



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:58 AM UTC

PDB ID : 3INK / pdb_00003ink
Title : UNRAVELING THE STRUCTURE OF INTERLEUKIN-2: REPLY
Authors : Mckay, D.B.; Brandhuber, B.J.
Deposited on : 1992-12-09
Resolution : 2.50 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

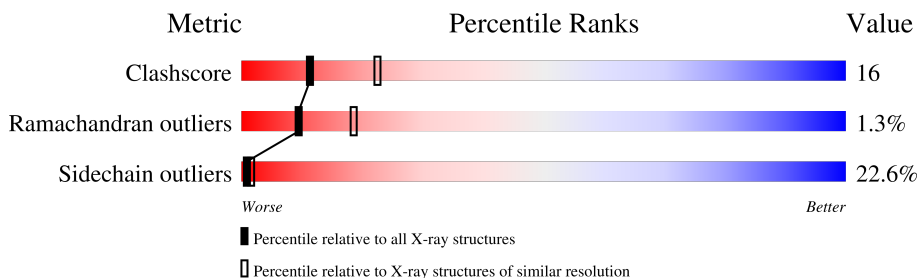
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	133	
1	D	133	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1996 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 INTERLEUKIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	122	Total	C	N	O	S	0	0	1
			998	643	167	183	5			
1	D	122	Total	C	N	O	S	0	0	1
			998	643	167	183	5			

There are 2 discrepancies between the modelled and reference sequences:

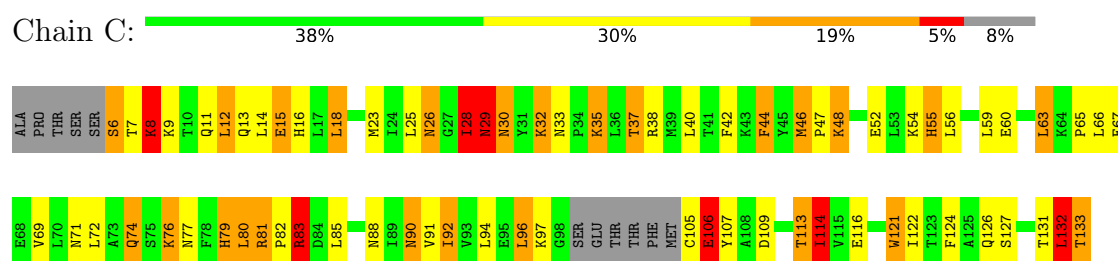
Chain	Residue	Modelled	Actual	Comment	Reference
C	125	ALA	CYS	conflict	UNP P60568
D	125	ALA	CYS	conflict	UNP P60568

3 Residue-property plots [i](#)

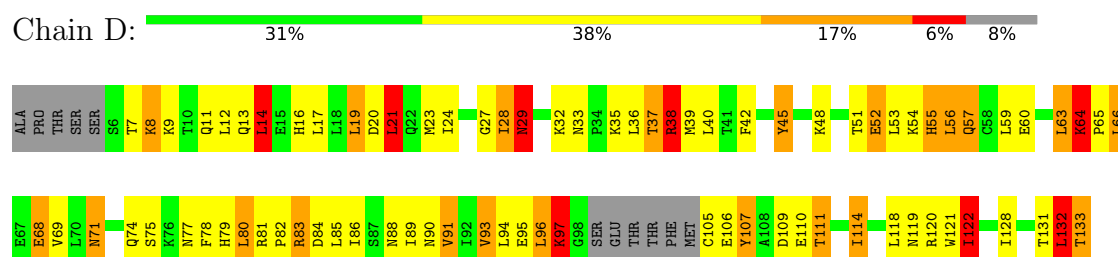
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: INTERLEUKIN-2



• Molecule 1: INTERLEUKIN-2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.80Å 40.10Å 33.70Å 90.00° 109.30° 93.20°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1996	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

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	C	1.35	6/1013 (0.6%)	2.37	59/1366 (4.3%)
1	D	1.40	9/1013 (0.9%)	2.42	61/1366 (4.5%)
All	All	1.38	15/2026 (0.7%)	2.39	120/2732 (4.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	97	LYS	C-N	-7.31	1.23	1.33
1	C	46	MET	CA-CB	-6.95	1.44	1.53
1	D	114	ILE	CA-CB	6.82	1.62	1.54
1	D	79	HIS	CD2-NE2	-6.70	1.30	1.37
1	C	55	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	79	HIS	CD2-NE2	-6.34	1.30	1.37
1	D	16	HIS	CD2-NE2	-5.76	1.31	1.37
1	D	55	HIS	CD2-NE2	-5.63	1.31	1.37
1	C	90	ASN	CA-CB	-5.62	1.44	1.53
1	D	55	HIS	CG-ND1	-5.58	1.32	1.38
1	D	59	LEU	CA-CB	5.28	1.63	1.54
1	C	97	LYS	C-N	-5.27	1.25	1.33
1	D	16	HIS	CA-CB	-5.25	1.44	1.53
1	C	79	HIS	CG-ND1	-5.20	1.32	1.38
1	D	91	VAL	CA-CB	5.01	1.61	1.54

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	LEU	N-CA-C	14.52	130.52	112.23
1	C	114	ILE	CB-CA-C	-11.30	96.63	112.22
1	D	114	ILE	CB-CA-C	-11.12	97.12	112.14
1	C	48	LYS	N-CA-C	-10.68	99.17	111.03
1	D	109	ASP	N-CA-C	10.24	122.53	111.36
1	D	122	ILE	N-CA-C	-10.07	100.75	110.42
1	D	59	LEU	N-CA-C	-9.97	99.96	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ASN	OD1-CG-ND2	-9.45	113.15	122.60
1	C	132	LEU	N-CA-CB	-8.92	97.98	110.65
1	D	114	ILE	N-CA-CB	8.84	122.57	110.54
1	C	59	LEU	N-CA-C	-8.53	100.59	112.45
1	D	42	PHE	O-C-N	8.24	132.62	123.22
1	C	42	PHE	CA-CB-CG	-8.23	105.57	113.80
1	D	68	GLU	CB-CG-CD	-7.97	99.04	112.60
1	D	33	ASN	CA-CB-CG	7.90	120.50	112.60
1	C	55	HIS	CB-CG-CD2	-7.90	120.94	131.20
1	C	114	ILE	N-CA-CB	7.83	122.33	110.58
1	C	16	HIS	CB-CG-CD2	-7.78	121.08	131.20
1	C	131	THR	N-CA-C	-7.69	104.03	113.41
1	C	26	ASN	CA-CB-CG	7.59	120.19	112.60
1	D	121	TRP	CG-CD2-CE3	7.40	141.30	133.90
1	C	44	PHE	CA-CB-CG	-7.34	106.46	113.80
1	C	124	PHE	N-CA-C	-7.31	103.39	111.36
1	C	76	LYS	N-CA-C	7.27	121.05	111.75
1	C	28	ILE	CB-CG1-CD1	-7.22	98.64	113.80
1	C	16	HIS	N-CA-C	-7.19	102.85	111.69
1	D	88	ASN	CA-CB-CG	7.14	119.75	112.60
1	C	96	LEU	N-CA-C	7.07	122.57	113.88
1	D	81	ARG	CA-C-O	-7.07	113.78	119.71
1	D	69	VAL	N-CA-C	-7.01	103.64	110.72
1	D	32	LYS	N-CA-C	-6.97	104.51	113.16
1	C	32	LYS	N-CA-C	-6.96	104.67	113.02
1	D	29	ASN	N-CA-C	6.96	125.62	110.80
1	D	8	LYS	CA-C-O	-6.90	113.10	120.42
1	D	88	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	C	121	TRP	CG-CD2-CE3	6.82	140.72	133.90
1	C	38	ARG	CB-CG-CD	6.76	126.85	111.30
1	D	109	ASP	CA-CB-CG	-6.75	105.85	112.60
1	C	109	ASP	N-CA-C	6.74	118.31	110.97
1	D	9	LYS	CA-CB-CG	-6.71	100.68	114.10
1	D	28	ILE	CB-CG1-CD1	-6.68	99.77	113.80
1	C	16	HIS	CB-CG-ND1	6.65	132.68	122.70
1	C	71	ASN	CB-CG-ND2	6.65	126.37	116.40
1	C	106	GLU	CB-CG-CD	6.58	123.79	112.60
1	D	64	LYS	CG-CD-CE	6.58	126.44	111.30
1	D	42	PHE	CA-C-N	6.58	130.91	121.50
1	D	42	PHE	C-N-CA	6.58	130.91	121.50
1	C	55	HIS	CB-CG-ND1	6.54	132.51	122.70
1	D	36	LEU	N-CA-C	6.51	118.93	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	LEU	CA-C-O	-6.51	112.11	119.79
1	C	56	LEU	N-CA-C	-6.48	105.24	113.01
1	D	7	THR	CA-CB-OG1	-6.45	99.92	109.60
1	C	83	ARG	CB-CG-CD	6.44	126.12	111.30
1	C	37	THR	CA-CB-CG2	-6.42	99.58	110.50
1	C	97	LYS	N-CA-CB	-6.42	99.59	110.50
1	C	8	LYS	CA-C-O	-6.37	113.17	120.24
1	D	14	LEU	O-C-N	-6.36	115.22	122.09
1	D	9	LYS	CB-CG-CD	6.31	125.82	111.30
1	D	83	ARG	NE-CZ-NH2	-6.27	113.56	119.20
1	D	75	SER	N-CA-C	6.25	120.47	112.34
1	D	38	ARG	N-CA-C	-6.22	103.81	111.40
1	D	33	ASN	CB-CA-C	6.21	116.66	110.33
1	C	30	ASN	CB-CG-ND2	6.14	125.61	116.40
1	C	80	LEU	N-CA-C	-6.13	99.81	109.50
1	D	74	GLN	CB-CG-CD	6.10	122.97	112.60
1	C	15	GLU	CA-CB-CG	6.08	126.26	114.10
1	C	71	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	D	79	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	D	56	LEU	N-CA-C	-6.05	105.88	113.20
1	C	126	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	C	6	SER	N-CA-C	-6.00	94.21	111.00
1	D	48	LYS	N-CA-C	-5.99	104.75	111.28
1	D	7	THR	N-CA-CB	-5.98	101.01	110.28
1	C	88	ASN	CB-CG-ND2	5.81	125.11	116.40
1	D	8	LYS	N-CA-C	-5.80	105.03	111.36
1	C	26	ASN	OD1-CG-ND2	-5.78	116.83	122.60
1	D	96	LEU	N-CA-CB	-5.77	101.42	110.30
1	D	55	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	D	37	THR	N-CA-CB	-5.73	101.39	110.22
1	D	71	ASN	CA-C-O	5.71	126.47	119.05
1	C	88	ASN	CA-CB-CG	5.70	118.30	112.60
1	C	32	LYS	CG-CD-CE	5.69	124.39	111.30
1	C	79	HIS	CB-CG-CD2	-5.69	123.80	131.20
1	D	21	LEU	O-C-N	-5.60	116.19	122.12
1	C	121	TRP	CB-CG-CD1	-5.59	118.51	126.90
1	C	133	THR	CA-CB-CG2	5.59	120.00	110.50
1	D	16	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	C	42	PHE	CA-C-O	-5.57	115.06	121.47
1	D	80	LEU	N-CA-C	-5.53	100.76	109.50
1	C	131	THR	CA-C-O	5.49	125.62	119.41
1	D	132	LEU	CA-C-N	5.46	131.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	LEU	C-N-CA	5.46	131.53	121.70
1	D	68	GLU	CA-CB-CG	5.46	125.01	114.10
1	D	19	LEU	CA-C-O	-5.41	114.69	120.42
1	C	8	LYS	O-C-N	-5.38	115.24	122.23
1	D	64	LYS	CB-CG-CD	5.32	123.53	111.30
1	C	13	GLN	CA-CB-CG	-5.29	103.53	114.10
1	D	24	ILE	N-CA-C	-5.27	105.40	110.72
1	D	121	TRP	CG-CD1-NE1	-5.26	103.36	110.20
1	D	45	TYR	CA-C-O	5.26	126.97	120.92
1	C	113	THR	OG1-CB-CG2	-5.26	98.78	109.30
1	D	90	ASN	CA-CB-CG	-5.26	107.34	112.60
1	C	91	VAL	N-CA-C	-5.24	105.74	110.82
1	C	133	THR	N-CA-CB	-5.24	102.60	111.50
1	D	84	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	71	ASN	CA-C-O	5.23	125.81	119.38
1	D	77	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	C	81	ARG	O-C-N	-5.16	116.71	121.30
1	C	35	LYS	CB-CG-CD	-5.15	99.45	111.30
1	C	18	LEU	N-CA-C	5.12	117.26	111.11
1	D	111	THR	CA-C-O	-5.12	116.06	121.94
1	C	94	LEU	N-CA-C	-5.11	105.80	111.36
1	C	29	ASN	N-CA-C	5.06	121.58	110.80
1	C	92	ILE	CB-CA-C	-5.06	105.31	112.14
1	D	20	ASP	N-CA-C	-5.06	105.77	111.28
1	C	28	ILE	CA-CB-CG1	5.04	118.97	110.40
1	D	121	TRP	CB-CG-CD1	-5.04	119.34	126.90
1	C	16	HIS	CA-C-O	-5.03	114.66	120.24
1	D	93	VAL	CG1-CB-CG2	-5.03	99.73	110.80
1	D	57	GLN	N-CA-C	-5.02	105.89	111.36

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	C	998	0	1039	31	0
1	D	998	0	1039	36	0
All	All	1996	0	2078	66	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 16.

All (66) 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:13:GLN:NE2	1:D:95:GLU:OE1	1.75	1.18
1:D:64:LYS:HG3	1:D:65:PRO:HD3	1.41	1.00
1:C:44:PHE:CE2	1:C:114:ILE:HD13	2.08	0.89
1:C:35:LYS:NZ	1:C:74:GLN:OE1	2.08	0.86
1:C:44:PHE:HE2	1:C:114:ILE:HD13	1.41	0.85
1:D:128:ILE:O	1:D:131:THR:OG1	1.96	0.81
1:D:52:GLU:H	1:D:55:HIS:CD2	2.08	0.71
1:D:13:GLN:HE21	1:D:95:GLU:CD	1.95	0.70
1:D:51:THR:H	1:D:55:HIS:CD2	2.10	0.70
1:D:105:CYS:SG	1:D:107:TYR:CE1	2.86	0.68
1:D:56:LEU:HB3	1:D:93:VAL:HG13	1.79	0.64
1:C:18:LEU:HD11	1:C:122:ILE:HG23	1.81	0.63
1:D:35:LYS:HA	1:D:38:ARG:HE	1.65	0.62
1:C:11:GLN:HB2	1:C:132:LEU:HD23	1.81	0.62
1:D:52:GLU:H	1:D:55:HIS:HD2	1.46	0.61
1:D:35:LYS:O	1:D:38:ARG:HG2	2.01	0.60
1:C:8:LYS:O	1:C:12:LEU:HB2	2.01	0.60
1:C:105:CYS:SG	1:C:107:TYR:CE1	2.95	0.60
1:C:82:PRO:HG2	1:C:83:ARG:HH11	1.68	0.59
1:C:81:ARG:HB3	1:C:83:ARG:HG2	1.85	0.58
1:D:64:LYS:HG3	1:D:65:PRO:CD	2.27	0.57
1:D:68:GLU:HA	1:D:71:ASN:ND2	2.20	0.56
1:C:23:MET:SD	1:C:79:HIS:HD2	2.31	0.54
1:C:28:ILE:C	1:C:33:ASN:HD22	2.16	0.53
1:D:52:GLU:OE1	1:D:54:LYS:HG2	2.10	0.51
1:C:47:PRO:HG3	1:C:121:TRP:CZ2	2.46	0.51
1:C:92:ILE:HG22	1:C:96:LEU:HD12	1.93	0.50
1:C:32:LYS:HE2	1:C:76:LYS:HD3	1.93	0.49
1:D:132:LEU:N	1:D:132:LEU:HD13	2.26	0.49
1:C:69:VAL:HG11	1:C:114:ILE:HD11	1.95	0.49
1:C:83:ARG:HD3	1:C:83:ARG:H	1.78	0.49
1:D:28:ILE:HG12	1:D:39:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:MET:SD	1:D:80:LEU:HD13	2.54	0.48
1:D:14:LEU:HD13	1:D:96:LEU:HD21	1.95	0.47
1:D:60:GLU:HA	1:D:63:LEU:HD22	1.95	0.47
1:D:51:THR:N	1:D:55:HIS:HD2	2.12	0.47
1:D:51:THR:N	1:D:55:HIS:CD2	2.81	0.47
1:D:66:LEU:HD13	1:D:86:ILE:HD11	1.96	0.47
1:D:13:GLN:CD	1:D:95:GLU:OE1	2.53	0.47
1:D:132:LEU:O	1:D:133:THR:HB	2.16	0.46
1:C:25:LEU:O	1:C:29:ASN:HB2	2.16	0.46
1:D:51:THR:H	1:D:55:HIS:HD2	1.60	0.46
1:C:52:GLU:O	1:C:55:HIS:HB2	2.16	0.46
1:D:53:LEU:O	1:D:97:LYS:HB3	2.17	0.45
1:C:18:LEU:CD1	1:C:122:ILE:HG23	2.44	0.44
1:D:13:GLN:HG2	1:D:95:GLU:OE1	2.18	0.44
1:D:89:ILE:O	1:D:93:VAL:HG23	2.17	0.44
1:C:114:ILE:H	1:C:114:ILE:HG12	1.69	0.44
1:C:28:ILE:HA	1:C:33:ASN:ND2	2.33	0.43
1:C:80:LEU:HB3	1:C:85:LEU:HG	2.01	0.43
1:C:83:ARG:H	1:C:83:ARG:CD	2.29	0.43
1:C:60:GLU:HA	1:C:63:LEU:HD22	2.00	0.43
1:C:46:MET:HE3	1:C:46:MET:HB3	1.91	0.42
1:D:17:LEU:HG	1:D:21:LEU:HD22	2.00	0.42
1:C:48:LYS:HB2	1:C:106:GLU:O	2.19	0.42
1:D:118:LEU:O	1:D:122:ILE:HD12	2.20	0.42
1:C:11:GLN:O	1:C:15:GLU:HG3	2.20	0.42
1:C:113:THR:CG2	1:C:116:GLU:H	2.33	0.42
1:D:23:MET:SD	1:D:80:LEU:CD1	3.08	0.41
1:D:27:GLY:HA3	1:D:78:PHE:CE1	2.55	0.41
1:C:80:LEU:HA	1:C:80:LEU:HD12	1.82	0.41
1:C:35:LYS:HD3	1:C:72:LEU:O	2.20	0.41
1:D:13:GLN:CG	1:D:95:GLU:OE1	2.68	0.41
1:D:78:PHE:CD2	1:D:82:PRO:HG3	2.55	0.41
1:D:8:LYS:O	1:D:12:LEU:HD13	2.21	0.40
1:C:83:ARG:HG3	1:D:45:TYR:OH	2.21	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	C	118/133 (89%)	111 (94%)	6 (5%)	1 (1%)	16	31
1	D	118/133 (89%)	111 (94%)	5 (4%)	2 (2%)	7	13
All	All	236/266 (89%)	222 (94%)	11 (5%)	3 (1%)	9	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	29	ASN
1	C	29	ASN
1	D	107	TYR

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	C	115/125 (92%)	90 (78%)	25 (22%)	1	2
1	D	115/125 (92%)	88 (76%)	27 (24%)	1	1
All	All	230/250 (92%)	178 (77%)	52 (23%)	1	1

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	SER
1	C	7	THR
1	C	8	LYS

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Mol	Chain	Res	Type
1	C	9	LYS
1	C	12	LEU
1	C	14	LEU
1	C	26	ASN
1	C	28	ILE
1	C	30	ASN
1	C	37	THR
1	C	40	LEU
1	C	54	LYS
1	C	63	LEU
1	C	65	PRO
1	C	66	LEU
1	C	67	GLU
1	C	74	GLN
1	C	77	ASN
1	C	83	ARG
1	C	90	ASN
1	C	106	GLU
1	C	114	ILE
1	C	127	SER
1	C	132	LEU
1	C	133	THR
1	D	11	GLN
1	D	14	LEU
1	D	19	LEU
1	D	21	LEU
1	D	29	ASN
1	D	37	THR
1	D	38	ARG
1	D	40	LEU
1	D	52	GLU
1	D	57	GLN
1	D	63	LEU
1	D	64	LYS
1	D	66	LEU
1	D	83	ARG
1	D	85	LEU
1	D	91	VAL
1	D	94	LEU
1	D	97	LYS
1	D	106	GLU
1	D	110	GLU

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Mol	Chain	Res	Type
1	D	111	THR
1	D	114	ILE
1	D	119	ASN
1	D	120	ARG
1	D	122	ILE
1	D	132	LEU
1	D	133	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	GLN
1	C	79	HIS
1	C	119	ASN
1	D	26	ASN
1	D	57	GLN
1	D	77	ASN
1	D	119	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.