



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 1RFB / pdb_00001rfb
Title : CRYSTAL STRUCTURE OF RECOMBINANT BOVINE INTERFERON-GAMMA AT 3.0 ANGSTROMS RESOLUTION
Authors : Samudzi, C.T.; Rubin, J.R.
Deposited on : 1993-06-30
Resolution : 3.00 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)	:	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

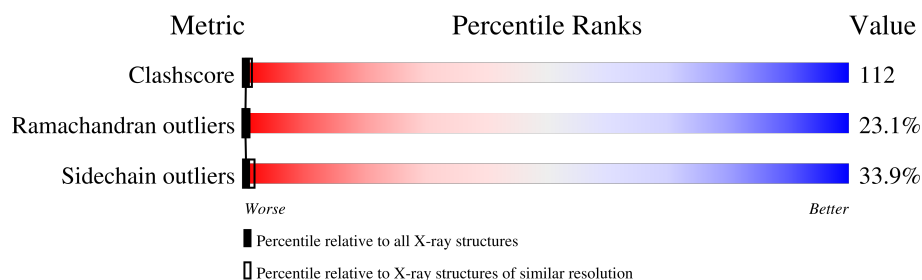
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	119	 7% 21% 34% 38%
1	B	119	 8% 25% 45% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2023 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 INTERFERON-GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			990	636	163	188	3			
1	B	119	Total	C	N	O	S	0	0	0
			990	636	163	188	3			

- Molecule 2 is water.

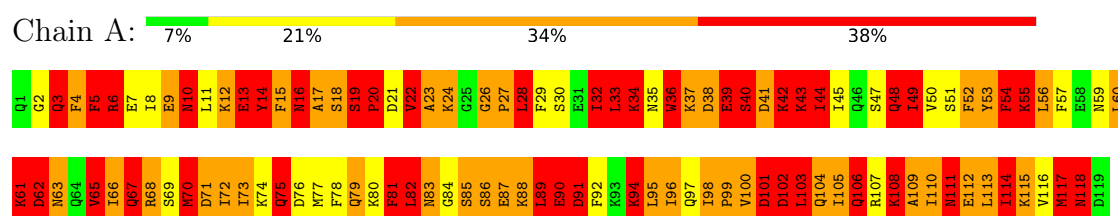
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	23	Total	O	0	0
			23	23		

3 Residue-property plots

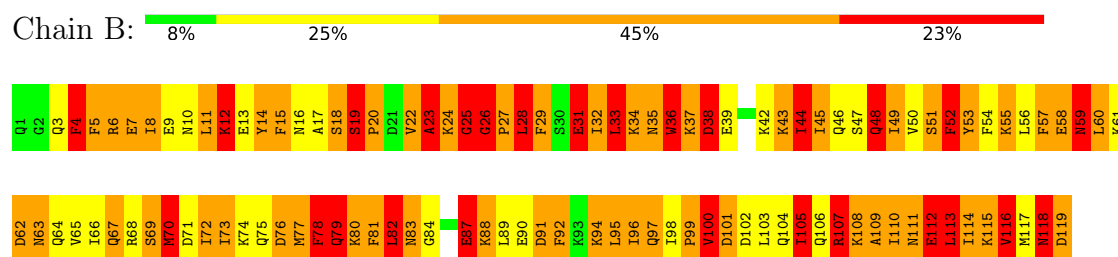
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: INTERFERON-GAMMA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	42.80Å 79.90Å 85.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2023	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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	A	1.31	4/1006 (0.4%)	3.31	138/1343 (10.3%)
1	B	1.26	5/1006 (0.5%)	3.06	100/1343 (7.4%)
All	All	1.29	9/2012 (0.4%)	3.19	238/2686 (8.9%)

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	B	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	GLY	C-O	9.78	1.37	1.24
1	B	20	PRO	N-CD	7.66	1.58	1.47
1	B	26	GLY	CA-C	-7.41	1.41	1.51
1	A	20	PRO	CA-CB	7.32	1.64	1.53
1	A	36	TRP	CA-CB	5.63	1.62	1.53
1	B	44	ILE	CA-CB	5.34	1.61	1.54
1	A	44	ILE	CA-CB	5.19	1.61	1.54
1	A	3	GLN	N-CA	-5.10	1.39	1.46
1	B	20	PRO	N-CA	-5.04	1.40	1.47

All (238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	GLY	CA-C-O	-27.50	82.19	121.52
1	A	15	PHE	CA-CB-CG	21.17	134.97	113.80
1	B	19	SER	CA-C-N	20.80	145.84	119.84
1	B	19	SER	C-N-CA	20.80	145.84	119.84
1	B	19	SER	CA-C-O	-20.66	91.86	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	PHE	CA-CB-CG	19.01	132.81	113.80
1	A	10	ASN	CA-CB-CG	18.68	131.28	112.60
1	A	81	PHE	CA-CB-CG	18.02	131.82	113.80
1	B	26	GLY	O-C-N	-16.88	104.89	121.77
1	A	2	GLY	CA-C-N	15.31	150.78	121.54
1	A	2	GLY	C-N-CA	15.31	150.78	121.54
1	A	22	VAL	N-CA-C	-15.23	90.26	109.30
1	B	20	PRO	CA-N-CD	-14.71	91.41	112.00
1	B	20	PRO	N-CA-CB	14.29	118.25	103.25
1	A	22	VAL	CA-C-O	-13.27	105.91	121.04
1	A	5	PHE	CA-CB-CG	13.06	126.86	113.80
1	B	102	ASP	CA-CB-CG	12.77	125.37	112.60
1	B	62	ASP	CA-CB-CG	12.60	125.20	112.60
1	B	78	PHE	CA-CB-CG	12.59	126.39	113.80
1	B	15	PHE	CA-CB-CG	12.54	126.34	113.80
1	A	83	ASN	CA-CB-CG	-12.47	100.13	112.60
1	A	20	PRO	N-CA-C	12.31	137.82	112.47
1	A	20	PRO	N-CA-CB	-12.07	90.57	103.25
1	A	49	ILE	CA-C-N	12.06	140.37	121.19
1	A	49	ILE	C-N-CA	12.06	140.37	121.19
1	A	36	TRP	CA-CB-CG	-11.68	91.42	113.60
1	A	6	ARG	N-CA-C	11.13	125.97	112.38
1	A	70	MET	N-CA-C	-11.07	99.29	111.36
1	B	58	GLU	CB-CG-CD	11.04	131.37	112.60
1	B	59	ASN	CA-CB-CG	10.48	123.08	112.60
1	A	13	GLU	CB-CG-CD	10.15	129.85	112.60
1	A	115	LYS	N-CA-C	9.93	124.05	111.24
1	A	52	PHE	CA-CB-CG	-9.70	104.10	113.80
1	B	78	PHE	N-CA-C	-9.55	100.85	111.07
1	B	19	SER	O-C-N	9.43	132.17	121.32
1	A	118	ASN	CA-C-N	9.33	138.49	121.70
1	A	118	ASN	C-N-CA	9.33	138.49	121.70
1	A	108	LYS	CA-C-N	9.25	133.05	120.38
1	A	108	LYS	C-N-CA	9.25	133.05	120.38
1	A	62	ASP	CA-C-N	9.21	139.14	121.54
1	A	62	ASP	C-N-CA	9.21	139.14	121.54
1	A	117	MET	N-CA-C	-9.13	96.97	110.48
1	A	91	ASP	N-CA-C	9.12	121.22	111.28
1	A	117	MET	CB-CA-C	9.01	126.05	109.46
1	A	88	LYS	CA-C-N	8.98	132.51	120.65
1	A	88	LYS	C-N-CA	8.98	132.51	120.65
1	A	82	LEU	CA-C-N	8.84	138.43	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	LEU	C-N-CA	8.84	138.43	121.54
1	A	118	ASN	CA-CB-CG	8.82	121.42	112.60
1	A	105	ILE	CA-C-N	8.69	138.14	121.54
1	A	105	ILE	C-N-CA	8.69	138.14	121.54
1	B	78	PHE	N-CA-CB	8.63	122.52	110.01
1	B	92	PHE	CA-CB-CG	-8.60	105.20	113.80
1	B	69	SER	CA-CB-OG	8.55	128.19	111.10
1	A	72	ILE	CA-C-O	-8.50	111.84	120.85
1	A	20	PRO	CB-CA-C	-8.47	97.58	111.56
1	A	75	GLN	CB-CG-CD	8.47	127.01	112.60
1	A	30	SER	N-CA-C	-8.45	102.15	111.36
1	B	82	LEU	N-CA-C	8.45	125.11	109.56
1	A	36	TRP	N-CA-C	8.42	128.72	110.80
1	B	35	ASN	CA-CB-CG	-8.40	104.20	112.60
1	A	103	LEU	CA-C-N	8.35	137.48	121.54
1	A	103	LEU	C-N-CA	8.35	137.48	121.54
1	A	3	GLN	N-CA-C	8.34	128.57	110.80
1	A	28	LEU	N-CA-C	8.31	128.50	110.80
1	A	89	LEU	N-CA-CB	-8.17	97.98	109.91
1	B	4	PHE	CA-C-N	7.93	131.70	120.28
1	B	4	PHE	C-N-CA	7.93	131.70	120.28
1	A	53	TYR	CA-C-N	7.92	131.69	120.28
1	A	53	TYR	C-N-CA	7.92	131.69	120.28
1	B	118	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	B	22	VAL	CB-CA-C	7.80	122.35	110.96
1	A	48	GLN	CB-CG-CD	7.68	125.65	112.60
1	A	83	ASN	N-CA-CB	7.62	123.38	110.49
1	B	81	PHE	CA-CB-CG	7.62	121.42	113.80
1	A	90	GLU	CA-C-N	7.60	130.47	120.28
1	A	90	GLU	C-N-CA	7.60	130.47	120.28
1	A	66	ILE	N-CA-CB	7.59	123.75	111.23
1	A	27	PRO	CA-C-N	7.56	135.99	121.54
1	A	27	PRO	C-N-CA	7.56	135.99	121.54
1	A	112	GLU	N-CA-C	7.55	122.15	112.34
1	A	109	ALA	N-CA-C	7.50	120.41	111.33
1	A	16	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	105	ILE	N-CA-CB	-7.49	100.69	112.07
1	B	38	ASP	CA-CB-CG	7.43	120.03	112.60
1	B	91	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	60	LEU	N-CA-C	7.37	122.74	112.72
1	A	90	GLU	CB-CG-CD	7.35	125.10	112.60
1	A	86	SER	N-CA-C	7.33	120.14	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	GLY	N-CA-C	7.29	127.22	112.34
1	A	79	GLN	CB-CG-CD	7.28	124.98	112.60
1	B	82	LEU	CA-C-O	-7.18	111.48	122.32
1	A	39	GLU	CA-C-N	7.17	135.23	121.54
1	A	39	GLU	C-N-CA	7.17	135.23	121.54
1	B	118	ASN	CA-CB-CG	7.15	119.75	112.60
1	B	110	ILE	N-CA-C	7.12	122.15	111.89
1	B	119	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	42	LYS	CA-C-N	7.10	135.10	121.54
1	A	42	LYS	C-N-CA	7.10	135.10	121.54
1	A	65	VAL	CA-C-O	-7.09	111.92	120.78
1	B	76	ASP	CA-CB-CG	-7.09	105.51	112.60
1	A	6	ARG	CA-C-O	-7.08	110.92	119.49
1	A	117	MET	N-CA-CB	-7.08	99.52	110.29
1	B	44	ILE	N-CA-C	7.05	124.00	109.34
1	B	107	ARG	CA-C-N	7.00	134.01	120.99
1	B	107	ARG	C-N-CA	7.00	134.01	120.99
1	B	99	PRO	CA-C-N	6.95	134.47	121.97
1	B	99	PRO	C-N-CA	6.95	134.47	121.97
1	B	18	SER	CA-C-O	-6.91	113.56	120.82
1	B	109	ALA	CA-C-N	6.79	132.20	120.86
1	B	109	ALA	C-N-CA	6.79	132.20	120.86
1	B	90	GLU	CA-C-N	6.75	134.44	121.54
1	B	90	GLU	C-N-CA	6.75	134.44	121.54
1	B	63	ASN	CA-CB-CG	-6.75	105.85	112.60
1	B	43	LYS	CA-C-N	6.72	134.07	121.97
1	B	43	LYS	C-N-CA	6.72	134.07	121.97
1	A	52	PHE	N-CA-CB	6.70	120.62	110.30
1	B	58	GLU	N-CA-CB	6.66	120.63	110.44
1	B	53	TYR	CB-CA-C	6.63	121.80	110.79
1	B	35	ASN	N-CA-C	6.61	120.33	112.93
1	A	104	GLN	CA-C-N	6.59	131.26	121.77
1	A	104	GLN	C-N-CA	6.59	131.26	121.77
1	A	60	LEU	CA-C-N	6.59	134.13	121.54
1	A	60	LEU	C-N-CA	6.59	134.13	121.54
1	B	15	PHE	CA-C-O	6.57	127.66	120.90
1	A	110	ILE	CA-C-N	6.56	134.07	121.54
1	A	110	ILE	C-N-CA	6.56	134.07	121.54
1	A	117	MET	CA-C-O	-6.56	113.93	121.47
1	A	113	LEU	CA-C-O	6.48	128.19	121.07
1	A	22	VAL	N-CA-CB	6.46	118.25	110.31
1	B	52	PHE	N-CA-C	-6.46	104.28	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	VAL	N-CA-C	6.46	122.78	109.34
1	A	36	TRP	CA-C-O	-6.45	111.29	120.51
1	A	70	MET	O-C-N	6.44	129.49	122.15
1	B	73	ILE	O-C-N	6.42	128.44	121.83
1	B	55	LYS	N-CA-CB	6.42	119.77	110.47
1	B	111	ASN	N-CA-C	6.39	119.56	111.69
1	B	58	GLU	N-CA-C	-6.39	105.23	113.16
1	B	83	ASN	CA-C-N	6.34	127.15	119.99
1	B	83	ASN	C-N-CA	6.34	127.15	119.99
1	A	94	LYS	CA-C-O	6.33	127.33	120.55
1	A	39	GLU	N-CA-C	6.33	118.50	107.49
1	A	111	ASN	CA-C-N	6.33	130.81	120.63
1	A	111	ASN	C-N-CA	6.33	130.81	120.63
1	B	60	LEU	N-CA-C	6.29	121.20	112.45
1	B	27	PRO	CA-C-N	6.29	133.55	121.54
1	B	27	PRO	C-N-CA	6.29	133.55	121.54
1	A	71	ASP	O-C-N	6.28	129.31	122.15
1	B	27	PRO	N-CA-CB	6.23	110.12	103.39
1	A	88	LYS	CA-C-O	6.20	127.10	120.10
1	B	92	PHE	N-CA-CB	6.20	119.90	110.42
1	A	67	GLN	CA-C-O	-6.19	111.66	120.51
1	A	17	ALA	CA-C-N	6.15	133.29	121.54
1	A	17	ALA	C-N-CA	6.15	133.29	121.54
1	A	55	LYS	N-CA-C	-6.14	105.44	113.17
1	A	26	GLY	CA-C-N	6.13	127.50	119.84
1	A	26	GLY	C-N-CA	6.13	127.50	119.84
1	A	61	LYS	N-CA-C	6.11	123.80	110.80
1	B	5	PHE	N-CA-C	6.09	118.72	111.71
1	B	31	GLU	CA-CB-CG	6.05	126.20	114.10
1	A	94	LYS	N-CA-C	-6.04	104.03	111.40
1	B	53	TYR	N-CA-C	-6.01	104.72	111.28
1	B	84	GLY	N-CA-C	6.01	119.92	112.64
1	A	12	LYS	N-CA-C	-6.00	104.54	112.34
1	A	10	ASN	CB-CA-C	5.99	120.69	110.74
1	B	33	LEU	N-CA-C	5.98	123.55	110.80
1	A	90	GLU	CA-CB-CG	5.98	126.06	114.10
1	A	15	PHE	N-CA-CB	5.95	119.25	110.33
1	B	87	GLU	N-CA-C	5.92	118.25	111.02
1	B	57	PHE	CB-CA-C	5.88	122.39	110.38
1	A	90	GLU	CB-CA-C	-5.88	98.72	110.42
1	A	41	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	98	ILE	N-CA-CB	-5.82	103.06	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	MET	CB-CA-C	5.81	120.55	110.68
1	B	112	GLU	CB-CG-CD	5.81	122.47	112.60
1	A	101	ASP	CA-C-O	5.80	127.45	121.07
1	B	62	ASP	CA-C-N	5.79	132.59	121.54
1	B	62	ASP	C-N-CA	5.79	132.59	121.54
1	B	18	SER	N-CA-C	5.77	117.24	111.07
1	B	77	MET	N-CA-C	5.77	118.34	111.71
1	B	47	SER	CA-C-N	5.73	129.02	120.31
1	B	47	SER	C-N-CA	5.73	129.02	120.31
1	B	80	LYS	N-CA-CB	5.72	119.19	110.39
1	A	89	LEU	CA-C-N	5.71	132.44	121.54
1	A	89	LEU	C-N-CA	5.71	132.44	121.54
1	A	38	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	39	GLU	CB-CA-C	-5.64	103.72	110.94
1	B	65	VAL	CB-CA-C	5.61	120.50	111.29
1	B	81	PHE	CA-C-O	-5.61	114.92	120.70
1	A	71	ASP	N-CA-C	-5.60	105.26	111.36
1	A	9	GLU	CA-C-O	5.60	126.42	120.10
1	B	12	LYS	CA-CB-CG	5.60	125.29	114.10
1	A	17	ALA	N-CA-C	5.59	122.71	110.80
1	A	35	ASN	CA-C-N	5.57	132.17	121.54
1	A	35	ASN	C-N-CA	5.57	132.17	121.54
1	A	44	ILE	CB-CA-C	-5.56	102.17	111.29
1	B	113	LEU	CB-CA-C	5.56	120.13	110.68
1	A	62	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	19	SER	C-N-CD	-5.53	102.32	125.00
1	B	48	GLN	OE1-CD-NE2	-5.50	117.09	122.60
1	A	99	PRO	N-CA-C	5.50	120.78	113.57
1	A	5	PHE	CA-C-N	5.47	129.36	120.60
1	A	5	PHE	C-N-CA	5.47	129.36	120.60
1	A	40	SER	N-CA-C	5.46	122.44	110.80
1	B	63	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	A	98	ILE	CA-C-N	5.42	124.94	119.19
1	A	98	ILE	C-N-CA	5.42	124.94	119.19
1	A	61	LYS	CA-C-N	5.39	131.84	121.54
1	A	61	LYS	C-N-CA	5.39	131.84	121.54
1	B	27	PRO	N-CD-CG	5.39	111.29	103.20
1	B	77	MET	CA-C-O	-5.39	114.01	120.10
1	B	25	GLY	N-CA-C	-5.37	100.46	113.18
1	A	70	MET	N-CA-CB	5.36	118.10	110.16
1	B	96	ILE	N-CA-C	5.34	116.06	110.62
1	A	114	ILE	N-CA-CB	-5.32	102.45	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ALA	CA-C-N	5.32	127.97	120.42
1	A	109	ALA	C-N-CA	5.32	127.97	120.42
1	A	71	ASP	CA-C-N	-5.30	112.90	120.42
1	A	71	ASP	C-N-CA	-5.30	112.90	120.42
1	B	98	ILE	CB-CA-C	5.29	120.99	111.36
1	A	54	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	14	TYR	N-CA-CB	5.20	118.34	110.28
1	A	41	ASP	N-CA-C	-5.20	104.11	110.61
1	A	85	SER	CA-C-N	5.20	127.77	120.28
1	A	85	SER	C-N-CA	5.20	127.77	120.28
1	B	20	PRO	CA-CB-CG	-5.18	94.67	104.50
1	B	49	ILE	CA-C-N	5.17	129.62	121.09
1	B	49	ILE	C-N-CA	5.17	129.62	121.09
1	B	118	ASN	CA-C-O	-5.16	113.14	120.51
1	A	41	ASP	CA-C-N	5.15	131.38	121.54
1	A	41	ASP	C-N-CA	5.15	131.38	121.54
1	B	23	ALA	CA-C-O	-5.15	113.14	120.51
1	B	79	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	B	110	ILE	CA-C-O	-5.13	113.82	120.03
1	A	9	GLU	N-CA-C	-5.12	105.82	111.71
1	B	116	VAL	CB-CA-C	-5.12	102.89	111.29
1	A	102	ASP	N-CA-CB	-5.11	101.86	110.49
1	A	72	ILE	CA-CB-CG2	5.09	119.15	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	19	SER	Peptide,Mainchain
1	B	26	GLY	Peptide,Mainchain

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	990	0	1001	244	1
1	B	990	0	1002	246	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	0	12	0
2	B	23	0	0	15	0
All	All	2023	0	2003	445	1

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 112.

All (445) 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:8:ILE:HA	2:A:443:HOH:O	1.42	1.17
1:A:19:SER:HB3	1:A:20:PRO:CD	1.74	1.16
1:A:19:SER:CB	1:A:20:PRO:HD3	1.75	1.16
1:A:8:ILE:HD13	1:A:69:SER:HB3	1.25	1.10
1:A:105:ILE:HD12	1:B:28:LEU:HG	1.28	1.09
1:A:44:ILE:HG23	1:B:82:LEU:HD13	1.30	1.06
1:B:8:ILE:HD12	1:B:72:ILE:CG2	1.87	1.04
1:B:79:GLN:HA	1:B:83:ASN:HB2	1.39	1.03
1:A:19:SER:HB3	1:A:20:PRO:HD3	1.02	1.02
1:A:22:VAL:O	1:A:24:LYS:N	1.92	1.01
1:A:3:GLN:HG3	1:A:4:PHE:H	1.23	0.99
1:B:3:GLN:HB3	1:B:6:ARG:NH1	1.76	0.99
1:A:28:LEU:O	1:A:32:ILE:HD13	1.64	0.98
1:A:114:ILE:HG23	2:A:407:HOH:O	1.64	0.97
1:B:118:ASN:O	1:B:119:ASP:HB2	1.59	0.97
1:B:28:LEU:O	1:B:32:ILE:HG12	1.65	0.97
1:A:69:SER:HA	1:A:72:ILE:HG22	1.46	0.96
1:B:37:LYS:H	1:B:37:LYS:HD3	1.27	0.96
1:A:61:LYS:HA	1:A:67:GLN:NE2	1.80	0.95
1:A:82:LEU:HD13	1:A:84:GLY:H	1.31	0.94
1:A:92:PHE:HA	1:A:95:LEU:HB2	1.51	0.92
1:A:117:MET:O	1:A:118:ASN:HB2	1.67	0.92
1:B:62:ASP:HB3	1:B:66:ILE:HB	1.50	0.89
1:A:18:SER:O	1:A:19:SER:HB2	1.70	0.89
1:A:36:TRP:HE1	1:A:45:ILE:HD13	1.34	0.89
1:A:47:SER:HB3	1:B:44:ILE:HD13	1.55	0.88
1:A:105:ILE:HG12	1:B:29:PHE:CD2	2.08	0.88
1:A:86:SER:HB3	2:A:416:HOH:O	1.74	0.86
1:A:44:ILE:HD12	1:A:45:ILE:HG13	1.59	0.85
1:B:88:LYS:HD2	1:B:91:ASP:HB2	1.57	0.84
1:A:8:ILE:HG22	2:A:401:HOH:O	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:GLU:HA	1:B:10:ASN:ND2	1.93	0.84
1:B:52:PHE:HE1	1:B:56:LEU:HD13	1.43	0.84
1:A:44:ILE:HG13	1:A:45:ILE:H	1.43	0.83
1:B:3:GLN:O	1:B:5:PHE:N	2.10	0.83
1:B:55:LYS:O	2:B:438:HOH:O	1.95	0.83
1:A:55:LYS:HB2	1:A:55:LYS:NZ	1.92	0.83
1:B:32:ILE:HG22	1:B:33:LEU:HD12	1.60	0.82
1:B:113:LEU:O	1:B:116:VAL:HG23	1.79	0.82
1:B:18:SER:O	1:B:19:SER:HB3	1.79	0.81
1:A:105:ILE:HD11	1:B:29:PHE:HB2	1.62	0.81
1:B:89:LEU:HD23	2:B:420:HOH:O	1.80	0.81
1:A:82:LEU:HD13	1:A:84:GLY:N	1.96	0.80
1:B:36:TRP:N	1:B:36:TRP:HE3	1.80	0.80
1:A:82:LEU:CD1	1:A:84:GLY:H	1.94	0.80
1:A:44:ILE:CG1	1:A:45:ILE:H	1.91	0.80
1:B:67:GLN:HG3	1:B:68:ARG:N	1.98	0.78
1:B:81:PHE:HB3	2:B:425:HOH:O	1.83	0.78
1:B:56:LEU:HD12	1:B:59:ASN:ND2	2.00	0.77
1:B:26:GLY:HA3	1:B:28:LEU:HD22	1.65	0.77
1:A:70:MET:HA	1:A:73:ILE:CD1	2.15	0.77
1:B:24:LYS:O	1:B:26:GLY:N	2.17	0.76
1:A:82:LEU:HB3	1:A:88:LYS:HD3	1.67	0.76
1:A:11:LEU:O	1:A:14:TYR:N	2.17	0.76
1:B:116:VAL:HG12	1:B:117:MET:HG3	1.66	0.76
1:A:11:LEU:HD13	1:A:14:TYR:HD2	1.50	0.76
1:A:108:LYS:NZ	1:A:110:ILE:HG23	2.00	0.76
1:B:64:GLN:HE21	1:B:68:ARG:NE	1.83	0.76
1:B:107:ARG:NH2	1:B:108:LYS:HA	2.01	0.76
1:A:3:GLN:CG	1:A:4:PHE:H	1.99	0.75
1:A:96:ILE:HG23	1:A:97:GLN:H	1.49	0.75
1:B:15:PHE:HZ	1:B:73:ILE:HD13	1.50	0.75
1:B:8:ILE:HD12	1:B:72:ILE:HG23	1.66	0.75
1:B:43:LYS:O	1:B:46:GLN:HG2	1.87	0.75
1:A:54:PHE:CE1	1:A:74:LYS:HG2	2.22	0.74
1:A:105:ILE:CD1	1:B:28:LEU:HG	2.12	0.74
1:A:82:LEU:N	1:A:88:LYS:HZ2	1.85	0.74
1:A:110:ILE:O	1:A:112:GLU:HG2	1.87	0.74
1:B:62:ASP:OD2	1:B:66:ILE:HD12	1.88	0.74
1:A:53:TYR:CE1	1:B:109:ALA:HA	2.23	0.73
1:B:28:LEU:HA	1:B:31:GLU:HG3	1.70	0.73
1:B:37:LYS:HD3	1:B:37:LYS:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:PHE:CZ	1:B:56:LEU:HD22	2.24	0.73
1:A:48:GLN:HE22	1:B:48:GLN:HE22	1.37	0.73
1:A:91:ASP:C	1:A:95:LEU:HD12	2.14	0.73
1:B:37:LYS:H	1:B:37:LYS:CD	1.95	0.73
1:A:62:ASP:OD1	1:A:65:VAL:HB	1.89	0.72
1:B:81:PHE:O	1:B:82:LEU:HD12	1.88	0.72
1:A:53:TYR:CZ	1:B:109:ALA:HA	2.24	0.72
1:B:12:LYS:HA	1:B:15:PHE:CD2	2.24	0.72
1:B:61:LYS:HB2	2:B:424:HOH:O	1.89	0.72
1:A:57:PHE:HB3	1:A:70:MET:HG3	1.71	0.72
1:B:35:ASN:O	1:B:38:ASP:OD1	2.07	0.72
1:B:8:ILE:HD12	1:B:72:ILE:HG22	1.72	0.71
1:A:43:LYS:HG3	1:A:44:ILE:H	1.55	0.71
1:A:105:ILE:HG12	1:B:29:PHE:HD2	1.56	0.70
1:A:112:GLU:HG3	1:B:80:LYS:HE2	1.71	0.70
1:A:81:PHE:HB3	1:A:88:LYS:HZ2	1.55	0.70
1:A:81:PHE:HB3	1:A:88:LYS:NZ	2.07	0.70
1:B:26:GLY:CA	1:B:28:LEU:HD22	2.21	0.70
1:B:50:VAL:O	1:B:54:PHE:HD1	1.73	0.70
1:A:7:GLU:O	1:A:10:ASN:OD1	2.08	0.70
2:A:426:HOH:O	1:B:50:VAL:HG22	1.91	0.69
1:B:8:ILE:HD13	2:B:409:HOH:O	1.92	0.69
1:B:32:ILE:O	1:B:36:TRP:CH2	2.45	0.69
1:B:36:TRP:N	1:B:36:TRP:CE3	2.61	0.69
1:B:108:LYS:HZ1	1:B:111:ASN:HB2	1.57	0.69
1:A:57:PHE:HD2	1:A:74:LYS:HB2	1.56	0.69
1:A:11:LEU:HD23	2:A:402:HOH:O	1.94	0.68
1:B:108:LYS:NZ	1:B:108:LYS:O	2.26	0.68
1:A:44:ILE:HD12	1:A:45:ILE:CG1	2.23	0.68
1:A:69:SER:CA	1:A:72:ILE:HG22	2.24	0.67
1:B:10:ASN:O	1:B:13:GLU:OE1	2.11	0.67
1:A:108:LYS:HZ1	1:A:110:ILE:HG23	1.59	0.67
1:B:36:TRP:HB3	2:B:403:HOH:O	1.95	0.67
1:A:44:ILE:HG23	1:B:82:LEU:CD1	2.18	0.67
1:B:12:LYS:HG3	1:B:15:PHE:HE2	1.59	0.67
1:B:46:GLN:HA	1:B:49:ILE:CD1	2.25	0.67
1:A:8:ILE:HD13	1:A:69:SER:CB	2.14	0.66
1:A:8:ILE:HD12	1:A:8:ILE:O	1.95	0.66
1:A:36:TRP:HE3	1:A:36:TRP:H	1.40	0.66
1:B:27:PRO:HG2	1:B:31:GLU:HG2	1.76	0.66
1:A:24:LYS:O	1:A:24:LYS:HE2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLN:O	1:B:79:GLN:NE2	2.28	0.66
1:B:12:LYS:HZ2	1:B:12:LYS:N	1.94	0.66
1:B:92:PHE:C	1:B:92:PHE:CD2	2.74	0.66
1:A:18:SER:O	1:A:19:SER:CB	2.43	0.65
1:B:16:ASN:OD1	1:B:17:ALA:N	2.29	0.65
1:A:82:LEU:H	1:A:88:LYS:NZ	1.93	0.65
1:A:3:GLN:C	1:A:5:PHE:H	2.04	0.65
1:A:104:GLN:HG3	1:B:56:LEU:HD11	1.78	0.65
1:A:82:LEU:HD12	1:A:88:LYS:CG	2.27	0.65
1:A:111:ASN:HD22	1:A:112:GLU:H	1.43	0.64
1:A:33:LEU:HD23	1:A:49:ILE:HD13	1.78	0.64
1:A:44:ILE:HG13	1:A:45:ILE:N	2.12	0.64
1:A:47:SER:HB3	1:B:44:ILE:CD1	2.26	0.64
1:A:82:LEU:HB3	1:A:88:LYS:NZ	2.13	0.64
1:B:61:LYS:O	1:B:61:LYS:HG2	1.95	0.64
1:A:57:PHE:CG	1:A:70:MET:HB2	2.32	0.64
1:A:76:ASP:O	1:A:79:GLN:HG2	1.98	0.64
1:B:42:LYS:HZ1	1:B:45:ILE:HG23	1.63	0.64
1:A:14:TYR:HB3	1:A:66:ILE:HD11	1.80	0.63
1:A:99:PRO:O	1:A:100:VAL:O	2.17	0.63
1:B:97:GLN:O	1:B:99:PRO:HD3	1.96	0.63
1:B:12:LYS:HZ3	1:B:73:ILE:HD11	1.62	0.63
1:B:13:GLU:HA	1:B:16:ASN:ND2	2.14	0.63
1:A:7:GLU:C	1:A:10:ASN:HB3	2.24	0.63
1:B:28:LEU:HD23	1:B:29:PHE:H	1.63	0.63
1:A:11:LEU:HD13	1:A:14:TYR:CD2	2.32	0.62
1:A:36:TRP:NE1	1:A:45:ILE:HD13	2.12	0.62
1:B:89:LEU:HD12	2:B:433:HOH:O	1.99	0.62
1:A:101:ASP:C	1:A:103:LEU:H	2.07	0.62
1:B:24:LYS:HD2	1:B:25:GLY:H	1.64	0.62
1:A:80:LYS:NZ	1:B:113:LEU:O	2.32	0.62
1:A:108:LYS:HB3	1:B:29:PHE:CE1	2.35	0.61
1:B:52:PHE:CE1	1:B:56:LEU:HD13	2.30	0.61
1:A:51:SER:O	1:A:55:LYS:NZ	2.34	0.61
1:A:69:SER:O	1:A:73:ILE:CD1	2.49	0.61
1:B:111:ASN:O	1:B:114:ILE:HG22	2.00	0.61
1:A:67:GLN:NE2	1:A:70:MET:SD	2.74	0.61
1:A:14:TYR:HB3	1:A:66:ILE:CD1	2.31	0.60
1:B:88:LYS:HD2	1:B:88:LYS:O	2.01	0.60
1:A:36:TRP:CE3	1:A:36:TRP:N	2.68	0.60
1:B:3:GLN:HB3	1:B:6:ARG:HH12	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HB2	1:A:55:LYS:HZ3	1.64	0.60
1:A:107:ARG:C	1:A:109:ALA:H	2.08	0.60
1:B:45:ILE:HG13	1:B:46:GLN:OE1	2.01	0.60
1:B:108:LYS:HZ3	1:B:108:LYS:CA	2.14	0.60
1:A:28:LEU:C	1:A:32:ILE:HD13	2.26	0.60
1:A:44:ILE:CG2	1:B:82:LEU:HD22	2.32	0.60
1:B:26:GLY:C	1:B:28:LEU:HD22	2.27	0.60
1:A:70:MET:HA	1:A:73:ILE:HD11	1.83	0.60
1:B:12:LYS:HG3	1:B:15:PHE:CE2	2.37	0.60
1:B:108:LYS:HA	1:B:108:LYS:HZ3	1.66	0.60
1:A:82:LEU:N	1:A:88:LYS:NZ	2.49	0.60
1:B:54:PHE:CE1	1:B:77:MET:HE3	2.36	0.60
1:B:76:ASP:HA	1:B:79:GLN:NE2	2.17	0.60
1:A:105:ILE:HB	2:A:429:HOH:O	2.02	0.60
1:A:40:SER:C	1:A:42:LYS:HZ3	2.09	0.59
1:B:11:LEU:HD22	1:B:69:SER:OG	2.02	0.59
1:B:46:GLN:O	1:B:49:ILE:HG12	2.02	0.59
1:B:36:TRP:CB	1:B:37:LYS:HD3	2.31	0.59
1:A:48:GLN:OE1	1:B:95:LEU:HD22	2.02	0.59
1:B:58:GLU:N	2:B:413:HOH:O	2.35	0.59
1:A:8:ILE:HG13	1:A:12:LYS:HZ1	1.68	0.59
1:A:53:TYR:O	1:A:56:LEU:HB3	2.02	0.59
1:A:44:ILE:HG12	1:B:82:LEU:HD22	1.85	0.59
1:B:3:GLN:C	1:B:5:PHE:H	2.09	0.59
1:A:3:GLN:HG3	1:A:4:PHE:N	2.05	0.59
1:B:23:ALA:O	1:B:24:LYS:HB2	2.02	0.59
1:A:57:PHE:HB3	1:A:70:MET:CG	2.32	0.59
1:B:24:LYS:C	1:B:26:GLY:N	2.57	0.59
1:B:83:ASN:O	1:B:83:ASN:ND2	2.33	0.59
1:A:36:TRP:HE1	1:A:45:ILE:CD1	2.11	0.58
1:A:82:LEU:HB3	1:A:88:LYS:CD	2.33	0.58
1:B:36:TRP:HB2	1:B:37:LYS:HD3	1.85	0.58
1:A:5:PHE:HA	1:A:9:GLU:OE2	2.03	0.58
1:A:36:TRP:CD1	1:A:45:ILE:HG21	2.38	0.58
1:B:24:LYS:C	1:B:26:GLY:H	2.09	0.58
1:B:108:LYS:NZ	1:B:111:ASN:HB2	2.19	0.58
1:B:107:ARG:HH21	1:B:108:LYS:HA	1.68	0.58
1:A:82:LEU:HD13	1:A:83:ASN:N	2.20	0.57
1:A:105:ILE:HD11	1:B:29:PHE:CB	2.33	0.57
1:B:70:MET:O	1:B:74:LYS:HB2	2.03	0.57
1:A:42:LYS:O	1:A:44:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:HA	1:A:10:ASN:OD1	2.05	0.57
1:B:107:ARG:NH2	1:B:108:LYS:HE2	2.20	0.57
1:A:82:LEU:HD12	1:A:88:LYS:HD3	1.87	0.56
1:A:44:ILE:HG12	1:B:82:LEU:CD2	2.35	0.56
1:B:15:PHE:CZ	1:B:73:ILE:HD13	2.36	0.56
1:A:92:PHE:N	1:A:95:LEU:HD12	2.20	0.56
1:B:92:PHE:HB3	2:B:433:HOH:O	2.05	0.56
1:B:107:ARG:C	1:B:107:ARG:HE	2.13	0.56
1:B:114:ILE:C	1:B:116:VAL:H	2.14	0.56
1:A:52:PHE:O	1:A:52:PHE:CD1	2.59	0.56
1:B:67:GLN:O	1:B:70:MET:HG2	2.06	0.56
1:A:42:LYS:HZ3	1:A:42:LYS:H	1.52	0.55
1:A:60:LEU:O	1:A:70:MET:HE1	2.06	0.55
1:A:61:LYS:O	1:A:63:ASN:N	2.39	0.55
1:A:22:VAL:HG13	1:A:24:LYS:HB2	1.87	0.55
1:B:62:ASP:CB	1:B:66:ILE:HB	2.32	0.55
1:A:57:PHE:CE2	1:A:73:ILE:HD13	2.41	0.55
1:B:111:ASN:O	1:B:113:LEU:N	2.40	0.55
1:A:87:GLU:OE1	1:A:87:GLU:HA	2.08	0.54
1:A:42:LYS:H	1:A:42:LYS:NZ	2.05	0.54
1:A:43:LYS:CG	1:A:44:ILE:H	2.20	0.54
1:B:45:ILE:HD12	1:B:49:ILE:HG23	1.90	0.54
1:B:116:VAL:HG12	1:B:117:MET:N	2.21	0.54
1:B:100:VAL:HG12	1:B:100:VAL:O	2.07	0.54
1:A:91:ASP:O	1:A:94:LYS:HB3	2.07	0.54
1:B:5:PHE:O	1:B:9:GLU:HG2	2.08	0.54
1:A:44:ILE:CG1	1:B:82:LEU:HD22	2.37	0.54
1:A:44:ILE:CG2	1:B:82:LEU:HD13	2.22	0.54
1:A:48:GLN:NE2	1:B:48:GLN:HE22	2.04	0.54
1:B:28:LEU:O	1:B:32:ILE:N	2.30	0.54
1:B:89:LEU:HA	2:B:433:HOH:O	2.07	0.54
1:B:24:LYS:CD	1:B:25:GLY:H	2.21	0.53
1:B:94:LYS:HE2	1:B:95:LEU:HD23	1.90	0.53
1:A:105:ILE:O	1:A:107:ARG:N	2.31	0.53
1:B:101:ASP:C	1:B:103:LEU:H	2.16	0.53
1:A:22:VAL:O	1:A:23:ALA:C	2.51	0.53
1:A:95:LEU:CD2	1:B:48:GLN:HB3	2.38	0.53
1:A:105:ILE:HD11	1:B:29:PHE:H	1.71	0.53
1:B:5:PHE:HB3	1:B:9:GLU:CD	2.33	0.53
1:B:107:ARG:HH21	1:B:110:ILE:HG22	1.73	0.53
1:A:82:LEU:HB3	1:A:88:LYS:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:SER:C	1:A:42:LYS:NZ	2.67	0.53
1:B:64:GLN:HE21	1:B:68:ARG:CZ	2.21	0.53
1:A:94:LYS:C	1:A:96:ILE:H	2.17	0.53
1:A:41:ASP:N	1:A:42:LYS:HZ3	2.07	0.53
1:B:91:ASP:O	1:B:95:LEU:HG	2.09	0.52
1:B:96:ILE:O	1:B:97:GLN:CB	2.57	0.52
1:B:112:GLU:CD	1:B:112:GLU:O	2.51	0.52
1:B:99:PRO:O	1:B:104:GLN:NE2	2.42	0.52
1:A:11:LEU:C	1:A:13:GLU:N	2.65	0.52
1:A:21:ASP:OD1	1:A:24:LYS:HB2	2.10	0.52
1:A:66:ILE:O	1:A:68:ARG:N	2.43	0.52
1:A:87:GLU:OE1	1:A:87:GLU:CA	2.57	0.52
1:B:100:VAL:O	1:B:101:ASP:O	2.28	0.52
1:B:5:PHE:N	1:B:5:PHE:CD1	2.76	0.52
1:B:5:PHE:HB3	1:B:9:GLU:CG	2.39	0.52
1:B:64:GLN:NE2	1:B:68:ARG:NE	2.55	0.52
1:A:33:LEU:CD2	1:A:49:ILE:HD13	2.40	0.51
1:B:79:GLN:HG3	1:B:83:ASN:OD1	2.11	0.51
1:B:96:ILE:O	1:B:97:GLN:HB3	2.10	0.51
1:A:9:GLU:O	1:A:12:LYS:HG2	2.10	0.51
1:A:61:LYS:CA	1:A:67:GLN:NE2	2.64	0.51
1:A:95:LEU:HD11	1:B:45:ILE:CG2	2.41	0.51
1:B:12:LYS:HZ2	1:B:12:LYS:H	1.57	0.51
1:B:101:ASP:N	1:B:104:GLN:OE1	2.43	0.51
1:B:117:MET:C	1:B:119:ASP:H	2.18	0.51
1:A:110:ILE:HD11	1:A:113:LEU:HD11	1.91	0.51
1:B:12:LYS:N	1:B:12:LYS:NZ	2.57	0.51
1:B:29:PHE:HZ	1:B:53:TYR:OH	1.92	0.51
1:A:6:ARG:O	1:A:10:ASN:HB2	2.11	0.51
1:B:76:ASP:O	1:B:79:GLN:HB2	2.10	0.51
1:A:16:ASN:O	1:A:17:ALA:HB3	2.11	0.51
1:A:86:SER:O	1:A:89:LEU:HB3	2.10	0.51
1:A:92:PHE:HA	1:A:95:LEU:HD12	1.93	0.51
1:B:12:LYS:HE3	1:B:15:PHE:CE2	2.46	0.51
1:A:54:PHE:CD1	1:A:74:LYS:HG2	2.45	0.51
1:A:111:ASN:ND2	1:A:112:GLU:H	2.08	0.51
1:A:43:LYS:CG	1:A:44:ILE:N	2.74	0.50
1:A:43:LYS:HE3	1:B:43:LYS:HB3	1.94	0.50
1:A:108:LYS:HZ3	1:A:110:ILE:HG23	1.77	0.50
1:B:4:PHE:CE1	1:B:8:ILE:HG21	2.47	0.50
1:B:12:LYS:HA	1:B:15:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:HA	1:A:74:LYS:HD2	1.94	0.50
2:A:437:HOH:O	1:B:15:PHE:HB2	2.10	0.50
1:B:44:ILE:HG13	1:B:45:ILE:N	2.27	0.50
1:B:56:LEU:HA	1:B:59:ASN:HD22	1.77	0.50
1:B:79:GLN:CG	1:B:83:ASN:OD1	2.59	0.50
1:A:11:LEU:HD22	1:A:14:TYR:CD2	2.46	0.50
1:A:70:MET:HA	1:A:73:ILE:HD12	1.92	0.50
1:B:37:LYS:O	1:B:39:GLU:N	2.45	0.50
1:B:59:ASN:OD1	1:B:60:LEU:HD23	2.12	0.50
1:A:112:GLU:CG	1:B:80:LYS:HE2	2.41	0.49
1:B:57:PHE:HB3	1:B:70:MET:HB2	1.94	0.49
1:A:70:MET:CA	1:A:73:ILE:HD12	2.42	0.49
1:A:77:MET:HA	1:A:80:LYS:HG2	1.92	0.49
1:A:105:ILE:CD1	1:B:29:PHE:HB2	2.39	0.49
1:A:105:ILE:CG1	1:B:29:PHE:CD2	2.89	0.49
1:A:106:GLN:C	1:B:29:PHE:HE2	2.21	0.49
1:A:19:SER:CB	1:A:20:PRO:CD	2.52	0.49
1:A:22:VAL:C	1:A:24:LYS:N	2.69	0.49
1:A:82:LEU:HD12	1:A:88:LYS:HG3	1.93	0.49
1:B:94:LYS:C	1:B:96:ILE:H	2.20	0.49
1:A:32:ILE:C	1:A:34:LYS:H	2.21	0.49
1:A:34:LYS:HE3	1:A:34:LYS:HA	1.94	0.49
1:A:52:PHE:O	1:A:56:LEU:HB2	2.13	0.49
1:A:66:ILE:O	1:A:67:GLN:C	2.56	0.49
1:A:106:GLN:O	1:A:109:ALA:HB2	2.12	0.49
1:B:18:SER:O	1:B:19:SER:CB	2.54	0.49
1:B:32:ILE:HG22	1:B:33:LEU:N	2.28	0.49
1:B:50:VAL:HA	1:B:53:TYR:HB2	1.94	0.49
1:A:63:ASN:O	1:A:63:ASN:ND2	2.46	0.49
1:A:110:ILE:HG13	2:A:435:HOH:O	2.13	0.49
1:A:56:LEU:HD12	1:A:57:PHE:CE1	2.48	0.49
1:A:61:LYS:HA	1:A:67:GLN:HE21	1.70	0.49
1:A:83:ASN:H	1:A:88:LYS:HZ3	1.60	0.48
1:A:117:MET:O	1:A:118:ASN:CB	2.46	0.48
1:A:91:ASP:O	1:A:95:LEU:HG	2.14	0.48
1:B:28:LEU:CA	1:B:31:GLU:HG3	2.42	0.48
1:A:8:ILE:HG13	1:A:12:LYS:NZ	2.29	0.48
1:A:88:LYS:O	1:A:91:ASP:OD1	2.31	0.48
2:A:410:HOH:O	1:B:56:LEU:HD21	2.13	0.48
1:A:14:TYR:HB3	1:A:66:ILE:CG1	2.42	0.48
1:A:14:TYR:HB3	1:A:66:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLN:C	1:B:79:GLN:HE22	2.19	0.48
1:B:101:ASP:C	1:B:103:LEU:N	2.69	0.48
1:A:29:PHE:HA	1:A:32:ILE:HB	1.96	0.48
1:A:95:LEU:HD22	1:B:48:GLN:HB3	1.96	0.48
1:B:28:LEU:C	1:B:32:ILE:HG12	2.35	0.48
1:B:92:PHE:O	1:B:92:PHE:CG	2.64	0.48
1:B:114:ILE:C	1:B:116:VAL:N	2.68	0.48
1:A:74:LYS:HA	1:A:77:MET:HG2	1.94	0.47
1:B:5:PHE:N	1:B:5:PHE:HD1	2.11	0.47
1:A:108:LYS:NZ	1:A:111:ASN:H	2.12	0.47
1:A:48:GLN:HE22	1:B:48:GLN:NE2	2.09	0.47
1:A:70:MET:HG2	1:A:71:ASP:N	2.30	0.47
1:B:46:GLN:O	1:B:49:ILE:CG1	2.62	0.47
1:B:56:LEU:HD12	1:B:59:ASN:HD22	1.78	0.47
1:A:67:GLN:O	1:A:70:MET:HG2	2.14	0.47
1:A:108:LYS:HZ2	1:A:111:ASN:H	1.62	0.47
1:B:62:ASP:O	1:B:67:GLN:N	2.43	0.47
1:A:42:LYS:HB3	2:A:422:HOH:O	2.13	0.47
1:A:37:LYS:O	1:A:37:LYS:HG2	2.15	0.47
1:A:43:LYS:NZ	1:A:115:LYS:NZ	2.63	0.47
1:B:6:ARG:H	1:B:6:ARG:HD3	1.79	0.47
1:A:57:PHE:CD1	1:A:70:MET:HB2	2.50	0.47
1:A:82:LEU:CB	1:A:88:LYS:HD3	2.42	0.47
1:B:11:LEU:CD1	2:B:411:HOH:O	2.63	0.47
1:B:105:ILE:O	1:B:107:ARG:N	2.43	0.47
1:A:53:TYR:O	1:A:56:LEU:CB	2.63	0.47
1:A:105:ILE:CD1	1:B:29:PHE:CB	2.92	0.47
1:A:44:ILE:HG21	1:B:82:LEU:HD22	1.97	0.46
1:A:95:LEU:HD11	1:B:45:ILE:HG21	1.97	0.46
1:B:24:LYS:CG	1:B:25:GLY:N	2.79	0.46
1:A:89:LEU:HD23	1:A:90:GLU:N	2.30	0.46
1:B:108:LYS:NZ	1:B:111:ASN:CB	2.78	0.46
1:A:92:PHE:CA	1:A:95:LEU:HD12	2.46	0.46
1:B:107:ARG:HH21	1:B:110:ILE:CG2	2.28	0.46
1:A:8:ILE:HG12	1:A:73:ILE:HG13	1.98	0.46
1:B:52:PHE:HA	1:B:55:LYS:HD2	1.96	0.46
1:A:6:ARG:NH2	2:A:401:HOH:O	2.48	0.46
1:A:104:GLN:HG2	1:A:104:GLN:O	2.15	0.46
1:A:55:LYS:HB2	1:A:55:LYS:HZ2	1.76	0.46
1:B:32:ILE:HG22	1:B:33:LEU:CD1	2.39	0.46
1:B:108:LYS:HZ3	1:B:108:LYS:C	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:GLN:HA	1:B:51:SER:HB2	1.97	0.46
1:A:80:LYS:NZ	1:B:113:LEU:HA	2.31	0.45
1:A:5:PHE:CG	1:A:6:ARG:N	2.84	0.45
1:B:26:GLY:HA3	1:B:28:LEU:CD2	2.40	0.45
1:B:77:MET:HG3	2:B:412:HOH:O	2.15	0.45
1:A:82:LEU:HD12	1:A:88:LYS:CD	2.46	0.45
1:B:56:LEU:HD12	1:B:59:ASN:HD21	1.75	0.45
1:A:26:GLY:HA2	1:A:27:PRO:HD3	1.59	0.45
1:A:8:ILE:O	1:A:12:LYS:NZ	2.49	0.45
1:A:70:MET:CG	1:A:71:ASP:N	2.79	0.45
1:B:37:LYS:O	1:B:38:ASP:C	2.59	0.45
1:B:76:ASP:C	1:B:79:GLN:HE21	2.25	0.45
1:B:10:ASN:C	1:B:10:ASN:OD1	2.59	0.45
1:B:108:LYS:O	1:B:109:ALA:C	2.58	0.45
1:B:107:ARG:HH22	1:B:108:LYS:HE2	1.81	0.45
1:B:110:ILE:O	1:B:110:ILE:HG13	2.17	0.45
1:B:115:LYS:HD2	1:B:115:LYS:O	2.16	0.45
1:A:102:ASP:O	1:A:103:LEU:HB2	2.16	0.45
1:B:36:TRP:HB2	1:B:37:LYS:CE	2.47	0.45
1:B:56:LEU:HA	1:B:59:ASN:ND2	2.32	0.45
1:A:52:PHE:O	1:A:52:PHE:CG	2.71	0.44
1:A:106:GLN:CA	1:B:29:PHE:HE2	2.30	0.44
1:B:15:PHE:C	1:B:17:ALA:N	2.74	0.44
1:A:91:ASP:O	1:A:94:LYS:CB	2.66	0.44
1:A:99:PRO:O	1:A:103:LEU:HB3	2.17	0.44
1:B:46:GLN:HA	1:B:49:ILE:HD11	1.97	0.44
1:A:50:VAL:HG12	1:A:81:PHE:CE1	2.53	0.43
1:A:52:PHE:CE1	1:A:55:LYS:HB3	2.53	0.43
1:A:79:GLN:HG3	1:A:80:LYS:HD2	2.00	0.43
1:B:59:ASN:ND2	2:B:438:HOH:O	2.48	0.43
1:A:70:MET:CA	1:A:73:ILE:CD1	2.92	0.43
1:B:68:ARG:O	1:B:71:ASP:HB3	2.18	0.43
1:A:48:GLN:HG2	1:B:95:LEU:CD2	2.48	0.43
1:B:46:GLN:C	1:B:49:ILE:HG12	2.44	0.43
1:B:78:PHE:CE1	1:B:89:LEU:HD13	2.53	0.43
1:A:105:ILE:HD11	1:B:29:PHE:N	2.34	0.43
1:B:34:LYS:CG	1:B:35:ASN:H	2.32	0.43
1:B:108:LYS:HZ1	1:B:111:ASN:CB	2.30	0.43
1:A:80:LYS:NZ	1:B:113:LEU:C	2.77	0.43
1:B:70:MET:HB3	1:B:70:MET:HE3	1.76	0.43
1:B:11:LEU:HD12	2:B:411:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LYS:HE3	1:B:15:PHE:CZ	2.54	0.42
1:B:11:LEU:O	1:B:14:TYR:HB2	2.19	0.42
1:A:108:LYS:HB3	1:B:29:PHE:CD1	2.55	0.42
1:A:33:LEU:HD23	1:A:49:ILE:CD1	2.48	0.42
1:A:113:LEU:HD11	1:B:5:PHE:HE2	1.84	0.42
1:B:76:ASP:HB3	2:B:412:HOH:O	2.19	0.42
1:A:11:LEU:O	1:A:14:TYR:HB2	2.20	0.42
1:A:87:GLU:OE1	1:A:87:GLU:N	2.52	0.42
1:B:11:LEU:O	1:B:12:LYS:C	2.62	0.42
1:B:101:ASP:H	1:B:104:GLN:HE22	1.66	0.42
1:B:110:ILE:O	1:B:110:ILE:CG1	2.67	0.42
1:B:46:GLN:NE2	1:B:49:ILE:HD13	2.35	0.42
1:B:87:GLU:O	1:B:89:LEU:N	2.52	0.42
1:A:106:GLN:O	1:A:107:ARG:C	2.63	0.42
1:A:91:ASP:O	1:A:95:LEU:CG	2.68	0.41
1:B:56:LEU:HD12	1:B:56:LEU:HA	1.84	0.41
1:B:76:ASP:CA	1:B:79:GLN:NE2	2.83	0.41
1:A:37:LYS:O	1:A:39:GLU:N	2.53	0.41
1:A:87:GLU:N	1:A:87:GLU:CD	2.79	0.41
1:B:100:VAL:C	1:B:101:ASP:O	2.62	0.41
1:B:67:GLN:CG	1:B:68:ARG:N	2.71	0.41
1:A:101:ASP:O	1:A:103:LEU:N	2.50	0.41
1:B:42:LYS:HG3	1:B:44:ILE:HG23	2.02	0.41
1:B:52:PHE:CE1	1:B:56:LEU:HD22	2.55	0.41
1:A:21:ASP:CG	1:A:22:VAL:O	2.64	0.41
1:A:42:LYS:HB2	1:A:43:LYS:H	1.33	0.41
1:A:56:LEU:HD22	1:A:56:LEU:HA	1.93	0.41
1:B:24:LYS:CD	1:B:25:GLY:N	2.84	0.41
1:A:7:GLU:CA	1:A:10:ASN:OD1	2.68	0.41
1:A:32:ILE:HG22	1:A:33:LEU:N	2.36	0.41
1:A:101:ASP:C	1:A:103:LEU:N	2.75	0.41
1:A:105:ILE:CD1	1:B:29:PHE:N	2.84	0.41
1:B:14:TYR:HD1	1:B:14:TYR:HA	1.76	0.41
1:B:67:GLN:HG3	1:B:68:ARG:H	1.80	0.41
1:B:107:ARG:NH2	1:B:110:ILE:CG2	2.84	0.41
1:A:44:ILE:HD12	1:A:45:ILE:CD1	2.50	0.41
1:A:61:LYS:C	1:A:67:GLN:HE21	2.29	0.41
1:A:62:ASP:OD1	1:A:66:ILE:N	2.48	0.40
1:A:71:ASP:O	1:A:75:GLN:HB2	2.20	0.40
1:B:111:ASN:C	1:B:113:LEU:H	2.29	0.40
1:A:6:ARG:H	1:A:6:ARG:HG3	1.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD22	1:A:29:PHE:CE1	2.55	0.40
1:A:32:ILE:O	1:A:36:TRP:CZ3	2.73	0.40
1:B:5:PHE:HB3	1:B:9:GLU:HG2	2.03	0.40
1:B:118:ASN:O	1:B:118:ASN:ND2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASN:O	1:B:68:ARG:NH1[3_655]	2.11	0.09

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	117/119 (98%)	65 (56%)	20 (17%)	32 (27%)	0	0
1	B	117/119 (98%)	64 (55%)	31 (26%)	22 (19%)	0	0
All	All	234/238 (98%)	129 (55%)	51 (22%)	54 (23%)	0	0

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	18	SER
1	A	19	SER
1	A	20	PRO
1	A	23	ALA
1	A	28	LEU
1	A	34	LYS
1	A	38	ASP
1	A	40	SER

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Mol	Chain	Res	Type
1	A	43	LYS
1	A	44	ILE
1	A	61	LYS
1	A	62	ASP
1	A	63	ASN
1	A	67	GLN
1	A	100	VAL
1	A	102	ASP
1	A	106	GLN
1	A	111	ASN
1	A	118	ASN
1	B	4	PHE
1	B	19	SER
1	B	20	PRO
1	B	28	LEU
1	B	32	ILE
1	B	63	ASN
1	B	100	VAL
1	B	106	GLN
1	B	112	GLU
1	A	3	GLN
1	A	42	LYS
1	A	96	ILE
1	A	103	LEU
1	A	114	ILE
1	B	23	ALA
1	B	33	LEU
1	B	44	ILE
1	B	95	LEU
1	B	97	GLN
1	B	101	ASP
1	A	33	LEU
1	B	24	LYS
1	B	38	ASP
1	B	88	LYS
1	B	105	ILE
1	B	34	LYS
1	B	36	TRP
1	A	32	ILE
1	A	36	TRP
1	A	95	LEU
1	A	98	ILE

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Mol	Chain	Res	Type
1	B	25	GLY
1	A	108	LYS
1	A	65	VAL

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	112/112 (100%)	71 (63%)	41 (37%)	0	1
1	B	112/112 (100%)	77 (69%)	35 (31%)	0	1
All	All	224/224 (100%)	148 (66%)	76 (34%)	0	1

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	6	ARG
1	A	10	ASN
1	A	13	GLU
1	A	14	TYR
1	A	15	PHE
1	A	16	ASN
1	A	19	SER
1	A	20	PRO
1	A	22	VAL
1	A	24	LYS
1	A	28	LEU
1	A	32	ILE
1	A	33	LEU
1	A	34	LYS
1	A	37	LYS
1	A	39	GLU
1	A	42	LYS
1	A	43	LYS
1	A	48	GLN

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Mol	Chain	Res	Type
1	A	49	ILE
1	A	54	PHE
1	A	55	LYS
1	A	56	LEU
1	A	68	ARG
1	A	70	MET
1	A	73	ILE
1	A	75	GLN
1	A	81	PHE
1	A	82	LEU
1	A	85	SER
1	A	87	GLU
1	A	89	LEU
1	A	90	GLU
1	A	91	ASP
1	A	94	LYS
1	A	101	ASP
1	A	106	GLN
1	A	111	ASN
1	A	116	VAL
1	A	117	MET
1	B	6	ARG
1	B	7	GLU
1	B	8	ILE
1	B	11	LEU
1	B	12	LYS
1	B	14	TYR
1	B	22	VAL
1	B	28	LEU
1	B	29	PHE
1	B	31	GLU
1	B	33	LEU
1	B	36	TRP
1	B	37	LYS
1	B	44	ILE
1	B	45	ILE
1	B	48	GLN
1	B	51	SER
1	B	52	PHE
1	B	59	ASN
1	B	67	GLN
1	B	70	MET

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Mol	Chain	Res	Type
1	B	72	ILE
1	B	78	PHE
1	B	79	GLN
1	B	82	LEU
1	B	87	GLU
1	B	94	LYS
1	B	105	ILE
1	B	107	ARG
1	B	108	LYS
1	B	113	LEU
1	B	114	ILE
1	B	115	LYS
1	B	116	VAL
1	B	118	ASN

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	63	ASN
1	A	67	GLN
1	A	79	GLN
1	A	106	GLN
1	A	111	ASN
1	B	35	ASN
1	B	48	GLN
1	B	64	GLN
1	B	79	GLN
1	B	111	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.