



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:12 PM UTC

PDB ID : 4BJL / pdb_00004bjl
Title : LOCW, A LAMBDA 1 TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN) CRYSTALLIZED IN DISTILLED WATER
Authors : Schiffer, M.; Huang, D.B.
Deposited on : 1995-05-26
Resolution : 2.40 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

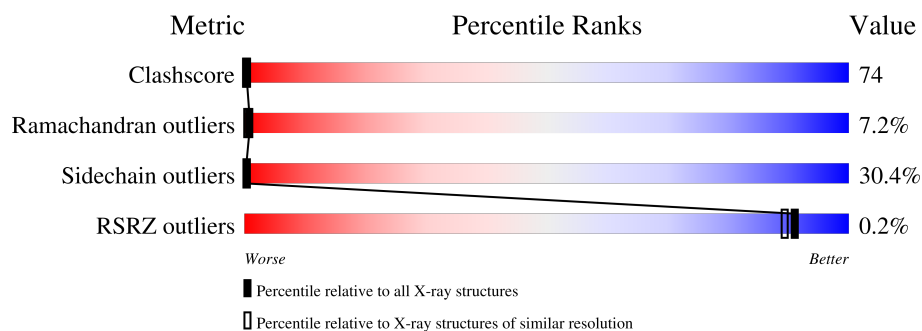
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 3460 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

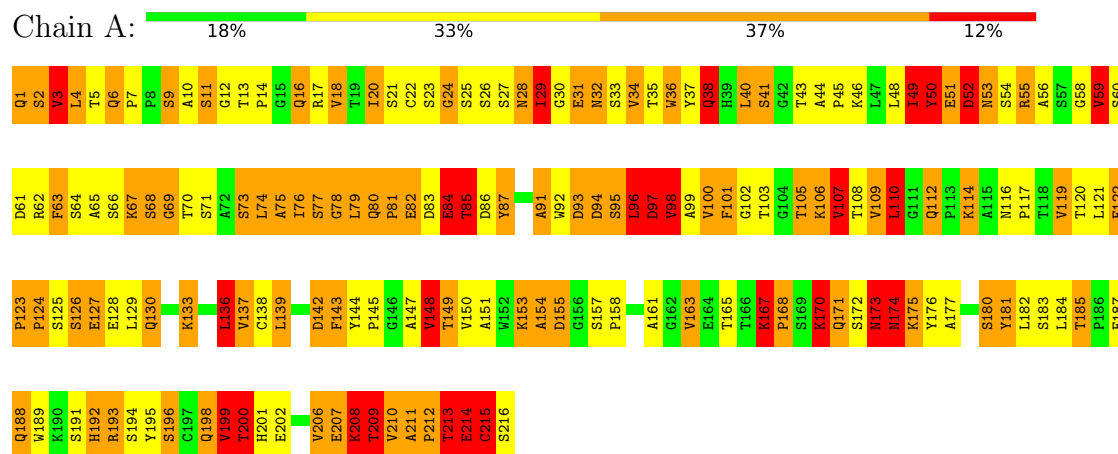
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	112	Total O 112 112	0	0
2	B	152	Total O 152 152	0	0

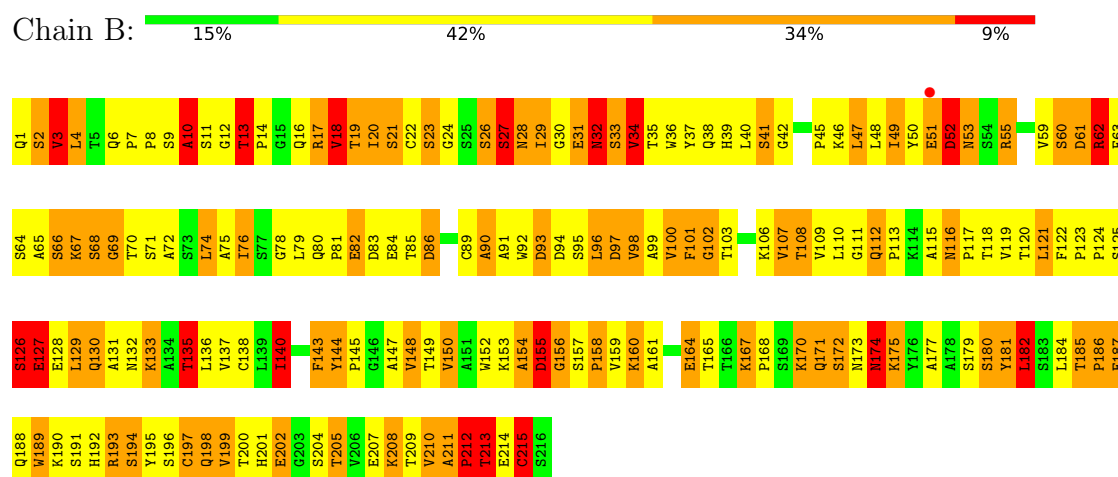
3 Residue-property plots

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	118.92Å 73.55Å 49.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	60.0 (10.00-2.40) 57.1 (10.00-2.40)	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}	0.155 , (Not available) 0.151 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 108.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3460	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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	1.31	4/1628 (0.2%)	2.57	140/2226 (6.3%)
1	B	1.33	3/1628 (0.2%)	2.58	140/2226 (6.3%)
All	All	1.32	7/3256 (0.2%)	2.58	280/4452 (6.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	THR	CA-CB	6.17	1.62	1.53
1	A	175	LYS	N-CA	5.84	1.52	1.45
1	B	213	THR	CA-CB	5.53	1.61	1.53
1	A	84	GLU	C-N	-5.31	1.28	1.33
1	B	102	GLY	N-CA	5.17	1.51	1.45
1	A	85	THR	CA-CB	5.06	1.61	1.54
1	A	80	GLN	CA-CB	-5.04	1.47	1.54

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	GLU	CA-CB-CG	16.66	147.42	114.10
1	A	142	ASP	N-CA-C	11.61	127.41	111.39
1	A	97	ASP	CA-CB-CG	11.26	123.86	112.60
1	A	198	GLN	OE1-CD-NE2	11.11	133.71	122.60
1	B	143	PHE	CA-CB-CG	10.84	124.64	113.80
1	B	173	ASN	N-CA-C	-10.32	100.63	113.02
1	A	154	ALA	CA-C-O	-9.54	109.69	120.66
1	A	94	ASP	CA-CB-CG	-9.50	103.10	112.60
1	B	96	LEU	N-CA-C	-9.31	102.73	114.56
1	A	91	ALA	CA-C-O	-9.27	111.54	121.36
1	B	7	PRO	O-C-N	9.23	125.49	121.15
1	B	64	SER	CA-C-O	-9.21	110.67	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	CYS	CA-C-O	-9.16	110.66	120.46
1	B	82	GLU	N-CA-C	9.14	124.22	112.34
1	A	6	GLN	OE1-CD-NE2	9.07	131.67	122.60
1	A	107	VAL	N-CA-CB	9.03	121.83	110.99
1	B	112	GLN	CB-CG-CD	8.96	127.83	112.60
1	B	140	ILE	O-C-N	8.87	131.64	123.03
1	A	188	GLN	N-CA-C	-8.82	101.67	111.28
1	B	61	ASP	N-CA-C	-8.72	102.81	113.19
1	A	163	VAL	CB-CA-C	8.71	124.65	111.68
1	B	211	ALA	O-C-N	8.68	130.22	121.72
1	A	97	ASP	N-CA-C	-8.62	92.44	110.80
1	A	175	LYS	CB-CA-C	8.52	123.86	109.80
1	A	161	ALA	CA-C-O	8.42	130.38	120.70
1	B	131	ALA	O-C-N	8.38	133.35	122.04
1	A	185	THR	O-C-N	8.12	130.98	121.39
1	B	96	LEU	CA-C-O	8.11	127.79	118.55
1	B	110	LEU	N-CA-C	8.05	119.84	111.14
1	A	176	TYR	O-C-N	7.99	131.96	122.85
1	B	157	SER	O-C-N	7.91	130.68	121.66
1	A	122	PHE	O-C-N	7.89	129.08	121.66
1	A	50	TYR	CA-CB-CG	7.88	128.08	113.90
1	B	194	SER	CA-C-N	7.83	135.21	122.29
1	B	194	SER	C-N-CA	7.83	135.21	122.29
1	A	12	GLY	CA-C-N	7.79	131.54	120.49
1	A	12	GLY	C-N-CA	7.79	131.54	120.49
1	A	53	ASN	CA-CB-CG	7.78	120.38	112.60
1	A	69	GLY	N-CA-C	-7.73	94.87	113.18
1	B	98	VAL	O-C-N	7.72	131.24	122.82
1	B	2	SER	CA-C-N	7.65	135.74	121.97
1	B	2	SER	C-N-CA	7.65	135.74	121.97
1	B	97	ASP	N-CA-CB	-7.63	100.48	111.84
1	A	107	VAL	O-C-N	7.62	131.49	123.03
1	B	155	ASP	CA-CB-CG	7.54	120.14	112.60
1	B	53	ASN	CA-CB-CG	-7.54	105.06	112.60
1	B	160	LYS	N-CA-CB	7.54	123.23	110.49
1	A	81	PRO	N-CA-C	7.51	123.27	114.03
1	B	121	LEU	CA-C-N	7.51	135.57	122.28
1	B	121	LEU	C-N-CA	7.51	135.57	122.28
1	B	180	SER	O-C-N	7.50	131.97	123.27
1	B	75	ALA	O-C-N	7.50	132.88	123.14
1	A	80	GLN	N-CA-C	-7.49	97.25	109.82
1	B	152	TRP	CA-CB-CG	7.45	127.75	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	GLN	CA-C-O	-7.43	112.51	121.28
1	A	185	THR	N-CA-C	-7.38	99.84	110.40
1	B	116	ASN	CA-CB-CG	7.33	119.93	112.60
1	A	188	GLN	N-CA-CB	7.31	120.87	110.12
1	A	153	LYS	CA-CB-CG	7.25	128.60	114.10
1	A	192	HIS	N-CA-C	7.18	120.24	110.55
1	A	206	VAL	O-C-N	7.14	130.74	123.10
1	A	176	TYR	CA-C-O	-7.08	113.46	121.81
1	A	127	GLU	N-CA-CB	7.06	121.30	109.78
1	A	199	VAL	CB-CA-C	7.06	119.72	110.12
1	A	193	ARG	CD-NE-CZ	7.03	134.24	124.40
1	B	125	SER	CA-CB-OG	7.00	125.09	111.10
1	B	126	SER	N-CA-C	-6.99	103.59	111.14
1	A	181	TYR	O-C-N	6.97	131.36	123.27
1	B	28	ASN	CA-CB-CG	6.94	119.54	112.60
1	B	131	ALA	N-CA-C	-6.92	102.26	113.19
1	A	66	SER	CA-C-O	-6.91	113.15	120.40
1	A	75	ALA	CA-C-O	-6.90	113.16	120.40
1	A	185	THR	CA-CB-OG1	-6.88	99.28	109.60
1	A	170	LYS	CB-CA-C	6.88	120.16	109.84
1	A	192	HIS	CA-CB-CG	-6.82	106.98	113.80
1	A	198	GLN	CB-CG-CD	-6.78	101.07	112.60
1	A	200	THR	CB-CA-C	6.78	121.45	109.72
1	A	196	SER	O-C-N	6.76	132.16	123.11
1	A	154	ALA	O-C-N	6.74	131.50	123.27
1	B	123	PRO	N-CA-C	-6.73	102.48	110.70
1	B	47	LEU	N-CA-C	-6.68	99.94	109.96
1	A	136	LEU	O-C-N	6.68	131.84	123.15
1	B	72	ALA	CA-C-O	-6.67	113.65	121.46
1	B	208	LYS	O-C-N	6.64	131.41	123.24
1	B	7	PRO	N-CA-C	-6.64	103.48	110.58
1	A	174	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	124	PRO	CA-C-N	6.61	130.72	120.75
1	A	124	PRO	C-N-CA	6.61	130.72	120.75
1	A	110	LEU	CB-CA-C	6.59	117.91	109.80
1	B	156	GLY	O-C-N	6.56	131.23	122.70
1	A	173	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	154	ALA	N-CA-C	-6.54	98.33	109.24
1	B	155	ASP	N-CA-CB	6.54	121.53	110.49
1	B	51	GLU	CA-CB-CG	6.52	127.15	114.10
1	B	181	TYR	CA-C-N	6.51	132.11	122.86
1	B	181	TYR	C-N-CA	6.51	132.11	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	SER	CA-C-N	6.48	131.99	122.08
1	B	95	SER	C-N-CA	6.48	131.99	122.08
1	B	38	GLN	N-CA-C	-6.48	99.65	109.95
1	B	18	VAL	CA-C-O	6.45	127.90	120.67
1	A	210	VAL	O-C-N	6.45	128.58	122.97
1	A	80	GLN	CA-C-O	-6.44	114.03	120.66
1	B	186	PRO	CB-CA-C	6.41	122.14	111.56
1	B	170	LYS	O-C-N	6.39	130.74	122.87
1	B	215	CYS	N-CA-CB	6.38	121.27	110.49
1	B	150	VAL	CB-CA-C	6.33	119.58	110.33
1	B	179	SER	CB-CA-C	6.32	120.72	109.65
1	B	214	GLU	CA-C-N	6.31	133.59	121.54
1	B	214	GLU	C-N-CA	6.31	133.59	121.54
1	B	170	LYS	N-CA-C	-6.29	101.11	110.23
1	B	144	TYR	CA-CB-CG	-6.28	102.59	113.90
1	A	142	ASP	N-CA-CB	-6.26	102.43	111.70
1	A	60	SER	CA-C-N	6.25	129.28	120.28
1	A	60	SER	C-N-CA	6.25	129.28	120.28
1	B	47	LEU	CB-CA-C	6.25	119.89	109.89
1	A	63	PHE	N-CA-CB	6.23	119.91	109.94
1	B	96	LEU	CA-C-N	-6.20	113.21	122.07
1	B	96	LEU	C-N-CA	-6.20	113.21	122.07
1	A	120	THR	O-C-N	6.19	131.29	123.12
1	A	84	GLU	CA-C-N	6.18	133.45	122.08
1	A	84	GLU	C-N-CA	6.18	133.45	122.08
1	B	32	ASN	CA-C-O	6.16	128.65	121.44
1	A	91	ALA	O-C-N	6.15	130.12	122.92
1	A	67	LYS	N-CA-C	-6.15	102.25	110.55
1	A	148	VAL	O-C-N	6.15	127.84	122.12
1	A	192	HIS	CA-C-N	6.14	128.78	120.44
1	A	192	HIS	C-N-CA	6.14	128.78	120.44
1	B	62	ARG	O-C-N	6.13	128.71	122.09
1	B	209	THR	O-C-N	6.12	130.74	123.27
1	B	112	GLN	CA-C-N	6.12	127.04	120.13
1	B	112	GLN	C-N-CA	6.12	127.04	120.13
1	A	199	VAL	CA-C-O	6.11	126.30	120.25
1	A	123	PRO	CB-CA-C	6.11	118.37	110.92
1	A	34	VAL	CB-CA-C	6.11	119.67	110.63
1	A	29	ILE	O-C-N	6.09	128.10	121.83
1	A	106	LYS	CA-C-N	-6.08	115.27	122.93
1	A	106	LYS	C-N-CA	-6.08	115.27	122.93
1	B	3	VAL	N-CA-C	6.08	121.98	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	CYS	O-C-N	6.07	130.78	123.13
1	B	158	PRO	N-CA-C	-6.02	102.42	111.57
1	B	138	CYS	N-CA-C	-6.02	97.34	107.99
1	A	55	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	B	171	GLN	CA-CB-CG	6.00	126.11	114.10
1	B	32	ASN	CA-C-N	6.00	129.64	120.82
1	B	32	ASN	C-N-CA	6.00	129.64	120.82
1	B	107	VAL	N-CA-C	-5.99	101.28	109.55
1	A	50	TYR	CB-CA-C	5.97	120.81	110.79
1	A	127	GLU	N-CA-C	-5.93	101.58	111.37
1	B	69	GLY	CA-C-N	5.92	132.09	121.66
1	B	69	GLY	C-N-CA	5.92	132.09	121.66
1	A	32	ASN	N-CA-C	5.86	118.45	110.55
1	A	59	VAL	CA-C-N	5.85	132.59	122.64
1	A	59	VAL	C-N-CA	5.85	132.59	122.64
1	B	3	VAL	CA-C-N	5.85	131.07	123.00
1	B	3	VAL	C-N-CA	5.85	131.07	123.00
1	B	198	GLN	CA-CB-CG	5.85	125.80	114.10
1	B	10	ALA	O-C-N	5.83	130.35	122.59
1	A	171	GLN	CB-CA-C	5.83	120.74	110.36
1	A	167	LYS	CA-CB-CG	5.80	125.69	114.10
1	B	193	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	B	32	ASN	CB-CA-C	5.79	121.66	109.79
1	A	80	GLN	CA-C-N	5.78	125.88	119.87
1	A	80	GLN	C-N-CA	5.78	125.88	119.87
1	B	34	VAL	CA-C-O	-5.78	115.16	121.92
1	A	158	PRO	CA-C-N	5.76	130.19	122.93
1	A	158	PRO	C-N-CA	5.76	130.19	122.93
1	B	180	SER	CA-C-O	-5.75	114.14	120.30
1	A	52	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	152	TRP	CA-C-N	5.74	131.98	122.33
1	B	152	TRP	C-N-CA	5.74	131.98	122.33
1	A	176	TYR	CA-CB-CG	-5.74	103.57	113.90
1	A	138	CYS	CA-C-N	-5.74	113.41	121.72
1	A	138	CYS	C-N-CA	-5.74	113.41	121.72
1	B	181	TYR	N-CA-CB	5.73	120.02	110.85
1	A	38	GLN	N-CA-C	-5.73	100.94	110.17
1	A	93	ASP	CA-C-N	5.72	132.47	121.54
1	A	93	ASP	C-N-CA	5.72	132.47	121.54
1	B	8	PRO	CA-C-N	5.72	131.21	122.11
1	B	8	PRO	C-N-CA	5.72	131.21	122.11
1	A	11	SER	O-C-N	5.72	129.68	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ASP	O-C-N	5.71	131.54	122.41
1	B	102	GLY	N-CA-C	-5.70	103.42	112.66
1	B	212	PRO	CA-C-N	5.68	131.75	121.06
1	B	212	PRO	C-N-CA	5.68	131.75	121.06
1	A	208	LYS	CB-CA-C	5.68	119.18	109.80
1	A	85	THR	N-CA-CB	-5.68	101.35	110.55
1	A	6	GLN	O-C-N	5.67	127.84	121.32
1	A	73	SER	N-CA-C	5.65	117.32	107.49
1	B	4	LEU	CA-C-N	5.63	130.14	122.19
1	B	4	LEU	C-N-CA	5.63	130.14	122.19
1	B	198	GLN	CB-CA-C	5.63	119.42	110.19
1	A	211	ALA	CA-C-N	5.60	126.84	119.84
1	A	211	ALA	C-N-CA	5.60	126.84	119.84
1	A	95	SER	N-CA-CB	5.59	119.93	110.49
1	A	63	PHE	O-C-N	5.58	130.07	122.82
1	B	51	GLU	CA-C-N	5.56	132.15	121.54
1	B	51	GLU	C-N-CA	5.56	132.15	121.54
1	B	51	GLU	CA-C-O	5.55	128.28	121.84
1	B	103	THR	CA-CB-OG1	-5.51	101.33	109.60
1	A	24	GLY	CA-C-O	-5.51	116.52	122.47
1	B	171	GLN	OE1-CD-NE2	-5.50	117.09	122.60
1	B	53	ASN	O-C-N	5.50	127.76	121.93
1	B	133	LYS	CA-C-O	-5.48	114.85	120.99
1	A	98	VAL	CA-C-N	5.46	129.69	122.42
1	A	98	VAL	C-N-CA	5.46	129.69	122.42
1	A	143	PHE	CA-CB-CG	5.46	119.26	113.80
1	A	139	LEU	CB-CA-C	5.46	119.24	110.29
1	B	116	ASN	O-C-N	5.45	128.03	121.60
1	A	122	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	27	SER	N-CA-CB	-5.44	102.12	110.12
1	B	118	THR	N-CA-CB	5.44	119.09	110.55
1	A	112	GLN	OE1-CD-NE2	5.44	128.04	122.60
1	B	154	ALA	CA-C-N	5.44	131.92	121.54
1	B	154	ALA	C-N-CA	5.44	131.92	121.54
1	B	93	ASP	CA-CB-CG	-5.43	107.17	112.60
1	B	86	ASP	N-CA-C	-5.43	102.49	110.52
1	B	121	LEU	CB-CA-C	5.42	119.64	109.71
1	A	87	TYR	O-C-N	5.42	130.19	123.14
1	A	130	GLN	O-C-N	5.42	129.94	122.46
1	A	43	THR	CA-CB-OG1	-5.40	101.50	109.60
1	B	51	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	49	ILE	CB-CA-C	5.38	118.16	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	VAL	CA-C-N	5.38	131.02	122.74
1	B	148	VAL	C-N-CA	5.38	131.02	122.74
1	B	159	VAL	CA-C-N	5.38	131.81	121.54
1	B	159	VAL	C-N-CA	5.38	131.81	121.54
1	B	74	LEU	CA-C-O	5.38	127.65	121.47
1	B	64	SER	N-CA-CB	-5.37	102.21	111.55
1	A	58	GLY	N-CA-C	-5.35	100.49	113.18
1	B	90	ALA	CA-C-N	5.35	130.74	121.64
1	B	90	ALA	C-N-CA	5.35	130.74	121.64
1	A	97	ASP	O-C-N	5.35	129.71	122.59
1	A	148	VAL	CA-C-O	-5.34	117.46	121.68
1	B	101	PHE	CA-CB-CG	5.32	119.11	113.80
1	A	36	TRP	CA-CB-CG	5.29	123.66	113.60
1	A	174	ASN	CA-C-N	-5.28	113.13	122.74
1	A	174	ASN	C-N-CA	-5.28	113.13	122.74
1	A	209	THR	N-CA-C	5.28	116.83	108.96
1	A	67	LYS	N-CA-CB	5.28	118.47	110.45
1	A	85	THR	CA-CB-CG2	5.28	119.47	110.50
1	A	133	LYS	CA-C-O	-5.26	115.65	121.33
1	B	12	GLY	CA-C-N	5.24	132.17	121.48
1	B	12	GLY	C-N-CA	5.24	132.17	121.48
1	B	152	TRP	N-CA-C	-5.24	101.63	109.95
1	B	32	ASN	CA-CB-CG	-5.23	107.37	112.60
1	B	26	SER	CA-C-N	5.21	127.27	120.28
1	B	26	SER	C-N-CA	5.21	127.27	120.28
1	B	185	THR	CB-CA-C	5.20	116.93	108.87
1	A	55	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	43	THR	CA-CB-CG2	5.19	119.33	110.50
1	B	199	VAL	CA-C-N	-5.19	115.68	123.00
1	B	199	VAL	C-N-CA	-5.19	115.68	123.00
1	A	214	GLU	CB-CG-CD	5.19	121.42	112.60
1	A	149	THR	CA-C-N	-5.18	114.98	122.45
1	A	149	THR	C-N-CA	-5.18	114.98	122.45
1	A	80	GLN	O-C-N	5.17	125.75	121.35
1	A	80	GLN	CB-CA-C	5.17	116.99	109.08
1	A	50	TYR	N-CA-C	5.17	117.70	111.40
1	B	66	SER	CA-C-N	5.16	132.96	121.81
1	B	66	SER	C-N-CA	5.16	132.96	121.81
1	A	215	CYS	CA-C-N	5.12	130.93	121.70
1	A	215	CYS	C-N-CA	5.12	130.93	121.70
1	A	136	LEU	N-CA-C	-5.10	101.61	109.52
1	A	49	ILE	N-CA-C	-5.09	101.08	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	SER	O-C-N	5.09	129.36	122.59
1	B	155	ASP	O-C-N	5.09	129.35	122.59
1	A	67	LYS	CA-C-O	-5.08	115.82	121.81
1	B	68	SER	N-CA-CB	5.08	119.07	110.49
1	B	155	ASP	CB-CA-C	-5.08	100.32	110.42
1	A	171	GLN	CA-C-N	5.06	127.38	120.54
1	A	171	GLN	C-N-CA	5.06	127.38	120.54
1	B	174	ASN	N-CA-CB	-5.04	104.51	112.63
1	B	182	LEU	CA-C-N	5.04	129.50	121.99
1	B	182	LEU	C-N-CA	5.04	129.50	121.99
1	A	130	GLN	CA-C-N	5.03	132.00	121.94
1	A	130	GLN	C-N-CA	5.03	132.00	121.94
1	B	135	THR	N-CA-C	-5.03	101.73	109.52
1	B	23	SER	CA-C-O	5.02	126.70	120.92
1	A	171	GLN	CA-CB-CG	5.02	124.13	114.10
1	A	213	THR	CA-C-O	5.01	127.68	120.51

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	260	0
1	B	1598	0	1537	220	0
2	A	112	0	0	15	0
2	B	152	0	0	27	0
All	All	3460	0	3073	464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

All (464) 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:38:GLN:HG3	1:A:85:THR:CG2	1.62	1.27
1:B:52:ASP:HB2	2:B:742:HOH:O	1.28	1.26
1:B:84:GLU:OE1	1:B:170:LYS:HE2	1.46	1.12
1:A:38:GLN:CG	1:A:85:THR:HG21	1.80	1.12
1:B:130:GLN:HE21	1:B:130:GLN:HA	1.00	1.11
1:A:170:LYS:H	1:A:170:LYS:HD3	1.18	1.08
1:A:13:THR:O	1:A:16:GLN:HB2	1.54	1.06
1:B:115:ALA:HB2	1:B:175:LYS:HE2	1.40	1.03
1:B:60:SER:HB2	1:B:62:ARG:HB2	1.41	1.02
1:A:74:LEU:HD13	1:A:76:ILE:HD11	1.44	0.99
1:A:170:LYS:H	1:A:170:LYS:CD	1.77	0.97
1:B:130:GLN:HA	1:B:130:GLN:NE2	1.75	0.97
1:A:24:GLY:H	1:A:29:ILE:HD11	1.29	0.96
1:A:38:GLN:HG3	1:A:85:THR:HG21	0.97	0.95
1:A:110:LEU:HD21	1:A:114:LYS:HB2	1.49	0.95
1:B:49:ILE:HD12	1:B:55:ARG:HA	1.48	0.94
1:B:136:LEU:HD13	1:B:182:LEU:HD23	1.50	0.94
1:B:62:ARG:NH2	1:B:76:ILE:HD11	1.83	0.92
1:B:46:LYS:NZ	1:B:59:VAL:HG22	1.86	0.91
1:A:148:VAL:HG23	1:A:199:VAL:HG23	1.52	0.90
1:A:99:ALA:HB3	2:A:544:HOH:O	1.69	0.90
1:B:119:VAL:HG21	1:B:199:VAL:HG11	1.54	0.90
1:B:121:LEU:CD2	1:B:210:VAL:HG22	2.03	0.89
1:B:46:LYS:HZ1	1:B:59:VAL:HG22	1.37	0.89
1:A:3:VAL:HA	1:A:100:VAL:HG12	1.54	0.88
1:B:130:GLN:HE21	1:B:130:GLN:CA	1.85	0.88
1:B:93:ASP:HB2	1:B:100:VAL:CG2	2.03	0.88
1:A:153:LYS:NZ	1:A:207:GLU:OE2	2.05	0.88
1:A:36:TRP:O	1:A:48:LEU:HB2	1.73	0.88
1:A:7:PRO:O	1:A:105:THR:HB	1.74	0.87
1:A:79:LEU:HD22	1:A:109:VAL:HG22	1.55	0.87
1:A:6:GLN:HG2	1:A:105:THR:CG2	2.04	0.87
1:A:2:SER:O	1:A:3:VAL:HB	1.74	0.86
1:A:29:ILE:O	1:A:67:LYS:NZ	2.08	0.86
1:B:115:ALA:CB	1:B:175:LYS:HE2	2.06	0.85
1:B:37:TYR:CE1	1:B:47:LEU:HD12	2.12	0.85
1:B:184:LEU:HD22	1:B:188:GLN:HB3	1.57	0.84
1:A:170:LYS:HD3	1:A:170:LYS:N	1.90	0.84
1:B:60:SER:C	1:B:62:ARG:H	1.80	0.84
1:B:86:ASP:OD1	1:B:106:LYS:HG3	1.78	0.84
1:A:92:TRP:HZ2	1:A:97:ASP:O	1.59	0.84
1:A:24:GLY:H	1:A:29:ILE:CD1	1.91	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HG12	1:B:101:PHE:O	1.78	0.83
1:A:93:ASP:N	1:A:98:VAL:O	2.10	0.83
1:A:30:GLY:O	1:A:31:GLU:HB2	1.78	0.83
1:A:92:TRP:CZ2	1:A:97:ASP:O	2.32	0.82
1:A:3:VAL:N	1:A:100:VAL:HG11	1.96	0.81
1:B:19:THR:HA	1:B:74:LEU:O	1.81	0.81
1:A:16:GLN:O	1:A:79:LEU:HB2	1.81	0.80
1:B:4:LEU:O	1:B:102:GLY:HA2	1.82	0.80
1:B:119:VAL:HG21	1:B:199:VAL:CG1	2.12	0.80
1:B:11:SER:HB3	1:B:108:THR:HG23	1.62	0.79
1:A:74:LEU:HD13	1:A:76:ILE:CD1	2.12	0.79
1:A:189:TRP:CZ2	1:A:212:PRO:HA	2.18	0.79
1:A:24:GLY:N	1:A:29:ILE:HD11	1.98	0.78
1:B:84:GLU:OE1	1:B:170:LYS:CE	2.28	0.78
1:B:124:PRO:HD3	1:B:136:LEU:HG	1.65	0.78
1:B:119:VAL:CG2	1:B:199:VAL:HG11	2.15	0.77
1:B:126:SER:O	1:B:127:GLU:C	2.27	0.77
1:B:62:ARG:HH22	1:B:83:ASP:CG	1.94	0.76
1:B:10:ALA:O	1:B:107:VAL:HA	1.85	0.76
1:A:128:GLU:OE2	1:A:133:LYS:HE3	1.85	0.76
1:A:20:ILE:CG2	1:A:105:THR:HG21	2.15	0.76
1:A:38:GLN:HG3	1:A:85:THR:HG23	1.67	0.76
1:A:6:GLN:NE2	1:A:87:TYR:O	2.20	0.75
1:A:62:ARG:NH2	1:A:83:ASP:OD1	2.18	0.75
1:A:148:VAL:HG22	1:A:149:THR:N	2.00	0.75
1:A:96:LEU:CB	1:A:98:VAL:HG22	2.17	0.75
1:B:84:GLU:HG2	1:B:109:VAL:H	1.50	0.75
1:B:126:SER:O	1:B:128:GLU:N	2.20	0.75
1:A:168:PRO:HD3	2:A:618:HOH:O	1.87	0.75
1:B:121:LEU:O	2:B:605:HOH:O	2.06	0.74
1:A:96:LEU:HB3	1:A:98:VAL:HG22	1.69	0.74
1:B:192:HIS:CD2	1:B:195:TYR:OH	2.41	0.74
1:B:121:LEU:HG	1:B:210:VAL:CG2	2.17	0.74
1:A:149:THR:HB	1:A:200:THR:HG23	1.70	0.73
1:A:63:PHE:CD2	1:A:76:ILE:HG13	2.23	0.73
1:B:201:HIS:O	1:B:202:GLU:HB2	1.87	0.73
1:A:119:VAL:HG11	1:A:199:VAL:CG1	2.19	0.72
1:A:148:VAL:CG2	1:A:199:VAL:HG23	2.18	0.72
1:A:119:VAL:HG11	1:A:199:VAL:HG13	1.71	0.72
1:B:144:TYR:CD1	1:B:144:TYR:C	2.67	0.72
1:B:170:LYS:HG2	2:B:828:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLU:C	1:A:215:CYS:SG	2.73	0.72
1:B:192:HIS:HD2	1:B:195:TYR:OH	1.73	0.72
1:B:13:THR:HG21	2:B:764:HOH:O	1.90	0.72
1:A:148:VAL:CG2	1:A:149:THR:N	2.52	0.71
1:B:126:SER:O	1:B:129:LEU:N	2.22	0.71
1:B:60:SER:C	1:B:62:ARG:N	2.48	0.71
1:B:160:LYS:HE3	2:B:543:HOH:O	1.91	0.71
1:A:181:TYR:OH	1:B:171:GLN:OE1	2.09	0.70
1:B:208:LYS:HD3	2:B:808:HOH:O	1.91	0.70
1:B:205:THR:CG2	2:B:874:HOH:O	2.39	0.69
1:A:51:GLU:O	1:A:52:ASP:HB2	1.92	0.69
1:B:52:ASP:C	2:B:742:HOH:O	2.36	0.69
1:A:25:SER:N	1:A:28:ASN:OD1	2.25	0.69
1:B:121:LEU:HG	1:B:210:VAL:HG22	1.73	0.68
1:B:147:ALA:O	1:B:148:VAL:HG13	1.92	0.68
1:B:136:LEU:HD11	1:B:184:LEU:HD12	1.74	0.68
1:A:94:ASP:C	1:A:96:LEU:H	1.99	0.68
1:B:65:ALA:HB2	1:B:74:LEU:HD12	1.74	0.68
1:B:93:ASP:HB2	1:B:100:VAL:HG21	1.75	0.68
1:B:121:LEU:CG	1:B:210:VAL:HG22	2.24	0.68
1:B:182:LEU:HD21	1:B:184:LEU:HD11	1.75	0.67
1:B:153:LYS:HA	1:B:158:PRO:HA	1.75	0.67
1:A:7:PRO:HD2	1:A:21:SER:O	1.95	0.67
1:A:2:SER:C	1:A:100:VAL:HG11	2.20	0.66
1:B:136:LEU:CD1	1:B:184:LEU:HD12	2.26	0.66
1:B:35:THR:HG23	1:B:49:ILE:O	1.94	0.66
1:A:112:GLN:HE22	1:A:175:LYS:HG2	1.60	0.66
1:A:171:GLN:HB2	1:B:164:GLU:HG2	1.76	0.66
1:A:18:VAL:O	1:A:75:ALA:HA	1.96	0.66
1:A:84:GLU:HB3	1:A:107:VAL:O	1.95	0.66
1:A:101:PHE:N	1:A:101:PHE:CD1	2.62	0.66
1:A:116:ASN:ND2	2:A:602:HOH:O	2.14	0.66
1:A:6:GLN:HG2	1:A:105:THR:HG22	1.78	0.66
1:A:62:ARG:HH22	1:A:83:ASP:CG	2.03	0.66
1:A:122:PHE:CE1	1:B:137:VAL:HG21	2.31	0.66
1:B:19:THR:C	1:B:20:ILE:HD13	2.21	0.65
1:A:171:GLN:NE2	1:B:181:TYR:OH	2.28	0.65
1:A:63:PHE:HD2	1:A:76:ILE:HG13	1.60	0.65
1:A:4:LEU:O	1:A:102:GLY:HA2	1.95	0.65
1:A:41:SER:HB3	2:A:560:HOH:O	1.96	0.65
1:B:37:TYR:CE1	1:B:47:LEU:CD1	2.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:THR:OG1	1:B:180:SER:OG	2.11	0.65
1:B:192:HIS:NE2	2:B:849:HOH:O	2.24	0.65
1:A:92:TRP:CZ2	1:A:97:ASP:C	2.75	0.64
1:A:34:VAL:HG23	1:A:67:LYS:HE2	1.79	0.64
1:A:70:THR:HG22	1:A:70:THR:O	1.98	0.64
1:B:187:GLU:O	1:B:188:GLN:C	2.40	0.64
1:B:196:SER:HA	1:B:208:LYS:O	1.96	0.64
1:A:209:THR:HG23	1:A:210:VAL:N	2.13	0.64
1:B:62:ARG:NH2	1:B:83:ASP:OD2	2.30	0.64
1:B:148:VAL:O	2:B:823:HOH:O	2.15	0.64
1:A:136:LEU:HD11	1:A:184:LEU:CD1	2.28	0.63
1:B:80:GLN:O	1:B:109:VAL:HG21	1.97	0.63
1:B:205:THR:HG21	2:B:874:HOH:O	1.96	0.63
1:A:38:GLN:HB2	1:A:87:TYR:CE2	2.33	0.63
1:A:117:PRO:HB3	1:A:143:PHE:HB3	1.79	0.63
1:B:20:ILE:HD13	1:B:20:ILE:N	2.13	0.63
1:B:211:ALA:O	1:B:213:THR:N	2.32	0.63
1:A:84:GLU:HA	1:A:107:VAL:HG22	1.81	0.62
1:A:150:VAL:HG12	1:A:151:ALA:N	2.13	0.62
1:B:96:LEU:O	1:B:97:ASP:C	2.41	0.62
1:A:48:LEU:HD11	1:A:87:TYR:CD2	2.35	0.62
1:A:126:SER:O	1:A:127:GLU:C	2.40	0.62
1:B:121:LEU:HD21	1:B:210:VAL:HG22	1.81	0.62
1:B:186:PRO:O	1:B:190:LYS:HG2	2.00	0.62
1:B:97:ASP:OD1	1:B:97:ASP:O	2.18	0.61
1:A:20:ILE:CG2	1:A:105:THR:CG2	2.78	0.61
1:A:24:GLY:O	1:A:70:THR:HG22	2.01	0.61
1:A:150:VAL:HG12	1:A:151:ALA:H	1.65	0.61
1:B:41:SER:HB3	2:B:720:HOH:O	1.98	0.61
1:B:184:LEU:CD2	1:B:188:GLN:HB3	2.28	0.61
1:A:36:TRP:O	1:A:48:LEU:N	2.29	0.61
1:A:144:TYR:HA	1:A:145:PRO:C	2.24	0.61
1:A:6:GLN:OE1	1:A:102:GLY:HA3	2.00	0.61
1:B:130:GLN:O	2:B:842:HOH:O	2.16	0.61
1:A:2:SER:HB3	1:A:100:VAL:HG11	1.81	0.61
1:A:182:LEU:HD11	2:A:614:HOH:O	2.01	0.61
1:B:113:PRO:O	2:B:804:HOH:O	2.16	0.61
1:A:76:ILE:HG22	1:A:76:ILE:O	2.00	0.61
1:A:92:TRP:CE3	1:A:99:ALA:HB2	2.36	0.61
1:A:22:CYS:O	1:A:29:ILE:CD1	2.47	0.60
1:B:48:LEU:HD23	1:B:74:LEU:HD21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:SER:C	1:A:27:SER:H	2.08	0.60
1:A:209:THR:CG2	1:A:210:VAL:N	2.65	0.60
1:B:189:TRP:CZ2	1:B:212:PRO:HA	2.36	0.60
1:A:6:GLN:HG2	1:A:105:THR:HG21	1.84	0.60
1:B:4:LEU:CD2	1:B:29:ILE:HD11	2.31	0.60
1:B:32:ASN:ND2	1:B:92:TRP:O	2.35	0.60
1:A:121:LEU:HD23	1:A:209:THR:HA	1.84	0.60
1:B:28:ASN:O	1:B:29:ILE:C	2.45	0.60
1:A:119:VAL:CG2	1:A:208:LYS:HB2	2.32	0.59
1:A:74:LEU:CD1	1:A:76:ILE:HD11	2.25	0.59
1:B:80:GLN:O	1:B:81:PRO:C	2.45	0.59
1:B:24:GLY:O	1:B:70:THR:HB	2.03	0.59
1:B:52:ASP:CB	2:B:742:HOH:O	2.10	0.59
1:A:121:LEU:HD23	1:A:209:THR:CA	2.33	0.59
1:A:184:LEU:HD22	1:A:189:TRP:HA	1.84	0.59
1:A:185:THR:OG1	1:A:188:GLN:HG3	2.02	0.59
1:B:90:ALA:HA	1:B:100:VAL:O	2.02	0.59
1:A:3:VAL:CA	1:A:100:VAL:HG12	2.29	0.59
1:B:50:TYR:O	1:B:51:GLU:C	2.44	0.59
1:B:4:LEU:HD21	1:B:29:ILE:HG13	1.85	0.58
1:B:145:PRO:HA	2:B:817:HOH:O	2.03	0.58
1:A:182:LEU:HD21	1:A:195:TYR:HE1	1.68	0.58
1:A:11:SER:OG	1:A:110:LEU:HD11	2.03	0.58
1:A:148:VAL:CG2	1:A:149:THR:H	2.15	0.58
1:B:76:ILE:HD12	1:B:76:ILE:C	2.29	0.58
1:A:119:VAL:HG22	1:A:208:LYS:HD3	1.86	0.58
1:B:18:VAL:HG22	1:B:76:ILE:CG2	2.32	0.58
1:B:191:SER:O	1:B:191:SER:OG	2.21	0.58
1:A:122:PHE:CZ	1:B:137:VAL:CG2	2.87	0.58
1:A:80:GLN:HG2	1:A:81:PRO:HD2	1.86	0.58
1:A:17:ARG:NH1	2:A:551:HOH:O	2.30	0.57
1:A:172:SER:C	1:A:174:ASN:H	2.12	0.57
1:A:49:ILE:HG21	1:A:65:ALA:HB3	1.86	0.57
1:A:119:VAL:HA	1:A:139:LEU:O	2.05	0.57
1:B:182:LEU:CD2	1:B:184:LEU:HD11	2.34	0.57
1:A:97:ASP:H	1:A:98:VAL:HG22	1.69	0.57
1:A:5:THR:O	1:A:22:CYS:HA	2.05	0.57
1:A:184:LEU:HD22	1:A:189:TRP:CA	2.33	0.57
1:A:45:PRO:HG2	1:B:101:PHE:CD2	2.40	0.56
1:A:93:ASP:HB2	1:A:100:VAL:HG23	1.87	0.56
1:A:82:GLU:HG3	2:A:555:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:GLU:O	1:B:53:ASN:N	2.31	0.56
1:B:35:THR:HG21	1:B:47:LEU:HD11	1.86	0.56
1:B:121:LEU:HG	1:B:210:VAL:HG21	1.88	0.56
1:A:29:ILE:HD12	1:A:71:SER:HA	1.88	0.56
1:A:24:GLY:O	1:A:70:THR:CG2	2.54	0.55
1:A:182:LEU:HD21	1:A:195:TYR:CE1	2.42	0.55
1:A:124:PRO:HB2	1:A:129:LEU:HD13	1.88	0.55
1:B:62:ARG:HH21	1:B:76:ILE:HD11	1.70	0.55
1:A:7:PRO:O	1:A:105:THR:CB	2.51	0.55
1:A:20:ILE:HD11	1:A:76:ILE:HD13	1.88	0.55
1:A:149:THR:O	1:A:199:VAL:HA	2.05	0.55
1:B:84:GLU:HG2	1:B:108:THR:HA	1.88	0.55
1:A:136:LEU:O	1:A:181:TYR:HA	2.06	0.55
1:B:49:ILE:HD11	1:B:55:ARG:HG3	1.87	0.55
1:A:6:GLN:HE21	1:A:105:THR:HG23	1.71	0.55
1:A:93:ASP:HB2	1:A:100:VAL:CG2	2.37	0.55
1:A:29:ILE:HG21	1:A:71:SER:CA	2.37	0.54
1:A:79:LEU:HD22	1:A:109:VAL:CG2	2.31	0.54
1:A:3:VAL:N	1:A:100:VAL:CG1	2.69	0.54
1:A:136:LEU:HD11	1:A:184:LEU:HD11	1.89	0.54
1:A:155:ASP:OD1	1:A:193:ARG:HB3	2.07	0.54
1:B:126:SER:C	1:B:128:GLU:N	2.64	0.54
1:A:212:PRO:O	2:A:624:HOH:O	2.18	0.54
1:B:93:ASP:O	1:B:97:ASP:N	2.41	0.54
1:A:37:TYR:HA	1:A:46:LYS:O	2.07	0.54
1:B:128:GLU:OE1	1:B:133:LYS:HE3	2.06	0.54
1:A:1:PCA:O	1:A:2:SER:CB	2.55	0.54
1:B:201:HIS:O	1:B:202:GLU:CB	2.54	0.54
1:B:33:SER:HA	1:B:52:ASP:OD1	2.07	0.53
1:B:49:ILE:CD1	1:B:55:ARG:HG3	2.38	0.53
1:B:155:ASP:OD1	1:B:193:ARG:HB2	2.08	0.53
1:B:200:THR:OG1	1:B:205:THR:OG1	2.20	0.53
1:A:3:VAL:CA	1:A:100:VAL:CG1	2.86	0.53
1:A:3:VAL:HA	1:A:100:VAL:CG1	2.32	0.53
1:A:121:LEU:CD2	1:A:209:THR:HA	2.39	0.53
1:A:62:ARG:O	1:A:77:SER:HB2	2.08	0.53
1:B:18:VAL:HG22	1:B:76:ILE:HG23	1.91	0.53
1:B:37:TYR:CD1	1:B:47:LEU:HA	2.44	0.53
1:A:184:LEU:CD2	1:A:189:TRP:HA	2.38	0.53
1:A:193:ARG:HB3	2:A:613:HOH:O	2.08	0.53
1:A:214:GLU:O	1:A:215:CYS:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD23	1:B:29:ILE:HD11	1.91	0.53
1:A:96:LEU:O	1:A:97:ASP:HB2	2.08	0.52
1:A:34:VAL:O	1:A:52:ASP:N	2.35	0.52
1:B:22:CYS:O	1:B:29:ILE:CD1	2.57	0.52
1:B:92:TRP:HA	1:B:99:ALA:HA	1.91	0.52
1:B:121:LEU:CG	1:B:210:VAL:CG2	2.84	0.52
1:B:130:GLN:HB2	2:B:867:HOH:O	2.09	0.52
1:A:44:ALA:CB	1:B:102:GLY:O	2.57	0.52
1:A:208:LYS:HE3	2:A:628:HOH:O	2.08	0.52
1:B:121:LEU:HD21	1:B:210:VAL:CG2	2.39	0.52
1:B:208:LYS:CD	2:B:808:HOH:O	2.53	0.52
1:A:215:CYS:O	1:A:216:SER:HB2	2.09	0.52
1:A:85:THR:HG22	1:A:86:ASP:O	2.10	0.51
1:B:51:GLU:C	1:B:53:ASN:H	2.16	0.51
1:B:92:TRP:HZ2	1:B:97:ASP:OD1	1.94	0.51
1:A:20:ILE:HG22	1:A:105:THR:HG21	1.91	0.51
1:B:29:ILE:HG12	1:B:34:VAL:HG23	1.92	0.51
1:B:187:GLU:O	1:B:191:SER:HB3	2.11	0.51
1:B:188:GLN:O	1:B:192:HIS:HD2	1.93	0.51
1:B:192:HIS:HD2	1:B:195:TYR:HH	1.57	0.51
1:A:136:LEU:HD12	1:A:136:LEU:N	2.26	0.51
1:B:172:SER:C	1:B:174:ASN:H	2.16	0.51
1:A:6:GLN:NE2	1:A:105:THR:HG23	2.26	0.51
1:A:11:SER:HB2	1:A:110:LEU:HD12	1.92	0.51
1:A:68:SER:C	1:A:69:GLY:O	2.51	0.51
1:A:48:LEU:HD11	1:A:87:TYR:HD2	1.76	0.50
1:A:84:GLU:HA	1:A:107:VAL:O	2.11	0.50
1:B:60:SER:HB2	1:B:62:ARG:CB	2.27	0.50
1:B:67:LYS:HA	1:B:71:SER:O	2.12	0.50
1:B:97:ASP:C	1:B:97:ASP:OD1	2.51	0.50
1:B:154:ALA:O	1:B:156:GLY:N	2.44	0.50
1:B:37:TYR:HA	1:B:46:LYS:O	2.11	0.50
1:B:132:ASN:HA	1:B:186:PRO:HG2	1.94	0.50
1:A:20:ILE:HD11	1:A:76:ILE:CD1	2.41	0.50
1:A:36:TRP:C	1:A:48:LEU:HB2	2.34	0.50
1:A:85:THR:CG2	1:A:86:ASP:H	2.24	0.50
1:A:85:THR:CG2	1:A:86:ASP:N	2.75	0.50
1:A:126:SER:O	1:A:130:GLN:HG3	2.12	0.50
1:A:92:TRP:CD1	1:A:93:ASP:O	2.66	0.49
1:A:6:GLN:CG	1:A:105:THR:HG22	2.42	0.49
1:B:182:LEU:HD21	1:B:184:LEU:CD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:HD11	1:A:87:TYR:CE2	2.48	0.49
1:A:82:GLU:HB2	2:A:542:HOH:O	2.11	0.49
1:B:93:ASP:HB2	1:B:100:VAL:HG23	1.92	0.49
1:B:144:TYR:CD1	1:B:145:PRO:N	2.81	0.49
1:A:14:PRO:HG3	1:A:109:VAL:CG1	2.43	0.49
1:B:35:THR:HG21	1:B:47:LEU:CD1	2.43	0.49
1:B:92:TRP:HZ3	2:B:771:HOH:O	1.95	0.49
1:A:33:SER:OG	1:A:51:GLU:OE1	2.31	0.49
1:A:44:ALA:HB2	1:B:102:GLY:O	2.13	0.49
1:A:188:GLN:O	1:A:191:SER:OG	2.28	0.49
1:B:140:ILE:HG22	1:B:143:PHE:CD2	2.48	0.49
1:A:94:ASP:C	1:A:96:LEU:N	2.70	0.48
1:A:17:ARG:NH1	2:A:523:HOH:O	2.46	0.48
1:B:135:THR:CG2	1:B:181:TYR:HD2	2.26	0.48
1:A:168:PRO:HA	1:A:177:ALA:O	2.14	0.48
1:A:182:LEU:CD2	1:A:195:TYR:CE1	2.96	0.48
1:B:40:LEU:HD13	1:B:85:THR:HG22	1.96	0.48
1:A:214:GLU:C	1:A:215:CYS:O	2.57	0.48
1:B:150:VAL:CG2	1:B:197:CYS:SG	3.01	0.48
1:A:165:THR:HG23	1:A:180:SER:HB2	1.94	0.48
1:B:196:SER:CA	1:B:208:LYS:O	2.62	0.48
1:A:48:LEU:CD1	1:A:87:TYR:HD2	2.26	0.48
1:A:81:PRO:HA	1:A:109:VAL:HG21	1.96	0.48
1:B:14:PRO:HD3	1:B:111:GLY:H	1.79	0.48
1:B:34:VAL:HG23	1:B:91:ALA:HB2	1.95	0.48
1:A:119:VAL:HG11	1:A:199:VAL:HG11	1.96	0.48
1:B:96:LEU:HB3	1:B:98:VAL:HG22	1.95	0.48
1:B:136:LEU:O	1:B:181:TYR:HA	2.14	0.48
1:B:197:CYS:O	1:B:207:GLU:HA	2.14	0.48
1:B:147:ALA:O	1:B:148:VAL:CG1	2.60	0.47
1:A:38:GLN:CG	1:A:85:THR:CG2	2.57	0.47
1:B:4:LEU:HD12	1:B:100:VAL:HB	1.97	0.47
1:B:175:LYS:HD3	2:B:844:HOH:O	2.13	0.47
1:A:49:ILE:CD1	1:A:49:ILE:N	2.78	0.47
1:B:4:LEU:HD22	1:B:22:CYS:SG	2.55	0.47
1:B:9:SER:HA	1:B:106:LYS:O	2.15	0.47
1:A:25:SER:O	1:A:27:SER:N	2.36	0.47
1:B:132:ASN:OD1	1:B:186:PRO:HD2	2.14	0.47
1:A:121:LEU:HD23	1:A:209:THR:C	2.40	0.47
1:A:155:ASP:OD1	1:A:193:ARG:CB	2.63	0.46
1:A:10:ALA:O	1:A:107:VAL:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PRO:HG2	1:B:101:PHE:CG	2.50	0.46
1:A:155:ASP:OD2	1:A:192:HIS:HD2	1.98	0.46
1:B:119:VAL:O	1:B:208:LYS:HE3	2.15	0.46
1:B:182:LEU:CD2	1:B:184:LEU:CD1	2.93	0.46
1:A:92:TRP:HA	1:A:99:ALA:HA	1.98	0.46
1:A:112:GLN:HE22	1:A:175:LYS:CG	2.26	0.46
1:A:122:PHE:CZ	1:B:137:VAL:HG21	2.50	0.46
1:B:35:THR:HG22	1:B:36:TRP:N	2.31	0.46
1:A:99:ALA:CB	2:A:544:HOH:O	2.44	0.46
1:A:29:ILE:HG21	1:A:71:SER:C	2.41	0.46
1:A:93:ASP:CB	1:A:98:VAL:O	2.63	0.46
1:A:182:LEU:CD2	1:A:195:TYR:HE1	2.29	0.46
1:B:92:TRP:CZ2	1:B:97:ASP:OD1	2.69	0.46
1:A:70:THR:C	1:A:71:SER:OG	2.59	0.46
1:A:93:ASP:CA	1:A:98:VAL:O	2.64	0.46
1:A:213:THR:HG21	1:B:215:CYS:SG	2.56	0.46
1:A:150:VAL:CG1	1:A:151:ALA:N	2.79	0.46
1:B:124:PRO:HB2	1:B:129:LEU:HD13	1.98	0.46
1:A:142:ASP:OD1	1:A:171:GLN:OE1	2.34	0.45
1:B:2:SER:OG	1:B:3:VAL:N	2.47	0.45
1:B:6:GLN:OE1	1:B:89:CYS:SG	2.74	0.45
1:B:32:ASN:ND2	1:B:32:ASN:N	2.61	0.45
1:A:11:SER:OG	1:A:110:LEU:CD1	2.65	0.45
1:B:119:VAL:C	1:B:208:LYS:HD2	2.41	0.45
1:B:121:LEU:CD2	1:B:210:VAL:CG2	2.83	0.45
1:B:187:GLU:O	1:B:189:TRP:N	2.49	0.45
1:B:65:ALA:HB2	1:B:74:LEU:CD1	2.42	0.45
1:B:185:THR:O	1:B:186:PRO:C	2.59	0.45
1:B:37:TYR:CZ	1:B:47:LEU:HD12	2.51	0.45
1:B:79:LEU:HD13	1:B:109:VAL:HG22	1.99	0.45
1:A:92:TRP:HD1	1:A:93:ASP:O	2.00	0.45
1:A:150:VAL:HA	1:A:198:GLN:O	2.16	0.45
1:A:167:LYS:O	1:A:168:PRO:C	2.60	0.45
1:B:53:ASN:ND2	2:B:742:HOH:O	2.49	0.45
1:A:5:THR:O	1:A:23:SER:N	2.48	0.45
1:B:62:ARG:CZ	1:B:76:ILE:HD11	2.46	0.45
1:A:20:ILE:CD1	1:A:74:LEU:HB3	2.48	0.44
1:B:49:ILE:CD1	1:B:55:ARG:HA	2.35	0.44
1:A:213:THR:HG23	1:A:214:GLU:O	2.16	0.44
1:A:36:TRP:O	1:A:48:LEU:CB	2.57	0.44
1:A:65:ALA:HA	1:A:73:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:HB2	1:A:147:ALA:HB3	2.00	0.44
1:A:80:GLN:HG2	1:A:81:PRO:CD	2.46	0.44
1:A:153:LYS:HA	1:A:157:SER:O	2.17	0.44
1:A:170:LYS:H	1:A:170:LYS:HD2	1.75	0.44
1:B:6:GLN:HA	1:B:21:SER:O	2.18	0.44
1:A:3:VAL:HG22	1:A:101:PHE:O	2.18	0.44
1:A:101:PHE:HB2	1:B:45:PRO:HD2	2.00	0.44
1:A:209:THR:HG23	1:A:210:VAL:H	1.82	0.44
1:A:125:SER:OG	2:B:605:HOH:O	2.21	0.44
1:A:184:LEU:HB3	1:A:185:THR:H	1.61	0.44
1:A:206:VAL:CG2	2:A:601:HOH:O	2.66	0.44
1:A:25:SER:C	1:A:27:SER:N	2.73	0.43
1:A:48:LEU:O	1:A:59:VAL:HG21	2.18	0.43
1:A:148:VAL:HG23	1:A:149:THR:H	1.81	0.43
1:A:50:TYR:N	1:A:54:SER:O	2.49	0.43
1:A:211:ALA:HA	1:A:212:PRO:HD3	1.72	0.43
1:B:17:ARG:HB2	2:B:739:HOH:O	2.18	0.43
1:B:185:THR:C	1:B:187:GLU:N	2.74	0.43
1:A:48:LEU:C	1:A:49:ILE:HD12	2.44	0.43
1:A:78:GLY:O	1:A:79:LEU:C	2.62	0.43
1:A:150:VAL:CG1	1:A:151:ALA:H	2.29	0.43
1:B:39:HIS:O	1:B:41:SER:N	2.52	0.43
1:A:14:PRO:HG3	1:A:109:VAL:HG13	2.00	0.43
1:A:24:GLY:HA3	1:A:29:ILE:CG1	2.48	0.43
1:A:32:ASN:O	1:A:67:LYS:NZ	2.48	0.43
1:B:63:PHE:HZ	2:B:718:HOH:O	2.01	0.43
1:B:128:GLU:O	1:B:133:LYS:O	2.37	0.43
1:A:76:ILE:N	1:A:76:ILE:HD12	2.34	0.43
1:A:91:ALA:O	1:A:99:ALA:HA	2.19	0.43
1:B:4:LEU:CD2	1:B:29:ILE:CD1	2.97	0.43
1:B:92:TRP:CD1	1:B:94:ASP:OD1	2.72	0.43
1:A:69:GLY:C	1:A:71:SER:H	2.27	0.42
1:A:172:SER:OG	1:A:173:ASN:N	2.52	0.42
1:A:20:ILE:HG23	1:A:105:THR:HG21	1.98	0.42
1:A:40:LEU:O	1:A:41:SER:C	2.61	0.42
1:A:137:VAL:HG21	1:B:122:PHE:CE2	2.54	0.42
1:B:53:ASN:N	2:B:742:HOH:O	2.51	0.42
1:A:49:ILE:N	1:A:49:ILE:HD12	2.35	0.42
1:A:171:GLN:HE21	1:B:164:GLU:HG2	1.84	0.42
1:B:40:LEU:O	1:B:42:GLY:N	2.53	0.42
1:B:82:GLU:HG3	1:B:174:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:SER:HB3	1:B:164:GLU:OE2	2.19	0.42
1:B:14:PRO:HD3	1:B:111:GLY:N	2.35	0.42
1:B:117:PRO:CD	1:B:201:HIS:CD2	3.02	0.42
1:A:151:ALA:O	1:A:198:GLN:HB3	2.20	0.42
1:A:213:THR:C	1:A:214:GLU:O	2.61	0.42
1:B:40:LEU:O	1:B:41:SER:C	2.63	0.42
1:B:60:SER:HB3	1:B:62:ARG:HG3	2.01	0.42
1:B:84:GLU:CG	1:B:109:VAL:H	2.25	0.42
1:A:170:LYS:CD	1:A:170:LYS:N	2.53	0.42
1:B:121:LEU:HD23	1:B:210:VAL:HG22	1.97	0.42
1:A:85:THR:HG23	1:A:86:ASP:H	1.85	0.42
1:B:119:VAL:O	1:B:208:LYS:HD2	2.19	0.42
1:A:55:ARG:HG2	1:A:56:ALA:O	2.20	0.42
1:A:154:ALA:O	1:A:157:SER:HB2	2.19	0.42
1:A:154:ALA:O	1:A:155:ASP:C	2.62	0.41
1:A:4:LEU:N	1:A:4:LEU:CD1	2.80	0.41
1:A:56:ALA:HB3	1:A:59:VAL:HG21	2.01	0.41
1:A:70:THR:O	1:A:70:THR:CG2	2.65	0.41
1:B:4:LEU:HD21	1:B:29:ILE:CG1	2.48	0.41
1:B:13:THR:O	1:B:16:GLN:HB3	2.20	0.41
1:B:27:SER:HB2	1:B:93:ASP:OD1	2.20	0.41
1:B:50:TYR:CE2	1:B:55:ARG:O	2.73	0.41
1:B:112:GLN:HB3	1:B:113:PRO:CD	2.50	0.41
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.91	0.41
1:A:184:LEU:HD21	1:A:195:TYR:CZ	2.56	0.41
1:B:49:ILE:HD12	1:B:49:ILE:HA	1.82	0.41
1:B:208:LYS:CE	2:B:808:HOH:O	2.69	0.41
1:B:174:ASN:HD22	1:B:174:ASN:HA	1.54	0.41
1:A:50:TYR:HD1	1:A:54:SER:O	2.03	0.41
1:A:136:LEU:HD12	1:A:182:LEU:O	2.21	0.41
1:A:148:VAL:CG2	1:A:199:VAL:CG2	2.95	0.41
1:A:68:SER:HB3	1:A:69:GLY:H	1.57	0.41
1:A:93:ASP:OD2	1:A:100:VAL:HG21	2.20	0.41
1:A:123:PRO:HG3	1:A:210:VAL:HG21	2.03	0.41
1:B:13:THR:HA	1:B:111:GLY:H	1.86	0.41
1:B:68:SER:HB3	2:B:729:HOH:O	2.21	0.41
1:A:32:ASN:O	1:A:67:LYS:CE	2.69	0.41
1:B:4:LEU:HD23	1:B:29:ILE:CD1	2.50	0.41
1:A:49:ILE:HG21	1:A:65:ALA:CB	2.50	0.41
1:A:116:ASN:HA	1:A:201:HIS:HD2	1.85	0.41
1:A:6:GLN:CG	1:A:105:THR:CG2	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:SER:CB	2:A:530:HOH:O	2.70	0.41
1:A:45:PRO:HD2	1:B:101:PHE:HB3	2.03	0.41
1:B:67:LYS:HE3	1:B:69:GLY:O	2.21	0.41
1:B:74:LEU:HD12	1:B:74:LEU:HA	1.97	0.41
1:B:117:PRO:HD3	1:B:201:HIS:CD2	2.56	0.41
1:A:4:LEU:HD12	1:A:4:LEU:HA	1.58	0.40
1:B:140:ILE:O	1:B:177:ALA:HA	2.21	0.40
1:B:167:LYS:HA	1:B:168:PRO:HD3	1.87	0.40
1:A:85:THR:HG22	1:A:87:TYR:CE1	2.57	0.40
1:B:46:LYS:HZ3	1:B:59:VAL:HG22	1.80	0.40
1:B:185:THR:O	1:B:187:GLU:N	2.54	0.40
1:A:86:ASP:N	1:A:86:ASP:OD1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/216 (99%)	174 (81%)	25 (12%)	15 (7%)	1	0
1	B	214/216 (99%)	171 (80%)	27 (13%)	16 (8%)	1	0
All	All	428/432 (99%)	345 (81%)	52 (12%)	31 (7%)	1	0

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	31	GLU
1	A	77	SER
1	A	96	LEU
1	A	97	ASP
1	A	214	GLU

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Mol	Chain	Res	Type
1	B	3	VAL
1	B	41	SER
1	B	52	ASP
1	B	55	ARG
1	A	202	GLU
1	A	215	CYS
1	B	29	ILE
1	B	78	GLY
1	B	127	GLU
1	B	189	TRP
1	B	212	PRO
1	A	79	LEU
1	A	155	ASP
1	A	213	THR
1	B	10	ALA
1	B	30	GLY
1	B	31	GLU
1	B	155	ASP
1	A	26	SER
1	A	52	ASP
1	B	161	ALA
1	B	187	GLU
1	B	215	CYS
1	A	78	GLY
1	A	168	PRO

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%)	118 (65%)	63 (35%)	0	0
1	B	181/181 (100%)	134 (74%)	47 (26%)	0	0
All	All	362/362 (100%)	252 (70%)	110 (30%)	0	0

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	VAL
1	A	4	LEU
1	A	9	SER
1	A	16	GLN
1	A	18	VAL
1	A	20	ILE
1	A	28	ASN
1	A	29	ILE
1	A	35	THR
1	A	38	GLN
1	A	40	LEU
1	A	41	SER
1	A	49	ILE
1	A	50	TYR
1	A	51	GLU
1	A	53	ASN
1	A	59	VAL
1	A	61	ASP
1	A	64	SER
1	A	68	SER
1	A	74	LEU
1	A	76	ILE
1	A	82	GLU
1	A	84	GLU
1	A	85	THR
1	A	95	SER
1	A	96	LEU
1	A	98	VAL
1	A	100	VAL
1	A	101	PHE
1	A	103	THR
1	A	105	THR
1	A	106	LYS
1	A	107	VAL
1	A	108	THR
1	A	109	VAL
1	A	110	LEU
1	A	114	LYS
1	A	119	VAL
1	A	126	SER
1	A	136	LEU
1	A	137	VAL

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Mol	Chain	Res	Type
1	A	148	VAL
1	A	163	VAL
1	A	167	LYS
1	A	170	LYS
1	A	173	ASN
1	A	174	ASN
1	A	180	SER
1	A	183	SER
1	A	187	GLU
1	A	194	SER
1	A	196	SER
1	A	199	VAL
1	A	200	THR
1	A	207	GLU
1	A	208	LYS
1	A	209	THR
1	A	212	PRO
1	A	213	THR
1	A	214	GLU
1	A	215	CYS
1	B	3	VAL
1	B	13	THR
1	B	17	ARG
1	B	18	VAL
1	B	19	THR
1	B	20	ILE
1	B	21	SER
1	B	23	SER
1	B	26	SER
1	B	27	SER
1	B	31	GLU
1	B	32	ASN
1	B	33	SER
1	B	34	VAL
1	B	49	ILE
1	B	52	ASP
1	B	60	SER
1	B	61	ASP
1	B	62	ARG
1	B	66	SER
1	B	67	LYS
1	B	76	ILE

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Mol	Chain	Res	Type
1	B	100	VAL
1	B	108	THR
1	B	116	ASN
1	B	120	THR
1	B	126	SER
1	B	127	GLU
1	B	129	LEU
1	B	130	GLN
1	B	135	THR
1	B	140	ILE
1	B	149	THR
1	B	164	GLU
1	B	167	LYS
1	B	172	SER
1	B	174	ASN
1	B	175	LYS
1	B	182	LEU
1	B	194	SER
1	B	197	CYS
1	B	198	GLN
1	B	202	GLU
1	B	204	SER
1	B	205	THR
1	B	210	VAL
1	B	213	THR

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	112	GLN
1	A	171	GLN
1	A	188	GLN
1	A	192	HIS
1	B	32	ASN
1	B	38	GLN
1	B	80	GLN
1	B	130	GLN
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	1.03	1 (16%)	7,8,12	1.60	2 (28%)
1	PCA	B	1	1	6,7,9	0.84	0	7,8,12	1.35	1 (14%)

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	2.40	1.29	1.20

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CA-C	3.35	117.25	112.66
1	B	1	PCA	CB-CA-C	2.75	116.43	112.66
1	A	1	PCA	O-C-CA	-2.11	119.35	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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](#)

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%)	-0.74	0	100 100	5, 22, 43, 56	0
1	B	215/216 (99%)	-0.85	1 (0%)	87 85	5, 20, 32, 52	0
All	All	430/432 (99%)	-0.79	1 (0%)	91 89	5, 21, 41, 56	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	GLU	2.4

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	0.80	0.09	42,42,42,42	0
1	PCA	A	1	7/9	0.90	0.13	40,41,42,42	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 ⓘ

There are no such residues in this entry.