



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 PM UTC

PDB ID : 1YUH / pdb_00001yuh
Title : FAB FRAGMENT
Authors : Yuhasz, S.C.; Amzel, L.M.; Parry, C.; Strand, M.
Deposited on : 1996-01-30
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

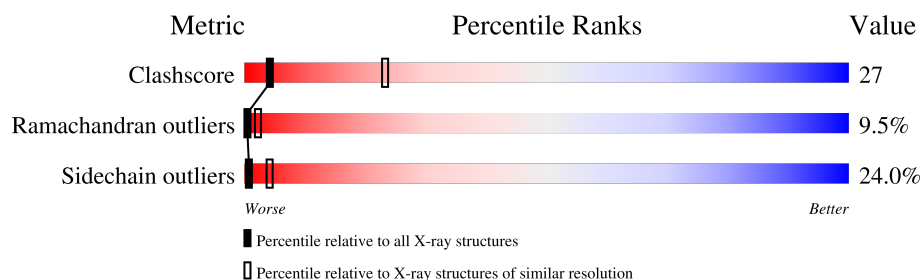
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	211	24% 37% 27% 12%
1	L	211	25% 42% 26% 8%
2	B	218	24% 36% 28% 12%
2	H	218	26% 44% 24% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6530 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 88C6/12 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1594	996	269	323	6			
1	A	211	Total	C	N	O	S	0	0	0
			1594	996	269	323	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	44	ARG	HIS	conflict	GB 387376
L	57	GLY	ALA	conflict	GB 387376
L	160	GLU	GLN	conflict	GB 387376
L	184	SER	THR	conflict	GB 387376
L	192	ALA	SER	conflict	GB 387376
A	44	ARG	HIS	conflict	GB 387376
A	57	GLY	ALA	conflict	GB 387376
A	160	GLU	GLN	conflict	GB 387376
A	184	SER	THR	conflict	GB 387376
A	192	ALA	SER	conflict	GB 387376

- Molecule 2 is a protein called 88C6/12 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1647	1046	273	319	9			
2	B	218	Total	C	N	O	S	0	0	0
			1647	1046	273	319	9			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	9	ALA	PRO	conflict	GB 3399661
H	20	LEU	MET	conflict	GB 3399661

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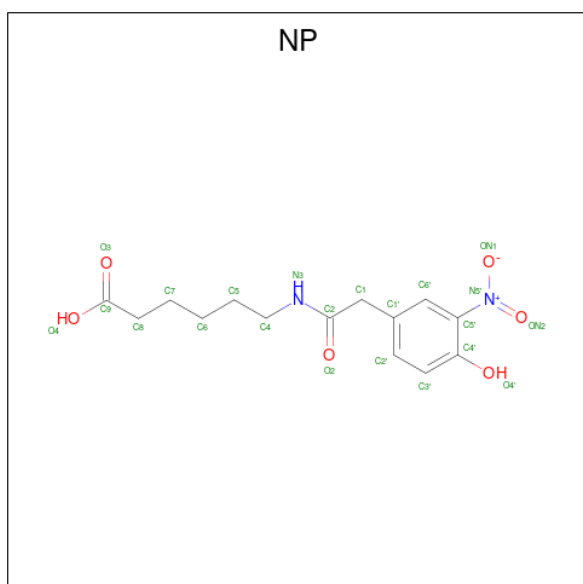
Chain	Residue	Modelled	Actual	Comment	Reference
H	33	LEU	VAL	conflict	GB 3399661
H	37	ILE	VAL	conflict	GB 3399661
H	40	ARG	LYS	conflict	GB 3399661
H	43	ARG	GLN	conflict	GB 3399661
H	50	ARG	TYR	conflict	GB 3399661
H	52	ASP	ASN	conflict	GB 3399661
H	54	ASN	TYR	conflict	GB 3399661
H	56	VAL	ASP	conflict	GB 3399661
H	57	VAL	GLY	conflict	GB 3399661
H	60	PHE	TYR	conflict	GB 3399661
H	66	SER	GLY	conflict	GB 3399661
H	72	VAL	SER	conflict	GB 3399661
H	75	PRO	SER	conflict	GB 3399661
H	97	ALA	VAL	conflict	GB 3399661
H	99	TYR	GLY	conflict	GB 3399661
H	100	ALA	GLY	conflict	GB 3399661
H	102	CYS	-	insertion	GB 3399661
H	?	-	TYR	deletion	GB 3399661
H	?	-	TYR	deletion	GB 3399661
H	?	-	ALA	deletion	GB 3399661
H	113	THR	SER	conflict	GB 3399661
H	120	ALA	LYS	conflict	GB 3399661
H	163	ALA	SER	conflict	GB 3399661
H	190	ALA	SER	conflict	GB 3399661
H	196	GLY	GLU	conflict	GB 3399661
H	210	ALA	LYS	conflict	GB 3399661
B	9	ALA	PRO	conflict	GB 3399661
B	20	LEU	MET	conflict	GB 3399661
B	33	LEU	VAL	conflict	GB 3399661
B	37	ILE	VAL	conflict	GB 3399661
B	40	ARG	LYS	conflict	GB 3399661
B	43	ARG	GLN	conflict	GB 3399661
B	50	ARG	TYR	conflict	GB 3399661
B	52	ASP	ASN	conflict	GB 3399661
B	54	ASN	TYR	conflict	GB 3399661
B	56	VAL	ASP	conflict	GB 3399661
B	57	VAL	GLY	conflict	GB 3399661
B	60	PHE	TYR	conflict	GB 3399661
B	66	SER	GLY	conflict	GB 3399661
B	72	VAL	SER	conflict	GB 3399661
B	75	PRO	SER	conflict	GB 3399661
B	97	ALA	VAL	conflict	GB 3399661

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Chain	Residue	Modelled	Actual	Comment	Reference
B	99	TYR	GLY	conflict	GB 3399661
B	100	ALA	GLY	conflict	GB 3399661
B	102	CYS	-	insertion	GB 3399661
B	?	-	TYR	deletion	GB 3399661
B	?	-	TYR	deletion	GB 3399661
B	?	-	ALA	deletion	GB 3399661
B	113	THR	SER	conflict	GB 3399661
B	120	ALA	LYS	conflict	GB 3399661
B	163	ALA	SER	conflict	GB 3399661
B	190	ALA	SER	conflict	GB 3399661
B	196	GLY	GLU	conflict	GB 3399661
B	210	ALA	LYS	conflict	GB 3399661

- Molecule 3 is 4-HYDROXY-3-NITROPHENYLACETYL-EPSILON-AMINOCAPROIC ACID (CCD ID: NP) (formula: $C_{14}H_{18}N_2O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			22	14	2	6		
3	B	1	Total	C	N	O	0	0
			22	14	2	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	3	Total	O	0	0
			3	3		

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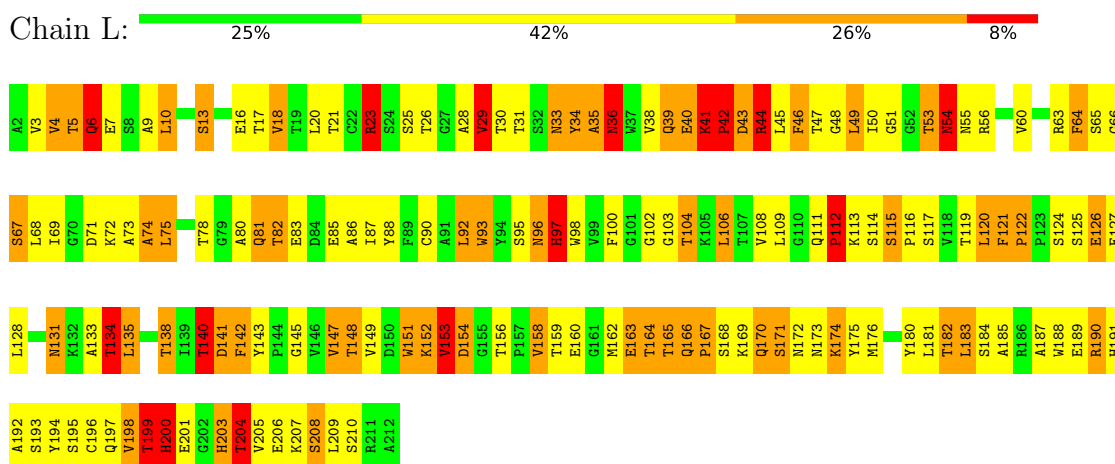
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		

3 Residue-property plots

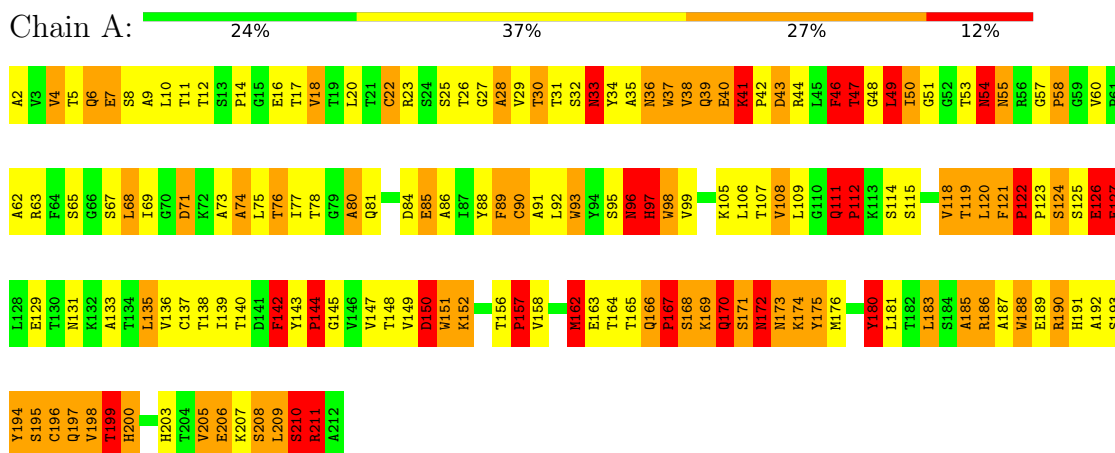
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

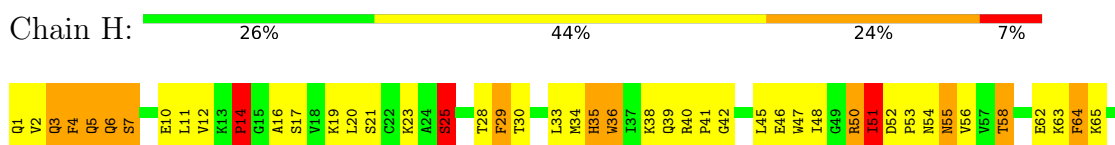
• Molecule 1: 88C6/12 FAB (LIGHT CHAIN)

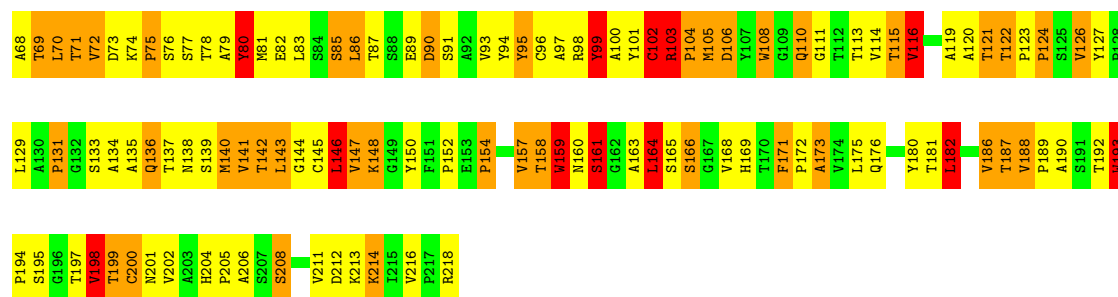


• Molecule 1: 88C6/12 FAB (LIGHT CHAIN)

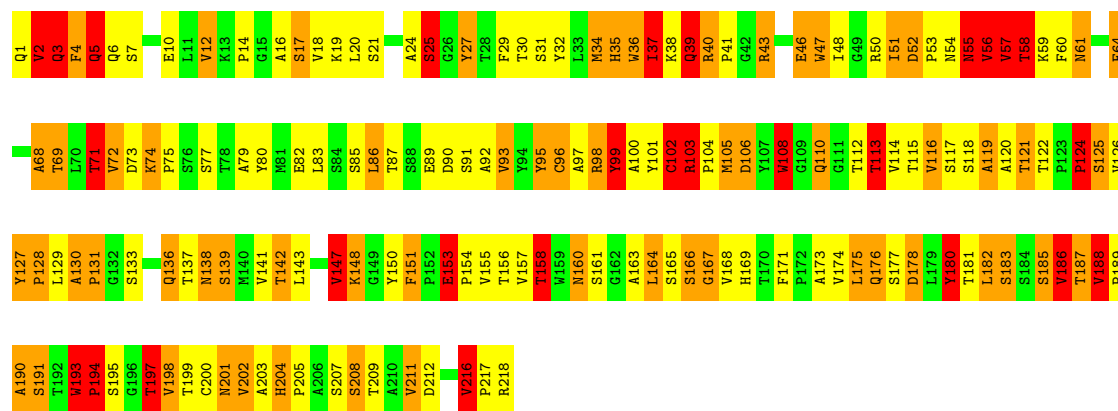
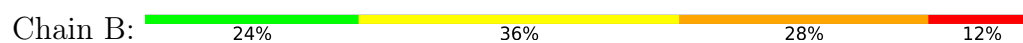


• Molecule 2: 88C6/12 FAB (HEAVY CHAIN)





● Molecule 2: 88C6/12 FAB (HEAVY CHAIN)



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	81.20Å 86.90Å 131.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.23	6/1630 (0.4%)	2.65	157/2224 (7.1%)
1	L	1.21	7/1630 (0.4%)	2.58	141/2224 (6.3%)
2	B	1.23	10/1691 (0.6%)	2.69	153/2311 (6.6%)
2	H	1.23	10/1691 (0.6%)	2.53	122/2311 (5.3%)
All	All	1.22	33/6642 (0.5%)	2.61	573/9070 (6.3%)

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	6
2	B	0	6
2	H	0	2
All	All	0	14

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	211	VAL	CA-CB	9.24	1.63	1.54
2	H	142	THR	CA-CB	7.94	1.64	1.53
2	B	198	VAL	CA-CB	7.26	1.61	1.53
1	L	97	HIS	CD2-NE2	-7.03	1.30	1.37
1	L	200	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	191	HIS	CD2-NE2	-6.80	1.30	1.37
2	B	169	HIS	CD2-NE2	-6.68	1.30	1.37
2	H	35	HIS	CD2-NE2	-6.67	1.30	1.37
1	L	138	THR	CA-CB	6.49	1.61	1.52
1	A	200	HIS	CD2-NE2	-6.47	1.30	1.37
2	B	204	HIS	CD2-NE2	-6.45	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	35	HIS	CD2-NE2	-6.33	1.30	1.37
1	L	97	HIS	CG-ND1	-6.33	1.31	1.38
2	H	204	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	203	HIS	CD2-NE2	-6.32	1.30	1.37
2	H	169	HIS	CD2-NE2	-6.25	1.30	1.37
2	H	115	THR	CA-CB	6.14	1.61	1.53
1	L	191	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	97	HIS	CD2-NE2	-6.03	1.31	1.37
2	H	72	VAL	CA-CB	6.03	1.63	1.54
2	B	113	THR	CA-CB	6.01	1.60	1.53
2	B	69	THR	CA-CB	5.95	1.61	1.53
2	B	126	VAL	CA-CB	5.89	1.60	1.53
1	A	18	VAL	CA-CB	5.83	1.61	1.54
2	H	108	TRP	NE1-CE2	-5.74	1.31	1.37
1	L	203	HIS	CD2-NE2	-5.74	1.31	1.37
2	H	157	VAL	CA-CB	5.72	1.59	1.53
2	H	35	HIS	CG-ND1	-5.62	1.32	1.38
2	B	142	THR	CA-CB	5.41	1.61	1.53
2	H	2	VAL	CA-CB	5.38	1.59	1.53
1	A	191	HIS	CG-ND1	-5.19	1.32	1.38
2	B	202	VAL	CA-CB	5.14	1.59	1.53
1	L	191	HIS	CG-ND1	-5.09	1.32	1.38

All (573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	157	VAL	N-CA-C	13.53	129.68	108.85
1	A	172	ASN	OD1-CG-ND2	-13.27	109.33	122.60
2	H	157	VAL	N-CA-C	12.86	126.83	107.15
1	L	43	ASP	CA-CB-CG	12.85	125.45	112.60
2	B	103	ARG	O-C-N	-12.45	110.95	121.54
2	B	164	LEU	N-CA-C	12.14	132.10	107.69
2	B	58	THR	N-CA-C	12.12	125.63	108.54
1	L	170	GLN	OE1-CD-NE2	-12.07	110.53	122.60
2	B	54	ASN	OD1-CG-ND2	-11.63	110.97	122.60
1	L	195	SER	N-CA-C	11.51	128.36	107.99
2	B	86	LEU	N-CA-C	11.48	126.43	110.24
2	B	95	TYR	N-CA-C	11.28	126.57	108.41
2	H	197	THR	N-CA-C	11.24	125.63	110.35
2	B	18	VAL	N-CA-C	11.11	124.58	109.80
2	B	197	THR	N-CA-C	11.08	126.58	109.96
1	L	39	GLN	OE1-CD-NE2	-10.97	111.63	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6	GLN	OE1-CD-NE2	-10.87	111.73	122.60
2	H	116	VAL	N-CA-C	10.69	117.64	106.21
2	B	126	VAL	N-CA-C	10.66	122.40	108.12
1	L	198	VAL	N-CA-C	10.65	123.24	107.80
1	A	46	PHE	N-CA-C	10.64	126.78	112.30
2	H	120	ALA	N-CA-C	10.55	125.88	110.59
2	H	55	ASN	OD1-CG-ND2	-10.40	112.20	122.60
2	B	72	VAL	N-CA-C	10.39	123.95	108.46
1	A	81	GLN	OE1-CD-NE2	-10.32	112.28	122.60
1	L	71	ASP	CA-CB-CG	10.31	122.91	112.60
2	H	136	GLN	OE1-CD-NE2	-10.28	112.32	122.60
1	A	198	VAL	N-CA-CB	-10.19	99.54	110.95
2	H	105	MET	N-CA-C	10.18	122.24	107.88
1	L	189	GLU	N-CA-C	10.14	132.41	110.80
1	A	170	GLN	N-CA-C	9.97	124.81	108.96
2	H	86	LEU	N-CA-C	9.92	125.17	110.48
2	H	123	PRO	N-CA-C	9.91	122.80	110.70
1	A	33	ASN	OD1-CG-ND2	-9.90	112.70	122.60
1	A	28	ALA	N-CA-C	9.83	123.56	108.42
1	L	175	TYR	N-CA-C	9.70	124.88	110.52
1	A	168	SER	N-CA-C	9.63	123.75	109.59
2	H	5	GLN	OE1-CD-NE2	-9.63	112.97	122.60
2	B	25	SER	N-CA-C	9.63	124.11	108.32
1	A	55	ASN	OD1-CG-ND2	-9.58	113.02	122.60
2	H	110	GLN	OE1-CD-NE2	-9.58	113.02	122.60
1	A	172	ASN	CB-CG-ND2	9.58	130.76	116.40
1	A	195	SER	N-CA-C	9.55	125.30	110.20
1	L	173	ASN	OD1-CG-ND2	-9.53	113.07	122.60
1	A	150	ASP	CA-CB-CG	9.51	122.11	112.60
1	L	10	LEU	N-CA-C	9.48	122.45	108.60
2	B	180	TYR	N-CA-C	9.43	123.48	109.24
2	H	163	ALA	N-CA-C	9.34	122.65	111.82
2	B	187	THR	N-CA-C	9.29	126.20	113.37
1	A	173	ASN	CA-CB-CG	9.28	121.88	112.60
2	B	198	VAL	N-CA-C	9.26	121.32	107.15
1	A	38	VAL	N-CA-C	9.14	120.01	110.05
1	L	134	THR	N-CA-C	9.13	123.79	108.90
2	B	153	GLU	N-CA-C	9.14	130.00	109.81
2	B	39	GLN	OE1-CD-NE2	-9.13	113.47	122.60
1	L	81	GLN	OE1-CD-NE2	-9.11	113.49	122.60
2	H	25	SER	N-CA-C	9.11	123.47	107.61
1	A	8	SER	N-CA-C	9.04	120.82	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	51	ILE	CB-CA-C	-9.03	98.25	110.98
1	L	126	GLU	N-CA-C	8.97	120.75	110.97
2	H	126	VAL	N-CA-C	8.92	120.61	108.84
1	L	5	THR	CA-C-O	8.84	130.77	120.70
2	H	198	VAL	N-CA-CB	-8.81	100.19	111.64
2	H	138	ASN	OD1-CG-ND2	-8.81	113.79	122.60
2	B	193	TRP	N-CA-C	8.77	122.83	110.20
1	A	6	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	A	131	ASN	CA-CB-CG	-8.66	103.94	112.60
2	B	208	SER	N-CA-C	8.61	129.14	110.80
1	A	114	SER	N-CA-C	8.61	123.16	110.17
1	A	142	PHE	N-CA-C	8.60	122.48	108.55
2	H	65	LYS	O-C-N	-8.57	113.03	122.12
1	A	199	THR	N-CA-C	8.57	123.39	109.59
2	H	72	VAL	N-CA-C	8.54	121.87	108.89
2	H	108	TRP	CG-CD2-CE3	8.48	142.38	133.90
2	H	90	ASP	CA-CB-CG	8.47	121.07	112.60
1	A	112	PRO	N-CA-C	8.45	129.87	112.47
2	B	5	GLN	OE1-CD-NE2	-8.43	114.17	122.60
2	B	202	VAL	N-CA-C	8.43	119.14	106.42
2	B	60	PHE	N-CA-C	8.43	121.40	110.53
1	L	36	ASN	N-CA-C	8.38	123.06	109.40
2	H	110	GLN	CG-CD-NE2	8.36	128.94	116.40
2	H	169	HIS	CB-CG-CD2	-8.36	120.33	131.20
2	H	80	TYR	N-CA-C	8.35	122.01	110.24
1	L	153	VAL	N-CA-C	8.29	124.35	113.07
2	H	58	THR	N-CA-C	8.29	122.41	108.90
1	A	36	ASN	N-CA-C	8.28	122.40	108.90
2	B	147	VAL	N-CA-C	8.27	120.43	107.28
1	L	172	ASN	OD1-CG-ND2	-8.25	114.35	122.60
2	B	105	MET	N-CA-C	8.21	120.94	107.73
1	L	134	THR	CA-C-O	8.19	129.20	120.36
1	A	55	ASN	CA-CB-CG	8.14	120.74	112.60
2	B	92	ALA	N-CA-C	8.13	118.97	108.24
1	A	173	ASN	OD1-CG-ND2	-8.13	114.47	122.60
1	L	40	GLU	CA-CB-CG	8.11	130.32	114.10
1	L	13	SER	N-CA-C	8.10	119.85	109.65
2	B	85	SER	N-CA-C	8.09	122.50	112.47
1	L	204	THR	N-CA-C	8.04	120.91	110.53
2	H	103	ARG	O-C-N	-8.04	115.78	121.65
2	B	61	ASN	OD1-CG-ND2	-8.01	114.59	122.60
2	B	102	CYS	N-CA-C	7.99	127.82	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	166	SER	N-CA-C	7.96	127.76	110.80
2	H	39	GLN	OE1-CD-NE2	-7.95	114.65	122.60
2	B	154	PRO	N-CA-C	7.95	123.50	110.55
2	B	37	ILE	N-CA-CB	-7.94	101.32	111.64
2	H	80	TYR	CA-CB-CG	7.92	128.15	113.90
2	H	171	PHE	CA-CB-CG	-7.91	105.89	113.80
1	A	37	TRP	N-CA-C	7.91	122.74	107.71
2	H	6	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	L	111	GLN	OE1-CD-NE2	-7.88	114.72	122.60
1	A	96	ASN	OD1-CG-ND2	-7.83	114.77	122.60
2	H	68	ALA	N-CA-C	7.81	122.57	109.76
2	H	202	VAL	CA-C-O	7.81	128.71	120.51
1	L	183	LEU	N-CA-C	7.81	121.03	109.24
1	A	199	THR	CA-CB-OG1	-7.79	97.92	109.60
1	L	141	ASP	CA-CB-CG	7.78	120.38	112.60
1	A	97	HIS	N-CA-C	7.77	121.16	108.26
2	B	202	VAL	N-CA-CB	-7.77	104.88	112.65
1	A	118	VAL	N-CA-C	7.76	118.98	110.21
2	B	68	ALA	N-CA-C	7.76	121.77	109.50
1	A	124	SER	N-CA-C	7.75	120.77	110.53
2	H	198	VAL	CA-C-O	7.74	128.44	120.39
1	L	140	THR	N-CA-C	7.73	120.65	109.14
1	A	55	ASN	CB-CG-ND2	7.72	127.97	116.40
1	L	92	LEU	N-CA-C	7.70	121.47	109.07
2	H	173	ALA	N-CA-C	7.70	121.87	110.48
1	L	33	ASN	CA-CB-CG	-7.69	104.91	112.60
2	B	106	ASP	CA-CB-CG	7.68	120.28	112.60
1	A	189	GLU	N-CA-C	7.66	123.94	111.37
1	L	46	PHE	CA-CB-CG	7.64	121.44	113.80
1	L	197	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	L	121	PHE	CA-CB-CG	-7.62	106.18	113.80
2	B	188	VAL	N-CA-C	7.60	125.29	108.88
2	H	164	LEU	N-CA-C	7.59	121.98	108.24
1	A	98	TRP	N-CA-C	7.58	120.66	110.35
2	B	122	THR	CA-CB-OG1	-7.57	98.25	109.60
2	B	157	VAL	N-CA-CB	-7.55	96.28	111.91
1	A	50	ILE	N-CA-C	7.55	118.75	107.80
1	L	185	ALA	N-CA-C	7.52	123.78	111.37
2	B	176	GLN	OE1-CD-NE2	-7.52	115.08	122.60
2	H	169	HIS	CA-CB-CG	7.48	121.28	113.80
1	L	5	THR	N-CA-C	7.47	122.34	107.62
2	B	138	ASN	OD1-CG-ND2	-7.47	115.13	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	GLN	N-CA-C	7.47	121.21	107.99
1	L	100	PHE	N-CA-C	7.45	121.61	109.76
1	L	170	GLN	CG-CD-NE2	7.45	127.58	116.40
1	A	39	GLN	N-CA-C	7.45	123.27	107.70
1	A	88	TYR	N-CA-C	7.45	121.52	108.56
1	A	81	GLN	N-CA-C	7.44	121.57	109.59
2	B	150	TYR	N-CA-C	7.39	121.53	109.85
2	H	133	SER	N-CA-C	7.37	120.87	109.60
2	B	90	ASP	CA-C-O	7.34	126.79	119.08
1	A	175	TYR	N-CA-C	7.34	121.73	110.36
1	A	111	GLN	N-CA-C	7.33	124.34	109.60
2	B	110	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	A	197	GLN	OE1-CD-NE2	-7.30	115.30	122.60
1	A	170	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	167	PRO	N-CA-C	7.28	127.47	112.47
2	B	211	VAL	N-CA-C	7.26	120.08	109.63
1	L	55	ASN	OD1-CG-ND2	-7.25	115.35	122.60
1	A	199	THR	CA-CB-CG2	7.24	122.80	110.50
1	A	194	TYR	N-CA-C	7.22	123.03	113.20
1	A	41	LYS	N-CA-C	7.22	125.76	109.81
1	A	122	PRO	O-C-N	-7.22	117.76	121.15
2	B	160	ASN	OD1-CG-ND2	-7.20	115.40	122.60
2	B	119	ALA	N-CA-C	7.20	120.26	109.25
1	A	71	ASP	CA-CB-CG	7.19	119.79	112.60
2	B	169	HIS	CB-CG-CD2	-7.17	121.88	131.20
1	L	46	PHE	O-C-N	-7.16	113.59	122.68
1	A	98	TRP	CG-CD2-CE3	7.13	141.03	133.90
1	A	57	GLY	CA-C-N	7.12	128.75	119.84
1	A	57	GLY	C-N-CA	7.12	128.75	119.84
2	H	169	HIS	CB-CG-ND1	7.12	133.37	122.70
1	A	10	LEU	N-CA-C	7.11	120.22	109.41
1	A	89	PHE	N-CA-C	7.09	120.43	108.23
2	B	200	CYS	N-CA-C	7.09	120.97	110.48
1	A	180	TYR	N-CA-C	7.09	120.28	108.73
1	L	81	GLN	CG-CD-NE2	7.08	127.03	116.40
1	A	43	ASP	N-CA-C	7.08	125.89	110.80
1	L	114	SER	O-C-N	-7.08	113.95	122.65
2	H	211	VAL	N-CA-C	7.06	124.03	109.34
2	B	43	ARG	N-CA-C	7.06	125.84	110.80
1	L	54	ASN	N-CA-C	7.04	124.59	114.39
2	H	85	SER	N-CA-C	7.04	125.79	110.80
2	B	55	ASN	OD1-CG-ND2	-7.03	115.57	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	171	SER	N-CA-C	7.02	125.75	110.80
1	L	208	SER	N-CA-C	6.99	119.38	108.96
2	H	188	VAL	N-CA-C	6.98	115.51	109.02
1	A	5	THR	CA-C-O	6.96	129.34	120.57
2	H	198	VAL	N-CA-C	6.95	117.90	107.75
2	H	169	HIS	CB-CA-C	-6.95	101.37	111.23
2	B	147	VAL	CA-CB-CG1	-6.94	98.60	110.40
2	H	124	PRO	N-CA-C	6.92	121.36	110.50
2	H	54	ASN	OD1-CG-ND2	-6.91	115.69	122.60
2	B	71	THR	O-C-N	-6.91	115.47	123.27
1	L	35	ALA	N-CA-C	6.91	125.51	110.80
1	A	170	GLN	CA-CB-CG	6.89	127.88	114.10
1	A	36	ASN	CA-CB-CG	-6.89	105.71	112.60
2	B	148	LYS	N-CA-C	6.88	119.83	110.55
1	L	54	ASN	OD1-CG-ND2	-6.87	115.73	122.60
2	B	141	VAL	N-CA-C	6.86	118.00	108.12
1	A	62	ALA	CA-C-N	6.86	134.64	121.54
1	A	62	ALA	C-N-CA	6.86	134.64	121.54
1	L	197	GLN	N-CA-C	6.85	119.91	108.20
2	B	136	GLN	OE1-CD-NE2	-6.85	115.75	122.60
2	B	190	ALA	CA-C-N	6.84	134.61	121.54
2	B	190	ALA	C-N-CA	6.84	134.61	121.54
2	B	201	ASN	OD1-CG-ND2	-6.84	115.76	122.60
1	A	140	THR	N-CA-C	6.83	120.81	109.95
2	H	127	TYR	N-CA-C	6.82	120.28	109.64
1	L	46	PHE	N-CA-C	6.81	119.97	107.99
2	B	191	SER	N-CA-C	6.81	125.30	110.80
1	A	38	VAL	CB-CA-C	-6.78	104.13	111.59
1	L	122	PRO	N-CA-C	6.78	118.97	110.70
1	A	111	GLN	OE1-CD-NE2	-6.78	115.82	122.60
1	L	142	PHE	N-CA-C	6.78	121.34	109.96
1	A	135	LEU	N-CA-C	6.77	120.54	109.24
2	B	21	SER	N-CA-C	6.76	119.41	108.32
1	L	56	ARG	N-CA-C	6.76	120.18	110.10
2	B	163	ALA	N-CA-C	6.76	125.20	110.80
1	A	47	THR	N-CA-C	6.75	125.19	110.80
1	L	54	ASN	O-C-N	-6.75	115.24	122.19
1	A	115	SER	O-C-N	-6.75	115.03	121.57
1	A	97	HIS	CA-CB-CG	6.74	120.54	113.80
1	A	121	PHE	CA-C-N	6.74	124.51	119.66
1	A	121	PHE	C-N-CA	6.74	124.51	119.66
2	H	136	GLN	CB-CG-CD	6.73	124.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLN	CB-CA-C	6.73	117.89	110.15
2	B	201	ASN	CA-CB-CG	6.73	119.33	112.60
2	H	154	PRO	N-CA-C	6.72	126.32	112.47
1	L	199	THR	N-CA-C	6.72	119.89	109.07
2	B	51	ILE	CB-CA-C	-6.71	101.25	110.77
1	L	55	ASN	N-CA-C	6.70	119.19	108.41
2	H	5	GLN	N-CA-C	6.69	119.34	108.63
2	H	172	PRO	O-C-N	-6.69	115.61	123.10
1	L	96	ASN	OD1-CG-ND2	-6.68	115.92	122.60
2	H	42	GLY	N-CA-C	6.68	124.25	115.36
2	H	148	LYS	N-CA-C	6.65	120.71	110.20
2	H	110	GLN	CA-CB-CG	6.65	127.41	114.10
1	L	50	ILE	CA-CB-CG1	6.64	121.69	110.40
2	B	98	ARG	N-CA-C	6.64	119.11	108.41
2	B	167	GLY	N-CA-C	6.64	124.80	115.43
2	B	17	SER	N-CA-C	6.63	119.66	107.99
1	A	166	GLN	CA-C-N	6.62	128.11	119.84
1	A	166	GLN	C-N-CA	6.62	128.11	119.84
2	H	175	LEU	N-CA-C	6.62	121.53	107.70
1	A	35	ALA	N-CA-C	6.61	120.07	110.42
2	B	124	PRO	N-CA-C	6.60	126.06	112.47
2	H	214	LYS	N-CA-C	6.57	120.58	110.20
2	B	64	PHE	CA-CB-CG	-6.57	107.23	113.80
1	L	50	ILE	CA-CB-CG2	-6.56	99.34	110.50
1	L	39	GLN	CG-CD-NE2	6.54	126.21	116.40
1	A	174	LYS	CA-C-O	-6.54	113.54	120.80
2	B	178	ASP	CA-CB-CG	6.53	119.13	112.60
2	B	52	ASP	CA-CB-CG	6.51	119.11	112.60
1	L	173	ASN	CA-CB-CG	6.50	119.10	112.60
2	H	159	TRP	CG-CD2-CE3	6.50	140.40	133.90
1	A	121	PHE	CA-CB-CG	6.50	120.30	113.80
1	A	131	ASN	OD1-CG-ND2	-6.49	116.11	122.60
2	B	204	HIS	CB-CG-CD2	-6.49	122.76	131.20
1	L	131	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	L	6	GLN	CG-CD-NE2	6.48	126.12	116.40
1	A	142	PHE	CA-CB-CG	6.48	120.28	113.80
1	L	25	SER	N-CA-C	6.47	118.87	111.11
2	H	39	GLN	CG-CD-NE2	6.47	126.10	116.40
2	H	176	GLN	OE1-CD-NE2	-6.46	116.14	122.60
2	H	55	ASN	CB-CG-ND2	6.46	126.09	116.40
1	A	4	VAL	CA-C-O	6.45	128.20	120.65
1	A	98	TRP	CB-CG-CD1	-6.45	117.22	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	116	PRO	O-C-N	-6.44	113.95	122.64
2	B	178	ASP	N-CA-C	6.41	124.46	110.80
2	B	130	ALA	N-CA-C	6.39	118.89	109.62
1	A	127	GLU	N-CA-C	6.39	124.41	110.80
1	L	116	PRO	N-CA-C	6.38	125.60	112.47
1	A	188	TRP	CG-CD2-CE3	6.37	140.27	133.90
2	H	134	ALA	N-CA-C	6.36	118.81	108.63
2	B	1	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	L	182	THR	N-CA-C	6.35	118.87	108.52
2	H	99	TYR	N-CA-C	6.35	118.84	108.55
1	A	208	SER	O-C-N	-6.35	116.60	123.26
1	L	7	GLU	O-C-N	-6.34	115.49	122.84
1	A	180	TYR	CA-C-O	6.34	127.14	120.36
1	A	22	CYS	N-CA-C	6.33	117.76	107.32
2	H	17	SER	O-C-N	-6.32	115.03	122.81
1	A	210	SER	N-CA-C	6.32	124.27	110.80
2	B	156	THR	CA-CB-OG1	-6.32	100.12	109.60
1	A	33	ASN	CB-CG-ND2	6.32	125.88	116.40
1	A	162	MET	N-CA-C	6.31	124.24	110.80
2	H	73	ASP	CA-CB-CG	6.31	118.91	112.60
2	H	180	TYR	N-CA-C	6.30	120.19	110.42
2	B	101	TYR	N-CA-C	-6.30	97.37	110.80
2	H	6	GLN	CB-CG-CD	6.30	123.32	112.60
1	A	80	ALA	N-CA-C	6.29	124.19	110.80
1	A	97	HIS	O-C-N	-6.29	115.23	123.28
2	H	141	VAL	N-CA-C	6.28	117.63	108.58
2	B	151	PHE	O-C-N	-6.28	117.07	121.65
1	L	131	ASN	CA-CB-CG	-6.27	106.33	112.60
2	B	73	ASP	N-CA-C	6.26	121.83	107.48
1	A	39	GLN	OE1-CD-NE2	-6.26	116.34	122.60
2	B	126	VAL	N-CA-CB	-6.26	104.77	111.46
2	B	5	GLN	CG-CD-NE2	6.24	125.76	116.40
2	H	16	ALA	O-C-N	-6.23	115.45	122.93
2	H	51	ILE	N-CA-CB	6.23	120.83	110.86
2	H	198	VAL	CA-CB-CG2	-6.22	99.82	110.40
2	B	37	ILE	N-CA-C	6.22	116.83	107.75
1	L	112	PRO	N-CA-C	6.21	125.27	112.47
2	H	63	LYS	N-CA-C	6.20	118.84	111.71
2	B	216	VAL	N-CA-C	6.19	115.35	108.05
2	B	218	ARG	N-CA-C	6.19	128.32	111.00
2	H	187	THR	N-CA-C	6.18	118.01	109.54
1	A	151	TRP	CG-CD2-CE3	6.18	140.08	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	39	GLN	N-CA-C	6.17	119.89	109.76
2	B	46	GLU	N-CA-C	6.17	118.82	108.02
1	L	148	THR	CA-CB-OG1	-6.17	100.35	109.60
1	L	23	ARG	CA-CB-CG	6.17	126.43	114.10
1	A	42	PRO	CA-N-CD	-6.16	103.38	112.00
2	B	108	TRP	CA-CB-CG	6.16	125.30	113.60
2	H	1	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	35	ALA	O-C-N	6.15	130.00	123.11
1	A	173	ASN	CB-CG-ND2	6.15	125.62	116.40
1	L	93	TRP	N-CA-CB	-6.14	101.33	110.24
1	A	164	THR	N-CA-C	6.14	117.90	109.18
2	B	165	SER	CA-C-O	6.14	127.07	120.20
1	L	182	THR	CA-CB-OG1	-6.13	100.41	109.60
2	H	64	PHE	N-CA-C	6.13	120.38	112.41
2	B	139	SER	N-CA-C	6.12	123.85	110.80
1	A	197	GLN	CA-C-O	6.12	127.01	120.46
2	H	102	CYS	N-CA-C	6.10	123.80	110.80
1	L	135	LEU	N-CA-C	6.10	118.67	108.73
2	B	193	TRP	CG-CD2-CE3	6.09	140.00	133.90
2	H	197	THR	CA-C-O	6.09	128.00	121.55
1	A	171	SER	N-CA-C	6.08	123.75	110.80
1	A	191	HIS	O-C-N	-6.08	116.92	123.42
2	B	198	VAL	N-CA-CB	-6.07	104.74	111.66
1	L	41	LYS	CA-C-N	6.06	127.42	119.84
1	L	41	LYS	C-N-CA	6.06	127.42	119.84
1	A	40	GLU	CA-CB-CG	6.06	126.22	114.10
1	L	38	VAL	N-CA-C	6.04	116.57	107.75
2	B	138	ASN	CA-CB-CG	6.04	118.64	112.60
1	L	28	ALA	N-CA-C	6.02	118.19	108.32
1	L	166	GLN	CA-C-N	6.02	127.36	119.84
1	L	166	GLN	C-N-CA	6.02	127.36	119.84
2	H	94	TYR	N-CA-C	6.02	119.05	109.24
2	B	125	SER	CA-C-O	6.01	126.94	120.63
1	A	84	ASP	N-CA-C	6.01	123.60	110.80
2	B	158	THR	N-CA-C	6.01	119.37	110.48
2	H	5	GLN	CG-CD-NE2	6.00	125.40	116.40
2	B	92	ALA	CA-C-O	6.00	127.35	121.05
2	H	50	ARG	CA-CB-CG	5.99	126.08	114.10
1	A	169	LYS	O-C-N	-5.99	114.63	122.59
2	B	89	GLU	CB-CG-CD	5.99	122.78	112.60
2	B	101	TYR	CA-CB-CG	5.97	124.65	113.90
2	H	119	ALA	N-CA-C	5.97	118.67	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	182	LEU	N-CA-C	5.97	118.55	107.99
2	B	99	TYR	CA-CB-CG	5.96	124.63	113.90
2	B	3	GLN	OE1-CD-NE2	-5.96	116.64	122.60
2	B	120	ALA	N-CA-C	5.95	119.60	110.20
1	A	81	GLN	CG-CD-NE2	5.94	125.31	116.40
1	L	117	SER	CA-CB-OG	5.93	122.97	111.10
1	L	193	SER	N-CA-C	5.93	118.78	107.75
2	H	85	SER	CA-C-O	5.92	128.97	120.51
1	A	188	TRP	CB-CG-CD1	-5.91	118.04	126.90
2	H	6	GLN	CA-CB-CG	-5.91	102.28	114.10
2	B	142	THR	N-CA-C	5.89	118.84	109.24
2	B	122	THR	CA-CB-CG2	5.88	120.50	110.50
1	L	111	GLN	CG-CD-NE2	5.88	125.21	116.40
1	A	136	VAL	CB-CA-C	-5.88	104.21	111.32
2	B	54	ASN	CA-CB-CG	5.87	118.47	112.60
1	A	183	LEU	N-CA-C	5.87	118.33	109.41
1	A	126	GLU	CA-CB-CG	5.86	125.83	114.10
2	B	173	ALA	N-CA-C	5.86	119.61	110.17
1	L	44	ARG	N-CA-C	5.86	123.28	110.80
2	H	108	TRP	CA-CB-CG	5.85	124.72	113.60
1	A	163	GLU	O-C-N	-5.85	116.55	123.22
1	A	206	GLU	N-CA-C	5.85	117.66	107.49
2	B	141	VAL	O-C-N	-5.84	116.89	123.20
1	A	74	ALA	N-CA-C	5.83	117.94	108.26
1	L	188	TRP	CG-CD2-CE3	5.83	139.73	133.90
1	L	151	TRP	CA-CB-CG	5.83	124.67	113.60
2	H	104	PRO	N-CA-C	-5.82	105.60	113.40
1	A	16	GLU	CB-CG-CD	5.82	122.50	112.60
2	H	7	SER	O-C-N	-5.81	114.86	122.59
1	L	160	GLU	N-CA-C	5.81	118.21	107.99
1	L	163	GLU	O-C-N	-5.81	116.44	123.29
1	A	203	HIS	CB-CG-CD2	-5.81	123.65	131.20
2	H	121	THR	CA-CB-CG2	5.79	120.35	110.50
2	H	204	HIS	CB-CG-CD2	-5.78	123.68	131.20
2	H	54	ASN	N-CA-C	5.78	117.66	111.36
2	H	182	LEU	O-C-N	-5.77	116.57	123.27
2	B	121	THR	N-CA-C	5.77	123.09	110.80
1	A	46	PHE	N-CA-CB	-5.77	101.92	111.49
1	L	113	LYS	N-CA-C	5.76	118.26	109.62
1	A	198	VAL	O-C-N	-5.76	116.38	122.83
1	L	42	PRO	CA-N-CD	-5.76	103.94	112.00
1	L	74	ALA	N-CA-C	5.75	117.80	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	165	SER	N-CA-C	5.75	119.11	111.75
1	L	36	ASN	OD1-CG-ND2	-5.74	116.86	122.60
1	A	6	GLN	CG-CD-NE2	5.74	125.00	116.40
2	B	199	THR	CA-CB-OG1	-5.74	101.00	109.60
1	A	58	PRO	N-CA-C	5.72	124.25	112.47
2	B	71	THR	N-CA-C	5.72	118.57	109.24
2	H	50	ARG	N-CA-C	5.72	118.48	107.44
2	B	157	VAL	CA-C-O	5.71	128.86	121.32
1	A	36	ASN	OD1-CG-ND2	-5.71	116.89	122.60
2	H	208	SER	N-CA-C	5.70	122.95	110.80
1	A	33	ASN	CA-CB-CG	5.70	118.30	112.60
1	L	152	LYS	CA-CB-CG	5.69	125.49	114.10
1	L	36	ASN	CB-CG-ND2	5.69	124.93	116.40
1	L	64	PHE	CA-CB-CG	5.68	119.48	113.80
1	L	47	THR	CA-C-O	5.68	126.96	120.54
1	L	54	ASN	N-CA-CB	-5.68	103.49	110.98
2	H	212	ASP	N-CA-C	5.67	118.43	108.56
2	H	3	GLN	OE1-CD-NE2	-5.67	116.93	122.60
2	B	36	TRP	CE2-CD2-CG	-5.67	100.39	107.20
2	B	16	ALA	CA-C-O	5.67	127.54	121.02
2	B	71	THR	N-CA-CB	-5.66	101.20	110.43
1	A	111	GLN	CA-C-N	5.64	126.89	119.84
1	A	111	GLN	C-N-CA	5.64	126.89	119.84
2	H	42	GLY	O-C-N	-5.64	115.22	122.39
2	B	12	VAL	N-CA-C	5.64	117.45	108.87
1	L	3	VAL	N-CA-C	-5.63	99.52	107.75
2	H	141	VAL	N-CA-CB	-5.63	104.58	110.72
2	B	197	THR	N-CA-CB	-5.62	101.47	109.85
1	L	47	THR	N-CA-C	5.62	118.79	109.46
1	A	185	ALA	N-CA-C	5.61	118.12	111.33
1	L	203	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	150	ASP	N-CA-C	5.60	117.92	110.53
2	H	122	THR	N-CA-C	5.60	122.50	108.40
2	H	71	THR	O-C-N	-5.59	116.54	123.36
1	A	198	VAL	N-CA-C	5.58	116.80	108.54
2	B	185	SER	N-CA-C	5.58	119.06	110.42
2	B	51	ILE	N-CA-C	5.58	115.89	107.75
1	L	33	ASN	N-CA-C	5.57	118.11	111.71
2	B	147	VAL	CB-CA-C	-5.56	103.76	110.99
2	B	198	VAL	CA-C-O	5.56	127.55	121.04
1	L	29	VAL	CA-C-O	5.55	127.72	120.78
1	L	47	THR	O-C-N	-5.55	116.89	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	MET	CA-C-O	5.55	126.35	120.36
2	H	108	TRP	CB-CG-CD1	-5.54	118.60	126.90
1	L	98	TRP	CG-CD2-CE3	5.53	139.43	133.90
2	B	93	VAL	O-C-N	-5.53	117.38	123.18
1	L	159	THR	CA-C-O	5.52	125.73	119.27
2	B	108	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	99	VAL	O-C-N	-5.51	118.01	122.97
1	L	115	SER	O-C-N	-5.51	114.98	121.32
1	L	151	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	199	THR	CB-CA-C	-5.51	99.46	109.38
2	H	199	THR	CA-CB-OG1	-5.50	101.36	109.60
2	B	39	GLN	CG-CD-NE2	5.50	124.65	116.40
2	H	186	VAL	O-C-N	-5.49	118.19	122.97
1	A	208	SER	N-CA-C	5.49	116.62	108.60
1	A	166	GLN	OE1-CD-NE2	-5.49	117.11	122.60
2	H	159	TRP	CE2-CD2-CG	-5.49	100.61	107.20
2	B	108	TRP	N-CA-CB	5.48	119.27	111.05
1	L	151	TRP	CB-CG-CD1	-5.47	118.70	126.90
1	A	99	VAL	CA-C-O	5.46	125.08	120.22
2	B	168	VAL	O-C-N	-5.46	115.75	122.57
1	L	49	LEU	N-CA-C	5.44	119.41	112.12
2	H	95	TYR	N-CA-C	5.44	117.77	108.90
2	H	182	LEU	N-CA-C	5.44	117.66	109.23
2	H	146	LEU	CA-CB-CG	5.43	135.32	116.30
1	L	156	THR	N-CA-C	5.42	121.79	109.81
2	B	193	TRP	CB-CG-CD1	-5.42	118.77	126.90
2	B	98	ARG	CA-CB-CG	5.42	124.93	114.10
1	A	93	TRP	CG-CD2-CE3	5.41	139.31	133.90
1	L	201	GLU	N-CA-CB	-5.40	104.04	112.41
2	B	141	VAL	N-CA-CB	-5.39	103.64	111.52
1	A	28	ALA	O-C-N	-5.39	118.12	123.46
1	A	62	ALA	CA-C-O	5.38	129.37	122.64
2	B	202	VAL	CA-C-O	5.38	126.80	121.09
1	A	209	LEU	CA-C-N	5.37	131.80	121.54
1	A	209	LEU	C-N-CA	5.37	131.80	121.54
1	L	3	VAL	O-C-N	-5.37	117.51	123.20
1	L	200	HIS	O-C-N	-5.36	117.06	123.27
2	B	116	VAL	N-CA-C	5.34	116.07	107.73
2	H	168	VAL	N-CA-C	5.33	116.45	109.58
2	B	194	PRO	N-CA-C	5.32	125.94	112.10
1	L	102	GLY	CA-C-O	5.32	127.82	119.31
1	L	164	THR	N-CA-C	5.32	116.73	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	HIS	N-CA-C	5.32	116.93	108.79
1	A	97	HIS	CB-CG-CD2	-5.31	124.29	131.20
2	B	85	SER	CA-C-N	5.31	128.39	120.90
2	B	85	SER	C-N-CA	5.31	128.39	120.90
2	H	165	SER	N-CA-C	5.31	117.06	111.28
1	A	98	TRP	CE2-CD2-CG	-5.30	100.84	107.20
1	L	53	THR	N-CA-CB	5.30	119.45	110.49
2	H	198	VAL	CB-CA-C	5.29	118.28	110.77
1	L	67	SER	N-CA-C	5.28	118.74	107.70
1	L	196	CYS	N-CA-C	5.28	116.85	108.67
1	L	203	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	L	153	VAL	CA-CB-CG1	5.27	119.36	110.40
1	L	36	ASN	CA-CB-CG	-5.27	107.33	112.60
1	A	54	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	B	36	TRP	CD1-CG-CD2	5.26	114.72	106.30
2	B	127	TYR	CB-CA-C	-5.26	104.96	110.33
2	H	64	PHE	CA-CB-CG	-5.26	108.54	113.80
1	L	188	TRP	CE2-CD2-CG	-5.25	100.89	107.20
1	L	80	ALA	N-CA-C	5.25	118.08	110.42
1	A	22	CYS	CB-CA-C	-5.25	104.82	111.70
2	H	86	LEU	CA-C-O	5.25	127.50	121.47
1	L	198	VAL	CA-CB-CG2	-5.24	101.48	110.40
2	B	27	TYR	N-CA-C	5.24	115.21	108.34
2	B	136	GLN	CG-CD-NE2	5.24	124.26	116.40
1	L	28	ALA	O-C-N	-5.23	117.45	123.42
1	L	135	LEU	CA-C-O	5.23	125.96	120.36
2	B	57	VAL	CG1-CB-CG2	-5.23	99.29	110.80
2	H	198	VAL	CA-CB-CG1	5.23	119.29	110.40
1	A	49	LEU	N-CA-C	5.22	120.70	110.56
2	B	36	TRP	CG-CD2-CE3	5.22	139.12	133.90
2	B	204	HIS	CB-CG-ND1	5.21	130.52	122.70
1	L	16	GLU	O-C-N	-5.21	116.71	122.86
1	L	127	GLU	CA-CB-CG	5.21	124.51	114.10
2	H	193	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	A	185	ALA	O-C-N	-5.20	116.60	122.12
1	A	152	LYS	N-CA-C	5.20	116.66	109.54
1	L	124	SER	N-CA-C	5.20	117.97	110.28
1	A	205	VAL	O-C-N	-5.19	117.52	122.97
1	A	151	TRP	CB-CG-CD1	-5.19	119.12	126.90
1	L	98	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	H	140	MET	N-CA-C	5.18	117.41	109.07
2	B	203	ALA	N-CA-C	5.18	117.93	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	28	THR	N-CA-C	5.17	117.51	108.52
1	L	165	THR	O-C-N	-5.16	116.19	123.11
1	A	20	LEU	N-CA-C	5.15	117.18	110.53
1	L	115	SER	N-CA-C	5.15	121.19	109.81
1	L	198	VAL	N-CA-CB	-5.15	104.97	111.46
2	B	217	PRO	O-C-N	5.14	128.58	122.98
1	L	4	VAL	N-CA-CB	-5.14	105.44	111.60
1	L	38	VAL	O-C-N	-5.13	117.76	123.20
1	A	168	SER	CA-CB-OG	5.13	121.37	111.10
1	A	151	TRP	CA-CB-CG	5.13	123.35	113.60
1	L	81	GLN	N-CA-C	5.13	117.92	109.72
2	B	51	ILE	CA-C-O	5.12	125.72	120.39
2	H	158	THR	O-C-N	-5.11	117.06	123.04
2	B	142	THR	O-C-N	-5.11	117.50	123.27
2	H	6	GLN	CG-CD-NE2	5.09	124.04	116.40
1	A	169	LYS	N-CA-C	5.09	121.65	110.80
2	B	186	VAL	N-CA-C	5.09	115.37	107.78
2	H	36	TRP	CG-CD2-CE3	5.09	138.99	133.90
2	B	60	PHE	O-C-N	-5.09	116.39	122.65
2	B	56	VAL	N-CA-C	5.09	119.92	109.34
1	L	158	VAL	CA-C-O	5.07	127.12	120.78
1	A	119	THR	CA-CB-OG1	-5.07	101.99	109.60
2	B	193	TRP	CE2-CD2-CG	-5.07	101.12	107.20
2	B	25	SER	CA-C-O	5.06	126.31	120.14
2	H	103	ARG	CA-C-O	-5.06	115.69	120.34
1	L	18	VAL	N-CA-C	5.05	115.02	108.35
1	A	25	SER	CA-C-O	5.05	125.86	120.20
2	B	40	ARG	CA-C-O	-5.05	114.92	120.17
2	H	54	ASN	CB-CG-ND2	5.04	123.97	116.40
2	B	175	LEU	N-CA-C	5.04	117.50	108.17
2	B	2	VAL	CB-CA-C	-5.04	103.02	111.29
2	B	100	ALA	N-CA-C	5.04	120.29	114.04
1	A	86	ALA	N-CA-C	5.03	115.95	108.60
1	A	193	SER	CA-CB-OG	5.03	121.16	111.10
1	L	151	TRP	CE2-CD2-CG	-5.03	101.16	107.20
2	B	218	ARG	N-CA-CB	-5.03	101.95	110.50
1	A	211	ARG	CA-CB-CG	5.03	124.15	114.10
2	H	68	ALA	CA-C-O	5.02	126.38	120.80
1	A	165	THR	N-CA-C	5.02	117.53	110.14
2	H	62	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	63	ARG	CA-CB-CG	5.02	124.14	114.10
1	A	115	SER	N-CA-C	-5.02	102.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	SER	CA-CB-OG	5.01	121.12	111.10
1	A	131	ASN	CB-CG-ND2	5.01	123.91	116.40
1	L	34	TYR	N-CA-CB	-5.01	104.69	112.30
1	L	125	SER	CA-C-N	5.01	127.26	120.65
1	L	125	SER	C-N-CA	5.01	127.26	120.65
2	B	96	CYS	CA-CB-SG	5.01	125.92	114.40
2	B	47	TRP	CG-CD2-CE3	5.00	138.91	133.90
2	H	54	ASN	CA-CB-CG	5.00	117.60	112.60
1	A	172	ASN	CA-CB-CG	5.00	117.60	112.60
1	L	64	PHE	CA-C-O	5.00	126.20	120.80
2	H	65	LYS	CB-CG-CD	-5.00	99.80	111.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	PRO	Peptide
1	A	143	TYR	Peptide
1	A	156	THR	Peptide
1	A	180	TYR	Sidechain
1	A	194	TYR	Sidechain
1	A	41	LYS	Peptide
2	B	103	ARG	Peptide
2	B	151	PHE	Peptide
2	B	171	PHE	Peptide
2	B	188	VAL	Peptide
2	B	193	TRP	Peptide
2	B	216	VAL	Peptide
2	H	193	TRP	Peptide
2	H	99	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	1594	0	1538	101	0
1	L	1594	0	1538	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1647	0	1622	106	0
2	H	1647	0	1622	110	0
3	B	22	0	16	2	0
3	H	22	0	16	1	0
4	H	1	0	0	0	0
4	L	3	0	0	0	0
All	All	6530	0	6352	351	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 27.

All (351) 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:150:ASP:HB2	1:A:197:GLN:HB3	1.38	1.02
2:H:105:MET:HG2	2:H:108:TRP:HE1	1.32	0.94
2:B:39:GLN:HB3	2:B:93:VAL:HB	1.55	0.88
2:H:19:LYS:HD2	2:H:80:TYR:HB3	1.57	0.86
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.58	0.86
1:A:37:TRP:HB2	1:A:50:ILE:HB	1.59	0.85
1:L:151:TRP:HD1	1:L:162:MET:SD	2.01	0.82
1:L:29:VAL:HG11	1:L:73:ALA:HB2	1.61	0.80
2:H:105:MET:HG2	2:H:108:TRP:NE1	1.96	0.80
2:H:30:THR:HA	2:H:53:PRO:HB2	1.66	0.78
2:H:5:GLN:HG2	2:H:23:LYS:HB3	1.64	0.77
2:H:69:THR:HG23	2:H:82:GLU:HB3	1.66	0.77
2:H:124:PRO:HB2	2:H:147:VAL:HG12	1.67	0.76
1:L:17:THR:HG22	1:L:78:THR:HA	1.66	0.76
1:A:49:LEU:HA	1:A:60:VAL:HG21	1.67	0.76
2:B:105:MET:HE3	2:B:108:TRP:CD1	2.20	0.76
2:B:30:THR:HA	2:B:53:PRO:HB2	1.68	0.75
2:B:91:SER:OG	2:B:115:THR:HA	1.88	0.74
2:H:126:VAL:HB	2:H:147:VAL:HG13	1.70	0.74
1:L:151:TRP:CD1	1:L:162:MET:SD	2.82	0.73
1:L:20:LEU:HD13	1:L:75:LEU:HD23	1.69	0.73
1:L:85:GLU:HB2	1:L:108:VAL:HG22	1.71	0.73
1:L:82:THR:HA	1:L:108:VAL:HG21	1.70	0.72
2:H:38:LYS:HB3	2:H:48:ILE:HD11	1.70	0.71
2:H:99:TYR:HD1	2:H:103:ARG:HG3	1.54	0.71
2:B:202:VAL:HG12	2:B:211:VAL:O	1.90	0.71
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:THR:HG22	2:B:82:GLU:HB3	1.72	0.70
1:L:48:GLY:HA3	2:H:105:MET:SD	2.31	0.69
1:A:120:LEU:HB3	1:A:137:CYS:HA	1.72	0.69
1:A:151:TRP:HD1	1:A:162:MET:HE1	1.57	0.69
1:A:39:GLN:HB3	1:A:47:THR:HB	1.73	0.69
1:A:121:PHE:HB2	2:B:129:LEU:HD23	1.74	0.69
2:B:147:VAL:HG11	2:B:202:VAL:HG21	1.73	0.69
2:B:24:ALA:HB1	2:B:27:TYR:HE1	1.57	0.68
2:B:50:ARG:NH1	3:B:996:NP:H6'	2.07	0.68
1:A:48:GLY:N	2:B:105:MET:HE1	2.09	0.68
2:H:105:MET:SD	2:H:106:ASP:C	2.77	0.68
1:L:190:ARG:HH11	1:L:190:ARG:HB3	1.59	0.68
1:A:133:ALA:HB3	1:A:183:LEU:HB2	1.77	0.67
1:A:135:LEU:HB2	1:A:181:LEU:HB3	1.77	0.67
2:H:105:MET:SD	2:H:105:MET:C	2.78	0.67
2:B:74:LYS:HA	2:B:77:SER:HA	1.77	0.66
1:L:13:SER:HB3	1:L:109:LEU:HD23	1.77	0.65
1:L:97:HIS:HB2	2:H:47:TRP:CZ3	2.32	0.65
1:A:93:TRP:CZ2	1:A:96:ASN:HA	2.31	0.65
1:L:53:THR:HG21	1:L:68:LEU:HD12	1.77	0.65
1:L:54:ASN:HA	1:L:66:GLY:HA3	1.78	0.65
2:B:52:ASP:HB3	2:B:57:VAL:HB	1.80	0.64
1:A:151:TRP:CD1	1:A:162:MET:HE1	2.33	0.64
2:B:3:GLN:NE2	2:B:5:GLN:HG3	2.13	0.64
2:H:173:ALA:HB2	2:H:182:LEU:HB2	1.79	0.64
1:A:2:ALA:N	1:A:26:THR:HG1	1.95	0.63
1:A:30:THR:HG23	1:A:32:SER:OG	1.98	0.63
2:B:27:TYR:CD2	2:B:32:TYR:HD2	2.16	0.63
1:L:33:ASN:O	1:L:93:TRP:HB3	1.98	0.63
1:A:152:LYS:HG2	1:A:157:PRO:HD3	1.80	0.63
1:A:118:VAL:HG22	1:A:139:ILE:HA	1.81	0.63
2:H:50:ARG:HH12	2:H:52:ASP:HB2	1.65	0.62
2:B:56:VAL:HG23	2:B:72:VAL:HG12	1.81	0.62
1:A:135:LEU:HD13	1:A:181:LEU:HG	1.81	0.62
2:B:99:TYR:CE2	2:B:102:CYS:HA	2.34	0.62
1:A:185:ALA:HB3	1:A:186:ARG:HH12	1.65	0.62
1:L:85:GLU:HG3	1:L:106:LEU:O	2.00	0.61
1:L:97:HIS:HB2	2:H:47:TRP:HZ3	1.63	0.61
2:H:12:VAL:HG13	2:H:116:VAL:HG13	1.80	0.61
2:B:27:TYR:HD2	2:B:32:TYR:HD2	1.47	0.61
2:B:99:TYR:CZ	2:B:102:CYS:HA	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLY:HA3	1:A:175:TYR:CD2	2.36	0.61
1:A:151:TRP:O	1:A:157:PRO:HA	2.00	0.61
1:L:41:LYS:HG2	1:L:42:PRO:HD2	1.83	0.61
2:H:34:MET:HB3	2:H:51:ILE:HG13	1.81	0.61
2:H:74:LYS:HB2	2:H:75:PRO:HD3	1.83	0.61
2:H:157:VAL:HG23	2:H:201:ASN:O	2.01	0.61
1:A:127:GLU:HB3	2:B:127:TYR:CE2	2.36	0.61
2:H:5:GLN:OE1	2:H:25:SER:HB2	2.01	0.60
2:H:29:PHE:CE2	2:H:74:LYS:HA	2.36	0.60
1:L:122:PRO:HB2	2:H:218:ARG:HH12	1.65	0.60
2:H:19:LYS:HE3	2:H:82:GLU:HB2	1.83	0.60
2:B:97:ALA:HB1	2:B:105:MET:HB3	1.84	0.60
1:A:192:ALA:HB1	1:A:210:SER:OG	2.02	0.60
1:A:14:PRO:HA	1:A:80:ALA:O	2.02	0.60
2:H:105:MET:HE2	2:H:108:TRP:HD1	1.67	0.60
1:A:36:ASN:HA	1:A:50:ILE:O	2.02	0.59
1:L:135:LEU:HB2	1:L:181:LEU:HB3	1.84	0.59
2:H:105:MET:SD	2:H:106:ASP:CA	2.90	0.59
1:A:12:THR:HG21	1:A:18:VAL:HB	1.84	0.59
2:B:55:ASN:ND2	2:B:57:VAL:HG23	2.17	0.59
1:A:198:VAL:HB	1:A:205:VAL:HB	1.84	0.59
1:L:199:THR:HG23	1:L:204:THR:HG23	1.84	0.59
2:H:50:ARG:NH1	2:H:52:ASP:HB2	2.16	0.59
1:A:107:THR:HG21	1:A:144:PRO:HG3	1.83	0.59
1:A:44:ARG:HH21	2:B:93:VAL:HG13	1.68	0.59
2:B:55:ASN:HD21	2:B:57:VAL:HG23	1.67	0.59
2:H:148:LYS:HG3	2:H:181:THR:HG23	1.85	0.59
1:A:183:LEU:HD22	1:A:187:ALA:HB1	1.85	0.59
2:H:99:TYR:HE1	2:H:102:CYS:N	2.01	0.59
1:L:121:PHE:CD2	2:H:129:LEU:HB3	2.37	0.59
2:H:52:ASP:HB3	2:H:55:ASN:OD1	2.03	0.59
2:B:143:LEU:HB2	2:B:186:VAL:HG12	1.85	0.58
1:A:120:LEU:HD11	1:A:208:SER:N	2.17	0.58
2:B:12:VAL:HG21	2:B:86:LEU:HD11	1.84	0.58
2:H:91:SER:OG	2:H:115:THR:HA	2.03	0.58
1:A:121:PHE:CD2	2:B:129:LEU:HB3	2.38	0.58
2:H:140:MET:HA	2:H:189:PRO:HA	1.84	0.58
2:H:105:MET:HG2	2:H:108:TRP:CD1	2.38	0.58
1:A:124:SER:HB3	2:B:129:LEU:HD12	1.83	0.58
2:H:33:LEU:HD11	2:H:50:ARG:HH11	1.69	0.58
1:A:53:THR:HG22	1:A:54:ASN:HD22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:ILE:HA	2:H:64:PHE:HD2	1.68	0.57
2:H:105:MET:SD	2:H:106:ASP:N	2.78	0.57
1:A:38:VAL:HG23	1:A:89:PHE:HB2	1.87	0.57
1:A:29:VAL:HA	1:A:33:ASN:HD21	1.70	0.57
2:H:129:LEU:HB2	2:H:144:GLY:O	2.05	0.56
1:A:180:TYR:OH	2:B:183:SER:HB2	2.05	0.56
2:B:19:LYS:HD3	2:B:82:GLU:HB2	1.86	0.56
2:B:17:SER:HB3	2:B:83:LEU:O	2.06	0.56
1:A:65:SER:HB2	1:A:76:THR:HB	1.86	0.56
2:H:3:GLN:HG2	2:H:25:SER:HB3	1.88	0.56
2:H:129:LEU:HA	2:H:218:ARG:NH2	2.21	0.56
2:H:161:SER:HA	2:H:201:ASN:OD1	2.06	0.56
2:B:40:ARG:HD3	2:B:41:PRO:HD3	1.88	0.56
1:L:147:VAL:HG23	1:L:200:HIS:HD2	1.70	0.55
1:L:164:THR:HG22	1:L:165:THR:N	2.21	0.55
2:H:48:ILE:HA	2:H:64:PHE:CD2	2.42	0.55
1:L:138:THR:HG23	2:H:171:PHE:HZ	1.70	0.55
1:A:34:TYR:CD1	2:B:102:CYS:HB2	2.41	0.55
1:L:49:LEU:HA	1:L:60:VAL:HG21	1.88	0.55
1:A:185:ALA:HB3	1:A:186:ARG:NH1	2.22	0.55
1:L:192:ALA:O	1:L:210:SER:HA	2.07	0.54
1:A:172:ASN:OD1	1:A:174:LYS:HE2	2.08	0.54
2:H:91:SER:HA	2:H:116:VAL:HG23	1.90	0.54
1:L:69:ILE:HG12	1:L:74:ALA:HB3	1.88	0.54
1:L:170:GLN:HG2	1:L:174:LYS:O	2.08	0.54
1:A:98:TRP:NE1	2:B:35:HIS:HE1	2.06	0.54
1:A:135:LEU:HD22	1:A:181:LEU:HD23	1.89	0.54
1:L:21:THR:HB	1:L:72:LYS:HD3	1.88	0.54
1:L:72:LYS:HZ3	1:L:74:ALA:HB2	1.73	0.54
1:L:36:ASN:ND2	1:L:51:GLY:HA2	2.23	0.54
1:L:190:ARG:HB3	1:L:190:ARG:NH1	2.21	0.54
2:H:50:ARG:NE	3:H:995:NP:H11	2.23	0.53
1:A:126:GLU:O	1:A:129:GLU:HG2	2.07	0.53
2:H:12:VAL:HG21	2:H:86:LEU:HD21	1.89	0.53
2:B:167:GLY:HA3	2:B:187:THR:OG1	2.07	0.53
2:H:97:ALA:HA	2:H:108:TRP:HA	1.91	0.53
1:L:51:GLY:HA3	2:H:103:ARG:HH12	1.73	0.53
1:A:69:ILE:HG13	1:A:74:ALA:HB3	1.91	0.53
1:A:124:SER:OG	2:B:127:TYR:HB3	2.08	0.53
2:H:19:LYS:CE	2:H:82:GLU:HB2	2.38	0.53
1:A:50:ILE:HG13	1:A:75:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:GLY:HA3	2:H:103:ARG:NH1	2.24	0.53
1:L:40:GLU:O	1:L:86:ALA:HB1	2.09	0.53
1:L:190:ARG:HD2	1:L:190:ARG:O	2.09	0.53
2:H:95:TYR:CG	2:H:108:TRP:HE3	2.27	0.52
1:A:142:PHE:CD1	1:A:142:PHE:N	2.77	0.52
2:H:47:TRP:HZ2	2:H:50:ARG:HB2	1.75	0.52
1:A:46:PHE:HB3	2:B:108:TRP:NE1	2.24	0.52
1:L:9:ALA:HA	1:L:104:THR:HG22	1.90	0.52
1:L:63:ARG:HH12	1:L:81:GLN:HE21	1.58	0.52
1:A:190:ARG:HA	1:A:211:ARG:NH1	2.25	0.52
1:L:134:THR:HG21	2:H:148:LYS:NZ	2.24	0.52
1:A:118:VAL:HG21	1:A:198:VAL:HG11	1.91	0.52
2:B:50:ARG:HH12	3:B:996:NP:H6'	1.73	0.52
1:L:87:ILE:HA	1:L:104:THR:O	2.09	0.51
1:L:158:VAL:HG11	1:L:181:LEU:HD11	1.91	0.51
2:H:76:SER:O	2:H:78:THR:HG23	2.10	0.51
2:H:103:ARG:HG2	2:H:103:ARG:HH11	1.75	0.51
1:A:147:VAL:HG23	1:A:199:THR:O	2.11	0.51
1:L:85:GLU:HB2	1:L:108:VAL:CG2	2.41	0.51
1:A:142:PHE:N	1:A:142:PHE:HD1	2.08	0.51
2:B:50:ARG:O	2:B:58:THR:HA	2.10	0.51
2:B:193:TRP:CD1	2:B:194:PRO:HA	2.46	0.51
2:B:95:TYR:HB3	2:B:108:TRP:HE3	1.76	0.51
2:B:24:ALA:HB1	2:B:27:TYR:CE1	2.41	0.50
2:H:51:ILE:CD1	2:H:79:ALA:HB1	2.41	0.50
2:H:140:MET:HB3	2:H:187:THR:HG22	1.92	0.50
2:H:86:LEU:HD12	2:H:90:ASP:OD1	2.11	0.50
2:B:193:TRP:NE1	2:B:198:VAL:H	2.10	0.50
2:H:146:LEU:HD11	2:H:148:LYS:HD2	1.94	0.50
1:A:51:GLY:HA3	2:B:103:ARG:HH12	1.77	0.50
2:B:105:MET:HE2	2:B:106:ASP:C	2.36	0.50
2:B:158:THR:O	2:B:201:ASN:HB2	2.12	0.50
2:B:50:ARG:HH21	2:B:59:LYS:HG3	1.77	0.50
2:H:36:TRP:HD1	2:H:70:LEU:HD21	1.76	0.49
2:B:117:SER:OG	2:B:119:ALA:HB3	2.12	0.49
1:A:36:ASN:OD1	2:B:103:ARG:HA	2.13	0.49
2:H:161:SER:HA	2:H:201:ASN:HD21	1.76	0.49
1:L:6:GLN:NE2	1:L:103:GLY:H	2.11	0.49
1:A:38:VAL:HG12	2:B:105:MET:SD	2.53	0.49
1:A:44:ARG:NH2	2:B:93:VAL:HG13	2.27	0.49
1:L:131:ASN:O	1:L:184:SER:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PRO:O	2:B:129:LEU:HG	2.12	0.49
1:A:23:ARG:HG2	1:A:23:ARG:HH11	1.77	0.49
2:B:153:GLU:HA	2:B:180:TYR:CE1	2.48	0.49
2:H:103:ARG:NH1	2:H:103:ARG:HG2	2.28	0.49
1:A:97:HIS:HA	2:B:47:TRP:CZ3	2.48	0.48
2:H:159:TRP:CH2	2:H:200:CYS:SG	3.07	0.48
1:A:28:ALA:HB1	1:A:71:ASP:HB2	1.94	0.48
1:A:209:LEU:HD12	2:B:133:SER:OG	2.13	0.48
2:B:175:LEU:HB3	2:B:180:TYR:HD2	1.77	0.48
1:L:69:ILE:HB	1:L:72:LYS:HZ2	1.78	0.48
2:H:45:LEU:HD13	2:H:108:TRP:HH2	1.78	0.48
1:A:36:ASN:CG	2:B:103:ARG:HA	2.39	0.48
1:L:46:PHE:O	2:H:105:MET:HE3	2.13	0.48
2:B:47:TRP:HZ2	2:B:50:ARG:HB2	1.77	0.48
2:B:193:TRP:HE1	2:B:198:VAL:H	1.60	0.48
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.32	0.48
2:H:99:TYR:CD1	2:H:103:ARG:HG3	2.42	0.48
1:A:120:LEU:HD21	1:A:207:LYS:O	2.14	0.48
1:A:111:GLN:HA	1:A:112:PRO:HD2	1.63	0.47
1:A:68:LEU:HA	1:A:73:ALA:HA	1.96	0.47
2:B:52:ASP:CB	2:B:57:VAL:HB	2.43	0.47
1:L:198:VAL:O	1:L:204:THR:HA	2.14	0.47
2:H:143:LEU:HD23	2:H:186:VAL:HG13	1.96	0.47
2:H:160:ASN:CB	2:H:164:LEU:HD22	2.44	0.47
1:L:147:VAL:HG23	1:L:200:HIS:CD2	2.48	0.47
2:H:14:PRO:HD3	2:H:116:VAL:HG12	1.96	0.47
1:A:29:VAL:HG22	1:A:92:LEU:HD21	1.97	0.47
1:A:147:VAL:HG22	1:A:148:THR:N	2.30	0.47
2:B:34:MET:HE3	2:B:79:ALA:HB2	1.95	0.47
2:B:56:VAL:HG23	2:B:72:VAL:CG1	2.44	0.47
1:L:34:TYR:CB	2:H:102:CYS:SG	3.02	0.47
2:H:12:VAL:O	2:H:116:VAL:HA	2.15	0.47
2:B:87:THR:O	2:B:116:VAL:HG11	2.14	0.47
2:B:131:PRO:HD2	2:B:143:LEU:HD13	1.96	0.47
2:H:161:SER:HA	2:H:201:ASN:ND2	2.30	0.47
1:A:38:VAL:CG2	1:A:89:PHE:HB2	2.45	0.47
1:L:164:THR:HG22	1:L:165:THR:H	1.80	0.47
1:A:4:VAL:HG13	1:A:22:CYS:SG	2.55	0.47
2:B:147:VAL:HG11	2:B:202:VAL:CG2	2.44	0.47
1:A:170:GLN:NE2	1:A:176:MET:HG2	2.30	0.46
1:L:44:ARG:HH12	2:H:111:GLY:HA3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:THR:HA	2:B:186:VAL:O	2.15	0.46
2:B:5:GLN:HE22	2:B:25:SER:HB2	1.81	0.46
2:H:33:LEU:HD23	2:H:99:TYR:OH	2.16	0.46
2:H:12:VAL:HG12	2:H:114:VAL:HG22	1.98	0.46
1:A:29:VAL:HA	1:A:33:ASN:ND2	2.30	0.46
2:B:4:PHE:CE2	2:B:96:CYS:SG	3.09	0.46
1:A:53:THR:HG23	1:A:68:LEU:HB2	1.98	0.46
1:L:49:LEU:HD11	1:L:64:PHE:CE1	2.51	0.46
2:H:193:TRP:HD1	2:H:198:VAL:HB	1.80	0.46
1:L:88:TYR:O	1:L:103:GLY:HA2	2.16	0.45
1:A:120:LEU:HD23	1:A:196:CYS:HB3	1.97	0.45
2:H:33:LEU:HD11	2:H:50:ARG:NH1	2.32	0.45
2:B:124:PRO:HB2	2:B:147:VAL:CG1	2.46	0.45
1:L:135:LEU:O	1:L:180:TYR:HA	2.17	0.45
2:H:160:ASN:H	2:H:164:LEU:CD2	2.30	0.45
2:H:160:ASN:H	2:H:164:LEU:HD22	1.81	0.45
1:A:40:GLU:HG2	1:A:89:PHE:HE2	1.81	0.45
2:B:125:SER:O	2:B:148:LYS:HB2	2.16	0.45
1:A:4:VAL:CG1	1:A:22:CYS:SG	3.04	0.45
2:H:38:LYS:HG2	2:H:46:GLU:HB2	1.98	0.45
2:B:95:TYR:HB3	2:B:108:TRP:CE3	2.51	0.45
2:H:126:VAL:O	2:H:213:LYS:HD3	2.17	0.45
2:B:188:VAL:HA	2:B:189:PRO:HD2	1.76	0.45
2:B:99:TYR:CD2	2:B:103:ARG:O	2.69	0.45
1:L:184:SER:O	1:L:187:ALA:HB3	2.17	0.44
1:A:11:THR:HG21	1:A:109:LEU:HD12	1.98	0.44
1:L:36:ASN:ND2	2:H:103:ARG:HA	2.32	0.44
1:L:142:PHE:HB2	1:L:200:HIS:NE2	2.33	0.44
2:H:87:THR:OG1	2:H:89:GLU:HB2	2.18	0.44
2:B:37:ILE:HG21	2:B:108:TRP:HZ3	1.82	0.44
1:L:166:GLN:HG2	1:L:167:PRO:HG2	2.00	0.44
2:H:19:LYS:HD2	2:H:80:TYR:CB	2.39	0.44
1:A:18:VAL:HG12	1:A:80:ALA:HB2	1.99	0.44
2:B:204:HIS:CE1	2:B:207:SER:OG	2.70	0.44
1:L:142:PHE:HB2	1:L:200:HIS:CE1	2.53	0.44
2:B:99:TYR:HD2	2:B:103:ARG:O	2.00	0.44
2:H:51:ILE:HD11	2:H:79:ALA:HB1	2.00	0.44
2:B:193:TRP:CD1	2:B:197:THR:HA	2.53	0.44
1:L:183:LEU:HD21	1:L:194:TYR:HE2	1.82	0.44
2:H:81:MET:HG2	2:H:83:LEU:CD1	2.47	0.43
2:B:124:PRO:HB2	2:B:147:VAL:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:HE2	1:A:147:VAL:HG11	1.82	0.43
2:B:29:PHE:CD2	2:B:74:LYS:HB3	2.53	0.43
2:B:30:THR:CG2	2:B:74:LYS:HG2	2.49	0.43
1:L:48:GLY:CA	2:H:105:MET:SD	3.02	0.43
1:L:153:VAL:HG22	1:L:194:TYR:CE2	2.54	0.43
2:B:130:ALA:HA	2:B:131:PRO:HD2	1.83	0.43
1:L:46:PHE:CE2	2:H:45:LEU:HD11	2.54	0.43
2:B:71:THR:O	2:B:80:TYR:HB2	2.18	0.43
2:B:131:PRO:CD	2:B:143:LEU:HD13	2.49	0.43
1:A:120:LEU:HD11	1:A:207:LYS:C	2.44	0.42
2:B:105:MET:HE3	2:B:108:TRP:NE1	2.32	0.42
2:H:33:LEU:HD23	2:H:99:TYR:CZ	2.54	0.42
2:H:50:ARG:O	2:H:58:THR:HA	2.18	0.42
2:H:126:VAL:HA	2:H:146:LEU:O	2.18	0.42
1:A:44:ARG:NH2	2:B:113:THR:HG23	2.34	0.42
1:A:170:GLN:HG2	1:A:172:ASN:ND2	2.34	0.42
2:B:4:PHE:HE2	2:B:96:CYS:SG	2.43	0.42
2:H:105:MET:HE2	2:H:108:TRP:CD1	2.51	0.42
2:H:141:VAL:HG12	2:H:188:VAL:O	2.19	0.42
2:B:61:ASN:HB3	2:B:64:PHE:HB2	2.00	0.42
1:L:166:GLN:HA	1:L:167:PRO:HD2	1.79	0.42
2:H:36:TRP:HA	2:H:95:TYR:O	2.20	0.42
1:A:127:GLU:HB3	2:B:127:TYR:CZ	2.54	0.42
2:B:36:TRP:CH2	2:B:96:CYS:HB3	2.55	0.42
1:A:172:ASN:OD1	1:A:174:LYS:HB2	2.19	0.42
1:L:121:PHE:O	1:L:209:LEU:HD11	2.20	0.42
2:H:6:GLN:HG3	2:H:21:SER:O	2.20	0.42
1:A:133:ALA:O	1:A:135:LEU:HD12	2.20	0.42
2:B:125:SER:N	2:B:148:LYS:O	2.53	0.42
2:B:148:LYS:HG2	2:B:181:THR:HG23	2.02	0.42
2:B:195:SER:O	2:B:197:THR:N	2.52	0.42
1:L:6:GLN:HE21	1:L:6:GLN:HB2	1.74	0.41
1:L:121:PHE:HD2	2:H:129:LEU:HB3	1.85	0.41
1:A:11:THR:HG22	1:A:12:THR:N	2.35	0.41
1:A:151:TRP:HA	1:A:195:SER:O	2.20	0.41
1:L:34:TYR:HB2	2:H:102:CYS:SG	2.61	0.41
2:H:140:MET:HE3	2:H:189:PRO:HG3	2.01	0.41
1:A:48:GLY:H	2:B:105:MET:HE1	1.82	0.41
1:L:5:THR:N	1:L:23:ARG:O	2.53	0.41
2:H:93:VAL:HA	2:H:113:THR:HA	2.02	0.41
1:A:85:GLU:OE2	1:A:108:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:ASN:CG	2:H:103:ARG:HA	2.45	0.41
2:H:4:PHE:HE1	2:H:96:CYS:SG	2.44	0.41
1:A:170:GLN:O	1:A:172:ASN:N	2.53	0.41
1:L:133:ALA:HB3	1:L:183:LEU:HD12	2.02	0.41
1:L:199:THR:HG22	1:L:203:HIS:N	2.35	0.41
1:A:22:CYS:HB3	1:A:73:ALA:HB3	2.03	0.41
1:A:98:TRP:CD1	2:B:35:HIS:HE1	2.38	0.41
1:A:158:VAL:HG11	1:A:181:LEU:HD13	2.02	0.41
2:B:136:GLN:O	2:B:138:ASN:N	2.53	0.41
1:L:143:TYR:HD2	1:L:174:LYS:HG3	1.85	0.41
1:A:34:TYR:HB3	2:B:102:CYS:HB3	2.03	0.41
1:A:152:LYS:NZ	1:A:197:GLN:NE2	2.69	0.41
2:B:3:GLN:HE21	2:B:5:GLN:HG3	1.85	0.41
2:H:199:THR:OG1	2:H:214:LYS:HG2	2.21	0.41
1:A:36:ASN:ND2	2:B:103:ARG:HA	2.36	0.41
1:A:44:ARG:HH21	2:B:93:VAL:CG1	2.33	0.41
1:L:120:LEU:HD13	1:L:151:TRP:CH2	2.56	0.41
1:L:122:PRO:HB2	2:H:218:ARG:NH1	2.34	0.41
1:A:9:ALA:HB1	1:A:105:LYS:HB2	2.03	0.41
2:B:193:TRP:CG	2:B:194:PRO:HA	2.56	0.41
1:L:140:THR:O	1:L:141:ASP:HB2	2.21	0.41
1:A:197:GLN:HB2	1:A:206:GLU:OE1	2.21	0.41
2:B:10:GLU:HB2	2:B:114:VAL:HG22	2.03	0.41
2:B:50:ARG:C	2:B:50:ARG:HD2	2.46	0.41
1:L:34:TYR:HB3	2:H:102:CYS:SG	2.61	0.40
1:L:96:ASN:O	1:L:97:HIS:HB3	2.21	0.40
1:A:18:VAL:HG13	1:A:77:ILE:HB	2.03	0.40
1:A:90:CYS:SG	1:A:91:ALA:N	2.94	0.40
2:B:2:VAL:HG11	2:B:98:ARG:HH12	1.85	0.40
2:B:68:ALA:HA	2:B:82:GLU:O	2.20	0.40
1:L:20:LEU:N	1:L:75:LEU:O	2.54	0.40
1:L:134:THR:HG21	2:H:148:LYS:HZ1	1.86	0.40
2:H:131:PRO:HG3	2:H:143:LEU:HD13	2.03	0.40
1:A:123:PRO:HG3	1:A:135:LEU:HG	2.04	0.40
2:B:127:TYR:HA	2:B:128:PRO:HD2	1.90	0.40
1:L:36:ASN:O	1:L:90:CYS:HA	2.22	0.40
2:H:193:TRP:CE3	2:H:194:PRO:HD3	2.57	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	207/211 (98%)	149 (72%)	41 (20%)	17 (8%)	0	3
1	L	207/211 (98%)	164 (79%)	28 (14%)	15 (7%)	1	4
2	B	214/218 (98%)	155 (72%)	35 (16%)	24 (11%)	0	1
2	H	214/218 (98%)	167 (78%)	23 (11%)	24 (11%)	0	1
All	All	842/858 (98%)	635 (75%)	127 (15%)	80 (10%)	0	2

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	112	PRO
1	L	154	ASP
1	L	167	PRO
1	L	171	SER
2	H	7	SER
2	H	139	SER
1	A	41	LYS
1	A	47	THR
1	A	112	PRO
1	A	127	GLU
1	A	169	LYS
1	A	171	SER
1	A	210	SER
2	B	57	VAL
2	B	121	THR
2	B	137	THR
2	B	139	SER
2	B	160	ASN
2	B	166	SER
2	B	176	GLN
2	B	190	ALA
2	B	191	SER

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Mol	Chain	Res	Type
2	B	205	PRO
1	L	95	SER
2	H	4	PHE
2	H	29	PHE
2	H	85	SER
2	H	100	ALA
2	H	102	CYS
2	H	135	ALA
2	H	137	THR
2	H	161	SER
1	A	43	ASP
1	A	95	SER
1	A	167	PRO
2	B	7	SER
2	B	102	CYS
1	L	35	ALA
1	L	42	PRO
1	L	82	THR
1	L	145	GLY
2	H	41	PRO
2	H	56	VAL
2	H	121	THR
1	A	7	GLU
1	A	27	GLY
1	A	157	PRO
1	A	162	MET
2	B	194	PRO
1	L	6	GLN
1	L	29	VAL
1	L	41	LYS
2	H	131	PRO
2	H	154	PRO
2	H	190	ALA
2	H	195	SER
1	A	54	ASN
2	B	55	ASN
2	B	56	VAL
2	B	110	GLN
2	B	153	GLU
2	B	161	SER
2	B	177	SER
2	B	178	ASP

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Mol	Chain	Res	Type
1	L	44	ARG
1	L	97	HIS
2	H	166	SER
2	H	205	PRO
2	H	206	ALA
2	B	208	SER
1	L	115	SER
2	H	77	SER
2	H	192	THR
2	H	208	SER
1	A	58	PRO
1	A	144	PRO
2	B	128	PRO
2	H	14	PRO
2	B	131	PRO
2	B	124	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	177/177 (100%)	133 (75%)	44 (25%)	0	4
1	L	177/177 (100%)	129 (73%)	48 (27%)	0	2
2	B	185/185 (100%)	141 (76%)	44 (24%)	1	4
2	H	185/185 (100%)	147 (80%)	38 (20%)	1	7
All	All	724/724 (100%)	550 (76%)	174 (24%)	1	4

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	4	VAL
1	L	6	GLN
1	L	10	LEU
1	L	18	VAL
1	L	23	ARG

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Mol	Chain	Res	Type
1	L	26	THR
1	L	30	THR
1	L	31	THR
1	L	36	ASN
1	L	39	GLN
1	L	41	LYS
1	L	43	ASP
1	L	45	LEU
1	L	54	ASN
1	L	65	SER
1	L	67	SER
1	L	75	LEU
1	L	83	GLU
1	L	92	LEU
1	L	104	THR
1	L	106	LEU
1	L	112	PRO
1	L	119	THR
1	L	120	LEU
1	L	126	GLU
1	L	128	LEU
1	L	134	THR
1	L	140	THR
1	L	147	VAL
1	L	148	THR
1	L	149	VAL
1	L	152	LYS
1	L	153	VAL
1	L	154	ASP
1	L	163	GLU
1	L	168	SER
1	L	169	LYS
1	L	174	LYS
1	L	176	MET
1	L	182	THR
1	L	190	ARG
1	L	199	THR
1	L	200	HIS
1	L	204	THR
1	L	205	VAL
1	L	206	GLU
1	L	207	LYS

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Mol	Chain	Res	Type
1	L	208	SER
2	H	10	GLU
2	H	11	LEU
2	H	14	PRO
2	H	20	LEU
2	H	25	SER
2	H	40	ARG
2	H	51	ILE
2	H	69	THR
2	H	70	LEU
2	H	71	THR
2	H	72	VAL
2	H	75	PRO
2	H	80	TYR
2	H	98	ARG
2	H	99	TYR
2	H	101	TYR
2	H	102	CYS
2	H	103	ARG
2	H	104	PRO
2	H	106	ASP
2	H	110	GLN
2	H	116	VAL
2	H	122	THR
2	H	136	GLN
2	H	142	THR
2	H	143	LEU
2	H	145	CYS
2	H	146	LEU
2	H	147	VAL
2	H	152	PRO
2	H	158	THR
2	H	159	TRP
2	H	161	SER
2	H	164	LEU
2	H	182	LEU
2	H	198	VAL
2	H	200	CYS
2	H	216	VAL
1	A	6	GLN
1	A	7	GLU
1	A	17	THR

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Mol	Chain	Res	Type
1	A	30	THR
1	A	31	THR
1	A	33	ASN
1	A	46	PHE
1	A	49	LEU
1	A	55	ASN
1	A	68	LEU
1	A	76	THR
1	A	78	THR
1	A	85	GLU
1	A	90	CYS
1	A	96	ASN
1	A	97	HIS
1	A	106	LEU
1	A	108	VAL
1	A	111	GLN
1	A	112	PRO
1	A	119	THR
1	A	120	LEU
1	A	125	SER
1	A	126	GLU
1	A	127	GLU
1	A	138	THR
1	A	142	PHE
1	A	144	PRO
1	A	149	VAL
1	A	150	ASP
1	A	157	PRO
1	A	166	GLN
1	A	167	PRO
1	A	168	SER
1	A	170	GLN
1	A	172	ASN
1	A	173	ASN
1	A	186	ARG
1	A	188	TRP
1	A	190	ARG
1	A	196	CYS
1	A	199	THR
1	A	200	HIS
1	A	211	ARG
2	B	2	VAL

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Mol	Chain	Res	Type
2	B	3	GLN
2	B	4	PHE
2	B	5	GLN
2	B	6	GLN
2	B	14	PRO
2	B	20	LEU
2	B	25	SER
2	B	31	SER
2	B	37	ILE
2	B	39	GLN
2	B	43	ARG
2	B	46	GLU
2	B	51	ILE
2	B	56	VAL
2	B	58	THR
2	B	71	THR
2	B	74	LYS
2	B	75	PRO
2	B	99	TYR
2	B	104	PRO
2	B	108	TRP
2	B	112	THR
2	B	113	THR
2	B	118	SER
2	B	147	VAL
2	B	153	GLU
2	B	155	VAL
2	B	158	THR
2	B	164	LEU
2	B	166	SER
2	B	174	VAL
2	B	180	TYR
2	B	182	LEU
2	B	183	SER
2	B	185	SER
2	B	186	VAL
2	B	188	VAL
2	B	193	TRP
2	B	194	PRO
2	B	197	THR
2	B	209	THR
2	B	212	ASP

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Mol	Chain	Res	Type
2	B	216	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	33	ASN
1	L	39	GLN
1	L	54	ASN
1	L	81	GLN
1	L	170	GLN
1	L	200	HIS
2	H	35	HIS
2	H	138	ASN
1	A	39	GLN
1	A	54	ASN
1	A	131	ASN
1	A	197	GLN
2	B	3	GLN
2	B	35	HIS
2	B	54	ASN
2	B	55	ASN
2	B	136	GLN
2	B	204	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NP	H	995	-	22,22,22	1.69	2 (9%)	24,28,28	9.01	8 (33%)
3	NP	B	996	-	22,22,22	1.82	3 (13%)	24,28,28	4.96	9 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NP	H	995	-	-	6/15/17/17	0/1/1/1
3	NP	B	996	-	-	10/15/17/17	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	996	NP	C5'-N5'	-6.40	1.34	1.45
3	H	995	NP	C5'-N5'	-5.48	1.35	1.45
3	H	995	NP	ON2-N5'	3.72	1.29	1.22
3	B	996	NP	ON2-N5'	3.23	1.28	1.22
3	B	996	NP	O4-C9	-2.22	1.23	1.30

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	995	NP	C1-C2-N3	30.42	158.28	116.06
3	H	995	NP	O2-C2-N3	-25.75	72.51	123.03
3	B	996	NP	O2-C2-C1	-19.62	79.46	121.99
3	H	995	NP	O2-C2-C1	-16.70	85.79	121.99
3	B	996	NP	C1-C2-N3	-7.48	105.68	116.06
3	B	996	NP	O2-C2-N3	-7.08	109.14	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	996	NP	C4-N3-C2	6.78	135.45	122.82
3	H	995	NP	C4-N3-C2	5.43	132.93	122.82
3	B	996	NP	C5-C4-N3	-4.24	100.30	112.20
3	H	995	NP	ON2-N5'-C5'	3.95	125.79	119.03
3	H	995	NP	O4-C9-C8	2.51	121.93	114.00
3	B	996	NP	C6-C5-C4	2.46	124.91	113.56
3	B	996	NP	C6'-C5'-C4'	-2.24	118.56	121.42
3	B	996	NP	ON2-N5'-C5'	2.22	122.83	119.03
3	B	996	NP	C5'-C6'-C1'	2.07	122.87	118.55
3	H	995	NP	C1'-C1-C2	-2.06	106.19	112.33
3	H	995	NP	O4'-C4'-C3'	-2.00	113.99	119.36

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	996	NP	C1-C2-N3-C4
3	B	996	NP	O2-C2-N3-C4
3	B	996	NP	C6-C7-C8-C9
3	H	995	NP	O2-C2-N3-C4
3	H	995	NP	C1'-C1-C2-O2
3	B	996	NP	C2-C1-C1'-C2'
3	B	996	NP	C2-C1-C1'-C6'
3	B	996	NP	C1'-C1-C2-O2
3	H	995	NP	C6-C7-C8-C9
3	H	995	NP	C5-C6-C7-C8
3	B	996	NP	C7-C8-C9-O3
3	H	995	NP	C7-C8-C9-O4
3	B	996	NP	C7-C8-C9-O4
3	H	995	NP	C7-C8-C9-O3
3	B	996	NP	C5-C6-C7-C8
3	B	996	NP	C4-C5-C6-C7

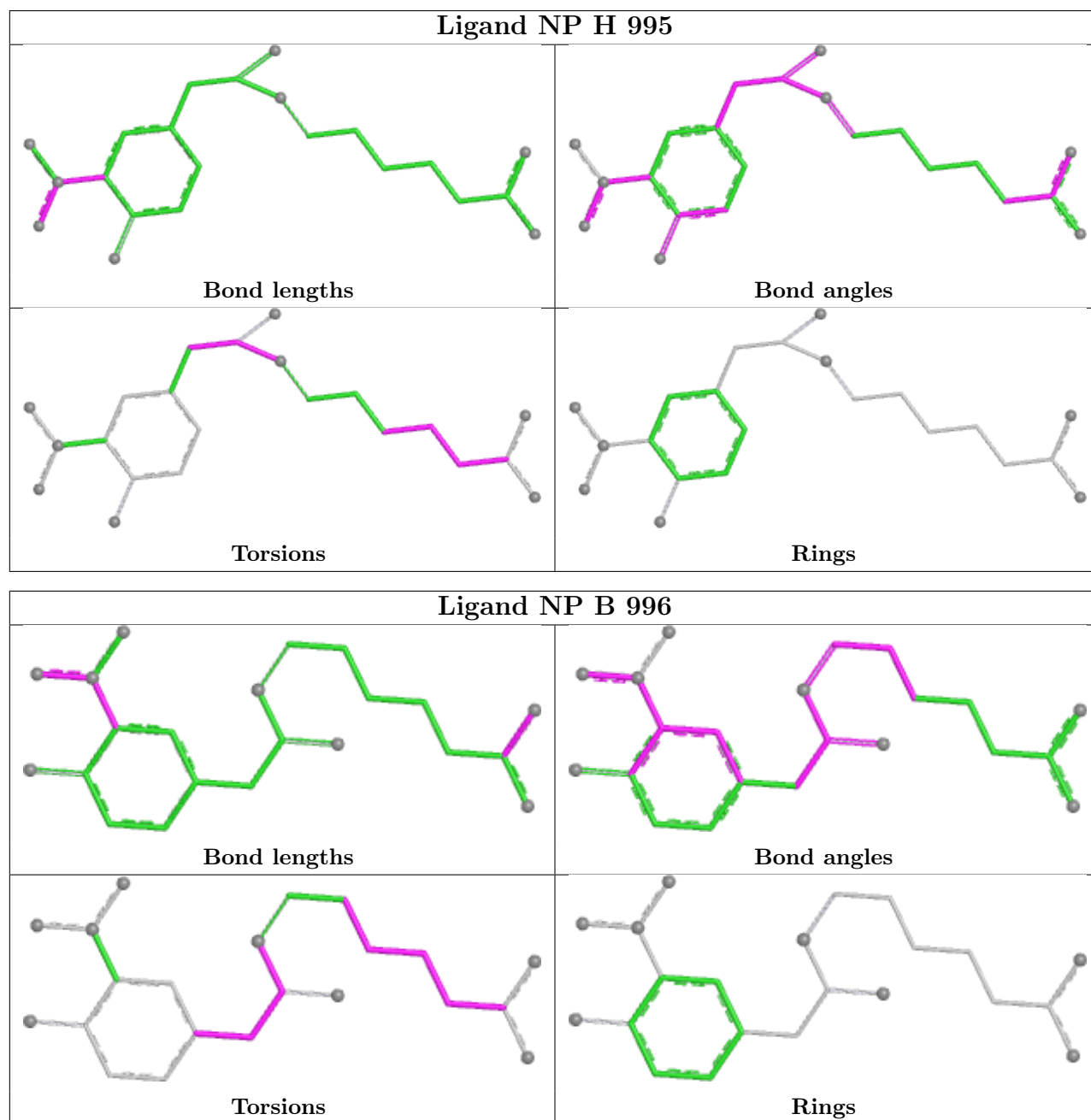
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	995	NP	1	0
3	B	996	NP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	H	1
1	A	1
1	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	117:SER	C	118:SER	N	3.13
1	H	117:SER	C	118:SER	N	3.12
1	A	109:LEU	C	110:GLY	N	3.02
1	L	109:LEU	C	110:GLY	N	2.88

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.