



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:04 AM UTC

PDB ID : 1BJM / pdb_00001bjm
Title : LOC NAKS, A LAMBDA 1 TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN) CRYSTALLIZED IN NAKSO4
Authors : Schiffer, M.; Huang, D.B.
Deposited on : 1995-05-26
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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
Mogul	:	2022.3.0, CSD as543be (2022)
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

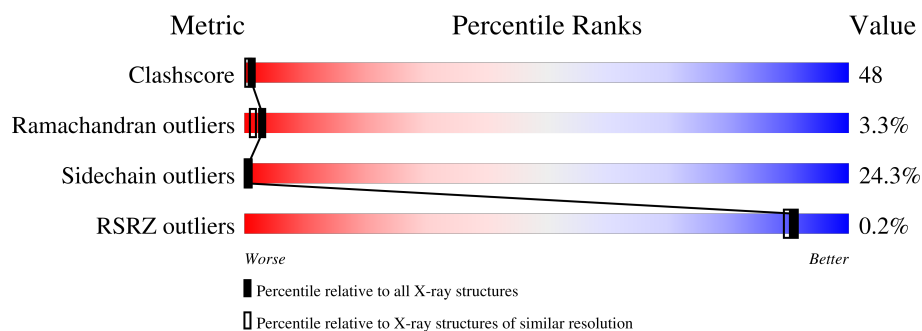
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	216	
1	B	216	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3494 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 LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1598	992	266	335	5			
1	B	216	Total	C	N	O	S	0	0	0
			1598	992	266	335	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	THR	ILE	conflict	PIR S25754
A	31	GLU	GLY	conflict	PIR S25754
A	33	SER	THR	conflict	PIR S25754
A	35	THR	ASN	conflict	PIR S25754
A	39	HIS	GLN	conflict	PIR S25754
A	41	SER	PRO	conflict	PIR S25754
A	43	THR	ARG	conflict	PIR S25754
A	50	TYR	HIS	conflict	PIR S25754
A	51	GLU	SER	conflict	PIR S25754
A	52	ASP	ASN	conflict	PIR S25754
A	54	SER	GLN	conflict	PIR S25754
A	56	ALA	PRO	conflict	PIR S25754
A	60	SER	PRO	conflict	PIR S25754
A	65	ALA	GLY	conflict	PIR S25754
A	81	PRO	SER	conflict	PIR S25754
A	85	THR	ALA	conflict	PIR S25754
A	?	-	ASN	deletion	PIR S25754
A	97	ASP	GLY	conflict	PIR S25754
A	98	VAL	ARG	conflict	PIR S25754
A	99	ALA	TYR	conflict	PIR S25754
B	19	THR	ILE	conflict	PIR S25754
B	31	GLU	GLY	conflict	PIR S25754
B	33	SER	THR	conflict	PIR S25754
B	35	THR	ASN	conflict	PIR S25754
B	39	HIS	GLN	conflict	PIR S25754

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Chain	Residue	Modelled	Actual	Comment	Reference
B	41	SER	PRO	conflict	PIR S25754
B	43	THR	ARG	conflict	PIR S25754
B	50	TYR	HIS	conflict	PIR S25754
B	51	GLU	SER	conflict	PIR S25754
B	52	ASP	ASN	conflict	PIR S25754
B	54	SER	GLN	conflict	PIR S25754
B	56	ALA	PRO	conflict	PIR S25754
B	60	SER	PRO	conflict	PIR S25754
B	65	ALA	GLY	conflict	PIR S25754
B	81	PRO	SER	conflict	PIR S25754
B	85	THR	ALA	conflict	PIR S25754
B	?	-	ASN	deletion	PIR S25754
B	97	ASP	GLY	conflict	PIR S25754
B	98	VAL	ARG	conflict	PIR S25754
B	99	ALA	TYR	conflict	PIR S25754

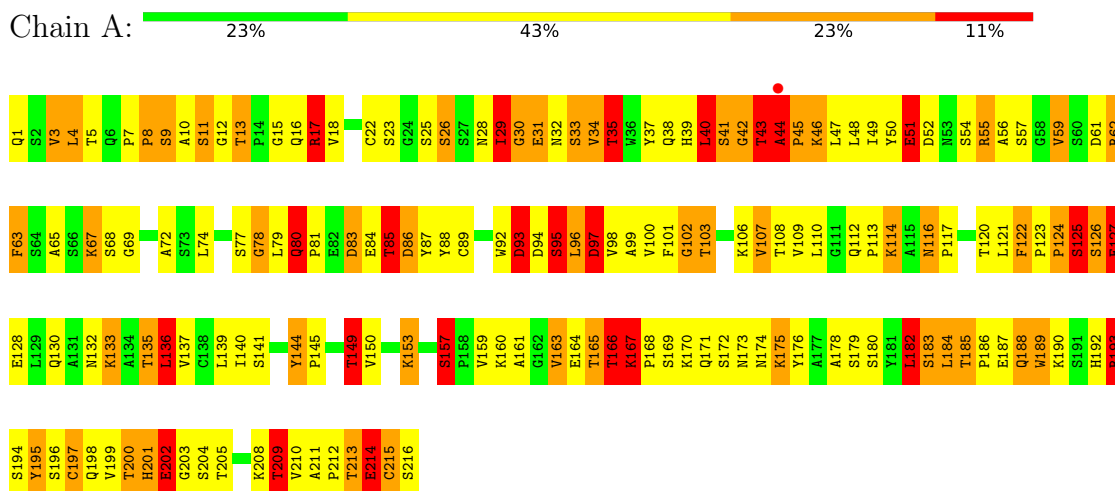
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	161	Total O 161 161	0	0
2	B	137	Total O 137 137	0	0

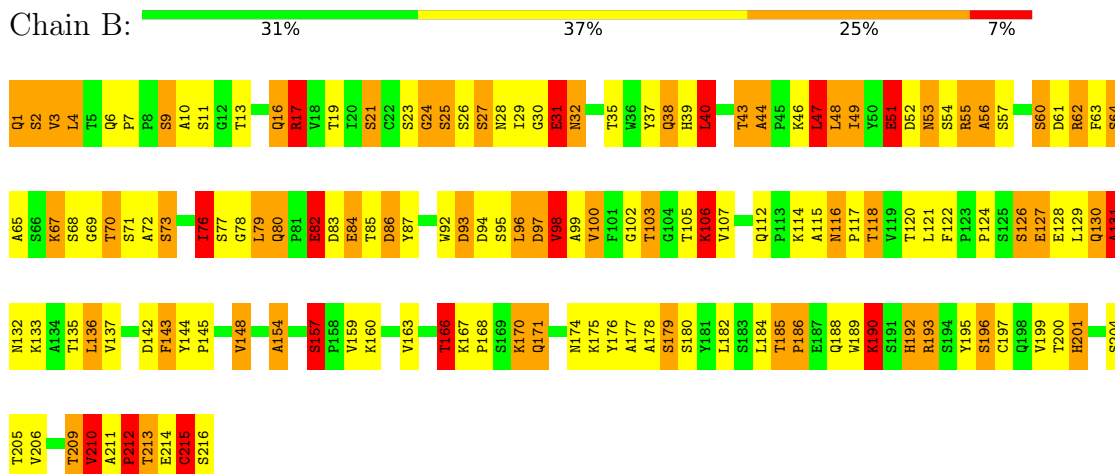
3 Residue-property plots

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: LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER



• Molecule 1: LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.87Å 72.62Å 63.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	76.3 (10.00-2.20) 72.7 (10.00-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.158 , (Not available) 0.156 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 88.3	EDS
L-test for twinning ¹	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3494	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: PCA

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	1.37	3/1628 (0.2%)	2.52	134/2226 (6.0%)
1	B	1.28	4/1628 (0.2%)	2.60	120/2226 (5.4%)
All	All	1.33	7/3256 (0.2%)	2.56	254/4452 (5.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	GLY	C-N	-13.46	1.14	1.33
1	B	24	GLY	N-CA	7.00	1.51	1.45
1	A	7	PRO	CA-C	6.57	1.55	1.51
1	A	125	SER	N-CA	6.24	1.53	1.45
1	B	2	SER	N-CA	-5.45	1.35	1.46
1	B	166	THR	CA-CB	5.16	1.61	1.53
1	B	103	THR	CB-OG1	5.01	1.51	1.43

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	CA-C-N	25.46	167.54	121.70
1	B	1	PCA	C-N-CA	25.46	167.54	121.70
1	A	127	GLU	CB-CG-CD	13.12	134.90	112.60
1	A	122	PHE	CA-CB-CG	12.98	126.78	113.80
1	A	97	ASP	CA-CB-CG	11.45	124.05	112.60
1	B	7	PRO	O-C-N	11.07	126.35	121.15
1	A	41	SER	CA-C-N	9.89	129.23	121.61
1	A	41	SER	C-N-CA	9.89	129.23	121.61
1	A	116	ASN	CB-CA-C	9.70	123.66	109.11
1	B	40	LEU	N-CA-C	-9.38	95.40	110.32
1	A	93	ASP	CA-CB-CG	-9.36	103.24	112.60
1	B	84	GLU	CB-CG-CD	9.16	128.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ASN	OD1-CG-ND2	9.10	131.70	122.60
1	B	106	LYS	CA-CB-CG	8.90	131.90	114.10
1	B	148	VAL	O-C-N	8.80	133.14	122.58
1	B	174	ASN	CA-CB-CG	-8.78	103.82	112.60
1	A	93	ASP	N-CA-C	8.74	129.43	110.80
1	A	95	SER	CA-C-O	-8.65	111.33	121.11
1	B	201	HIS	CA-CB-CG	8.65	122.45	113.80
1	B	94	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	96	LEU	N-CA-C	8.46	122.43	110.50
1	A	4	LEU	CA-C-O	8.35	130.06	120.96
1	A	157	SER	O-C-N	8.35	129.40	121.38
1	A	94	ASP	CA-C-N	8.34	135.90	122.81
1	A	94	ASP	C-N-CA	8.34	135.90	122.81
1	B	180	SER	CA-C-O	-8.24	111.17	120.32
1	B	7	PRO	N-CA-C	-8.24	101.77	110.58
1	B	69	GLY	CA-C-N	8.20	137.23	122.38
1	B	69	GLY	C-N-CA	8.20	137.23	122.38
1	A	122	PHE	O-C-N	8.14	130.43	121.23
1	B	100	VAL	CB-CA-C	8.14	122.33	110.77
1	B	148	VAL	CA-C-O	-8.11	113.30	121.49
1	A	159	VAL	N-CA-CB	8.10	122.11	111.90
1	A	95	SER	N-CA-C	-8.03	96.87	109.72
1	B	100	VAL	N-CA-CB	-7.94	101.31	111.64
1	A	63	PHE	O-C-N	7.91	132.45	123.27
1	B	40	LEU	CA-C-O	-7.77	112.04	121.36
1	A	7	PRO	O-C-N	7.76	124.88	121.31
1	A	95	SER	N-CA-CB	7.70	124.24	111.08
1	B	3	VAL	CA-C-N	7.68	133.81	123.05
1	B	3	VAL	C-N-CA	7.68	133.81	123.05
1	A	3	VAL	CA-C-N	7.66	132.00	121.05
1	A	3	VAL	C-N-CA	7.66	132.00	121.05
1	B	130	GLN	N-CA-C	-7.66	101.84	112.25
1	A	44	ALA	O-C-N	7.58	130.04	121.32
1	A	188	GLN	N-CA-C	-7.55	103.02	111.71
1	B	137	VAL	O-C-N	7.52	131.32	123.20
1	B	116	ASN	CA-CB-CG	7.50	120.10	112.60
1	B	55	ARG	CA-C-O	-7.47	112.50	120.80
1	A	166	THR	CA-CB-CG2	7.45	123.16	110.50
1	B	23	SER	CA-C-N	-7.44	114.01	122.42
1	B	23	SER	C-N-CA	-7.44	114.01	122.42
1	B	199	VAL	N-CA-CB	-7.43	101.15	111.25
1	B	9	SER	CA-C-O	7.41	129.81	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	THR	N-CA-CB	-7.41	98.22	110.23
1	A	213	THR	CB-CA-C	7.36	121.75	109.38
1	B	171	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	A	3	VAL	N-CA-CB	-7.27	99.23	111.23
1	B	31	GLU	CB-CG-CD	7.16	124.78	112.60
1	A	55	ARG	CD-NE-CZ	7.16	134.42	124.40
1	A	136	LEU	CA-C-N	-7.13	113.21	123.06
1	A	136	LEU	C-N-CA	-7.13	113.21	123.06
1	B	16	GLN	OE1-CD-NE2	7.13	129.73	122.60
1	A	86	ASP	CB-CA-C	7.04	121.55	109.51
1	B	178	ALA	CA-C-O	-6.98	113.98	121.38
1	A	9	SER	CA-C-N	6.96	134.18	121.94
1	A	9	SER	C-N-CA	6.96	134.18	121.94
1	B	62	ARG	CA-CB-CG	6.95	128.00	114.10
1	B	76	ILE	N-CA-CB	6.95	119.34	111.21
1	A	103	THR	CA-CB-OG1	-6.91	99.23	109.60
1	B	56	ALA	CA-C-O	-6.84	113.61	121.47
1	A	193	ARG	CD-NE-CZ	6.81	133.93	124.40
1	A	17	ARG	NE-CZ-NH2	6.77	125.29	119.20
1	A	46	LYS	CA-CB-CG	6.74	127.58	114.10
1	B	154	ALA	CB-CA-C	6.72	120.49	110.14
1	B	212	PRO	CA-C-N	6.72	134.38	121.54
1	B	212	PRO	C-N-CA	6.72	134.38	121.54
1	A	83	ASP	O-C-N	6.69	131.19	122.42
1	B	115	ALA	CA-C-N	6.65	129.59	120.67
1	B	115	ALA	C-N-CA	6.65	129.59	120.67
1	B	100	VAL	CA-CB-CG1	6.61	121.63	110.40
1	A	201	HIS	CB-CA-C	-6.57	102.82	111.42
1	A	137	VAL	CB-CA-C	6.53	120.35	110.62
1	A	94	ASP	CA-CB-CG	-6.51	106.09	112.60
1	A	34	VAL	O-C-N	6.50	130.20	123.18
1	A	7	PRO	N-CA-C	-6.44	104.28	110.47
1	A	26	SER	N-CA-C	-6.41	101.94	111.81
1	A	126	SER	CA-C-O	6.40	127.20	120.42
1	B	3	VAL	CA-C-O	6.38	127.89	121.64
1	A	205	THR	CA-CB-OG1	-6.36	100.06	109.60
1	B	179	SER	CA-C-O	-6.36	114.47	121.33
1	A	163	VAL	O-C-N	6.34	130.03	123.18
1	B	192	HIS	CA-CB-CG	-6.34	107.46	113.80
1	B	200	THR	CA-C-O	-6.33	113.48	120.38
1	B	210	VAL	CB-CA-C	6.30	120.20	110.50
1	B	180	SER	O-C-N	6.29	130.67	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	SER	N-CA-C	-6.27	103.15	111.24
1	A	201	HIS	N-CA-C	6.24	117.65	107.23
1	B	213	THR	N-CA-CB	6.23	121.01	110.49
1	A	8	PRO	CA-C-N	6.18	132.30	122.59
1	A	8	PRO	C-N-CA	6.18	132.30	122.59
1	B	60	SER	N-CA-CB	-6.15	101.95	110.38
1	B	82	GLU	CB-CG-CD	6.15	123.06	112.60
1	B	4	LEU	CA-C-O	6.13	127.07	120.32
1	B	55	ARG	CD-NE-CZ	-6.13	115.82	124.40
1	A	11	SER	N-CA-CB	-6.12	102.26	111.56
1	A	83	ASP	CA-CB-CG	6.10	118.70	112.60
1	B	179	SER	O-C-N	6.09	130.20	123.25
1	A	80	GLN	CB-CA-C	6.08	118.94	108.91
1	B	121	LEU	CA-C-O	-6.03	113.91	120.36
1	B	7	PRO	N-CA-CB	6.03	106.35	103.22
1	A	163	VAL	N-CA-CB	6.03	121.88	111.39
1	A	197	CYS	CA-C-O	-6.03	113.81	120.38
1	A	17	ARG	NE-CZ-NH1	-6.02	115.48	121.50
1	A	85	THR	N-CA-CB	-6.01	102.06	111.56
1	A	127	GLU	CG-CD-OE1	5.98	132.16	118.40
1	B	49	ILE	CA-C-O	5.96	127.35	120.67
1	A	72	ALA	CA-C-O	-5.96	115.06	121.38
1	A	52	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	131	ALA	CA-C-N	5.91	130.56	122.34
1	B	131	ALA	C-N-CA	5.91	130.56	122.34
1	A	84	GLU	CA-C-N	5.91	131.56	121.87
1	A	84	GLU	C-N-CA	5.91	131.56	121.87
1	A	80	GLN	CA-C-N	5.89	125.59	119.82
1	A	80	GLN	C-N-CA	5.89	125.59	119.82
1	A	133	LYS	N-CA-CB	5.88	121.15	111.62
1	A	187	GLU	N-CA-C	-5.88	106.73	114.31
1	B	11	SER	CA-C-O	5.87	127.50	120.28
1	A	185	THR	N-CA-C	-5.86	102.77	110.39
1	B	3	VAL	N-CA-C	5.86	117.15	108.65
1	A	8	PRO	O-C-N	-5.85	114.92	122.23
1	B	1	PCA	O-C-N	-5.84	113.66	123.00
1	B	93	ASP	CA-C-N	5.84	128.03	120.44
1	B	93	ASP	C-N-CA	5.84	128.03	120.44
1	A	195	TYR	CA-C-O	-5.82	113.97	120.66
1	B	84	GLU	CG-CD-OE1	5.80	131.75	118.40
1	B	200	THR	O-C-N	5.80	130.14	123.29
1	A	139	LEU	CB-CA-C	5.80	119.29	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	GLU	CA-C-O	-5.80	114.35	121.02
1	A	45	PRO	N-CA-C	-5.76	100.61	112.47
1	B	47	LEU	N-CA-CB	-5.76	101.27	109.85
1	A	135	THR	O-C-N	5.76	130.38	123.36
1	A	29	ILE	CA-C-O	5.74	127.96	120.78
1	A	161	ALA	N-CA-C	5.74	118.02	109.59
1	B	132	ASN	N-CA-C	5.73	119.55	111.52
1	A	149	THR	CA-CB-CG2	5.72	120.22	110.50
1	B	166	THR	CA-CB-CG2	5.71	120.21	110.50
1	B	63	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	70	THR	CA-C-N	5.69	131.47	122.94
1	B	70	THR	C-N-CA	5.69	131.47	122.94
1	B	105	THR	O-C-N	5.67	129.95	123.31
1	A	54	SER	CB-CA-C	5.65	120.20	110.77
1	B	86	ASP	O-C-N	5.64	130.37	123.21
1	B	73	SER	O-C-N	5.61	129.78	123.27
1	A	96	LEU	CA-C-N	5.61	130.92	122.68
1	A	96	LEU	C-N-CA	5.61	130.92	122.68
1	B	118	THR	O-C-N	5.60	129.60	123.27
1	B	55	ARG	O-C-N	5.59	129.73	123.19
1	B	148	VAL	CA-CB-CG1	5.57	119.87	110.40
1	A	102	GLY	N-CA-C	-5.55	104.13	112.89
1	B	190	LYS	N-CA-C	5.55	117.13	111.14
1	A	39	HIS	N-CA-C	5.54	119.28	107.70
1	A	167	LYS	CB-CA-C	5.54	117.34	109.08
1	B	47	LEU	CA-C-O	-5.54	114.44	120.81
1	B	40	LEU	CB-CA-C	5.53	118.97	109.51
1	A	59	VAL	CB-CA-C	5.52	119.25	111.63
1	B	60	SER	CA-CB-OG	5.52	122.14	111.10
1	A	141	SER	CA-C-N	5.52	130.79	122.68
1	A	141	SER	C-N-CA	5.52	130.79	122.68
1	B	31	GLU	CA-C-O	-5.52	113.32	119.67
1	A	165	THR	CB-CA-C	5.51	119.30	109.65
1	A	12	GLY	CA-C-O	-5.50	115.84	121.61
1	B	17	ARG	CA-C-N	5.49	130.18	123.10
1	B	17	ARG	C-N-CA	5.49	130.18	123.10
1	A	89	CYS	N-CA-C	-5.48	102.35	110.46
1	A	51	GLU	CB-CG-CD	5.48	121.91	112.60
1	A	13	THR	CB-CA-C	5.47	119.34	109.45
1	A	33	SER	CA-C-O	-5.46	114.99	121.16
1	A	176	TYR	N-CA-C	5.46	118.99	110.32
1	A	144	TYR	CA-C-O	-5.45	112.69	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	A	200	THR	CA-CB-OG1	-5.44	101.44	109.60
1	B	184	LEU	O-C-N	5.43	130.24	122.74
1	A	42	GLY	N-CA-C	-5.43	102.53	111.38
1	B	99	ALA	N-CA-C	-5.43	100.45	109.46
1	B	38	GLN	N-CA-C	-5.42	100.57	109.40
1	A	124	PRO	CA-C-O	-5.40	115.20	121.95
1	B	135	THR	N-CA-CB	5.39	120.76	111.00
1	A	176	TYR	CA-CB-CG	-5.35	104.26	113.90
1	A	168	PRO	CA-C-N	-5.34	113.48	122.29
1	A	168	PRO	C-N-CA	-5.34	113.48	122.29
1	A	194	SER	O-C-N	5.33	128.27	123.26
1	B	166	THR	CA-CB-OG1	-5.33	101.60	109.60
1	A	61	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	67	LYS	CA-C-O	-5.32	115.38	121.40
1	A	93	ASP	CA-C-N	5.31	127.83	120.29
1	A	93	ASP	C-N-CA	5.31	127.83	120.29
1	B	186	PRO	CA-C-N	5.30	127.65	120.44
1	B	186	PRO	C-N-CA	5.30	127.65	120.44
1	A	3	VAL	N-CA-C	5.30	120.36	109.34
1	B	70	THR	CA-CB-CG2	5.30	119.50	110.50
1	B	197	CYS	CA-CB-SG	-5.29	102.23	114.40
1	B	143	PHE	CA-C-O	5.29	127.14	121.16
1	B	159	VAL	N-CA-CB	5.28	117.94	111.60
1	A	63	PHE	CA-C-O	-5.28	114.66	120.30
1	A	40	LEU	N-CA-C	-5.27	102.71	110.52
1	A	40	LEU	CA-C-O	-5.26	115.52	121.72
1	A	136	LEU	O-C-N	5.26	129.14	123.10
1	B	65	ALA	O-C-N	5.25	129.58	122.96
1	A	51	GLU	CA-C-N	5.25	131.57	121.54
1	A	51	GLU	C-N-CA	5.25	131.57	121.54
1	A	103	THR	N-CA-CB	-5.23	101.43	110.32
1	A	126	SER	CA-C-N	5.23	127.55	120.65
1	A	126	SER	C-N-CA	5.23	127.55	120.65
1	B	98	VAL	O-C-N	5.22	129.10	122.57
1	B	48	LEU	O-C-N	5.22	129.13	122.03
1	B	142	ASP	N-CA-CB	-5.22	104.24	112.13
1	A	40	LEU	N-CA-CB	5.22	118.81	110.46
1	A	209	THR	CA-CB-OG1	-5.21	101.79	109.60
1	B	19	THR	CA-C-O	5.18	125.96	120.36
1	A	7	PRO	CA-C-N	5.18	124.50	118.85
1	A	7	PRO	C-N-CA	5.18	124.50	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	THR	N-CA-C	5.18	121.84	110.80
1	A	202	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	214	GLU	CA-C-N	5.17	131.16	123.05
1	A	214	GLU	C-N-CA	5.17	131.16	123.05
1	B	64	SER	O-C-N	5.17	129.26	123.27
1	B	51	GLU	CG-CD-OE2	5.16	130.28	118.40
1	B	80	GLN	N-CA-C	-5.16	102.66	110.50
1	B	49	ILE	CA-C-N	-5.15	114.11	122.36
1	B	49	ILE	C-N-CA	-5.15	114.11	122.36
1	A	32	ASN	O-C-N	5.14	128.41	121.83
1	A	80	GLN	CA-CB-CG	5.14	124.38	114.10
1	A	182	LEU	CB-CA-C	5.14	118.38	110.62
1	A	40	LEU	CB-CA-C	5.13	118.81	109.83
1	B	87	TYR	CA-C-N	5.12	130.63	122.94
1	B	87	TYR	C-N-CA	5.12	130.63	122.94
1	A	17	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	35	THR	N-CA-CB	-5.11	102.67	110.85
1	B	185	THR	N-CA-CB	5.10	117.13	109.88
1	A	83	ASP	N-CA-CB	5.10	118.12	110.53
1	B	157	SER	CA-C-O	5.08	125.73	120.25
1	A	94	ASP	N-CA-C	5.07	116.88	111.36
1	A	149	THR	N-CA-CB	5.05	119.55	110.80
1	A	195	TYR	N-CA-CB	-5.05	101.85	111.00
1	A	117	PRO	O-C-N	5.04	129.29	123.14
1	B	21	SER	CB-CA-C	5.04	118.02	109.50
1	A	189	TRP	CA-CB-CG	5.04	123.18	113.60
1	B	196	SER	CA-C-O	5.03	126.73	120.54
1	B	84	GLU	CA-CB-CG	5.03	124.15	114.10
1	B	205	THR	CA-CB-OG1	-5.03	102.06	109.60
1	A	200	THR	CA-CB-CG2	5.01	119.03	110.50
1	B	136	LEU	O-C-N	5.00	129.56	123.21
1	B	171	GLN	N-CA-C	-5.00	103.06	110.46

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	1598	0	1535	167	0
1	B	1598	0	1536	139	1
2	A	161	0	0	49	0
2	B	137	0	0	25	1
All	All	3494	0	3071	300	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 48.

All (300) 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:30:GLY:O	1:A:31:GLU:HB2	1.49	1.12
1:A:95:SER:HB2	2:A:566:HOH:O	1.49	1.11
1:A:192:HIS:CE1	2:A:651:HOH:O	2.03	1.11
1:B:212:PRO:HG3	2:B:841:HOH:O	1.52	1.09
1:A:47:LEU:HD21	1:A:50:TYR:HB3	1.39	1.04
1:A:8:PRO:HG3	1:A:149:THR:HG22	1.42	1.02
1:B:192:HIS:O	1:B:212:PRO:HG2	1.59	1.00
2:A:688:HOH:O	1:B:166:THR:CG2	2.09	0.99
1:B:40:LEU:HD12	1:B:40:LEU:H	1.26	0.99
1:A:92:TRP:O	1:A:93:ASP:HB2	1.63	0.98
1:B:214:GLU:O	1:B:215:CYS:HB2	1.63	0.97
1:B:62:ARG:NH2	1:B:83:ASP:OD2	2.02	0.92
2:A:632:HOH:O	1:B:171:GLN:HA	1.70	0.92
1:A:59:VAL:HA	2:A:549:HOH:O	1.69	0.91
1:A:193:ARG:HA	2:A:653:HOH:O	1.70	0.91
1:A:166:THR:HG23	2:A:631:HOH:O	1.70	0.90
1:A:164:GLU:OE1	2:A:632:HOH:O	1.90	0.89
1:B:40:LEU:HD13	1:B:43:THR:OG1	1.73	0.89
1:A:126:SER:O	1:A:130:GLN:HG3	1.71	0.89
1:B:17:ARG:HB3	1:B:77:SER:HA	1.54	0.88
1:A:40:LEU:HD22	1:A:41:SER:H	1.38	0.87
1:B:25:SER:HB3	2:B:714:HOH:O	1.72	0.87
1:A:48:LEU:C	1:A:49:ILE:HD12	2.00	0.86
1:B:52:ASP:OD1	1:B:67:LYS:HD2	1.77	0.85
1:B:185:THR:OG1	1:B:188:GLN:OE1	1.95	0.84
1:B:28:ASN:HA	1:B:92:TRP:O	1.78	0.83
1:A:167:LYS:NZ	1:A:167:LYS:HB3	1.94	0.82
1:A:29:ILE:HG22	1:A:69:GLY:O	1.80	0.81
1:A:4:LEU:HB2	1:A:102:GLY:HA2	1.63	0.81
1:B:51:GLU:OE1	2:B:745:HOH:O	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:O	1:A:31:GLU:N	2.15	0.80
1:B:32:ASN:ND2	1:B:92:TRP:O	2.15	0.80
1:A:189:TRP:CZ2	1:A:212:PRO:HA	2.17	0.80
1:A:17:ARG:HG2	1:A:77:SER:HA	1.63	0.79
1:B:16:GLN:HG2	1:B:17:ARG:H	1.47	0.79
1:B:144:TYR:OH	2:B:818:HOH:O	2.00	0.79
1:B:95:SER:OG	1:B:96:LEU:HD22	1.83	0.79
1:B:9:SER:HB2	2:B:706:HOH:O	1.81	0.78
1:A:133:LYS:HE2	2:A:640:HOH:O	1.83	0.78
1:A:96:LEU:HD11	2:A:562:HOH:O	1.85	0.77
1:B:163:VAL:HG22	1:B:182:LEU:HD13	1.64	0.77
1:B:167:LYS:HD3	1:B:167:LYS:N	1.99	0.77
1:A:112:GLN:NE2	2:A:600:HOH:O	2.17	0.76
1:A:11:SER:HB2	1:A:108:THR:O	1.85	0.76
1:A:192:HIS:NE2	2:A:651:HOH:O	2.11	0.76
1:B:163:VAL:HB	2:B:882:HOH:O	1.87	0.75
1:A:93:ASP:O	2:A:574:HOH:O	2.04	0.74
1:B:157:SER:OG	2:B:826:HOH:O	2.02	0.74
1:B:16:GLN:HG2	1:B:17:ARG:N	2.04	0.73
1:B:133:LYS:HE2	2:B:606:HOH:O	1.87	0.72
1:A:86:ASP:OD1	1:A:106:LYS:HG3	1.90	0.72
1:A:190:LYS:HE3	2:A:646:HOH:O	1.88	0.72
1:A:167:LYS:HG3	2:A:837:HOH:O	1.89	0.72
1:B:62:ARG:HH21	1:B:83:ASP:CG	1.97	0.72
1:A:18:VAL:HA	2:A:530:HOH:O	1.87	0.72
1:A:103:THR:HG22	2:A:525:HOH:O	1.89	0.72
1:B:62:ARG:NH2	1:B:83:ASP:CG	2.47	0.72
1:A:175:LYS:HE3	2:A:601:HOH:O	1.90	0.71
1:A:48:LEU:HD22	1:A:59:VAL:HG11	1.73	0.71
1:A:35:THR:HG23	1:A:47:LEU:CD1	2.21	0.71
2:A:718:HOH:O	1:B:35:THR:HG23	1.90	0.71
1:B:40:LEU:HD13	1:B:43:THR:CB	2.22	0.70
1:A:125:SER:HB2	1:A:127:GLU:CD	2.18	0.69
1:B:31:GLU:O	2:B:716:HOH:O	2.11	0.69
1:A:40:LEU:C	1:A:42:GLY:H	2.00	0.69
1:A:173:ASN:O	1:A:174:ASN:HB2	1.93	0.68
1:B:86:ASP:OD2	2:B:719:HOH:O	2.09	0.68
1:A:150:VAL:HG22	1:A:199:VAL:HG22	1.76	0.68
1:B:189:TRP:HZ3	1:B:195:TYR:CD2	2.12	0.67
1:B:43:THR:O	1:B:44:ALA:CB	2.42	0.66
1:B:185:THR:CB	1:B:188:GLN:OE1	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:TRP:CZ3	1:B:195:TYR:HD2	2.14	0.66
1:A:45:PRO:HD2	2:A:540:HOH:O	1.94	0.66
1:B:4:LEU:HD13	1:B:100:VAL:HG12	1.77	0.66
1:A:96:LEU:CD1	2:A:562:HOH:O	2.41	0.65
1:A:38:GLN:HG3	1:A:85:THR:HG21	1.78	0.65
1:A:145:PRO:HD2	2:A:614:HOH:O	1.96	0.65
1:A:125:SER:HB2	1:A:127:GLU:HG2	1.79	0.64
1:B:163:VAL:CG2	1:B:182:LEU:HD13	2.27	0.64
1:B:195:TYR:N	1:B:210:VAL:O	2.27	0.64
1:B:212:PRO:CG	2:B:841:HOH:O	2.24	0.63
1:B:189:TRP:CZ3	1:B:195:TYR:CD2	2.85	0.63
1:A:4:LEU:HB2	1:A:102:GLY:CA	2.27	0.63
1:A:78:GLY:O	1:A:80:GLN:NE2	2.30	0.62
1:B:93:ASP:OD2	2:B:701:HOH:O	2.16	0.62
1:A:103:THR:CG2	2:A:525:HOH:O	2.46	0.62
1:B:117:PRO:HD3	1:B:201:HIS:CD2	2.34	0.62
1:A:153:LYS:HD3	1:A:196:SER:OG	1.99	0.62
1:A:1:PCA:HA	2:A:522:HOH:O	1.99	0.62
1:A:22:CYS:SG	1:A:29:ILE:HD11	2.39	0.62
1:B:190:LYS:HA	1:B:190:LYS:HE2	1.80	0.62
1:B:24:GLY:HA3	1:B:29:ILE:HD12	1.81	0.61
1:B:62:ARG:NH2	1:B:83:ASP:OD1	2.33	0.61
1:A:30:GLY:O	1:A:31:GLU:CB	2.37	0.61
1:B:40:LEU:CD1	1:B:43:THR:OG1	2.47	0.61
1:B:160:LYS:HE3	2:B:829:HOH:O	1.99	0.61
1:B:26:SER:HA	1:B:30:GLY:HA3	1.82	0.61
1:B:185:THR:HG23	1:B:188:GLN:OE1	2.01	0.61
1:A:29:ILE:HG23	1:A:67:LYS:HD3	1.83	0.61
1:B:157:SER:HB2	2:B:825:HOH:O	2.00	0.60
1:A:62:ARG:HH22	1:A:83:ASP:CG	2.09	0.60
1:A:11:SER:CB	1:A:108:THR:O	2.48	0.60
1:B:98:VAL:HG12	2:B:743:HOH:O	2.01	0.60
1:A:40:LEU:CD2	1:A:41:SER:H	2.14	0.60
1:B:16:GLN:CG	1:B:17:ARG:H	2.15	0.60
1:A:167:LYS:NZ	1:A:167:LYS:CB	2.64	0.59
1:B:189:TRP:HZ3	1:B:195:TYR:HD2	1.45	0.59
1:A:35:THR:HG23	1:A:47:LEU:HD12	1.85	0.59
1:B:93:ASP:OD1	1:B:96:LEU:HB2	2.03	0.59
1:A:192:HIS:HE1	2:A:651:HOH:O	1.62	0.58
1:A:38:GLN:HE21	1:A:85:THR:HG21	1.67	0.58
1:B:28:ASN:O	1:B:32:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HD12	1:B:40:LEU:N	2.08	0.58
1:A:15:GLY:N	1:A:79:LEU:O	2.26	0.58
1:A:169:SER:HB2	2:A:637:HOH:O	2.03	0.58
1:A:215:CYS:HA	1:B:216:SER:C	2.28	0.58
1:B:171:GLN:HG3	1:B:175:LYS:O	2.04	0.58
1:A:167:LYS:HB3	1:A:167:LYS:HZ3	1.66	0.57
1:B:40:LEU:H	1:B:40:LEU:CD1	2.04	0.57
1:B:10:ALA:HB3	1:B:107:VAL:HG22	1.85	0.57
1:A:160:LYS:NZ	2:A:521:HOH:O	2.36	0.56
1:A:16:GLN:HG2	1:A:17:ARG:H	1.69	0.56
1:B:17:ARG:HA	1:B:76:ILE:O	2.04	0.56
1:A:30:GLY:HA2	1:A:69:GLY:O	2.06	0.56
1:A:140:ILE:CD1	1:A:150:VAL:HG21	2.36	0.56
1:A:92:TRP:O	1:A:93:ASP:CB	2.48	0.56
1:A:140:ILE:HD11	1:A:150:VAL:HG21	1.87	0.56
1:A:214:GLU:CA	1:A:214:GLU:OE1	2.53	0.56
1:A:215:CYS:H	1:B:216:SER:C	2.13	0.56
1:B:6:GLN:OE1	1:B:102:GLY:HA3	2.05	0.56
1:A:43:THR:O	1:A:44:ALA:CB	2.54	0.56
1:A:114:LYS:O	2:A:655:HOH:O	2.18	0.56
1:B:39:HIS:CD2	1:B:40:LEU:O	2.59	0.55
1:B:185:THR:CG2	1:B:188:GLN:OE1	2.53	0.55
1:A:3:VAL:HG12	1:A:100:VAL:HG13	1.88	0.55
1:A:40:LEU:HD22	1:A:41:SER:N	2.15	0.55
1:A:182:LEU:CD1	1:A:184:LEU:HD11	2.36	0.55
1:B:168:PRO:HD3	2:B:834:HOH:O	2.06	0.55
1:B:133:LYS:CE	2:B:606:HOH:O	2.48	0.55
1:A:112:GLN:HB2	1:A:113:PRO:HD2	1.89	0.54
1:B:188:GLN:O	1:B:192:HIS:HD2	1.91	0.54
1:A:79:LEU:HD21	1:A:109:VAL:HG22	1.87	0.54
1:A:116:ASN:OD1	2:A:603:HOH:O	2.18	0.54
1:B:55:ARG:HD3	1:B:60:SER:O	2.08	0.54
1:B:49:ILE:HA	1:B:54:SER:O	2.07	0.54
1:B:116:ASN:HA	1:B:201:HIS:HD2	1.72	0.53
1:A:29:ILE:HG22	1:A:30:GLY:N	2.23	0.53
1:A:186:PRO:O	2:A:646:HOH:O	2.19	0.53
1:A:195:TYR:CD2	2:A:661:HOH:O	2.59	0.53
1:A:167:LYS:HE3	2:A:636:HOH:O	2.08	0.53
1:A:79:LEU:CD2	1:A:109:VAL:HG22	2.40	0.52
1:B:185:THR:HB	1:B:186:PRO:HD2	1.90	0.52
1:A:145:PRO:CD	2:A:614:HOH:O	2.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:PHE:CE2	1:B:148:VAL:HG13	2.43	0.52
1:A:35:THR:HG22	1:A:37:TYR:CE1	2.44	0.52
1:A:190:LYS:CE	2:A:646:HOH:O	2.54	0.52
1:B:193:ARG:HA	1:B:212:PRO:HD2	1.92	0.52
1:A:130:GLN:HG2	2:A:609:HOH:O	2.09	0.51
1:B:13:THR:O	1:B:16:GLN:HB3	2.10	0.51
1:B:93:ASP:O	1:B:97:ASP:N	2.43	0.51
1:B:129:LEU:C	1:B:131:ALA:H	2.16	0.51
2:A:612:HOH:O	1:B:118:THR:CG2	2.59	0.51
1:A:135:THR:O	1:B:122:PHE:CZ	2.64	0.51
1:A:169:SER:HB3	2:A:831:HOH:O	2.11	0.50
1:B:16:GLN:CG	1:B:17:ARG:N	2.73	0.50
1:B:40:LEU:CD1	1:B:40:LEU:N	2.72	0.50
1:A:3:VAL:HB	1:A:101:PHE:O	2.11	0.50
1:B:84:GLU:O	1:B:85:THR:HG22	2.11	0.50
1:A:40:LEU:C	1:A:42:GLY:N	2.69	0.50
1:A:125:SER:HB2	1:A:127:GLU:CG	2.42	0.50
1:A:183:SER:O	1:A:184:LEU:HD12	2.12	0.50
1:B:126:SER:O	1:B:128:GLU:N	2.44	0.50
1:A:33:SER:OG	1:A:51:GLU:HA	2.10	0.50
1:A:49:ILE:HD12	1:A:49:ILE:N	2.27	0.50
1:B:78:GLY:O	1:B:79:LEU:C	2.54	0.50
1:A:214:GLU:OE1	1:A:214:GLU:HA	2.10	0.50
1:B:193:ARG:C	1:B:212:PRO:HD2	2.37	0.50
1:A:43:THR:HG22	2:B:741:HOH:O	2.11	0.50
1:A:201:HIS:O	1:A:202:GLU:C	2.53	0.49
1:A:87:TYR:CE1	1:A:107:VAL:HG13	2.47	0.49
1:A:166:THR:CG2	2:A:631:HOH:O	2.42	0.49
1:A:203:GLY:C	2:A:656:HOH:O	2.54	0.49
2:A:688:HOH:O	1:B:166:THR:HG23	1.91	0.49
1:B:93:ASP:CG	1:B:96:LEU:HB2	2.38	0.49
1:A:38:GLN:HB2	1:A:48:LEU:HD11	1.93	0.49
1:A:43:THR:O	1:A:44:ALA:HB2	2.13	0.49
1:B:80:GLN:O	1:B:83:ASP:HB2	2.12	0.49
1:B:1:PCA:N	1:B:96:LEU:HD21	2.27	0.49
1:A:35:THR:HG23	1:A:47:LEU:HD11	1.91	0.49
1:A:196:SER:HA	1:A:208:LYS:O	2.13	0.49
1:A:80:GLN:HB2	1:A:81:PRO:HD2	1.94	0.49
1:A:112:GLN:HB2	1:A:113:PRO:CD	2.43	0.49
1:B:128:GLU:O	1:B:128:GLU:HG2	2.13	0.49
1:B:154:ALA:HB2	1:B:195:TYR:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:SER:O	1:B:127:GLU:C	2.56	0.48
1:B:17:ARG:HH11	1:B:17:ARG:HG2	1.78	0.48
1:B:43:THR:O	1:B:44:ALA:HB3	2.12	0.48
1:A:157:SER:HB3	2:A:635:HOH:O	2.13	0.48
1:B:145:PRO:O	1:B:201:HIS:HE1	1.96	0.48
1:B:196:SER:HB3	1:B:209:THR:HB	1.96	0.47
1:A:95:SER:C	2:A:566:HOH:O	2.56	0.47
1:B:84:GLU:O	1:B:85:THR:CG2	2.62	0.47
1:B:96:LEU:HD13	1:B:96:LEU:HA	1.39	0.47
1:A:124:PRO:HD3	1:A:136:LEU:HD22	1.96	0.47
1:B:154:ALA:CB	1:B:195:TYR:CE1	2.97	0.47
1:A:9:SER:HA	1:A:106:LYS:O	2.14	0.47
1:B:47:LEU:HD13	1:B:56:ALA:HB2	1.95	0.47
1:A:65:ALA:HB2	1:A:74:LEU:HD12	1.97	0.47
1:A:85:THR:HG23	1:A:86:ASP:O	2.15	0.47
1:A:197:CYS:N	1:A:208:LYS:O	2.47	0.47
1:A:107:VAL:O	1:A:107:VAL:CG2	2.58	0.47
1:A:107:VAL:O	1:A:107:VAL:HG22	2.15	0.47
1:A:135:THR:O	1:B:122:PHE:HZ	1.98	0.47
1:A:166:THR:HB	1:A:179:SER:O	2.15	0.47
1:A:126:SER:O	1:A:130:GLN:CG	2.54	0.46
1:B:193:ARG:O	1:B:212:PRO:HD2	2.16	0.46
1:A:62:ARG:NH2	1:A:83:ASP:OD2	2.47	0.46
1:A:183:SER:C	1:A:184:LEU:CD1	2.88	0.46
1:A:182:LEU:CD1	1:A:184:LEU:CD1	2.93	0.46
1:A:99:ALA:HB3	1:B:37:TYR:OH	2.16	0.46
1:B:93:ASP:OD1	1:B:96:LEU:HD23	2.15	0.46
1:B:171:GLN:OE1	1:B:177:ALA:HB2	2.15	0.46
1:B:163:VAL:CB	2:B:882:HOH:O	2.56	0.45
1:A:56:ALA:O	1:A:57:SER:C	2.58	0.45
1:A:112:GLN:HG3	1:A:144:TYR:CD2	2.51	0.45
1:B:211:ALA:HA	1:B:212:PRO:HD3	1.85	0.45
1:A:213:THR:O	1:B:216:SER:O	2.34	0.45
1:B:27:SER:O	1:B:32:ASN:ND2	2.47	0.45
1:A:85:THR:HG23	1:A:86:ASP:N	2.32	0.45
1:A:130:GLN:NE2	2:A:609:HOH:O	2.32	0.45
1:A:166:THR:HG22	1:A:178:ALA:HA	1.98	0.45
1:A:211:ALA:HA	1:A:212:PRO:HD3	1.77	0.45
1:A:81:PRO:C	1:A:83:ASP:H	2.24	0.45
2:A:631:HOH:O	1:B:166:THR:HG23	2.17	0.45
1:A:10:ALA:O	1:A:107:VAL:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HA	1:A:186:PRO:HG2	1.99	0.44
1:B:117:PRO:HB3	1:B:143:PHE:HB3	1.98	0.44
1:B:40:LEU:HB2	1:B:43:THR:OG1	2.16	0.44
1:B:43:THR:O	1:B:44:ALA:HB2	2.18	0.44
1:B:56:ALA:O	1:B:57:SER:C	2.61	0.44
1:B:103:THR:HG22	2:B:705:HOH:O	2.18	0.44
1:A:29:ILE:C	1:A:31:GLU:N	2.75	0.44
1:A:153:LYS:HD3	1:A:196:SER:HG	1.80	0.44
1:A:35:THR:CG2	1:A:37:TYR:CZ	3.01	0.44
1:B:95:SER:OG	1:B:96:LEU:CD2	2.58	0.44
1:B:196:SER:HB2	1:B:209:THR:HG22	1.98	0.44
1:A:171:GLN:HA	1:A:171:GLN:NE2	2.32	0.43
1:A:18:VAL:HG13	2:A:530:HOH:O	2.17	0.43
1:A:37:TYR:N	1:A:88:TYR:O	2.38	0.43
1:A:48:LEU:HB3	1:A:49:ILE:HD12	2.00	0.43
1:A:87:TYR:CE1	1:A:107:VAL:CG1	3.01	0.43
1:A:183:SER:C	1:A:184:LEU:HD12	2.44	0.43
1:A:170:LYS:HE3	1:A:170:LYS:HB2	1.76	0.43
1:A:87:TYR:CD1	1:A:107:VAL:HG13	2.53	0.43
1:A:116:ASN:ND2	1:A:204:SER:OG	2.52	0.42
1:A:128:GLU:HG2	1:A:133:LYS:HB2	2.00	0.42
1:A:93:ASP:OD1	1:A:97:ASP:HA	2.19	0.42
1:A:182:LEU:HD12	1:A:184:LEU:CD1	2.49	0.42
1:B:52:ASP:HB3	2:B:728:HOH:O	2.19	0.42
1:B:96:LEU:HD22	1:B:96:LEU:N	2.34	0.42
1:A:175:LYS:N	1:A:175:LYS:CD	2.83	0.42
1:A:120:THR:HG22	1:A:122:PHE:CE1	2.54	0.42
1:A:165:THR:HG23	1:A:180:SER:HB2	2.00	0.42
1:B:53:ASN:C	1:B:53:ASN:HD22	2.27	0.42
1:A:85:THR:HG22	1:A:87:TYR:CE1	2.54	0.42
1:B:24:GLY:CA	1:B:29:ILE:HD12	2.49	0.42
1:A:55:ARG:NH1	1:A:63:PHE:O	2.49	0.42
1:A:122:PHE:HA	1:A:123:PRO:HD2	1.88	0.42
1:A:216:SER:C	2:B:658:HOH:O	2.62	0.42
1:B:128:GLU:O	1:B:133:LYS:O	2.38	0.42
1:B:144:TYR:CD1	1:B:145:PRO:HA	2.55	0.42
1:A:29:ILE:CG2	1:A:69:GLY:O	2.62	0.42
1:A:40:LEU:HG	1:A:85:THR:OG1	2.20	0.42
1:A:150:VAL:HA	1:A:198:GLN:O	2.20	0.42
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.88	0.41
1:B:124:PRO:HD3	1:B:136:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HZ2	1:A:153:LYS:HG2	1.48	0.41
1:A:78:GLY:O	1:A:79:LEU:C	2.62	0.41
1:A:171:GLN:NE2	2:A:832:HOH:O	2.54	0.41
2:A:688:HOH:O	1:B:166:THR:HG21	2.00	0.41
1:A:128:GLU:CG	1:A:133:LYS:HE3	2.50	0.41
1:B:9:SER:HB2	1:B:106:LYS:HD3	2.01	0.41
1:B:68:SER:N	1:B:71:SER:O	2.40	0.41
1:A:48:LEU:CB	1:A:49:ILE:HD12	2.51	0.41
1:B:67:LYS:HA	1:B:71:SER:O	2.21	0.41
1:B:196:SER:CB	1:B:209:THR:HG22	2.51	0.41
1:B:214:GLU:HB3	2:B:853:HOH:O	2.20	0.41
1:A:196:SER:CA	1:A:208:LYS:O	2.69	0.41
2:A:560:HOH:O	1:B:39:HIS:HE1	2.04	0.41
1:B:170:LYS:HD2	1:B:176:TYR:CZ	2.56	0.40
1:A:35:THR:CG2	1:A:37:TYR:CE1	3.03	0.40
1:A:116:ASN:HD22	1:A:201:HIS:HD2	1.68	0.40
1:B:82:GLU:H	1:B:82:GLU:HG3	1.51	0.40
1:A:35:THR:HG21	1:A:37:TYR:OH	2.20	0.40
1:B:3:VAL:O	2:B:702:HOH:O	2.22	0.40
1:B:154:ALA:HB2	1:B:195:TYR:CD1	2.57	0.40
1:A:196:SER:HA	1:A:209:THR:HA	2.04	0.40
2:A:612:HOH:O	1:B:118:THR:HG23	2.21	0.40
1:B:64:SER:HA	2:B:729:HOH:O	2.21	0.40
1:B:67:LYS:HA	1:B:72:ALA:HA	2.03	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:B:127:GLU:OE1	2:B:803:HOH:O[3_545]	2.15	0.05

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	214/216 (99%)	188 (88%)	19 (9%)	7 (3%)	3	1
1	B	214/216 (99%)	191 (89%)	16 (8%)	7 (3%)	3	1
All	All	428/432 (99%)	379 (89%)	35 (8%)	14 (3%)	3	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	ALA
1	A	93	ASP
1	B	2	SER
1	B	44	ALA
1	B	213	THR
1	B	215	CYS
1	A	30	GLY
1	A	31	GLU
1	A	214	GLU
1	A	43	THR
1	B	127	GLU
1	B	212	PRO
1	B	131	ALA
1	A	78	GLY

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	181/181 (100%)	133 (74%)	48 (26%)	0	0
1	B	181/181 (100%)	141 (78%)	40 (22%)	1	1
All	All	362/362 (100%)	274 (76%)	88 (24%)	1	0

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	13	THR
1	A	17	ARG
1	A	23	SER
1	A	25	SER
1	A	26	SER
1	A	28	ASN
1	A	29	ILE
1	A	34	VAL
1	A	35	THR
1	A	40	LEU
1	A	43	THR
1	A	46	LYS
1	A	51	GLU
1	A	62	ARG
1	A	68	SER
1	A	80	GLN
1	A	85	THR
1	A	93	ASP
1	A	95	SER
1	A	97	ASP
1	A	98	VAL
1	A	107	VAL
1	A	110	LEU
1	A	114	LYS
1	A	121	LEU
1	A	125	SER
1	A	127	GLU
1	A	136	LEU
1	A	149	THR
1	A	153	LYS
1	A	157	SER
1	A	163	VAL
1	A	166	THR
1	A	167	LYS
1	A	172	SER
1	A	175	LYS
1	A	182	LEU
1	A	183	SER
1	A	184	LEU
1	A	185	THR
1	A	188	GLN
1	A	193	ARG

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Mol	Chain	Res	Type
1	A	200	THR
1	A	202	GLU
1	A	209	THR
1	A	210	VAL
1	A	215	CYS
1	B	17	ARG
1	B	21	SER
1	B	25	SER
1	B	27	SER
1	B	31	GLU
1	B	32	ASN
1	B	38	GLN
1	B	40	LEU
1	B	43	THR
1	B	46	LYS
1	B	47	LEU
1	B	48	LEU
1	B	51	GLU
1	B	53	ASN
1	B	61	ASP
1	B	67	LYS
1	B	70	THR
1	B	73	SER
1	B	76	ILE
1	B	79	LEU
1	B	82	GLU
1	B	96	LEU
1	B	97	ASP
1	B	98	VAL
1	B	106	LYS
1	B	112	GLN
1	B	114	LYS
1	B	120	THR
1	B	130	GLN
1	B	157	SER
1	B	166	THR
1	B	170	LYS
1	B	179	SER
1	B	190	LYS
1	B	193	ARG
1	B	204	SER
1	B	206	VAL

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Mol	Chain	Res	Type
1	B	209	THR
1	B	210	VAL
1	B	215	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	53	ASN
1	A	116	ASN
1	A	171	GLN
1	A	201	HIS
1	B	32	ASN
1	B	39	HIS
1	B	53	ASN
1	B	116	ASN
1	B	192	HIS
1	B	201	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PCA	B	1	1	6,7,9	0.69	0	7,8,12	1.76	2 (28%)
1	PCA	A	1	1	6,7,9	0.85	0	7,8,12	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	B	1	1	-	0/0/9/13	0/1/1/1
1	PCA	A	1	1	-	0/0/9/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	PCA	CB-CA-C	2.91	116.64	112.66
1	B	1	PCA	O-C-CA	2.70	131.70	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	PCA	1	0
1	A	1	PCA	1	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	42:GLY	C	43:THR	N	1.14

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	215/216 (99%)	-0.66	1 (0%) 87 85	8, 22, 45, 55	0
1	B	215/216 (99%)	-0.76	0 100 100	5, 21, 35, 53	0
All	All	430/432 (99%)	-0.71	1 (0%) 91 90	5, 21, 42, 55	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	ALA	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	B	1	7/9	0.68	0.13	45,47,48,48	0
1	PCA	A	1	7/9	0.73	0.10	44,44,45,45	0

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.