



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:50 AM UTC

PDB ID : 1LIL / pdb_00001lil
Title : BENICE JONES PROTEIN CLE, A LAMBDA III IMMUNOGLOBULIN
LIGHT-CHAIN DIMER
Authors : Schiffer, M.; Huang, D.B.
Deposited on : 1996-05-13
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

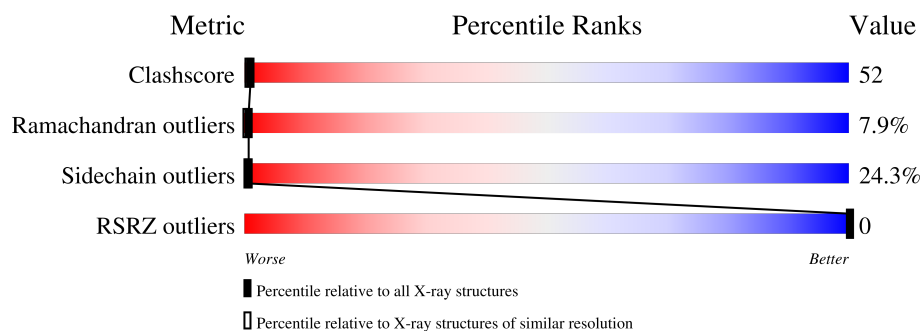
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

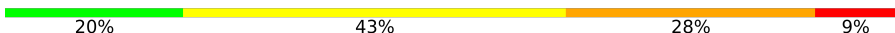
The reported resolution of this entry is 2.65 Å.

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	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	212	
1	B	212	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3314 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 LAMBDA III BENICE JONES PROTEIN CLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1595	994	267	328	6			
1	B	212	Total	C	N	O	S	0	0	0
			1595	994	267	328	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	VAL	LEU	conflict	UNP P01842
A	11	LEU	VAL	conflict	UNP P01842
A	20	ARG	SER	conflict	UNP P01842
A	26	GLU	ASP	conflict	UNP P01842
A	27	LYS	THR	conflict	UNP P01842
A	31	ALA	LYS	conflict	UNP P01842
A	33	VAL	ALA	conflict	UNP P01842
A	39	ARG	LYS	conflict	UNP P01842
A	42	GLN	HIS	conflict	UNP P01842
A	46	VAL	LEU	conflict	UNP P01842
A	49	TYR	PHE	conflict	UNP P01842
A	52	ASN	SER	conflict	UNP P01842
A	53	ARG	LYS	conflict	UNP P01842
A	66	SER	ASN	conflict	UNP P01842
A	80	THR	ALA	conflict	UNP P01842
A	81	LEU	MET	conflict	UNP P01842
A	90	VAL	ALA	conflict	UNP P01842
A	94	ASN	-	insertion	UNP P01842
A	95	ALA	-	insertion	UNP P01842
A	?	-	THR	deletion	UNP P01842
A	96	VAL	ALA	conflict	UNP P01842
B	4	VAL	LEU	conflict	UNP P01842
B	11	LEU	VAL	conflict	UNP P01842
B	20	ARG	SER	conflict	UNP P01842
B	26	GLU	ASP	conflict	UNP P01842

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	LYS	THR	conflict	UNP P01842
B	31	ALA	LYS	conflict	UNP P01842
B	33	VAL	ALA	conflict	UNP P01842
B	39	ARG	LYS	conflict	UNP P01842
B	42	GLN	HIS	conflict	UNP P01842
B	46	VAL	LEU	conflict	UNP P01842
B	49	TYR	PHE	conflict	UNP P01842
B	52	ASN	SER	conflict	UNP P01842
B	53	ARG	LYS	conflict	UNP P01842
B	66	SER	ASN	conflict	UNP P01842
B	80	THR	ALA	conflict	UNP P01842
B	81	LEU	MET	conflict	UNP P01842
B	90	VAL	ALA	conflict	UNP P01842
B	94	ASN	-	insertion	UNP P01842
B	95	ALA	-	insertion	UNP P01842
B	?	-	THR	deletion	UNP P01842
B	96	VAL	ALA	conflict	UNP P01842

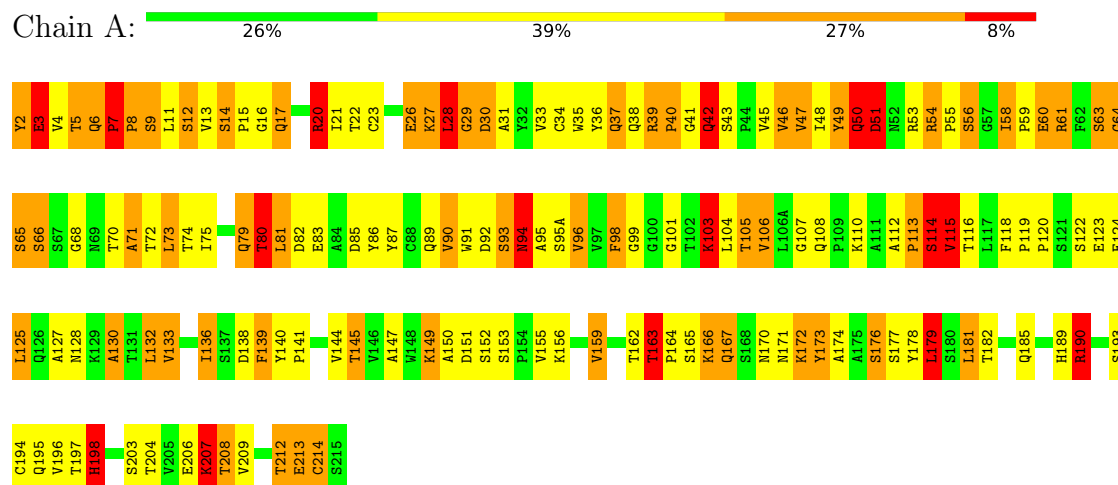
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	64	Total O 64 64	0	0

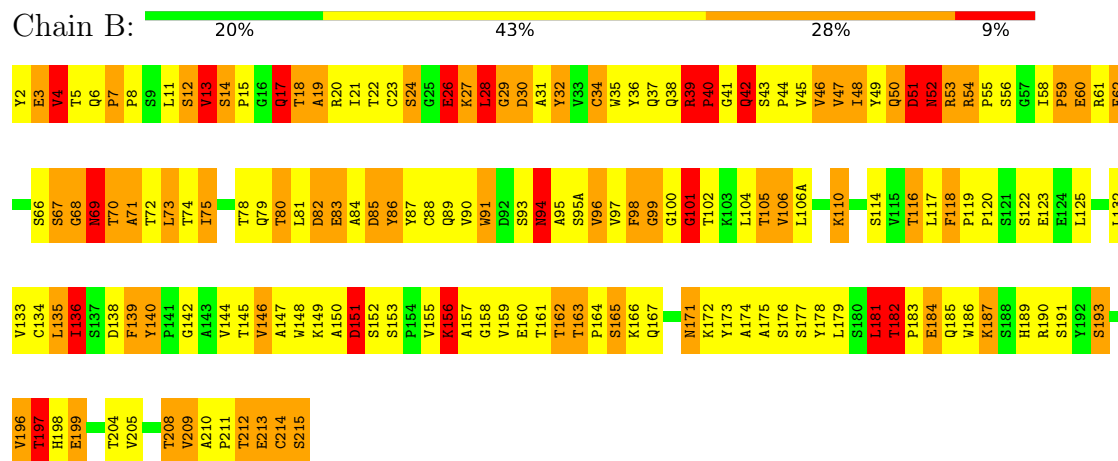
3 Residue-property plots

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: LAMBDA III BENICE JONES PROTEIN CLE



• Molecule 1: LAMBDA III BENICE JONES PROTEIN CLE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.17Å 72.54Å 49.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.65 10.00 – 2.66	Depositor EDS
% Data completeness (in resolution range)	71.0 (10.00-2.65) 71.1 (10.00-2.66)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.190 , 0.340 0.178 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 108.1	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3314	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.23	3/1634 (0.2%)	2.24	85/2234 (3.8%)
1	B	1.24	3/1634 (0.2%)	2.45	107/2234 (4.8%)
All	All	1.24	6/3268 (0.2%)	2.35	192/4468 (4.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	GLN	CB-CG	6.80	1.72	1.52
1	B	197	THR	CA-CB	5.78	1.60	1.53
1	B	67	SER	N-CA	5.62	1.49	1.46
1	B	32	TYR	N-CA	5.57	1.52	1.46
1	A	29	GLY	CA-C	5.33	1.55	1.52
1	A	106	VAL	N-CA	5.23	1.52	1.46

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASP	CA-CB-CG	21.50	134.10	112.60
1	B	118	PHE	CA-CB-CG	12.37	126.17	113.80
1	A	30	ASP	CA-CB-CG	11.55	124.15	112.60
1	B	163	THR	N-CA-C	-10.43	96.50	109.65
1	B	139	PHE	CA-CB-CG	9.85	123.65	113.80
1	A	79	GLN	CA-CB-CG	9.26	132.63	114.10
1	B	32	TYR	CA-C-O	-9.13	111.14	121.19
1	B	189	HIS	CA-CB-CG	-9.11	104.69	113.80
1	B	106	VAL	CB-CA-C	8.92	123.43	111.21
1	B	67	SER	O-C-N	8.82	128.47	122.03
1	A	95(A)	SER	N-CA-C	8.31	123.53	110.32
1	A	203	SER	N-CA-C	8.28	122.57	107.99
1	B	14	SER	O-C-N	8.23	127.66	121.65
1	A	213	GLU	N-CA-C	8.22	123.58	111.34
1	A	38	GLN	CA-CB-CG	8.17	130.44	114.10
1	B	4	VAL	CA-C-O	-8.11	110.65	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	VAL	O-C-N	8.10	131.94	123.20
1	B	159	VAL	N-CA-C	8.07	120.20	108.58
1	A	151	ASP	CB-CA-C	8.02	123.12	111.73
1	B	196	VAL	CA-C-O	7.94	127.29	120.22
1	A	198	HIS	CA-CB-CG	7.87	121.67	113.80
1	B	181	LEU	O-C-N	7.83	131.48	123.26
1	B	26	GLU	CA-CB-CG	7.82	129.75	114.10
1	A	61	ARG	N-CA-C	-7.82	103.72	113.18
1	B	34	CYS	N-CA-C	7.73	121.21	109.23
1	A	56	SER	N-CA-C	7.72	122.60	110.32
1	A	113	PRO	N-CA-C	7.71	123.12	110.55
1	B	39	ARG	CB-CA-C	7.70	122.19	109.56
1	B	26	GLU	CB-CG-CD	7.67	125.64	112.60
1	A	66	SER	N-CA-C	7.63	121.56	107.60
1	B	39	ARG	NE-CZ-NH2	7.53	125.97	119.20
1	B	54	ARG	NE-CZ-NH1	-7.49	114.01	121.50
1	A	99	GLY	N-CA-C	-7.42	104.17	112.33
1	A	172	LYS	N-CA-CB	7.40	122.11	110.56
1	A	39	ARG	CA-C-N	7.39	129.08	119.84
1	A	39	ARG	C-N-CA	7.39	129.08	119.84
1	A	106	VAL	N-CA-C	-7.34	99.23	109.21
1	A	49	TYR	CA-CB-CG	7.33	127.09	113.90
1	B	212	THR	CA-C-N	7.29	135.47	121.54
1	B	212	THR	C-N-CA	7.29	135.47	121.54
1	A	207	LYS	CA-C-O	-7.24	113.73	121.99
1	B	15	PRO	CA-C-O	-7.15	113.01	121.95
1	B	51	ASP	CA-CB-CG	7.12	119.72	112.60
1	A	136	ILE	N-CA-CB	-7.08	103.58	112.15
1	A	179	LEU	O-C-N	7.07	131.88	123.33
1	B	69	ASN	CA-CB-CG	7.05	119.65	112.60
1	B	46	VAL	CA-C-O	-7.00	112.87	120.85
1	B	178	TYR	CA-CB-CG	6.99	126.47	113.90
1	B	62	PHE	CA-CB-CG	6.97	120.78	113.80
1	A	114	SER	N-CA-C	-6.96	98.61	109.25
1	B	84	ALA	O-C-N	6.93	130.79	122.75
1	B	7	PRO	CA-C-N	6.91	127.20	119.32
1	B	7	PRO	C-N-CA	6.91	127.20	119.32
1	B	68	GLY	N-CA-C	-6.90	96.82	113.18
1	A	45	VAL	CA-C-O	-6.88	113.27	120.64
1	B	54	ARG	CD-NE-CZ	-6.88	114.76	124.40
1	A	96	VAL	CA-C-O	6.88	128.57	121.28
1	A	156	LYS	O-C-N	6.84	131.05	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	SER	CA-C-O	-6.81	112.61	120.31
1	B	70	THR	N-CA-C	6.79	119.49	108.76
1	A	37	GLN	CA-C-O	-6.78	113.38	120.70
1	A	3	GLU	CA-C-O	-6.74	113.06	120.81
1	B	30	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	213	GLU	CB-CA-C	-6.71	102.05	112.31
1	B	18	THR	CA-CB-CG2	6.68	121.85	110.50
1	A	29	GLY	N-CA-C	-6.63	99.42	110.95
1	A	47	VAL	CB-CA-C	6.61	118.08	110.88
1	B	32	TYR	N-CA-C	-6.59	100.67	110.23
1	B	85	ASP	CB-CA-C	6.59	121.13	109.72
1	B	99	GLY	N-CA-C	-6.56	100.01	111.62
1	B	156	LYS	CA-C-N	6.54	131.42	122.19
1	B	156	LYS	C-N-CA	6.54	131.42	122.19
1	A	159	VAL	N-CA-C	-6.50	100.59	109.37
1	B	53	ARG	NE-CZ-NH2	6.49	125.04	119.20
1	A	172	LYS	N-CA-C	-6.49	100.36	110.42
1	B	18	THR	CA-CB-OG1	-6.44	99.94	109.60
1	B	28	LEU	CA-C-N	6.39	128.13	120.14
1	B	28	LEU	C-N-CA	6.39	128.13	120.14
1	A	40	PRO	CA-N-CD	-6.37	103.08	112.00
1	A	64	GLY	CA-C-O	-6.36	114.83	121.63
1	A	43	SER	O-C-N	6.35	127.09	121.18
1	B	40	PRO	CB-CA-C	6.35	122.03	111.56
1	B	83	GLU	N-CA-C	-6.35	100.50	109.96
1	B	82	ASP	O-C-N	6.33	129.13	122.23
1	A	190	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	A	90	VAL	CB-CA-C	-6.32	103.32	111.53
1	B	14	SER	CA-C-O	-6.30	114.54	120.34
1	B	52	ASN	N-CA-C	6.30	120.67	112.92
1	B	184	GLU	CA-CB-CG	6.30	126.69	114.10
1	A	79	GLN	CG-CD-NE2	6.29	125.83	116.40
1	B	31	ALA	N-CA-C	6.28	118.75	108.52
1	B	191	SER	N-CA-C	6.28	117.77	108.60
1	B	110	LYS	CB-CA-C	6.26	120.83	109.62
1	B	110	LYS	N-CA-C	-6.26	101.84	110.35
1	B	145	THR	CA-CB-OG1	-6.25	100.22	109.60
1	B	178	TYR	N-CA-CB	6.19	122.21	111.13
1	B	98	PHE	CA-CB-CG	6.18	119.98	113.80
1	A	65	SER	N-CA-C	6.17	117.25	108.74
1	A	190	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	B	166	LYS	N-CA-C	6.14	118.80	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	GLN	O-C-N	6.09	129.51	122.99
1	B	45	VAL	CB-CA-C	6.08	119.86	110.50
1	A	93	SER	CA-C-N	6.07	133.14	121.54
1	A	93	SER	C-N-CA	6.07	133.14	121.54
1	A	14	SER	CB-CA-C	6.06	117.89	108.61
1	A	94	ASN	N-CA-C	6.06	123.70	110.80
1	B	43	SER	O-C-N	6.06	126.81	121.18
1	B	59	PRO	CA-C-N	6.04	133.08	121.54
1	B	59	PRO	C-N-CA	6.04	133.08	121.54
1	A	12	SER	CA-C-O	-5.92	115.57	122.37
1	B	3	GLU	N-CA-C	5.91	119.11	109.59
1	B	184	GLU	CA-C-O	5.91	126.51	119.60
1	B	171	ASN	CA-CB-CG	5.90	118.50	112.60
1	A	6	GLN	N-CA-C	5.89	117.08	109.72
1	B	182	THR	CB-CA-C	-5.87	100.31	109.11
1	A	30	ASP	N-CA-CB	5.83	120.35	110.49
1	B	29	GLY	N-CA-C	5.81	120.85	113.24
1	A	139	PHE	CA-CB-CG	5.80	119.60	113.80
1	B	163	THR	O-C-N	5.79	127.56	121.42
1	B	120	PRO	O-C-N	5.75	129.62	123.01
1	B	205	VAL	O-C-N	5.74	129.74	123.09
1	A	79	GLN	CB-CA-C	-5.70	100.60	111.48
1	B	178	TYR	O-C-N	5.70	130.22	123.33
1	A	106	VAL	CB-CA-C	5.69	119.42	111.34
1	B	71	ALA	CA-C-O	-5.67	114.70	121.56
1	B	78	THR	N-CA-C	-5.67	101.89	110.28
1	A	20	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	173	TYR	CA-CB-CG	-5.62	103.79	113.90
1	A	167	GLN	N-CA-C	-5.60	103.52	110.41
1	B	182	THR	CA-C-O	-5.59	114.89	120.64
1	A	79	GLN	CG-CD-OE1	-5.57	109.67	120.80
1	A	190	ARG	O-C-N	5.57	129.84	122.43
1	B	182	THR	O-C-N	5.57	128.71	121.64
1	A	7	PRO	CA-C-N	5.54	126.76	119.84
1	A	7	PRO	C-N-CA	5.54	126.76	119.84
1	B	205	VAL	N-CA-CB	5.54	120.44	111.36
1	B	52	ASN	O-C-N	-5.51	115.73	122.34
1	A	209	VAL	O-C-N	5.49	128.87	123.00
1	B	190	ARG	N-CA-C	-5.45	105.36	112.23
1	B	162	THR	CB-CA-C	-5.45	101.41	109.90
1	B	26	GLU	N-CA-CB	5.44	118.04	110.26
1	B	3	GLU	CB-CG-CD	5.44	121.84	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	VAL	O-C-N	5.43	127.85	122.04
1	A	26	GLU	N-CA-C	5.41	117.18	111.28
1	A	5	THR	N-CA-C	5.39	117.99	108.24
1	B	140	TYR	CA-CB-CG	-5.37	104.24	113.90
1	B	19	ALA	CA-C-N	5.35	131.47	123.23
1	B	19	ALA	C-N-CA	5.35	131.47	123.23
1	A	9	SER	CA-C-O	-5.34	115.53	121.51
1	A	125	LEU	N-CA-C	5.32	117.16	111.36
1	A	145	THR	CA-CB-OG1	-5.31	101.64	109.60
1	B	82	ASP	N-CA-C	-5.30	105.52	113.89
1	A	118	PHE	CB-CA-C	-5.29	102.80	109.31
1	B	213	GLU	N-CA-C	5.29	122.06	110.80
1	B	13	VAL	CB-CA-C	5.28	119.96	111.29
1	B	42	GLN	CB-CG-CD	-5.28	103.62	112.60
1	A	71	ALA	CA-C-O	-5.25	115.08	120.54
1	B	18	THR	CB-CA-C	5.24	120.06	109.68
1	A	194	CYS	CA-C-O	-5.24	115.05	120.70
1	A	145	THR	CB-CA-C	5.22	117.87	110.24
1	B	34	CYS	CA-CB-SG	-5.21	102.42	114.40
1	A	56	SER	CA-C-O	5.21	127.61	121.36
1	A	26	GLU	CB-CG-CD	5.21	121.46	112.60
1	A	176	SER	O-C-N	5.21	129.18	123.25
1	A	85	ASP	O-C-N	5.20	129.41	123.27
1	B	46	VAL	CA-C-N	-5.19	115.97	121.84
1	B	46	VAL	C-N-CA	-5.19	115.97	121.84
1	B	101	GLY	CA-C-N	5.17	131.02	122.33
1	B	101	GLY	C-N-CA	5.17	131.02	122.33
1	B	86	TYR	O-C-N	5.16	129.26	123.27
1	B	99	GLY	CA-C-O	-5.16	116.64	121.18
1	B	17	GLN	N-CA-CB	5.16	119.21	110.49
1	B	136	ILE	CA-C-O	-5.14	115.42	121.64
1	A	151	ASP	N-CA-C	-5.13	104.81	111.74
1	B	8	PRO	N-CA-C	5.12	121.38	113.75
1	B	209	VAL	O-C-N	5.12	128.80	123.02
1	A	177	SER	CA-C-O	-5.11	115.27	120.99
1	A	3	GLU	CB-CA-C	-5.09	101.75	109.89
1	B	208	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	132	LEU	N-CA-C	-5.07	101.45	109.96
1	A	58	ILE	O-C-N	5.06	126.87	121.10
1	B	52	ASN	N-CA-CB	-5.06	103.17	110.56
1	B	46	VAL	N-CA-C	-5.05	102.22	108.89
1	A	80	THR	N-CA-CB	5.05	117.63	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	VAL	N-CA-CB	-5.05	105.64	112.10
1	A	55	PRO	CA-C-O	-5.04	114.49	121.90
1	A	163	THR	O-C-N	5.04	126.92	121.23
1	A	197	THR	CA-C-O	-5.04	115.40	120.84
1	B	102	THR	CA-C-O	-5.03	114.10	120.28
1	A	98	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	42	GLN	CG-CD-NE2	-5.02	108.87	116.40
1	A	27	LYS	CA-C-O	-5.01	115.51	121.32

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	1595	0	1533	147	0
1	B	1595	0	1533	183	1
2	A	60	0	0	9	2
2	B	64	0	0	12	1
All	All	3314	0	3066	326	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 52.

All (326) 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:B:36:TYR:CE1	1:B:46:VAL:HG22	1.69	1.26
1:B:199:GLU:HA	2:B:409:HOH:O	1.35	1.25
1:A:47:VAL:O	1:A:48:ILE:HD13	1.43	1.14
1:A:87:TYR:HB3	1:A:98:PHE:CE1	1.83	1.13
1:A:87:TYR:HB3	1:A:98:PHE:HE1	1.00	1.07
1:A:50:GLN:O	1:A:51:ASP:HB2	1.55	1.05
1:A:36:TYR:CE1	1:A:46:VAL:HG12	1.94	1.01
1:B:36:TYR:HE1	1:B:46:VAL:CG2	1.75	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:SER:HB3	1:B:208:THR:HG22	1.44	1.00
1:A:87:TYR:CB	1:A:98:PHE:HE1	1.76	0.97
1:B:132:LEU:HD12	1:B:179:LEU:HD23	1.45	0.97
1:B:123:GLU:HG3	2:B:370:HOH:O	1.63	0.97
1:B:193:SER:CB	1:B:208:THR:HG22	1.93	0.97
1:A:28:LEU:HD21	1:A:71:ALA:HB2	1.47	0.95
1:B:181:LEU:HD22	1:B:185:GLN:HB3	1.49	0.94
1:B:156:LYS:HZ3	1:B:157:ALA:HB3	1.34	0.93
1:A:31:ALA:HA	1:A:91:TRP:O	1.69	0.91
1:B:34:CYS:SG	1:B:49:TYR:HA	2.10	0.90
1:B:3:GLU:HG2	1:B:4:VAL:O	1.70	0.90
1:B:67:SER:OG	1:B:68:GLY:N	2.01	0.88
1:B:91:TRP:HZ3	1:B:95:ALA:C	1.82	0.88
1:A:136:ILE:HG22	1:A:139:PHE:CE2	2.10	0.86
1:A:49:TYR:C	1:A:51:ASP:H	1.78	0.86
1:A:27:LYS:O	1:A:29:GLY:N	2.10	0.84
1:B:156:LYS:NZ	1:B:157:ALA:HB3	1.92	0.82
1:B:54:ARG:HD3	1:B:58:ILE:HG22	1.62	0.82
1:B:139:PHE:CE2	1:B:144:VAL:HG13	2.16	0.80
1:B:162:THR:O	2:B:463:HOH:O	2.01	0.79
1:B:156:LYS:HG2	1:B:157:ALA:N	1.98	0.79
1:A:6:GLN:NE2	1:A:86:TYR:O	2.15	0.79
1:A:11:LEU:HD23	1:A:21:ILE:HG12	1.64	0.78
1:B:91:TRP:CZ3	1:B:95:ALA:C	2.63	0.77
1:A:60:GLU:HB3	2:A:309:HOH:O	1.84	0.76
1:A:50:GLN:NE2	1:A:53:ARG:HG3	2.01	0.76
1:B:91:TRP:CH2	1:B:95:ALA:HA	2.21	0.76
1:A:190:ARG:NE	1:A:190:ARG:HA	2.00	0.75
1:B:47:VAL:HG12	1:B:58:ILE:CD1	2.17	0.75
1:B:32:TYR:CD1	1:B:50:GLN:HG2	2.22	0.75
1:B:4:VAL:HG21	1:B:90:VAL:HG21	1.69	0.74
1:B:90:VAL:O	1:B:96:VAL:HA	1.87	0.74
1:A:4:VAL:CG1	1:A:23:CYS:SG	2.76	0.73
1:A:28:LEU:CD2	1:A:71:ALA:HB2	2.19	0.73
1:A:173:TYR:N	1:A:173:TYR:CD1	2.56	0.73
1:A:167:GLN:HG3	1:A:170:ASN:OD1	1.88	0.73
1:A:22:THR:OG1	1:A:70:THR:HG23	1.89	0.73
1:B:52:ASN:OD1	2:B:427:HOH:O	2.06	0.72
1:B:156:LYS:HG2	1:B:157:ALA:H	1.53	0.72
1:A:173:TYR:N	1:A:173:TYR:HD1	1.88	0.72
1:B:117:LEU:HD23	1:B:208:THR:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:THR:C	1:B:184:GLU:H	1.97	0.71
1:B:156:LYS:H	1:B:156:LYS:HD3	1.55	0.71
1:B:39:ARG:HD2	1:B:40:PRO:HD2	1.71	0.71
1:A:115:VAL:HG12	1:A:207:LYS:HG3	1.72	0.70
1:B:23:CYS:O	1:B:70:THR:HG23	1.91	0.70
1:A:9:SER:OG	1:A:141:PRO:HG2	1.90	0.70
1:A:65:SER:O	1:A:71:ALA:HA	1.92	0.69
1:A:49:TYR:C	1:A:51:ASP:N	2.46	0.69
1:B:11:LEU:O	1:B:104:LEU:HD12	1.93	0.69
1:A:20:ARG:HH11	1:A:20:ARG:HB2	1.57	0.69
1:A:7:PRO:O	1:A:101:GLY:O	2.10	0.69
1:A:149:LYS:HA	1:A:153:SER:O	1.92	0.68
1:A:47:VAL:O	1:A:48:ILE:CD1	2.33	0.68
1:B:119:PRO:HA	1:B:132:LEU:HD23	1.75	0.67
1:B:156:LYS:CG	1:B:157:ALA:H	2.07	0.67
1:A:166:LYS:HD3	2:A:377:HOH:O	1.95	0.67
1:A:31:ALA:HB1	1:A:90:VAL:HG13	1.76	0.67
1:A:50:GLN:O	1:A:51:ASP:CB	2.41	0.67
1:A:133:VAL:HG21	1:B:118:PHE:CE1	2.30	0.67
1:A:36:TYR:HE2	1:A:89:GLN:NE2	1.92	0.66
1:A:103:LYS:HB2	1:A:103:LYS:NZ	2.10	0.66
1:B:47:VAL:HG12	1:B:58:ILE:HD11	1.77	0.66
1:B:117:LEU:HD23	1:B:208:THR:CA	2.24	0.66
1:A:20:ARG:HH11	1:A:20:ARG:CG	2.10	0.65
1:A:115:VAL:O	1:A:207:LYS:HG3	1.96	0.65
1:B:39:ARG:NH2	1:B:81:LEU:HD23	2.11	0.65
1:A:95:ALA:HA	2:A:320:HOH:O	1.96	0.65
1:A:54:ARG:HH21	1:A:60:GLU:HG2	1.60	0.65
1:A:58:ILE:CG2	1:A:59:PRO:HD2	2.27	0.65
1:B:136:ILE:HD13	1:B:136:ILE:N	2.11	0.65
1:A:11:LEU:CD2	1:A:21:ILE:HG12	2.26	0.65
1:B:193:SER:HB3	1:B:208:THR:CG2	2.26	0.64
1:A:27:LYS:C	1:A:29:GLY:H	2.05	0.64
1:A:49:TYR:O	1:A:51:ASP:N	2.31	0.64
1:A:54:ARG:NH2	1:A:60:GLU:HG2	2.12	0.63
1:A:2:TYR:N	1:A:2:TYR:CD1	2.65	0.63
1:A:14:SER:N	1:A:17:GLN:OE1	2.30	0.63
1:B:60:GLU:OE1	2:B:414:HOH:O	2.15	0.63
1:B:80:THR:C	1:B:82:ASP:H	2.06	0.63
1:A:90:VAL:HG12	1:A:90:VAL:O	1.98	0.63
1:A:130:ALA:O	1:A:181:LEU:HD12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLN:HE21	1:A:53:ARG:HB2	1.62	0.63
1:B:91:TRP:CZ3	1:B:95:ALA:HA	2.34	0.63
1:A:21:ILE:O	1:A:73:LEU:N	2.26	0.63
1:B:61:ARG:NH2	1:B:82:ASP:OD1	2.32	0.63
1:A:3:GLU:HB2	1:A:26:GLU:OE2	1.98	0.62
1:A:34:CYS:HA	1:A:48:ILE:O	1.99	0.62
1:B:41:GLY:O	1:B:42:GLN:NE2	2.31	0.62
1:B:181:LEU:HB3	1:B:185:GLN:HB2	1.81	0.62
1:A:8:PRO:HG2	1:A:198:HIS:O	1.99	0.62
1:B:12:SER:HB2	1:B:106(A):LEU:HD21	1.80	0.62
1:B:117:LEU:CD2	1:B:208:THR:HA	2.29	0.62
1:A:33:VAL:HA	1:A:89:GLN:O	1.99	0.62
1:A:50:GLN:HE22	1:A:53:ARG:HG3	1.62	0.61
1:A:54:ARG:NH1	1:A:63:SER:HA	2.15	0.61
1:B:13:VAL:CG1	1:B:14:SER:H	2.14	0.61
1:A:123:GLU:OE2	1:B:209:VAL:HG12	2.01	0.61
1:A:13:VAL:HG22	1:A:14:SER:N	2.16	0.61
1:A:58:ILE:HG23	1:A:59:PRO:HD2	1.81	0.61
1:A:181:LEU:HD12	1:A:181:LEU:O	2.00	0.61
1:B:13:VAL:HG12	1:B:14:SER:H	1.65	0.61
1:A:145:THR:O	1:A:196:VAL:HA	2.01	0.61
1:B:140:TYR:CD1	1:B:140:TYR:C	2.79	0.60
1:A:36:TYR:HE1	1:A:46:VAL:HG12	1.63	0.60
1:B:22:THR:HG22	1:B:72:THR:OG1	2.01	0.60
1:B:36:TYR:HE1	1:B:46:VAL:HG22	0.78	0.60
1:B:164:PRO:HA	1:B:174:ALA:O	2.01	0.60
1:A:3:GLU:CB	1:A:26:GLU:OE2	2.49	0.60
1:B:2:TYR:CD2	1:B:97:VAL:HG22	2.36	0.59
1:A:112:ALA:HB1	1:A:113:PRO:HD2	1.85	0.59
1:B:91:TRP:CD2	1:B:96:VAL:HG23	2.37	0.59
1:B:91:TRP:CE3	1:B:96:VAL:HG23	2.37	0.59
1:B:37:GLN:HE21	1:B:86:TYR:HE1	1.49	0.59
1:B:181:LEU:HD23	1:B:185:GLN:OE1	2.03	0.59
1:B:156:LYS:HZ2	1:B:157:ALA:H	1.49	0.59
1:B:182:THR:HB	1:B:184:GLU:HB2	1.83	0.58
1:A:50:GLN:NE2	1:A:53:ARG:CG	2.66	0.58
1:B:210:ALA:O	1:B:212:THR:N	2.36	0.58
1:A:20:ARG:HH11	1:A:20:ARG:HG2	1.69	0.58
1:A:20:ARG:HH11	1:A:20:ARG:CB	2.16	0.58
1:B:148:TRP:HE1	1:B:177:SER:HB3	1.69	0.58
1:B:167:GLN:HB2	1:B:172:LYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG11	1:A:179:LEU:HD11	1.86	0.57
1:B:3:GLU:CD	1:B:100:GLY:H	2.11	0.57
1:B:81:LEU:HD23	1:B:171:ASN:OD1	2.05	0.57
1:B:39:ARG:O	1:B:41:GLY:N	2.39	0.56
1:B:47:VAL:HG12	1:B:58:ILE:HD12	1.87	0.56
1:B:182:THR:HB	1:B:184:GLU:H	1.70	0.56
1:B:197:THR:HG23	1:B:204:THR:OG1	2.05	0.56
1:B:61:ARG:O	1:B:75:ILE:HA	2.05	0.56
1:A:136:ILE:HG22	1:A:139:PHE:HE2	1.63	0.56
1:B:39:ARG:O	1:B:40:PRO:C	2.48	0.56
1:A:136:ILE:HG22	1:A:139:PHE:CD2	2.40	0.56
1:B:142:GLY:HA3	1:B:173:TYR:CE2	2.41	0.56
1:B:150:ALA:O	1:B:151:ASP:C	2.47	0.56
1:A:11:LEU:HD23	1:A:21:ILE:CG1	2.32	0.56
1:B:6:GLN:HG3	1:B:23:CYS:SG	2.46	0.55
1:A:3:GLU:HB2	1:A:26:GLU:CD	2.31	0.55
1:B:3:GLU:HB3	2:B:428:HOH:O	2.05	0.55
1:B:155:VAL:HG11	1:B:179:LEU:HD11	1.88	0.55
1:B:50:GLN:O	1:B:52:ASN:N	2.38	0.55
1:B:68:GLY:O	1:B:70:THR:N	2.40	0.55
1:B:139:PHE:CD2	1:B:144:VAL:HG13	2.41	0.55
1:B:41:GLY:O	1:B:42:GLN:HB2	2.06	0.55
1:A:14:SER:O	1:A:16:GLY:N	2.40	0.55
1:A:4:VAL:HG13	1:A:23:CYS:SG	2.47	0.55
1:B:59:PRO:HD2	1:B:62:PHE:HE1	1.72	0.54
1:B:70:THR:HG22	1:B:71:ALA:O	2.07	0.54
1:B:91:TRP:CZ3	1:B:95:ALA:CA	2.90	0.54
1:A:120:PRO:HB2	1:A:125:LEU:CD1	2.37	0.54
1:A:60:GLU:OE1	1:A:60:GLU:O	2.25	0.54
1:B:165:SER:O	1:B:173:TYR:HA	2.08	0.54
1:B:35:TRP:HD1	1:B:48:ILE:HG22	1.73	0.53
1:B:210:ALA:C	1:B:212:THR:H	2.16	0.53
1:A:163:THR:HG22	1:A:163:THR:O	2.08	0.53
1:A:36:TYR:CE2	1:A:89:GLN:NE2	2.75	0.53
1:A:136:ILE:CG2	1:A:139:PHE:CE2	2.89	0.53
1:B:150:ALA:HB2	1:B:155:VAL:CG2	2.39	0.53
1:B:2:TYR:CE2	1:B:97:VAL:HG22	2.44	0.53
1:B:156:LYS:HD3	1:B:156:LYS:N	2.23	0.53
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.40	0.53
1:B:122:SER:O	1:B:125:LEU:N	2.42	0.53
1:A:119:PRO:HB2	1:A:120:PRO:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:HB	1:B:175:ALA:HA	1.89	0.53
1:A:94:ASN:N	1:A:94:ASN:HD22	2.06	0.52
1:B:46:VAL:HG12	1:B:55:PRO:HG3	1.92	0.52
1:B:146:VAL:HG12	1:B:147:ALA:N	2.24	0.52
1:A:13:VAL:HG22	1:A:14:SER:O	2.10	0.52
1:A:87:TYR:CB	1:A:98:PHE:CE1	2.64	0.51
1:B:34:CYS:SG	1:B:49:TYR:HB2	2.49	0.51
1:A:60:GLU:CB	2:A:309:HOH:O	2.52	0.51
1:A:140:TYR:CD1	1:A:141:PRO:HA	2.45	0.51
1:B:91:TRP:HH2	1:B:95:ALA:HA	1.75	0.51
1:A:208:THR:HG22	2:A:374:HOH:O	2.09	0.51
1:A:123:GLU:O	1:A:124:GLU:C	2.53	0.51
1:A:103:LYS:HB2	1:A:103:LYS:HZ3	1.73	0.51
1:B:34:CYS:SG	1:B:49:TYR:CA	2.91	0.51
1:B:161:THR:HA	1:B:176:SER:O	2.11	0.51
1:B:182:THR:C	1:B:184:GLU:N	2.60	0.51
1:A:39:ARG:O	1:A:42:GLN:HB2	2.10	0.51
1:B:4:VAL:HA	2:B:412:HOH:O	2.10	0.50
1:B:19:ALA:O	1:B:74:THR:HA	2.11	0.50
1:B:156:LYS:HZ2	1:B:157:ALA:N	2.09	0.50
1:B:181:LEU:HB3	1:B:185:GLN:CB	2.41	0.50
1:B:41:GLY:O	2:B:410:HOH:O	2.20	0.50
1:B:146:VAL:HG13	1:B:196:VAL:HG22	1.94	0.50
1:A:50:GLN:HE21	1:A:53:ARG:CB	2.25	0.50
1:A:20:ARG:HB2	1:A:20:ARG:NH1	2.26	0.50
1:B:3:GLU:CG	1:B:4:VAL:O	2.53	0.50
1:A:182:THR:OG1	1:A:185:GLN:HG3	2.12	0.50
1:B:21:ILE:O	1:B:73:LEU:N	2.35	0.50
1:B:146:VAL:HG12	1:B:147:ALA:H	1.76	0.50
1:B:34:CYS:O	1:B:88:CYS:HA	2.12	0.50
1:B:116:THR:O	1:B:134:CYS:HA	2.11	0.50
1:A:60:GLU:O	1:A:60:GLU:CD	2.54	0.49
1:A:47:VAL:C	1:A:48:ILE:HD13	2.32	0.49
1:A:115:VAL:HG12	1:A:207:LYS:CG	2.39	0.49
1:A:34:CYS:HB2	1:A:89:GLN:HB3	1.94	0.49
1:A:195:GLN:HB2	1:A:206:GLU:OE1	2.12	0.49
1:B:24:SER:OG	1:B:70:THR:OG1	2.31	0.49
1:B:27:LYS:O	1:B:29:GLY:N	2.45	0.49
1:B:79:GLN:O	1:B:106:VAL:HG21	2.13	0.49
1:A:3:GLU:HB2	1:A:26:GLU:CG	2.43	0.48
1:B:2:TYR:HD1	2:B:456:HOH:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:GLN:HB3	2:A:306:HOH:O	2.12	0.48
1:B:36:TYR:CE1	1:B:46:VAL:CG2	2.65	0.48
1:B:155:VAL:HG11	1:B:179:LEU:CD1	2.43	0.48
1:A:4:VAL:HG11	1:A:23:CYS:SG	2.54	0.48
1:B:183:PRO:O	1:B:187:LYS:HG2	2.13	0.48
1:B:22:THR:HG22	1:B:72:THR:HA	1.96	0.47
1:B:156:LYS:CE	1:B:157:ALA:HB3	2.43	0.47
1:A:147:ALA:HB3	1:A:195:GLN:HB3	1.96	0.47
1:B:162:THR:HG22	1:B:163:THR:O	2.15	0.47
1:B:49:TYR:HD2	1:B:55:PRO:HD3	1.78	0.47
1:B:114:SER:HB3	2:B:462:HOH:O	2.15	0.47
1:A:12:SER:HA	1:A:105:THR:O	2.15	0.46
1:A:212:THR:HG22	1:B:215:SER:OXT	2.15	0.46
1:B:27:LYS:C	1:B:29:GLY:N	2.73	0.46
1:B:67:SER:O	2:B:404:HOH:O	2.21	0.46
1:B:69:ASN:C	1:B:70:THR:HG1	2.22	0.46
1:B:20:ARG:HG3	1:B:72:THR:HG23	1.98	0.46
1:B:158:GLY:O	1:B:179:LEU:HA	2.15	0.46
1:A:92:ASP:O	1:A:94:ASN:ND2	2.49	0.46
1:A:164:PRO:HA	1:A:174:ALA:O	2.15	0.46
1:B:135:LEU:C	1:B:136:ILE:HD13	2.41	0.46
1:B:54:ARG:HH11	1:B:54:ARG:HD2	1.48	0.46
1:B:70:THR:HG22	1:B:71:ALA:N	2.31	0.46
1:B:13:VAL:O	1:B:106(A):LEU:HB2	2.16	0.46
1:B:91:TRP:HZ3	1:B:95:ALA:CA	2.26	0.46
1:A:3:GLU:HB3	1:A:26:GLU:OE2	2.15	0.45
1:A:58:ILE:CG2	1:A:59:PRO:CD	2.95	0.45
1:B:160:GLU:O	1:B:177:SER:HA	2.16	0.45
1:B:13:VAL:HG12	1:B:14:SER:N	2.29	0.45
1:B:42:GLN:OE1	1:B:42:GLN:HA	2.16	0.45
1:A:110:LYS:HB3	1:A:110:LYS:HE2	1.78	0.45
1:A:112:ALA:HB1	1:A:113:PRO:CD	2.46	0.45
1:A:127:ALA:O	1:A:128:ASN:CB	2.64	0.45
1:B:47:VAL:HA	1:B:58:ILE:HG13	1.97	0.45
1:A:34:CYS:SG	2:A:331:HOH:O	2.61	0.45
1:B:34:CYS:SG	1:B:49:TYR:CB	3.05	0.45
1:A:120:PRO:HB2	1:A:125:LEU:HD13	1.99	0.45
1:A:163:THR:O	1:A:164:PRO:C	2.58	0.45
1:A:181:LEU:CD1	1:A:181:LEU:C	2.89	0.45
1:B:22:THR:HG22	1:B:72:THR:CB	2.47	0.45
1:A:58:ILE:HG22	1:A:59:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLN:HB3	1:B:18:THR:H	1.51	0.45
1:A:64:GLY:HA2	1:A:72:THR:O	2.17	0.45
1:B:91:TRP:CZ3	1:B:95:ALA:O	2.69	0.45
1:B:59:PRO:HD2	1:B:62:PHE:CE1	2.51	0.45
1:A:149:LYS:CA	1:A:153:SER:O	2.62	0.44
1:B:13:VAL:CG1	1:B:14:SER:N	2.79	0.44
1:A:14:SER:CB	1:A:17:GLN:OE1	2.65	0.44
1:A:13:VAL:CG2	1:A:14:SER:N	2.81	0.44
1:A:165:SER:O	1:A:173:TYR:HA	2.16	0.44
1:B:66:SER:HA	1:B:70:THR:O	2.17	0.44
1:A:213:GLU:N	1:B:215:SER:OXT	2.50	0.44
2:A:476:HOH:O	1:B:163:THR:HG21	2.18	0.44
1:A:13:VAL:O	1:A:106:VAL:HA	2.18	0.44
1:B:39:ARG:NH2	1:B:81:LEU:CD2	2.80	0.44
1:B:193:SER:OG	1:B:208:THR:HG22	2.16	0.44
1:A:11:LEU:HD21	1:A:20:ARG:H	1.83	0.44
1:A:207:LYS:HB3	1:A:207:LYS:HE2	1.65	0.44
1:A:163:THR:O	1:A:163:THR:CG2	2.65	0.43
1:A:14:SER:HB2	1:A:17:GLN:OE1	2.18	0.43
1:A:80:THR:HG23	1:A:83:GLU:OE1	2.18	0.43
1:B:3:GLU:HG3	1:B:99:GLY:HA2	2.00	0.43
1:B:87:TYR:CE1	1:B:101:GLY:HA3	2.54	0.43
1:A:167:GLN:N	1:A:172:LYS:O	2.50	0.43
1:B:193:SER:CA	1:B:208:THR:HG22	2.48	0.43
1:B:32:TYR:CE1	1:B:50:GLN:HG2	2.54	0.43
1:B:91:TRP:CE3	1:B:95(A):SER:O	2.72	0.43
1:A:75:ILE:HD13	1:A:75:ILE:HG21	1.83	0.43
1:B:136:ILE:N	1:B:136:ILE:CD1	2.76	0.43
1:A:50:GLN:HE21	1:A:53:ARG:CG	2.32	0.42
1:A:114:SER:O	1:A:136:ILE:HA	2.19	0.42
1:B:26:GLU:C	1:B:27:LYS:HG2	2.43	0.42
1:B:39:ARG:HH21	1:B:81:LEU:CD2	2.31	0.42
1:B:114:SER:CB	2:B:462:HOH:O	2.67	0.42
1:B:11:LEU:O	1:B:104:LEU:HA	2.19	0.42
1:B:94:ASN:O	1:B:95:ALA:HB3	2.20	0.42
1:A:91:TRP:CD2	1:A:96:VAL:HG12	2.55	0.42
1:B:6:GLN:HG2	1:B:7:PRO:HD2	2.02	0.42
1:B:54:ARG:HA	1:B:55:PRO:HD2	1.67	0.42
1:B:89:GLN:HE21	1:B:89:GLN:HB3	1.41	0.42
1:B:96:VAL:O	1:B:96:VAL:HG12	2.19	0.42
1:A:21:ILE:HD11	1:A:104:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:TRP:CE2	1:A:73:LEU:HB2	2.55	0.42
1:A:159:VAL:HA	1:A:178:TYR:O	2.19	0.42
1:A:162:THR:OG1	1:A:176:SER:N	2.47	0.42
1:A:166:LYS:HD2	1:A:171:ASN:OD1	2.20	0.42
1:B:27:LYS:C	1:B:29:GLY:H	2.27	0.42
1:A:115:VAL:HG12	1:A:115:VAL:O	2.20	0.42
1:B:13:VAL:O	1:B:106(A):LEU:CD2	2.68	0.42
1:B:37:GLN:HA	1:B:85:ASP:O	2.20	0.42
1:B:2:TYR:N	1:B:2:TYR:CD1	2.87	0.42
1:B:11:LEU:HD22	1:B:21:ILE:HG12	2.02	0.42
1:B:97:VAL:CG1	1:B:98:PHE:N	2.83	0.41
1:A:36:TYR:CD1	1:A:46:VAL:HG12	2.50	0.41
1:A:213:GLU:C	1:A:214:CYS:SG	3.04	0.41
1:B:36:TYR:HE2	1:B:89:GLN:NE2	2.19	0.41
1:B:12:SER:C	1:B:13:VAL:HG23	2.45	0.41
1:B:20:ARG:HA	1:B:73:LEU:O	2.20	0.41
1:B:93:SER:OG	1:B:94:ASN:OD1	2.38	0.41
1:B:156:LYS:NZ	1:B:157:ALA:CB	2.75	0.41
1:B:156:LYS:CD	1:B:157:ALA:H	2.34	0.41
1:B:182:THR:O	1:B:184:GLU:N	2.54	0.41
1:B:52:ASN:ND2	1:B:53:ARG:HG2	2.36	0.41
1:B:136:ILE:O	1:B:174:ALA:HA	2.20	0.41
1:B:83:GLU:OE1	1:B:105:THR:HG22	2.21	0.41
1:B:52:ASN:ND2	1:B:52:ASN:C	2.79	0.40
1:A:39:ARG:HB3	2:A:312:HOH:O	2.21	0.40
1:A:136:ILE:CG2	1:A:139:PHE:HE2	2.33	0.40
1:B:37:GLN:O	1:B:44:PRO:HA	2.20	0.40
1:B:122:SER:HA	1:B:125:LEU:HD12	2.03	0.40
1:A:20:ARG:HD3	1:A:20:ARG:HA	1.71	0.40
1:A:80:THR:C	1:A:82:ASP:H	2.29	0.40
1:A:150:ALA:HB1	1:A:189:HIS:CD2	2.57	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)
2:A:375:HOH:O	2:B:479:HOH:O[2_655]	2.12	0.08
1:B:215:SER:O	2:A:310:HOH:O[4_456]	2.16	0.04

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	210/212 (99%)	161 (77%)	33 (16%)	16 (8%)	1	0
1	B	210/212 (99%)	166 (79%)	27 (13%)	17 (8%)	1	0
All	All	420/424 (99%)	327 (78%)	60 (14%)	33 (8%)	1	0

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	30	ASP
1	A	40	PRO
1	B	40	PRO
1	B	69	ASN
1	B	213	GLU
1	B	214	CYS
1	A	15	PRO
1	A	41	GLY
1	A	51	ASP
1	A	68	GLY
1	A	81	LEU
1	A	103	LYS
1	A	130	ALA
1	B	17	GLN
1	B	28	LEU
1	B	42	GLN
1	B	94	ASN
1	B	101	GLY
1	B	211	PRO
1	A	8	PRO
1	B	27	LYS
1	B	51	ASP
1	B	60	GLU
1	A	50	GLN

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Mol	Chain	Res	Type
1	A	107	GLY
1	B	138	ASP
1	B	186	TRP
1	A	93	SER
1	B	198	HIS
1	A	198	HIS
1	A	7	PRO
1	B	13	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	181/181 (100%)	136 (75%)	45 (25%)	0	0
1	B	181/181 (100%)	138 (76%)	43 (24%)	1	0
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	2	TYR
1	A	3	GLU
1	A	5	THR
1	A	17	GLN
1	A	20	ARG
1	A	28	LEU
1	A	37	GLN
1	A	42	GLN
1	A	46	VAL
1	A	50	GLN
1	A	51	ASP
1	A	54	ARG
1	A	56	SER
1	A	60	GLU
1	A	66	SER

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Mol	Chain	Res	Type
1	A	73	LEU
1	A	74	THR
1	A	79	GLN
1	A	80	THR
1	A	81	LEU
1	A	94	ASN
1	A	103	LYS
1	A	105	THR
1	A	108	GLN
1	A	114	SER
1	A	115	VAL
1	A	116	THR
1	A	122	SER
1	A	132	LEU
1	A	133	VAL
1	A	138	ASP
1	A	144	VAL
1	A	149	LYS
1	A	152	SER
1	A	163	THR
1	A	166	LYS
1	A	179	LEU
1	A	181	LEU
1	A	190	ARG
1	A	193	SER
1	A	204	THR
1	A	207	LYS
1	A	208	THR
1	A	212	THR
1	A	214	CYS
1	B	4	VAL
1	B	5	THR
1	B	12	SER
1	B	24	SER
1	B	26	GLU
1	B	28	LEU
1	B	30	ASP
1	B	38	GLN
1	B	39	ARG
1	B	40	PRO
1	B	42	GLN
1	B	48	ILE

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Mol	Chain	Res	Type
1	B	50	GLN
1	B	51	ASP
1	B	52	ASN
1	B	56	SER
1	B	69	ASN
1	B	73	LEU
1	B	75	ILE
1	B	80	THR
1	B	91	TRP
1	B	94	ASN
1	B	96	VAL
1	B	105	THR
1	B	110	LYS
1	B	116	THR
1	B	135	LEU
1	B	136	ILE
1	B	146	VAL
1	B	149	LYS
1	B	151	ASP
1	B	152	SER
1	B	153	SER
1	B	156	LYS
1	B	165	SER
1	B	181	LEU
1	B	182	THR
1	B	187	LYS
1	B	193	SER
1	B	197	THR
1	B	199	GLU
1	B	214	CYS
1	B	215	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	37	GLN
1	A	50	GLN
1	A	52	ASN
1	A	79	GLN
1	A	89	GLN
1	A	94	ASN
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	189	HIS
1	B	52	ASN
1	B	89	GLN
1	B	198	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	212/212 (100%)	-0.46	0 100 100	16, 16, 16, 16	0
1	B	212/212 (100%)	-0.44	0 100 100	16, 16, 16, 16	0
All	All	424/424 (100%)	-0.45	0 100 100	16, 16, 16, 16	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.