



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:55 AM UTC

PDB ID : 3BJL / pdb_00003bjl
Title : LOC, A LAMBDA 1 TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN) CRYSTALLIZED IN AMMONIUM SULFATE
Authors : Schiffer, M.; Huang, D.B.
Deposited on : 1995-05-26
Resolution : 2.30 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
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

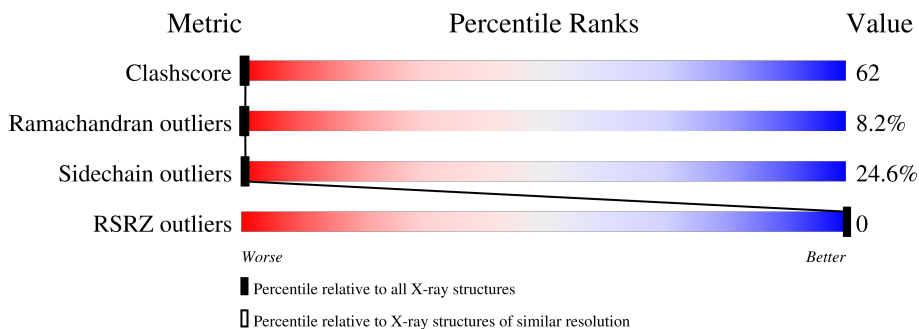
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

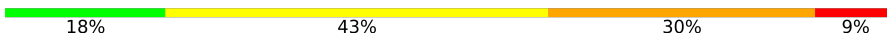
The reported resolution of this entry is 2.30 Å.

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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 3560 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

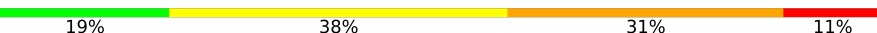
- Molecule 2 is water.

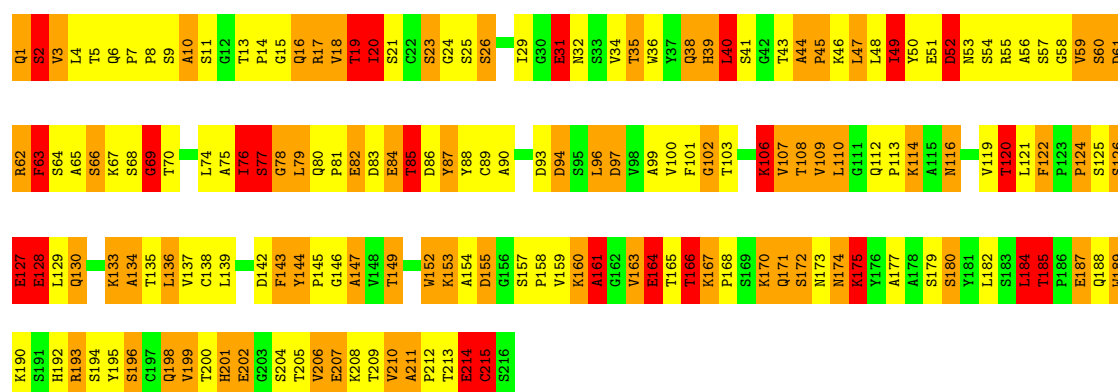
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	175	Total O 175 175	0	0
2	B	189	Total O 189 189	0	0

3 Residue-property plots

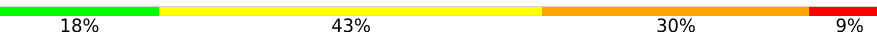
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

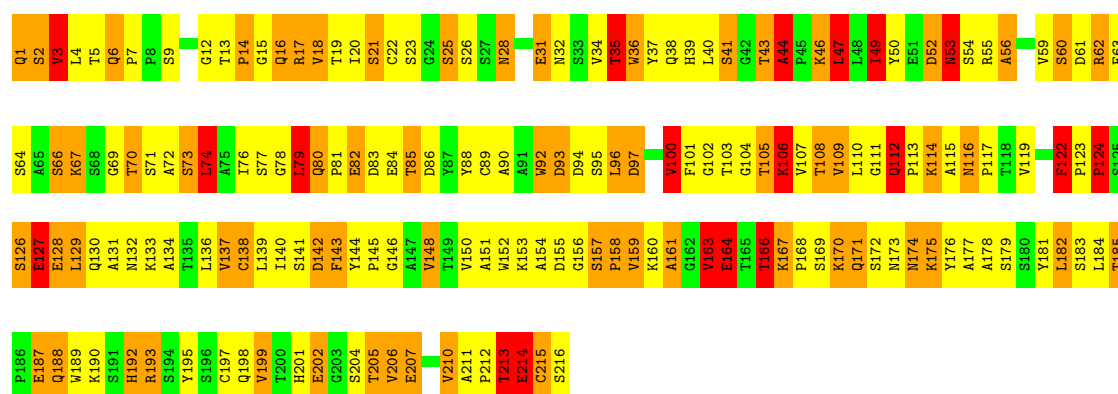
• Molecule 1: LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.30Å 72.40Å 46.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	76.6 (10.00-2.30) 72.2 (10.00-2.41)	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}	0.165 , (Not available) 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 118.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3560	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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	1.27	1/1628 (0.1%)	2.60	141/2226 (6.3%)
1	B	1.33	2/1628 (0.1%)	2.57	129/2226 (5.8%)
All	All	1.30	3/3256 (0.1%)	2.59	270/4452 (6.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	THR	CA-CB	5.98	1.61	1.53
1	B	34	VAL	C-N	-5.08	1.26	1.33
1	B	213	THR	CA-CB	5.03	1.61	1.53

All (270) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	PHE	CA-CB-CG	16.24	130.04	113.80
1	B	17	ARG	CD-NE-CZ	13.34	143.08	124.40
1	B	132	ASN	CA-CB-CG	12.29	124.89	112.60
1	A	94	ASP	CA-CB-CG	12.29	124.89	112.60
1	A	142	ASP	CA-CB-CG	-11.12	101.48	112.60
1	A	69	GLY	CA-C-N	11.06	139.79	122.86
1	A	69	GLY	C-N-CA	11.06	139.79	122.86
1	B	116	ASN	CB-CA-C	10.94	123.89	108.68
1	A	53	ASN	CA-CB-CG	10.55	123.15	112.60
1	A	2	SER	CA-C-N	10.42	140.72	121.97
1	A	2	SER	C-N-CA	10.42	140.72	121.97
1	A	88	TYR	CA-C-O	-9.75	109.70	121.11
1	A	199	VAL	CB-CA-C	-9.75	98.82	110.91
1	B	143	PHE	CA-CB-CG	9.66	123.46	113.80
1	B	97	ASP	CA-CB-CG	-9.65	102.94	112.60
1	B	138	CYS	CA-C-O	-9.62	110.53	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	GLU	N-CA-C	-9.53	101.77	113.97
1	A	32	ASN	CA-CB-CG	9.50	122.10	112.60
1	B	70	THR	CA-C-O	9.45	129.47	118.79
1	B	213	THR	CA-C-N	9.29	139.28	121.54
1	B	213	THR	C-N-CA	9.29	139.28	121.54
1	A	61	ASP	CA-CB-CG	9.14	121.74	112.60
1	A	52	ASP	CA-C-N	9.04	135.81	120.72
1	A	52	ASP	C-N-CA	9.04	135.81	120.72
1	A	6	GLN	OE1-CD-NE2	9.02	131.62	122.60
1	A	157	SER	N-CA-C	-9.00	98.47	109.72
1	A	114	LYS	CA-C-O	-8.99	112.02	121.55
1	A	128	GLU	N-CA-C	-8.93	102.97	114.04
1	A	77	SER	CA-C-O	-8.67	111.45	122.63
1	A	120	THR	CA-C-O	-8.65	111.04	120.30
1	B	35	THR	N-CA-CB	-8.63	95.82	110.83
1	B	62	ARG	CD-NE-CZ	-8.62	112.33	124.40
1	A	128	GLU	CB-CG-CD	8.41	126.90	112.60
1	A	20	ILE	CB-CA-C	-8.38	100.82	110.96
1	A	20	ILE	O-C-N	8.28	133.04	122.94
1	B	60	SER	O-C-N	8.22	132.37	122.75
1	A	161	ALA	O-C-N	8.07	133.33	122.59
1	A	101	PHE	CA-CB-CG	-8.06	105.73	113.80
1	A	106	LYS	CA-CB-CG	8.04	130.18	114.10
1	A	87	TYR	CA-C-O	-7.97	112.09	120.70
1	B	34	VAL	CA-C-N	7.79	134.63	122.94
1	B	34	VAL	C-N-CA	7.79	134.63	122.94
1	A	163	VAL	CB-CA-C	7.76	121.85	111.21
1	A	108	THR	CA-C-O	-7.74	111.94	120.38
1	A	192	HIS	CA-CB-CG	-7.74	106.06	113.80
1	B	82	GLU	CB-CG-CD	7.72	125.73	112.60
1	B	166	THR	CA-C-O	-7.70	113.40	121.87
1	B	197	CYS	CA-C-O	-7.70	111.99	120.38
1	A	185	THR	N-CA-C	-7.61	98.82	110.32
1	A	20	ILE	CA-C-O	-7.61	111.75	120.65
1	A	24	GLY	O-C-N	7.55	130.94	123.31
1	B	205	THR	CA-C-O	-7.53	110.79	119.98
1	A	25	SER	CA-C-N	7.43	130.54	120.44
1	A	25	SER	C-N-CA	7.43	130.54	120.44
1	A	80	GLN	O-C-N	7.41	128.75	121.57
1	A	133	LYS	CA-C-O	-7.38	113.06	121.40
1	A	122	PHE	CA-CB-CG	7.37	121.17	113.80
1	B	214	GLU	CA-C-N	7.28	135.44	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	GLU	C-N-CA	7.28	135.44	121.54
1	B	31	GLU	CA-C-O	-7.27	111.09	119.60
1	A	49	ILE	N-CA-C	7.27	119.45	107.24
1	B	62	ARG	NE-CZ-NH1	-7.16	114.34	121.50
1	A	116	ASN	CA-C-O	7.16	127.04	120.60
1	A	133	LYS	CA-CB-CG	7.13	128.35	114.10
1	B	148	VAL	CA-C-O	-7.06	114.72	121.64
1	A	96	LEU	N-CA-C	-7.05	103.35	112.23
1	B	44	ALA	O-C-N	7.01	129.38	121.32
1	B	7	PRO	N-CA-C	-7.00	102.16	110.70
1	B	210	VAL	CA-C-O	6.96	128.02	120.43
1	A	174	ASN	N-CA-CB	-6.94	107.16	114.10
1	B	112	GLN	N-CA-CB	6.94	119.35	109.78
1	B	23	SER	N-CA-C	6.92	120.01	108.73
1	B	129	LEU	N-CA-C	-6.88	104.70	113.23
1	B	47	LEU	CA-C-O	-6.88	113.46	121.16
1	B	114	LYS	N-CA-C	-6.88	100.81	110.50
1	B	62	ARG	NE-CZ-NH2	6.81	125.33	119.20
1	A	19	THR	CA-C-N	6.81	130.88	122.37
1	A	19	THR	C-N-CA	6.81	130.88	122.37
1	A	143	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	200	THR	CA-C-O	-6.74	113.42	120.70
1	B	128	GLU	N-CA-CB	6.72	120.01	110.67
1	A	106	LYS	CA-C-O	-6.71	113.06	120.38
1	B	182	LEU	O-C-N	6.71	131.17	123.31
1	B	167	LYS	N-CA-CB	6.69	120.20	109.90
1	A	97	ASP	CA-CB-CG	-6.64	105.96	112.60
1	B	214	GLU	N-CA-CB	6.64	121.71	110.49
1	A	149	THR	CA-C-O	-6.63	113.20	120.30
1	B	25	SER	O-C-N	-6.63	114.53	123.15
1	B	38	GLN	CA-C-N	-6.60	113.68	122.99
1	B	38	GLN	C-N-CA	-6.60	113.68	122.99
1	A	161	ALA	CA-C-O	-6.60	111.08	120.51
1	A	7	PRO	CA-C-N	6.56	125.79	118.97
1	A	7	PRO	C-N-CA	6.56	125.79	118.97
1	B	112	GLN	N-CA-C	-6.55	100.56	110.39
1	A	74	LEU	CA-C-O	-6.54	113.25	120.38
1	A	114	LYS	N-CA-C	-6.53	101.46	110.35
1	A	215	CYS	N-CA-CB	6.49	121.46	110.49
1	A	61	ASP	N-CA-C	-6.43	105.15	112.87
1	B	15	GLY	N-CA-C	6.42	123.55	115.21
1	A	63	PHE	CA-C-O	6.40	128.84	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	VAL	O-C-N	6.40	131.48	122.59
1	B	192	HIS	CA-CB-CG	-6.38	107.42	113.80
1	A	49	ILE	CB-CA-C	-6.38	103.14	110.73
1	B	86	ASP	CA-C-O	-6.37	113.77	121.28
1	B	19	THR	CA-CB-OG1	-6.35	100.08	109.60
1	B	61	ASP	O-C-N	6.34	131.12	122.37
1	B	187	GLU	O-C-N	6.34	129.59	122.11
1	B	202	GLU	N-CA-C	6.33	120.39	111.52
1	A	164	GLU	CB-CG-CD	6.32	123.35	112.60
1	A	80	GLN	CB-CG-CD	6.32	123.34	112.60
1	B	73	SER	O-C-N	6.30	131.04	123.36
1	B	193	ARG	NE-CZ-NH1	-6.30	115.20	121.50
1	B	93	ASP	CA-CB-CG	-6.29	106.31	112.60
1	A	136	LEU	CA-C-O	-6.25	114.04	121.66
1	A	175	LYS	CA-C-O	-6.21	114.49	121.81
1	A	3	VAL	CA-C-N	6.19	131.26	122.72
1	A	3	VAL	C-N-CA	6.19	131.26	122.72
1	B	100	VAL	CB-CA-C	6.11	119.60	110.98
1	A	90	ALA	O-C-N	-6.11	116.43	123.33
1	B	207	GLU	CA-CB-CG	6.10	126.29	114.10
1	A	53	ASN	CA-C-O	-6.09	111.89	119.38
1	A	152	TRP	CA-CB-CG	6.05	125.10	113.60
1	A	201	HIS	CA-CB-CG	6.02	119.82	113.80
1	B	82	GLU	CA-CB-CG	6.01	126.12	114.10
1	B	60	SER	CA-C-O	-5.99	115.28	121.87
1	B	202	GLU	CB-CA-C	-5.98	103.85	111.86
1	B	28	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	199	VAL	N-CA-C	5.96	116.76	107.28
1	B	105	THR	CA-CB-OG1	-5.96	100.67	109.60
1	A	23	SER	CA-C-O	5.95	127.02	120.71
1	A	121	LEU	CB-CA-C	5.94	119.54	109.50
1	A	39	HIS	N-CA-CB	5.94	119.95	111.05
1	B	164	GLU	O-C-N	5.92	130.28	123.29
1	B	205	THR	CA-CB-OG1	-5.92	100.72	109.60
1	A	31	GLU	CB-CG-CD	5.90	122.62	112.60
1	B	86	ASP	O-C-N	5.88	129.86	123.10
1	A	184	LEU	N-CA-CB	-5.87	102.01	110.87
1	A	174	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	86	ASP	CA-C-O	-5.85	114.19	120.92
1	A	29	ILE	CA-C-O	-5.84	115.34	121.41
1	B	109	VAL	CB-CA-C	5.84	119.48	111.31
1	A	187	GLU	CB-CG-CD	5.83	122.52	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PHE	O-C-N	5.83	129.92	123.33
1	A	129	LEU	N-CA-C	-5.79	104.93	112.23
1	A	54	SER	N-CA-C	5.79	118.67	109.24
1	B	79	LEU	N-CA-C	5.78	118.73	110.24
1	B	157	SER	CB-CA-C	5.76	117.54	108.84
1	A	134	ALA	CA-C-O	-5.76	112.26	120.15
1	A	160	LYS	CB-CA-C	5.75	119.31	110.62
1	A	214	GLU	CA-C-N	5.75	132.53	121.54
1	A	214	GLU	C-N-CA	5.75	132.53	121.54
1	B	177	ALA	CA-C-O	-5.75	113.64	120.43
1	A	144	TYR	CB-CA-C	5.74	118.07	109.63
1	B	163	VAL	N-CA-C	5.74	116.12	107.80
1	A	196	SER	CA-C-O	-5.72	114.53	120.70
1	B	108	THR	CA-C-N	-5.71	115.45	122.93
1	B	108	THR	C-N-CA	-5.71	115.45	122.93
1	B	49	ILE	CA-C-O	-5.71	114.66	121.28
1	B	163	VAL	CA-C-O	5.70	126.63	120.53
1	B	124	PRO	CA-C-O	-5.67	115.14	121.32
1	A	38	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	102	GLY	N-CA-C	-5.64	104.05	113.02
1	B	17	ARG	O-C-N	5.62	129.82	123.42
1	A	25	SER	CA-C-O	5.59	128.45	121.46
1	B	178	ALA	N-CA-CB	5.58	120.66	111.62
1	B	112	GLN	CA-CB-CG	5.57	125.25	114.10
1	A	82	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	166	THR	CA-CB-CG2	5.55	119.94	110.50
1	A	80	GLN	CA-C-O	-5.54	113.81	120.41
1	B	31	GLU	N-CA-C	5.54	120.16	112.90
1	A	164	GLU	CA-C-O	-5.51	114.21	120.32
1	A	58	GLY	N-CA-C	-5.49	107.39	115.30
1	A	138	CYS	O-C-N	5.49	129.43	122.84
1	A	59	VAL	N-CA-CB	5.48	118.18	111.60
1	B	56	ALA	N-CA-C	-5.47	103.28	110.33
1	B	139	LEU	CA-C-O	-5.46	114.81	121.36
1	A	142	ASP	O-C-N	5.46	129.85	122.59
1	A	167	LYS	CB-CA-C	5.46	115.91	109.47
1	B	84	GLU	CB-CG-CD	5.46	121.88	112.60
1	A	85	THR	N-CA-CB	-5.45	102.62	111.24
1	B	67	LYS	CA-C-N	5.45	127.86	120.44
1	B	67	LYS	C-N-CA	5.45	127.86	120.44
1	B	157	SER	CA-C-N	5.45	126.66	119.84
1	B	157	SER	C-N-CA	5.45	126.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	CYS	CA-C-N	-5.45	113.13	120.87
1	A	138	CYS	C-N-CA	-5.45	113.13	120.87
1	A	29	ILE	N-CA-CB	5.44	116.33	110.62
1	A	101	PHE	N-CA-C	5.43	118.84	110.42
1	A	133	LYS	O-C-N	5.43	129.75	123.17
1	A	196	SER	O-C-N	5.43	130.29	123.23
1	A	40	LEU	O-C-N	5.43	129.81	122.59
1	A	167	LYS	N-CA-C	-5.43	101.17	109.64
1	B	36	TRP	CA-C-O	-5.41	114.86	120.70
1	B	82	GLU	N-CA-C	-5.39	105.34	112.94
1	B	21	SER	CA-CB-OG	-5.39	100.32	111.10
1	B	158	PRO	N-CA-C	5.38	123.55	112.47
1	A	163	VAL	CA-CB-CG1	5.36	119.52	110.40
1	B	167	LYS	CA-C-N	5.36	125.66	119.93
1	B	167	LYS	C-N-CA	5.36	125.66	119.93
1	B	1	PCA	CA-C-N	5.34	131.31	121.70
1	B	1	PCA	C-N-CA	5.34	131.31	121.70
1	A	175	LYS	CA-CB-CG	5.33	124.77	114.10
1	A	84	GLU	O-C-N	5.33	129.68	122.59
1	A	139	LEU	N-CA-C	-5.33	102.40	110.28
1	A	26	SER	O-C-N	5.32	127.83	122.09
1	A	211	ALA	CA-C-N	5.32	126.49	119.84
1	A	211	ALA	C-N-CA	5.32	126.49	119.84
1	B	174	ASN	CA-C-O	5.32	126.60	120.32
1	B	106	LYS	O-C-N	5.32	129.62	123.30
1	B	25	SER	CA-C-O	5.30	127.65	121.44
1	A	39	HIS	CA-C-N	5.29	131.65	121.54
1	A	39	HIS	C-N-CA	5.29	131.65	121.54
1	B	142	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	210	VAL	CB-CA-C	5.29	118.63	110.28
1	B	47	LEU	CA-CB-CG	5.28	134.76	116.30
1	B	53	ASN	N-CA-C	5.25	121.42	114.12
1	A	31	GLU	N-CA-CB	5.24	119.35	110.49
1	A	147	ALA	CA-C-N	5.24	130.13	122.69
1	A	147	ALA	C-N-CA	5.24	130.13	122.69
1	B	14	PRO	CB-CA-C	5.23	118.29	111.64
1	B	167	LYS	N-CA-C	-5.23	102.04	109.62
1	B	207	GLU	CG-CD-OE1	-5.21	106.41	118.40
1	B	169	SER	O-C-N	5.21	129.64	123.24
1	B	74	LEU	N-CA-C	-5.19	100.72	109.07
1	B	122	PHE	O-C-N	5.18	127.38	121.94
1	A	124	PRO	CA-C-O	-5.18	115.35	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	VAL	O-C-N	5.17	128.83	122.83
1	B	166	THR	CA-CB-OG1	-5.17	101.84	109.60
1	B	6	GLN	O-C-N	5.17	126.58	121.57
1	B	85	THR	CA-C-O	-5.15	115.56	120.56
1	B	193	ARG	NE-CZ-NH2	5.15	123.84	119.20
1	A	166	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	97	ASP	CA-C-N	5.13	127.86	122.11
1	B	97	ASP	C-N-CA	5.13	127.86	122.11
1	B	79	LEU	N-CA-CB	-5.13	101.53	109.48
1	A	21	SER	CA-C-O	-5.12	115.38	121.89
1	B	79	LEU	CA-C-O	5.12	126.54	120.96
1	A	120	THR	O-C-N	5.11	129.20	123.27
1	A	198	GLN	CA-C-N	5.11	128.96	122.37
1	A	198	GLN	C-N-CA	5.11	128.96	122.37
1	B	146	GLY	N-CA-C	5.11	125.29	113.18
1	B	92	TRP	CA-C-N	-5.11	115.90	123.05
1	B	92	TRP	C-N-CA	-5.11	115.90	123.05
1	A	62	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	B	206	VAL	CA-CB-CG1	5.10	119.07	110.40
1	A	26	SER	CA-C-O	-5.10	115.45	120.70
1	A	175	LYS	N-CA-C	-5.09	103.67	110.55
1	B	214	GLU	CB-CG-CD	5.09	121.26	112.60
1	B	127	GLU	CB-CG-CD	5.08	121.24	112.60
1	B	206	VAL	N-CA-CB	5.08	120.22	111.39
1	B	207	GLU	N-CA-CB	5.07	120.18	111.00
1	A	189	TRP	CB-CA-C	5.07	119.31	110.79
1	A	16	GLN	OE1-CD-NE2	5.07	127.67	122.60
1	A	130	GLN	CA-C-N	5.06	130.74	122.65
1	A	130	GLN	C-N-CA	5.06	130.74	122.65
1	A	10	ALA	N-CA-C	-5.06	101.39	109.23
1	A	187	GLU	N-CA-CB	5.05	117.60	110.13
1	B	5	THR	N-CA-C	5.04	121.54	110.80
1	B	115	ALA	N-CA-C	-5.04	100.49	109.06
1	A	76	ILE	N-CA-C	-5.04	99.87	107.73
1	A	16	GLN	CB-CG-CD	-5.04	104.03	112.60
1	B	23	SER	CA-C-O	5.03	125.74	120.36
1	B	207	GLU	CG-CD-OE2	5.03	129.96	118.40
1	B	141	SER	N-CA-C	5.02	117.52	110.14
1	B	199	VAL	CA-C-N	5.02	130.20	122.77
1	B	199	VAL	C-N-CA	5.02	130.20	122.77
1	A	207	GLU	CB-CA-C	-5.01	100.45	110.42
1	A	34	VAL	CA-C-N	5.01	130.45	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	VAL	C-N-CA	5.01	130.45	122.94
1	B	56	ALA	CA-C-O	-5.00	116.38	122.03

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	1536	189	1
1	B	1598	0	1536	216	2
2	A	175	0	0	35	1
2	B	189	0	0	25	0
All	All	3560	0	3072	389	2

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 62.

All (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:632:HOH:O	1:B:166:THR:HG21	1.40	1.20
1:B:79:LEU:HD21	1:B:109:VAL:HG22	1.20	1.15
1:A:31:GLU:HG3	2:A:530:HOH:O	1.45	1.12
1:B:114:LYS:HE3	1:B:202:GLU:HG3	1.23	1.11
1:B:128:GLU:HG3	1:B:133:LYS:HD3	1.31	1.10
1:A:214:GLU:HG2	2:A:690:HOH:O	1.55	1.06
1:B:35:THR:CG2	1:B:90:ALA:HB3	1.87	1.03
1:A:187:GLU:HG3	2:A:646:HOH:O	1.59	1.02
1:B:17:ARG:HD3	2:B:711:HOH:O	1.64	0.98
1:B:35:THR:HG23	1:B:37:TYR:CE1	2.00	0.96
1:B:35:THR:HG22	1:B:90:ALA:HB3	1.45	0.94
1:B:81:PRO:HB3	1:B:112:GLN:HG3	1.49	0.94
1:A:47:LEU:HD12	1:A:48:LEU:N	1.83	0.92
1:B:20:ILE:HD13	1:B:74:LEU:HD23	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:O	1:A:174:ASN:HB2	1.74	0.87
1:B:2:SER:HA	1:B:103:THR:HG22	1.55	0.86
1:A:172:SER:HB3	1:B:164:GLU:OE2	1.75	0.86
2:A:632:HOH:O	1:B:166:THR:CG2	2.09	0.86
1:A:114:LYS:HE3	2:A:526:HOH:O	1.74	0.86
1:B:128:GLU:CG	1:B:133:LYS:HD3	2.07	0.85
1:B:79:LEU:HD23	1:B:79:LEU:C	2.03	0.84
1:A:116:ASN:OD1	1:A:204:SER:HB2	1.79	0.83
1:A:38:GLN:HG2	1:A:85:THR:HG21	1.60	0.83
1:B:55:ARG:HD2	2:B:725:HOH:O	1.79	0.83
1:B:112:GLN:HB2	1:B:144:TYR:CE2	2.14	0.83
1:B:39:HIS:O	1:B:85:THR:HB	1.80	0.82
1:B:124:PRO:HD3	1:B:136:LEU:CD2	2.10	0.81
1:A:3:VAL:O	2:A:522:HOH:O	1.99	0.80
1:B:14:PRO:HA	1:B:79:LEU:O	1.81	0.80
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.47	0.80
1:B:35:THR:HG21	1:B:90:ALA:HB3	1.64	0.80
1:B:171:GLN:HG3	1:B:175:LYS:O	1.80	0.79
1:B:123:PRO:HA	1:B:136:LEU:CD2	2.13	0.79
1:A:137:VAL:CG2	1:B:122:PHE:CZ	2.66	0.78
1:A:198:GLN:NE2	2:A:654:HOH:O	2.16	0.78
1:A:154:ALA:O	1:A:155:ASP:HB2	1.82	0.78
1:B:12:GLY:O	1:B:110:LEU:HB2	1.82	0.78
1:B:13:THR:HG23	2:B:801:HOH:O	1.82	0.78
1:A:119:VAL:HG22	1:A:199:VAL:HG21	1.64	0.78
1:A:35:THR:HG21	2:A:567:HOH:O	1.85	0.77
1:B:110:LEU:HD12	2:B:750:HOH:O	1.83	0.77
1:A:127:GLU:OE1	1:A:127:GLU:N	2.18	0.76
1:A:49:ILE:HD12	1:A:55:ARG:HA	1.68	0.76
1:A:184:LEU:HD23	1:A:189:TRP:HB2	1.65	0.76
1:B:79:LEU:HD21	1:B:109:VAL:CG2	2.09	0.76
1:B:128:GLU:HG2	1:B:133:LYS:O	1.87	0.75
1:B:62:ARG:HH21	1:B:83:ASP:CG	1.95	0.75
1:B:158:PRO:O	1:B:160:LYS:N	2.19	0.74
1:B:215:CYS:HA	2:B:864:HOH:O	1.87	0.74
1:B:62:ARG:HG3	1:B:62:ARG:NH1	2.03	0.74
1:A:17:ARG:HG2	1:A:77:SER:HA	1.70	0.74
1:A:153:LYS:HA	1:A:158:PRO:HA	1.70	0.73
1:B:127:GLU:O	1:B:127:GLU:HG3	1.86	0.73
1:A:49:ILE:HG22	1:A:49:ILE:O	1.89	0.73
1:B:124:PRO:HD3	1:B:136:LEU:HD21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LYS:HE3	1:B:202:GLU:CG	2.12	0.73
1:A:2:SER:O	2:A:521:HOH:O	2.05	0.73
1:A:44:ALA:H	1:A:45:PRO:HD3	1.52	0.72
1:B:81:PRO:HB3	1:B:112:GLN:CG	2.20	0.72
1:B:119:VAL:HG22	1:B:199:VAL:HG21	1.71	0.72
1:A:126:SER:O	1:A:130:GLN:N	2.22	0.72
1:A:137:VAL:HG21	1:B:122:PHE:CE1	2.25	0.72
1:A:62:ARG:NH2	1:A:83:ASP:OD1	2.23	0.71
1:A:50:TYR:HD1	1:A:51:GLU:HG3	1.55	0.71
1:B:40:LEU:CD2	1:B:85:THR:HG21	2.20	0.71
1:A:119:VAL:O	1:A:208:LYS:HE3	1.90	0.71
1:B:213:THR:HG22	1:B:214:GLU:H	1.54	0.71
1:A:93:ASP:O	1:A:97:ASP:CA	2.39	0.71
1:A:126:SER:C	1:A:128:GLU:H	1.98	0.71
1:A:49:ILE:HG21	1:A:52:ASP:O	1.91	0.70
1:A:93:ASP:O	1:A:97:ASP:HA	1.90	0.70
1:B:119:VAL:CG2	1:B:199:VAL:HG21	2.20	0.70
1:A:8:PRO:HG3	1:A:149:THR:OG1	1.92	0.70
1:A:116:ASN:OD1	1:A:204:SER:CB	2.39	0.70
1:B:35:THR:CG2	1:B:37:TYR:CE1	2.74	0.70
1:B:171:GLN:NE2	1:B:173:ASN:OD1	2.22	0.70
1:B:213:THR:HG22	1:B:214:GLU:N	2.06	0.69
1:B:40:LEU:HG	1:B:85:THR:HG21	1.74	0.69
1:A:20:ILE:HD12	1:A:20:ILE:N	2.07	0.69
1:A:85:THR:HG22	1:A:87:TYR:CE1	2.26	0.69
1:B:20:ILE:CD1	1:B:74:LEU:HD23	2.23	0.69
1:B:20:ILE:HG23	1:B:105:THR:HG21	1.74	0.68
1:A:57:SER:HB2	2:A:581:HOH:O	1.93	0.68
1:B:184:LEU:HB2	1:B:188:GLN:HG2	1.74	0.68
1:A:93:ASP:O	1:A:97:ASP:N	2.26	0.68
1:A:206:VAL:HG12	1:A:207:GLU:H	1.57	0.68
1:A:44:ALA:O	1:A:46:LYS:N	2.27	0.68
1:B:47:LEU:HD13	1:B:56:ALA:HB2	1.75	0.68
1:B:79:LEU:HD23	1:B:80:GLN:N	2.09	0.68
1:B:35:THR:HG23	1:B:37:TYR:HE1	1.56	0.68
1:A:103:THR:OG1	2:A:591:HOH:O	2.11	0.67
1:A:201:HIS:O	1:A:202:GLU:C	2.38	0.67
1:B:63:PHE:CE1	1:B:76:ILE:HG12	2.29	0.67
1:B:136:LEU:O	1:B:181:TYR:HA	1.95	0.67
1:A:136:LEU:HD23	1:A:152:TRP:HZ3	1.60	0.67
1:A:207:GLU:OE2	2:A:658:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:HD22	1:A:201:HIS:HD2	1.42	0.67
1:B:62:ARG:HH11	1:B:62:ARG:CG	2.02	0.67
1:A:13:THR:OG1	1:A:16:GLN:NE2	2.28	0.66
1:B:80:GLN:O	1:B:83:ASP:HB2	1.93	0.66
1:B:35:THR:CG2	1:B:37:TYR:HE1	2.07	0.66
1:A:4:LEU:HG	1:A:100:VAL:HG12	1.75	0.66
1:B:79:LEU:C	1:B:79:LEU:CD2	2.69	0.66
1:A:160:LYS:O	1:A:161:ALA:HB2	1.95	0.65
1:B:114:LYS:CE	1:B:202:GLU:HG3	2.13	0.65
1:A:190:LYS:O	2:A:651:HOH:O	2.14	0.65
1:B:159:VAL:HG11	1:B:195:TYR:HE1	1.62	0.65
1:B:79:LEU:CD2	1:B:109:VAL:HG22	2.12	0.65
1:B:163:VAL:HG23	1:B:182:LEU:CD1	2.27	0.65
1:A:185:THR:H	1:A:188:GLN:HB2	1.61	0.64
1:B:96:LEU:HD23	1:B:96:LEU:H	1.63	0.64
1:A:116:ASN:ND2	1:A:201:HIS:HD2	1.95	0.64
1:B:81:PRO:O	1:B:174:ASN:HB2	1.98	0.64
1:A:66:SER:OG	1:A:67:LYS:N	2.29	0.64
1:A:171:GLN:NE2	1:A:173:ASN:OD1	2.26	0.64
1:B:170:LYS:HD3	1:B:174:ASN:OD1	1.97	0.64
1:A:50:TYR:CD1	1:A:51:GLU:HG3	2.33	0.64
1:B:40:LEU:O	1:B:41:SER:C	2.40	0.63
1:B:213:THR:CG2	1:B:214:GLU:H	2.10	0.63
1:B:153:LYS:HA	1:B:157:SER:O	1.98	0.63
1:A:99:ALA:CB	1:B:101:PHE:HZ	2.11	0.63
1:B:31:GLU:OE1	1:B:94:ASP:OD2	2.17	0.63
1:A:160:LYS:O	1:A:161:ALA:CB	2.46	0.63
1:B:214:GLU:CD	1:B:215:CYS:H	2.06	0.62
1:A:47:LEU:HD12	1:A:47:LEU:C	2.24	0.62
1:B:97:ASP:OD1	2:B:742:HOH:O	2.16	0.62
1:A:96:LEU:O	1:A:97:ASP:HB3	2.00	0.62
1:A:84:GLU:HA	1:A:107:VAL:O	2.00	0.61
1:B:176:TYR:HE2	2:B:849:HOH:O	1.83	0.61
1:A:18:VAL:HG11	1:A:79:LEU:HD22	1.82	0.61
1:A:137:VAL:HG21	1:B:122:PHE:CZ	2.34	0.61
1:A:10:ALA:O	1:A:11:SER:HB3	2.00	0.60
1:A:119:VAL:HG12	1:A:208:LYS:CG	2.31	0.60
1:B:123:PRO:HA	1:B:136:LEU:HD23	1.82	0.60
1:B:117:PRO:HB3	1:B:143:PHE:HB3	1.84	0.60
1:B:119:VAL:HG13	1:B:138:CYS:SG	2.42	0.60
1:B:124:PRO:HD3	1:B:136:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HA	2:A:525:HOH:O	2.01	0.60
1:A:114:LYS:CE	2:A:526:HOH:O	2.43	0.59
1:A:173:ASN:OD1	1:A:175:LYS:HB2	2.02	0.59
1:B:22:CYS:O	1:B:71:SER:HA	2.03	0.59
1:A:40:LEU:HD13	2:A:595:HOH:O	2.02	0.59
1:A:9:SER:OG	1:A:202:GLU:HG3	2.01	0.59
1:A:11:SER:HB2	1:A:108:THR:O	2.03	0.58
1:A:136:LEU:HD23	1:A:152:TRP:CZ3	2.39	0.58
1:A:195:TYR:HB2	1:A:210:VAL:HG12	1.85	0.58
1:B:53:ASN:C	1:B:53:ASN:HD22	2.11	0.58
1:A:39:HIS:CG	1:A:40:LEU:H	2.22	0.58
1:A:44:ALA:N	1:A:45:PRO:CD	2.66	0.57
1:B:20:ILE:N	1:B:74:LEU:O	2.35	0.57
1:B:184:LEU:HB2	1:B:188:GLN:CG	2.34	0.57
1:B:46:LYS:HD3	2:B:721:HOH:O	2.05	0.57
1:A:44:ALA:H	1:A:45:PRO:CD	2.17	0.57
1:A:19:THR:O	1:A:19:THR:OG1	2.23	0.57
1:A:208:LYS:NZ	2:A:659:HOH:O	2.35	0.57
1:A:4:LEU:O	1:A:102:GLY:HA2	2.04	0.57
1:A:116:ASN:HD22	1:A:201:HIS:CD2	2.22	0.57
1:B:82:GLU:CD	2:B:738:HOH:O	2.48	0.57
1:A:153:LYS:HE3	2:A:658:HOH:O	2.05	0.56
1:A:214:GLU:HA	1:A:214:GLU:OE1	2.04	0.56
1:A:76:ILE:HG21	1:A:79:LEU:HD12	1.87	0.56
1:B:20:ILE:HD13	1:B:74:LEU:CD2	2.31	0.56
1:B:3:VAL:CG1	1:B:100:VAL:CG1	2.84	0.56
1:B:3:VAL:HG11	1:B:100:VAL:HG13	1.86	0.56
1:A:136:LEU:HD22	1:A:182:LEU:HD23	1.88	0.56
1:A:128:GLU:HB2	2:A:609:HOH:O	2.05	0.56
1:B:40:LEU:CG	1:B:85:THR:HG21	2.36	0.55
1:A:36:TRP:HB2	1:A:49:ILE:HB	1.87	0.55
1:A:124:PRO:CG	1:A:134:ALA:HB1	2.37	0.55
1:A:49:ILE:CG2	1:A:52:ASP:O	2.54	0.55
1:A:126:SER:C	1:A:128:GLU:N	2.61	0.55
1:A:48:LEU:O	1:A:49:ILE:HD13	2.07	0.55
1:A:190:LYS:HD3	2:A:683:HOH:O	2.06	0.54
1:B:119:VAL:HG21	1:B:199:VAL:CG2	2.37	0.54
1:A:153:LYS:HD3	2:A:658:HOH:O	2.08	0.54
1:B:163:VAL:HG23	1:B:182:LEU:HD12	1.89	0.54
1:A:214:GLU:CD	1:B:215:CYS:O	2.49	0.54
1:A:205:THR:HG22	1:A:205:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:PRO:HG3	1:B:134:ALA:HB1	1.90	0.54
1:B:62:ARG:NH2	1:B:83:ASP:OD2	2.34	0.54
1:B:153:LYS:HG2	1:B:157:SER:C	2.32	0.54
1:B:185:THR:OG1	1:B:188:GLN:HB3	2.07	0.54
1:A:68:SER:OG	1:A:69:GLY:N	2.41	0.54
1:A:60:SER:C	1:A:62:ARG:H	2.14	0.53
1:A:38:GLN:CG	1:A:85:THR:HG21	2.37	0.53
1:A:119:VAL:HG12	1:A:208:LYS:HG2	1.89	0.53
1:B:4:LEU:HB3	1:B:102:GLY:HA2	1.91	0.53
1:B:13:THR:O	1:B:14:PRO:C	2.51	0.53
1:B:35:THR:HG22	1:B:90:ALA:CB	2.31	0.53
1:B:142:ASP:OD2	2:B:827:HOH:O	2.19	0.53
1:B:78:GLY:O	1:B:80:GLN:OE1	2.27	0.53
1:B:140:ILE:CD1	1:B:150:VAL:HG21	2.38	0.53
1:B:185:THR:OG1	1:B:188:GLN:CB	2.56	0.53
1:A:136:LEU:HD13	1:A:184:LEU:HD22	1.90	0.53
1:B:40:LEU:HD23	1:B:85:THR:CG2	2.39	0.53
1:B:128:GLU:O	1:B:133:LYS:HB3	2.09	0.53
1:A:13:THR:O	1:A:16:GLN:HB3	2.08	0.53
1:B:17:ARG:HD2	2:B:764:HOH:O	2.08	0.53
1:B:159:VAL:HG11	1:B:195:TYR:CE1	2.43	0.53
1:B:166:THR:HG23	1:B:167:LYS:O	2.09	0.53
1:A:119:VAL:CG2	1:A:199:VAL:HG21	2.37	0.53
1:A:119:VAL:HG12	1:A:208:LYS:HG3	1.90	0.53
1:A:137:VAL:HG23	1:B:122:PHE:CZ	2.44	0.53
1:A:212:PRO:O	1:A:213:THR:HG23	2.08	0.53
1:B:53:ASN:HD22	1:B:54:SER:N	2.07	0.53
1:B:145:PRO:O	1:B:201:HIS:HE1	1.91	0.53
1:B:168:PRO:HD3	2:B:841:HOH:O	2.08	0.53
1:A:119:VAL:CG1	1:A:208:LYS:HG2	2.39	0.52
1:A:124:PRO:HB3	1:A:134:ALA:HA	1.91	0.52
1:B:144:TYR:CD1	1:B:145:PRO:HA	2.45	0.52
1:B:12:GLY:O	1:B:110:LEU:CB	2.55	0.52
1:B:124:PRO:CG	1:B:134:ALA:HB1	2.40	0.52
1:A:116:ASN:ND2	1:A:201:HIS:CD2	2.77	0.52
1:B:43:THR:O	1:B:44:ALA:CB	2.58	0.52
1:B:142:ASP:CG	2:B:827:HOH:O	2.52	0.52
1:A:2:SER:CA	2:A:521:HOH:O	2.58	0.51
1:A:45:PRO:O	1:B:1:PCA:HG3	2.10	0.51
1:A:96:LEU:O	1:A:97:ASP:CB	2.59	0.51
1:A:125:SER:OG	2:A:609:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ASP:O	1:A:65:ALA:HB3	2.10	0.51
1:B:93:ASP:HB2	1:B:100:VAL:HG21	1.93	0.51
1:A:15:GLY:O	1:A:78:GLY:HA2	2.11	0.51
1:A:153:LYS:CD	2:A:658:HOH:O	2.59	0.50
1:B:32:ASN:ND2	1:B:92:TRP:O	2.39	0.50
1:B:80:GLN:O	1:B:109:VAL:HG21	2.11	0.50
1:A:39:HIS:CD2	1:A:40:LEU:H	2.29	0.50
1:B:22:CYS:HB2	1:B:36:TRP:CH2	2.46	0.50
1:B:28:ASN:HA	1:B:92:TRP:O	2.11	0.50
1:A:214:GLU:OE2	1:B:215:CYS:O	2.29	0.50
1:B:96:LEU:N	1:B:96:LEU:CD2	2.75	0.50
1:A:20:ILE:N	1:A:20:ILE:CD1	2.73	0.50
1:A:120:THR:HG23	1:B:133:LYS:HZ3	1.76	0.50
1:B:112:GLN:HB2	1:B:144:TYR:HE2	1.70	0.50
1:A:144:TYR:CD1	1:A:145:PRO:HA	2.47	0.49
1:B:211:ALA:HB3	2:B:862:HOH:O	2.12	0.49
1:B:82:GLU:HA	1:B:174:ASN:HD22	1.76	0.49
1:A:198:GLN:CD	2:A:654:HOH:O	2.54	0.49
1:B:154:ALA:O	1:B:155:ASP:C	2.55	0.49
1:B:55:ARG:NH2	2:B:726:HOH:O	2.43	0.49
1:A:110:LEU:HD11	1:A:114:LYS:HG2	1.93	0.49
1:B:3:VAL:HG12	1:B:100:VAL:CG1	2.43	0.49
1:A:206:VAL:HG12	1:A:207:GLU:N	2.28	0.49
1:A:2:SER:C	2:A:521:HOH:O	2.54	0.49
1:B:52:ASP:OD1	1:B:67:LYS:HE3	2.13	0.49
1:B:104:GLY:O	2:B:746:HOH:O	2.19	0.49
1:B:9:SER:HB2	1:B:106:LYS:NZ	2.28	0.49
1:A:49:ILE:CD1	1:A:55:ARG:HA	2.42	0.48
1:A:60:SER:C	1:A:62:ARG:N	2.67	0.48
1:B:96:LEU:HD23	1:B:96:LEU:N	2.27	0.48
1:B:161:ALA:HB3	2:B:836:HOH:O	2.12	0.48
1:A:19:THR:HA	1:A:75:ALA:HA	1.95	0.48
1:A:10:ALA:O	1:A:107:VAL:HA	2.14	0.48
1:A:128:GLU:O	1:A:133:LYS:O	2.32	0.48
1:B:93:ASP:HB2	1:B:100:VAL:CG2	2.42	0.48
1:B:192:HIS:HE1	2:B:889:HOH:O	1.97	0.48
1:B:6:GLN:NE2	1:B:105:THR:OG1	2.47	0.48
1:A:164:GLU:OE1	1:B:172:SER:OG	2.32	0.48
1:A:1:PCA:HG3	1:B:46:LYS:HG2	1.95	0.48
1:A:16:GLN:O	1:A:79:LEU:HB2	2.14	0.48
1:A:18:VAL:CG1	1:A:79:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:HG23	1:B:182:LEU:HD13	1.96	0.47
1:B:187:GLU:C	1:B:189:TRP:N	2.71	0.47
1:A:119:VAL:HG22	1:A:199:VAL:CG2	2.38	0.47
1:A:194:SER:HB2	1:A:209:THR:HG23	1.96	0.47
1:A:112:GLN:NE2	1:A:175:LYS:NZ	2.62	0.47
1:A:48:LEU:C	1:A:49:ILE:HD13	2.39	0.47
1:A:126:SER:O	1:A:128:GLU:N	2.48	0.47
1:B:199:VAL:O	1:B:205:THR:HA	2.14	0.47
1:A:2:SER:CB	2:A:521:HOH:O	2.62	0.47
1:A:9:SER:HB3	1:A:147:ALA:HB3	1.96	0.47
1:A:124:PRO:HG2	1:A:134:ALA:HB1	1.97	0.47
1:B:95:SER:O	1:B:96:LEU:C	2.58	0.47
1:B:36:TRP:HA	1:B:88:TYR:O	2.15	0.46
1:B:49:ILE:HA	1:B:54:SER:O	2.15	0.46
1:B:107:VAL:HG12	1:B:108:THR:N	2.29	0.46
1:B:53:ASN:ND2	1:B:54:SER:OG	2.48	0.46
1:B:152:TRP:O	1:B:158:PRO:HA	2.15	0.46
1:A:112:GLN:HG3	1:A:113:PRO:HD2	1.98	0.46
1:A:63:PHE:CD1	1:A:63:PHE:N	2.82	0.46
1:A:182:LEU:HG	1:A:184:LEU:HD13	1.98	0.46
1:B:4:LEU:O	1:B:102:GLY:HA2	2.15	0.46
1:B:204:SER:C	1:B:205:THR:OG1	2.59	0.46
1:A:20:ILE:HD12	1:A:20:ILE:H	1.78	0.46
1:A:20:ILE:CD1	1:A:20:ILE:H	2.29	0.46
1:A:106:LYS:HG2	1:A:147:ALA:HB2	1.97	0.46
1:A:133:LYS:HB2	1:A:133:LYS:HE3	1.52	0.46
1:A:167:LYS:HD3	1:A:168:PRO:O	2.16	0.46
1:A:39:HIS:CG	1:A:40:LEU:N	2.83	0.46
1:B:18:VAL:HG22	2:B:786:HOH:O	2.16	0.46
1:B:40:LEU:CD2	1:B:85:THR:CG2	2.91	0.46
1:A:81:PRO:C	1:A:83:ASP:H	2.23	0.46
1:A:164:GLU:O	1:A:180:SER:HA	2.15	0.46
1:A:119:VAL:CG2	1:A:199:VAL:CG2	2.93	0.46
1:A:193:ARG:O	1:A:211:ALA:HB2	2.16	0.46
1:B:2:SER:O	1:B:3:VAL:HG22	2.15	0.46
1:A:207:GLU:HG3	1:A:208:LYS:N	2.29	0.45
1:A:171:GLN:HG2	1:A:177:ALA:HB2	1.97	0.45
1:A:114:LYS:NZ	2:A:602:HOH:O	2.49	0.45
1:B:50:TYR:N	1:B:54:SER:O	2.41	0.45
1:A:170:LYS:HB3	1:A:170:LYS:HE3	1.60	0.45
1:A:196:SER:HA	1:A:208:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:NH1	1:B:62:ARG:CG	2.62	0.45
1:A:108:THR:HG21	1:A:145:PRO:HB3	1.98	0.45
1:B:117:PRO:HD3	1:B:201:HIS:CG	2.51	0.45
1:A:109:VAL:HG12	1:A:109:VAL:O	2.15	0.45
1:B:40:LEU:HD23	1:B:85:THR:HG21	1.98	0.45
1:B:117:PRO:HD3	1:B:201:HIS:CD2	2.52	0.45
1:B:161:ALA:CB	2:B:836:HOH:O	2.65	0.45
1:A:1:PCA:HG3	1:B:46:LYS:CG	2.47	0.44
1:A:64:SER:HB2	2:A:542:HOH:O	2.16	0.44
1:A:35:THR:HA	1:A:49:ILE:O	2.17	0.44
1:A:154:ALA:O	1:A:155:ASP:CB	2.58	0.44
1:B:129:LEU:C	1:B:131:ALA:H	2.25	0.44
1:B:157:SER:HA	1:B:158:PRO:HD3	1.74	0.44
1:A:40:LEU:CD1	2:A:595:HOH:O	2.65	0.44
1:A:78:GLY:O	1:A:79:LEU:C	2.59	0.44
1:B:193:ARG:HA	2:B:856:HOH:O	2.16	0.44
1:B:198:GLN:NE2	1:B:207:GLU:OE1	2.51	0.44
1:B:3:VAL:HG11	1:B:100:VAL:CG1	2.47	0.44
1:B:145:PRO:O	1:B:201:HIS:CE1	2.71	0.44
1:A:59:VAL:O	1:A:59:VAL:HG12	2.18	0.44
1:A:190:LYS:NZ	2:A:650:HOH:O	2.49	0.44
1:B:81:PRO:CB	1:B:112:GLN:HG3	2.34	0.44
1:B:112:GLN:HB3	1:B:113:PRO:HD2	2.00	0.44
1:A:214:GLU:HG3	1:B:215:CYS:SG	2.58	0.43
1:B:184:LEU:CD1	1:B:189:TRP:HB2	2.48	0.43
1:B:189:TRP:CZ2	1:B:212:PRO:HA	2.53	0.43
1:B:43:THR:O	1:B:44:ALA:HB2	2.17	0.43
1:B:136:LEU:HD12	1:B:182:LEU:HD23	1.99	0.43
1:B:184:LEU:HB2	1:B:188:GLN:CD	2.43	0.43
1:A:31:GLU:CG	2:A:530:HOH:O	2.27	0.43
1:B:150:VAL:HA	1:B:198:GLN:O	2.19	0.43
1:B:151:ALA:HA	1:B:160:LYS:HE3	2.01	0.43
1:B:214:GLU:CG	1:B:215:CYS:N	2.81	0.43
1:B:90:ALA:HA	1:B:100:VAL:O	2.18	0.43
1:B:142:ASP:CA	1:B:175:LYS:HD2	2.48	0.43
1:A:143:PHE:CE1	1:A:146:GLY:HA2	2.54	0.43
1:B:126:SER:O	1:B:130:GLN:N	2.51	0.43
1:B:127:GLU:O	1:B:127:GLU:CG	2.64	0.43
1:A:116:ASN:HA	1:A:201:HIS:HD2	1.84	0.43
1:A:14:PRO:C	1:A:16:GLN:H	2.27	0.42
1:A:137:VAL:HG11	1:B:137:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LEU:HB2	1:B:43:THR:OG1	2.19	0.42
1:B:55:ARG:HB3	1:B:59:VAL:HB	2.01	0.42
1:B:116:ASN:N	1:B:116:ASN:HD22	2.17	0.42
1:A:44:ALA:O	1:A:45:PRO:C	2.62	0.42
1:A:55:ARG:HB3	1:A:59:VAL:HG11	2.01	0.42
1:A:152:TRP:HE1	1:A:180:SER:HG	1.62	0.42
1:B:96:LEU:H	1:B:96:LEU:CD2	2.30	0.42
1:B:22:CYS:N	1:B:72:ALA:O	2.53	0.42
1:B:170:LYS:HE3	1:B:170:LYS:HB2	1.70	0.42
1:B:82:GLU:CG	2:B:738:HOH:O	2.67	0.42
1:B:152:TRP:H	1:B:160:LYS:HE3	1.83	0.42
1:A:47:LEU:HD12	1:A:48:LEU:H	1.73	0.42
1:B:142:ASP:HA	1:B:175:LYS:HD2	2.01	0.42
1:A:120:THR:HG23	1:B:133:LYS:NZ	2.34	0.42
1:B:171:GLN:HB3	2:B:844:HOH:O	2.19	0.42
1:A:116:ASN:HA	1:A:201:HIS:CD2	2.55	0.42
1:A:133:LYS:CD	2:A:617:HOH:O	2.67	0.42
1:B:166:THR:HG23	1:B:167:LYS:N	2.33	0.42
1:B:127:GLU:HA	1:B:130:GLN:CD	2.45	0.42
1:A:165:THR:HG23	1:A:180:SER:HB2	2.01	0.41
1:B:1:PCA:O	1:B:2:SER:OG	2.35	0.41
1:B:18:VAL:HG12	1:B:76:ILE:HD12	2.02	0.41
1:B:123:PRO:HA	1:B:136:LEU:HD21	1.95	0.41
1:B:127:GLU:HA	1:B:130:GLN:HB2	2.02	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.83	0.41
1:B:119:VAL:HG21	1:B:199:VAL:HG21	1.93	0.41
1:A:196:SER:CA	1:A:208:LYS:O	2.68	0.41
1:B:175:LYS:HZ3	1:B:175:LYS:HG3	1.55	0.41
1:B:185:THR:OG1	1:B:188:GLN:HB2	2.20	0.41
1:A:112:GLN:O	1:A:113:PRO:C	2.62	0.41
1:A:126:SER:O	1:A:130:GLN:HB2	2.20	0.41
1:A:153:LYS:CE	2:A:658:HOH:O	2.65	0.41
1:B:187:GLU:O	1:B:189:TRP:N	2.54	0.41
1:B:187:GLU:O	1:B:190:LYS:N	2.52	0.41
1:B:16:GLN:HB3	1:B:17:ARG:H	1.43	0.41
1:B:49:ILE:HG23	1:B:50:TYR:N	2.36	0.41
1:B:66:SER:O	1:B:72:ALA:HA	2.20	0.41
1:B:124:PRO:HB2	1:B:129:LEU:HD11	2.03	0.41
1:B:159:VAL:HG13	1:B:159:VAL:O	2.20	0.41
1:A:127:GLU:HA	1:A:130:GLN:HB2	2.03	0.41
1:A:166:THR:CG2	1:A:167:LYS:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:SER:HB2	2:B:714:HOH:O	2.21	0.41
1:B:171:GLN:HA	2:B:844:HOH:O	2.21	0.40
1:A:36:TRP:CZ3	1:A:89:CYS:HB3	2.56	0.40
1:B:55:ARG:C	1:B:56:ALA:O	2.61	0.40
1:A:16:GLN:HE21	1:A:16:GLN:HB2	1.45	0.40
1:B:9:SER:HB2	1:B:106:LYS:HZ1	1.85	0.40

All (2) 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:3:VAL:CG1	2:A:704:HOH:O[2_664]	1.75	0.45
1:A:51:GLU:OE1	1:B:54:SER:OG[2_664]	2.18	0.02

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	214/216 (99%)	172 (80%)	21 (10%)	21 (10%)	0	0
1	B	214/216 (99%)	179 (84%)	21 (10%)	14 (6%)	1	0
All	All	428/432 (99%)	351 (82%)	42 (10%)	35 (8%)	0	0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	110	LEU
1	A	161	ALA
1	A	202	GLU
1	B	2	SER
1	B	16	GLN

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Mol	Chain	Res	Type
1	B	44	ALA
1	B	213	THR
1	B	214	GLU
1	A	31	GLU
1	A	44	ALA
1	A	45	PRO
1	A	56	ALA
1	A	69	GLY
1	A	171	GLN
1	B	3	VAL
1	B	111	GLY
1	B	156	GLY
1	B	159	VAL
1	B	215	CYS
1	A	40	LEU
1	A	79	LEU
1	A	127	GLU
1	A	155	ASP
1	A	214	GLU
1	B	41	SER
1	B	188	GLN
1	A	41	SER
1	A	82	GLU
1	A	166	THR
1	A	215	CYS
1	B	161	ALA
1	A	52	ASP
1	B	69	GLY
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%)	135 (75%)	46 (25%)	0	0
1	B	181/181 (100%)	138 (76%)	43 (24%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	362/362 (100%)	273 (75%)	89 (25%)	1 0

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	5	THR
1	A	17	ARG
1	A	18	VAL
1	A	19	THR
1	A	20	ILE
1	A	23	SER
1	A	26	SER
1	A	35	THR
1	A	40	LEU
1	A	47	LEU
1	A	49	ILE
1	A	60	SER
1	A	61	ASP
1	A	63	PHE
1	A	66	SER
1	A	76	ILE
1	A	77	SER
1	A	85	THR
1	A	94	ASP
1	A	106	LYS
1	A	107	VAL
1	A	109	VAL
1	A	120	THR
1	A	122	PHE
1	A	126	SER
1	A	127	GLU
1	A	128	GLU
1	A	135	THR
1	A	153	LYS
1	A	159	VAL
1	A	163	VAL
1	A	164	GLU
1	A	166	THR
1	A	170	LYS
1	A	172	SER
1	A	175	LYS

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Mol	Chain	Res	Type
1	A	179	SER
1	A	180	SER
1	A	184	LEU
1	A	185	THR
1	A	193	ARG
1	A	206	VAL
1	A	210	VAL
1	A	214	GLU
1	A	215	CYS
1	B	3	VAL
1	B	18	VAL
1	B	25	SER
1	B	26	SER
1	B	35	THR
1	B	43	THR
1	B	46	LYS
1	B	47	LEU
1	B	49	ILE
1	B	52	ASP
1	B	53	ASN
1	B	60	SER
1	B	64	SER
1	B	66	SER
1	B	70	THR
1	B	73	SER
1	B	74	LEU
1	B	77	SER
1	B	79	LEU
1	B	80	GLN
1	B	89	CYS
1	B	96	LEU
1	B	100	VAL
1	B	106	LYS
1	B	112	GLN
1	B	122	PHE
1	B	124	PRO
1	B	126	SER
1	B	127	GLU
1	B	137	VAL
1	B	148	VAL
1	B	163	VAL
1	B	164	GLU

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Mol	Chain	Res	Type
1	B	166	THR
1	B	170	LYS
1	B	171	GLN
1	B	175	LYS
1	B	179	SER
1	B	183	SER
1	B	185	THR
1	B	206	VAL
1	B	210	VAL
1	B	216	SER

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	16	GLN
1	A	39	HIS
1	A	112	GLN
1	A	174	ASN
1	A	201	HIS
1	B	16	GLN
1	B	53	ASN
1	B	116	ASN
1	B	174	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	A	1	1	6,7,9	0.97	1 (16%)	7,8,12	1.59	2 (28%)
1	PCA	B	1	1	6,7,9	0.64	0	7,8,12	1.49	3 (42%)

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	A	1	1	-	0/0/9/13	0/1/1/1
1	PCA	B	1	1	-	0/0/9/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	2.30	1.28	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	O-C-CA	-3.20	116.55	124.77
1	B	1	PCA	CG-CD-N	-2.24	99.43	105.72
1	B	1	PCA	O-C-CA	-2.23	119.04	124.77
1	A	1	PCA	CD-N-CA	2.16	112.71	107.21
1	B	1	PCA	CB-CA-C	2.14	115.59	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	2	0
1	B	1	PCA	2	0

5.5 Carbohydrates [i](#)

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 [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%)	-0.72	0 100 100	16, 32, 50, 69	0
1	B	215/216 (99%)	-0.70	0 100 100	14, 31, 49, 72	0
All	All	430/432 (99%)	-0.71	0 100 100	14, 32, 50, 72	0

There are no RSRZ outliers to report.

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	0.85	0.07	47,48,48,49	0
1	PCA	A	1	7/9	0.86	0.09	46,46,46,47	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.