45
1:D:154:ARG:HH11	1:D:159:SER:HB3	1.81	0.45
1:C:70:ASP:HB3	1:C:75:ARG:HG3	1.99	0.45
1:C:90:ARG:CZ	1:C:107:ASP:OD2	2.64	0.45
1:B:137:TYR:OH	1:B:166:ILE:HD13	2.16	0.45
1:D:120:GLN:HG3	1:D:121:PRO:HD2	1.97	0.45
1:A:86:ILE:HA	1:A:87:PRO:C	2.40	0.45
1:B:115:LYS:C	1:B:116:MET:SD	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:O	1:D:143:GLN:HG3	2.17	0.45
1:A:53:VAL:HG23	1:A:192:PHE:CZ	2.52	0.44
1:A:183:TYR:HE2	1:B:86:ILE:C	2.25	0.44
1:D:147:THR:HG22	1:D:169:VAL:HG21	1.99	0.44
1:C:114:SER:HA	1:C:214:GLN:O	2.18	0.44
1:C:180:THR:HA	1:C:186:ILE:HD12	1.99	0.44
1:B:82:ARG:HG2	1:B:91:LEU:HD11	1.96	0.44
1:C:82:ARG:HD3	1:C:91:LEU:HD21	1.99	0.44
1:D:134:GLU:O	1:D:135:ASP:HB2	2.16	0.44
1:D:154:ARG:HB2	1:D:161:GLU:HG2	2.00	0.44
1:A:135:ASP:OD2	1:B:51:ARG:NH2	2.44	0.44
1:C:89:LYS:HB3	1:C:220:GLU:HG2	1.99	0.44
1:B:84:ALA:C	1:B:85:LEU:O	2.58	0.43
1:B:85:LEU:HD23	1:B:86:ILE:N	2.33	0.43
1:C:82:ARG:NH2	2:C:304:HOH:O	2.51	0.43
1:C:146:ILE:HD12	1:D:144:GLU:O	2.18	0.43
1:C:110:THR:CG2	1:C:112:GLN:HB2	2.47	0.43
1:D:138:SER:HG	1:D:145:GLN:CD	2.26	0.43
1:A:59:SER:HB2	1:A:61:ARG:HD3	2.01	0.43
1:A:83:LYS:CE	1:B:134:GLU:O	2.66	0.43
1:B:143:GLN:N	1:B:143:GLN:OE1	2.52	0.43
1:D:162:THR:HG21	2:D:327:HOH:O	2.19	0.43
1:A:183:TYR:CD1	1:A:183:TYR:N	2.86	0.43
1:A:142:PRO:O	1:A:143:GLN:CB	2.66	0.43
1:C:107:ASP:CG	1:C:110:THR:HG22	2.44	0.43
1:B:115:LYS:O	1:B:116:MET:SD	2.77	0.42
1:D:74:GLN:O	1:D:98:TYR:HB2	2.19	0.42
1:D:114:SER:HA	1:D:213:ALA:HB1	2.00	0.42
1:C:173:TYR:CE2	1:D:141:GLY:HA2	2.55	0.42
1:B:160:TYR:CD1	1:B:160:TYR:O	2.73	0.42
1:A:49:GLU:HG2	1:A:68:SER:HA	2.01	0.42
2:C:303:HOH:O	1:D:176:GLN:CD	2.63	0.42
1:B:112:GLN:NE2	2:B:305:HOH:O	2.51	0.42
1:C:126:ASP:OD1	1:C:126:ASP:C	2.62	0.42
1:C:181:ILE:N	1:C:186:ILE:HD11	2.35	0.42
1:D:75:ARG:HG3	1:D:75:ARG:O	2.19	0.42
1:A:51:ARG:NH2	1:B:135:ASP:OD2	2.38	0.41
1:C:82:ARG:HA	1:C:82:ARG:HD2	1.69	0.41
1:D:104:PHE:HA	1:D:114:SER:O	2.20	0.41
1:A:53:VAL:HG23	1:A:192:PHE:HZ	1.84	0.41
1:B:110:THR:HG23	1:B:112:GLN:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:PHE:CE2	1:C:206:PRO:HG3	2.56	0.41
1:C:207:PRO:O	1:C:208:SER:C	2.62	0.41
1:B:53:VAL:HG23	1:B:192:PHE:CZ	2.55	0.41
1:A:204:PHE:O	1:A:206:PRO:HD3	2.21	0.41
1:D:51:ARG:HD3	1:D:193:ASP:OD2	2.21	0.41
1:A:154:ARG:HD2	1:A:159:SER:OG	2.21	0.41
1:D:70:ASP:OD2	1:D:75:ARG:HD2	2.21	0.40
1:C:202:SER:O	1:C:203:VAL:C	2.64	0.40
1:B:49:GLU:HG2	1:B:68:SER:HA	2.03	0.40
1:C:132:THR:OG1	1:C:154:ARG:O	2.27	0.40
1:A:158:ARG:C	1:B:86:ILE:HD11	2.46	0.40
1:A:210:CYS:O	1:A:213:ALA:HB2	2.22	0.40
1:C:53:VAL:HG23	1:C:192:PHE:HZ	1.87	0.40
1:C:89:LYS:HA	1:C:220:GLU:O	2.22	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	183/198 (92%)	173 (94%)	10 (6%)	0	100	100
1	B	181/198 (91%)	169 (93%)	10 (6%)	2 (1%)	11	7
1	C	183/198 (92%)	168 (92%)	11 (6%)	4 (2%)	5	2
1	D	177/198 (89%)	159 (90%)	16 (9%)	2 (1%)	11	7
All	All	724/792 (91%)	669 (92%)	47 (6%)	8 (1%)	11	7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	83	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	SER
1	D	90	ARG
1	C	159	SER
1	C	83	LYS
1	C	209	THR
1	D	84	ALA
1	C	119	THR

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	171/182 (94%)	152 (89%)	19 (11%)	6	3
1	B	169/182 (93%)	150 (89%)	19 (11%)	6	3
1	C	171/182 (94%)	153 (90%)	18 (10%)	6	4
1	D	167/182 (92%)	151 (90%)	16 (10%)	8	5
All	All	678/728 (93%)	606 (89%)	72 (11%)	6	4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
1	A	75	ARG
1	A	91	LEU
1	A	111	LYS
1	A	116	MET
1	A	119	THR
1	A	120	GLN
1	A	143	GLN
1	A	153	ASP
1	A	154	ARG
1	A	155	LYS
1	A	158	ARG
1	A	161	GLU
1	A	162	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	180	THR
1	A	183	TYR
1	A	186	ILE
1	A	208	SER
1	A	212	MET
1	B	67	LEU
1	B	75	ARG
1	B	82	ARG
1	B	86	ILE
1	B	90	ARG
1	B	99	LYS
1	B	100	ASP
1	B	143	GLN
1	B	145	GLN
1	B	155	LYS
1	B	158	ARG
1	B	159	SER
1	B	160	TYR
1	B	162	THR
1	B	187	LEU
1	B	196	LEU
1	B	212	MET
1	B	215	LEU
1	B	220	GLU
1	C	57	GLN
1	C	61	ARG
1	C	75	ARG
1	C	82	ARG
1	C	86	ILE
1	C	90	ARG
1	C	116	MET
1	C	118	LEU
1	C	125	LEU
1	C	126	ASP
1	C	137	TYR
1	C	138	SER
1	C	158	ARG
1	C	160	TYR
1	C	162	THR
1	C	181	ILE
1	C	187	LEU
1	C	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	82	ARG
1	D	89	LYS
1	D	90	ARG
1	D	99	LYS
1	D	100	ASP
1	D	110	THR
1	D	117	THR
1	D	152	SER
1	D	159	SER
1	D	160	TYR
1	D	171	ASP
1	D	184	SER
1	D	196	LEU
1	D	215	LEU
1	D	216	GLU
1	D	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	112	GLN
1	A	120	GLN
1	A	136	GLN
1	A	149	GLN
1	A	182	ASN
1	B	56	GLN
1	B	145	GLN
1	B	182	ASN
1	C	112	GLN
1	C	176	GLN
1	C	214	GLN
1	D	47	GLN
1	D	74	GLN
1	D	136	GLN
1	D	149	GLN
1	D	176	GLN
1	D	195	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	185/198 (93%)	-0.77	0 100 100	29, 49, 88, 142	0
1	B	183/198 (92%)	-0.82	2 (1%) 78 77	30, 48, 96, 182	0
1	C	184/198 (92%)	-0.88	0 100 100	30, 47, 84, 155	1 (0%)
1	D	180/198 (90%)	-0.76	0 100 100	29, 50, 100, 131	1 (0%)
All	All	732/792 (92%)	-0.81	2 (0%) 90 89	29, 49, 97, 182	2 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ALA	3.0
1	B	159	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.