



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:15 AM UTC

PDB ID : 1AIF / pdb_00001aif
Title : ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB FROM MOUSE
Authors : Ban, N.; Escobar, C.; Hasel, K.; Day, J.; Greenwood, A.; McPherson, A.
Deposited on : 1994-11-14
Resolution : 2.90 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
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

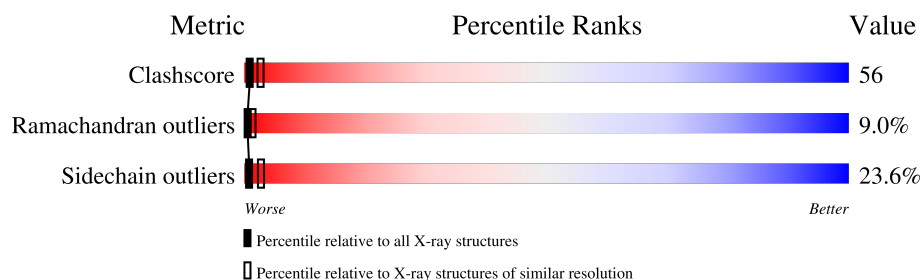
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

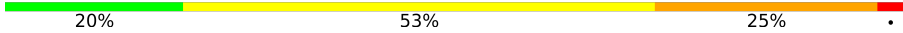
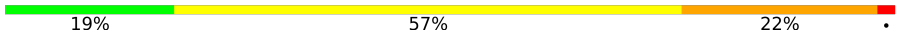
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	215	
1	L	215	
2	B	218	
2	H	218	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6662 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 ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1655	1029	273	345	8			
1	A	215	Total	C	N	O	S	0	0	0
			1655	1029	273	345	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	ASP	GLN	conflict	UNP P01837
L	3	GLN	VAL	conflict	UNP P01837
L	10	PHE	ILE	conflict	UNP P01837
L	12	ALA	SER	conflict	UNP P01837
L	18	LYS	ARG	conflict	UNP P01837
L	21	ILE	MET	conflict	UNP P01837
L	25	VAL	ALA	conflict	UNP P01837
L	26	SER	ASN	conflict	UNP P01837
L	28	SER	-	insertion	UNP P01837
L	29	ILE	-	insertion	UNP P01837
L	31	SER	VAL	conflict	UNP P01837
L	33	ASN	TYR	conflict	UNP P01837
L	34	LEU	MET	conflict	UNP P01837
L	42	GLU	GLY	conflict	UNP P01837
L	47	PRO	ARG	conflict	UNP P01837
L	51	GLY	ASP	conflict	UNP P01837
L	54	ASN	LYS	conflict	UNP P01837
L	61	VAL	ALA	conflict	UNP P01837
L	93	ASN	SER	conflict	UNP P01837
L	95	TYR	HIS	conflict	UNP P01837
L	114	PRO	GLN	conflict	UNP P01837
A	1	ASP	GLN	conflict	UNP P01837
A	3	GLN	VAL	conflict	UNP P01837
A	10	PHE	ILE	conflict	UNP P01837

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	SER	conflict	UNP P01837
A	18	LYS	ARG	conflict	UNP P01837
A	21	ILE	MET	conflict	UNP P01837
A	25	VAL	ALA	conflict	UNP P01837
A	26	SER	ASN	conflict	UNP P01837
A	28	SER	-	insertion	UNP P01837
A	29	ILE	-	insertion	UNP P01837
A	31	SER	VAL	conflict	UNP P01837
A	33	ASN	TYR	conflict	UNP P01837
A	34	LEU	MET	conflict	UNP P01837
A	42	GLU	GLY	conflict	UNP P01837
A	47	PRO	ARG	conflict	UNP P01837
A	51	GLY	ASP	conflict	UNP P01837
A	54	ASN	LYS	conflict	UNP P01837
A	61	VAL	ALA	conflict	UNP P01837
A	93	ASN	SER	conflict	UNP P01837
A	95	TYR	HIS	conflict	UNP P01837
A	114	PRO	GLN	conflict	UNP P01837

- Molecule 2 is a protein called ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1676	1066	277	325	8			
2	B	218	Total	C	N	O	S	0	0	0
			1676	1066	277	325	8			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	GLN	GLU	conflict	GB 1042226
H	20	LEU	VAL	conflict	GB 1042226
H	28	THR	ALA	conflict	GB 1042226
H	30	ASN	SER	conflict	GB 1042226
H	31	ASN	TYR	conflict	GB 1042226
H	35	SER	ASN	conflict	GB 1042226
H	43	LYS	ARG	conflict	GB 1042226
H	48	VAL	ILE	conflict	GB 1042226
H	53	LEU	PHE	conflict	GB 1042226
H	54	ASN	LYS	conflict	GB 1042226
H	56	ASP	-	insertion	GB 1042226

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Chain	Residue	Modelled	Actual	Comment	Reference
H	58	PHE	ASN	conflict	GB 1042226
H	59	ALA	TYR	conflict	GB 1042226
H	69	LYS	ARG	conflict	GB 1042226
H	71	ILE	THR	conflict	GB 1042226
H	80	ARG	SER	conflict	GB 1042226
H	81	LEU	VAL	conflict	GB 1042226
H	87	SER	ASN	conflict	GB 1042226
H	99	VAL	-	insertion	GB 1042226
H	100	LEU	THR	conflict	GB 1042226
H	102	PRO	GLU	conflict	GB 1042226
H	103	LEU	GLY	conflict	GB 1042226
H	104	PHE	ILE	conflict	GB 1042226
H	107	ALA	PRO	conflict	GB 1042226
H	108	VAL	PHE	conflict	GB 1042226
H	109	ASP	ALA	conflict	GB 1042226
H	116	SER	LEU	conflict	GB 1042226
H	121	SER	ALA	conflict	GB 1042226
H	?	-	SER	deletion	GB 1042226
H	196	ARG	-	insertion	GB 1042226
B	5	GLN	GLU	conflict	GB 1042226
B	20	LEU	VAL	conflict	GB 1042226
B	28	THR	ALA	conflict	GB 1042226
B	30	ASN	SER	conflict	GB 1042226
B	31	ASN	TYR	conflict	GB 1042226
B	35	SER	ASN	conflict	GB 1042226
B	43	LYS	ARG	conflict	GB 1042226
B	48	VAL	ILE	conflict	GB 1042226
B	53	LEU	PHE	conflict	GB 1042226
B	54	ASN	LYS	conflict	GB 1042226
B	56	ASP	-	insertion	GB 1042226
B	58	PHE	ASN	conflict	GB 1042226
B	59	ALA	TYR	conflict	GB 1042226
B	69	LYS	ARG	conflict	GB 1042226
B	71	ILE	THR	conflict	GB 1042226
B	80	ARG	SER	conflict	GB 1042226
B	81	LEU	VAL	conflict	GB 1042226
B	87	SER	ASN	conflict	GB 1042226
B	99	VAL	-	insertion	GB 1042226
B	100	LEU	THR	conflict	GB 1042226
B	102	PRO	GLU	conflict	GB 1042226
B	103	LEU	GLY	conflict	GB 1042226
B	104	PHE	ILE	conflict	GB 1042226

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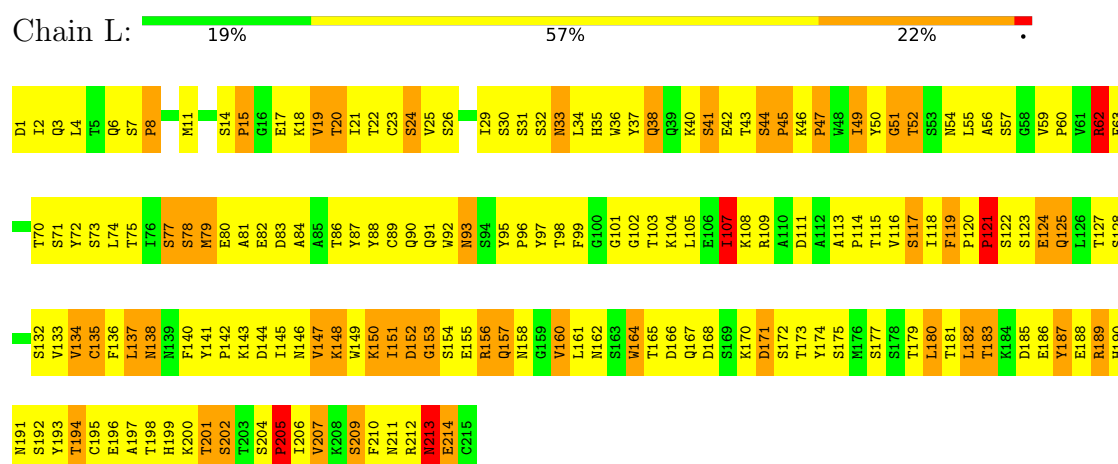
Chain	Residue	Modelled	Actual	Comment	Reference
B	107	ALA	PRO	conflict	GB 1042226
B	108	VAL	PHE	conflict	GB 1042226
B	109	ASP	ALA	conflict	GB 1042226
B	116	SER	LEU	conflict	GB 1042226
B	121	SER	ALA	conflict	GB 1042226
B	?	-	SER	deletion	GB 1042226
B	196	ARG	-	insertion	GB 1042226

3 Residue-property plots

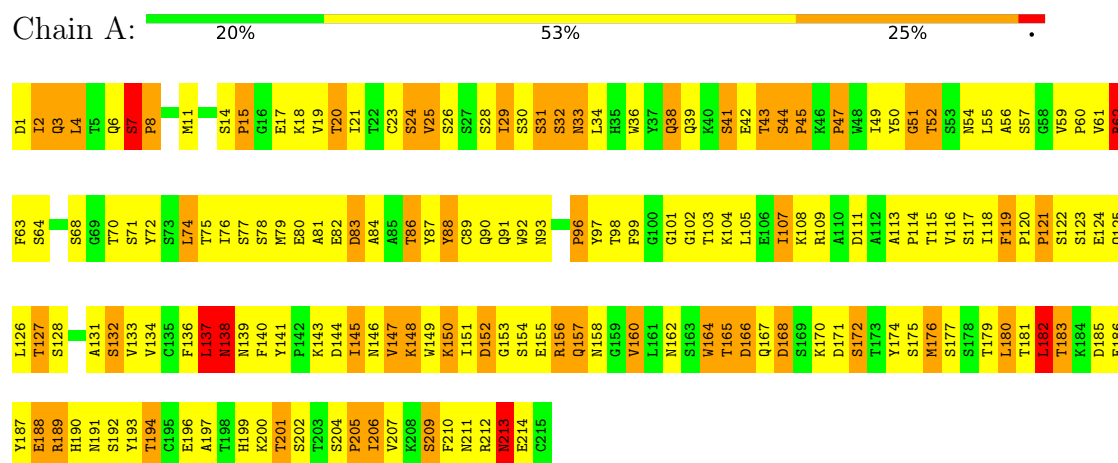
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

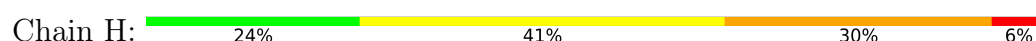
• Molecule 1: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (LIGHT CHAIN)

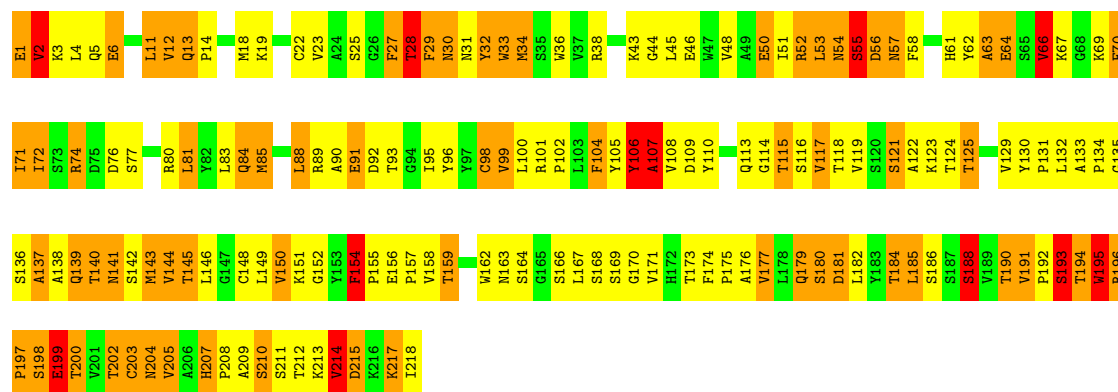


• Molecule 1: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (LIGHT CHAIN)



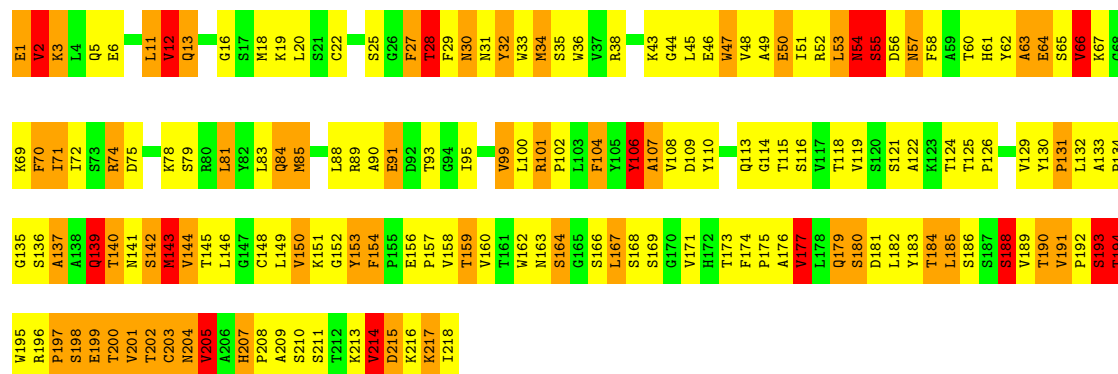
• Molecule 2: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (HEAVY CHAIN)





● Molecule 2: ANTI-IDIOTYPIC FAB 409.5.3 (IGG2A) FAB (HEAVY CHAIN)

Chain B: 23% 45% 24% 7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.20 Å 71.20 Å 75.80 Å 85.30° 121.40° 116.50°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.0 (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6662	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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	1.14	4/1696 (0.2%)	1.55	40/2306 (1.7%)
1	L	1.16	2/1696 (0.1%)	1.51	31/2306 (1.3%)
2	B	1.28	6/1721 (0.3%)	1.64	39/2347 (1.7%)
2	H	1.33	5/1721 (0.3%)	1.67	37/2347 (1.6%)
All	All	1.23	17/6834 (0.2%)	1.59	147/9306 (1.6%)

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
1	A	0	1
2	B	0	2
2	H	0	2
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	194	THR	CA-CB	12.70	1.69	1.53
2	B	194	THR	CA-CB	9.23	1.64	1.53
1	L	195	CYS	CA-C	7.09	1.59	1.53
2	B	217	LYS	CA-C	6.65	1.60	1.52
2	H	217	LYS	CA-C	6.58	1.60	1.52
1	A	52	THR	CA-CB	-5.82	1.44	1.53
2	H	29	PHE	CA-C	-5.79	1.45	1.53
2	B	3	LYS	CA-C	5.75	1.59	1.53
1	A	2	ILE	CA-C	5.74	1.59	1.52
1	A	201	THR	CA-CB	5.58	1.60	1.52
2	B	101	ARG	CA-C	-5.58	1.47	1.52
2	H	23	VAL	CA-CB	5.35	1.61	1.54
1	L	81	ALA	CA-CB	-5.35	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	143	MET	SD-CE	5.35	1.93	1.79
1	A	137	LEU	CA-C	-5.25	1.47	1.53
2	B	142	SER	CA-C	5.19	1.59	1.52
2	H	195	TRP	C-O	5.17	1.30	1.23

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	134	PRO	N-CA-C	15.29	133.89	113.40
2	B	134	PRO	N-CA-C	13.11	130.96	113.40
1	L	201	THR	N-CA-C	12.62	126.35	112.97
2	H	154	PHE	CA-C-N	-12.02	107.40	119.78
2	H	154	PHE	C-N-CA	-12.02	107.40	119.78
1	A	113	ALA	CA-C-N	11.97	131.70	120.21
1	A	113	ALA	C-N-CA	11.97	131.70	120.21
2	B	154	PHE	CA-C-N	-11.40	108.04	119.78
2	B	154	PHE	C-N-CA	-11.40	108.04	119.78
2	H	215	ASP	N-CA-C	10.46	122.49	108.38
2	B	28	THR	N-CA-C	-10.29	88.87	110.80
1	L	113	ALA	CA-C-N	10.22	130.02	120.21
1	L	113	ALA	C-N-CA	10.22	130.02	120.21
2	B	197	PRO	N-CA-C	-10.15	91.57	112.47
2	B	53	LEU	N-CA-C	9.79	125.43	113.38
2	B	207	HIS	CA-C-N	9.75	132.02	119.84
2	B	207	HIS	C-N-CA	9.75	132.02	119.84
2	H	207	HIS	CA-C-N	9.70	131.96	119.84
2	H	207	HIS	C-N-CA	9.70	131.96	119.84
2	B	215	ASP	N-CA-C	9.61	120.93	108.24
2	H	28	THR	N-CA-C	-9.46	90.64	110.80
1	A	128	SER	N-CA-C	-9.25	101.78	113.43
1	A	3	GLN	N-CA-C	9.02	123.10	108.41
2	B	104	PHE	N-CA-C	-8.97	99.38	110.41
2	H	154	PHE	N-CA-C	8.81	129.28	109.81
2	H	104	PHE	N-CA-C	-8.69	99.72	110.41
1	A	201	THR	N-CA-C	8.66	124.50	112.72
2	H	13	GLN	N-CA-C	-8.62	97.86	109.84
1	L	128	SER	N-CA-C	-8.62	102.69	113.55
1	A	201	THR	CB-CA-C	-8.57	100.68	111.22
1	A	138	ASN	N-CA-C	7.93	122.94	110.17
2	B	154	PHE	N-CA-C	7.87	127.20	109.81
2	B	195	TRP	N-CA-C	-7.81	98.59	110.30
2	H	197	PRO	N-CA-C	-7.71	91.88	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLY	N-CA-C	-7.63	98.33	112.37
1	A	125	GLN	N-CA-C	7.62	120.25	111.11
2	H	173	THR	N-CA-C	-7.60	100.29	110.55
1	L	3	GLN	N-CA-C	7.51	121.14	108.90
1	A	62	ARG	N-CA-C	-7.45	103.78	113.17
1	A	183	THR	N-CA-C	-7.34	98.95	109.96
1	L	132	SER	N-CA-C	7.30	120.31	108.34
1	A	44	SER	N-CA-C	7.21	119.76	110.39
1	L	213	ASN	N-CA-C	-7.14	105.18	114.04
2	H	210	SER	N-CA-C	7.14	127.56	113.29
1	L	183	THR	N-CA-C	-7.05	99.85	110.28
2	B	210	SER	N-CA-C	6.96	125.63	110.80
1	L	14	SER	CA-C-N	-6.95	112.32	119.83
1	L	14	SER	C-N-CA	-6.95	112.32	119.83
2	H	53	LEU	N-CA-C	6.94	121.06	112.59
1	L	6	GLN	N-CA-C	6.88	119.74	108.52
1	A	43	THR	N-CA-C	6.72	117.14	108.34
2	H	74	ARG	CA-C-N	-6.58	113.71	122.99
2	H	74	ARG	C-N-CA	-6.58	113.71	122.99
1	L	52	THR	N-CA-C	-6.58	105.16	113.72
1	L	51	GLY	N-CA-C	-6.54	100.85	112.22
2	B	2	VAL	CB-CA-C	-6.52	100.59	111.29
1	L	62	ARG	N-CA-C	-6.52	105.08	113.16
2	B	13	GLN	N-CA-C	-6.45	100.87	109.84
1	A	166	ASP	N-CA-C	-6.45	101.85	110.55
2	H	88	LEU	N-CA-C	6.43	118.60	110.24
2	B	44	GLY	N-CA-C	-6.36	100.20	112.02
2	B	88	LEU	N-CA-C	6.33	119.42	110.23
1	L	81	ALA	N-CA-C	6.32	120.82	113.18
1	A	180	LEU	N-CA-C	-6.29	99.44	109.76
1	A	134	VAL	N-CA-C	6.28	117.83	108.23
1	A	132	SER	N-CA-C	6.26	118.61	108.34
2	H	156	GLU	CA-C-N	-6.24	113.09	119.83
2	H	156	GLU	C-N-CA	-6.24	113.09	119.83
2	H	106	TYR	N-CA-C	6.24	119.67	109.06
2	H	144	VAL	N-CA-C	6.19	118.84	108.81
1	A	7	SER	N-CA-C	-6.19	100.63	109.24
1	A	187	TYR	N-CA-C	6.19	117.90	111.03
2	H	63	ALA	N-CA-C	6.18	118.17	108.96
2	B	173	THR	N-CA-C	-6.17	100.52	110.32
1	A	64	SER	N-CA-C	6.16	119.57	108.48
1	L	108	LYS	N-CA-C	6.13	119.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	GLU	N-CA-C	6.12	121.84	113.16
1	L	138	ASN	N-CA-C	6.11	119.78	109.76
2	B	74	ARG	CA-C-N	-6.08	114.42	122.99
2	B	74	ARG	C-N-CA	-6.08	114.42	122.99
2	H	56	ASP	N-CA-C	-6.07	100.85	109.96
2	B	156	GLU	CA-C-N	-6.05	113.29	119.83
2	B	156	GLU	C-N-CA	-6.05	113.29	119.83
2	H	107	ALA	N-CA-C	-6.05	97.92	110.80
1	L	125	GLN	N-CA-C	6.00	118.31	111.11
2	H	205	VAL	N-CA-C	5.99	117.38	108.46
1	A	71	SER	N-CA-C	5.94	118.50	107.99
2	B	106	TYR	N-CA-C	5.92	118.88	108.75
2	B	63	ALA	N-CA-C	5.89	117.20	108.60
2	B	142	SER	N-CA-C	5.88	118.34	108.23
2	H	105	TYR	N-CA-C	-5.79	104.66	110.97
1	A	168	ASP	N-CA-C	-5.79	103.02	110.19
1	A	188	GLU	N-CA-C	-5.78	104.98	111.28
1	A	204	SER	CA-C-N	5.75	127.03	119.84
1	A	204	SER	C-N-CA	5.75	127.03	119.84
1	L	207	VAL	N-CA-C	5.72	121.23	109.34
1	A	145	ILE	N-CA-C	5.70	117.88	108.99
2	H	199	GLU	CA-C-N	-5.70	111.20	120.71
2	H	199	GLU	C-N-CA	-5.70	111.20	120.71
2	B	122	ALA	N-CA-C	5.67	117.36	109.31
1	L	201	THR	CB-CA-C	-5.64	102.54	111.17
1	A	83	ASP	N-CA-C	-5.63	106.07	113.17
1	A	108	LYS	N-CA-C	5.62	118.39	109.96
2	B	12	VAL	CB-CA-C	-5.61	100.66	110.71
1	A	6	GLN	N-CA-C	5.58	117.61	108.52
2	B	177	VAL	CB-CA-C	-5.57	103.54	111.34
1	L	24	SER	N-CA-C	5.56	117.44	108.32
2	H	139	GLN	N-CA-C	5.55	120.55	113.55
1	L	44	SER	N-CA-C	5.54	117.59	110.39
2	H	156	GLU	N-CA-C	5.53	122.02	109.81
1	A	24	SER	N-CA-C	5.51	118.40	108.48
2	H	188	SER	N-CA-C	5.51	116.78	108.46
2	B	201	VAL	N-CA-C	5.51	120.79	109.34
2	B	144	VAL	N-CA-C	5.50	117.71	108.81
1	A	74	LEU	N-CA-C	-5.46	99.77	109.06
1	L	107	ILE	N-CA-C	5.45	115.71	107.80
1	L	71	SER	N-CA-C	5.45	117.63	107.99
1	L	134	VAL	N-CA-C	5.40	116.49	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	101	GLY	N-CA-C	-5.31	107.74	114.16
1	A	147	VAL	N-CA-C	5.30	116.00	108.42
2	B	205	VAL	N-CA-C	5.30	116.29	108.45
1	L	180	LEU	N-CA-C	-5.26	100.73	109.46
2	B	47	TRP	N-CA-C	-5.26	101.86	109.59
2	B	107	ALA	N-CA-C	-5.25	99.61	110.80
1	A	4	LEU	N-CA-C	-5.22	101.64	109.95
2	B	52	ARG	N-CA-C	5.20	117.08	108.13
2	B	188	SER	N-CA-C	5.19	116.29	108.46
1	L	49	ILE	N-CA-C	5.18	115.36	108.11
2	H	44	GLY	N-CA-C	-5.15	101.04	112.17
2	B	54	ASN	N-CA-C	5.15	121.76	110.80
1	A	101	GLY	N-CA-C	-5.13	107.96	114.16
1	A	81	ALA	N-CA-C	5.12	119.24	112.89
1	A	164	TRP	N-CA-C	5.12	117.32	109.95
2	H	12	VAL	CB-CA-C	-5.10	101.89	110.71
2	H	117	VAL	N-CA-C	-5.09	100.78	108.12
1	A	213	ASN	N-CA-C	-5.09	107.02	113.43
1	L	19	VAL	N-CA-C	5.08	116.84	108.97
2	H	52	ARG	N-CA-C	5.08	116.86	108.13
1	L	135	CYS	N-CA-C	5.08	116.97	107.99
2	H	211	SER	N-CA-C	5.08	117.58	109.81
2	B	153	TYR	N-CA-C	-5.06	101.60	109.14
1	A	182	LEU	CA-C-N	5.04	128.01	120.95
1	A	182	LEU	C-N-CA	5.04	128.01	120.95
2	H	33	TRP	N-CA-C	-5.03	101.09	108.79
2	B	139	GLN	N-CA-C	5.02	119.36	112.68
1	A	86	THR	N-CA-C	-5.02	100.23	108.41
1	L	187	TYR	N-CA-C	5.01	116.59	111.03

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	TYR	Sidechain
2	B	28	THR	Mainchain
2	B	32	TYR	Sidechain
2	H	196	ARG	Mainchain
2	H	32	TYR	Sidechain

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	1655	0	1562	178	0
1	L	1655	0	1562	194	0
2	B	1676	0	1637	200	0
2	H	1676	0	1637	200	0
All	All	6662	0	6398	728	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 56.

All (728) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:VAL:HG13	2:H:66:VAL:HG11	1.34	1.08
2:B:48:VAL:HG13	2:B:66:VAL:HG11	1.34	1.05
2:B:53:LEU:HG	2:B:53:LEU:O	1.58	1.00
1:L:15:PRO:HG3	1:L:107:ILE:HD11	1.41	0.98
2:B:142:SER:HB2	2:B:193:SER:HB3	1.47	0.94
1:L:180:LEU:HG	1:L:182:LEU:HD21	1.45	0.94
1:L:145:ILE:HD11	1:L:199:HIS:HD2	1.32	0.93
1:A:15:PRO:HG3	1:A:107:ILE:HD11	1.47	0.93
1:A:38:GLN:HG3	1:A:87:TYR:CE2	2.05	0.91
1:L:4:LEU:HD23	1:L:23:CYS:SG	2.10	0.91
2:H:51:ILE:HB	2:H:72:ILE:HG12	1.55	0.89
2:H:152:GLY:HA2	2:H:182:LEU:HG	1.55	0.88
1:A:144:ASP:C	1:A:145:ILE:HD12	1.99	0.88
2:H:142:SER:HB2	2:H:193:SER:HB3	1.56	0.86
2:H:101:ARG:HD2	2:H:102:PRO:HD2	1.56	0.86
1:L:92:TRP:HA	1:L:97:TYR:CD1	2.11	0.86
1:L:50:TYR:O	1:L:54:ASN:HB2	1.75	0.86
2:H:4:LEU:HD23	2:H:98:CYS:SG	2.16	0.85
2:B:33:TRP:CE2	2:B:101:ARG:HB3	2.11	0.85
1:L:49:ILE:HG23	1:L:54:ASN:O	1.77	0.85
1:L:38:GLN:HG3	1:L:87:TYR:CE2	2.12	0.85
2:H:53:LEU:O	2:H:53:LEU:HG	1.74	0.85
1:A:31:SER:HA	1:A:72:TYR:HE2	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:O	1:A:54:ASN:HB2	1.77	0.84
1:L:144:ASP:C	1:L:145:ILE:HD12	2.02	0.84
2:B:33:TRP:CZ2	2:B:101:ARG:HB3	2.13	0.83
2:B:50:GLU:HG2	2:B:51:ILE:O	1.78	0.82
1:L:164:TRP:O	2:H:175:PRO:HD2	1.80	0.82
1:A:49:ILE:HG23	1:A:54:ASN:O	1.81	0.81
2:B:191:VAL:HB	2:B:192:PRO:HD2	1.62	0.81
1:A:213:ASN:HB2	2:B:136:SER:HB3	1.63	0.81
1:L:145:ILE:HD11	1:L:199:HIS:CD2	2.16	0.80
1:L:31:SER:HA	1:L:72:TYR:HE2	1.46	0.80
1:A:164:TRP:O	2:B:175:PRO:HD2	1.82	0.80
2:H:36:TRP:CD1	2:H:83:LEU:HD13	2.17	0.79
1:A:151:ILE:HG22	1:A:193:TYR:HA	1.64	0.79
1:L:168:ASP:HB3	1:L:172:SER:H	1.47	0.79
2:H:93:THR:HG23	2:H:118:THR:HA	1.65	0.79
2:H:74:ARG:HB2	2:H:81:LEU:HA	1.65	0.79
1:L:157:GLN:HE22	1:L:158:ASN:HD21	1.29	0.78
1:L:114:PRO:HB3	1:L:140:PHE:HB3	1.64	0.78
1:A:50:TYR:CD1	2:B:108:VAL:HB	2.18	0.78
1:L:213:ASN:HB2	2:H:136:SER:HB3	1.65	0.78
1:A:11:MET:HB3	1:A:105:LEU:HD12	1.66	0.78
2:B:53:LEU:O	2:B:55:SER:N	2.17	0.78
1:A:4:LEU:HD23	1:A:23:CYS:SG	2.24	0.78
1:L:74:LEU:HD23	1:L:75:THR:N	1.98	0.77
1:A:157:GLN:HE22	1:A:158:ASN:HD21	1.30	0.77
1:L:213:ASN:HD22	2:H:136:SER:HB3	1.48	0.77
1:L:4:LEU:HD11	1:L:91:GLN:HB2	1.67	0.76
2:H:33:TRP:CE2	2:H:101:ARG:HB3	2.20	0.76
2:H:54:ASN:O	2:H:55:SER:HB2	1.84	0.76
2:H:1:GLU:O	2:H:2:VAL:HG13	1.86	0.76
1:A:120:PRO:HB3	1:A:210:PHE:CE2	2.21	0.76
2:B:148:CYS:O	2:B:186:SER:HB2	1.86	0.76
1:L:147:VAL:HG22	1:L:197:ALA:HA	1.67	0.76
2:H:204:ASN:H	2:H:204:ASN:ND2	1.82	0.76
1:L:180:LEU:HG	1:L:182:LEU:CD2	2.15	0.76
1:A:31:SER:HA	1:A:72:TYR:CE2	2.21	0.75
2:B:33:TRP:HE1	2:B:101:ARG:HG3	1.51	0.75
1:A:114:PRO:HB3	1:A:140:PHE:HB3	1.68	0.75
2:H:34:MET:SD	2:H:74:ARG:NH1	2.59	0.75
2:B:102:PRO:HB2	2:B:104:PHE:CE1	2.20	0.75
1:L:213:ASN:HB2	2:H:136:SER:CB	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ASN:ND2	2:B:204:ASN:H	1.82	0.75
2:B:133:ALA:CB	2:B:218:ILE:HG22	2.17	0.74
1:L:50:TYR:CD1	2:H:108:VAL:HB	2.23	0.74
1:A:90:GLN:NE2	1:A:99:PHE:CZ	2.55	0.74
1:A:180:LEU:HG	1:A:182:LEU:HD21	1.68	0.73
2:B:32:TYR:CE2	2:B:53:LEU:HD22	2.24	0.73
1:A:181:THR:C	1:A:182:LEU:HD23	2.14	0.73
2:B:143:MET:N	2:B:193:SER:HA	2.04	0.73
2:B:33:TRP:HE1	2:B:101:ARG:CG	2.00	0.73
1:L:213:ASN:ND2	2:H:136:SER:HB3	2.04	0.72
2:H:50:GLU:HG2	2:H:51:ILE:O	1.89	0.72
1:L:116:VAL:HG22	1:L:137:LEU:HD23	1.71	0.72
2:B:137:ALA:HB1	2:B:139:GLN:CD	2.13	0.72
1:L:120:PRO:HB3	1:L:210:PHE:CE2	2.24	0.72
2:B:160:VAL:HG22	2:B:205:VAL:HG22	1.71	0.72
2:H:27:PHE:CD1	2:H:27:PHE:C	2.68	0.72
1:A:25:VAL:HG12	1:A:26:SER:H	1.55	0.72
1:L:145:ILE:CD1	1:L:199:HIS:HD2	2.00	0.72
1:L:146:ASN:OD1	1:L:198:THR:HG23	1.90	0.72
1:A:182:LEU:HD13	1:A:186:GLU:HG2	1.72	0.72
2:H:19:LYS:NZ	2:H:84:GLN:HG3	2.05	0.71
1:A:4:LEU:HD23	1:A:89:CYS:SG	2.30	0.71
2:B:51:ILE:N	2:B:72:ILE:HD13	2.05	0.71
1:L:177:SER:HB3	2:H:174:PHE:CE2	2.24	0.71
2:H:33:TRP:CZ2	2:H:101:ARG:HB3	2.26	0.71
1:L:199:HIS:O	1:L:201:THR:N	2.25	0.70
2:B:6:GLU:HB3	2:B:22:CYS:HB3	1.73	0.70
2:B:101:ARG:HD2	2:B:102:PRO:HD2	1.72	0.70
2:H:202:THR:HG22	2:H:215:ASP:O	1.91	0.70
1:A:74:LEU:HD23	1:A:75:THR:N	2.07	0.70
1:L:181:THR:C	1:L:182:LEU:HD23	2.17	0.70
1:L:161:LEU:HD11	2:H:179:GLN:NE2	2.06	0.70
1:L:212:ARG:HG2	1:L:214:GLU:OE2	1.91	0.70
2:H:101:ARG:NH1	2:H:108:VAL:HA	2.07	0.70
2:B:72:ILE:HA	2:B:83:LEU:HD12	1.73	0.69
2:B:31:ASN:OD1	2:B:54:ASN:O	2.10	0.69
1:L:180:LEU:CG	1:L:182:LEU:HD21	2.22	0.69
2:H:137:ALA:HB1	2:H:139:GLN:CD	2.18	0.69
1:A:2:ILE:CD1	1:A:96:PRO:HD2	2.22	0.69
1:A:20:THR:HB	1:A:75:THR:OG1	1.93	0.69
1:A:147:VAL:HG22	1:A:197:ALA:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ALA:HB1	2:B:139:GLN:NE2	2.08	0.69
1:L:36:TRP:HB2	1:L:49:ILE:HB	1.73	0.69
2:H:38:ARG:HG2	2:H:48:VAL:CG2	2.23	0.69
1:A:127:THR:HG23	1:A:127:THR:O	1.92	0.68
1:L:4:LEU:HD23	1:L:89:CYS:SG	2.34	0.68
1:L:157:GLN:NE2	1:L:158:ASN:HD21	1.92	0.68
2:H:102:PRO:HB2	2:H:104:PHE:CE1	2.29	0.68
1:A:157:GLN:NE2	1:A:158:ASN:HD21	1.92	0.68
1:L:8:PRO:O	1:L:103:THR:HG23	1.94	0.68
1:A:133:VAL:HG23	1:A:133:VAL:O	1.94	0.67
2:B:69:LYS:C	2:B:70:PHE:HD1	2.03	0.67
2:H:88:LEU:HD22	2:H:92:ASP:HB2	1.77	0.67
2:H:11:LEU:HB2	2:H:118:THR:HB	1.77	0.67
2:B:101:ARG:NH1	2:B:108:VAL:HA	2.10	0.67
2:H:74:ARG:HD2	2:H:81:LEU:HB2	1.75	0.66
2:H:69:LYS:C	2:H:70:PHE:HD1	2.03	0.66
1:A:2:ILE:HD11	1:A:96:PRO:HD2	1.77	0.66
1:A:168:ASP:HB3	1:A:172:SER:H	1.60	0.66
1:A:156:ARG:HG3	1:A:156:ARG:O	1.94	0.66
2:B:152:GLY:HA2	2:B:182:LEU:HG	1.77	0.66
2:H:101:ARG:HB2	2:H:109:ASP:HB3	1.78	0.66
1:A:145:ILE:HD11	1:A:199:HIS:HD2	1.60	0.66
2:H:33:TRP:O	2:H:34:MET:HG2	1.96	0.66
2:B:1:GLU:O	2:B:2:VAL:HG13	1.96	0.66
1:A:36:TRP:HB2	1:A:49:ILE:HB	1.77	0.65
1:A:15:PRO:CG	1:A:107:ILE:HD11	2.24	0.65
2:B:11:LEU:HB2	2:B:118:THR:HB	1.78	0.65
2:B:57:ASN:CG	2:B:58:PHE:H	2.04	0.65
2:B:152:GLY:HA2	2:B:182:LEU:CG	2.26	0.65
1:A:29:ILE:HD12	1:A:30:SER:N	2.11	0.65
1:L:213:ASN:HB2	2:H:136:SER:OG	1.97	0.65
2:B:196:ARG:HB3	2:B:197:PRO:HD2	1.77	0.65
1:A:19:VAL:O	1:A:75:THR:HA	1.97	0.64
1:L:151:ILE:HG22	1:L:193:TYR:HA	1.79	0.64
2:H:101:ARG:HB2	2:H:109:ASP:CB	2.27	0.64
2:B:51:ILE:H	2:B:72:ILE:HD13	1.61	0.64
1:A:177:SER:HB3	2:B:174:PHE:CE2	2.33	0.64
1:L:189:ARG:NH1	1:A:1:ASP:H1	1.96	0.64
2:B:191:VAL:HB	2:B:192:PRO:CD	2.26	0.64
1:A:52:THR:HG23	1:A:72:TYR:HD2	1.63	0.64
2:H:53:LEU:O	2:H:55:SER:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:TRP:CZ3	2:B:203:CYS:HB2	2.33	0.64
1:L:21:ILE:CG2	1:L:103:THR:HG21	2.28	0.64
2:B:33:TRP:NE1	2:B:101:ARG:CG	2.61	0.63
2:B:34:MET:SD	2:B:74:ARG:NH1	2.71	0.63
2:B:102:PRO:HB2	2:B:104:PHE:CD1	2.32	0.63
1:L:50:TYR:HE1	1:L:56:ALA:HA	1.63	0.63
2:H:72:ILE:HA	2:H:83:LEU:HD12	1.81	0.63
1:A:191:ASN:OD1	1:A:211:ASN:HA	1.98	0.63
2:B:5:GLN:O	2:B:22:CYS:HA	1.98	0.63
2:H:31:ASN:OD1	2:H:54:ASN:O	2.17	0.63
1:A:199:HIS:O	1:A:201:THR:N	2.32	0.63
2:B:197:PRO:C	2:B:199:GLU:N	2.55	0.63
1:L:31:SER:HA	1:L:72:TYR:CE2	2.29	0.63
2:H:203:CYS:SG	2:H:203:CYS:O	2.56	0.63
2:B:93:THR:HG23	2:B:118:THR:HA	1.80	0.62
2:B:163:ASN:N	2:B:204:ASN:HD21	1.96	0.62
1:A:25:VAL:HG12	1:A:26:SER:N	2.15	0.62
2:H:137:ALA:HB1	2:H:139:GLN:NE2	2.14	0.62
1:A:157:GLN:NE2	1:A:158:ASN:ND2	2.46	0.62
2:B:166:SER:OG	2:B:167:LEU:HD23	1.99	0.62
2:H:163:ASN:N	2:H:204:ASN:HD21	1.97	0.62
1:A:4:LEU:HD11	1:A:91:GLN:HB2	1.82	0.62
1:A:88:TYR:CD1	1:A:102:GLY:HA3	2.34	0.62
2:B:129:VAL:O	2:B:130:TYR:CD1	2.53	0.62
1:L:191:ASN:OD1	1:L:211:ASN:HA	1.99	0.62
2:H:143:MET:N	2:H:193:SER:HA	2.14	0.61
2:H:179:GLN:O	2:H:180:SER:HB3	2.00	0.61
1:A:145:ILE:HD12	1:A:145:ILE:N	2.14	0.61
1:A:119:PHE:CD1	1:A:119:PHE:N	2.68	0.61
2:H:99:VAL:HG23	2:H:110:TYR:O	2.01	0.61
2:H:191:VAL:HB	2:H:192:PRO:HD2	1.83	0.61
2:B:145:THR:O	2:B:146:LEU:HD23	2.00	0.61
1:A:33:ASN:HD22	1:A:92:TRP:C	2.09	0.61
1:L:146:ASN:O	1:L:147:VAL:HG23	2.00	0.61
2:B:150:VAL:O	2:B:184:THR:HA	2.01	0.61
1:L:21:ILE:HG13	1:L:21:ILE:O	2.00	0.61
1:L:45:PRO:HG2	2:H:45:LEU:HD21	1.82	0.61
2:B:19:LYS:NZ	2:B:84:GLN:HG3	2.16	0.61
1:L:157:GLN:NE2	1:L:158:ASN:ND2	2.49	0.60
2:B:101:ARG:HB2	2:B:109:ASP:CB	2.30	0.60
2:H:67:LYS:C	2:H:69:LYS:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:TRP:O	2:B:34:MET:HG2	2.00	0.60
2:H:19:LYS:HZ2	2:H:84:GLN:HG3	1.65	0.60
1:A:119:PHE:HD2	2:B:133:ALA:O	1.84	0.60
2:B:197:PRO:HB2	2:B:199:GLU:OE1	2.02	0.60
1:A:150:LYS:HA	1:A:155:GLU:HA	1.82	0.60
1:A:194:THR:HA	1:A:209:SER:HB3	1.83	0.60
2:H:179:GLN:O	2:H:179:GLN:HG2	2.00	0.60
1:L:62:ARG:NH1	1:L:80:GLU:HB2	2.16	0.60
2:H:27:PHE:HE2	2:H:32:TYR:CD2	2.19	0.60
2:B:75:ASP:HB2	2:B:78:LYS:HD2	1.84	0.60
1:L:20:THR:HA	1:L:74:LEU:O	2.02	0.60
1:L:41:SER:O	1:L:42:GLU:HB2	2.01	0.60
2:H:197:PRO:C	2:H:199:GLU:N	2.60	0.60
1:L:156:ARG:O	1:L:156:ARG:HG3	1.99	0.60
1:L:2:ILE:HD11	1:L:96:PRO:HD2	1.84	0.59
2:B:176:ALA:HB2	2:B:185:LEU:HD12	1.84	0.59
2:B:74:ARG:HB2	2:B:81:LEU:HA	1.85	0.59
1:A:213:ASN:HD22	2:B:136:SER:HB3	1.68	0.59
2:B:197:PRO:C	2:B:199:GLU:H	2.10	0.59
1:A:109:ARG:HD3	1:A:172:SER:O	2.02	0.59
2:H:27:PHE:CZ	2:H:74:ARG:NH2	2.71	0.59
2:H:29:PHE:O	2:H:30:ASN:C	2.45	0.59
2:B:51:ILE:HB	2:B:72:ILE:HG12	1.83	0.59
1:L:33:ASN:ND2	1:L:92:TRP:O	2.35	0.59
1:L:197:ALA:O	1:L:206:ILE:HD12	2.01	0.59
2:H:71:ILE:HD12	2:H:72:ILE:O	2.02	0.59
2:H:162:TRP:CD1	2:H:171:VAL:HG23	2.38	0.59
1:L:181:THR:HG23	1:L:181:THR:O	2.01	0.59
1:A:15:PRO:HG3	1:A:107:ILE:CD1	2.27	0.59
2:H:3:LYS:HB2	2:H:25:SER:HB3	1.83	0.59
1:A:33:ASN:ND2	1:A:92:TRP:O	2.35	0.59
2:B:179:GLN:O	2:B:180:SER:HB3	2.02	0.59
1:L:125:GLN:HG3	2:H:130:TYR:CZ	2.37	0.58
1:A:132:SER:HB2	1:A:180:LEU:O	2.03	0.58
1:A:213:ASN:HB2	2:B:136:SER:CB	2.33	0.58
2:B:19:LYS:HG3	2:B:84:GLN:CG	2.34	0.58
1:L:19:VAL:O	1:L:75:THR:HA	2.03	0.58
1:L:20:THR:HB	1:L:75:THR:OG1	2.03	0.58
1:L:150:LYS:HA	1:L:155:GLU:HA	1.85	0.58
1:A:119:PHE:H	1:A:119:PHE:HD1	1.51	0.58
2:H:101:ARG:HD2	2:H:102:PRO:CD	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:152:GLY:HA2	2:H:182:LEU:CG	2.32	0.57
1:L:90:GLN:NE2	1:L:99:PHE:CZ	2.72	0.57
2:B:143:MET:CA	2:B:193:SER:HA	2.33	0.57
1:L:133:VAL:HG11	1:L:193:TYR:HD2	1.69	0.57
1:A:189:ARG:HE	1:A:190:HIS:CE1	2.23	0.57
2:B:33:TRP:NE1	2:B:101:ARG:HG3	2.19	0.57
1:L:33:ASN:HD22	1:L:92:TRP:C	2.12	0.57
1:L:165:THR:O	1:L:174:TYR:HD1	1.88	0.57
2:B:33:TRP:CD1	2:B:101:ARG:O	2.58	0.57
2:B:114:GLY:O	2:B:115:THR:HG23	2.04	0.57
1:L:52:THR:HG23	1:L:72:TYR:HD2	1.70	0.57
2:H:32:TYR:CE2	2:H:53:LEU:HD22	2.39	0.57
2:H:34:MET:CE	2:H:74:ARG:HH11	2.18	0.57
1:L:136:PHE:CE2	2:H:188:SER:HB2	2.40	0.57
1:L:21:ILE:HG22	1:L:103:THR:HG21	1.86	0.57
1:L:55:LEU:HD22	1:L:59:VAL:HG11	1.87	0.57
2:B:3:LYS:HB2	2:B:25:SER:HB3	1.87	0.57
1:A:182:LEU:HD13	1:A:186:GLU:CG	2.35	0.56
1:L:24:SER:HA	1:L:70:THR:O	2.05	0.56
1:L:119:PHE:CD1	1:L:119:PHE:N	2.73	0.56
1:A:55:LEU:HD22	1:A:59:VAL:HG11	1.87	0.56
1:A:160:VAL:HG12	1:A:162:ASN:ND2	2.21	0.56
2:B:69:LYS:HB2	2:B:70:PHE:CD1	2.41	0.56
2:B:102:PRO:HB2	2:B:104:PHE:HE1	1.70	0.56
1:A:24:SER:HA	1:A:70:THR:O	2.04	0.56
2:B:145:THR:C	2:B:146:LEU:HD23	2.31	0.56
2:B:162:TRP:CD1	2:B:171:VAL:HG23	2.40	0.56
1:A:165:THR:O	1:A:174:TYR:HD1	1.87	0.56
2:H:57:ASN:CG	2:H:58:PHE:H	2.13	0.56
1:A:92:TRP:HA	1:A:97:TYR:CD1	2.40	0.56
2:B:176:ALA:HB2	2:B:185:LEU:CD1	2.36	0.56
1:L:111:ASP:HA	1:L:141:TYR:HD1	1.71	0.56
1:L:151:ILE:HD11	1:L:156:ARG:HG2	1.87	0.56
1:L:88:TYR:CD2	1:L:102:GLY:HA3	2.41	0.55
1:L:160:VAL:HG12	1:L:162:ASN:ND2	2.21	0.55
2:B:29:PHE:O	2:B:31:ASN:N	2.39	0.55
1:L:74:LEU:HD23	1:L:74:LEU:C	2.31	0.55
1:L:92:TRP:HA	1:L:97:TYR:CE1	2.42	0.55
2:H:101:ARG:HH22	2:H:106:TYR:HD1	1.54	0.55
1:L:2:ILE:CD1	1:L:96:PRO:HD2	2.36	0.55
1:L:133:VAL:HG23	1:L:133:VAL:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:168:ASP:HB3	1:L:172:SER:N	2.16	0.55
2:H:129:VAL:HG12	2:H:130:TYR:N	2.21	0.55
1:A:206:ILE:N	1:A:206:ILE:HD12	2.22	0.55
2:B:33:TRP:CZ2	2:B:101:ARG:CB	2.88	0.55
1:A:50:TYR:HE1	1:A:56:ALA:HA	1.71	0.55
1:A:160:VAL:HA	1:A:179:THR:O	2.06	0.55
1:L:189:ARG:HH22	1:A:1:ASP:HB2	1.72	0.55
2:H:218:ILE:OXT	2:H:218:ILE:HG12	2.07	0.55
1:A:126:LEU:HD23	1:A:131:ALA:HB2	1.89	0.55
1:A:157:GLN:HE22	1:A:158:ASN:ND2	2.00	0.55
2:B:12:VAL:HG11	2:B:16:GLY:HA3	1.88	0.55
1:A:62:ARG:NH1	1:A:83:ASP:OD2	2.39	0.55
1:L:213:ASN:CB	2:H:136:SER:HB3	2.37	0.55
2:B:19:LYS:HG3	2:B:84:GLN:HG2	1.88	0.55
2:B:63:ALA:O	2:B:64:GLU:C	2.50	0.55
2:H:69:LYS:C	2:H:70:PHE:CD1	2.85	0.54
2:B:101:ARG:HD2	2:B:102:PRO:CD	2.36	0.54
2:H:166:SER:O	2:H:167:LEU:HD22	2.08	0.54
1:A:211:ASN:O	1:A:212:ARG:HG3	2.08	0.54
1:L:157:GLN:HE22	1:L:158:ASN:ND2	1.99	0.54
1:L:185:ASP:O	1:L:189:ARG:HB2	2.08	0.54
2:B:100:LEU:C	2:B:100:LEU:HD12	2.32	0.54
2:B:198:SER:O	2:B:200:THR:N	2.41	0.54
2:B:27:PHE:CD1	2:B:27:PHE:C	2.84	0.54
2:B:29:PHE:O	2:B:30:ASN:C	2.50	0.54
1:L:165:THR:HG22	1:L:175:SER:H	1.72	0.54
2:H:53:LEU:O	2:H:54:ASN:C	2.50	0.54
2:B:143:MET:HA	2:B:193:SER:HA	1.88	0.54
1:L:25:VAL:HG12	1:L:26:SER:H	1.73	0.54
2:H:6:GLU:HB3	2:H:22:CYS:HB3	1.88	0.54
2:B:12:VAL:HG22	2:B:18:MET:HE3	1.89	0.54
2:B:99:VAL:HG23	2:B:110:TYR:O	2.07	0.54
1:L:145:ILE:CG1	1:L:199:HIS:HD2	2.21	0.54
2:H:32:TYR:HA	2:H:102:PRO:HA	1.90	0.53
2:H:163:ASN:O	2:H:164:SER:C	2.51	0.53
1:A:213:ASN:CG	2:B:135:GLY:O	2.51	0.53
1:L:133:VAL:HG11	1:L:193:TYR:CD2	2.44	0.53
1:A:199:HIS:CE1	1:A:201:THR:HG23	2.43	0.53
2:B:53:LEU:O	2:B:53:LEU:CG	2.41	0.53
2:B:196:ARG:C	2:B:198:SER:N	2.65	0.53
2:H:133:ALA:CB	2:H:218:ILE:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ARG:HH22	2:B:106:TYR:HD1	1.55	0.53
2:B:129:VAL:HG21	2:B:213:LYS:HB3	1.90	0.53
1:L:213:ASN:CG	2:H:135:GLY:O	2.50	0.53
2:H:197:PRO:C	2:H:199:GLU:H	2.16	0.53
1:A:157:GLN:H	1:A:157:GLN:HE21	1.57	0.53
2:B:153:TYR:CE1	2:B:183:TYR:HB2	2.44	0.53
1:L:82:GLU:OE1	1:L:82:GLU:N	2.42	0.53
2:H:27:PHE:CD1	2:H:27:PHE:O	2.63	0.53
2:H:29:PHE:O	2:H:31:ASN:N	2.42	0.53
2:H:27:PHE:O	2:H:27:PHE:HD1	1.90	0.52
2:B:197:PRO:O	2:B:199:GLU:N	2.41	0.52
2:H:33:TRP:C	2:H:34:MET:HG2	2.34	0.52
1:A:121:PRO:HD3	1:A:133:VAL:HG12	1.91	0.52
2:B:129:VAL:HG12	2:B:130:TYR:N	2.24	0.52
1:A:34:LEU:O	1:A:51:GLY:O	2.27	0.52
2:B:101:ARG:NH1	2:B:107:ALA:O	2.43	0.52
2:H:32:TYR:CD1	2:H:33:TRP:N	2.78	0.52
2:H:124:THR:HG22	2:H:125:THR:N	2.23	0.52
2:B:101:ARG:HB2	2:B:109:ASP:HB3	1.90	0.52
2:B:131:PRO:HA	2:B:217:LYS:HZ2	1.74	0.52
2:H:43:LYS:HE2	2:H:46:GLU:CB	2.40	0.52
2:H:177:VAL:HG23	2:H:184:THR:O	2.09	0.52
1:A:41:SER:O	1:A:42:GLU:CB	2.58	0.52
2:B:35:SER:HB2	2:B:49:ALA:O	2.09	0.52
1:L:141:TYR:HB2	1:L:173:THR:HG22	1.90	0.52
1:A:17:GLU:HG2	1:A:18:LYS:H	1.74	0.52
1:L:95:TYR:CE2	2:H:61:HIS:HB2	2.45	0.52
2:H:145:THR:C	2:H:146:LEU:HD23	2.35	0.52
1:A:133:VAL:O	1:A:149:TRP:CH2	2.63	0.51
1:A:21:ILE:O	1:A:21:ILE:HG13	2.08	0.51
1:L:133:VAL:O	1:L:149:TRP:CH2	2.64	0.51
2:H:5:GLN:O	2:H:22:CYS:HA	2.10	0.51
1:A:62:ARG:NH1	1:A:80:GLU:HB2	2.25	0.51
1:L:30:SER:O	1:L:31:SER:C	2.53	0.51
1:L:116:VAL:HG22	1:L:137:LEU:CD2	2.39	0.51
2:B:12:VAL:CG1	2:B:16:GLY:HA3	2.40	0.51
2:B:19:LYS:HZ3	2:B:84:GLN:HG3	1.73	0.51
2:B:126:PRO:O	2:B:152:GLY:O	2.28	0.51
1:L:79:MET:SD	1:L:105:LEU:HD21	2.51	0.51
2:H:19:LYS:HZ3	2:H:84:GLN:HG3	1.75	0.51
2:H:196:ARG:C	2:H:198:SER:N	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:90:GLN:OE1	1:L:92:TRP:CZ2	2.64	0.51
1:L:189:ARG:NH1	1:A:1:ASP:N	2.58	0.51
1:A:168:ASP:HB3	1:A:172:SER:N	2.26	0.51
2:B:133:ALA:HB3	2:B:218:ILE:HG22	1.92	0.51
1:L:21:ILE:HG21	1:L:103:THR:HG21	1.93	0.51
2:H:28:THR:CG2	2:H:28:THR:O	2.58	0.51
2:B:67:LYS:C	2:B:69:LYS:H	2.18	0.51
1:L:145:ILE:HD12	1:L:145:ILE:N	2.25	0.51
2:B:36:TRP:CD1	2:B:83:LEU:HD13	2.46	0.51
1:L:144:ASP:O	1:L:145:ILE:HD12	2.11	0.50
1:L:189:ARG:HH12	1:A:1:ASP:H1	1.57	0.50
2:H:158:VAL:HG22	2:H:159:THR:N	2.27	0.50
1:A:168:ASP:OD1	1:A:170:LYS:N	2.45	0.50
2:H:32:TYR:CD1	2:H:32:TYR:C	2.90	0.50
1:A:21:ILE:CG2	1:A:103:THR:HG21	2.40	0.50
2:H:32:TYR:HD1	2:H:33:TRP:N	2.09	0.50
1:L:118:ILE:HG23	1:L:118:ILE:O	2.12	0.50
2:H:70:PHE:CD1	2:H:70:PHE:N	2.79	0.50
1:L:119:PHE:CE2	2:H:145:THR:O	2.65	0.50
1:A:52:THR:HG23	1:A:72:TYR:CD2	2.46	0.50
2:B:142:SER:C	2:B:193:SER:HA	2.36	0.50
2:H:43:LYS:HE2	2:H:46:GLU:HB3	1.94	0.50
1:A:50:TYR:CE1	2:B:108:VAL:HB	2.47	0.50
1:A:145:ILE:CG2	1:A:146:ASN:N	2.74	0.50
2:B:57:ASN:CG	2:B:58:PHE:N	2.70	0.50
2:B:163:ASN:O	2:B:164:SER:C	2.55	0.50
1:L:50:TYR:CG	2:H:108:VAL:HB	2.46	0.50
1:L:109:ARG:HD3	1:L:172:SER:O	2.12	0.50
2:H:22:CYS:SG	2:H:81:LEU:HD12	2.51	0.50
2:H:213:LYS:O	2:H:214:VAL:HG23	2.11	0.50
1:A:199:HIS:CE1	1:A:201:THR:HG1	2.30	0.50
2:H:143:MET:HA	2:H:193:SER:HA	1.93	0.49
1:A:52:THR:CG2	1:A:72:TYR:HD2	2.24	0.49
1:L:119:PHE:HD1	1:L:119:PHE:H	1.60	0.49
2:H:131:PRO:O	2:H:132:LEU:HD23	2.12	0.49
2:B:116:SER:HB3	2:B:157:PRO:HG3	1.94	0.49
1:L:2:ILE:HD12	1:L:96:PRO:O	2.12	0.49
1:L:92:TRP:CE3	1:L:97:TYR:CD2	3.00	0.49
2:H:214:VAL:HG13	2:H:215:ASP:N	2.26	0.49
2:B:48:VAL:CG1	2:B:66:VAL:HG11	2.25	0.49
1:A:191:ASN:OD1	1:A:211:ASN:CA	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:LEU:C	2:B:185:LEU:HD23	2.37	0.49
2:H:101:ARG:NH1	2:H:107:ALA:O	2.45	0.49
2:B:74:ARG:HD2	2:B:81:LEU:HB2	1.93	0.49
2:B:142:SER:CB	2:B:193:SER:HB3	2.32	0.49
2:B:153:TYR:N	2:B:153:TYR:CD1	2.77	0.49
2:H:33:TRP:HE1	2:H:101:ARG:HG3	1.77	0.49
2:B:32:TYR:CD1	2:B:32:TYR:C	2.91	0.49
1:L:25:VAL:HG12	1:L:26:SER:N	2.27	0.49
1:L:206:ILE:HD12	1:L:206:ILE:N	2.28	0.49
2:H:2:VAL:HG21	2:H:110:TYR:CD2	2.47	0.49
2:H:139:GLN:O	2:H:141:ASN:N	2.45	0.49
1:A:72:TYR:N	1:A:72:TYR:CD1	2.80	0.49
1:A:185:ASP:O	1:A:189:ARG:HB2	2.12	0.49
2:H:143:MET:CA	2:H:193:SER:HA	2.43	0.49
2:H:149:LEU:HA	2:H:186:SER:HB3	1.93	0.49
2:H:204:ASN:H	2:H:204:ASN:HD22	1.60	0.49
2:B:33:TRP:C	2:B:34:MET:HG2	2.37	0.49
1:L:35:HIS:CD2	1:L:92:TRP:NE1	2.81	0.49
1:L:125:GLN:HB2	2:H:130:TYR:CE1	2.48	0.49
1:L:180:LEU:CD2	1:L:182:LEU:HD21	2.41	0.49
2:H:197:PRO:O	2:H:199:GLU:N	2.46	0.49
1:A:118:ILE:HG12	1:A:118:ILE:O	2.11	0.49
1:L:72:TYR:CD1	1:L:72:TYR:N	2.80	0.49
2:H:124:THR:CG2	2:H:125:THR:N	2.75	0.49
2:H:150:VAL:O	2:H:184:THR:HA	2.13	0.49
2:B:70:PHE:CD1	2:B:70:PHE:N	2.81	0.49
1:L:145:ILE:CG1	1:L:199:HIS:CD2	2.96	0.48
2:H:72:ILE:HD11	2:H:81:LEU:HD21	1.95	0.48
2:B:133:ALA:HB1	2:B:218:ILE:HG22	1.92	0.48
1:A:136:PHE:CE2	2:B:188:SER:HB2	2.49	0.48
1:A:152:ASP:O	1:A:154:SER:N	2.45	0.48
2:B:51:ILE:HD11	2:B:58:PHE:CD2	2.47	0.48
2:B:144:VAL:O	2:B:190:THR:HA	2.14	0.48
1:L:21:ILE:HD11	1:L:74:LEU:HD13	1.93	0.48
2:H:53:LEU:O	2:H:53:LEU:CG	2.52	0.48
2:H:62:TYR:OH	2:H:72:ILE:HG22	2.13	0.48
1:A:180:LEU:CG	1:A:182:LEU:HD21	2.39	0.48
2:B:101:ARG:NH2	2:B:106:TYR:HD1	2.12	0.48
1:A:55:LEU:HD22	1:A:59:VAL:CG1	2.43	0.48
2:B:177:VAL:HG23	2:B:184:THR:O	2.14	0.48
1:L:4:LEU:CD2	1:L:89:CYS:SG	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:55:LEU:HD22	1:L:59:VAL:CG1	2.43	0.48
1:L:191:ASN:OD1	1:L:211:ASN:CA	2.60	0.48
2:H:36:TRP:CD1	2:H:72:ILE:HD12	2.49	0.48
1:A:79:MET:SD	1:A:105:LEU:HD21	2.54	0.48
1:A:45:PRO:HG2	2:B:45:LEU:HD21	1.94	0.48
2:B:47:TRP:NE1	2:B:49:ALA:O	2.47	0.48
1:L:199:HIS:CE1	1:L:201:THR:HG1	2.29	0.48
2:H:38:ARG:HG2	2:H:48:VAL:HG23	1.95	0.48
2:H:185:LEU:C	2:H:185:LEU:HD23	2.39	0.48
2:B:102:PRO:CB	2:B:104:PHE:CE1	2.95	0.48
1:L:90:GLN:HG3	1:L:99:PHE:CD2	2.49	0.48
1:L:122:SER:O	1:L:123:SER:C	2.57	0.48
1:L:133:VAL:CG2	1:L:180:LEU:HB3	2.43	0.47
2:H:63:ALA:H	2:H:66:VAL:HG23	1.78	0.47
2:H:145:THR:O	2:H:146:LEU:HD23	2.15	0.47
1:A:91:GLN:OE1	1:A:93:ASN:N	2.47	0.47
1:A:152:ASP:N	1:A:152:ASP:OD1	2.47	0.47
2:B:204:ASN:H	2:B:204:ASN:HD22	1.58	0.47
2:H:85:MET:HE1	2:H:96:TYR:CZ	2.49	0.47
2:H:88:LEU:HD22	2:H:92:ASP:CB	2.42	0.47
2:H:148:CYS:O	2:H:186:SER:HB2	2.14	0.47
1:A:116:VAL:HG22	1:A:137:LEU:HD23	1.95	0.47
2:B:139:GLN:O	2:B:141:ASN:N	2.47	0.47
2:B:189:VAL:O	2:B:189:VAL:HG13	2.14	0.47
1:A:162:ASN:HB3	1:A:176:MET:CE	2.44	0.47
1:L:60:PRO:HG2	1:L:63:PHE:CE1	2.49	0.47
1:L:199:HIS:CE1	1:L:201:THR:HG23	2.50	0.47
2:H:144:VAL:O	2:H:190:THR:HA	2.14	0.47
2:H:195:TRP:H	2:H:195:TRP:CD1	2.33	0.47
1:A:133:VAL:HG11	1:A:193:TYR:HD2	1.79	0.47
1:L:115:THR:HG22	1:L:115:THR:O	2.14	0.47
1:L:147:VAL:O	1:L:148:LYS:HD2	2.15	0.47
2:H:102:PRO:CB	2:H:104:PHE:CE1	2.98	0.47
2:H:180:SER:O	2:H:181:ASP:C	2.58	0.47
1:A:30:SER:O	1:A:31:SER:C	2.57	0.47
1:A:31:SER:C	1:A:52:THR:OG1	2.57	0.47
1:A:44:SER:O	1:A:45:PRO:C	2.57	0.47
2:B:27:PHE:CE1	2:B:74:ARG:NH2	2.83	0.47
2:B:63:ALA:O	2:B:65:SER:N	2.47	0.47
2:B:213:LYS:O	2:B:214:VAL:HG23	2.15	0.47
2:H:176:ALA:HB2	2:H:185:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:THR:HA	1:A:74:LEU:O	2.14	0.47
1:A:181:THR:O	1:A:182:LEU:HD23	2.14	0.47
1:A:213:ASN:ND2	2:B:136:SER:HB3	2.30	0.47
2:H:198:SER:O	2:H:200:THR:N	2.48	0.47
2:H:214:VAL:CG1	2:H:215:ASP:N	2.76	0.47
1:A:20:THR:HG22	1:A:75:THR:HG23	1.97	0.47
1:A:180:LEU:HG	1:A:182:LEU:CD2	2.42	0.47
2:H:34:MET:SD	2:H:100:LEU:HB2	2.56	0.47
2:H:101:ARG:NH2	2:H:107:ALA:O	2.48	0.47
1:A:127:THR:O	1:A:127:THR:CG2	2.63	0.47
1:A:199:HIS:CE1	1:A:201:THR:OG1	2.68	0.47
1:L:34:LEU:O	1:L:51:GLY:O	2.33	0.46
2:H:131:PRO:HA	2:H:217:LYS:HZ3	1.80	0.46
2:B:202:THR:HG22	2:B:215:ASP:O	2.15	0.46
2:H:33:TRP:HE1	2:H:101:ARG:CG	2.27	0.46
2:H:36:TRP:CZ2	2:H:81:LEU:HD13	2.50	0.46
1:A:52:THR:CG2	1:A:72:TYR:CD2	2.99	0.46
1:A:188:GLU:O	1:A:190:HIS:N	2.49	0.46
1:A:191:ASN:O	1:A:193:TYR:HD1	1.98	0.46
2:B:125:THR:O	2:B:153:TYR:HA	2.16	0.46
1:L:23:CYS:N	1:L:72:TYR:O	2.48	0.46
1:L:193:TYR:HB3	1:L:210:PHE:CE1	2.51	0.46
2:H:2:VAL:HG11	2:H:110:TYR:CG	2.50	0.46
2:H:102:PRO:HB2	2:H:104:PHE:CD1	2.51	0.46
1:L:125:GLN:HG3	2:H:130:TYR:OH	2.16	0.46
2:H:114:GLY:O	2:H:115:THR:HG23	2.15	0.46
1:A:50:TYR:CG	2:B:108:VAL:HB	2.51	0.46
1:A:145:ILE:HG22	1:A:146:ASN:N	2.30	0.46
2:B:131:PRO:HA	2:B:217:LYS:NZ	2.30	0.46
2:B:152:GLY:HA2	2:B:182:LEU:CD1	2.46	0.46
1:L:157:GLN:O	1:L:158:ASN:ND2	2.48	0.46
2:B:19:LYS:HG3	2:B:84:GLN:HG3	1.97	0.46
2:B:196:ARG:O	2:B:198:SER:N	2.48	0.46
2:H:71:ILE:HG13	2:H:71:ILE:O	2.15	0.46
1:A:126:LEU:HD23	1:A:131:ALA:CB	2.46	0.46
2:B:27:PHE:CZ	2:B:74:ARG:NH2	2.83	0.46
1:L:90:GLN:CD	1:L:99:PHE:CZ	2.94	0.46
2:H:89:ARG:C	2:H:119:VAL:HG11	2.40	0.46
1:A:21:ILE:HD11	1:A:74:LEU:HD13	1.97	0.46
1:A:133:VAL:HG11	1:A:193:TYR:CD2	2.50	0.46
1:L:41:SER:O	1:L:42:GLU:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:ALA:HB3	2:H:218:ILE:HG22	1.96	0.46
2:H:138:ALA:CB	2:H:144:VAL:HG23	2.46	0.46
2:B:36:TRP:CE2	2:B:83:LEU:HB2	2.51	0.46
2:B:81:LEU:C	2:B:81:LEU:HD22	2.41	0.46
1:A:120:PRO:HB3	1:A:210:PHE:CZ	2.51	0.45
2:B:2:VAL:HG11	2:B:110:TYR:CG	2.51	0.45
1:A:139:ASN:N	1:A:139:ASN:HD22	2.13	0.45
2:B:32:TYR:HD1	2:B:33:TRP:N	2.15	0.45
2:B:36:TRP:CZ2	2:B:81:LEU:HD13	2.52	0.45
1:L:196:GLU:HA	1:L:206:ILE:O	2.16	0.45
1:A:23:CYS:N	1:A:72:TYR:O	2.45	0.45
1:A:32:SER:O	2:B:106:TYR:OH	2.34	0.45
1:A:162:ASN:HB3	1:A:176:MET:HE3	1.96	0.45
2:B:28:THR:O	2:B:28:THR:CG2	2.63	0.45
2:B:152:GLY:HA2	2:B:182:LEU:HD11	1.98	0.45
2:B:216:LYS:O	2:B:216:LYS:HG3	2.16	0.45
1:L:19:VAL:O	1:L:75:THR:HG23	2.16	0.45
1:L:171:ASP:OD1	1:L:173:THR:HG23	2.17	0.45
2:B:32:TYR:CD1	2:B:33:TRP:N	2.85	0.45
2:H:131:PRO:HA	2:H:217:LYS:NZ	2.32	0.45
1:A:8:PRO:O	1:A:103:THR:HG23	2.16	0.45
1:A:31:SER:OG	1:A:68:SER:HA	2.17	0.45
2:B:43:LYS:HE2	2:B:46:GLU:HB3	1.98	0.45
2:B:203:CYS:O	2:B:203:CYS:SG	2.74	0.45
2:B:53:LEU:O	2:B:54:ASN:C	2.59	0.45
2:B:102:PRO:CB	2:B:104:PHE:HE1	2.29	0.45
1:L:91:GLN:NE2	1:L:97:TYR:HA	2.32	0.45
2:H:69:LYS:HB2	2:H:70:PHE:CD1	2.52	0.45
1:A:147:VAL:C	1:A:148:LYS:HD2	2.41	0.45
2:H:166:SER:OG	2:H:167:LEU:HD23	2.17	0.45
1:A:150:LYS:NZ	1:A:196:GLU:OE1	2.46	0.45
2:B:32:TYR:HA	2:B:102:PRO:HA	1.99	0.45
2:B:69:LYS:HB2	2:B:70:PHE:CE1	2.52	0.45
2:B:148:CYS:O	2:B:186:SER:CB	2.62	0.45
2:H:33:TRP:NE1	2:H:101:ARG:CG	2.80	0.45
2:H:195:TRP:H	2:H:195:TRP:HD1	1.65	0.45
1:A:190:HIS:HB2	1:A:193:TYR:CE1	2.51	0.45
2:B:158:VAL:C	2:B:159:THR:HG22	2.40	0.45
1:L:171:ASP:OD1	1:L:173:THR:OG1	2.34	0.45
2:H:139:GLN:O	2:H:140:THR:C	2.59	0.45
1:A:119:PHE:CD2	2:B:132:LEU:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:O	1:A:149:TRP:CZ2	2.70	0.45
2:B:34:MET:SD	2:B:100:LEU:HB2	2.57	0.45
2:H:154:PHE:O	2:H:155:PRO:C	2.56	0.44
2:H:163:ASN:H	2:H:204:ASN:HD21	1.63	0.44
2:B:20:LEU:HD23	2:B:85:MET:SD	2.57	0.44
1:L:34:LEU:HG	1:L:72:TYR:CD2	2.51	0.44
1:L:152:ASP:O	1:L:154:SER:N	2.50	0.44
1:A:90:GLN:OE1	1:A:92:TRP:CZ2	2.70	0.44
2:H:102:PRO:HG2	2:H:104:PHE:HD1	1.82	0.44
2:B:51:ILE:HG13	2:B:60:THR:HG22	1.99	0.44
2:H:28:THR:O	2:H:28:THR:HG22	2.17	0.44
1:A:3:GLN:OE1	1:A:3:GLN:N	2.50	0.44
2:B:143:MET:HA	2:B:193:SER:N	2.32	0.44
2:B:152:GLY:CA	2:B:182:LEU:HD11	2.48	0.44
2:H:209:ALA:O	2:H:210:SER:OG	2.32	0.44
1:A:62:ARG:HH12	1:A:80:GLU:HB2	1.81	0.44
1:L:90:GLN:HG3	1:L:99:PHE:CE2	2.52	0.44
2:B:69:LYS:C	2:B:70:PHE:CD1	2.90	0.44
2:B:192:PRO:HG2	2:B:196:ARG:HD2	2.00	0.44
1:L:2:ILE:O	1:L:98:THR:HG21	2.18	0.44
1:L:35:HIS:CD2	1:L:92:TRP:HE1	2.35	0.44
2:H:133:ALA:HB2	2:H:218:ILE:H	1.83	0.44
2:H:168:SER:O	2:H:170:GLY:N	2.51	0.44
1:A:82:GLU:N	1:A:82:GLU:OE1	2.51	0.44
1:A:145:ILE:HD11	1:A:199:HIS:CD2	2.48	0.44
1:A:186:GLU:OE2	1:A:190:HIS:CE1	2.71	0.44
2:B:90:ALA:O	2:B:91:GLU:C	2.61	0.44
2:H:33:TRP:CZ2	2:H:101:ARG:CB	3.00	0.43
2:H:53:LEU:C	2:H:55:SER:N	2.75	0.43
1:A:116:VAL:HG22	1:A:137:LEU:CD2	2.48	0.43
1:A:116:VAL:HG12	1:A:117:SER:N	2.32	0.43
2:H:207:HIS:HA	2:H:208:PRO:HD2	1.63	0.43
1:A:191:ASN:OD1	1:A:191:ASN:C	2.61	0.43
2:B:62:TYR:OH	2:B:71:ILE:HA	2.18	0.43
1:L:29:ILE:HD12	1:L:30:SER:O	2.18	0.43
1:L:29:ILE:HB	1:L:93:ASN:OD1	2.19	0.43
1:L:191:ASN:OD1	1:L:191:ASN:C	2.60	0.43
1:L:194:THR:HA	1:L:209:SER:HB3	2.00	0.43
1:A:138:ASN:O	1:A:139:ASN:HB2	2.16	0.43
2:B:198:SER:O	2:B:201:VAL:N	2.51	0.43
1:L:133:VAL:CG2	1:L:149:TRP:CZ3	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:ASN:CG	2:H:58:PHE:N	2.77	0.43
2:H:100:LEU:HD12	2:H:100:LEU:C	2.44	0.43
1:A:17:GLU:HG2	1:A:18:LYS:N	2.34	0.43
1:A:109:ARG:O	1:A:141:TYR:CE1	2.71	0.43
1:A:157:GLN:HE21	1:A:157:GLN:N	2.15	0.43
1:L:62:ARG:HB2	1:L:77:SER:HB2	2.00	0.43
2:H:124:THR:HG21	2:H:209:ALA:HB1	2.00	0.43
1:A:21:ILE:HG21	1:A:103:THR:HG21	2.00	0.43
2:B:71:ILE:HD12	2:B:72:ILE:O	2.18	0.43
2:B:194:THR:O	2:B:196:ARG:HG3	2.18	0.43
2:B:207:HIS:HA	2:B:208:PRO:HD2	1.74	0.43
1:L:119:PHE:CZ	2:H:145:THR:O	2.72	0.43
1:A:145:ILE:CD1	1:A:199:HIS:HD2	2.30	0.43
2:B:191:VAL:CB	2:B:192:PRO:CD	2.94	0.43
1:L:17:GLU:HG2	1:L:18:LYS:H	1.83	0.43
1:L:123:SER:O	1:L:124:GLU:C	2.61	0.43
1:L:151:ILE:HA	1:L:192:SER:O	2.19	0.43
2:H:11:LEU:CD2	2:H:155:PRO:HB3	2.48	0.43
1:A:160:VAL:HG12	1:A:162:ASN:HD21	1.84	0.43
1:A:199:HIS:CE1	1:A:201:THR:CG2	3.02	0.43
2:B:89:ARG:C	2:B:119:VAL:HG11	2.43	0.43
2:H:63:ALA:O	2:H:64:GLU:C	2.61	0.43
2:H:191:VAL:HB	2:H:192:PRO:CD	2.49	0.43
1:A:190:HIS:HB2	1:A:193:TYR:HE1	1.84	0.43
2:B:132:LEU:C	2:B:133:ALA:O	2.58	0.43
1:L:1:ASP:N	1:A:189:ARG:NH1	2.67	0.43
1:L:109:ARG:O	1:L:141:TYR:CE1	2.72	0.43
1:L:120:PRO:HB2	1:L:121:PRO:HD2	2.00	0.43
2:H:116:SER:HB3	2:H:157:PRO:HG3	1.99	0.43
2:B:27:PHE:HE2	2:B:32:TYR:CD2	2.36	0.43
2:B:33:TRP:CE2	2:B:101:ARG:CB	2.93	0.43
2:B:129:VAL:HG12	2:B:130:TYR:H	1.84	0.43
1:L:92:TRP:HE3	1:L:97:TYR:CD2	2.37	0.42
1:L:186:GLU:OE2	1:L:190:HIS:HE1	2.02	0.42
2:H:11:LEU:HA	2:H:118:THR:O	2.19	0.42
1:A:90:GLN:CD	1:A:99:PHE:CE2	2.97	0.42
1:A:122:SER:O	1:A:123:SER:C	2.62	0.42
2:B:35:SER:HA	2:B:50:GLU:HA	2.01	0.42
1:L:38:GLN:O	1:L:46:LYS:HB3	2.19	0.42
2:H:136:SER:O	2:H:137:ALA:HB2	2.18	0.42
1:L:31:SER:C	1:L:52:THR:OG1	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HD12	1:A:96:PRO:O	2.19	0.42
1:A:115:THR:O	1:A:115:THR:HG22	2.18	0.42
2:H:202:THR:HA	2:H:215:ASP:O	2.18	0.42
1:A:160:VAL:CG1	1:A:162:ASN:HD21	2.33	0.42
1:L:186:GLU:OE2	1:L:190:HIS:CE1	2.72	0.42
2:H:18:MET:O	2:H:84:GLN:HG2	2.19	0.42
2:H:102:PRO:CB	2:H:104:PHE:HE1	2.32	0.42
1:L:135:CYS:CB	1:L:149:TRP:CZ2	3.03	0.42
2:H:34:MET:CE	2:H:74:ARG:NH1	2.82	0.42
2:H:101:ARG:NH1	2:H:108:VAL:CA	2.80	0.42
2:H:166:SER:C	2:H:167:LEU:HD22	2.45	0.42
1:A:60:PRO:HG2	1:A:63:PHE:CE2	2.54	0.42
2:H:14:PRO:HD3	2:H:121:SER:HA	2.01	0.42
2:H:29:PHE:HD1	2:H:29:PHE:HA	1.72	0.42
2:B:71:ILE:O	2:B:71:ILE:HG13	2.18	0.42
1:L:171:ASP:CG	1:L:173:THR:HG1	2.27	0.42
1:L:181:THR:O	1:L:181:THR:CG2	2.67	0.42
2:H:101:ARG:CZ	2:H:107:ALA:O	2.67	0.42
2:H:129:VAL:HG21	2:H:213:LYS:HB3	2.02	0.42
2:H:34:MET:HE3	2:H:34:MET:HB3	1.95	0.42
2:H:101:ARG:NH2	2:H:106:TYR:HD1	2.18	0.42
2:H:129:VAL:HG12	2:H:130:TYR:H	1.84	0.42
2:B:139:GLN:O	2:B:140:THR:C	2.62	0.42
1:L:134:VAL:HG22	1:L:179:THR:HG23	2.02	0.42
1:L:189:ARG:HE	1:L:190:HIS:CE1	2.38	0.42
1:L:199:HIS:CE1	1:L:201:THR:CG2	3.03	0.42
2:H:90:ALA:O	2:H:91:GLU:C	2.63	0.42
2:H:123:LYS:HD2	2:H:124:THR:H	1.84	0.42
1:A:74:LEU:HD23	1:A:74:LEU:C	2.45	0.42
1:A:88:TYR:CD1	1:A:102:GLY:CA	3.00	0.42
1:L:74:LEU:C	1:L:74:LEU:CD2	2.93	0.41
1:L:119:PHE:HD2	2:H:133:ALA:O	2.03	0.41
2:H:145:THR:HG23	2:H:190:THR:HG23	2.02	0.41
1:A:2:ILE:O	1:A:98:THR:HG21	2.20	0.41
2:B:34:MET:CE	2:B:74:ARG:HH11	2.33	0.41
2:B:131:PRO:O	2:B:132:LEU:HD23	2.19	0.41
2:H:132:LEU:C	2:H:133:ALA:O	2.61	0.41
1:A:111:ASP:HA	1:A:141:TYR:HD1	1.84	0.41
1:L:78:SER:O	1:L:79:MET:C	2.60	0.41
1:A:196:GLU:HA	1:A:206:ILE:O	2.21	0.41
2:B:177:VAL:HG23	2:B:184:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:187:TYR:O	1:L:188:GLU:C	2.64	0.41
2:H:67:LYS:C	2:H:69:LYS:N	2.74	0.41
1:A:55:LEU:HB3	1:A:59:VAL:HB	2.03	0.41
1:A:63:PHE:CE1	1:A:76:ILE:HG12	2.55	0.41
1:L:168:ASP:OD2	1:L:170:LYS:N	2.51	0.41
1:A:165:THR:HG22	1:A:175:SER:H	1.84	0.41
1:A:199:HIS:ND1	1:A:201:THR:OG1	2.46	0.41
2:B:133:ALA:HB2	2:B:218:ILE:H	1.85	0.41
2:B:153:TYR:CZ	2:B:183:TYR:HB2	2.56	0.41
2:B:124:THR:HG21	2:B:209:ALA:HB1	2.01	0.41
2:B:184:THR:O	2:B:184:THR:HG23	2.20	0.41
1:L:52:THR:O	1:L:52:THR:HG22	2.19	0.41
1:L:40:LYS:O	1:L:41:SER:C	2.63	0.41
1:L:50:TYR:CE1	1:L:56:ALA:HA	2.49	0.41
1:L:60:PRO:HG2	1:L:63:PHE:CD1	2.56	0.41
1:L:125:GLN:O	1:L:125:GLN:HG2	2.20	0.41
1:L:133:VAL:HG23	1:L:180:LEU:HB3	2.03	0.41
1:L:153:GLY:O	1:L:155:GLU:N	2.54	0.41
2:H:179:GLN:O	2:H:179:GLN:CG	2.69	0.41
1:A:194:THR:CA	1:A:209:SER:HB3	2.49	0.41
2:B:180:SER:O	2:B:181:ASP:C	2.63	0.41
1:L:142:PRO:O	1:L:145:ILE:HD13	2.21	0.41
1:L:62:ARG:NH1	1:L:83:ASP:OD2	2.54	0.40
1:L:95:TYR:CE2	2:H:61:HIS:CB	3.05	0.40
1:L:161:LEU:HA	1:L:161:LEU:HD23	1.80	0.40
2:H:74:ARG:HG3	2:H:80:ARG:O	2.21	0.40
2:H:93:THR:HG23	2:H:117:VAL:O	2.21	0.40
1:A:7:SER:HA	1:A:8:PRO:HA	1.84	0.40
1:A:136:PHE:CE2	2:B:188:SER:CB	3.03	0.40
2:B:60:THR:O	2:B:61:HIS:CG	2.74	0.40
1:L:37:TYR:HE2	1:L:90:GLN:OE1	2.03	0.40
1:L:92:TRP:HE3	1:L:97:TYR:CE2	2.40	0.40
1:L:116:VAL:HG12	1:L:117:SER:N	2.36	0.40
1:A:90:GLN:HG3	1:A:99:PHE:CD2	2.57	0.40
1:L:44:SER:O	1:L:45:PRO:C	2.64	0.40
1:L:177:SER:HB3	2:H:174:PHE:CD2	2.55	0.40
1:L:204:SER:O	1:L:205:PRO:O	2.39	0.40
2:B:47:TRP:HE1	2:B:50:GLU:HB2	1.86	0.40
2:B:149:LEU:HA	2:B:186:SER:HB3	2.02	0.40
2:B:150:VAL:HG23	2:B:185:LEU:O	2.21	0.40
2:B:168:SER:O	2:B:171:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:ARG:HB3	2:B:197:PRO:CD	2.43	0.40
1:L:22:THR:HA	1:L:73:SER:HA	2.03	0.40
2:H:76:ASP:O	2:H:77:SER:C	2.63	0.40
2:B:19:LYS:HZ2	2:B:84:GLN:HG3	1.86	0.40
1:L:87:TYR:CD1	1:L:87:TYR:N	2.90	0.40
1:L:190:HIS:HB2	1:L:193:TYR:CE1	2.56	0.40
1:A:157:GLN:O	1:A:158:ASN:ND2	2.55	0.40
2:B:197:PRO:C	2:B:199:GLU:HG3	2.46	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	213/215 (99%)	160 (75%)	34 (16%)	19 (9%)	0	1
1	L	213/215 (99%)	164 (77%)	34 (16%)	15 (7%)	1	2
2	B	216/218 (99%)	161 (74%)	36 (17%)	19 (9%)	0	1
2	H	216/218 (99%)	161 (74%)	31 (14%)	24 (11%)	0	1
All	All	858/866 (99%)	646 (75%)	135 (16%)	77 (9%)	0	1

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	200	LYS
1	L	202	SER
1	L	205	PRO
2	H	30	ASN
2	H	54	ASN
2	H	55	SER
2	H	64	GLU

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Mol	Chain	Res	Type
2	H	140	THR
2	H	169	SER
2	H	180	SER
2	H	193	SER
1	A	200	LYS
1	A	202	SER
1	A	205	PRO
2	B	30	ASN
2	B	54	ASN
2	B	55	SER
2	B	64	GLU
2	B	140	THR
2	B	169	SER
2	B	191	VAL
2	B	193	SER
1	L	41	SER
1	L	77	SER
1	L	84	ALA
1	L	160	VAL
1	L	189	ARG
2	H	50	GLU
2	H	122	ALA
2	H	143	MET
2	H	198	SER
2	H	199	GLU
1	A	41	SER
1	A	84	ALA
1	A	160	VAL
1	A	189	ARG
2	B	50	GLU
2	B	180	SER
2	B	199	GLU
1	L	153	GLY
1	L	167	GLN
2	H	107	ALA
1	A	32	SER
1	A	57	SER
1	A	77	SER
1	A	167	GLN
2	B	143	MET
2	B	198	SER
1	L	32	SER

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Mol	Chain	Res	Type
1	L	57	SER
2	H	57	ASN
2	H	66	VAL
2	H	137	ALA
2	H	214	VAL
1	A	121	PRO
2	B	57	ASN
2	B	154	PHE
1	L	121	PRO
2	H	91	GLU
2	H	154	PHE
2	H	191	VAL
1	A	153	GLY
2	B	137	ALA
2	H	141	ASN
2	H	212	THR
1	A	31	SER
1	A	47	PRO
1	A	192	SER
2	B	2	VAL
2	B	66	VAL
2	B	214	VAL
2	H	2	VAL
1	A	29	ILE
1	A	61	VAL
1	L	47	PRO
1	A	8	PRO
1	L	8	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	190/190 (100%)	147 (77%)	43 (23%)	1	3
1	L	190/190 (100%)	147 (77%)	43 (23%)	1	3
2	B	189/189 (100%)	143 (76%)	46 (24%)	1	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	189/189 (100%)	142 (75%)	47 (25%)	0	2
All	All	758/758 (100%)	579 (76%)	179 (24%)	1	3

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	11	MET
1	L	15	PRO
1	L	20	THR
1	L	33	ASN
1	L	38	GLN
1	L	43	THR
1	L	45	PRO
1	L	47	PRO
1	L	62	ARG
1	L	78	SER
1	L	79	MET
1	L	86	THR
1	L	93	ASN
1	L	104	LYS
1	L	107	ILE
1	L	117	SER
1	L	119	PHE
1	L	121	PRO
1	L	124	GLU
1	L	127	THR
1	L	137	LEU
1	L	138	ASN
1	L	143	LYS
1	L	147	VAL
1	L	148	LYS
1	L	150	LYS
1	L	151	ILE
1	L	152	ASP
1	L	156	ARG
1	L	157	GLN
1	L	164	TRP
1	L	166	ASP
1	L	171	ASP
1	L	182	LEU
1	L	183	THR

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Mol	Chain	Res	Type
1	L	194	THR
1	L	202	SER
1	L	205	PRO
1	L	207	VAL
1	L	209	SER
1	L	213	ASN
1	L	214	GLU
2	H	1	GLU
2	H	2	VAL
2	H	6	GLU
2	H	11	LEU
2	H	12	VAL
2	H	13	GLN
2	H	27	PHE
2	H	28	THR
2	H	34	MET
2	H	52	ARG
2	H	55	SER
2	H	56	ASP
2	H	66	VAL
2	H	70	PHE
2	H	71	ILE
2	H	72	ILE
2	H	81	LEU
2	H	84	GLN
2	H	85	MET
2	H	95	ILE
2	H	98	CYS
2	H	99	VAL
2	H	106	TYR
2	H	113	GLN
2	H	115	THR
2	H	121	SER
2	H	125	THR
2	H	145	THR
2	H	150	VAL
2	H	151	LYS
2	H	159	THR
2	H	177	VAL
2	H	179	GLN
2	H	181	ASP
2	H	184	THR

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Mol	Chain	Res	Type
2	H	185	LEU
2	H	188	SER
2	H	190	THR
2	H	193	SER
2	H	194	THR
2	H	195	TRP
2	H	200	THR
2	H	202	THR
2	H	203	CYS
2	H	204	ASN
2	H	205	VAL
2	H	214	VAL
1	A	7	SER
1	A	14	SER
1	A	15	PRO
1	A	20	THR
1	A	25	VAL
1	A	28	SER
1	A	33	ASN
1	A	38	GLN
1	A	39	GLN
1	A	43	THR
1	A	45	PRO
1	A	47	PRO
1	A	62	ARG
1	A	78	SER
1	A	86	THR
1	A	96	PRO
1	A	104	LYS
1	A	107	ILE
1	A	119	PHE
1	A	124	GLU
1	A	127	THR
1	A	137	LEU
1	A	138	ASN
1	A	143	LYS
1	A	148	LYS
1	A	150	LYS
1	A	152	ASP
1	A	156	ARG
1	A	157	GLN
1	A	165	THR

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Mol	Chain	Res	Type
1	A	166	ASP
1	A	171	ASP
1	A	172	SER
1	A	176	MET
1	A	182	LEU
1	A	183	THR
1	A	194	THR
1	A	205	PRO
1	A	206	ILE
1	A	207	VAL
1	A	209	SER
1	A	213	ASN
1	A	214	GLU
2	B	1	GLU
2	B	2	VAL
2	B	11	LEU
2	B	12	VAL
2	B	13	GLN
2	B	27	PHE
2	B	28	THR
2	B	34	MET
2	B	38	ARG
2	B	55	SER
2	B	56	ASP
2	B	66	VAL
2	B	70	PHE
2	B	71	ILE
2	B	79	SER
2	B	81	LEU
2	B	84	GLN
2	B	85	MET
2	B	91	GLU
2	B	95	ILE
2	B	99	VAL
2	B	106	TYR
2	B	113	GLN
2	B	121	SER
2	B	131	PRO
2	B	139	GLN
2	B	150	VAL
2	B	151	LYS
2	B	159	THR

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Mol	Chain	Res	Type
2	B	164	SER
2	B	167	LEU
2	B	177	VAL
2	B	179	GLN
2	B	184	THR
2	B	185	LEU
2	B	188	SER
2	B	190	THR
2	B	193	SER
2	B	194	THR
2	B	200	THR
2	B	202	THR
2	B	203	CYS
2	B	204	ASN
2	B	205	VAL
2	B	211	SER
2	B	214	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	33	ASN
1	L	35	HIS
1	L	139	ASN
1	L	157	GLN
1	L	158	ASN
1	L	213	ASN
2	H	54	ASN
2	H	139	GLN
2	H	172	HIS
2	H	179	GLN
2	H	204	ASN
2	H	207	HIS
1	A	33	ASN
1	A	35	HIS
1	A	39	GLN
1	A	138	ASN
1	A	139	ASN
1	A	146	ASN
1	A	157	GLN
1	A	158	ASN
1	A	190	HIS

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Mol	Chain	Res	Type
1	A	213	ASN
2	B	39	GLN
2	B	163	ASN
2	B	172	HIS
2	B	179	GLN
2	B	204	ASN
2	B	207	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.