



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 AM UTC

PDB ID : 4FAB / pdb_00004fab
Title : THREE-DIMENSIONAL STRUCTURE OF A FLUORESCCEIN-FAB COM-
PLEX CRYSTALLIZED IN 2-METHYL-2,4-PENTANEDIOL
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Deposited on : 1989-04-10
Resolution : 2.70 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

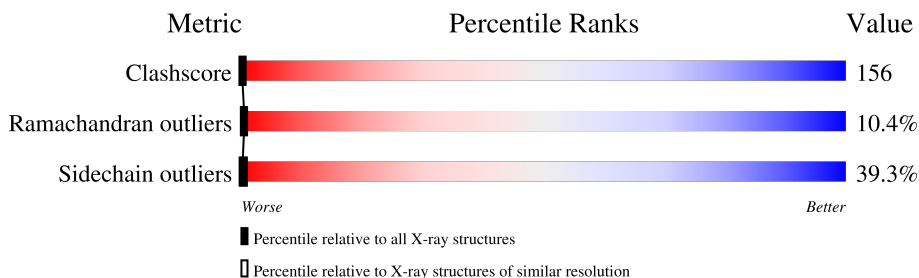
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	L	219	
2	H	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLU	H	218	-	-	X	-
4	MPD	H	219	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3395 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 IGG2A-KAPPA 4-4-20 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1700	1060	291	342	7			

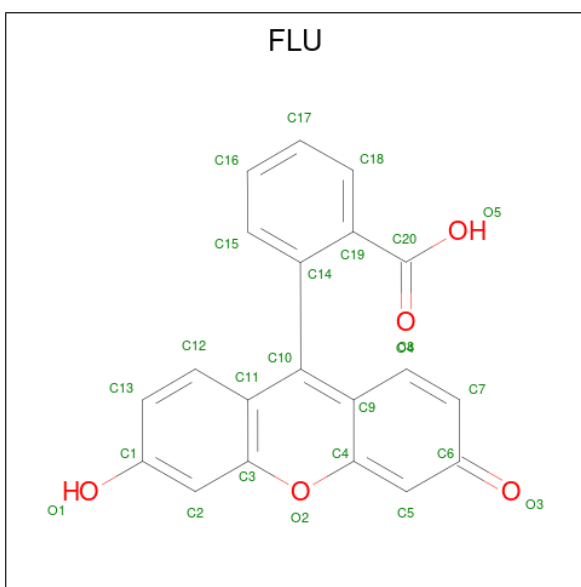
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	VAL	ILE	conflict	GB 1589925
L	7	THR	SER	conflict	GB 1589925
L	29	LEU	VAL	conflict	GB 1589925
L	33	GLN	ASN	conflict	GB 1589925
L	39	ARG	GLU	conflict	GB 1589925
L	41	TYR	PHE	conflict	GB 1589925
L	51	VAL	LEU	conflict	GB 1589925
L	92	PHE	TYR	conflict	GB 1589925
L	94	SER	PHE	conflict	GB 1589925
L	96	SER	ALA	conflict	GB 1589925
L	97	THR	SER	conflict	GB 1589925
L	217	ASN	GLY	conflict	GB 1589925

- Molecule 2 is a protein called IGG2A-KAPPA 4-4-20 FAB (HEAVY CHAIN).

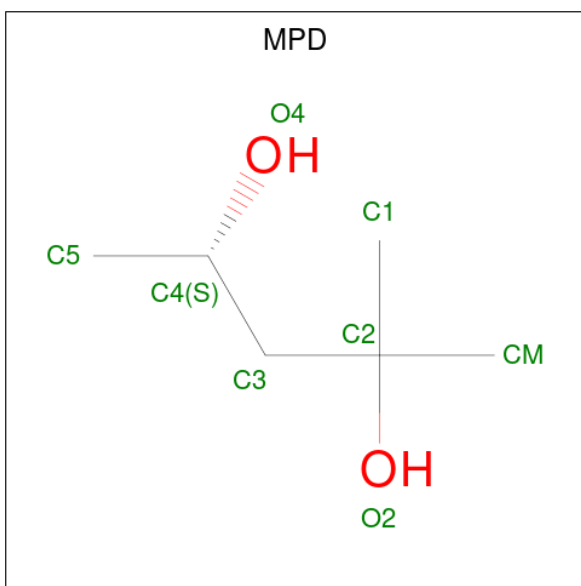
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1662	1050	269	333	10			

- Molecule 3 is 2-(6-HYDROXY-3-OXO-3H-XANTHEN-9-YL)-BENZOIC ACID (CCD ID: FLU) (formula: C₂₀H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			25	20	5		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



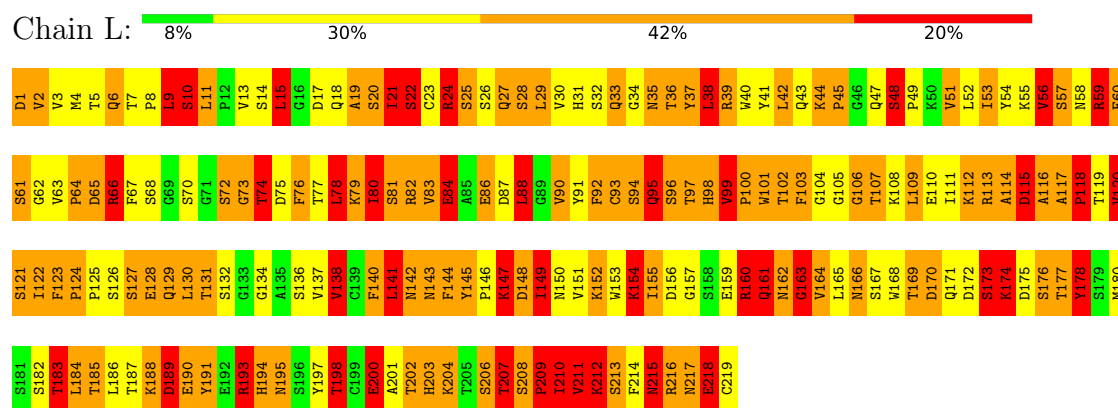
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			8	6	2		

3 Residue-property plots

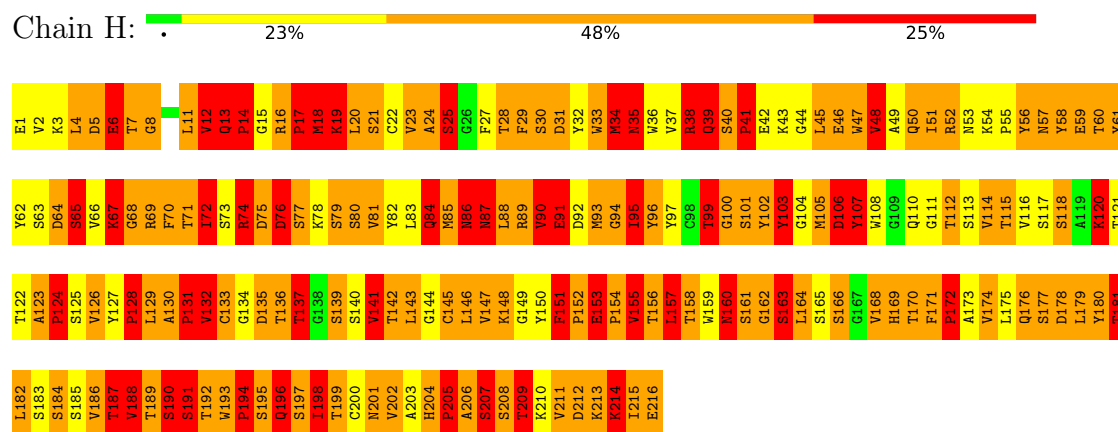
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: IGG2A-KAPPA 4-4-20 FAB (LIGHT CHAIN)



• Molecule 2: IGG2A-KAPPA 4-4-20 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 1	Depositor
Cell constants a, b, c, α , β , γ	58.30Å 43.90Å 42.50Å 82.10° 87.30° 84.60°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3395	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	L	1.62	19/1739 (1.1%)	3.03	217/2359 (9.2%)
2	H	1.76	31/1706 (1.8%)	3.22	250/2326 (10.7%)
All	All	1.69	50/3445 (1.5%)	3.13	467/4685 (10.0%)

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	L	0	2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	204	HIS	N-CA	8.41	1.55	1.46
2	H	215	ILE	N-CA	7.78	1.55	1.46
2	H	196	GLN	N-CA	7.55	1.55	1.46
1	L	23	CYS	N-CA	7.43	1.55	1.46
2	H	196	GLN	CA-CB	-7.29	1.41	1.53
2	H	72	ILE	CA-CB	7.20	1.62	1.54
2	H	8	GLY	N-CA	-7.16	1.34	1.45
2	H	56	TYR	CA-CB	6.72	1.64	1.53
1	L	78	LEU	CA-CB	-6.64	1.43	1.53
2	H	209	THR	CA-CB	6.62	1.64	1.53
1	L	173	SER	C-O	6.52	1.28	1.24
2	H	142	THR	CA-C	6.29	1.60	1.52
1	L	115	ASP	C-O	6.28	1.31	1.24
1	L	78	LEU	N-CA	6.26	1.53	1.45
2	H	177	SER	N-CA	6.22	1.54	1.46
1	L	74	THR	CB-OG1	6.17	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	5	THR	CA-CB	6.13	1.63	1.53
1	L	149	ILE	CA-C	6.13	1.60	1.53
1	L	114	ALA	CA-C	6.04	1.55	1.52
1	L	34	GLY	N-CA	5.91	1.53	1.45
2	H	181	THR	N-CA	5.85	1.53	1.46
2	H	13	GLN	CA-CB	-5.78	1.45	1.53
1	L	116	ALA	CA-CB	5.76	1.63	1.53
2	H	132	VAL	N-CA	5.73	1.51	1.46
2	H	162	GLY	N-CA	5.71	1.53	1.45
1	L	84	GLU	CA-CB	-5.68	1.44	1.53
2	H	163	SER	C-O	5.67	1.31	1.24
2	H	13	GLN	N-CA	5.66	1.55	1.45
1	L	140	PHE	CA-C	5.65	1.59	1.52
2	H	52	ARG	CA-C	-5.54	1.50	1.53
1	L	177	THR	CA-CB	5.49	1.61	1.53
2	H	110	GLN	CA-CB	-5.49	1.46	1.54
1	L	81	SER	N-CA	5.47	1.52	1.46
2	H	35	ASN	N-CA	5.42	1.52	1.46
1	L	84	GLU	CA-C	5.41	1.59	1.52
2	H	14	PRO	N-CA	5.41	1.54	1.47
2	H	100	GLY	N-CA	5.35	1.50	1.44
2	H	153	GLU	CA-CB	5.34	1.61	1.53
1	L	194	HIS	N-CA	5.33	1.52	1.45
2	H	135	ASP	C-O	5.30	1.29	1.24
2	H	132	VAL	CA-C	-5.25	1.47	1.52
2	H	78	LYS	N-CA	5.25	1.52	1.46
1	L	119	THR	N-CA	5.19	1.52	1.46
2	H	94	GLY	N-CA	5.14	1.50	1.45
2	H	157	LEU	N-CA	5.14	1.52	1.45
2	H	48	VAL	C-O	5.13	1.30	1.24
2	H	45	LEU	N-CA	5.11	1.52	1.46
2	H	170	THR	CA-CB	5.10	1.60	1.53
2	H	199	THR	CA-CB	5.06	1.61	1.53
1	L	99	VAL	N-CA	5.04	1.52	1.46

All (467) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	204	HIS	CA-CB-CG	27.67	141.47	113.80
1	L	142	ASN	CA-CB-CG	23.09	135.69	112.60
2	H	35	ASN	CA-CB-CG	18.70	131.30	112.60
2	H	196	GLN	CA-CB-CG	18.45	151.00	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	SER	CA-CB-OG	17.30	145.71	111.10
1	L	115	ASP	CA-CB-CG	17.20	129.80	112.60
2	H	106	ASP	CA-CB-CG	-16.40	96.20	112.60
2	H	160	ASN	CA-CB-CG	-15.57	97.03	112.60
1	L	35	ASN	CA-CB-CG	-15.43	97.17	112.60
2	H	16	ARG	CA-CB-CG	14.60	143.30	114.10
2	H	91	GLU	CB-CG-CD	14.23	136.80	112.60
2	H	215	ILE	CB-CA-C	13.61	125.93	111.23
2	H	110	GLN	N-CA-C	-13.61	96.76	114.31
1	L	58	ASN	CA-CB-CG	-13.40	99.20	112.60
1	L	84	GLU	CA-CB-CG	13.09	140.28	114.10
1	L	58	ASN	OD1-CG-ND2	13.02	135.62	122.60
2	H	87	ASN	CA-CB-CG	12.92	125.52	112.60
2	H	142	THR	N-CA-CB	12.73	131.18	110.69
2	H	110	GLN	CA-CB-CG	12.59	139.28	114.10
1	L	149	ILE	N-CA-CB	12.56	126.52	112.45
1	L	66	ARG	CD-NE-CZ	12.44	141.81	124.40
1	L	207	THR	N-CA-CB	12.38	131.41	110.49
2	H	132	VAL	CB-CA-C	11.77	121.52	111.05
2	H	15	GLY	N-CA-C	11.76	141.06	113.18
2	H	181	THR	CB-CA-C	11.54	129.85	109.65
1	L	217	ASN	CA-CB-CG	-11.49	101.11	112.60
1	L	1	ASP	CA-CB-CG	11.35	123.95	112.60
2	H	76	ASP	CA-CB-CG	11.31	123.91	112.60
1	L	65	ASP	CA-CB-CG	-11.17	101.43	112.60
1	L	92	PHE	CA-CB-CG	11.11	124.91	113.80
2	H	71	THR	CA-C-O	11.09	134.18	120.54
1	L	170	ASP	CA-C-O	-11.09	108.72	121.47
1	L	115	ASP	CA-C-O	-11.08	104.67	120.51
2	H	110	GLN	N-CA-CB	10.92	125.43	110.90
1	L	193	ARG	NE-CZ-NH2	-10.89	109.40	119.20
2	H	7	THR	CA-C-O	10.87	132.23	120.38
2	H	160	ASN	N-CA-C	10.79	125.10	107.73
2	H	33	TRP	CA-CB-CG	10.77	134.07	113.60
2	H	195	SER	O-C-N	10.76	133.15	122.07
2	H	31	ASP	CA-CB-CG	-10.66	101.94	112.60
2	H	84	GLN	CB-CG-CD	10.66	130.72	112.60
1	L	21	ILE	CB-CA-C	10.60	126.62	110.83
1	L	116	ALA	N-CA-C	10.54	133.26	110.80
2	H	5	ASP	CA-CB-CG	-10.37	102.23	112.60
2	H	132	VAL	N-CA-CB	-10.32	103.18	111.64
1	L	215	ASN	CA-CB-CG	10.31	122.91	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	160	ASN	OD1-CG-ND2	10.22	132.82	122.60
1	L	210	ILE	CB-CA-C	-10.19	98.63	110.96
2	H	195	SER	CA-C-O	-10.09	110.23	120.82
2	H	71	THR	CA-C-N	10.06	135.60	122.93
2	H	71	THR	C-N-CA	10.06	135.60	122.93
2	H	16	ARG	CD-NE-CZ	10.00	138.39	124.40
1	L	114	ALA	CA-C-O	9.93	125.60	119.55
1	L	173	SER	CA-C-O	-9.87	110.98	120.56
1	L	60	PHE	CA-CB-CG	-9.83	103.97	113.80
1	L	170	ASP	CA-CB-CG	9.81	122.41	112.60
2	H	38	ARG	CD-NE-CZ	9.79	138.10	124.40
2	H	197	SER	N-CA-C	9.67	120.66	108.19
1	L	113	ARG	CD-NE-CZ	9.63	137.88	124.40
2	H	90	VAL	CA-C-O	-9.63	108.74	120.78
2	H	14	PRO	CB-CA-C	9.58	127.37	111.56
2	H	8	GLY	N-CA-C	9.54	135.80	113.18
2	H	84	GLN	OE1-CD-NE2	-9.53	113.07	122.60
2	H	1	GLU	CB-CG-CD	9.47	128.70	112.60
1	L	138	VAL	N-CA-C	9.27	121.83	108.48
1	L	124	PRO	O-C-N	9.24	125.49	121.15
2	H	16	ARG	NE-CZ-NH1	9.13	130.63	121.50
2	H	78	LYS	N-CA-C	-8.95	91.73	110.80
2	H	154	PRO	N-CA-C	8.87	127.76	113.12
1	L	84	GLU	N-CA-CB	8.83	123.71	110.29
2	H	17	PRO	N-CA-C	8.80	130.59	112.47
1	L	218	GLU	CA-C-O	8.79	130.80	120.43
2	H	132	VAL	CA-C-O	-8.78	112.99	120.80
1	L	193	ARG	N-CA-CB	8.77	123.49	110.33
1	L	190	GLU	CA-CB-CG	8.75	131.60	114.10
2	H	213	LYS	CB-CA-C	8.73	127.63	109.38
2	H	153	GLU	N-CA-C	8.68	128.99	109.81
1	L	162	ASN	CB-CA-C	8.66	126.41	110.56
1	L	113	ARG	CA-CB-CG	8.45	131.01	114.10
2	H	57	ASN	CA-CB-CG	-8.41	104.19	112.60
2	H	188	VAL	CA-C-O	-8.40	112.85	121.67
1	L	129	GLN	N-CA-C	-8.38	102.09	111.14
2	H	58	TYR	N-CA-C	-8.35	100.73	111.92
1	L	84	GLU	N-CA-C	-8.34	98.14	110.48
2	H	205	PRO	N-CA-C	-8.32	101.57	113.47
1	L	149	ILE	O-C-N	8.31	131.64	122.92
1	L	200	GLU	CA-CB-CG	8.26	130.61	114.10
2	H	209	THR	N-CA-C	8.24	119.50	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	171	GLN	CA-C-O	-8.21	111.59	121.28
1	L	171	GLN	CB-CG-CD	8.19	126.52	112.60
1	L	22	SER	CA-C-N	-8.18	111.45	122.99
1	L	22	SER	C-N-CA	-8.18	111.45	122.99
1	L	80	ILE	N-CA-C	-8.17	96.81	108.58
1	L	95	GLN	CB-CG-CD	8.14	126.43	112.60
2	H	131	PRO	CA-C-N	-8.13	114.54	123.16
2	H	131	PRO	C-N-CA	-8.13	114.54	123.16
2	H	169	HIS	CA-CB-CG	-8.12	105.68	113.80
2	H	13	GLN	CA-CB-CG	8.12	130.33	114.10
1	L	174	LYS	N-CA-C	8.10	128.04	110.80
1	L	171	GLN	O-C-N	8.02	132.33	123.10
2	H	41	PRO	N-CA-CB	-7.96	94.89	103.25
2	H	118	SER	CA-CB-OG	7.94	126.98	111.10
1	L	156	ASP	CA-C-O	7.92	130.07	120.57
2	H	107	TYR	CA-C-O	7.88	130.01	121.11
1	L	207	THR	O-C-N	7.88	133.07	122.59
2	H	84	GLN	CB-CA-C	7.88	122.41	111.23
2	H	135	ASP	CA-CB-CG	7.87	120.47	112.60
1	L	19	ALA	CA-C-O	7.84	130.15	121.06
2	H	17	PRO	N-CA-CB	-7.83	95.03	103.25
2	H	74	ARG	NE-CZ-NH2	-7.82	112.16	119.20
2	H	7	THR	CA-C-N	7.80	136.69	121.41
2	H	7	THR	C-N-CA	7.80	136.69	121.41
2	H	214	LYS	CA-C-N	-7.77	110.98	122.01
2	H	214	LYS	C-N-CA	-7.77	110.98	122.01
1	L	160	ARG	CD-NE-CZ	7.68	135.16	124.40
1	L	142	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	L	20	SER	N-CA-C	-7.66	95.93	108.41
2	H	130	ALA	N-CA-C	7.65	119.28	109.65
1	L	210	ILE	CA-C-O	-7.64	111.71	120.65
2	H	196	GLN	N-CA-CB	7.63	123.39	110.49
1	L	116	ALA	N-CA-CB	-7.59	97.66	110.49
1	L	113	ARG	NE-CZ-NH2	7.59	126.03	119.20
2	H	6	GLU	CA-C-O	7.58	128.69	120.58
1	L	164	VAL	N-CA-C	7.54	118.99	107.99
2	H	23	VAL	N-CA-CB	-7.49	100.90	111.99
1	L	171	GLN	N-CA-CB	7.48	122.82	110.63
2	H	194	PRO	CA-C-N	7.48	130.16	120.44
2	H	194	PRO	C-N-CA	7.48	130.16	120.44
2	H	88	LEU	CB-CA-C	7.46	121.03	109.84
1	L	83	VAL	N-CA-CB	-7.45	103.85	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	THR	CB-CA-C	7.40	122.52	109.72
2	H	187	THR	N-CA-C	-7.39	97.21	108.96
1	L	127	SER	CB-CA-C	7.39	122.33	110.96
2	H	139	SER	CA-C-N	7.38	133.39	123.05
2	H	139	SER	C-N-CA	7.38	133.39	123.05
1	L	45	PRO	N-CA-C	7.37	122.38	111.03
1	L	113	ARG	CB-CG-CD	7.34	128.19	111.30
1	L	48	SER	N-CA-C	-7.34	99.52	110.24
1	L	166	ASN	CA-CB-CG	-7.34	105.26	112.60
2	H	153	GLU	CG-CD-OE1	7.32	135.24	118.40
2	H	190	SER	N-CA-C	7.32	126.39	110.80
2	H	56	TYR	CA-CB-CG	-7.28	100.80	113.90
1	L	25	SER	N-CA-C	7.28	126.30	110.80
2	H	176	GLN	O-C-N	7.27	131.66	122.93
1	L	103	PHE	CA-C-O	-7.27	113.01	120.71
2	H	81	VAL	O-C-N	7.27	131.08	122.36
1	L	193	ARG	CD-NE-CZ	-7.25	114.25	124.40
2	H	19	LYS	CB-CA-C	-7.25	97.19	109.72
2	H	135	ASP	CA-C-O	-7.24	111.81	120.56
2	H	13	GLN	CB-CA-C	7.20	119.62	108.61
2	H	123	ALA	O-C-N	7.19	126.98	121.88
2	H	67	LYS	CA-CB-CG	7.18	128.46	114.10
1	L	130	LEU	CB-CA-C	7.16	122.11	110.88
2	H	141	VAL	CB-CA-C	7.16	121.49	110.83
1	L	171	GLN	CB-CA-C	-7.12	97.46	109.50
2	H	74	ARG	N-CA-C	7.09	120.22	109.23
2	H	19	LYS	N-CA-CB	7.09	121.70	110.57
2	H	195	SER	CA-C-N	-7.03	108.11	121.54
2	H	195	SER	C-N-CA	-7.03	108.11	121.54
1	L	10	SER	CA-C-O	-7.02	113.22	121.44
1	L	21	ILE	N-CA-C	-6.99	98.38	108.17
2	H	46	GLU	CA-C-O	-6.98	113.27	121.44
1	L	22	SER	O-C-N	6.98	131.16	123.13
1	L	176	SER	N-CA-CB	-6.96	101.63	112.41
2	H	58	TYR	O-C-N	6.96	131.65	122.47
2	H	177	SER	CA-C-O	-6.95	110.57	120.51
2	H	17	PRO	CA-C-O	6.94	133.24	120.60
1	L	140	PHE	N-CA-CB	6.94	121.67	110.77
1	L	209	PRO	CA-C-N	6.94	131.04	122.37
1	L	209	PRO	C-N-CA	6.94	131.04	122.37
2	H	209	THR	N-CA-CB	-6.88	100.37	111.24
1	L	147	LYS	CA-C-O	-6.87	113.63	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	162	ASN	CA-CB-CG	-6.84	105.76	112.60
2	H	58	TYR	CA-C-O	-6.84	112.50	120.98
1	L	78	LEU	CB-CA-C	6.80	121.94	109.71
2	H	91	GLU	CG-CD-OE1	6.79	134.03	118.40
2	H	38	ARG	CG-CD-NE	6.79	126.94	112.00
1	L	157	GLY	CA-C-O	-6.76	111.73	119.10
2	H	19	LYS	CB-CG-CD	6.76	126.84	111.30
2	H	45	LEU	CB-CA-C	6.70	121.11	109.65
2	H	155	VAL	CB-CA-C	-6.69	104.23	111.59
1	L	123	PHE	CA-C-N	6.67	124.47	119.66
1	L	123	PHE	C-N-CA	6.67	124.47	119.66
1	L	177	THR	CA-CB-OG1	-6.67	99.60	109.60
1	L	9	LEU	N-CA-CB	6.64	120.29	110.33
1	L	97	THR	N-CA-CB	6.62	121.46	110.33
2	H	16	ARG	CB-CG-CD	6.60	126.48	111.30
1	L	36	THR	CB-CA-C	6.59	120.14	110.26
2	H	163	SER	CA-C-O	-6.58	111.10	120.51
1	L	24	ARG	N-CA-CB	6.57	123.12	111.69
1	L	145	TYR	CA-CB-CG	-6.57	102.08	113.90
2	H	110	GLN	O-C-N	6.57	129.56	122.34
2	H	143	LEU	CA-C-O	-6.54	113.06	120.32
1	L	176	SER	CA-C-N	6.53	133.24	122.07
1	L	176	SER	C-N-CA	6.53	133.24	122.07
1	L	83	VAL	N-CA-C	6.52	116.63	107.37
2	H	17	PRO	CA-C-N	6.51	133.97	121.54
2	H	17	PRO	C-N-CA	6.51	133.97	121.54
2	H	115	THR	CA-C-O	-6.49	113.69	120.70
1	L	127	SER	N-CA-C	-6.48	103.91	110.97
1	L	88	LEU	CA-C-O	-6.47	113.37	120.81
1	L	120	VAL	N-CA-C	-6.47	101.19	109.80
2	H	198	ILE	CA-C-O	6.46	128.86	120.78
1	L	149	ILE	CB-CA-C	-6.46	102.30	111.34
1	L	120	VAL	O-C-N	6.45	129.48	122.57
2	H	137	THR	N-CA-CB	-6.44	99.61	110.49
2	H	172	PRO	CB-CA-C	6.43	119.75	111.46
2	H	17	PRO	O-C-N	-6.43	113.97	122.64
2	H	157	LEU	CB-CA-C	6.42	122.64	110.51
1	L	210	ILE	N-CA-CB	6.41	118.31	111.00
2	H	196	GLN	CA-C-O	-6.41	111.34	120.51
1	L	98	HIS	N-CA-C	6.40	120.34	107.41
1	L	198	THR	CA-C-O	6.40	128.28	120.60
2	H	61	TYR	N-CA-CB	6.39	122.00	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	176	SER	CB-CA-C	6.37	121.74	111.36
1	L	212	LYS	CA-CB-CG	6.37	126.83	114.10
2	H	89	ARG	CD-NE-CZ	-6.36	115.49	124.40
2	H	175	LEU	CA-C-O	6.36	127.38	120.58
1	L	130	LEU	N-CA-C	-6.36	104.27	111.07
1	L	97	THR	CB-CA-C	-6.35	99.64	110.24
2	H	71	THR	O-C-N	-6.35	115.98	123.41
1	L	72	SER	N-CA-CB	6.33	121.19	110.49
1	L	117	ALA	O-C-N	6.32	127.60	121.66
2	H	16	ARG	N-CA-C	6.31	123.76	109.81
1	L	203	HIS	N-CA-C	6.26	118.92	109.41
1	L	53	ILE	N-CA-C	6.23	116.58	108.35
1	L	141	LEU	N-CA-CB	-6.22	100.12	110.39
2	H	189	THR	CA-C-N	6.22	133.42	121.54
2	H	189	THR	C-N-CA	6.22	133.42	121.54
2	H	213	LYS	N-CA-C	-6.21	99.69	109.50
2	H	95	ILE	N-CA-CB	6.21	120.80	110.86
2	H	153	GLU	CG-CD-OE2	-6.20	104.13	118.40
2	H	184	SER	CA-C-O	-6.20	113.87	121.06
1	L	34	GLY	N-CA-C	-6.18	98.53	113.18
1	L	178	TYR	CA-CB-CG	6.18	125.02	113.90
1	L	102	THR	N-CA-C	6.18	118.69	108.99
1	L	80	ILE	O-C-N	6.16	129.98	122.95
1	L	48	SER	O-C-N	6.14	129.44	121.64
1	L	74	THR	CA-CB-CG2	6.13	120.92	110.50
1	L	74	THR	CA-CB-OG1	-6.13	100.40	109.60
1	L	95	GLN	N-CA-CB	6.13	121.41	110.80
2	H	126	VAL	CA-C-O	6.12	127.08	120.53
1	L	33	GLN	OE1-CD-NE2	6.11	128.71	122.60
1	L	189	ASP	CA-CB-CG	6.11	118.71	112.60
2	H	70	PHE	CA-C-O	-6.11	114.44	121.47
1	L	193	ARG	O-C-N	6.11	131.03	122.36
1	L	193	ARG	CB-CA-C	-6.10	97.41	109.67
2	H	18	MET	CA-C-N	6.08	131.39	123.00
2	H	18	MET	C-N-CA	6.08	131.39	123.00
2	H	6	GLU	N-CA-CB	6.08	119.87	110.21
1	L	103	PHE	CA-CB-CG	-6.08	107.72	113.80
2	H	89	ARG	NE-CZ-NH2	6.07	124.67	119.20
2	H	176	GLN	CA-C-O	-6.07	114.08	120.58
1	L	116	ALA	CA-C-O	6.07	129.18	120.51
2	H	126	VAL	N-CA-C	6.07	116.59	107.80
1	L	143	ASN	CA-CB-CG	-6.06	106.54	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	19	LYS	N-CA-C	-6.06	99.32	109.07
1	L	24	ARG	CB-CG-CD	6.05	125.21	111.30
1	L	184	LEU	O-C-N	6.03	130.09	123.27
2	H	39	GLN	O-C-N	6.03	130.27	123.28
1	L	138	VAL	N-CA-CB	-6.01	100.94	111.39
1	L	129	GLN	O-C-N	6.00	128.57	122.09
2	H	84	GLN	CG-CD-NE2	6.00	125.41	116.40
2	H	78	LYS	CA-C-O	6.00	129.09	120.51
2	H	160	ASN	CB-CG-ND2	-5.98	107.42	116.40
2	H	173	ALA	N-CA-C	-5.98	102.64	110.53
1	L	161	GLN	CA-C-O	5.97	129.05	120.51
1	L	154	LYS	CB-CA-C	-5.97	101.60	110.62
1	L	77	THR	CA-C-N	-5.96	112.42	122.92
1	L	77	THR	C-N-CA	-5.96	112.42	122.92
2	H	88	LEU	CA-C-O	5.96	127.45	120.96
2	H	12	VAL	O-C-N	5.93	129.98	122.57
2	H	178	ASP	N-CA-C	5.93	119.82	112.59
2	H	180	TYR	N-CA-C	5.93	119.75	110.32
1	L	191	TYR	N-CA-CB	5.92	118.60	110.01
2	H	99	THR	CA-CB-OG1	-5.92	100.73	109.60
1	L	95	GLN	CA-CB-CG	5.92	125.93	114.10
1	L	27	GLN	CA-C-O	-5.91	114.96	121.28
2	H	95	ILE	N-CA-C	-5.91	99.91	108.71
2	H	21	SER	N-CA-CB	-5.91	100.94	110.69
1	L	174	LYS	CB-CA-C	-5.91	98.67	110.42
2	H	80	SER	CB-CA-C	5.90	120.37	109.70
2	H	152	PRO	CA-C-N	5.89	136.18	121.80
2	H	152	PRO	C-N-CA	5.89	136.18	121.80
2	H	110	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	L	160	ARG	CB-CG-CD	5.87	124.79	111.30
1	L	143	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	L	59	ARG	CA-C-O	-5.84	114.20	120.92
1	L	166	ASN	OD1-CG-ND2	5.83	128.44	122.60
1	L	120	VAL	CA-C-O	-5.83	115.59	121.59
1	L	157	GLY	O-C-N	5.83	130.05	122.42
2	H	189	THR	CA-C-O	5.83	127.91	121.56
2	H	214	LYS	O-C-N	5.82	130.46	123.36
2	H	39	GLN	CA-CB-CG	5.82	125.73	114.10
1	L	86	GLU	N-CA-C	-5.81	105.03	111.71
2	H	148	LYS	CA-CB-CG	5.80	125.69	114.10
2	H	135	ASP	CB-CA-C	5.79	121.87	111.03
1	L	210	ILE	O-C-N	5.79	130.00	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	86	ASN	N-CA-C	-5.79	98.47	110.80
1	L	163	GLY	N-CA-C	5.78	126.87	113.18
1	L	143	ASN	N-CA-C	5.77	117.66	110.91
1	L	36	THR	CA-C-N	-5.75	114.63	123.14
1	L	36	THR	C-N-CA	-5.75	114.63	123.14
1	L	218	GLU	CA-C-N	5.74	132.03	121.70
1	L	218	GLU	C-N-CA	5.74	132.03	121.70
2	H	47	TRP	CA-CB-CG	5.74	124.50	113.60
2	H	89	ARG	N-CA-C	-5.72	98.01	108.02
1	L	106	GLY	N-CA-C	-5.72	103.46	112.61
2	H	162	GLY	N-CA-C	-5.72	99.63	113.18
2	H	195	SER	N-CA-CB	5.72	118.30	110.01
2	H	28	THR	CA-C-O	-5.72	112.33	120.51
1	L	210	ILE	CA-CB-CG1	5.71	120.11	110.40
2	H	71	THR	N-CA-CB	5.71	121.47	111.13
2	H	113	SER	CA-C-O	5.71	127.55	121.05
1	L	97	THR	O-C-N	5.69	129.65	122.19
1	L	190	GLU	N-CA-CB	5.69	118.98	110.22
2	H	86	ASN	CA-CB-CG	-5.69	106.91	112.60
2	H	136	THR	N-CA-CB	5.68	120.08	110.49
1	L	6	GLN	N-CA-C	5.67	118.72	109.24
1	L	130	LEU	O-C-N	5.66	127.90	122.07
2	H	52	ARG	N-CA-C	5.65	114.17	108.75
2	H	87	ASN	OD1-CG-ND2	-5.64	116.96	122.60
2	H	81	VAL	CA-C-O	-5.64	115.61	121.93
2	H	212	ASP	CA-CB-CG	-5.63	106.97	112.60
1	L	78	LEU	N-CA-C	-5.63	101.41	110.14
1	L	189	ASP	CB-CA-C	5.63	119.68	110.95
2	H	107	TYR	CB-CA-C	5.62	120.41	109.33
1	L	193	ARG	CA-C-N	-5.62	113.00	123.05
1	L	193	ARG	C-N-CA	-5.62	113.00	123.05
2	H	154	PRO	CA-C-N	5.60	128.96	120.95
2	H	154	PRO	C-N-CA	5.60	128.96	120.95
2	H	87	ASN	CB-CG-OD1	5.60	132.00	120.80
1	L	22	SER	CA-C-O	-5.60	114.16	120.43
2	H	163	SER	N-CA-C	5.60	122.72	110.80
2	H	13	GLN	CA-C-O	-5.58	114.89	120.63
1	L	95	GLN	O-C-N	5.57	129.83	123.31
1	L	217	ASN	CA-C-O	-5.57	114.97	120.82
2	H	124	PRO	N-CA-CB	-5.57	97.90	103.19
1	L	200	GLU	CA-C-N	5.56	131.74	122.73
1	L	200	GLU	C-N-CA	5.56	131.74	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	131	THR	N-CA-C	-5.56	106.81	113.21
1	L	42	LEU	N-CA-C	-5.56	100.64	109.59
2	H	168	VAL	N-CA-CB	5.56	116.78	110.72
1	L	77	THR	CA-CB-OG1	-5.55	101.27	109.60
1	L	193	ARG	CG-CD-NE	-5.55	99.79	112.00
2	H	132	VAL	N-CA-C	5.54	116.00	111.62
2	H	192	THR	N-CA-C	-5.54	102.29	111.37
2	H	56	TYR	N-CA-CB	-5.54	102.25	110.61
1	L	80	ILE	CA-C-N	-5.53	114.31	122.83
1	L	80	ILE	C-N-CA	-5.53	114.31	122.83
1	L	64	PRO	CA-C-N	5.53	127.95	120.38
1	L	64	PRO	C-N-CA	5.53	127.95	120.38
2	H	14	PRO	CA-C-O	-5.52	110.55	120.60
2	H	114	VAL	O-C-N	5.50	128.91	123.18
1	L	44	LYS	O-C-N	5.50	126.15	121.20
1	L	156	ASP	CB-CA-C	5.50	119.91	111.39
1	L	24	ARG	CA-CB-CG	5.49	125.08	114.10
2	H	118	SER	CA-C-O	5.49	125.40	119.15
1	L	57	SER	O-C-N	5.48	129.00	122.27
1	L	81	SER	N-CA-C	-5.47	106.38	112.57
2	H	177	SER	N-CA-C	-5.47	99.14	110.80
1	L	194	HIS	CA-CB-CG	-5.47	108.33	113.80
2	H	13	GLN	O-C-N	5.47	132.47	121.59
1	L	11	LEU	O-C-N	5.47	127.61	121.32
2	H	93	MET	N-CA-C	5.46	117.54	108.20
1	L	90	VAL	CB-CA-C	5.46	118.67	110.98
2	H	166	SER	CB-CA-C	5.46	122.83	110.67
2	H	191	SER	CB-CA-C	5.45	121.27	110.42
1	L	79	LYS	CA-CB-CG	5.45	125.00	114.10
1	L	147	LYS	CA-CB-CG	5.45	124.99	114.10
2	H	33	TRP	N-CA-CB	-5.45	102.56	110.84
1	L	48	SER	CB-CA-C	5.44	117.28	109.11
1	L	216	ARG	CD-NE-CZ	5.43	132.00	124.40
2	H	4	LEU	CB-CA-C	5.42	119.63	109.71
2	H	25	SER	CB-CA-C	-5.42	102.11	110.78
1	L	183	THR	N-CA-C	5.41	117.25	108.26
2	H	2	VAL	CA-C-O	-5.41	114.02	120.78
2	H	19	LYS	O-C-N	5.40	129.66	123.29
2	H	169	HIS	CB-CA-C	5.40	118.89	111.23
2	H	96	TYR	N-CA-C	-5.39	100.38	109.07
1	L	111	ILE	N-CA-C	-5.39	102.63	109.58
1	L	218	GLU	O-C-N	-5.38	117.34	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	28	SER	CA-CB-OG	-5.37	100.36	111.10
2	H	130	ALA	N-CA-CB	-5.37	101.26	110.01
1	L	37	TYR	CA-CB-CG	5.37	123.56	113.90
1	L	72	SER	CA-C-O	5.37	128.19	120.51
2	H	128	PRO	N-CA-CB	-5.37	97.62	103.25
1	L	93	CYS	N-CA-CB	5.35	119.17	110.77
2	H	196	GLN	CB-CA-C	5.35	121.07	110.42
1	L	74	THR	N-CA-C	-5.34	105.41	112.94
2	H	16	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	L	75	ASP	N-CA-CB	-5.34	101.84	110.81
2	H	118	SER	CB-CA-C	5.34	118.94	109.65
2	H	89	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	H	95	ILE	O-C-N	5.33	128.58	122.93
2	H	190	SER	CA-C-O	5.32	128.12	120.51
1	L	57	SER	CA-C-O	-5.32	113.86	119.97
2	H	2	VAL	CA-C-N	-5.32	113.23	122.37
2	H	2	VAL	C-N-CA	-5.32	113.23	122.37
2	H	16	ARG	N-CA-CB	-5.32	100.91	110.37
2	H	154	PRO	CA-C-O	-5.32	117.29	121.38
2	H	207	SER	CA-C-O	-5.31	112.92	120.51
1	L	149	ILE	N-CA-C	-5.30	102.35	108.82
1	L	144	PHE	CA-CB-CG	5.29	119.09	113.80
2	H	2	VAL	O-C-N	5.29	129.18	122.57
1	L	84	GLU	O-C-N	5.29	128.93	122.96
1	L	74	THR	N-CA-CB	-5.29	102.26	110.98
2	H	196	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	L	140	PHE	CB-CA-C	-5.28	101.69	110.14
1	L	200	GLU	CB-CG-CD	5.25	121.53	112.60
1	L	38	LEU	CA-C-O	5.25	126.38	119.98
1	L	37	TYR	CB-CA-C	5.24	120.22	111.22
2	H	120	LYS	CA-C-O	-5.24	114.99	121.06
1	L	108	LYS	N-CA-C	5.22	117.26	108.96
2	H	202	VAL	CA-C-O	-5.22	114.43	121.32
2	H	40	SER	O-C-N	5.21	127.32	121.32
1	L	101	TRP	O-C-N	5.21	129.52	122.59
2	H	25	SER	N-CA-C	5.21	117.11	108.20
1	L	94	SER	CA-C-O	-5.21	115.37	121.46
1	L	217	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	L	118	PRO	CA-C-N	-5.20	115.50	122.42
1	L	118	PRO	C-N-CA	-5.20	115.50	122.42
1	L	22	SER	CB-CA-C	-5.20	101.54	110.22
2	H	84	GLN	CA-C-O	5.19	127.48	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	99	THR	CA-CB-CG2	5.19	119.33	110.50
2	H	2	VAL	CB-CA-C	-5.18	102.79	111.29
2	H	91	GLU	CA-CB-CG	5.18	124.46	114.10
2	H	186	VAL	CA-C-N	-5.18	115.30	122.30
2	H	186	VAL	C-N-CA	-5.18	115.30	122.30
1	L	190	GLU	O-C-N	5.17	128.27	122.22
2	H	120	LYS	CG-CD-CE	5.17	123.19	111.30
2	H	39	GLN	CA-C-O	-5.16	114.33	120.89
2	H	187	THR	CA-CB-CG2	5.16	119.27	110.50
2	H	34	MET	O-C-N	5.15	129.65	123.16
2	H	77	SER	N-CA-C	5.15	116.78	108.08
2	H	14	PRO	N-CA-C	-5.13	101.89	112.47
2	H	143	LEU	O-C-N	5.13	129.32	123.31
2	H	177	SER	CB-CA-C	5.13	120.64	110.42
2	H	198	ILE	CB-CA-C	5.13	119.70	111.29
1	L	35	ASN	N-CA-CB	-5.12	101.84	110.49
2	H	76	ASP	CA-C-N	5.11	131.51	122.66
2	H	76	ASP	C-N-CA	5.11	131.51	122.66
2	H	146	LEU	CA-C-O	-5.11	114.86	120.43
2	H	7	THR	O-C-N	-5.11	117.27	123.29
1	L	127	SER	CA-CB-OG	5.10	121.31	111.10
2	H	204	HIS	CA-C-O	5.10	125.90	120.08
2	H	48	VAL	N-CA-CB	-5.10	102.82	111.23
2	H	56	TYR	CA-C-O	5.10	125.39	119.32
1	L	113	ARG	NH1-CZ-NH2	-5.10	112.67	119.30
2	H	148	LYS	N-CA-C	5.10	117.16	109.41
2	H	187	THR	N-CA-CB	5.08	118.70	110.17
1	L	177	THR	CB-CA-C	-5.08	100.83	109.51
2	H	24	ALA	N-CA-C	5.07	118.45	107.49
2	H	207	SER	O-C-N	5.07	129.34	122.59
2	H	103	TYR	CA-CB-CG	-5.07	104.77	113.90
2	H	129	LEU	CA-C-N	5.07	130.57	120.94
2	H	129	LEU	C-N-CA	5.07	130.57	120.94
2	H	148	LYS	N-CA-CB	-5.06	103.38	111.43
2	H	126	VAL	N-CA-CB	-5.06	105.09	111.46
1	L	5	THR	N-CA-C	5.04	118.24	110.42
2	H	31	ASP	N-CA-C	5.04	120.32	113.37
2	H	151	PHE	N-CA-CB	5.03	119.32	110.37
1	L	78	LEU	N-CA-CB	5.01	118.57	110.85
2	H	78	LYS	CB-CG-CD	5.01	122.83	111.30
1	L	144	PHE	CB-CA-C	5.01	119.66	110.24
1	L	80	ILE	CA-C-O	-5.01	115.05	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	L	211	VAL	O-C-N	5.00	128.35	123.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	193	ARG	Sidechain
1	L	39	ARG	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	L	1700	0	1641	384	2
2	H	1662	0	1597	685	3
3	H	25	0	10	12	0
4	H	8	0	14	24	0
All	All	3395	0	3262	1040	4

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 156.

All (1040) 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:31:ASP:HA	2:H:53:ASN:ND2	1.41	1.32
1:L:214:PHE:HB2	2:H:133:CYS:SG	1.75	1.27
1:L:190:GLU:HA	1:L:193:ARG:NH2	1.47	1.27
2:H:51:ILE:HD11	2:H:72:ILE:CD1	1.68	1.24
2:H:38:ARG:NH1	2:H:96:TYR:OH	1.72	1.20
2:H:137:THR:O	2:H:141:VAL:HG22	1.41	1.18
2:H:62:TYR:CE1	2:H:71:THR:HA	1.79	1.18
1:L:193:ARG:HB2	1:L:193:ARG:CZ	1.67	1.18
2:H:153:GLU:OE2	2:H:180:TYR:CZ	1.99	1.15
2:H:20:LEU:HD13	2:H:85:MET:CE	1.78	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.27	1.14
2:H:131:PRO:HD3	2:H:143:LEU:HD23	1.19	1.14
2:H:20:LEU:HD13	2:H:85:MET:HE3	1.27	1.13
2:H:69:ARG:HB3	2:H:87:ASN:ND2	1.63	1.13
1:L:174:LYS:HG3	1:L:175:ASP:H	0.98	1.11
2:H:93:MET:HE3	2:H:116:VAL:H	1.14	1.11
2:H:105:MET:HG3	2:H:106:ASP:N	1.45	1.11
2:H:39:GLN:HB3	2:H:45:LEU:HD23	1.29	1.10
2:H:157:LEU:HD12	2:H:158:THR:N	1.65	1.10
2:H:27:PHE:HZ	2:H:34:MET:HE1	1.18	1.09
1:L:146:PRO:HG2	1:L:204:LYS:HG3	1.29	1.09
2:H:205:PRO:O	2:H:207:SER:N	1.86	1.08
2:H:131:PRO:HD3	2:H:143:LEU:CD2	1.82	1.08
1:L:144:PHE:CE1	1:L:149:ILE:HD11	1.88	1.08
2:H:51:ILE:CG1	2:H:72:ILE:HG13	1.83	1.07
1:L:174:LYS:CG	1:L:175:ASP:H	1.64	1.07
2:H:161:SER:HB3	2:H:197:SER:OG	1.54	1.07
1:L:149:ILE:HG22	1:L:150:ASN:H	1.13	1.07
2:H:27:PHE:CZ	2:H:34:MET:HE1	1.89	1.06
2:H:160:ASN:HB3	2:H:199:THR:OG1	1.54	1.06
2:H:86:ASN:O	2:H:87:ASN:HB3	1.48	1.06
2:H:206:ALA:O	2:H:207:SER:HB3	1.52	1.05
1:L:155:ILE:H	1:L:159:GLU:HB2	1.17	1.05
2:H:51:ILE:HD11	2:H:72:ILE:HD12	1.38	1.05
2:H:106:ASP:HB2	4:H:219:MPD:HM3	1.37	1.05
1:L:122:ILE:HG22	1:L:212:LYS:HG3	1.37	1.04
2:H:157:LEU:CD1	2:H:158:THR:H	1.69	1.04
1:L:190:GLU:HA	1:L:193:ARG:HH21	1.02	1.04
2:H:29:PHE:CG	2:H:79:SER:HB2	1.93	1.03
2:H:29:PHE:CD1	2:H:79:SER:HB2	1.94	1.03
2:H:158:THR:HG22	2:H:201:ASN:HB2	1.40	1.03
1:L:168:TRP:HE1	1:L:180:MET:HE3	1.21	1.03
2:H:105:MET:CG	2:H:106:ASP:H	1.71	1.03
1:L:194:HIS:O	1:L:216:ARG:HD3	1.58	1.03
1:L:2:VAL:HG22	1:L:26:SER:HB3	1.39	1.02
2:H:143:LEU:HD22	2:H:215:ILE:HG21	1.36	1.02
2:H:189:THR:O	2:H:194:PRO:HD3	1.58	1.02
1:L:32:SER:O	1:L:35:ASN:ND2	1.92	1.02
1:L:52:LEU:HA	1:L:63:VAL:HG21	1.35	1.02
2:H:87:ASN:O	2:H:89:ARG:NH1	1.93	1.02
2:H:190:SER:C	2:H:194:PRO:HG2	1.84	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:SER:O	2:H:198:ILE:HB	1.53	1.02
2:H:161:SER:HB2	2:H:198:ILE:HA	1.42	1.02
2:H:69:ARG:CB	2:H:87:ASN:HD21	1.73	1.01
2:H:90:VAL:HA	2:H:116:VAL:HG11	1.43	1.01
2:H:40:SER:HB2	2:H:43:LYS:HG3	1.43	1.00
2:H:51:ILE:HD11	2:H:72:ILE:CG1	1.91	1.00
2:H:106:ASP:CB	4:H:219:MPD:HM3	1.92	0.99
2:H:164:LEU:HB2	2:H:193:TRP:CZ2	1.97	0.99
2:H:62:TYR:CZ	2:H:72:ILE:HG22	1.98	0.98
1:L:120:VAL:HG11	1:L:212:LYS:HB2	1.46	0.98
2:H:64:ASP:HA	2:H:67:LYS:HD3	1.46	0.98
1:L:219:CYS:OXT	2:H:133:CYS:HB3	1.64	0.97
2:H:137:THR:HA	2:H:141:VAL:HG13	1.45	0.97
2:H:169:HIS:NE2	2:H:185:SER:OG	1.94	0.97
2:H:124:PRO:CB	2:H:150:TYR:HB3	1.94	0.97
1:L:197:TYR:HB2	1:L:214:PHE:CE2	2.00	0.97
2:H:162:GLY:HA2	2:H:197:SER:H	1.30	0.97
2:H:158:THR:CG2	2:H:201:ASN:HB2	1.94	0.96
2:H:160:ASN:O	2:H:198:ILE:HA	1.64	0.96
2:H:17:PRO:O	2:H:85:MET:C	2.08	0.96
2:H:157:LEU:HD12	2:H:158:THR:H	0.82	0.96
2:H:159:TRP:CE3	2:H:198:ILE:HD11	1.99	0.96
2:H:191:SER:C	2:H:194:PRO:HD2	1.91	0.95
1:L:31:HIS:HB2	1:L:97:THR:HG23	1.47	0.95
1:L:174:LYS:HD2	1:L:175:ASP:HB3	1.46	0.95
2:H:64:ASP:CA	2:H:67:LYS:HD3	1.95	0.95
2:H:5:ASP:C	2:H:5:ASP:OD2	2.10	0.95
1:L:42:LEU:HD21	1:L:44:LYS:HZ3	1.29	0.95
2:H:31:ASP:CA	2:H:53:ASN:ND2	2.29	0.94
2:H:45:LEU:HD13	2:H:108:TRP:CH2	2.02	0.94
2:H:51:ILE:HG23	2:H:60:THR:HG22	1.47	0.94
1:L:215:ASN:O	1:L:218:GLU:N	2.01	0.94
2:H:93:MET:HE2	2:H:115:THR:HG23	1.47	0.94
2:H:61:TYR:OH	2:H:67:LYS:HE3	1.66	0.94
2:H:191:SER:HA	2:H:194:PRO:HB2	1.45	0.94
2:H:20:LEU:HD13	2:H:85:MET:SD	2.08	0.94
2:H:31:ASP:HA	2:H:53:ASN:HD22	1.32	0.93
2:H:164:LEU:HD12	2:H:165:SER:N	1.82	0.93
2:H:162:GLY:O	2:H:163:SER:HB2	1.68	0.93
2:H:23:VAL:HG22	2:H:80:SER:HB3	1.51	0.93
2:H:40:SER:HB2	2:H:43:LYS:CG	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:CD1	2:H:72:ILE:HG13	2.00	0.92
2:H:200:CYS:C	2:H:201:ASN:HD22	1.76	0.92
2:H:41:PRO:HD2	2:H:94:GLY:HA2	1.51	0.92
2:H:90:VAL:HG12	2:H:116:VAL:HG22	1.52	0.92
1:L:215:ASN:H	1:L:219:CYS:HB3	1.32	0.92
2:H:62:TYR:HE1	2:H:71:THR:HA	1.29	0.92
2:H:54:LYS:HB2	2:H:55:PRO:HD3	1.52	0.92
1:L:174:LYS:HG3	1:L:175:ASP:N	1.80	0.91
2:H:214:LYS:NZ	2:H:214:LYS:HB3	1.83	0.91
2:H:19:LYS:HG3	2:H:19:LYS:O	1.46	0.91
1:L:195:ASN:HA	1:L:216:ARG:HB2	1.53	0.91
1:L:198:THR:HB	1:L:213:SER:OG	1.71	0.91
2:H:92:ASP:O	2:H:96:TYR:OH	1.89	0.90
2:H:16:ARG:N	2:H:17:PRO:HD3	1.86	0.90
2:H:19:LYS:O	2:H:19:LYS:CG	2.17	0.90
1:L:41:TYR:HE2	1:L:51:VAL:HG12	1.37	0.90
1:L:193:ARG:CZ	1:L:193:ARG:CB	2.50	0.90
2:H:12:VAL:O	2:H:116:VAL:HG23	1.72	0.90
2:H:171:PHE:CD1	2:H:171:PHE:N	2.34	0.90
2:H:40:SER:HA	2:H:94:GLY:HA3	1.54	0.90
1:L:124:PRO:HD2	2:H:132:VAL:HG11	1.54	0.90
2:H:77:SER:O	2:H:79:SER:OG	1.91	0.89
2:H:85:MET:O	2:H:88:LEU:HG	1.73	0.89
2:H:39:GLN:HB2	2:H:44:GLY:C	1.96	0.89
2:H:40:SER:O	2:H:43:LYS:HB2	1.72	0.89
2:H:130:ALA:O	2:H:132:VAL:HG12	1.73	0.89
2:H:51:ILE:HD11	2:H:72:ILE:HG13	1.54	0.89
2:H:161:SER:HB2	2:H:198:ILE:CA	2.01	0.89
2:H:163:SER:O	2:H:193:TRP:CZ2	2.26	0.89
1:L:41:TYR:CE2	1:L:51:VAL:HG12	2.07	0.88
2:H:16:ARG:H	2:H:17:PRO:HD3	1.35	0.88
2:H:203:ALA:HA	2:H:210:LYS:HA	1.56	0.88
2:H:17:PRO:HA	2:H:86:ASN:HA	1.56	0.88
2:H:29:PHE:HB2	2:H:79:SER:OG	1.71	0.88
2:H:31:ASP:HA	2:H:53:ASN:HD21	1.14	0.88
2:H:40:SER:HA	2:H:94:GLY:CA	2.04	0.88
1:L:203:HIS:CE1	1:L:204:LYS:HG2	2.07	0.88
2:H:69:ARG:HB3	2:H:87:ASN:HD21	1.29	0.88
2:H:108:TRP:HE1	4:H:219:MPD:H31	1.39	0.87
1:L:214:PHE:CB	2:H:133:CYS:SG	2.62	0.87
1:L:29:LEU:HD13	1:L:95:GLN:HB2	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:149:ILE:HG22	1:L:150:ASN:N	1.89	0.87
1:L:168:TRP:NE1	1:L:180:MET:HE3	1.88	0.87
1:L:215:ASN:CB	1:L:218:GLU:O	2.22	0.87
2:H:61:TYR:CZ	2:H:67:LYS:HE3	2.10	0.87
2:H:171:PHE:N	2:H:171:PHE:HD1	1.69	0.86
1:L:6:GLN:HE21	1:L:21:ILE:HD11	1.40	0.86
2:H:85:MET:HB2	2:H:88:LEU:HD21	1.56	0.86
2:H:198:ILE:HD13	2:H:199:THR:N	1.90	0.86
2:H:176:GLN:HG2	2:H:177:SER:OG	1.73	0.86
1:L:120:VAL:CG1	1:L:212:LYS:HB2	2.06	0.86
2:H:159:TRP:HE3	2:H:198:ILE:HD11	1.41	0.85
1:L:144:PHE:CE1	1:L:149:ILE:CD1	2.59	0.85
2:H:182:LEU:HG	2:H:183:SER:N	1.90	0.85
1:L:144:PHE:CD1	1:L:149:ILE:HD11	2.11	0.85
2:H:158:THR:HG22	2:H:201:ASN:CB	2.05	0.85
1:L:146:PRO:HG2	1:L:204:LYS:CG	2.07	0.85
2:H:93:MET:HE3	2:H:116:VAL:N	1.91	0.85
2:H:69:ARG:CA	2:H:87:ASN:HD21	1.90	0.84
2:H:193:TRP:N	2:H:194:PRO:CD	2.41	0.84
1:L:52:LEU:HA	1:L:63:VAL:CG2	2.08	0.84
2:H:199:THR:HG22	2:H:214:LYS:HG3	1.56	0.84
2:H:62:TYR:OH	2:H:71:THR:HB	1.76	0.84
1:L:190:GLU:CA	1:L:193:ARG:NH2	2.39	0.84
2:H:162:GLY:C	2:H:196:GLN:HE21	1.86	0.84
2:H:64:ASP:N	2:H:67:LYS:HD3	1.93	0.83
1:L:29:LEU:HD13	1:L:95:GLN:CB	2.07	0.83
1:L:120:VAL:CG2	1:L:141:LEU:HD23	2.07	0.83
1:L:59:ARG:HH11	1:L:59:ARG:HG2	1.44	0.83
2:H:28:THR:O	2:H:29:PHE:C	2.21	0.83
1:L:81:SER:O	1:L:82:ARG:HB3	1.79	0.83
2:H:164:LEU:HB2	2:H:193:TRP:HZ2	1.39	0.83
2:H:17:PRO:HG2	2:H:88:LEU:HD12	1.59	0.83
1:L:146:PRO:CG	1:L:204:LYS:HG3	2.08	0.83
2:H:38:ARG:HG2	2:H:96:TYR:CE2	2.14	0.83
2:H:190:SER:OG	2:H:191:SER:N	2.02	0.83
1:L:142:ASN:OD1	2:H:169:HIS:NE2	2.12	0.82
1:L:218:GLU:N	1:L:218:GLU:OE1	2.12	0.82
2:H:136:THR:OG1	2:H:140:SER:OG	1.85	0.82
2:H:164:LEU:HD12	2:H:165:SER:H	1.41	0.82
1:L:165:LEU:HD21	2:H:174:VAL:CG1	2.09	0.82
2:H:51:ILE:HG12	2:H:72:ILE:HG23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:SER:HA	2:H:194:PRO:CB	2.09	0.82
1:L:1:ASP:CG	1:L:100:PRO:HG3	2.05	0.82
1:L:7:THR:O	1:L:22:SER:HB2	1.80	0.82
2:H:205:PRO:C	2:H:207:SER:H	1.88	0.82
1:L:17:ASP:O	1:L:82:ARG:HA	1.78	0.81
2:H:45:LEU:HD13	2:H:108:TRP:HH2	1.40	0.81
2:H:127:TYR:HD2	2:H:146:LEU:CD2	1.94	0.81
2:H:29:PHE:CG	2:H:79:SER:CB	2.63	0.81
2:H:6:GLU:HB2	2:H:112:THR:HB	1.61	0.81
1:L:94:SER:HA	1:L:102:THR:O	1.81	0.81
1:L:161:GLN:CD	1:L:162:ASN:H	1.89	0.81
1:L:174:LYS:CG	1:L:175:ASP:N	2.35	0.81
2:H:70:PHE:CZ	2:H:85:MET:HB3	2.15	0.81
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.16	0.81
2:H:31:ASP:C	2:H:53:ASN:ND2	2.39	0.81
2:H:106:ASP:HB2	4:H:219:MPD:CM	2.11	0.81
2:H:106:ASP:CG	4:H:219:MPD:HM3	2.06	0.81
1:L:206:SER:OG	1:L:208:SER:O	1.98	0.80
2:H:90:VAL:HG12	2:H:116:VAL:CG2	2.10	0.80
2:H:136:THR:HG23	2:H:140:SER:O	1.80	0.80
2:H:12:VAL:HG11	2:H:17:PRO:HG2	1.61	0.80
2:H:120:LYS:CD	2:H:120:LYS:H	1.94	0.80
2:H:20:LEU:CD1	2:H:85:MET:HE3	2.10	0.80
1:L:124:PRO:HB3	1:L:214:PHE:CE1	2.17	0.80
2:H:191:SER:N	2:H:194:PRO:HG2	1.97	0.80
1:L:42:LEU:HD21	1:L:44:LYS:NZ	1.96	0.79
2:H:126:VAL:HG22	2:H:147:VAL:HB	1.65	0.79
2:H:189:THR:O	2:H:194:PRO:CD	2.30	0.79
2:H:171:PHE:HD1	2:H:171:PHE:H	1.28	0.79
2:H:62:TYR:CE1	2:H:71:THR:CA	2.64	0.79
2:H:124:PRO:HB3	2:H:150:TYR:CB	2.09	0.79
1:L:88:LEU:HD12	1:L:172:ASP:OD1	1.83	0.79
1:L:149:ILE:CG2	1:L:150:ASN:H	1.92	0.79
1:L:2:VAL:HG12	1:L:4:MET:HG2	1.65	0.78
2:H:100:GLY:O	2:H:106:ASP:HB2	1.83	0.78
2:H:99:THR:HB	4:H:219:MPD:CM	2.14	0.78
1:L:18:GLN:HG3	1:L:80:ILE:O	1.83	0.78
2:H:14:PRO:HG3	2:H:90:VAL:CG1	2.13	0.78
2:H:5:ASP:OD2	2:H:6:GLU:N	2.16	0.78
2:H:69:ARG:C	2:H:87:ASN:HD21	1.91	0.78
1:L:155:ILE:N	1:L:159:GLU:HB2	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:TYR:CD1	2:H:62:TYR:N	2.51	0.78
2:H:86:ASN:O	2:H:87:ASN:CB	2.28	0.78
1:L:215:ASN:HB2	1:L:218:GLU:O	1.84	0.78
2:H:39:GLN:HB2	2:H:44:GLY:O	1.83	0.78
2:H:103:TYR:CD1	3:H:218:FLU:H18	2.19	0.78
1:L:141:LEU:HD12	1:L:180:MET:HB3	1.65	0.77
2:H:61:TYR:CE1	2:H:62:TYR:C	2.62	0.77
2:H:120:LYS:CD	2:H:120:LYS:N	2.46	0.77
1:L:148:ASP:C	1:L:149:ILE:HD12	2.09	0.77
2:H:90:VAL:HA	2:H:116:VAL:CG1	2.15	0.77
2:H:120:LYS:O	2:H:120:LYS:HD3	1.85	0.77
1:L:166:ASN:OD1	1:L:182:SER:HB2	1.84	0.77
2:H:93:MET:HE2	2:H:115:THR:CG2	2.15	0.77
2:H:153:GLU:OE2	2:H:180:TYR:CE2	2.38	0.77
1:L:38:LEU:C	1:L:38:LEU:HD12	2.11	0.77
1:L:120:VAL:HG23	1:L:141:LEU:HD23	1.66	0.76
1:L:129:GLN:HG2	1:L:134:GLY:O	1.85	0.76
2:H:51:ILE:HG12	2:H:72:ILE:CG2	2.15	0.76
2:H:211:VAL:HG23	2:H:212:ASP:N	2.00	0.76
2:H:27:PHE:HZ	2:H:34:MET:CE	1.97	0.76
2:H:39:GLN:O	2:H:39:GLN:HG2	1.85	0.76
2:H:43:LYS:NZ	2:H:91:GLU:OE1	2.19	0.76
2:H:207:SER:O	2:H:208:SER:C	2.29	0.76
1:L:147:LYS:O	1:L:149:ILE:CD1	2.34	0.76
1:L:174:LYS:HD2	1:L:175:ASP:CB	2.16	0.75
2:H:105:MET:CG	2:H:106:ASP:N	2.33	0.75
2:H:188:VAL:HG22	2:H:193:TRP:HD1	1.51	0.75
1:L:6:GLN:NE2	1:L:21:ILE:HD11	2.02	0.75
1:L:130:LEU:HD22	1:L:188:LYS:HG3	1.69	0.75
1:L:149:ILE:HD12	1:L:149:ILE:N	1.99	0.75
2:H:62:TYR:O	2:H:67:LYS:HD2	1.86	0.75
1:L:217:ASN:HB3	1:L:218:GLU:OE1	1.86	0.75
2:H:193:TRP:N	2:H:194:PRO:HD2	2.02	0.75
1:L:215:ASN:HB3	1:L:218:GLU:O	1.87	0.75
2:H:17:PRO:CA	2:H:86:ASN:HA	2.17	0.75
2:H:190:SER:O	2:H:194:PRO:HG2	1.86	0.75
2:H:64:ASP:N	2:H:64:ASP:OD1	2.15	0.74
1:L:33:GLN:HA	1:L:35:ASN:HD21	1.53	0.74
2:H:71:THR:C	2:H:83:LEU:HD12	2.12	0.74
2:H:3:LYS:C	2:H:4:LEU:HD12	2.13	0.74
2:H:49:ALA:HB1	2:H:72:ILE:HB	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:GLN:CA	1:L:35:ASN:HD21	2.01	0.74
1:L:96:SER:HB3	3:H:218:FLU:O3	1.88	0.74
1:L:149:ILE:CD1	1:L:149:ILE:N	2.50	0.74
2:H:120:LYS:N	2:H:120:LYS:HD2	2.02	0.74
1:L:53:ILE:CG2	1:L:56:VAL:O	2.37	0.73
1:L:96:SER:CB	3:H:218:FLU:O3	2.36	0.73
1:L:11:LEU:HD23	1:L:109:LEU:HD11	1.70	0.73
1:L:160:ARG:O	1:L:161:GLN:O	2.06	0.73
2:H:120:LYS:H	2:H:120:LYS:HD3	1.52	0.73
2:H:155:VAL:HG23	2:H:156:THR:N	2.01	0.73
2:H:54:LYS:HG2	2:H:58:TYR:OH	1.87	0.73
2:H:85:MET:CB	2:H:88:LEU:HD21	2.18	0.73
2:H:203:ALA:HB2	2:H:210:LYS:HB2	1.69	0.73
1:L:154:LYS:O	1:L:198:THR:HG23	1.88	0.73
1:L:37:TYR:HB2	1:L:97:THR:OG1	1.88	0.73
2:H:17:PRO:O	2:H:85:MET:O	2.07	0.73
2:H:90:VAL:HG12	2:H:116:VAL:HG13	1.71	0.73
2:H:127:TYR:HD2	2:H:146:LEU:HD22	1.52	0.73
2:H:150:TYR:CZ	2:H:155:VAL:CG1	2.71	0.73
1:L:161:GLN:OE1	1:L:162:ASN:N	2.20	0.72
2:H:14:PRO:HG3	2:H:90:VAL:HG11	1.69	0.72
2:H:86:ASN:O	2:H:86:ASN:ND2	2.22	0.72
2:H:63:SER:O	2:H:67:LYS:N	2.21	0.72
4:H:219:MPD:H52	4:H:219:MPD:O2	1.90	0.72
1:L:100:PRO:O	2:H:47:TRP:CE3	2.41	0.72
1:L:124:PRO:CD	2:H:132:VAL:HG11	2.19	0.72
2:H:163:SER:C	2:H:193:TRP:CZ2	2.67	0.72
2:H:69:ARG:CB	2:H:87:ASN:ND2	2.37	0.72
2:H:205:PRO:C	2:H:207:SER:N	2.45	0.72
2:H:163:SER:O	2:H:193:TRP:HZ2	1.71	0.72
1:L:1:ASP:HA	1:L:100:PRO:CD	2.17	0.72
2:H:136:THR:C	2:H:140:SER:O	2.33	0.72
2:H:71:THR:O	2:H:84:GLN:NE2	2.23	0.72
2:H:64:ASP:O	2:H:66:VAL:N	2.22	0.72
1:L:32:SER:C	1:L:35:ASN:ND2	2.48	0.71
1:L:193:ARG:HB2	1:L:193:ARG:NH1	2.03	0.71
2:H:142:THR:HA	2:H:186:VAL:O	1.90	0.71
1:L:165:LEU:CD2	2:H:174:VAL:CG1	2.69	0.71
2:H:124:PRO:HA	2:H:148:LYS:O	1.90	0.71
1:L:55:LYS:HD3	2:H:104:GLY:HA3	1.72	0.71
1:L:65:ASP:O	1:L:65:ASP:OD2	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:CD1	2:H:72:ILE:HD13	2.24	0.71
1:L:4:MET:CE	1:L:95:GLN:HB3	2.21	0.71
2:H:40:SER:OG	2:H:93:MET:O	2.08	0.70
2:H:93:MET:HG3	2:H:115:THR:HA	1.71	0.70
2:H:153:GLU:CB	2:H:154:PRO:HD3	2.21	0.70
2:H:29:PHE:CB	2:H:79:SER:CB	2.69	0.70
1:L:19:ALA:O	1:L:79:LYS:HA	1.91	0.70
2:H:20:LEU:HD22	2:H:85:MET:HE1	1.73	0.70
2:H:77:SER:C	2:H:79:SER:N	2.45	0.70
2:H:99:THR:CB	4:H:219:MPD:HO2	2.03	0.70
1:L:120:VAL:CG1	1:L:212:LYS:HG2	2.21	0.70
1:L:161:GLN:CG	1:L:162:ASN:N	2.53	0.70
2:H:168:VAL:HA	2:H:185:SER:O	1.91	0.70
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.27	0.70
2:H:51:ILE:HG23	2:H:60:THR:CG2	2.20	0.70
2:H:128:PRO:HG2	2:H:128:PRO:O	1.92	0.70
2:H:135:ASP:O	2:H:136:THR:C	2.35	0.70
2:H:153:GLU:HB3	2:H:154:PRO:HD3	1.72	0.70
2:H:162:GLY:C	2:H:196:GLN:NE2	2.50	0.70
2:H:164:LEU:N	2:H:193:TRP:HE1	1.87	0.70
2:H:37:VAL:HG13	2:H:46:GLU:O	1.92	0.70
1:L:29:LEU:CD1	1:L:95:GLN:HB3	2.22	0.69
1:L:29:LEU:CD1	1:L:95:GLN:CB	2.70	0.69
1:L:84:GLU:O	1:L:87:ASP:HB2	1.92	0.69
2:H:103:TYR:H	3:H:218:FLU:C17	2.04	0.69
1:L:67:PHE:CZ	1:L:87:ASP:OD1	2.45	0.69
1:L:129:GLN:O	1:L:132:SER:HB2	1.93	0.69
2:H:40:SER:C	2:H:43:LYS:HB2	2.16	0.69
2:H:153:GLU:OE2	2:H:180:TYR:OH	2.11	0.69
1:L:24:ARG:HE	1:L:24:ARG:C	2.01	0.69
2:H:6:GLU:HG3	2:H:111:GLY:HA2	1.72	0.69
2:H:35:ASN:ND2	2:H:99:THR:OG1	2.26	0.69
2:H:164:LEU:CD1	2:H:165:SER:H	2.04	0.69
2:H:169:HIS:O	2:H:171:PHE:HE1	1.76	0.69
1:L:65:ASP:C	1:L:67:PHE:H	2.00	0.69
2:H:3:LYS:O	2:H:24:ALA:HA	1.93	0.69
2:H:11:LEU:O	2:H:12:VAL:HG23	1.92	0.69
2:H:23:VAL:HG22	2:H:80:SER:CB	2.22	0.69
2:H:62:TYR:CZ	2:H:71:THR:HB	2.28	0.69
2:H:106:ASP:OD1	4:H:219:MPD:HM3	1.93	0.69
1:L:161:GLN:HG3	1:L:162:ASN:N	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:ARG:CG	1:L:193:ARG:O	2.40	0.68
2:H:12:VAL:HG11	2:H:17:PRO:CG	2.23	0.68
2:H:124:PRO:CA	2:H:150:TYR:HB3	2.22	0.68
2:H:214:LYS:HB3	2:H:214:LYS:HZ3	1.56	0.68
2:H:32:TYR:CD2	2:H:101:SER:O	2.46	0.68
2:H:178:ASP:OD1	2:H:178:ASP:O	2.11	0.68
1:L:152:LYS:HZ3	1:L:154:LYS:HE2	1.58	0.68
2:H:99:THR:OG1	4:H:219:MPD:O2	2.06	0.68
1:L:51:VAL:HG21	2:H:105:MET:CE	2.23	0.68
1:L:59:ARG:HD3	1:L:63:VAL:CG1	2.22	0.68
2:H:191:SER:CA	2:H:194:PRO:HG2	2.24	0.68
1:L:115:ASP:OD2	1:L:175:ASP:O	2.11	0.68
1:L:120:VAL:HG12	1:L:212:LYS:HG2	1.74	0.68
2:H:51:ILE:HG12	2:H:72:ILE:HG13	1.75	0.68
2:H:162:GLY:CA	2:H:197:SER:H	2.04	0.68
1:L:33:GLN:C	1:L:35:ASN:H	2.01	0.67
1:L:100:PRO:O	1:L:101:TRP:HB2	1.92	0.67
1:L:122:ILE:HG13	1:L:123:PHE:N	2.09	0.67
1:L:122:ILE:HG13	1:L:123:PHE:H	1.58	0.67
2:H:6:GLU:N	2:H:6:GLU:OE2	2.27	0.67
2:H:199:THR:HG22	2:H:214:LYS:CG	2.24	0.67
2:H:6:GLU:CG	2:H:111:GLY:HA2	2.23	0.67
2:H:17:PRO:CG	2:H:88:LEU:HD12	2.24	0.67
2:H:51:ILE:HG13	2:H:72:ILE:HG13	1.72	0.67
2:H:105:MET:HG3	2:H:106:ASP:H	0.75	0.67
2:H:162:GLY:N	2:H:197:SER:C	2.53	0.67
1:L:52:LEU:CA	1:L:63:VAL:HG21	2.17	0.67
1:L:51:VAL:HG21	2:H:105:MET:HE1	1.77	0.66
2:H:24:ALA:HB1	2:H:27:PHE:CE2	2.30	0.66
2:H:160:ASN:O	2:H:198:ILE:HG12	1.95	0.66
1:L:39:ARG:NH2	1:L:96:SER:OG	2.28	0.66
2:H:64:ASP:O	2:H:65:SER:C	2.38	0.66
2:H:130:ALA:O	2:H:132:VAL:CG1	2.43	0.66
1:L:32:SER:C	1:L:35:ASN:HD21	2.01	0.66
1:L:60:PHE:CE1	1:L:61:SER:HB3	2.30	0.66
1:L:190:GLU:HA	1:L:193:ARG:HH22	1.58	0.66
1:L:191:TYR:CE1	1:L:216:ARG:HG3	2.31	0.66
2:H:20:LEU:CD1	2:H:85:MET:SD	2.83	0.66
1:L:174:LYS:HZ1	1:L:175:ASP:CG	2.03	0.66
2:H:90:VAL:HG12	2:H:116:VAL:CG1	2.25	0.66
1:L:193:ARG:NH2	1:L:193:ARG:HB2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:11:LEU:HD21	1:L:19:ALA:HB2	1.78	0.66
2:H:11:LEU:HD21	2:H:151:PHE:HZ	1.60	0.66
2:H:40:SER:N	2:H:43:LYS:HB2	2.10	0.66
1:L:165:LEU:HD21	2:H:174:VAL:HG12	1.77	0.65
2:H:169:HIS:CD2	2:H:185:SER:OG	2.49	0.65
2:H:191:SER:CA	2:H:194:PRO:CG	2.74	0.65
1:L:98:HIS:O	1:L:99:VAL:C	2.39	0.65
2:H:3:LYS:O	2:H:4:LEU:HD12	1.95	0.65
2:H:207:SER:OG	2:H:208:SER:N	2.23	0.65
2:H:61:TYR:CE1	2:H:63:SER:HA	2.31	0.65
2:H:62:TYR:CE1	2:H:72:ILE:N	2.62	0.65
1:L:113:ARG:NH1	1:L:175:ASP:HA	2.12	0.65
1:L:38:LEU:HD12	1:L:39:ARG:N	2.11	0.65
2:H:212:ASP:O	2:H:213:LYS:HG2	1.96	0.65
1:L:4:MET:HE2	1:L:95:GLN:HB3	1.77	0.65
2:H:64:ASP:CG	2:H:67:LYS:HZ2	2.05	0.65
2:H:151:PHE:CE2	2:H:152:PRO:HB3	2.32	0.65
2:H:39:GLN:HB3	2:H:45:LEU:CD2	2.18	0.65
2:H:40:SER:HA	2:H:94:GLY:HA2	1.78	0.65
2:H:13:GLN:C	2:H:14:PRO:O	2.30	0.65
2:H:62:TYR:HE1	2:H:71:THR:CA	2.04	0.65
2:H:146:LEU:HD21	2:H:148:LYS:HE3	1.77	0.65
2:H:147:VAL:HG22	2:H:147:VAL:O	1.96	0.65
2:H:164:LEU:N	2:H:193:TRP:NE1	2.45	0.65
2:H:191:SER:HA	2:H:194:PRO:CG	2.27	0.65
2:H:36:TRP:O	2:H:48:VAL:HB	1.97	0.64
2:H:70:PHE:O	2:H:71:THR:CG2	2.45	0.64
1:L:21:ILE:HD13	1:L:21:ILE:C	2.23	0.64
2:H:40:SER:CB	2:H:93:MET:O	2.46	0.64
2:H:62:TYR:OH	2:H:72:ILE:N	2.30	0.64
1:L:103:PHE:N	1:L:103:PHE:CD1	2.65	0.64
1:L:155:ILE:HG23	1:L:197:TYR:CE1	2.32	0.64
2:H:136:THR:CG2	2:H:137:THR:N	2.59	0.64
2:H:158:THR:CG2	2:H:201:ASN:CB	2.69	0.64
2:H:203:ALA:HB2	2:H:210:LYS:HE3	1.80	0.64
2:H:209:THR:HG23	2:H:210:LYS:N	2.11	0.64
2:H:22:CYS:HB2	2:H:36:TRP:CZ2	2.33	0.64
2:H:203:ALA:CB	2:H:210:LYS:HB2	2.26	0.64
1:L:8:PRO:HG2	1:L:10:SER:O	1.97	0.64
2:H:122:THR:HG22	2:H:123:ALA:H	1.62	0.64
2:H:161:SER:HB3	2:H:197:SER:HG	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:169:HIS:O	2:H:171:PHE:CE1	2.51	0.64
2:H:214:LYS:NZ	2:H:214:LYS:CB	2.61	0.64
1:L:161:GLN:CG	1:L:162:ASN:H	2.12	0.63
2:H:28:THR:O	2:H:30:SER:N	2.32	0.63
1:L:124:PRO:CD	2:H:132:VAL:CG1	2.77	0.63
1:L:155:ILE:HB	1:L:159:GLU:HG3	1.79	0.63
1:L:141:LEU:CD1	1:L:180:MET:HB3	2.29	0.63
1:L:204:LYS:HD2	1:L:204:LYS:N	2.12	0.63
2:H:70:PHE:CE2	2:H:85:MET:HG2	2.33	0.63
1:L:44:LYS:NZ	1:L:86:GLU:O	2.32	0.63
1:L:120:VAL:HG12	1:L:212:LYS:CG	2.29	0.63
2:H:164:LEU:CD1	2:H:165:SER:N	2.60	0.63
2:H:5:ASP:O	2:H:22:CYS:HA	1.98	0.63
2:H:52:ARG:O	2:H:74:ARG:NH2	2.32	0.63
2:H:137:THR:CA	2:H:141:VAL:HG13	2.25	0.63
2:H:5:ASP:OD2	2:H:6:GLU:C	2.42	0.62
2:H:24:ALA:HB3	2:H:29:PHE:CE1	2.33	0.62
2:H:103:TYR:H	3:H:218:FLU:C18	2.12	0.62
2:H:150:TYR:CE2	2:H:155:VAL:CG1	2.81	0.62
2:H:211:VAL:CG2	2:H:212:ASP:N	2.60	0.62
1:L:59:ARG:NH2	1:L:67:PHE:O	2.28	0.62
2:H:13:GLN:O	2:H:14:PRO:C	2.41	0.62
2:H:35:ASN:HB2	2:H:49:ALA:O	1.99	0.62
2:H:48:VAL:HG12	2:H:49:ALA:N	2.14	0.62
2:H:103:TYR:O	3:H:218:FLU:O4	2.18	0.62
2:H:151:PHE:CD2	2:H:151:PHE:C	2.77	0.62
2:H:17:PRO:HD2	2:H:88:LEU:HD12	1.82	0.62
2:H:77:SER:O	2:H:79:SER:N	2.31	0.62
2:H:157:LEU:HD22	2:H:202:VAL:HG22	1.81	0.62
2:H:191:SER:O	2:H:192:THR:C	2.40	0.62
1:L:10:SER:OG	1:L:11:LEU:N	2.30	0.62
1:L:53:ILE:HG21	1:L:56:VAL:O	2.00	0.62
1:L:136:SER:HA	1:L:184:LEU:O	2.00	0.62
2:H:101:SER:O	2:H:102:TYR:HB2	1.99	0.62
2:H:164:LEU:CG	2:H:165:SER:H	2.13	0.62
2:H:147:VAL:O	2:H:147:VAL:CG2	2.46	0.62
2:H:198:ILE:HD13	2:H:198:ILE:C	2.23	0.62
1:L:51:VAL:CG2	2:H:105:MET:HE1	2.30	0.62
1:L:59:ARG:HD3	1:L:63:VAL:HG12	1.81	0.62
2:H:99:THR:HB	4:H:219:MPD:HM1	1.81	0.62
1:L:189:ASP:C	1:L:193:ARG:HH22	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:38:ARG:HG2	2:H:96:TYR:CD2	2.35	0.62
2:H:193:TRP:CE3	2:H:196:GLN:OE1	2.53	0.62
1:L:4:MET:HG3	1:L:102:THR:HB	1.82	0.61
1:L:113:ARG:HG3	1:L:176:SER:HB2	1.82	0.61
2:H:136:THR:O	2:H:137:THR:C	2.44	0.61
1:L:21:ILE:HD13	1:L:22:SER:N	2.15	0.61
1:L:21:ILE:CG1	1:L:107:THR:HG21	2.31	0.61
2:H:22:CYS:CB	2:H:36:TRP:CZ2	2.83	0.61
2:H:40:SER:CA	2:H:43:LYS:HB2	2.29	0.61
1:L:52:LEU:HB2	1:L:53:ILE:HD12	1.82	0.61
1:L:215:ASN:N	1:L:219:CYS:HB3	2.09	0.61
2:H:64:ASP:CG	2:H:67:LYS:NZ	2.58	0.61
2:H:201:ASN:HD22	2:H:201:ASN:N	1.97	0.61
2:H:57:ASN:O	2:H:58:TYR:HB2	2.00	0.61
2:H:117:SER:HB2	2:H:178:ASP:OD1	2.00	0.61
1:L:11:LEU:HD23	1:L:109:LEU:CD1	2.31	0.61
1:L:81:SER:O	1:L:82:ARG:CB	2.48	0.61
1:L:82:ARG:O	1:L:82:ARG:HG3	2.00	0.61
2:H:82:TYR:HB3	2:H:84:GLN:OE1	1.99	0.61
1:L:15:LEU:HD13	1:L:15:LEU:N	2.15	0.61
1:L:203:HIS:CG	1:L:204:LYS:N	2.67	0.61
2:H:21:SER:HA	2:H:82:TYR:CD1	2.35	0.61
2:H:20:LEU:CD1	2:H:85:MET:CE	2.67	0.61
2:H:61:TYR:OH	2:H:67:LYS:CE	2.45	0.61
2:H:62:TYR:HE1	2:H:72:ILE:H	1.45	0.61
2:H:64:ASP:N	2:H:67:LYS:CD	2.64	0.61
2:H:61:TYR:HE1	2:H:63:SER:HA	1.66	0.61
2:H:75:ASP:O	2:H:79:SER:HA	2.01	0.61
2:H:99:THR:CB	4:H:219:MPD:O2	2.49	0.61
1:L:3:VAL:N	1:L:26:SER:HB2	2.16	0.61
2:H:13:GLN:O	2:H:14:PRO:O	2.17	0.61
2:H:204:HIS:CD2	2:H:206:ALA:HB3	2.35	0.61
1:L:91:TYR:CE2	1:L:109:LEU:HD23	2.36	0.60
1:L:164:VAL:HA	1:L:183:THR:O	2.01	0.60
2:H:39:GLN:O	2:H:40:SER:C	2.44	0.60
2:H:56:TYR:O	2:H:59:GLU:OE2	2.19	0.60
2:H:69:ARG:CA	2:H:87:ASN:ND2	2.62	0.60
1:L:161:GLN:HG3	1:L:163:GLY:N	2.17	0.60
1:L:38:LEU:HD23	1:L:76:PHE:CZ	2.36	0.60
2:H:206:ALA:O	2:H:207:SER:CB	2.35	0.60
1:L:128:GLU:O	1:L:132:SER:OG	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:TYR:HE1	2:H:72:ILE:N	2.00	0.60
2:H:152:PRO:HD2	2:H:206:ALA:HB1	1.84	0.60
1:L:28:SER:C	1:L:30:VAL:H	2.10	0.60
2:H:93:MET:CE	2:H:115:THR:CG2	2.79	0.60
2:H:160:ASN:O	2:H:198:ILE:CG1	2.49	0.60
1:L:1:ASP:HA	1:L:100:PRO:HD3	1.84	0.60
1:L:95:GLN:O	1:L:101:TRP:HA	2.01	0.60
1:L:56:VAL:CG2	1:L:57:SER:N	2.65	0.60
1:L:78:LEU:HD22	1:L:79:LYS:N	2.17	0.60
1:L:122:ILE:CG2	1:L:212:LYS:HG3	2.23	0.60
1:L:130:LEU:C	1:L:132:SER:H	2.08	0.60
1:L:6:GLN:OE1	1:L:92:PHE:HA	2.02	0.59
1:L:39:ARG:NH1	4:H:219:MPD:H32	2.16	0.59
2:H:17:PRO:CD	2:H:88:LEU:HD12	2.32	0.59
1:L:120:VAL:CG1	1:L:212:LYS:CB	2.78	0.59
2:H:31:ASP:CA	2:H:53:ASN:HD21	2.00	0.59
1:L:27:GLN:C	1:L:74:THR:HG23	2.27	0.59
2:H:99:THR:HB	4:H:219:MPD:HM2	1.83	0.59
2:H:150:TYR:CE1	2:H:155:VAL:HG11	2.37	0.59
1:L:165:LEU:CD2	2:H:174:VAL:HG11	2.32	0.59
1:L:174:LYS:NZ	1:L:175:ASP:CG	2.60	0.59
2:H:11:LEU:HD21	2:H:151:PHE:CZ	2.37	0.59
2:H:51:ILE:CG2	2:H:60:THR:HG22	2.28	0.59
1:L:52:LEU:C	1:L:53:ILE:HD12	2.28	0.59
1:L:54:TYR:CD1	2:H:105:MET:HE3	2.38	0.59
2:H:66:VAL:O	2:H:67:LYS:O	2.21	0.59
2:H:90:VAL:CG1	2:H:116:VAL:HG22	2.28	0.59
2:H:143:LEU:HD22	2:H:215:ILE:CG2	2.24	0.59
1:L:161:GLN:HG3	1:L:163:GLY:H	1.67	0.59
1:L:200:GLU:HB2	1:L:211:VAL:HG12	1.83	0.59
2:H:27:PHE:CE1	2:H:34:MET:HE1	2.37	0.59
1:L:15:LEU:HD22	1:L:15:LEU:H	1.68	0.59
2:H:81:VAL:HG22	2:H:82:TYR:N	2.16	0.59
1:L:116:ALA:HB1	1:L:143:ASN:O	2.03	0.59
1:L:90:VAL:HG12	1:L:92:PHE:CE1	2.38	0.58
1:L:120:VAL:CG1	1:L:212:LYS:CG	2.80	0.58
1:L:124:PRO:HD3	2:H:132:VAL:HG13	1.84	0.58
2:H:87:ASN:O	2:H:89:ARG:CZ	2.50	0.58
1:L:52:LEU:CB	1:L:53:ILE:HD12	2.33	0.58
1:L:155:ILE:HG23	1:L:197:TYR:CD1	2.39	0.58
2:H:90:VAL:CG1	2:H:116:VAL:HG13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:TYR:CD2	2:H:146:LEU:CD2	2.83	0.58
2:H:62:TYR:OH	2:H:72:ILE:O	2.20	0.58
2:H:161:SER:HB2	2:H:198:ILE:N	2.18	0.58
2:H:164:LEU:HB2	2:H:193:TRP:CE2	2.38	0.58
2:H:40:SER:HB3	2:H:93:MET:O	2.04	0.58
2:H:117:SER:HB2	2:H:178:ASP:CG	2.29	0.58
1:L:65:ASP:C	1:L:67:PHE:N	2.60	0.58
2:H:31:ASP:CA	2:H:53:ASN:HD22	2.04	0.58
1:L:18:GLN:OE1	1:L:81:SER:HA	2.03	0.58
2:H:162:GLY:HA2	2:H:197:SER:N	2.10	0.58
1:L:59:ARG:CD	1:L:63:VAL:HG12	2.33	0.58
1:L:66:ARG:HD2	1:L:80:ILE:CG2	2.33	0.58
1:L:193:ARG:O	1:L:193:ARG:HG3	2.04	0.58
2:H:39:GLN:O	2:H:39:GLN:CG	2.50	0.58
2:H:134:GLY:O	2:H:137:THR:CB	2.52	0.58
2:H:150:TYR:CZ	2:H:155:VAL:HG13	2.39	0.58
1:L:29:LEU:HD11	1:L:95:GLN:HB3	1.86	0.57
1:L:129:GLN:CG	1:L:134:GLY:O	2.52	0.57
2:H:153:GLU:CD	2:H:180:TYR:CZ	2.81	0.57
4:H:219:MPD:O2	4:H:219:MPD:C5	2.51	0.57
2:H:70:PHE:CE1	2:H:85:MET:HB3	2.39	0.57
2:H:90:VAL:O	2:H:92:ASP:N	2.37	0.57
2:H:91:GLU:HG3	2:H:91:GLU:O	2.04	0.57
2:H:33:TRP:CE2	2:H:52:ARG:HD3	2.40	0.57
2:H:40:SER:OG	2:H:43:LYS:HE2	2.05	0.57
2:H:69:ARG:C	2:H:87:ASN:ND2	2.61	0.57
2:H:90:VAL:C	2:H:92:ASP:H	2.11	0.57
1:L:124:PRO:HD3	2:H:132:VAL:CG1	2.33	0.57
1:L:210:ILE:O	1:L:210:ILE:HG22	2.00	0.57
2:H:73:SER:O	2:H:81:VAL:HG23	2.04	0.57
2:H:6:GLU:CG	2:H:111:GLY:CA	2.83	0.57
2:H:17:PRO:O	2:H:86:ASN:N	2.37	0.57
2:H:108:TRP:CD1	4:H:219:MPD:HM1	2.40	0.57
1:L:2:VAL:HG13	1:L:26:SER:HB2	1.86	0.57
1:L:203:HIS:CG	1:L:204:LYS:H	2.22	0.57
1:L:215:ASN:O	1:L:216:ARG:C	2.47	0.57
2:H:45:LEU:HD21	2:H:97:TYR:HE1	1.70	0.57
2:H:106:ASP:CB	4:H:219:MPD:H11	2.34	0.57
2:H:29:PHE:HB2	2:H:79:SER:CB	2.34	0.56
2:H:33:TRP:CZ2	2:H:52:ARG:HD3	2.40	0.56
2:H:36:TRP:CD1	2:H:72:ILE:CD1	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:ARG:HB3	2:H:87:ASN:CG	2.28	0.56
2:H:134:GLY:C	2:H:137:THR:OG1	2.47	0.56
2:H:209:THR:CG2	2:H:210:LYS:N	2.67	0.56
1:L:59:ARG:HG2	1:L:59:ARG:NH1	2.18	0.56
1:L:161:GLN:HG2	1:L:184:LEU:HD11	1.87	0.56
2:H:33:TRP:CD1	2:H:50:GLN:OE1	2.59	0.56
2:H:136:THR:CG2	2:H:137:THR:H	2.17	0.56
2:H:158:THR:HG22	2:H:201:ASN:O	2.04	0.56
2:H:197:SER:O	2:H:198:ILE:CB	2.40	0.56
1:L:31:HIS:CB	1:L:97:THR:HG23	2.29	0.56
2:H:24:ALA:HB3	2:H:29:PHE:CD1	2.40	0.56
2:H:38:ARG:O	2:H:45:LEU:HA	2.05	0.56
2:H:90:VAL:CB	2:H:116:VAL:HG13	2.35	0.56
2:H:155:VAL:CG2	2:H:156:THR:N	2.63	0.56
2:H:162:GLY:O	2:H:163:SER:CB	2.48	0.56
1:L:136:SER:OG	2:H:148:LYS:NZ	2.38	0.56
1:L:147:LYS:HB3	1:L:178:TYR:CE2	2.40	0.56
1:L:154:LYS:HB3	1:L:198:THR:HG23	1.87	0.56
2:H:162:GLY:CA	2:H:197:SER:O	2.53	0.56
2:H:151:PHE:CD2	2:H:152:PRO:N	2.74	0.56
1:L:21:ILE:HG12	1:L:107:THR:HG21	1.88	0.56
1:L:117:ALA:HB1	1:L:118:PRO:HD2	1.88	0.56
1:L:184:LEU:HD12	1:L:185:THR:H	1.69	0.56
2:H:66:VAL:HB	2:H:70:PHE:HB2	1.88	0.55
2:H:189:THR:OG1	2:H:193:TRP:HB2	2.05	0.55
1:L:49:PRO:HG2	2:H:45:LEU:HD11	1.87	0.55
2:H:29:PHE:CB	2:H:79:SER:OG	2.48	0.55
2:H:121:THR:HG22	2:H:151:PHE:HE2	1.70	0.55
1:L:11:LEU:HG	1:L:13:VAL:HG13	1.88	0.55
1:L:30:VAL:HG22	1:L:36:THR:OG1	2.06	0.55
1:L:110:GLU:OE1	1:L:178:TYR:OH	2.11	0.55
1:L:120:VAL:HG22	1:L:141:LEU:HD23	1.88	0.55
1:L:194:HIS:C	1:L:197:TYR:OH	2.49	0.55
1:L:202:THR:HG23	1:L:209:PRO:HD3	1.87	0.55
2:H:136:THR:HG23	2:H:137:THR:N	2.21	0.55
1:L:91:TYR:CD2	1:L:109:LEU:HD23	2.41	0.55
2:H:169:HIS:CE1	2:H:185:SER:OG	2.58	0.55
2:H:6:GLU:HG2	2:H:111:GLY:C	2.31	0.55
1:L:3:VAL:HG12	1:L:24:ARG:NH2	2.22	0.55
1:L:21:ILE:HD12	1:L:40:TRP:CZ3	2.41	0.55
2:H:158:THR:HG23	2:H:201:ASN:HB2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:SER:HB3	2:H:197:SER:CB	2.36	0.55
2:H:179:LEU:N	2:H:179:LEU:HD23	2.21	0.55
2:H:100:GLY:O	4:H:219:MPD:H12	2.06	0.55
2:H:63:SER:C	2:H:67:LYS:HD2	2.32	0.55
2:H:66:VAL:O	2:H:67:LYS:C	2.49	0.54
2:H:159:TRP:CE3	2:H:198:ILE:CD1	2.83	0.54
2:H:188:VAL:HG22	2:H:193:TRP:CD1	2.39	0.54
1:L:96:SER:O	3:H:218:FLU:H5	2.07	0.54
2:H:106:ASP:HB3	4:H:219:MPD:H11	1.88	0.54
1:L:94:SER:CA	1:L:102:THR:O	2.55	0.54
2:H:22:CYS:O	2:H:80:SER:HB2	2.07	0.54
2:H:162:GLY:N	2:H:197:SER:O	2.41	0.54
1:L:56:VAL:HG22	1:L:57:SER:H	1.72	0.54
2:H:162:GLY:H	2:H:197:SER:C	2.14	0.54
2:H:76:ASP:O	2:H:79:SER:HA	2.07	0.54
2:H:144:GLY:HA2	2:H:184:SER:O	2.08	0.54
1:L:104:GLY:O	1:L:106:GLY:N	2.40	0.54
2:H:27:PHE:CE1	2:H:32:TYR:CD2	2.96	0.54
2:H:198:ILE:C	2:H:198:ILE:CD1	2.81	0.54
1:L:67:PHE:CE2	1:L:80:ILE:HD13	2.43	0.54
2:H:63:SER:C	2:H:67:LYS:CD	2.80	0.54
1:L:138:VAL:HG11	2:H:129:LEU:HD13	1.90	0.54
2:H:99:THR:CB	4:H:219:MPD:HM2	2.38	0.54
2:H:193:TRP:H	2:H:194:PRO:CD	2.19	0.54
2:H:120:LYS:O	2:H:122:THR:OG1	2.25	0.53
2:H:207:SER:O	2:H:208:SER:O	2.26	0.53
2:H:61:TYR:CE1	2:H:62:TYR:O	2.61	0.53
2:H:90:VAL:C	2:H:92:ASP:N	2.67	0.53
1:L:42:LEU:CD2	1:L:44:LYS:HZ3	2.13	0.53
2:H:93:MET:HB2	2:H:116:VAL:HG12	1.90	0.53
1:L:161:GLN:OE1	1:L:162:ASN:HB2	2.08	0.53
2:H:61:TYR:CD1	2:H:61:TYR:C	2.87	0.53
2:H:81:VAL:HG22	2:H:82:TYR:H	1.73	0.53
2:H:126:VAL:HG12	2:H:213:LYS:HG3	1.90	0.53
2:H:153:GLU:OE2	2:H:153:GLU:CA	2.55	0.53
1:L:8:PRO:O	1:L:107:THR:OG1	2.22	0.53
1:L:118:PRO:HB3	1:L:144:PHE:CD2	2.44	0.53
1:L:130:LEU:CD2	1:L:188:LYS:HG3	2.38	0.53
1:L:138:VAL:HG12	1:L:138:VAL:O	2.08	0.53
1:L:29:LEU:HD21	1:L:95:GLN:HG2	1.90	0.53
2:H:54:LYS:HG2	2:H:58:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:168:TRP:CD1	1:L:180:MET:HG3	2.44	0.53
1:L:123:PHE:CE2	1:L:140:PHE:CE1	2.97	0.53
1:L:152:LYS:NZ	1:L:154:LYS:HE2	2.24	0.53
2:H:39:GLN:C	2:H:40:SER:O	2.46	0.53
2:H:45:LEU:HD21	2:H:97:TYR:CE1	2.44	0.53
2:H:142:THR:HG22	2:H:187:THR:N	2.24	0.53
2:H:161:SER:CB	2:H:198:ILE:N	2.71	0.53
2:H:16:ARG:HH21	2:H:86:ASN:HB2	1.74	0.53
2:H:38:ARG:NH1	2:H:96:TYR:CZ	2.61	0.53
2:H:45:LEU:CD1	2:H:108:TRP:CH2	2.86	0.53
2:H:83:LEU:HD23	2:H:85:MET:HE2	1.91	0.53
1:L:123:PHE:CD2	1:L:138:VAL:HG12	2.44	0.52
2:H:124:PRO:N	2:H:150:TYR:HB3	2.23	0.52
2:H:163:SER:C	2:H:193:TRP:CE2	2.87	0.52
2:H:195:SER:C	2:H:196:GLN:O	2.52	0.52
2:H:120:LYS:H	2:H:120:LYS:HD2	1.65	0.52
1:L:4:MET:HE2	1:L:95:GLN:CB	2.38	0.52
1:L:29:LEU:CD2	1:L:95:GLN:HG2	2.40	0.52
1:L:62:GLY:O	1:L:63:VAL:C	2.52	0.52
2:H:49:ALA:HB1	2:H:72:ILE:CB	2.38	0.52
2:H:191:SER:CA	2:H:194:PRO:HD2	2.38	0.52
1:L:54:TYR:HB3	2:H:105:MET:HE3	1.92	0.52
2:H:99:THR:CB	4:H:219:MPD:CM	2.87	0.52
2:H:150:TYR:CE2	2:H:155:VAL:HG12	2.44	0.52
2:H:57:ASN:O	2:H:58:TYR:CB	2.58	0.52
1:L:78:LEU:HD22	1:L:79:LYS:H	1.75	0.52
2:H:136:THR:HG22	2:H:137:THR:H	1.75	0.52
2:H:70:PHE:CZ	2:H:85:MET:CB	2.91	0.52
2:H:131:PRO:HD3	2:H:143:LEU:HD21	1.84	0.52
2:H:20:LEU:HD22	2:H:85:MET:CE	2.39	0.52
2:H:117:SER:HB2	2:H:178:ASP:OD2	2.09	0.52
1:L:44:LYS:O	1:L:47:GLN:HB2	2.09	0.51
2:H:108:TRP:NE1	4:H:219:MPD:H31	2.17	0.51
2:H:190:SER:C	2:H:191:SER:OG	2.53	0.51
1:L:35:ASN:ND2	1:L:35:ASN:N	2.44	0.51
1:L:38:LEU:HD23	1:L:76:PHE:CE2	2.45	0.51
1:L:43:GLN:HE22	2:H:39:GLN:HE22	1.56	0.51
2:H:61:TYR:CE2	2:H:67:LYS:HE3	2.45	0.51
2:H:21:SER:HB2	2:H:82:TYR:HE1	1.74	0.51
1:L:2:VAL:CG2	1:L:26:SER:HB3	2.27	0.51
1:L:35:ASN:O	1:L:37:TYR:CD2	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:184:LEU:HD12	1:L:185:THR:N	2.25	0.51
2:H:169:HIS:ND1	2:H:169:HIS:N	2.58	0.51
1:L:147:LYS:HB3	1:L:178:TYR:CZ	2.45	0.51
2:H:38:ARG:NH1	2:H:96:TYR:CE2	2.78	0.51
2:H:70:PHE:O	2:H:71:THR:HG22	2.11	0.51
1:L:194:HIS:C	1:L:197:TYR:HH	2.19	0.51
2:H:153:GLU:CD	2:H:180:TYR:HH	2.19	0.51
1:L:152:LYS:HZ2	1:L:200:GLU:HG2	1.76	0.51
2:H:22:CYS:C	2:H:23:VAL:HG23	2.35	0.51
2:H:150:TYR:CZ	2:H:180:TYR:HB2	2.46	0.51
2:H:176:GLN:O	2:H:177:SER:C	2.54	0.51
2:H:49:ALA:CB	2:H:72:ILE:HB	2.41	0.50
2:H:72:ILE:HD12	2:H:81:VAL:CG2	2.41	0.50
2:H:139:SER:O	2:H:190:SER:CA	2.59	0.50
2:H:203:ALA:CB	2:H:210:LYS:CB	2.88	0.50
2:H:106:ASP:OD1	2:H:106:ASP:C	2.52	0.50
1:L:59:ARG:HH11	1:L:59:ARG:CG	2.15	0.50
2:H:20:LEU:HB2	2:H:85:MET:HE3	1.94	0.50
2:H:62:TYR:CE2	2:H:72:ILE:HG22	2.45	0.50
2:H:164:LEU:CB	2:H:193:TRP:HE1	2.24	0.50
1:L:204:LYS:C	1:L:206:SER:H	2.18	0.50
2:H:82:TYR:CB	2:H:84:GLN:OE1	2.59	0.50
2:H:12:VAL:CG1	2:H:17:PRO:CG	2.90	0.50
2:H:193:TRP:CE3	2:H:196:GLN:NE2	2.80	0.50
2:H:193:TRP:H	2:H:194:PRO:HD2	1.77	0.50
1:L:28:SER:O	1:L:30:VAL:N	2.43	0.50
2:H:203:ALA:HA	2:H:210:LYS:CA	2.35	0.50
1:L:154:LYS:NZ	1:L:200:GLU:CD	2.69	0.50
2:H:176:GLN:HG2	2:H:177:SER:HG	1.74	0.50
2:H:189:THR:OG1	2:H:192:THR:OG1	2.25	0.50
2:H:121:THR:HA	2:H:151:PHE:HD2	1.77	0.50
1:L:91:TYR:O	1:L:106:GLY:HA2	2.12	0.50
2:H:35:ASN:CB	2:H:49:ALA:O	2.59	0.50
2:H:64:ASP:OD1	2:H:67:LYS:NZ	2.42	0.50
2:H:121:THR:HA	2:H:151:PHE:CD2	2.47	0.50
1:L:124:PRO:HG3	1:L:214:PHE:CD1	2.46	0.49
2:H:40:SER:HB2	2:H:43:LYS:CD	2.41	0.49
2:H:92:ASP:O	2:H:96:TYR:CZ	2.64	0.49
1:L:24:ARG:C	1:L:24:ARG:NE	2.69	0.49
1:L:141:LEU:HD11	1:L:151:VAL:HG21	1.93	0.49
2:H:204:HIS:O	2:H:207:SER:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:ASN:O	1:L:201:ALA:HA	2.12	0.49
1:L:165:LEU:CD2	2:H:174:VAL:HG12	2.37	0.49
2:H:36:TRP:HD1	2:H:72:ILE:CD1	2.24	0.49
2:H:70:PHE:CE2	2:H:85:MET:CG	2.94	0.49
2:H:71:THR:O	2:H:83:LEU:HA	2.11	0.49
1:L:66:ARG:HD3	1:L:82:ARG:O	2.12	0.49
1:L:145:TYR:CE2	1:L:178:TYR:OH	2.65	0.49
2:H:28:THR:OG1	2:H:31:ASP:HB2	2.12	0.49
2:H:81:VAL:CG2	2:H:82:TYR:H	2.26	0.49
1:L:165:LEU:HD21	2:H:174:VAL:CB	2.41	0.49
2:H:17:PRO:HG2	2:H:88:LEU:CD1	2.37	0.49
2:H:80:SER:HG	2:H:82:TYR:HH	1.58	0.49
1:L:38:LEU:C	1:L:38:LEU:CD1	2.83	0.49
2:H:62:TYR:OH	2:H:72:ILE:HG22	2.11	0.49
1:L:7:THR:OG1	1:L:22:SER:CB	2.60	0.49
1:L:60:PHE:CD1	1:L:61:SER:N	2.80	0.49
1:L:87:ASP:O	1:L:91:TYR:OH	2.19	0.49
2:H:75:ASP:O	2:H:76:ASP:O	2.30	0.49
2:H:123:ALA:HB1	2:H:124:PRO:HD2	1.93	0.49
1:L:183:THR:O	1:L:183:THR:HG22	2.12	0.49
2:H:142:THR:HG22	2:H:187:THR:CA	2.43	0.49
2:H:215:ILE:O	2:H:216:GLU:CB	2.61	0.49
1:L:3:VAL:H	1:L:26:SER:HB2	1.76	0.49
1:L:125:PRO:HG3	1:L:191:TYR:CE2	2.47	0.49
2:H:134:GLY:O	2:H:137:THR:OG1	2.31	0.49
1:L:51:VAL:HG21	2:H:105:MET:HE2	1.94	0.49
2:H:93:MET:CE	2:H:115:THR:HG23	2.30	0.49
1:L:15:LEU:HA	1:L:83:VAL:O	2.12	0.48
1:L:28:SER:HA	1:L:73:GLY:O	2.12	0.48
1:L:29:LEU:HD12	1:L:38:LEU:HB2	1.95	0.48
1:L:93:CYS:O	1:L:93:CYS:SG	2.70	0.48
2:H:20:LEU:O	2:H:82:TYR:HA	2.13	0.48
2:H:153:GLU:CD	2:H:180:TYR:OH	2.56	0.48
2:H:22:CYS:HB3	2:H:36:TRP:CZ2	2.48	0.48
2:H:29:PHE:CZ	2:H:34:MET:SD	3.06	0.48
1:L:9:LEU:H	1:L:9:LEU:HD22	1.77	0.48
1:L:31:HIS:HB2	1:L:37:TYR:HD2	1.78	0.48
1:L:40:TRP:CE2	1:L:78:LEU:HB3	2.49	0.48
1:L:56:VAL:HG22	1:L:57:SER:N	2.28	0.48
2:H:61:TYR:CD1	2:H:62:TYR:C	2.91	0.48
2:H:61:TYR:CG	2:H:62:TYR:N	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:180:TYR:C	2:H:181:THR:HG22	2.37	0.48
1:L:2:VAL:HG13	1:L:26:SER:CB	2.43	0.48
1:L:11:LEU:HD21	1:L:19:ALA:CB	2.44	0.48
1:L:123:PHE:HD2	1:L:138:VAL:HG12	1.78	0.48
1:L:168:TRP:NE1	1:L:180:MET:CE	2.70	0.48
2:H:54:LYS:HB2	2:H:55:PRO:CD	2.32	0.48
1:L:15:LEU:HD12	1:L:83:VAL:HG12	1.96	0.48
2:H:69:ARG:O	2:H:87:ASN:ND2	2.46	0.48
1:L:54:TYR:CD1	2:H:105:MET:CE	2.97	0.48
2:H:51:ILE:CD1	2:H:72:ILE:CD1	2.64	0.48
2:H:81:VAL:CG2	2:H:82:TYR:N	2.77	0.48
2:H:89:ARG:O	2:H:92:ASP:OD2	2.32	0.48
2:H:151:PHE:CZ	2:H:152:PRO:HB3	2.49	0.48
1:L:165:LEU:HD21	2:H:174:VAL:HB	1.95	0.48
2:H:16:ARG:N	2:H:17:PRO:CD	2.68	0.48
2:H:48:VAL:CG1	2:H:49:ALA:N	2.77	0.48
2:H:70:PHE:O	2:H:71:THR:HG23	2.12	0.48
2:H:128:PRO:O	2:H:128:PRO:CG	2.56	0.48
2:H:191:SER:N	2:H:194:PRO:CG	2.71	0.48
2:H:127:TYR:CD2	2:H:146:LEU:HD22	2.42	0.48
2:H:212:ASP:C	2:H:213:LYS:HG2	2.38	0.48
2:H:145:CYS:O	2:H:183:SER:HA	2.13	0.47
1:L:118:PRO:O	1:L:118:PRO:HG2	2.14	0.47
1:L:160:ARG:O	1:L:161:GLN:C	2.57	0.47
2:H:85:MET:HB2	2:H:88:LEU:CD2	2.35	0.47
2:H:162:GLY:H	2:H:197:SER:CA	2.27	0.47
1:L:149:ILE:CG2	1:L:150:ASN:N	2.57	0.47
2:H:57:ASN:C	2:H:58:TYR:CD2	2.93	0.47
2:H:77:SER:C	2:H:79:SER:HG	2.09	0.47
1:L:155:ILE:HG13	1:L:159:GLU:CB	2.44	0.47
2:H:22:CYS:O	2:H:80:SER:HA	2.14	0.47
2:H:161:SER:O	2:H:162:GLY:C	2.57	0.47
1:L:31:HIS:HB3	1:L:35:ASN:O	2.15	0.47
1:L:168:TRP:C	1:L:169:THR:HG22	2.38	0.47
1:L:218:GLU:N	1:L:218:GLU:CD	2.73	0.47
2:H:40:SER:HG	2:H:93:MET:C	2.20	0.47
2:H:28:THR:C	2:H:30:SER:N	2.71	0.47
1:L:174:LYS:HG3	1:L:175:ASP:OD1	2.15	0.47
1:L:174:LYS:CE	1:L:175:ASP:CG	2.88	0.47
2:H:4:LEU:HD12	2:H:4:LEU:N	2.30	0.47
2:H:4:LEU:HD21	2:H:100:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:95:GLN:O	1:L:95:GLN:NE2	2.48	0.46
1:L:136:SER:CA	1:L:184:LEU:O	2.62	0.46
1:L:147:LYS:O	1:L:149:ILE:HD13	2.11	0.46
2:H:41:PRO:C	2:H:43:LYS:H	2.23	0.46
2:H:92:ASP:C	2:H:96:TYR:HH	2.04	0.46
2:H:191:SER:C	2:H:194:PRO:CD	2.76	0.46
1:L:38:LEU:HD23	1:L:76:PHE:CE1	2.51	0.46
1:L:145:TYR:CD1	1:L:146:PRO:HA	2.51	0.46
2:H:29:PHE:CE1	2:H:34:MET:HE2	2.50	0.46
2:H:90:VAL:HB	2:H:116:VAL:HG13	1.97	0.46
1:L:30:VAL:O	1:L:30:VAL:HG12	2.15	0.46
1:L:94:SER:OG	1:L:95:GLN:N	2.48	0.46
2:H:21:SER:CB	2:H:82:TYR:HE1	2.28	0.46
2:H:131:PRO:O	2:H:131:PRO:HG2	2.16	0.46
2:H:139:SER:O	2:H:190:SER:HA	2.14	0.46
2:H:89:ARG:HH11	2:H:89:ARG:CG	2.26	0.46
1:L:166:ASN:OD1	1:L:182:SER:CB	2.61	0.46
2:H:103:TYR:HA	3:H:218:FLU:C18	2.45	0.46
2:H:6:GLU:HG3	2:H:112:THR:N	2.31	0.46
2:H:69:ARG:NH2	2:H:87:ASN:OD1	2.46	0.46
1:L:7:THR:OG1	1:L:22:SER:HB2	2.15	0.46
1:L:29:LEU:HD23	1:L:98:HIS:CD2	2.51	0.46
1:L:154:LYS:CB	1:L:198:THR:HG23	2.46	0.46
2:H:40:SER:HB2	2:H:43:LYS:CB	2.46	0.46
2:H:40:SER:OG	2:H:93:MET:C	2.59	0.46
2:H:49:ALA:HB1	2:H:72:ILE:HG12	1.98	0.46
2:H:157:LEU:HD12	2:H:158:THR:O	2.16	0.46
2:H:89:ARG:NH1	2:H:89:ARG:HG2	2.30	0.45
2:H:136:THR:CG2	2:H:140:SER:O	2.60	0.45
1:L:6:GLN:HA	1:L:22:SER:O	2.16	0.45
1:L:120:VAL:C	1:L:121:SER:OG	2.59	0.45
1:L:130:LEU:C	1:L:132:SER:N	2.74	0.45
2:H:17:PRO:N	2:H:87:ASN:H	2.14	0.45
2:H:29:PHE:O	2:H:30:SER:C	2.58	0.45
2:H:39:GLN:O	2:H:40:SER:O	2.33	0.45
1:L:59:ARG:NH1	1:L:59:ARG:CG	2.74	0.45
1:L:114:ALA:O	1:L:145:TYR:HB3	2.16	0.45
1:L:136:SER:HB3	1:L:185:THR:HG23	1.98	0.45
2:H:38:ARG:NE	2:H:48:VAL:CG2	2.80	0.45
2:H:149:GLY:O	2:H:179:LEU:HD12	2.17	0.45
1:L:115:ASP:O	1:L:116:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:ASN:OD1	2:H:169:HIS:CD2	2.70	0.45
2:H:36:TRP:HA	2:H:97:TYR:O	2.15	0.45
2:H:58:TYR:C	2:H:59:GLU:O	2.60	0.45
2:H:85:MET:CB	2:H:88:LEU:CD2	2.93	0.45
2:H:105:MET:O	2:H:106:ASP:HB3	2.16	0.45
2:H:161:SER:CB	2:H:197:SER:OG	2.45	0.45
1:L:65:ASP:OD2	1:L:65:ASP:C	2.49	0.45
1:L:66:ARG:HD2	1:L:80:ILE:HG22	1.98	0.45
1:L:44:LYS:HE3	1:L:86:GLU:O	2.17	0.45
1:L:95:GLN:HE21	1:L:102:THR:N	2.14	0.45
2:H:72:ILE:HA	2:H:82:TYR:O	2.16	0.45
2:H:166:SER:CB	2:H:188:VAL:HG23	2.47	0.45
1:L:3:VAL:HG12	1:L:24:ARG:HH22	1.82	0.45
1:L:169:THR:CG2	2:H:171:PHE:CD2	3.00	0.45
2:H:32:TYR:CE2	2:H:101:SER:O	2.70	0.45
2:H:62:TYR:HH	2:H:72:ILE:HG22	1.82	0.45
2:H:100:GLY:O	2:H:106:ASP:CB	2.59	0.45
2:H:123:ALA:HB2	2:H:208:SER:HB3	1.98	0.45
1:L:28:SER:C	1:L:30:VAL:N	2.74	0.45
1:L:123:PHE:CE2	1:L:140:PHE:HE1	2.35	0.45
2:H:120:LYS:N	2:H:120:LYS:HD3	2.21	0.45
2:H:164:LEU:CA	2:H:193:TRP:HE1	2.29	0.45
3:H:218:FLU:C15	3:H:218:FLU:H8	2.45	0.45
1:L:44:LYS:CE	1:L:86:GLU:O	2.66	0.44
1:L:53:ILE:HG23	1:L:56:VAL:O	2.14	0.44
2:H:49:ALA:CB	2:H:72:ILE:HG12	2.47	0.44
2:H:57:ASN:O	2:H:58:TYR:CD2	2.70	0.44
2:H:159:TRP:CD1	2:H:168:VAL:HG11	2.52	0.44
1:L:200:GLU:HB2	1:L:211:VAL:CG1	2.46	0.44
1:L:217:ASN:HB3	1:L:218:GLU:CD	2.41	0.44
2:H:40:SER:N	2:H:43:LYS:CB	2.79	0.44
2:H:164:LEU:CB	2:H:193:TRP:NE1	2.80	0.44
1:L:1:ASP:HA	1:L:100:PRO:HD2	1.95	0.44
1:L:124:PRO:HD2	2:H:132:VAL:CG1	2.33	0.44
1:L:153:TRP:HZ2	1:L:182:SER:HG	1.63	0.44
2:H:30:SER:HA	2:H:76:ASP:OD1	2.17	0.44
2:H:150:TYR:CZ	2:H:155:VAL:HG11	2.47	0.44
1:L:13:VAL:O	1:L:112:LYS:HB3	2.18	0.44
1:L:123:PHE:HA	1:L:124:PRO:HD3	1.77	0.44
1:L:204:LYS:HD2	1:L:204:LYS:H	1.80	0.44
2:H:51:ILE:CD1	2:H:72:ILE:CG1	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:116:VAL:HG13	2:H:116:VAL:O	2.18	0.44
2:H:153:GLU:HB3	2:H:154:PRO:CD	2.43	0.44
2:H:198:ILE:HD13	2:H:199:THR:H	1.79	0.44
3:H:218:FLU:C15	3:H:218:FLU:C8	2.94	0.44
1:L:82:ARG:O	1:L:82:ARG:CG	2.64	0.44
1:L:204:LYS:C	1:L:206:SER:N	2.72	0.44
2:H:192:THR:N	2:H:194:PRO:HD2	2.31	0.44
1:L:141:LEU:HD13	1:L:180:MET:SD	2.58	0.44
2:H:70:PHE:CZ	2:H:85:MET:CG	3.01	0.44
2:H:191:SER:CA	2:H:194:PRO:CD	2.95	0.44
1:L:24:ARG:HB2	1:L:74:THR:O	2.18	0.44
2:H:31:ASP:C	2:H:53:ASN:HD21	2.13	0.44
2:H:150:TYR:CD2	2:H:150:TYR:C	2.96	0.44
2:H:6:GLU:CG	2:H:112:THR:N	2.80	0.43
2:H:51:ILE:CD1	2:H:72:ILE:HD12	2.27	0.43
2:H:157:LEU:HD11	2:H:200:CYS:SG	2.58	0.43
1:L:55:LYS:CD	2:H:104:GLY:HA3	2.44	0.43
2:H:37:VAL:CG1	2:H:46:GLU:O	2.65	0.43
2:H:18:MET:HE1	2:H:114:VAL:HG22	2.00	0.43
2:H:19:LYS:CE	2:H:82:TYR:CD1	3.01	0.43
2:H:40:SER:O	2:H:43:LYS:CB	2.54	0.43
2:H:146:LEU:C	2:H:146:LEU:HD23	2.43	0.43
2:H:193:TRP:CE3	2:H:196:GLN:CD	2.95	0.43
1:L:96:SER:HB2	3:H:218:FLU:O3	2.18	0.43
2:H:27:PHE:CZ	2:H:34:MET:CE	2.79	0.43
2:H:57:ASN:O	2:H:58:TYR:HD2	2.01	0.43
2:H:178:ASP:C	2:H:179:LEU:HD23	2.44	0.43
2:H:124:PRO:O	2:H:124:PRO:HG2	2.19	0.43
1:L:60:PHE:CZ	1:L:61:SER:HB3	2.54	0.43
1:L:141:LEU:HD12	1:L:180:MET:O	2.18	0.43
1:L:197:TYR:CB	1:L:214:PHE:CE2	2.87	0.43
2:H:3:LYS:HG2	2:H:25:SER:O	2.18	0.43
2:H:72:ILE:CG2	2:H:72:ILE:O	2.67	0.43
2:H:189:THR:O	2:H:194:PRO:CG	2.66	0.43
2:H:6:GLU:HG2	2:H:111:GLY:CA	2.49	0.43
2:H:90:VAL:HG12	2:H:116:VAL:CB	2.49	0.43
2:H:150:TYR:CE2	2:H:180:TYR:HB2	2.52	0.43
2:H:160:ASN:CB	2:H:199:THR:OG1	2.45	0.43
2:H:35:ASN:HB3	2:H:50:GLN:HA	2.00	0.43
2:H:61:TYR:CE1	2:H:63:SER:N	2.86	0.43
2:H:61:TYR:HE1	2:H:63:SER:CA	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:48:SER:HA	1:L:49:PRO:HD3	1.83	0.43
1:L:59:ARG:HD3	1:L:63:VAL:HG11	1.99	0.43
2:H:19:LYS:HE2	2:H:82:TYR:CD1	2.54	0.43
2:H:70:PHE:CD2	2:H:83:LEU:HD21	2.54	0.43
1:L:161:GLN:CG	1:L:184:LEU:HD11	2.49	0.42
2:H:12:VAL:O	2:H:116:VAL:HA	2.19	0.42
2:H:70:PHE:CZ	2:H:85:MET:SD	3.11	0.42
2:H:188:VAL:CG2	2:H:193:TRP:HD1	2.27	0.42
2:H:130:ALA:O	2:H:131:PRO:C	2.62	0.42
1:L:21:ILE:C	1:L:21:ILE:CD1	2.91	0.42
1:L:65:ASP:O	1:L:67:PHE:N	2.52	0.42
1:L:68:SER:O	1:L:78:LEU:HA	2.19	0.42
2:H:166:SER:HB3	2:H:187:THR:O	2.19	0.42
1:L:98:HIS:C	1:L:99:VAL:O	2.62	0.42
1:L:129:GLN:O	1:L:132:SER:CB	2.64	0.42
2:H:63:SER:O	2:H:64:ASP:C	2.63	0.42
2:H:64:ASP:C	2:H:66:VAL:N	2.77	0.42
2:H:91:GLU:C	2:H:93:MET:H	2.26	0.42
1:L:112:LYS:O	1:L:112:LYS:HG3	2.13	0.42
1:L:153:TRP:NE1	1:L:182:SER:OG	2.53	0.42
2:H:72:ILE:N	2:H:83:LEU:HD12	2.34	0.42
1:L:190:GLU:N	1:L:193:ARG:HH22	2.17	0.42
2:H:50:GLN:HG2	2:H:51:ILE:N	2.34	0.42
2:H:51:ILE:HA	2:H:59:GLU:O	2.20	0.42
2:H:103:TYR:CE1	3:H:218:FLU:H18	2.54	0.42
2:H:143:LEU:CD1	2:H:198:ILE:HG21	2.50	0.42
2:H:170:THR:OG1	2:H:184:SER:OG	2.37	0.42
1:L:21:ILE:HD12	1:L:40:TRP:CH2	2.55	0.42
2:H:137:THR:HA	2:H:141:VAL:CG1	2.33	0.42
1:L:41:TYR:CE2	1:L:51:VAL:CG1	2.91	0.42
2:H:6:GLU:CG	2:H:111:GLY:C	2.92	0.42
2:H:12:VAL:CG1	2:H:17:PRO:HG3	2.49	0.42
2:H:63:SER:C	2:H:67:LYS:HD3	2.40	0.42
2:H:136:THR:O	2:H:140:SER:O	2.37	0.42
2:H:37:VAL:HG21	4:H:219:MPD:H53	2.02	0.42
2:H:95:ILE:N	2:H:95:ILE:HD12	2.35	0.42
2:H:159:TRP:CD1	2:H:168:VAL:CG1	3.03	0.42
1:L:63:VAL:HA	1:L:64:PRO:HD3	1.81	0.41
1:L:149:ILE:N	1:L:149:ILE:HD13	2.34	0.41
2:H:54:LYS:HE3	2:H:58:TYR:OH	2.20	0.41
2:H:131:PRO:CD	2:H:143:LEU:HD23	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:LEU:CD1	2:H:158:THR:N	2.50	0.41
1:L:60:PHE:CE1	1:L:61:SER:CB	3.02	0.41
1:L:152:LYS:NZ	1:L:152:LYS:CB	2.83	0.41
2:H:127:TYR:HA	2:H:128:PRO:HD3	1.90	0.41
1:L:152:LYS:HE2	1:L:152:LYS:HB3	1.95	0.41
1:L:155:ILE:HG13	1:L:159:GLU:HB2	2.01	0.41
2:H:58:TYR:O	2:H:59:GLU:C	2.61	0.41
2:H:70:PHE:CE2	2:H:85:MET:SD	3.13	0.41
2:H:210:LYS:O	2:H:210:LYS:CG	2.68	0.41
1:L:39:ARG:HH11	1:L:39:ARG:HD2	1.56	0.41
1:L:215:ASN:HB3	1:L:218:GLU:OE1	2.20	0.41
1:L:147:LYS:HA	1:L:178:TYR:CD2	2.56	0.41
1:L:172:ASP:C	1:L:173:SER:OG	2.63	0.41
1:L:88:LEU:CD1	1:L:172:ASP:OD1	2.62	0.41
1:L:191:TYR:CE1	1:L:216:ARG:CG	3.03	0.41
1:L:198:THR:CB	1:L:213:SER:OG	2.58	0.41
2:H:106:ASP:OD1	4:H:219:MPD:CM	2.65	0.41
2:H:90:VAL:CA	2:H:116:VAL:CG1	2.93	0.41
1:L:144:PHE:HE1	1:L:147:LYS:O	2.03	0.41
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.98	0.41
1:L:9:LEU:H	1:L:9:LEU:CD2	2.34	0.41
1:L:154:LYS:NZ	1:L:200:GLU:OE2	2.50	0.41
1:L:174:LYS:CD	1:L:175:ASP:H	2.27	0.41
2:H:61:TYR:CE1	2:H:63:SER:CA	3.02	0.41
2:H:72:ILE:HG23	2:H:72:ILE:O	2.21	0.41
2:H:124:PRO:HB3	2:H:150:TYR:CG	2.55	0.41
2:H:191:SER:N	2:H:194:PRO:HD2	2.35	0.41
1:L:175:ASP:OD2	1:L:177:THR:CG2	2.69	0.41
2:H:54:LYS:CB	2:H:55:PRO:CD	2.98	0.41
2:H:70:PHE:HD2	2:H:83:LEU:HD21	1.86	0.41
2:H:85:MET:O	2:H:87:ASN:N	2.53	0.41
2:H:107:TYR:HD2	2:H:107:TYR:HA	1.39	0.40
2:H:145:CYS:HB3	2:H:157:LEU:HD21	2.03	0.40
2:H:147:VAL:HG13	2:H:182:LEU:HD23	2.03	0.40
1:L:203:HIS:H	1:L:206:SER:HB2	1.86	0.40
2:H:165:SER:O	2:H:165:SER:OG	2.27	0.40
1:L:95:GLN:NE2	1:L:101:TRP:HA	2.36	0.40
1:L:187:THR:OG1	1:L:190:GLU:N	2.42	0.40
2:H:3:LYS:CG	2:H:25:SER:O	2.70	0.40
2:H:122:THR:O	2:H:204:HIS:HE1	2.04	0.40
2:H:142:THR:HG22	2:H:186:VAL:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:159:TRP:CZ3	2:H:198:ILE:CD1	3.05	0.40
1:L:184:LEU:HD12	1:L:184:LEU:HA	1.79	0.40
2:H:40:SER:CB	2:H:43:LYS:CD	3.00	0.40
2:H:67:LYS:HB3	2:H:68:GLY:H	1.26	0.40
2:H:92:ASP:O	2:H:96:TYR:CE1	2.74	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:SER:CB	1:L:216:ARG:NH2[1_645]	1.99	0.21
2:H:16:ARG:NH1	2:H:135:ASP:OD2[1_546]	2.07	0.13
1:L:70:SER:OG	2:H:209:THR:OG1[1_655]	2.14	0.06
2:H:16:ARG:CG	2:H:135:ASP:OD1[1_546]	2.14	0.06

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	L	217/219 (99%)	173 (80%)	29 (13%)	15 (7%)		
2	H	214/216 (99%)	145 (68%)	39 (18%)	30 (14%)		
All	All	431/435 (99%)	318 (74%)	68 (16%)	45 (10%)		

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	73	GLY
1	L	82	ARG
1	L	105	GLY
1	L	161	GLN
1	L	174	LYS

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Mol	Chain	Res	Type
1	L	206	SER
1	L	207	THR
2	H	17	PRO
2	H	18	MET
2	H	41	PRO
2	H	65	SER
2	H	67	LYS
2	H	76	ASP
2	H	87	ASN
2	H	102	TYR
2	H	137	THR
2	H	153	GLU
2	H	163	SER
2	H	190	SER
2	H	198	ILE
2	H	206	ALA
2	H	207	SER
2	H	208	SER
1	L	15	LEU
1	L	29	LEU
1	L	160	ARG
1	L	163	GLY
2	H	8	GLY
2	H	30	SER
2	H	91	GLU
2	H	196	GLN
1	L	56	VAL
1	L	61	SER
1	L	66	ARG
2	H	68	GLY
2	H	161	SER
2	H	29	PHE
2	H	86	ASN
2	H	103	TYR
1	L	115	ASP
2	H	106	ASP
2	H	128	PRO
2	H	90	VAL
2	H	14	PRO
2	H	131	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	L	197/197 (100%)	122 (62%)	75 (38%)	0	0
2	H	190/190 (100%)	113 (60%)	77 (40%)	0	0
All	All	387/387 (100%)	235 (61%)	152 (39%)	0	0

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	VAL
1	L	9	LEU
1	L	10	SER
1	L	14	SER
1	L	15	LEU
1	L	20	SER
1	L	21	ILE
1	L	22	SER
1	L	24	ARG
1	L	25	SER
1	L	38	LEU
1	L	45	PRO
1	L	48	SER
1	L	51	VAL
1	L	56	VAL
1	L	59	ARG
1	L	66	ARG
1	L	72	SER
1	L	74	THR
1	L	76	PHE
1	L	78	LEU
1	L	80	ILE
1	L	84	GLU
1	L	88	LEU
1	L	95	GLN
1	L	96	SER
1	L	99	VAL

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Mol	Chain	Res	Type
1	L	100	PRO
1	L	107	THR
1	L	109	LEU
1	L	112	LYS
1	L	115	ASP
1	L	118	PRO
1	L	120	VAL
1	L	121	SER
1	L	122	ILE
1	L	126	SER
1	L	127	SER
1	L	128	GLU
1	L	131	THR
1	L	137	VAL
1	L	138	VAL
1	L	141	LEU
1	L	147	LYS
1	L	148	ASP
1	L	149	ILE
1	L	152	LYS
1	L	154	LYS
1	L	155	ILE
1	L	160	ARG
1	L	167	SER
1	L	169	THR
1	L	170	ASP
1	L	173	SER
1	L	174	LYS
1	L	178	TYR
1	L	183	THR
1	L	185	THR
1	L	186	LEU
1	L	188	LYS
1	L	189	ASP
1	L	195	ASN
1	L	198	THR
1	L	200	GLU
1	L	202	THR
1	L	204	LYS
1	L	207	THR
1	L	208	SER
1	L	209	PRO

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Mol	Chain	Res	Type
1	L	210	ILE
1	L	211	VAL
1	L	212	LYS
1	L	213	SER
1	L	215	ASN
1	L	218	GLU
2	H	6	GLU
2	H	7	THR
2	H	11	LEU
2	H	12	VAL
2	H	13	GLN
2	H	14	PRO
2	H	17	PRO
2	H	18	MET
2	H	19	LYS
2	H	20	LEU
2	H	25	SER
2	H	34	MET
2	H	35	ASN
2	H	38	ARG
2	H	39	GLN
2	H	41	PRO
2	H	42	GLU
2	H	48	VAL
2	H	50	GLN
2	H	51	ILE
2	H	59	GLU
2	H	60	THR
2	H	64	ASP
2	H	65	SER
2	H	67	LYS
2	H	69	ARG
2	H	72	ILE
2	H	74	ARG
2	H	75	ASP
2	H	79	SER
2	H	84	GLN
2	H	85	MET
2	H	87	ASN
2	H	95	ILE
2	H	99	THR
2	H	101	SER

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Mol	Chain	Res	Type
2	H	105	MET
2	H	107	TYR
2	H	112	THR
2	H	118	SER
2	H	120	LYS
2	H	124	PRO
2	H	125	SER
2	H	128	PRO
2	H	132	VAL
2	H	133	CYS
2	H	141	VAL
2	H	145	CYS
2	H	147	VAL
2	H	151	PHE
2	H	153	GLU
2	H	155	VAL
2	H	156	THR
2	H	157	LEU
2	H	158	THR
2	H	160	ASN
2	H	164	LEU
2	H	171	PHE
2	H	172	PRO
2	H	174	VAL
2	H	179	LEU
2	H	181	THR
2	H	182	LEU
2	H	187	THR
2	H	188	VAL
2	H	190	SER
2	H	191	SER
2	H	193	TRP
2	H	194	PRO
2	H	196	GLN
2	H	198	ILE
2	H	201	ASN
2	H	205	PRO
2	H	209	THR
2	H	211	VAL
2	H	214	LYS
2	H	216	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	35	ASN
1	L	43	GLN
1	L	98	HIS
2	H	13	GLN
2	H	35	ASN
2	H	50	GLN
2	H	53	ASN
2	H	110	GLN
2	H	160	ASN
2	H	196	GLN
2	H	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	FLU	H	218	-	28,28,28	2.75	10 (35%)	41,41,41	1.89	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	H	219	-	7,7,7	0.89	0	9,10,10	1.09	1 (11%)

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	FLU	H	218	-	-	4/6/12/12	0/4/4/4
4	MPD	H	219	-	-	0/5/5/5	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	218	FLU	C14-C10	-8.68	1.38	1.49
3	H	218	FLU	C19-C20	-6.73	1.35	1.49
3	H	218	FLU	O3-C6	3.83	1.36	1.24
3	H	218	FLU	C5-C6	-3.56	1.37	1.45
3	H	218	FLU	C17-C16	3.27	1.45	1.38
3	H	218	FLU	C12-C11	-2.75	1.35	1.39
3	H	218	FLU	C18-C19	2.22	1.43	1.39
3	H	218	FLU	C13-C1	2.17	1.43	1.39
3	H	218	FLU	C15-C14	-2.17	1.36	1.39
3	H	218	FLU	C17-C18	-2.05	1.35	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	218	FLU	O3-C6-C5	-5.77	113.22	121.43
3	H	218	FLU	O5-C20-O4	-3.80	115.19	123.35
3	H	218	FLU	O3-C6-C7	3.19	126.71	121.56
3	H	218	FLU	C7-C6-C5	2.91	120.07	117.12
3	H	218	FLU	C18-C19-C14	2.90	122.51	119.26
3	H	218	FLU	C8-C9-C10	-2.56	118.61	123.90
3	H	218	FLU	O4-C20-C19	2.55	128.06	121.97
3	H	218	FLU	C8-C9-C4	2.49	120.60	115.59
3	H	218	FLU	C17-C16-C15	2.48	123.30	120.24
3	H	218	FLU	C4-C5-C6	-2.32	118.27	120.66
3	H	218	FLU	C15-C14-C10	-2.28	113.98	118.36
4	H	219	MPD	CM-C2-C1	-2.26	105.57	110.63

There are no chirality outliers.

All (4) torsion outliers are listed below:

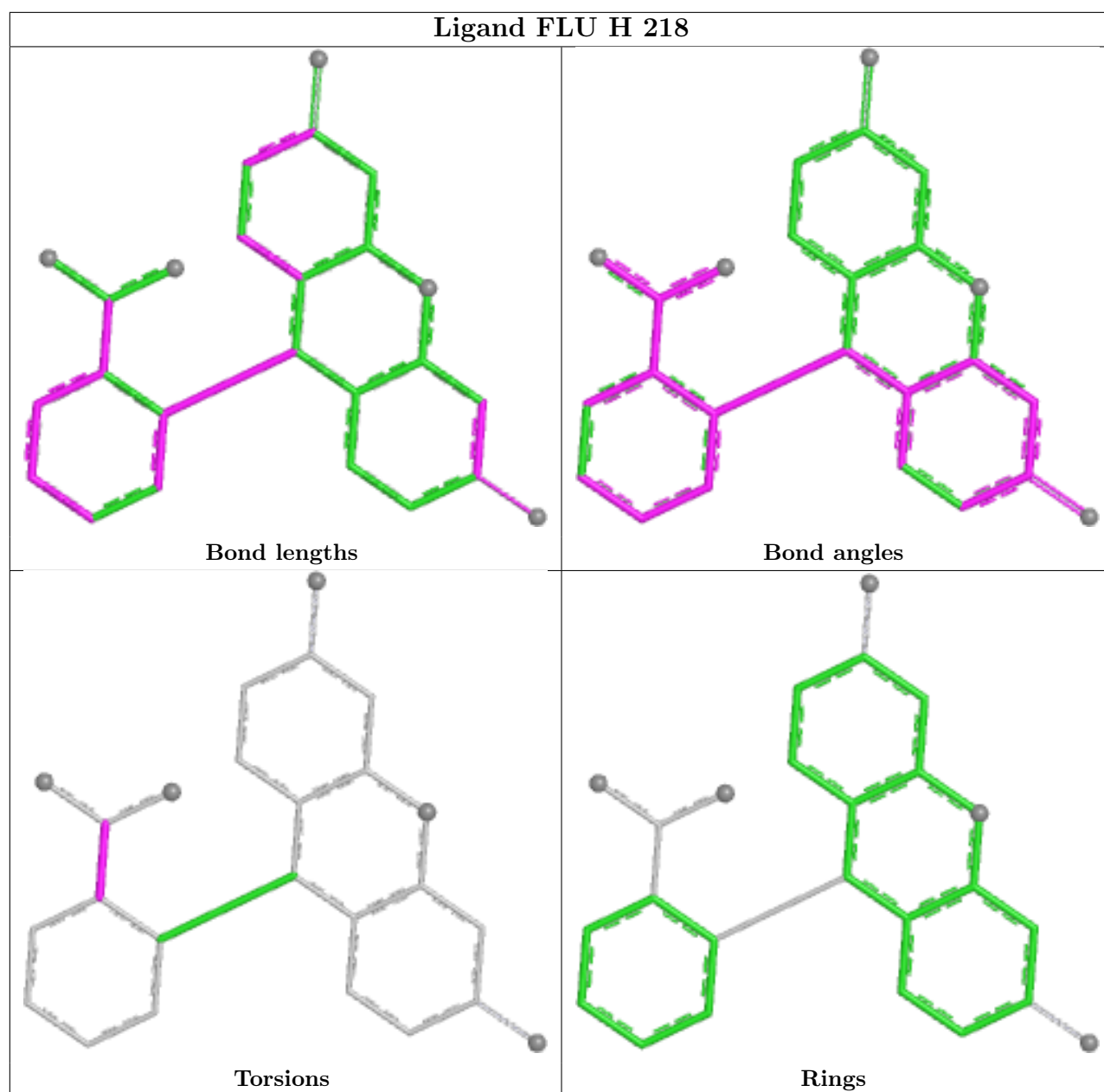
Mol	Chain	Res	Type	Atoms
3	H	218	FLU	C18-C19-C20-O4
3	H	218	FLU	C14-C19-C20-O4
3	H	218	FLU	C18-C19-C20-O5
3	H	218	FLU	C14-C19-C20-O5

There are no ring outliers.

2 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	218	FLU	12	0
4	H	219	MPD	24	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](#)

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.