



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 11:36 AM UTC

PDB ID : 1DM0 / pdb_00001dm0
Title : SHIGA TOXIN
Authors : Fraser, M.E.; Chernaia, M.M.; Kozlov, Y.V.; James, M.N.
Deposited on : 1999-12-13
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

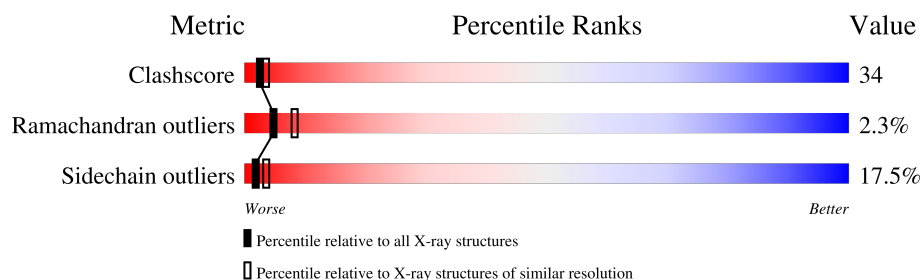
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	39% 38% 12% • 8%
1	L	287	26% 46% 16% • 9%
2	B	69	36% 42% 19% •
2	C	69	42% 46% 10% •
2	D	69	54% 39% 7%
2	E	69	46% 36% 17%
2	F	69	38% 43% 16% •
2	G	69	48% 39% 12% •

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Mol	Chain	Length	Quality of chain
2	H	69	26%54%20%
2	I	69	39%43%14%
2	J	69	32%42%25%
2	K	69	38%49%13%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9538 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 SHIGA TOXIN A SUBUNIT.

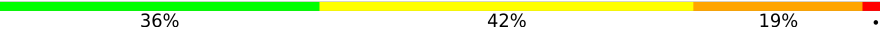
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2046	1284	363	390	9			
1	L	262	Total	C	N	O	S	0	0	0
			2030	1276	361	384	9			

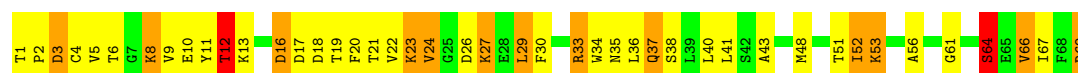
- Molecule 2 is a protein called SHIGA TOXIN B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	F	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	G	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	H	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	I	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	J	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
2	K	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

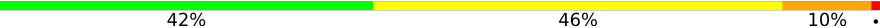
- Molecule 3 is water.

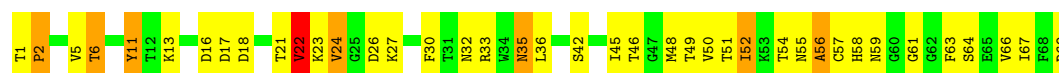
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	L	11	Total 11	O 11	0	0
3	B	1	Total 1	O 1	0	0
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0
3	E	5	Total 5	O 5	0	0
3	F	3	Total 3	O 3	0	0
3	G	4	Total 4	O 4	0	0
3	H	1	Total 1	O 1	0	0
3	I	2	Total 2	O 2	0	0
3	J	5	Total 5	O 5	0	0
3	K	10	Total 10	O 10	0	0

Chain B: 



• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain C: 



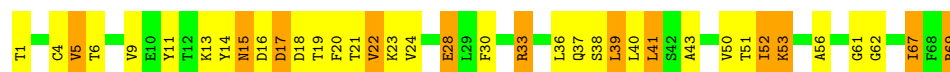
• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain D: 



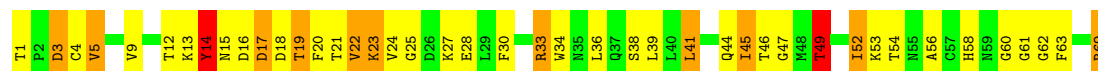
• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain E: 



• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain F: 



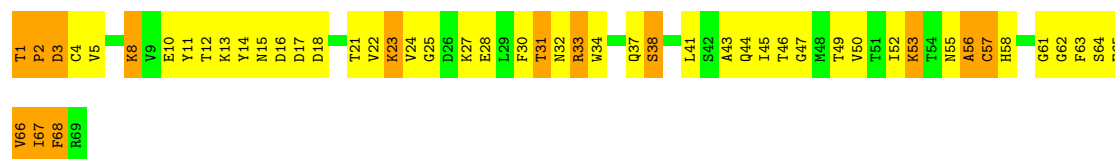
• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain G: 

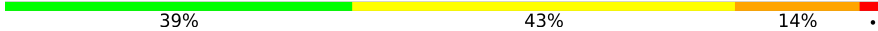


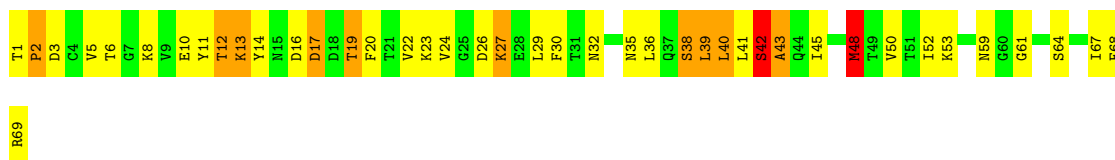
• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain H: 



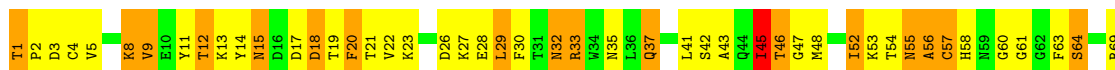
• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain I:  39% 43% 14% .

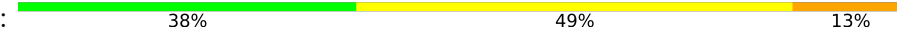


• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain J:  32% 42% 25% .



• Molecule 2: SHIGA TOXIN B SUBUNIT

Chain K:  38% 49% 13%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.05Å 147.46Å 83.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.1 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR	Depositor
R, R_{free}	0.206 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.37	7/2078 (0.3%)	1.60	38/2815 (1.3%)
1	L	1.18	6/2062 (0.3%)	1.54	34/2793 (1.2%)
2	B	1.41	4/549 (0.7%)	1.54	6/742 (0.8%)
2	C	1.46	4/549 (0.7%)	1.49	4/742 (0.5%)
2	D	1.41	2/549 (0.4%)	1.54	3/742 (0.4%)
2	E	1.59	2/549 (0.4%)	1.67	9/742 (1.2%)
2	F	1.41	2/549 (0.4%)	1.67	9/742 (1.2%)
2	G	1.50	3/549 (0.5%)	1.51	8/742 (1.1%)
2	H	1.36	2/549 (0.4%)	1.39	5/742 (0.7%)
2	I	1.32	0/549	1.54	12/742 (1.6%)
2	J	1.43	2/549 (0.4%)	1.59	10/742 (1.3%)
2	K	1.69	6/549 (1.1%)	1.71	11/742 (1.5%)
All	All	1.38	40/9630 (0.4%)	1.57	149/13028 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	67	ILE	CA-CB	-11.16	1.41	1.54
1	A	40	MET	SD-CE	10.10	2.04	1.79
2	K	24	VAL	CA-CB	-8.91	1.42	1.54
2	C	56	ALA	CA-CB	-7.17	1.44	1.53
2	B	48	MET	SD-CE	-6.86	1.62	1.79
2	E	50	VAL	C-O	-6.74	1.17	1.24
2	K	52	ILE	CA-CB	-6.65	1.46	1.54
2	K	66	VAL	CA-CB	-6.41	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	9	VAL	CA-CB	6.37	1.61	1.54
2	H	68	PHE	CA-CB	6.33	1.61	1.53
1	L	176	ARG	CD-NE	6.10	1.54	1.46
1	A	234	GLY	C-O	-6.04	1.17	1.23
1	A	143	MET	SD-CE	-6.04	1.64	1.79
1	L	104	THR	CA-CB	6.04	1.62	1.53
2	D	48	MET	SD-CE	-6.02	1.64	1.79
2	K	57	CYS	CA-C	-5.90	1.46	1.53
2	J	45	ILE	CA-CB	-5.88	1.46	1.54
2	F	22	VAL	C-O	-5.71	1.18	1.24
1	A	271	THR	CA-C	-5.67	1.45	1.52
1	A	194	ALA	CA-CB	-5.61	1.44	1.53
2	K	65	GLU	CA-C	-5.58	1.46	1.52
2	C	2	PRO	CA-C	-5.53	1.47	1.52
2	D	43	ALA	CA-CB	-5.53	1.44	1.53
2	K	45	ILE	CA-CB	-5.53	1.48	1.54
2	G	48	MET	SD-CE	-5.48	1.65	1.79
2	B	21	THR	CA-CB	5.46	1.61	1.53
2	C	45	ILE	CA-CB	5.42	1.61	1.54
2	B	64	SER	CA-C	-5.42	1.45	1.52
2	G	45	ILE	CA-CB	-5.38	1.47	1.54
1	A	210	LEU	CA-C	-5.37	1.46	1.52
2	B	37	GLN	C-O	-5.35	1.17	1.24
1	L	14	VAL	CA-CB	-5.30	1.47	1.54
2	C	48	MET	SD-CE	-5.29	1.66	1.79
1	L	39	LEU	CA-C	-5.24	1.46	1.52
2	F	38	SER	N-CA	-5.22	1.40	1.46
1	A	30	THR	CA-CB	5.19	1.61	1.53
1	L	221	VAL	C-O	-5.13	1.18	1.24
1	L	143	MET	SD-CE	-5.10	1.66	1.79
2	G	65	GLU	C-O	-5.07	1.18	1.24
2	E	17	ASP	CA-C	-5.06	1.44	1.52

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LEU	N-CA-C	11.75	124.09	111.28
1	L	74	ASN	N-CA-C	10.36	122.15	111.07
2	F	60	GLY	N-CA-C	-10.25	101.59	114.92
2	E	39	LEU	N-CA-C	-9.78	98.86	112.45
2	K	10	GLU	N-CA-C	9.75	121.91	111.28
2	F	19	THR	N-CA-C	-9.44	96.50	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	24	VAL	N-CA-C	-8.94	94.28	108.86
2	D	15	ASN	N-CA-C	8.33	121.80	110.55
2	J	43	ALA	N-CA-C	-8.30	102.31	111.36
2	C	24	VAL	CB-CA-C	-8.23	100.53	111.81
2	D	24	VAL	CB-CA-C	-7.96	100.65	110.99
1	A	73	ARG	N-CA-C	7.95	120.71	111.02
2	C	22	VAL	CB-CA-C	-7.92	98.82	110.62
2	K	8	LYS	N-CA-C	-7.85	98.90	110.52
2	K	19	THR	N-CA-C	-7.85	97.46	109.95
1	A	197	VAL	N-CA-C	7.79	117.89	110.42
1	A	194	ALA	N-CA-C	-7.73	102.18	111.69
2	B	16	ASP	N-CA-C	7.68	122.32	112.34
1	L	28	LEU	N-CA-C	-7.68	96.72	109.46
1	L	175	GLN	N-CA-C	-7.62	102.11	111.40
1	A	163	THR	N-CA-C	7.40	119.13	111.14
2	I	43	ALA	N-CA-C	-7.35	103.35	111.36
1	L	231	ALA	N-CA-C	-7.34	102.98	112.23
1	A	160	ARG	N-CA-C	7.34	119.28	111.28
1	L	34	GLY	N-CA-C	-7.27	103.16	115.08
2	J	28	GLU	N-CA-C	-7.19	96.81	108.52
2	K	45	ILE	N-CA-C	7.12	117.26	110.42
2	E	67	ILE	N-CA-C	-7.10	97.20	107.78
1	L	38	LEU	N-CA-C	-7.07	101.19	110.53
1	L	154	VAL	N-CA-C	-7.06	102.26	111.09
1	L	143	MET	N-CA-C	-7.03	103.62	111.71
2	B	26	ASP	N-CA-C	-6.98	104.42	114.12
1	L	280	SER	N-CA-C	6.83	119.74	111.82
2	G	26	ASP	N-CA-C	-6.77	104.99	113.18
1	L	104	THR	N-CA-C	-6.73	99.61	110.32
2	I	39	LEU	N-CA-C	-6.71	103.89	111.07
1	L	73	ARG	N-CA-C	6.71	122.37	111.37
2	J	60	GLY	N-CA-C	-6.56	107.27	115.08
2	J	1	THR	C-N-CD	-6.55	98.13	125.00
1	A	137	THR	CB-CA-C	-6.38	100.60	110.81
2	D	61	GLY	N-CA-C	-6.36	104.62	111.93
1	A	278	ASP	N-CA-C	-6.33	98.88	109.07
2	J	20	PHE	CB-CA-C	-6.33	102.78	111.95
1	A	41	ILE	CB-CA-C	-6.29	104.67	111.59
1	A	151	THR	N-CA-C	6.29	118.64	110.53
2	B	3	ASP	N-CA-C	-6.29	102.23	110.53
2	F	14	TYR	N-CA-C	-6.27	98.51	108.73
1	A	65	ASN	N-CA-C	6.26	121.69	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	42	SER	N-CA-C	-6.25	104.36	112.23
1	L	19	VAL	CB-CA-C	-6.24	103.84	112.02
2	C	56	ALA	N-CA-C	-6.22	104.74	113.20
2	E	28	GLU	N-CA-C	-6.19	98.31	108.41
2	H	10	GLU	N-CA-C	6.19	117.83	111.14
2	E	15	ASN	N-CA-C	6.19	118.51	110.53
2	B	29	LEU	N-CA-C	6.15	118.83	110.35
1	L	216	GLN	N-CA-C	-6.12	102.29	110.24
1	A	231	ALA	N-CA-C	-6.10	104.91	112.90
2	B	12	THR	N-CA-C	-6.08	99.99	109.72
2	F	56	ALA	N-CA-C	-6.06	104.01	112.25
1	A	149	SER	N-CA-C	6.06	118.11	110.24
2	F	33	ARG	N-CA-C	6.05	118.10	110.24
2	E	41	LEU	N-CA-CB	6.05	119.70	110.14
1	A	146	SER	N-CA-C	-6.02	99.18	109.24
1	L	181	THR	N-CA-C	6.02	123.63	110.80
1	A	74	ASN	N-CA-C	6.02	117.84	111.28
2	I	67	ILE	CB-CA-C	-6.01	103.58	110.73
1	A	209	VAL	N-CA-C	6.00	116.20	110.74
2	I	19	THR	N-CA-C	-6.00	101.61	110.48
2	J	21	THR	CB-CA-C	-5.99	100.55	109.90
2	K	64	SER	CB-CA-C	-5.96	98.56	110.42
2	I	17	ASP	N-CA-C	-5.94	105.94	112.72
1	L	213	TYR	N-CA-C	5.93	119.06	110.28
2	G	4	CYS	CA-C-N	-5.90	114.06	121.96
2	G	4	CYS	C-N-CA	-5.90	114.06	121.96
2	B	43	ALA	N-CA-C	-5.89	104.99	111.82
2	G	37	GLN	N-CA-C	5.89	117.37	111.07
1	L	180	THR	N-CA-C	-5.88	104.56	110.97
1	A	154	VAL	N-CA-C	-5.85	104.62	111.00
1	A	12	THR	N-CA-C	-5.85	104.90	111.28
1	A	271	THR	CB-CA-C	-5.85	100.10	109.75
1	L	146	SER	N-CA-C	-5.84	98.56	108.26
2	F	3	ASP	N-CA-C	-5.84	101.76	110.23
1	L	266	ARG	N-CA-C	-5.83	105.00	111.36
1	A	159	LEU	N-CA-C	-5.82	104.85	111.07
1	A	24	ILE	N-CA-C	5.80	117.68	112.17
2	K	5	VAL	N-CA-C	5.78	116.18	108.27
1	A	20	ILE	N-CA-C	5.76	116.49	110.62
1	L	6	ASP	N-CA-C	5.74	117.82	108.63
1	L	224	ILE	CB-CA-C	-5.73	103.36	111.21
1	A	203	TRP	N-CA-C	5.69	117.94	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	THR	CB-CA-C	-5.69	100.24	110.36
1	A	224	ILE	N-CA-C	5.68	116.07	108.11
2	E	69	ARG	NE-CZ-NH1	-5.68	115.82	121.50
2	K	15	ASN	N-CA-C	5.66	118.89	110.52
2	E	43	ALA	N-CA-C	-5.64	105.14	111.28
1	L	17	LEU	N-CA-C	-5.63	104.15	111.02
2	F	47	GLY	N-CA-C	5.63	123.65	115.32
2	I	20	PHE	N-CA-C	-5.62	100.24	109.40
2	J	55	ASN	N-CA-C	-5.62	103.95	112.04
2	G	14	TYR	N-CA-C	-5.53	100.97	109.76
1	A	198	ASP	CB-CA-C	-5.51	101.31	110.68
2	I	24	VAL	CB-CA-C	-5.50	102.49	110.63
1	A	280	SER	N-CA-C	5.47	117.24	111.28
2	G	27	LYS	N-CA-C	5.46	118.83	110.20
1	A	36	THR	N-CA-C	-5.45	101.28	109.95
1	L	14	VAL	CB-CA-C	-5.45	104.78	112.14
2	K	10	GLU	CB-CA-C	5.43	119.81	110.79
2	F	49	THR	N-CA-C	-5.43	100.84	109.96
2	I	40	LEU	N-CA-C	5.43	116.89	110.97
1	L	168	ALA	N-CA-C	-5.42	106.66	113.28
1	L	66	ASN	N-CA-C	5.38	119.54	112.92
1	L	241	ASN	N-CA-C	-5.38	97.73	107.75
1	L	192	MET	N-CA-C	5.38	116.89	109.15
2	J	8	LYS	N-CA-C	-5.33	103.35	110.55
1	A	147	GLY	N-CA-C	5.33	118.24	111.85
2	J	37	GLN	CB-CA-C	-5.31	101.97	110.79
1	A	238	LEU	N-CA-C	5.31	118.11	109.24
2	H	66	VAL	CA-C-N	-5.31	116.61	123.19
2	H	66	VAL	C-N-CA	-5.31	116.61	123.19
1	A	225	SER	CA-CB-OG	-5.30	100.51	111.10
1	A	112	SER	N-CA-C	5.28	119.72	113.28
2	G	22	VAL	CB-CA-C	-5.28	102.75	110.62
1	L	239	ILE	CB-CA-C	-5.26	103.32	110.90
2	E	20	PHE	CB-CA-C	-5.24	101.11	109.75
2	I	48	MET	N-CA-C	-5.22	102.03	110.32
2	H	2	PRO	CB-CA-C	-5.19	104.76	111.46
2	J	21	THR	N-CA-C	5.19	117.84	110.10
2	C	11	TYR	N-CA-C	-5.17	100.45	108.42
1	A	180	THR	N-CA-C	5.17	121.82	110.80
2	G	47	GLY	N-CA-C	5.17	122.24	115.47
2	I	8	LYS	N-CA-C	-5.17	102.88	110.52
2	H	43	ALA	N-CA-C	-5.16	105.73	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	285	ILE	N-CA-C	5.15	120.12	113.07
2	I	42	SER	N-CA-C	-5.14	106.70	113.12
2	K	32	ASN	N-CA-C	-5.13	105.71	112.94
1	L	22	SER	N-CA-C	-5.12	106.14	112.38
1	L	156	ARG	N-CA-C	5.12	116.86	111.28
1	A	136	THR	N-CA-C	-5.09	105.42	110.97
1	L	159	LEU	N-CA-C	-5.09	105.00	111.11
2	E	17	ASP	N-CA-C	-5.09	106.91	113.02
1	A	263	ALA	N-CA-C	5.09	121.65	110.80
1	L	20	ILE	CB-CA-C	-5.08	105.38	112.04
2	K	1	THR	N-CA-C	-5.08	96.77	111.00
1	A	232	ILE	N-CA-C	-5.08	105.54	110.42
1	L	119	ARG	N-CA-C	-5.08	105.74	111.28
1	A	14	VAL	CB-CA-C	-5.07	104.30	112.16
1	L	160	ARG	N-CA-C	5.06	116.48	111.07
2	I	3	ASP	N-CA-C	-5.04	102.82	110.24
1	A	104	THR	N-CA-C	-5.02	103.09	110.52

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	14	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	2046	0	2040	126	0
1	L	2030	0	2032	213	0
2	B	540	0	527	36	0
2	C	540	0	527	31	0
2	D	540	0	527	30	0
2	E	540	0	527	21	0
2	F	540	0	527	43	0
2	G	540	0	527	28	0
2	H	540	0	527	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	540	0	527	35	0
2	J	540	0	527	53	0
2	K	540	0	527	21	0
3	A	12	0	0	1	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
3	E	5	0	0	1	0
3	F	3	0	0	0	0
3	G	4	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	J	5	0	0	1	0
3	K	10	0	0	0	0
3	L	11	0	0	1	0
All	All	9538	0	9342	647	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 34.

All (647) 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:40:MET:SD	1:A:40:MET:CE	2.04	1.45
1:L:60:GLU:HG2	1:L:61:GLU:HG2	1.31	1.13
2:J:33:ARG:HH12	2:J:64:SER:HB3	1.07	1.06
1:A:128:MET:HE1	1:A:159:LEU:HB3	1.39	1.04
1:A:151:THR:HG22	1:A:154:VAL:HG23	1.41	1.02
1:A:121:ALA:HB1	1:A:156:ARG:HG2	1.39	1.02
1:A:40:MET:HE2	1:A:241:ASN:HA	1.39	1.01
2:F:14:TYR:HE1	2:F:41:LEU:HD11	1.20	1.01
1:L:125:ARG:HG3	1:L:125:ARG:HH11	1.27	0.99
2:H:67:ILE:HG13	2:I:13:LYS:HG3	1.43	0.99
2:I:48:MET:HE1	2:I:68:PHE:HB3	1.48	0.95
1:L:285:ILE:HD12	2:J:45:ILE:HG21	1.50	0.92
1:L:123:ILE:HD13	1:L:156:ARG:HG2	1.51	0.91
2:J:33:ARG:NH1	2:J:64:SER:HB3	1.85	0.91
1:A:216:GLN:H	1:A:216:GLN:HE21	1.19	0.90
1:A:287:MET:HE3	2:D:38:SER:HB2	1.55	0.89
1:L:123:ILE:CD1	1:L:156:ARG:HG2	2.03	0.88
1:L:64:PHE:CE2	1:L:140:LEU:HD21	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:SER:HA	1:L:132:ARG:HH22	1.37	0.87
1:A:31:ILE:HG23	1:A:229:ILE:HD11	1.57	0.86
1:A:214:HIS:H	1:A:216:GLN:HE22	1.23	0.85
2:H:67:ILE:CG1	2:I:13:LYS:HG3	2.07	0.85
2:F:14:TYR:CE1	2:F:41:LEU:HD11	2.10	0.84
2:F:69:ARG:HG2	2:F:69:ARG:HH11	1.43	0.84
1:L:32:SER:H	1:L:229:ILE:HD11	1.43	0.84
1:L:64:PHE:HE2	1:L:140:LEU:HD21	1.39	0.84
1:A:151:THR:CG2	1:A:154:VAL:HG23	2.09	0.83
1:L:67:LEU:HD11	1:L:142:LEU:HD13	1.60	0.82
1:A:131:ASN:HA	1:A:181:THR:HG21	1.61	0.81
1:L:6:ASP:HA	1:L:55:ARG:O	1.81	0.80
1:L:60:GLU:CG	1:L:61:GLU:HG2	2.10	0.79
2:C:67:ILE:HG13	2:D:13:LYS:HG3	1.63	0.79
2:J:32:ASN:H	2:J:32:ASN:HD22	1.29	0.79
1:L:31:ILE:HD12	1:L:38:LEU:HD22	1.65	0.79
1:L:91:ARG:HD2	1:L:95:PHE:O	1.83	0.79
1:A:216:GLN:HE21	1:A:216:GLN:N	1.80	0.78
1:A:285:ILE:HD12	2:F:45:ILE:HG22	1.66	0.78
1:L:41:ILE:HG13	1:L:238:LEU:HD21	1.66	0.78
1:L:165:THR:O	1:L:169:LEU:HB2	1.84	0.78
1:L:40:MET:SD	1:L:241:ASN:HA	2.24	0.77
1:L:285:ILE:CD1	2:J:45:ILE:HG21	2.14	0.77
1:A:5:LEU:HD23	1:A:7:PHE:CE1	2.20	0.76
2:B:8:LYS:NZ	2:B:8:LYS:HB3	2.00	0.75
2:D:22:VAL:CG1	2:D:24:VAL:HG23	2.17	0.75
2:G:5:VAL:HG22	2:G:24:VAL:HG12	1.69	0.75
1:L:95:PHE:HB3	1:L:98:VAL:CG2	2.17	0.75
2:J:56:ALA:HB1	2:J:61:GLY:HA2	1.68	0.74
1:L:138:SER:HB3	1:L:161:PHE:HE2	1.51	0.74
1:A:7:PHE:O	1:A:132:ARG:NH2	2.20	0.74
1:A:203:TRP:CZ3	1:A:240:LEU:HD21	2.23	0.74
1:L:58:ASP:HB3	1:L:62:GLY:HA2	1.70	0.73
1:L:58:ASP:HB3	1:L:62:GLY:CA	2.18	0.73
1:L:7:PHE:CD2	1:L:135:LEU:HD21	2.24	0.73
2:D:4:CYS:HB2	2:D:54:THR:HG22	1.71	0.72
2:F:69:ARG:HG2	2:F:69:ARG:NH1	2.03	0.72
1:L:8:SER:HA	1:L:132:ARG:NH2	2.03	0.72
1:L:83:ASN:OD1	1:L:85:THR:HB	1.88	0.72
1:L:95:PHE:HB3	1:L:98:VAL:HG21	1.69	0.72
2:J:33:ARG:HH11	2:J:33:ARG:CG	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:67:ILE:HG12	2:H:13:LYS:HG3	1.72	0.71
2:I:26:ASP:OD1	2:I:27:LYS:HG2	1.89	0.71
1:L:8:SER:CA	1:L:132:ARG:HH22	2.03	0.71
2:H:1:THR:HG23	2:H:2:PRO:CD	2.20	0.71
1:L:175:GLN:HG2	1:L:176:ARG:N	2.04	0.71
2:D:22:VAL:HG11	2:D:24:VAL:HG23	1.73	0.71
1:A:285:ILE:HD12	2:F:45:ILE:CG2	2.21	0.70
1:L:38:LEU:CD1	1:L:236:VAL:HG12	2.21	0.70
1:L:20:ILE:O	1:L:23:ALA:HB3	1.91	0.70
1:A:151:THR:HG22	1:A:154:VAL:CG2	2.21	0.70
1:L:90:TYR:OH	1:L:146:SER:HA	1.92	0.70
2:J:17:ASP:OD1	2:J:19:THR:HG23	1.91	0.70
1:A:6:ASP:HA	1:A:55:ARG:O	1.92	0.69
1:L:131:ASN:HA	1:L:181:THR:HG21	1.74	0.69
2:F:12:THR:HG22	2:F:22:VAL:HG12	1.72	0.69
1:A:61:GLU:HB3	1:A:63:ARG:HG2	1.74	0.69
1:A:131:ASN:HD22	1:A:189:SER:HB2	1.57	0.69
1:L:26:THR:HB	1:L:27:PRO:HD2	1.73	0.69
1:L:154:VAL:O	1:L:158:MET:HB2	1.92	0.69
2:H:18:ASP:HB3	2:H:34:TRP:CH2	2.27	0.69
2:G:20:PHE:CD1	2:G:37:GLN:HG2	2.27	0.69
1:A:287:MET:CE	2:D:38:SER:HB2	2.23	0.68
1:L:85:THR:HG22	1:L:86:ASN:N	2.07	0.68
1:L:121:ALA:HB1	1:L:123:ILE:HG12	1.75	0.68
1:L:203:TRP:CH2	1:L:240:LEU:HG	2.28	0.68
2:G:42:SER:O	2:G:46:THR:HG23	1.93	0.68
1:A:137:THR:HG22	1:A:138:SER:N	2.08	0.68
1:A:108:LEU:HA	1:A:148:THR:O	1.94	0.68
1:L:91:ARG:NH1	1:L:98:VAL:O	2.26	0.68
2:H:5:VAL:HG22	2:H:24:VAL:HG12	1.76	0.68
1:L:51:ALA:HB2	1:L:100:PHE:CE2	2.28	0.68
1:A:68:ARG:HD2	1:A:84:ARG:HD3	1.75	0.68
2:C:26:ASP:OD1	2:C:27:LYS:HD3	1.94	0.68
2:D:17:ASP:OD1	2:D:19:THR:HG23	1.94	0.68
2:G:41:LEU:HD12	2:G:44:GLN:NE2	2.08	0.68
1:L:176:ARG:NH1	1:L:234:GLY:O	2.27	0.67
2:G:48:MET:HE1	2:G:68:PHE:HB3	1.76	0.67
2:J:17:ASP:CG	2:J:19:THR:HG23	2.19	0.67
2:I:10:GLU:HB3	2:I:23:LYS:HG3	1.75	0.67
2:K:51:THR:OG1	2:K:69:ARG:NH1	2.27	0.67
1:L:60:GLU:N	1:L:60:GLU:OE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:THR:HG22	2:H:53:LYS:HB3	1.76	0.67
1:A:165:THR:O	1:A:169:LEU:HB2	1.94	0.67
1:A:129:GLN:HA	1:A:190:TYR:O	1.94	0.67
1:A:5:LEU:HD23	1:A:7:PHE:CZ	2.29	0.67
2:C:33:ARG:NH2	2:D:16:ASP:O	2.26	0.67
1:A:64:PHE:C	1:A:65:ASN:HD22	2.02	0.67
2:J:27:LYS:HD2	2:J:57:CYS:O	1.95	0.67
2:D:33:ARG:NH2	2:E:16:ASP:O	2.29	0.66
2:J:45:ILE:HG22	2:J:46:THR:N	2.09	0.66
2:B:33:ARG:NH2	2:C:16:ASP:O	2.29	0.66
1:A:173:GLN:HB2	1:A:235:SER:HA	1.78	0.66
1:A:173:GLN:NE2	1:A:196:ASP:OD1	2.28	0.66
2:B:16:ASP:O	2:F:33:ARG:NH2	2.29	0.66
2:G:33:ARG:NH2	2:H:16:ASP:O	2.29	0.65
1:L:210:LEU:N	1:L:211:PRO:HD2	2.11	0.65
1:L:8:SER:O	1:L:132:ARG:NH1	2.27	0.65
1:L:41:ILE:CG1	1:L:238:LEU:HD21	2.27	0.65
1:L:179:ARG:O	1:L:179:ARG:HG2	1.95	0.65
1:L:239:ILE:HG12	1:L:239:ILE:O	1.95	0.65
2:J:11:TYR:CE2	2:J:23:LYS:HD3	2.32	0.65
2:C:1:THR:CG2	2:C:2:PRO:HD2	2.26	0.64
1:L:130:ILE:HG22	1:L:131:ASN:N	2.13	0.64
2:J:35:ASN:ND2	2:K:37:GLN:OE1	2.29	0.64
1:L:125:ARG:HH11	1:L:125:ARG:CG	2.09	0.63
1:L:141:ASP:HB3	1:L:153:SER:OG	1.99	0.63
2:F:5:VAL:CG2	2:F:25:GLY:HA3	2.28	0.63
1:L:202:ASN:N	1:L:202:ASN:ND2	2.46	0.63
1:L:130:ILE:HG22	1:L:131:ASN:H	1.64	0.63
1:L:152:GLN:O	1:L:155:ALA:HB3	1.98	0.63
2:E:11:TYR:CE2	2:E:23:LYS:HD3	2.34	0.62
2:F:27:LYS:CE	2:F:58:HIS:HA	2.29	0.62
2:G:5:VAL:HG21	2:G:24:VAL:O	1.99	0.62
2:G:55:ASN:O	2:G:57:CYS:N	2.33	0.62
2:H:13:LYS:HE3	2:H:15:ASN:OD1	1.99	0.62
1:A:223:ARG:NH2	2:E:9:VAL:O	2.31	0.62
2:J:45:ILE:O	2:J:47:GLY:N	2.31	0.62
1:L:172:ARG:O	1:L:176:ARG:HB2	2.00	0.62
1:L:207:SER:OG	1:L:239:ILE:HB	2.00	0.62
2:C:33:ARG:NH1	2:C:64:SER:HB3	2.15	0.62
1:A:269:GLY:HA2	1:A:277:TRP:O	2.00	0.62
1:A:66:ASN:HB3	1:A:84:ARG:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:THR:HG21	2:B:53:LYS:O	2.00	0.62
2:H:12:THR:HG23	2:H:44:GLN:HE21	1.64	0.62
1:L:138:SER:HB3	1:L:161:PHE:CE2	2.33	0.61
1:A:9:THR:N	1:A:12:THR:OG1	2.30	0.61
2:H:12:THR:HG23	2:H:44:GLN:NE2	2.14	0.61
1:A:61:GLU:HA	1:A:61:GLU:OE1	2.00	0.61
2:J:32:ASN:HD22	2:J:32:ASN:N	1.98	0.61
2:B:56:ALA:O	2:B:61:GLY:HA3	2.01	0.61
1:L:51:ALA:HB2	1:L:100:PHE:HE2	1.65	0.61
2:J:56:ALA:O	2:J:61:GLY:HA3	2.01	0.61
1:L:139:TYR:O	1:L:143:MET:HG2	2.00	0.61
2:G:45:ILE:HG12	2:K:48:MET:HE2	1.81	0.61
1:L:125:ARG:HG3	1:L:125:ARG:NH1	2.07	0.60
1:L:172:ARG:HH21	1:L:237:ALA:HA	1.66	0.60
1:L:9:THR:O	1:L:12:THR:N	2.31	0.60
1:L:67:LEU:CD1	1:L:142:LEU:HD13	2.29	0.60
2:H:65:GLU:HA	2:I:14:TYR:O	2.01	0.60
1:L:24:ILE:HD11	1:L:76:LEU:HD21	1.83	0.60
1:A:50:PHE:HE1	1:A:52:VAL:CG2	2.15	0.60
1:A:270:ILE:HD12	1:A:279:SER:HA	1.82	0.60
2:H:34:TRP:H	2:H:34:TRP:CD1	2.19	0.60
2:B:10:GLU:HB3	2:B:23:LYS:HG2	1.84	0.60
2:F:17:ASP:O	2:J:32:ASN:HB2	2.02	0.60
2:B:34:TRP:CZ3	2:F:34:TRP:HD1	2.19	0.59
1:L:39:LEU:HB3	1:L:238:LEU:HD12	1.83	0.59
1:L:123:ILE:HD11	1:L:156:ARG:HG2	1.84	0.59
1:A:41:ILE:HG22	1:A:42:ASP:N	2.17	0.59
2:I:48:MET:CE	2:I:68:PHE:HB3	2.29	0.59
1:L:30:THR:HG21	1:L:213:TYR:O	2.01	0.59
1:A:167:GLU:OE1	1:A:167:GLU:HA	2.03	0.59
1:L:136:THR:O	1:L:140:LEU:HG	2.03	0.59
1:L:284:ALA:HB2	2:H:46:THR:HG23	1.84	0.59
1:L:41:ILE:HG13	1:L:238:LEU:CD2	2.33	0.59
2:D:24:VAL:HG21	2:D:52:ILE:HD12	1.84	0.59
2:F:52:ILE:HG23	2:F:63:PHE:CD1	2.37	0.59
1:A:148:THR:HG23	1:A:149:SER:N	2.18	0.58
2:F:21:THR:CG2	2:F:28:GLU:HG2	2.33	0.58
2:F:41:LEU:O	2:F:45:ILE:HD12	2.03	0.58
1:L:20:ILE:C	1:L:23:ALA:HB3	2.28	0.58
1:L:223:ARG:O	1:L:223:ARG:HG2	2.03	0.58
2:E:4:CYS:HB3	2:E:52:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ALA:HB1	1:A:179:ARG:HG2	1.84	0.58
2:H:56:ALA:O	2:H:58:HIS:N	2.34	0.58
1:L:167:GLU:OE1	1:L:170:ARG:NH1	2.36	0.58
2:D:1:THR:CG2	2:D:2:PRO:HD2	2.34	0.58
1:A:31:ILE:HG23	1:A:229:ILE:CD1	2.33	0.58
2:B:6:THR:OG1	2:B:51:THR:HG23	2.04	0.58
2:C:1:THR:HG23	2:C:2:PRO:HD2	1.85	0.57
2:I:36:LEU:HD21	2:J:14:TYR:CD2	2.39	0.57
1:L:5:LEU:HD12	1:L:16:SER:CB	2.34	0.57
1:L:38:LEU:HD12	1:L:236:VAL:HG12	1.86	0.57
1:L:180:THR:O	1:L:182:LEU:N	2.36	0.57
1:A:198:ASP:O	1:A:202:ASN:ND2	2.38	0.57
2:J:26:ASP:C	2:J:27:LYS:HG2	2.29	0.57
2:H:56:ALA:O	2:H:61:GLY:HA3	2.04	0.57
1:A:50:PHE:HE1	1:A:52:VAL:HG23	1.69	0.57
1:L:4:THR:HG23	1:L:55:ARG:HB3	1.85	0.57
1:L:100:PHE:CD1	1:L:101:PRO:HD2	2.40	0.57
2:B:12:THR:HB	2:B:20:PHE:CZ	2.39	0.57
2:F:49:THR:HG22	2:F:69:ARG:HD2	1.87	0.57
1:A:214:HIS:H	1:A:216:GLN:NE2	1.99	0.57
1:L:120:VAL:HG12	1:L:152:GLN:HA	1.87	0.57
1:L:193:THR:O	1:L:196:ASP:HB2	2.05	0.57
1:A:83:ASN:O	1:A:85:THR:N	2.38	0.56
2:D:30:PHE:O	2:D:62:GLY:HA2	2.05	0.56
1:L:202:ASN:HD22	1:L:202:ASN:H	1.53	0.56
1:L:270:ILE:HD12	1:L:279:SER:HA	1.86	0.56
1:L:273:ASN:O	1:L:274:LYS:HB2	2.05	0.56
2:G:33:ARG:NH1	2:G:64:SER:OG	2.37	0.56
1:L:14:VAL:O	1:L:18:ASN:ND2	2.38	0.56
1:L:69:LEU:CD2	1:L:158:MET:HE1	2.36	0.56
2:D:24:VAL:HG21	2:D:52:ILE:CD1	2.35	0.56
2:H:41:LEU:O	2:H:45:ILE:HG13	2.04	0.56
2:K:31:THR:OG1	2:K:33:ARG:HG2	2.06	0.56
1:L:7:PHE:CE2	1:L:135:LEU:HD21	2.39	0.56
1:A:152:GLN:O	1:A:156:ARG:HG3	2.06	0.56
1:L:114:TYR:O	1:L:118:GLN:HB2	2.05	0.56
2:F:14:TYR:CE1	2:F:20:PHE:CE1	2.94	0.56
2:J:32:ASN:H	2:J:32:ASN:ND2	2.02	0.56
2:F:16:ASP:O	2:F:18:ASP:N	2.39	0.56
1:A:64:PHE:CE1	1:A:140:LEU:HD21	2.41	0.55
2:E:33:ARG:NH2	2:F:15:ASN:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1:THR:HG23	2:H:2:PRO:HD2	1.87	0.55
1:A:216:GLN:H	1:A:216:GLN:NE2	1.98	0.55
1:L:5:LEU:HD23	1:L:7:PHE:CE1	2.42	0.55
1:L:24:ILE:CD1	1:L:76:LEU:HD21	2.37	0.55
2:J:32:ASN:N	2:J:32:ASN:ND2	2.53	0.55
1:A:121:ALA:CB	1:A:156:ARG:HG2	2.25	0.55
1:L:20:ILE:HA	1:L:23:ALA:HB3	1.89	0.55
1:L:5:LEU:HG	1:L:7:PHE:CE1	2.42	0.55
1:A:17:LEU:O	1:A:21:ARG:HG3	2.06	0.55
2:C:56:ALA:O	2:C:58:HIS:N	2.37	0.55
2:J:1:THR:CG2	2:J:54:THR:HA	2.37	0.55
1:L:58:ASP:HB3	1:L:62:GLY:HA3	1.87	0.54
1:L:217:ASP:OD1	1:L:217:ASP:N	2.39	0.54
1:A:26:THR:HB	1:A:27:PRO:HD2	1.88	0.54
1:A:64:PHE:HE1	1:A:140:LEU:HD21	1.73	0.54
1:A:216:GLN:N	1:A:216:GLN:NE2	2.51	0.54
2:B:5:VAL:HG12	2:B:52:ILE:HB	1.90	0.54
2:E:33:ARG:HH22	2:F:14:TYR:HD2	1.54	0.54
2:J:26:ASP:CG	2:J:27:LYS:HZ2	2.14	0.54
1:L:108:LEU:HA	1:L:148:THR:O	2.06	0.54
2:F:5:VAL:HG21	2:F:25:GLY:HA3	1.89	0.54
2:I:41:LEU:HD23	2:I:41:LEU:O	2.08	0.54
1:L:210:LEU:HD21	1:L:232:ILE:HD13	1.90	0.54
2:B:5:VAL:CG2	2:B:24:VAL:HG12	2.38	0.54
2:D:1:THR:HG21	2:D:54:THR:HA	1.89	0.54
1:L:38:LEU:HD11	1:L:236:VAL:HG12	1.90	0.54
2:C:6:THR:HG1	2:C:51:THR:HG1	1.55	0.54
2:C:50:VAL:HA	2:C:67:ILE:O	2.07	0.54
2:E:41:LEU:O	2:E:41:LEU:HG	2.08	0.54
2:K:18:ASP:OD1	2:K:18:ASP:N	2.41	0.54
1:L:67:LEU:HD11	1:L:142:LEU:CD1	2.35	0.54
2:H:1:THR:HG23	2:H:2:PRO:N	2.21	0.54
2:I:22:VAL:HG22	2:I:23:LYS:N	2.21	0.54
2:C:66:VAL:HG12	2:C:67:ILE:N	2.23	0.54
2:B:20:PHE:CD1	2:B:37:GLN:HG2	2.42	0.53
1:L:287:MET:HE1	2:H:38:SER:HA	1.90	0.53
2:D:1:THR:HG22	2:D:2:PRO:HD2	1.90	0.53
2:F:14:TYR:CE1	2:F:20:PHE:HE1	2.27	0.53
1:A:170:ARG:HD3	1:A:203:TRP:CD2	2.43	0.53
1:A:220:ARG:HD3	3:E:71:HOH:O	2.08	0.53
1:L:26:THR:HB	1:L:27:PRO:CD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:ASN:C	2:C:57:CYS:H	2.17	0.53
2:F:27:LYS:HE2	2:F:58:HIS:HA	1.91	0.53
1:L:121:ALA:CB	1:L:123:ILE:HG12	2.38	0.53
2:C:5:VAL:HG21	2:C:24:VAL:O	2.08	0.53
1:A:94:ASP:OD1	1:A:94:ASP:N	2.41	0.53
1:L:217:ASP:O	1:L:218:SER:HB2	2.08	0.53
2:E:22:VAL:HG21	2:E:40:LEU:HD13	1.91	0.53
1:L:60:GLU:HG2	1:L:61:GLU:CG	2.23	0.53
2:E:5:VAL:HG13	2:E:24:VAL:HG12	1.91	0.53
1:A:24:ILE:HG22	1:A:73:ARG:HH11	1.74	0.52
1:A:156:ARG:O	1:A:160:ARG:HG3	2.09	0.52
1:L:75:ASN:HB2	1:L:77:TYR:CD2	2.45	0.52
1:L:115:THR:O	1:L:119:ARG:HB2	2.09	0.52
2:F:17:ASP:OD1	2:F:19:THR:OG1	2.26	0.52
2:I:48:MET:HE1	2:I:68:PHE:CD2	2.45	0.52
1:A:278:ASP:OD2	1:A:280:SER:HB2	2.10	0.52
1:L:125:ARG:NH2	1:L:200:THR:OG1	2.41	0.52
1:L:140:LEU:O	1:L:142:LEU:N	2.43	0.52
2:H:18:ASP:HB3	2:H:34:TRP:CZ2	2.45	0.52
1:L:190:TYR:CD1	1:L:191:VAL:N	2.78	0.52
2:G:23:LYS:O	2:G:23:LYS:HG3	2.10	0.52
1:L:14:VAL:HG12	1:L:18:ASN:ND2	2.25	0.52
1:L:66:ASN:C	1:L:143:MET:HE1	2.34	0.52
1:L:195:GLU:CD	1:L:195:GLU:H	2.16	0.52
1:L:8:SER:C	1:L:132:ARG:HH22	2.18	0.52
1:L:58:ASP:CB	1:L:62:GLY:HA2	2.38	0.52
2:B:5:VAL:HG22	2:B:24:VAL:HG12	1.91	0.52
1:A:189:SER:N	3:A:293:HOH:O	2.42	0.51
2:E:36:LEU:O	2:E:38:SER:N	2.43	0.51
2:F:3:ASP:HA	2:F:53:LYS:HG2	1.92	0.51
2:I:48:MET:HE1	2:I:68:PHE:HD2	1.75	0.51
1:L:166:ALA:O	1:L:169:LEU:N	2.41	0.51
2:G:13:LYS:HB3	2:K:67:ILE:HA	1.93	0.51
2:K:66:VAL:HG12	2:K:67:ILE:N	2.24	0.51
2:D:56:ALA:O	2:D:61:GLY:HA3	2.10	0.51
1:A:8:SER:HB2	1:A:12:THR:HG21	1.91	0.51
1:A:29:GLN:O	1:A:29:GLN:HG2	2.10	0.51
2:E:17:ASP:O	2:E:18:ASP:HB2	2.10	0.51
1:A:142:LEU:HD23	1:A:154:VAL:HG13	1.92	0.51
1:L:94:ASP:CG	1:L:111:ASP:HB2	2.36	0.51
2:H:55:ASN:O	2:H:57:CYS:N	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:THR:HG22	1:A:95:PHE:CD1	2.46	0.51
2:C:51:THR:HB	2:C:67:ILE:HB	1.92	0.51
2:H:34:TRP:H	2:H:34:TRP:HD1	1.59	0.51
1:A:70:ILE:HD11	1:A:82:VAL:HG21	1.93	0.51
2:I:10:GLU:HB3	2:I:23:LYS:O	2.10	0.51
2:G:48:MET:CE	2:G:68:PHE:HB3	2.40	0.51
1:A:181:THR:O	1:A:181:THR:HG22	2.11	0.50
1:L:210:LEU:CD2	1:L:232:ILE:HD13	2.41	0.50
1:L:116:THR:O	1:L:120:VAL:HG23	2.11	0.50
2:H:55:ASN:C	2:H:57:CYS:H	2.17	0.50
1:L:77:TYR:OH	1:L:258:PRO:O	2.28	0.50
1:L:140:LEU:O	1:L:143:MET:N	2.44	0.50
2:F:9:VAL:HB	2:F:44:GLN:HG3	1.93	0.50
2:H:63:PHE:HE2	2:H:66:VAL:HG21	1.77	0.50
2:J:48:MET:HE3	2:K:45:ILE:CG1	2.41	0.50
2:G:16:ASP:O	2:G:16:ASP:OD1	2.30	0.50
2:K:1:THR:CG2	2:K:54:THR:HA	2.41	0.50
1:A:271:THR:HG22	1:A:272:HIS:N	2.26	0.50
2:B:8:LYS:HB3	2:B:8:LYS:HZ2	1.76	0.50
1:A:75:ASN:HB2	1:A:77:TYR:CD2	2.47	0.50
1:L:180:THR:OG1	1:L:181:THR:N	2.44	0.50
2:J:37:GLN:HG3	3:J:70:HOH:O	2.12	0.50
1:A:120:VAL:HG12	1:A:152:GLN:HA	1.93	0.50
1:L:100:PHE:O	1:L:103:THR:OG1	2.28	0.50
2:C:67:ILE:CG1	2:D:13:LYS:HG3	2.36	0.50
2:H:33:ARG:NH2	2:I:16:ASP:OD1	2.45	0.50
1:A:173:GLN:HG2	1:A:173:GLN:O	2.10	0.49
2:H:11:TYR:CD1	2:H:11:TYR:C	2.90	0.49
1:A:175:GLN:HG2	1:A:176:ARG:N	2.28	0.49
1:A:287:MET:HE3	2:D:38:SER:CB	2.37	0.49
2:B:11:TYR:CE2	2:B:23:LYS:HD3	2.48	0.49
2:J:20:PHE:CD1	2:J:37:GLN:HG2	2.48	0.49
2:K:49:THR:O	2:K:69:ARG:HB2	2.11	0.49
2:H:17:ASP:O	2:H:18:ASP:HB2	2.12	0.49
2:J:55:ASN:O	2:J:57:CYS:N	2.37	0.49
1:A:27:PRO:HA	1:A:39:LEU:HD23	1.95	0.49
1:L:19:VAL:O	1:L:23:ALA:HB2	2.12	0.49
1:L:20:ILE:CA	1:L:23:ALA:HB3	2.43	0.49
1:L:28:LEU:HD21	1:L:40:MET:HE3	1.94	0.49
1:L:47:ASP:OD2	1:L:72:GLU:OE2	2.29	0.49
2:D:4:CYS:CB	2:D:54:THR:HG22	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:67:ILE:HA	2:F:12:THR:O	2.12	0.49
2:H:1:THR:CB	2:H:2:PRO:HD2	2.43	0.49
2:J:30:PHE:N	2:J:30:PHE:CD1	2.81	0.49
1:A:170:ARG:HG2	1:A:203:TRP:CE2	2.47	0.49
1:L:10:ALA:HB1	1:L:179:ARG:CG	2.41	0.49
1:L:130:ILE:CG2	1:L:131:ASN:H	2.25	0.49
2:D:44:GLN:HA	3:D:73:HOH:O	2.12	0.49
2:H:34:TRP:CD1	2:H:34:TRP:N	2.80	0.49
2:H:63:PHE:HE2	2:H:66:VAL:CG2	2.26	0.49
1:A:12:THR:O	1:A:16:SER:OG	2.30	0.49
1:L:139:TYR:CZ	1:L:143:MET:HE2	2.48	0.49
2:G:16:ASP:O	2:K:33:ARG:NH2	2.46	0.49
2:K:9:VAL:HG12	2:K:9:VAL:O	2.13	0.49
1:L:13:TYR:CE2	1:L:178:PHE:HD2	2.30	0.49
1:L:39:LEU:CB	1:L:238:LEU:HD12	2.42	0.49
2:B:1:THR:HG23	2:B:2:PRO:HD2	1.95	0.49
2:C:30:PHE:CD1	2:C:30:PHE:C	2.91	0.49
1:L:56:GLY:O	1:L:132:ARG:NH2	2.45	0.49
1:L:205:ARG:NH2	1:L:281:THR:OG1	2.45	0.49
1:L:11:LYS:O	1:L:15:ASP:OD2	2.31	0.48
1:L:92:PHE:HB3	1:L:94:ASP:OD1	2.13	0.48
2:B:18:ASP:HB3	2:B:34:TRP:CH2	2.48	0.48
2:F:19:THR:HG22	2:F:20:PHE:H	1.78	0.48
2:J:11:TYR:OH	2:J:23:LYS:HD2	2.13	0.48
1:L:30:THR:HG21	3:L:298:HOH:O	2.13	0.48
2:F:21:THR:HG21	2:F:28:GLU:HG2	1.95	0.48
2:I:10:GLU:OE2	2:I:23:LYS:HE3	2.13	0.48
1:L:4:THR:CG2	1:L:55:ARG:HB3	2.42	0.48
2:I:11:TYR:CE2	2:I:23:LYS:HG2	2.49	0.48
2:J:17:ASP:O	2:J:18:ASP:HB2	2.14	0.48
2:K:43:ALA:HA	2:K:48:MET:HG3	1.96	0.48
2:K:54:THR:OG1	2:K:55:ASN:N	2.46	0.48
1:A:31:ILE:HG22	1:A:233:LEU:HD21	1.96	0.48
1:A:50:PHE:CE1	1:A:52:VAL:HG23	2.47	0.48
1:A:210:LEU:N	1:A:211:PRO:HD2	2.28	0.48
1:L:38:LEU:HD11	1:L:236:VAL:CG1	2.44	0.48
2:E:17:ASP:OD1	2:E:19:THR:HG23	2.14	0.48
2:J:33:ARG:HH12	2:J:64:SER:CB	2.00	0.48
2:K:16:ASP:O	2:K:18:ASP:OD1	2.32	0.48
2:J:33:ARG:HH11	2:J:33:ARG:HG2	1.77	0.48
2:K:29:LEU:HD23	2:K:58:HIS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:65:GLU:OE1	2:I:13:LYS:NZ	2.45	0.48
2:J:12:THR:CG2	2:J:22:VAL:HG23	2.44	0.48
2:J:56:ALA:HB1	2:J:61:GLY:CA	2.41	0.48
2:H:31:THR:OG1	2:H:32:ASN:N	2.47	0.48
1:A:27:PRO:HA	1:A:39:LEU:HA	1.96	0.47
1:L:203:TRP:HE1	1:L:239:ILE:HA	1.79	0.47
2:C:36:LEU:HD23	2:C:36:LEU:HA	1.63	0.47
1:A:11:LYS:O	1:A:15:ASP:HB2	2.14	0.47
1:L:130:ILE:CG2	1:L:178:PHE:HE1	2.27	0.47
1:L:202:ASN:N	1:L:202:ASN:HD22	2.11	0.47
2:B:17:ASP:OD1	2:B:19:THR:HG23	2.14	0.47
2:F:16:ASP:O	2:F:18:ASP:OD1	2.32	0.47
2:J:45:ILE:C	2:J:47:GLY:H	2.21	0.47
1:L:213:TYR:CD1	1:L:213:TYR:C	2.92	0.47
2:H:8:LYS:HE3	2:H:47:GLY:O	2.15	0.47
1:A:170:ARG:HG2	1:A:203:TRP:CZ2	2.50	0.47
2:I:16:ASP:OD1	2:I:16:ASP:O	2.31	0.47
1:L:75:ASN:HB3	1:L:260:MET:HG3	1.96	0.47
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.44	0.47
2:B:27:LYS:HA	2:B:27:LYS:HD3	1.56	0.47
1:A:285:ILE:HD11	2:F:46:THR:HG22	1.97	0.47
1:L:203:TRP:CZ2	1:L:240:LEU:HG	2.49	0.47
1:L:210:LEU:N	1:L:211:PRO:CD	2.78	0.47
2:B:30:PHE:CD2	2:B:30:PHE:C	2.93	0.47
1:L:72:GLU:HB3	1:L:77:TYR:HB2	1.97	0.46
1:A:108:LEU:HD23	1:A:148:THR:O	2.15	0.46
2:H:12:THR:CG2	2:H:44:GLN:NE2	2.78	0.46
1:A:48:ASN:OD1	1:A:73:ARG:HB3	2.16	0.46
2:B:8:LYS:HB3	2:B:8:LYS:HZ3	1.77	0.46
2:C:1:THR:HG22	2:C:2:PRO:HD2	1.97	0.46
2:C:35:ASN:OD1	2:C:35:ASN:N	2.43	0.46
2:G:23:LYS:HE2	2:G:25:GLY:O	2.16	0.46
2:G:39:LEU:HD23	2:G:39:LEU:N	2.30	0.46
2:H:1:THR:CG2	2:H:2:PRO:N	2.78	0.46
2:J:12:THR:CG2	2:J:20:PHE:CE2	2.98	0.46
1:A:39:LEU:HB2	1:A:238:LEU:HD12	1.98	0.46
1:L:201:LEU:HA	1:L:201:LEU:HD23	1.51	0.46
2:F:52:ILE:CG2	2:F:63:PHE:CD1	2.98	0.46
2:H:34:TRP:O	2:H:37:GLN:HG3	2.16	0.46
1:L:5:LEU:HD12	1:L:16:SER:HB3	1.97	0.46
1:L:191:VAL:HG23	1:L:191:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:PHE:CD1	2:G:30:PHE:C	2.94	0.46
1:L:130:ILE:CG2	1:L:131:ASN:N	2.78	0.46
1:L:216:GLN:C	1:L:218:SER:H	2.22	0.46
2:I:27:LYS:HA	2:I:59:ASN:HD21	1.80	0.46
1:A:203:TRP:CH2	1:A:240:LEU:CD2	2.99	0.46
1:L:213:TYR:CG	1:L:214:HIS:N	2.84	0.46
2:B:1:THR:HG21	2:B:53:LYS:C	2.41	0.46
2:B:33:ARG:NH1	2:B:64:SER:OG	2.49	0.46
2:B:8:LYS:NZ	2:B:8:LYS:CB	2.76	0.46
2:J:29:LEU:HD23	2:J:61:GLY:HA3	1.98	0.46
1:A:66:ASN:O	1:A:143:MET:HE1	2.16	0.46
2:G:11:TYR:CD1	2:G:11:TYR:C	2.94	0.46
2:J:42:SER:O	2:J:46:THR:HG23	2.17	0.46
1:A:5:LEU:CD2	1:A:7:PHE:CZ	2.97	0.45
2:C:56:ALA:O	2:C:61:GLY:HA3	2.16	0.45
2:F:52:ILE:CG2	2:F:63:PHE:CG	2.99	0.45
2:H:12:THR:OG1	2:H:44:GLN:NE2	2.43	0.45
1:L:100:PHE:CD1	1:L:101:PRO:CD	2.99	0.45
1:L:270:ILE:HD12	1:L:279:SER:CA	2.46	0.45
1:A:118:GLN:OE1	1:A:124:SER:HA	2.15	0.45
2:B:36:LEU:CD2	2:B:66:VAL:HG21	2.47	0.45
2:G:22:VAL:O	2:G:22:VAL:HG12	2.07	0.45
2:H:18:ASP:CB	2:H:34:TRP:CH2	2.97	0.45
2:J:9:VAL:HG13	2:J:22:VAL:HG22	1.99	0.45
1:L:5:LEU:CD2	1:L:7:PHE:CE1	2.99	0.45
1:L:139:TYR:OH	1:L:143:MET:HE2	2.16	0.45
2:D:11:TYR:CD1	2:D:11:TYR:C	2.93	0.45
2:F:17:ASP:O	2:F:18:ASP:HB2	2.16	0.45
2:G:55:ASN:C	2:G:57:CYS:N	2.75	0.45
2:J:1:THR:HG21	2:J:54:THR:HA	1.97	0.45
1:A:148:THR:CG2	1:A:149:SER:N	2.79	0.45
1:L:10:ALA:HB1	1:L:179:ARG:HG2	1.98	0.45
1:L:217:ASP:CG	1:L:274:LYS:HD2	2.41	0.45
2:B:16:ASP:O	2:B:16:ASP:OD1	2.34	0.45
2:C:22:VAL:HG23	2:C:63:PHE:HE2	1.81	0.45
1:L:41:ILE:O	1:L:41:ILE:HG22	2.17	0.45
2:B:34:TRP:CE3	2:F:34:TRP:HD1	2.35	0.45
2:G:51:THR:HB	2:G:67:ILE:HB	1.97	0.45
1:A:10:ALA:HB1	1:A:179:ARG:CG	2.46	0.45
2:E:6:THR:HA	2:E:51:THR:HA	1.99	0.45
2:K:30:PHE:CD1	2:K:30:PHE:C	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:ASP:OD1	2:I:19:THR:OG1	2.29	0.45
2:I:36:LEU:CD2	2:I:39:LEU:HD12	2.47	0.45
2:K:11:TYR:OH	2:K:28:GLU:OE1	2.28	0.45
1:L:130:ILE:CG2	1:L:178:PHE:CE1	3.00	0.45
2:J:4:CYS:O	2:J:57:CYS:SG	2.75	0.45
1:L:14:VAL:HG12	1:L:18:ASN:HD22	1.82	0.44
1:A:99:THR:HG23	1:A:100:PHE:N	2.32	0.44
1:A:281:THR:O	1:A:285:ILE:HG23	2.18	0.44
1:L:31:ILE:O	1:L:32:SER:HB2	2.18	0.44
1:L:159:LEU:HD23	1:L:159:LEU:HA	1.73	0.44
1:L:260:MET:HE2	1:L:260:MET:HB3	1.62	0.44
1:L:262:PRO:O	1:L:263:ALA:O	2.35	0.44
1:A:70:ILE:HD11	1:A:82:VAL:CG2	2.48	0.44
1:L:40:MET:CG	1:L:241:ASN:HB2	2.48	0.44
1:L:92:PHE:CD2	1:L:112:SER:HB3	2.51	0.44
2:D:65:GLU:HA	2:E:14:TYR:O	2.16	0.44
2:E:36:LEU:O	2:E:39:LEU:N	2.43	0.44
1:L:213:TYR:CD1	1:L:214:HIS:N	2.86	0.44
2:H:1:THR:HG23	2:H:2:PRO:CG	2.47	0.44
1:A:71:VAL:HG22	1:A:78:VAL:HG22	2.00	0.44
1:A:83:ASN:HB3	1:A:86:ASN:OD1	2.17	0.44
1:A:139:TYR:CE1	1:A:143:MET:HG3	2.53	0.44
1:A:270:ILE:HD11	1:A:279:SER:CB	2.48	0.44
1:L:3:PHE:CD1	1:L:3:PHE:N	2.84	0.44
1:L:171:PHE:CE1	1:L:199:LEU:HG	2.53	0.44
1:L:107:THR:HG22	1:L:108:LEU:O	2.17	0.44
2:F:16:ASP:C	2:F:18:ASP:H	2.25	0.44
2:I:1:THR:HA	2:I:2:PRO:HD3	1.35	0.44
2:J:15:ASN:ND2	2:J:19:THR:OG1	2.50	0.44
1:A:202:ASN:ND2	1:A:224:ILE:HD12	2.32	0.44
2:E:56:ALA:O	2:E:61:GLY:HA3	2.17	0.44
2:B:36:LEU:HD22	2:B:66:VAL:HG21	1.99	0.44
2:H:12:THR:CG2	2:H:44:GLN:HE21	2.29	0.44
2:J:14:TYR:CD1	2:J:14:TYR:C	2.96	0.44
1:A:6:ASP:OD1	1:A:8:SER:OG	2.29	0.44
1:L:3:PHE:O	1:L:52:VAL:HA	2.18	0.44
2:D:1:THR:CG2	2:D:54:THR:HA	2.48	0.44
2:E:30:PHE:O	2:E:62:GLY:HA2	2.18	0.44
2:F:17:ASP:OD1	2:F:19:THR:N	2.50	0.44
1:A:2:GLU:HA	1:A:51:ALA:O	2.18	0.43
2:H:5:VAL:CG2	2:H:24:VAL:HG12	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:PHE:CD1	1:A:50:PHE:C	2.96	0.43
1:A:79:THR:HG22	1:A:95:PHE:CE1	2.53	0.43
2:F:23:LYS:HA	2:F:27:LYS:O	2.19	0.43
1:A:142:LEU:CD2	1:A:154:VAL:HG13	2.49	0.43
2:B:41:LEU:HD22	2:F:39:LEU:HD23	2.01	0.43
2:B:69:ARG:HE	2:B:69:ARG:HB2	1.58	0.43
2:C:24:VAL:HG21	2:C:52:ILE:HG13	2.00	0.43
2:J:29:LEU:HB3	2:J:61:GLY:O	2.19	0.43
1:L:75:ASN:HB2	1:L:77:TYR:CE2	2.53	0.43
2:C:33:ARG:NH2	2:D:18:ASP:OD1	2.49	0.43
2:G:13:LYS:HE3	2:G:13:LYS:HB2	1.63	0.43
2:I:48:MET:CE	2:I:68:PHE:HD2	2.32	0.43
1:A:273:ASN:O	1:A:274:LYS:HB2	2.18	0.43
2:C:1:THR:HG21	2:C:54:THR:HA	2.00	0.43
1:L:25:GLY:C	1:L:39:LEU:HD23	2.43	0.43
1:L:167:GLU:OE1	1:L:167:GLU:HA	2.18	0.43
2:G:23:LYS:HD2	2:G:27:LYS:O	2.19	0.43
2:H:30:PHE:O	2:H:62:GLY:HA2	2.19	0.43
2:I:30:PHE:CD1	2:I:30:PHE:C	2.95	0.43
1:A:65:ASN:HD22	1:A:65:ASN:N	2.17	0.43
1:L:66:ASN:O	1:L:143:MET:HE1	2.19	0.43
1:L:66:ASN:CB	1:L:143:MET:CE	2.97	0.43
2:D:41:LEU:HA	2:D:41:LEU:HD12	1.68	0.43
2:F:4:CYS:CB	2:F:54:THR:HG22	2.49	0.43
2:H:23:LYS:HD2	2:H:28:GLU:HB2	2.01	0.43
2:J:11:TYR:CE2	2:J:23:LYS:CD	3.00	0.43
1:L:58:ASP:CG	1:L:62:GLY:HA2	2.44	0.43
1:L:139:TYR:CD1	1:L:139:TYR:C	2.97	0.43
1:L:203:TRP:NE1	1:L:239:ILE:HA	2.34	0.43
1:L:217:ASP:OD2	1:L:274:LYS:HD2	2.18	0.43
2:E:53:LYS:HZ3	2:E:53:LYS:HG2	1.65	0.43
1:L:8:SER:HA	1:L:56:GLY:O	2.19	0.43
2:I:27:LYS:HA	2:I:59:ASN:ND2	2.34	0.43
2:J:11:TYR:CZ	2:J:23:LYS:HD2	2.54	0.43
1:A:270:ILE:HD12	1:A:279:SER:CA	2.49	0.42
1:L:70:ILE:HD12	1:L:100:PHE:CE2	2.53	0.42
2:C:33:ARG:HH21	2:D:18:ASP:CG	2.25	0.42
1:A:57:ILE:HG21	1:A:136:THR:HA	2.01	0.42
1:L:79:THR:OG1	1:L:98:VAL:HG11	2.20	0.42
1:L:130:ILE:HG21	1:L:178:PHE:CE1	2.54	0.42
1:L:57:ILE:O	1:L:57:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:ASP:OD1	1:L:60:GLU:OE1	2.37	0.42
1:L:171:PHE:CD1	1:L:199:LEU:HG	2.55	0.42
1:L:198:ASP:O	1:L:201:LEU:N	2.50	0.42
2:C:42:SER:O	2:C:46:THR:HG23	2.19	0.42
2:K:1:THR:HG21	2:K:54:THR:HA	2.00	0.42
1:L:151:THR:OG1	1:L:154:VAL:HG23	2.18	0.42
2:B:3:ASP:OD1	2:B:53:LYS:NZ	2.52	0.42
2:H:2:PRO:O	2:H:3:ASP:O	2.38	0.42
2:H:68:PHE:HB2	2:I:12:THR:OG1	2.19	0.42
2:I:38:SER:O	2:I:42:SER:HB2	2.19	0.42
1:L:55:ARG:O	1:L:55:ARG:HG2	2.20	0.42
1:L:80:GLY:HA3	1:L:90:TYR:O	2.19	0.42
1:L:137:THR:O	1:L:140:LEU:N	2.52	0.42
2:I:40:LEU:C	2:I:42:SER:H	2.26	0.42
2:K:12:THR:HB	2:K:20:PHE:CZ	2.54	0.42
2:B:9:VAL:H	2:B:9:VAL:HG23	1.65	0.42
1:L:193:THR:O	1:L:197:VAL:HG23	2.20	0.42
2:D:14:TYR:CD1	2:D:14:TYR:C	2.97	0.42
2:E:53:LYS:HE2	2:E:67:ILE:HD11	2.01	0.42
1:A:70:ILE:HG12	1:A:82:VAL:HG23	2.02	0.42
1:A:109:SER:HB3	1:A:149:SER:HA	2.02	0.42
1:L:32:SER:HA	1:L:36:THR:O	2.19	0.42
2:B:18:ASP:HB3	2:B:34:TRP:HH2	1.84	0.42
2:B:22:VAL:HG21	2:B:40:LEU:HD13	2.01	0.42
2:H:1:THR:CG2	2:H:2:PRO:HD2	2.50	0.42
2:I:5:VAL:O	2:I:6:THR:OG1	2.34	0.42
2:I:29:LEU:HD23	2:I:61:GLY:CA	2.50	0.42
1:L:14:VAL:CG1	1:L:18:ASN:ND2	2.82	0.42
1:L:217:ASP:OD1	1:L:274:LYS:HD2	2.20	0.42
2:B:1:THR:HG22	2:B:53:LYS:HB3	2.01	0.42
2:H:23:LYS:HZ2	2:H:23:LYS:HG2	1.60	0.42
2:J:58:HIS:O	2:J:61:GLY:N	2.47	0.42
1:A:165:THR:HG22	1:A:166:ALA:N	2.35	0.42
1:A:270:ILE:CD1	1:A:279:SER:CB	2.97	0.42
1:L:40:MET:SD	1:L:241:ASN:CB	3.08	0.42
1:L:100:PHE:HD1	1:L:100:PHE:HA	1.73	0.42
1:L:275:ILE:HG22	1:L:277:TRP:CD1	2.54	0.42
2:C:5:VAL:HG22	2:C:6:THR:N	2.34	0.42
2:J:3:ASP:OD1	2:J:53:LYS:NZ	2.44	0.42
2:J:45:ILE:C	2:J:47:GLY:N	2.77	0.41
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:HD13	1:A:285:ILE:HG21	1.79	0.41
2:G:12:THR:HB	2:G:20:PHE:CE2	2.55	0.41
2:H:67:ILE:HG12	2:I:13:LYS:HG3	1.95	0.41
2:C:55:ASN:C	2:C:57:CYS:N	2.77	0.41
2:F:30:PHE:O	2:F:62:GLY:HA2	2.20	0.41
1:A:41:ILE:HG13	1:A:239:ILE:O	2.20	0.41
1:L:10:ALA:HB2	1:L:179:ARG:O	2.21	0.41
2:D:36:LEU:HA	2:D:36:LEU:HD23	1.51	0.41
1:A:125:ARG:NH2	1:A:197:VAL:HG13	2.36	0.41
1:L:172:ARG:NH2	1:L:237:ALA:CB	2.83	0.41
1:L:216:GLN:C	1:L:218:SER:N	2.76	0.41
2:C:33:ARG:NH1	2:C:64:SER:CB	2.83	0.41
2:H:1:THR:HG23	2:H:2:PRO:HG2	2.01	0.41
2:H:24:VAL:HG21	2:H:52:ILE:HD12	2.02	0.41
2:I:40:LEU:HD23	2:I:40:LEU:HA	1.83	0.41
2:I:43:ALA:HB1	2:I:48:MET:HB2	2.02	0.41
1:A:216:GLN:HB3	1:A:274:LYS:O	2.21	0.41
1:L:138:SER:OG	1:L:157:ALA:HA	2.20	0.41
2:D:33:ARG:CZ	2:D:64:SER:OG	2.69	0.41
2:H:14:TYR:OH	2:H:18:ASP:OD1	2.30	0.41
2:J:20:PHE:CG	2:J:37:GLN:HG2	2.55	0.41
1:L:266:ARG:NH2	2:G:48:MET:HA	2.36	0.41
2:J:69:ARG:HH11	2:J:69:ARG:HG2	1.86	0.41
1:A:121:ALA:HB2	1:A:156:ARG:N	2.36	0.41
1:A:205:ARG:NH1	1:A:278:ASP:OD2	2.52	0.41
2:E:16:ASP:C	2:E:18:ASP:H	2.28	0.41
1:A:241:ASN:ND2	1:A:241:ASN:C	2.77	0.41
1:L:7:PHE:CD2	1:L:135:LEU:CD2	3.00	0.41
1:L:172:ARG:HB2	1:L:237:ALA:HB2	2.01	0.41
2:B:34:TRP:CZ3	2:F:34:TRP:CD1	3.05	0.41
2:G:27:LYS:HE2	2:G:58:HIS:HA	2.03	0.41
1:L:50:PHE:CD1	1:L:50:PHE:C	2.98	0.41
2:C:11:TYR:CD1	2:C:11:TYR:C	2.99	0.41
2:C:17:ASP:O	2:C:18:ASP:HB2	2.20	0.41
2:D:36:LEU:O	2:D:40:LEU:HB2	2.21	0.41
1:A:41:ILE:CG2	1:A:42:ASP:N	2.82	0.40
1:L:21:ARG:C	1:L:23:ALA:N	2.78	0.40
2:F:58:HIS:O	2:F:61:GLY:N	2.43	0.40
2:H:1:THR:OG1	2:H:2:PRO:HD2	2.20	0.40
2:K:63:PHE:CD1	2:K:63:PHE:C	2.99	0.40
1:A:260:MET:HB3	1:A:260:MET:HE2	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:LEU:HD23	1:L:7:PHE:CZ	2.56	0.40
1:L:60:GLU:CD	1:L:61:GLU:HG2	2.45	0.40
1:L:284:ALA:HB2	2:H:46:THR:CG2	2.51	0.40
2:H:22:VAL:O	2:H:22:VAL:HG13	2.21	0.40
1:L:13:TYR:O	1:L:17:LEU:HG	2.21	0.40
1:L:58:ASP:O	1:L:62:GLY:HA3	2.20	0.40
2:I:41:LEU:O	2:I:45:ILE:HG13	2.21	0.40
2:J:12:THR:HG21	2:J:20:PHE:CE2	2.56	0.40
1:A:197:VAL:O	1:A:201:LEU:HG	2.21	0.40
1:L:67:LEU:CD1	1:L:142:LEU:CD1	2.99	0.40
1:L:224:ILE:HG21	1:L:224:ILE:HD13	1.85	0.40
1:L:20:ILE:O	1:L:24:ILE:N	2.32	0.40
2:I:48:MET:HE3	2:I:48:MET:HB3	1.79	0.40
2:J:52:ILE:HD13	2:J:63:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/287 (89%)	232 (91%)	20 (8%)	4 (2%)	7	14
1	L	254/287 (88%)	211 (83%)	34 (13%)	9 (4%)	3	4
2	B	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
2	C	67/69 (97%)	61 (91%)	6 (9%)	0	100	100
2	D	67/69 (97%)	63 (94%)	4 (6%)	0	100	100
2	E	67/69 (97%)	63 (94%)	3 (4%)	1 (2%)	8	16
2	F	67/69 (97%)	61 (91%)	5 (8%)	1 (2%)	8	16
2	G	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
2	H	67/69 (97%)	55 (82%)	7 (10%)	5 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	67/69 (97%)	59 (88%)	7 (10%)	1 (2%)	8	16
2	J	67/69 (97%)	57 (85%)	4 (6%)	6 (9%)	0	0
2	K	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
All	All	1180/1264 (93%)	1053 (89%)	100 (8%)	27 (2%)	5	8

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ARG
1	L	141	ASP
1	L	181	THR
1	L	263	ALA
2	F	17	ASP
2	J	2	PRO
2	J	56	ALA
1	L	32	SER
1	L	179	ARG
2	H	3	ASP
2	H	56	ALA
2	J	45	ILE
2	J	46	THR
1	A	48	ASN
2	H	4	CYS
2	H	25	GLY
2	J	18	ASP
2	J	57	CYS
1	L	214	HIS
2	E	37	GLN
2	H	57	CYS
1	A	266	ARG
1	L	264	ASP
1	A	8	SER
1	L	265	GLY
1	L	59	PRO
2	I	2	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	229/246 (93%)	194 (85%)	35 (15%)	3	5
1	L	227/246 (92%)	187 (82%)	40 (18%)	2	3
2	B	61/61 (100%)	44 (72%)	17 (28%)	0	1
2	C	61/61 (100%)	50 (82%)	11 (18%)	2	3
2	D	61/61 (100%)	55 (90%)	6 (10%)	7	16
2	E	61/61 (100%)	50 (82%)	11 (18%)	2	3
2	F	61/61 (100%)	50 (82%)	11 (18%)	2	3
2	G	61/61 (100%)	53 (87%)	8 (13%)	4	8
2	H	61/61 (100%)	49 (80%)	12 (20%)	1	2
2	I	61/61 (100%)	48 (79%)	13 (21%)	1	2
2	J	61/61 (100%)	50 (82%)	11 (18%)	2	3
2	K	61/61 (100%)	49 (80%)	12 (20%)	1	2
All	All	1066/1102 (97%)	879 (82%)	187 (18%)	2	3

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	2	GLU
1	A	11	LYS
1	A	16	SER
1	A	19	VAL
1	A	21	ARG
1	A	24	ILE
1	A	27	PRO
1	A	49	LEU
1	A	55	ARG
1	A	57	ILE
1	A	61	GLU
1	A	65	ASN
1	A	66	ASN
1	A	73	ARG
1	A	85	THR
1	A	94	ASP
1	A	99	THR
1	A	132	ARG

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Mol	Chain	Res	Type
1	A	137	THR
1	A	144	SER
1	A	150	LEU
1	A	153	SER
1	A	154	VAL
1	A	160	ARG
1	A	175	GLN
1	A	208	SER
1	A	216	GLN
1	A	224	ILE
1	A	233	LEU
1	A	241	ASN
1	A	242	CYS
1	A	268	ARG
1	A	275	ILE
1	A	280	SER
1	L	2	GLU
1	L	3	PHE
1	L	28	LEU
1	L	31	ILE
1	L	33	SER
1	L	38	LEU
1	L	39	LEU
1	L	41	ILE
1	L	49	LEU
1	L	55	ARG
1	L	57	ILE
1	L	61	GLU
1	L	85	THR
1	L	87	ASN
1	L	100	PHE
1	L	115	THR
1	L	117	LEU
1	L	119	ARG
1	L	125	ARG
1	L	149	SER
1	L	152	GLN
1	L	158	MET
1	L	172	ARG
1	L	174	ILE
1	L	175	GLN
1	L	182	LEU

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Mol	Chain	Res	Type
1	L	192	MET
1	L	193	THR
1	L	198	ASP
1	L	202	ASN
1	L	217	ASP
1	L	236	VAL
1	L	238	LEU
1	L	239	ILE
1	L	241	ASN
1	L	260	MET
1	L	268	ARG
1	L	273	ASN
1	L	274	LYS
1	L	276	LEU
2	B	4	CYS
2	B	8	LYS
2	B	12	THR
2	B	13	LYS
2	B	23	LYS
2	B	24	VAL
2	B	27	LYS
2	B	29	LEU
2	B	33	ARG
2	B	35	ASN
2	B	38	SER
2	B	52	ILE
2	B	53	LYS
2	B	64	SER
2	B	66	VAL
2	B	67	ILE
2	B	69	ARG
2	C	6	THR
2	C	13	LYS
2	C	21	THR
2	C	22	VAL
2	C	23	LYS
2	C	32	ASN
2	C	35	ASN
2	C	49	THR
2	C	52	ILE
2	C	59	ASN
2	C	69	ARG

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Mol	Chain	Res	Type
2	D	12	THR
2	D	13	LYS
2	D	22	VAL
2	D	33	ARG
2	D	45	ILE
2	D	69	ARG
2	E	1	THR
2	E	5	VAL
2	E	13	LYS
2	E	15	ASN
2	E	21	THR
2	E	22	VAL
2	E	28	GLU
2	E	33	ARG
2	E	52	ILE
2	E	53	LYS
2	E	69	ARG
2	F	1	THR
2	F	5	VAL
2	F	13	LYS
2	F	14	TYR
2	F	23	LYS
2	F	36	LEU
2	F	41	LEU
2	F	45	ILE
2	F	49	THR
2	F	52	ILE
2	F	69	ARG
2	G	13	LYS
2	G	22	VAL
2	G	23	LYS
2	G	26	ASP
2	G	29	LEU
2	G	38	SER
2	G	46	THR
2	G	53	LYS
2	H	1	THR
2	H	8	LYS
2	H	21	THR
2	H	23	LYS
2	H	27	LYS
2	H	31	THR

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Mol	Chain	Res	Type
2	H	33	ARG
2	H	38	SER
2	H	49	THR
2	H	50	VAL
2	H	53	LYS
2	H	64	SER
2	I	12	THR
2	I	13	LYS
2	I	27	LYS
2	I	32	ASN
2	I	35	ASN
2	I	38	SER
2	I	42	SER
2	I	48	MET
2	I	50	VAL
2	I	52	ILE
2	I	53	LYS
2	I	64	SER
2	I	69	ARG
2	J	5	VAL
2	J	8	LYS
2	J	12	THR
2	J	13	LYS
2	J	15	ASN
2	J	29	LEU
2	J	32	ASN
2	J	33	ARG
2	J	41	LEU
2	J	52	ILE
2	J	64	SER
2	K	5	VAL
2	K	18	ASP
2	K	21	THR
2	K	22	VAL
2	K	27	LYS
2	K	29	LEU
2	K	33	ARG
2	K	38	SER
2	K	39	LEU
2	K	49	THR
2	K	53	LYS
2	K	54	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	65	ASN
1	A	202	ASN
1	A	216	GLN
1	A	241	ASN
1	A	272	HIS
1	L	18	ASN
1	L	74	ASN
1	L	87	ASN
1	L	202	ASN
1	L	272	HIS
2	B	35	ASN
2	B	59	ASN
2	C	58	HIS
2	D	55	ASN
2	E	15	ASN
2	E	58	HIS
2	F	15	ASN
2	G	35	ASN
2	G	44	GLN
2	G	59	ASN
2	H	44	GLN
2	I	32	ASN
2	I	35	ASN
2	I	55	ASN
2	I	59	ASN
2	J	15	ASN
2	J	32	ASN
2	J	59	ASN
2	K	55	ASN
2	K	59	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.