



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:39 AM UTC

PDB ID : 3MCG / pdb_00003mcg
Title : THREE-DIMENSIONAL STRUCTURE OF A LIGHT CHAIN DIMER
CRYSTALLIZED IN WATER. CONFORMATIONAL FLEXIBILITY OF A
MOLECULE IN TWO CRYSTAL FORMS
Authors : Ely, K.R.; Herron, J.N.; Edmundson, A.B.
Deposited on : 1989-05-09
Resolution : 2.00 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

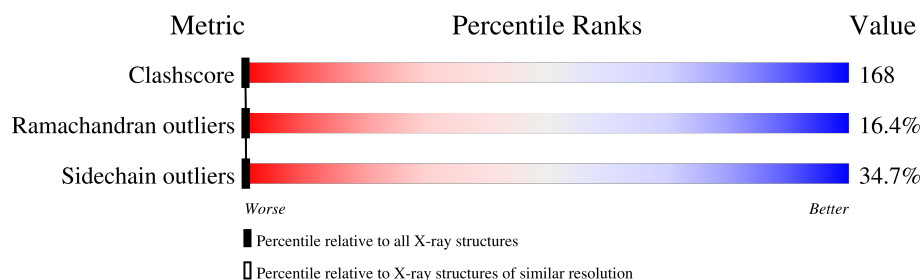
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	1	216	
1	2	216	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3478 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 IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	216	Total	C	N	O	S	0	0	0
			1606	1000	266	335	5			
1	2	216	Total	C	N	O	S	0	0	0
			1606	1000	266	335	5			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	20	ILE	PHE	conflict	PIR S14675
1	23	THR	SER	conflict	PIR S14675
1	29	VAL	ILE	conflict	PIR S14675
1	31	GLY	ASN	conflict	PIR S14675
1	39	GLN	ARG	conflict	PIR S14675
1	42	ALA	PRO	conflict	PIR S14675
1	48	VAL	LEU	conflict	PIR S14675
1	49	ILE	MET	conflict	PIR S14675
1	54	ASN	THR	conflict	PIR S14675
1	62	ASP	ASN	conflict	PIR S14675
1	94	GLU	ALA	conflict	PIR S14675
1	97	ASP	ASN	conflict	PIR S14675
1	98	ASN	SER	conflict	PIR S14675
1	99	PHE	LEU	conflict	PIR S14675
1	100	VAL	ILE	conflict	PIR S14675
1	103	THR	GLY	conflict	PIR S14675
1	106	LYS	ARG	conflict	PIR S14675
1	107	VAL	LEU	conflict	PIR S14675
1	116	ASN	ALA	conflict	PIR S14675
1	118	THR	SER	conflict	PIR S14675
1	156	GLY	SER	conflict	PIR S14675
1	167	LYS	THR	conflict	PIR S14675
2	20	ILE	PHE	conflict	PIR S14675
2	23	THR	SER	conflict	PIR S14675

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Chain	Residue	Modelled	Actual	Comment	Reference
2	29	VAL	ILE	conflict	PIR S14675
2	31	GLY	ASN	conflict	PIR S14675
2	39	GLN	ARG	conflict	PIR S14675
2	42	ALA	PRO	conflict	PIR S14675
2	48	VAL	LEU	conflict	PIR S14675
2	49	ILE	MET	conflict	PIR S14675
2	54	ASN	THR	conflict	PIR S14675
2	62	ASP	ASN	conflict	PIR S14675
2	94	GLU	ALA	conflict	PIR S14675
2	97	ASP	ASN	conflict	PIR S14675
2	98	ASN	SER	conflict	PIR S14675
2	99	PHE	LEU	conflict	PIR S14675
2	100	VAL	ILE	conflict	PIR S14675
2	103	THR	GLY	conflict	PIR S14675
2	106	LYS	ARG	conflict	PIR S14675
2	107	VAL	LEU	conflict	PIR S14675
2	116	ASN	ALA	conflict	PIR S14675
2	118	THR	SER	conflict	PIR S14675
2	156	GLY	SER	conflict	PIR S14675
2	167	LYS	THR	conflict	PIR S14675

- Molecule 2 is water.

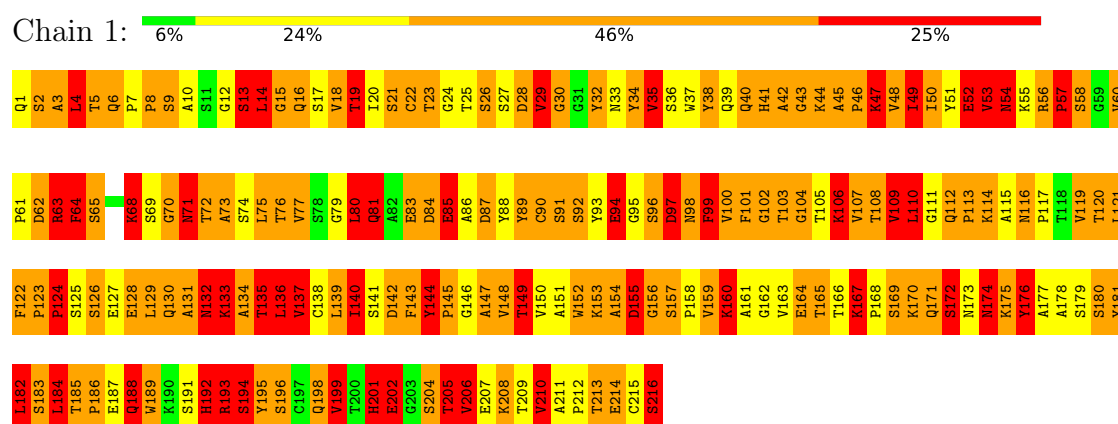
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	123	Total O 123 123	0	0
2	2	143	Total O 143 143	0	0

3 Residue-property plots

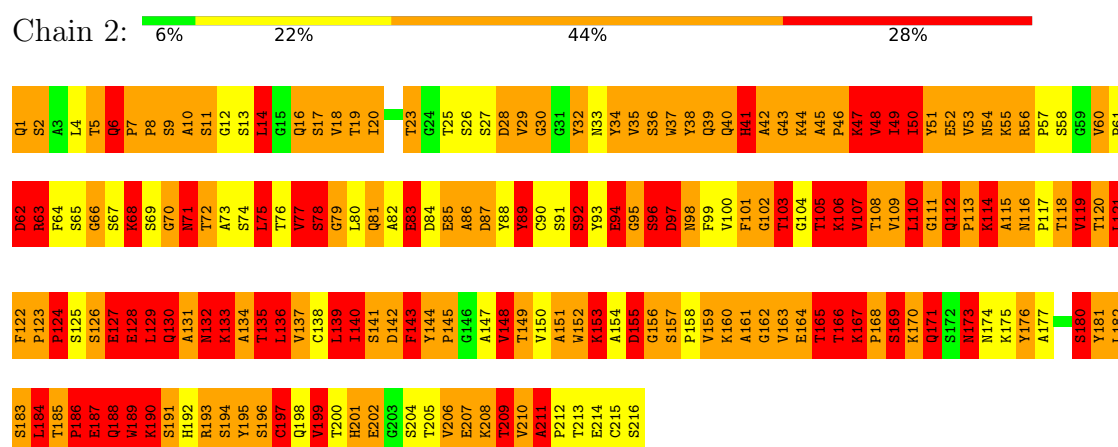
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT 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 2	Depositor
Cell constants a, b, c, α , β , γ	72.80Å 81.90Å 71.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3478	wwPDB-VP
Average B, all atoms (Å ²)	7.0	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: PCA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	1.83	25/1637 (1.5%)	3.32	248/2233 (11.1%)
1	2	1.76	24/1637 (1.5%)	3.31	261/2233 (11.7%)
All	All	1.80	49/3274 (1.5%)	3.32	509/4466 (11.4%)

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	1	1	0

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	136	LEU	N-CA	10.16	1.58	1.46
1	1	199	VAL	N-CA	7.91	1.56	1.46
1	1	103	THR	N-CA	7.91	1.55	1.45
1	1	116	ASN	CA-CB	7.24	1.64	1.53
1	2	79	GLY	N-CA	7.09	1.55	1.45
1	1	176	TYR	N-CA	7.01	1.54	1.46
1	1	135	THR	CA-CB	6.64	1.62	1.53
1	1	175	LYS	C-O	6.54	1.31	1.24
1	2	108	THR	CB-OG1	6.52	1.54	1.43
1	2	34	TYR	C-N	-6.51	1.24	1.33
1	1	35	VAL	N-CA	6.45	1.54	1.46
1	1	136	LEU	CA-CB	-6.39	1.42	1.53
1	2	138	CYS	N-CA	6.37	1.53	1.46
1	2	87	ASP	CA-CB	6.28	1.62	1.53
1	1	81	GLN	N-CA	6.21	1.53	1.46
1	2	110	LEU	N-CA	6.10	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	46	PRO	CA-CB	-6.04	1.47	1.54
1	1	5	THR	CA-CB	6.03	1.60	1.52
1	2	196	SER	N-CA	5.99	1.53	1.45
1	1	72	THR	CA-C	5.91	1.59	1.52
1	2	129	LEU	C-O	5.90	1.30	1.24
1	1	147	ALA	C-O	5.87	1.31	1.23
1	2	140	ILE	CA-C	5.82	1.59	1.52
1	2	185	THR	CA-CB	5.70	1.62	1.53
1	2	77	VAL	N-CA	5.69	1.53	1.46
1	1	92	SER	CA-CB	5.63	1.60	1.53
1	2	124	PRO	CA-CB	5.63	1.61	1.53
1	1	108	THR	C-N	-5.59	1.26	1.33
1	2	32	TYR	CA-CB	-5.54	1.44	1.53
1	1	108	THR	CA-CB	5.53	1.62	1.53
1	2	118	THR	CA-CB	5.50	1.62	1.53
1	2	83	GLU	N-CA	5.49	1.52	1.45
1	2	209	THR	N-CA	5.45	1.52	1.45
1	2	106	LYS	CA-CB	-5.40	1.44	1.53
1	1	202	GLU	N-CA	5.38	1.52	1.46
1	2	77	VAL	CA-CB	-5.35	1.47	1.54
1	2	167	LYS	CA-CB	-5.29	1.45	1.53
1	2	60	VAL	N-CA	5.25	1.53	1.46
1	1	180	SER	C-O	5.23	1.30	1.23
1	2	116	ASN	CA-C	5.20	1.60	1.52
1	1	167	LYS	CA-C	5.18	1.58	1.53
1	1	101	PHE	CA-C	5.17	1.59	1.52
1	2	197	CYS	CA-C	5.15	1.59	1.52
1	2	30	GLY	N-CA	5.10	1.52	1.45
1	1	159	VAL	CA-C	5.09	1.59	1.52
1	2	152	TRP	C-N	-5.05	1.26	1.33
1	1	134	ALA	C-O	5.04	1.30	1.24
1	1	201	HIS	N-CA	5.03	1.52	1.46
1	1	153	LYS	N-CA	5.02	1.52	1.45

All (509) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	140	ILE	N-CA-CB	25.02	137.99	110.72
1	1	71	ASN	CA-CB-CG	23.83	136.43	112.60
1	1	143	PHE	CA-CB-CG	22.70	136.50	113.80
1	2	71	ASN	CA-CB-CG	22.69	135.29	112.60
1	1	101	PHE	CA-CB-CG	18.13	131.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	103	THR	CB-CA-C	18.09	141.75	110.45
1	1	136	LEU	CA-CB-CG	17.24	176.65	116.30
1	1	99	PHE	CA-CB-CG	16.54	130.34	113.80
1	2	116	ASN	O-C-N	15.44	132.25	121.14
1	2	116	ASN	N-CA-CB	14.93	131.32	109.82
1	1	40	GLN	CA-CB-CG	14.45	143.01	114.10
1	1	87	ASP	CA-CB-CG	14.09	126.69	112.60
1	2	40	GLN	CA-CB-CG	14.03	142.15	114.10
1	1	155	ASP	CA-CB-CG	13.82	126.42	112.60
1	1	136	LEU	CB-CA-C	13.58	134.55	109.71
1	2	83	GLU	CB-CG-CD	12.63	134.07	112.60
1	2	7	PRO	CB-CA-C	12.30	125.93	110.92
1	2	94	GLU	CB-CG-CD	12.09	133.15	112.60
1	2	87	ASP	N-CA-C	12.09	127.97	109.96
1	1	176	TYR	CB-CA-C	12.04	132.19	110.16
1	2	116	ASN	CA-CB-CG	11.87	124.47	112.60
1	2	141	SER	CA-C-O	-11.85	107.87	120.55
1	2	40	GLN	CB-CG-CD	11.73	132.54	112.60
1	1	29	VAL	CB-CA-C	11.69	130.47	111.29
1	1	33	ASN	CA-C-O	-11.51	106.90	121.17
1	1	159	VAL	N-CA-CB	11.47	130.18	111.36
1	1	98	ASN	CA-CB-CG	11.29	123.89	112.60
1	2	130	GLN	OE1-CD-NE2	10.73	133.33	122.60
1	2	206	VAL	CB-CA-C	10.64	126.72	110.55
1	1	199	VAL	N-CA-C	-10.53	94.81	109.45
1	2	41	HIS	CA-CB-CG	10.47	124.27	113.80
1	2	40	GLN	OE1-CD-NE2	-10.43	112.17	122.60
1	2	142	ASP	N-CA-C	10.40	122.54	107.88
1	1	114	LYS	N-CA-C	-10.34	95.27	110.06
1	1	72	THR	N-CA-CB	10.16	128.51	110.83
1	2	139	LEU	CA-C-O	-10.12	109.77	120.40
1	2	28	ASP	N-CA-C	10.11	122.25	111.03
1	1	149	THR	N-CA-CB	9.88	124.49	109.97
1	2	167	LYS	N-CA-CB	9.87	127.95	110.37
1	1	148	VAL	N-CA-C	9.81	129.75	109.34
1	1	49	ILE	N-CA-C	-9.73	103.23	112.96
1	2	62	ASP	CA-CB-CG	9.72	122.32	112.60
1	2	173	ASN	OD1-CG-ND2	9.71	132.31	122.60
1	2	113	PRO	CB-CA-C	-9.70	103.72	111.87
1	2	124	PRO	N-CA-C	9.64	132.32	112.47
1	1	71	ASN	OD1-CG-ND2	-9.62	112.98	122.60
1	1	87	ASP	O-C-N	9.55	133.75	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	16	GLN	N-CA-C	9.52	117.89	108.75
1	1	87	ASP	N-CA-C	-9.48	95.25	110.32
1	2	77	VAL	N-CA-C	-9.46	94.08	107.80
1	1	182	LEU	CB-CA-C	9.46	128.08	109.35
1	2	129	LEU	CB-CA-C	9.45	125.83	110.90
1	1	4	LEU	CB-CA-C	9.42	129.16	110.42
1	2	132	ASN	CA-CB-CG	9.38	121.98	112.60
1	1	68	LYS	CA-CB-CG	9.37	132.84	114.10
1	1	201	HIS	CA-CB-CG	9.33	123.13	113.80
1	2	190	LYS	CA-C-O	-9.32	110.56	120.63
1	2	199	VAL	N-CA-CB	-9.32	103.02	112.06
1	2	10	ALA	CA-C-O	9.32	132.27	121.28
1	2	50	ILE	N-CA-CB	9.24	126.48	111.23
1	1	58	SER	N-CA-C	9.22	123.04	111.69
1	1	144	TYR	N-CA-CB	9.21	126.77	110.37
1	1	33	ASN	OD1-CG-ND2	9.19	131.79	122.60
1	2	106	LYS	CA-CB-CG	9.16	132.43	114.10
1	2	190	LYS	N-CA-CB	9.15	123.78	110.06
1	1	63	ARG	CD-NE-CZ	9.11	137.16	124.40
1	2	106	LYS	N-CA-CB	9.10	125.87	110.49
1	1	19	THR	CA-CB-OG1	-9.09	95.96	109.60
1	1	48	VAL	CB-CA-C	9.06	121.68	111.08
1	1	26	SER	N-CA-C	-9.02	102.43	113.97
1	1	46	PRO	CB-CA-C	9.00	119.43	111.87
1	2	210	VAL	N-CA-CB	8.96	126.15	111.45
1	2	77	VAL	CB-CA-C	8.91	123.97	110.96
1	1	2	SER	N-CA-CB	8.84	125.52	110.50
1	1	97	ASP	N-CA-C	-8.82	100.26	111.90
1	1	64	PHE	CA-C-O	-8.79	110.89	120.30
1	2	173	ASN	CA-CB-CG	-8.77	103.83	112.60
1	1	199	VAL	CA-C-O	-8.77	111.01	121.80
1	2	141	SER	N-CA-C	-8.74	100.73	111.40
1	2	87	ASP	N-CA-CB	-8.72	95.73	109.51
1	2	28	ASP	CA-CB-CG	-8.66	103.94	112.60
1	2	138	CYS	CA-CB-SG	8.66	134.31	114.40
1	2	136	LEU	N-CA-CB	-8.65	95.89	110.16
1	2	68	LYS	CB-CG-CD	8.64	131.17	111.30
1	2	114	LYS	CA-CB-CG	8.61	131.32	114.10
1	2	121	LEU	CA-C-O	-8.61	111.04	121.11
1	2	122	PHE	O-C-N	8.60	127.83	121.12
1	1	90	CYS	CA-C-O	-8.58	111.08	120.43
1	1	128	GLU	N-CA-CB	8.55	122.64	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	214	GLU	N-CA-C	8.53	122.86	109.81
1	2	197	CYS	N-CA-CB	8.53	124.59	110.52
1	2	108	THR	CA-CB-OG1	-8.52	96.83	109.60
1	1	206	VAL	N-CA-CB	8.50	125.26	111.23
1	1	128	GLU	CA-C-O	-8.48	111.89	120.80
1	1	116	ASN	N-CA-C	8.48	123.11	110.39
1	2	87	ASP	CA-CB-CG	-8.47	104.13	112.60
1	2	209	THR	CA-C-O	-8.47	111.19	121.36
1	1	136	LEU	N-CA-C	-8.45	95.12	108.90
1	1	14	LEU	CA-CB-CG	8.45	145.86	116.30
1	1	87	ASP	CA-C-O	-8.42	111.26	121.36
1	2	141	SER	N-CA-CB	8.41	122.58	110.13
1	1	199	VAL	CB-CA-C	8.40	123.08	111.49
1	2	191	SER	N-CA-CB	8.36	124.61	110.49
1	1	92	SER	CA-C-O	-8.35	111.42	120.36
1	1	192	HIS	CA-C-N	8.34	131.97	120.63
1	1	192	HIS	C-N-CA	8.34	131.97	120.63
1	2	159	VAL	CA-C-O	-8.34	110.36	120.78
1	1	210	VAL	N-CA-CB	8.32	125.87	111.39
1	2	5	THR	CB-CA-C	8.31	122.87	109.90
1	1	133	LYS	CA-CB-CG	8.31	130.71	114.10
1	2	9	SER	CA-C-O	8.26	130.22	120.14
1	1	194	SER	CB-CA-C	-8.22	96.76	109.99
1	1	167	LYS	N-CA-CB	8.22	121.83	109.75
1	2	155	ASP	CA-CB-CG	-8.20	104.40	112.60
1	2	14	LEU	CA-C-O	8.16	127.38	118.65
1	1	76	THR	N-CA-CB	8.15	123.53	110.65
1	1	4	LEU	CA-C-O	8.13	132.14	120.51
1	1	114	LYS	CA-CB-CG	8.12	130.35	114.10
1	2	195	TYR	N-CA-C	8.11	121.74	108.52
1	2	206	VAL	CA-CB-CG2	8.10	124.17	110.40
1	2	120	THR	CB-CA-C	8.08	123.53	109.80
1	2	95	GLY	N-CA-C	8.07	132.30	113.18
1	1	130	GLN	OE1-CD-NE2	-8.06	114.54	122.60
1	1	174	ASN	O-C-N	8.05	133.29	122.59
1	2	144	TYR	N-CA-C	8.04	123.69	112.75
1	1	145	PRO	CB-CA-C	8.02	124.80	111.56
1	2	97	ASP	CA-C-O	-7.95	109.14	120.51
1	1	161	ALA	CB-CA-C	7.94	121.65	109.34
1	2	139	LEU	CA-C-N	-7.91	112.17	122.37
1	2	139	LEU	C-N-CA	-7.91	112.17	122.37
1	2	186	PRO	CA-C-N	7.90	131.66	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	186	PRO	C-N-CA	7.90	131.66	120.28
1	2	187	GLU	CA-C-O	7.88	129.00	120.10
1	2	32	TYR	CA-CB-CG	7.85	128.03	113.90
1	2	7	PRO	N-CA-C	-7.82	101.16	110.70
1	1	119	VAL	CA-C-O	7.78	129.86	120.84
1	2	169	SER	CA-C-O	7.76	131.60	120.51
1	2	5	THR	CA-C-O	7.75	129.76	120.92
1	2	195	TYR	CA-C-O	-7.74	111.80	120.32
1	1	90	CYS	CB-CA-C	-7.71	97.04	109.75
1	2	127	GLU	CA-C-O	7.68	131.50	120.51
1	1	33	ASN	O-C-N	7.66	132.31	121.97
1	1	210	VAL	O-C-N	7.64	131.43	123.18
1	1	62	ASP	CA-CB-CG	-7.62	104.98	112.60
1	2	23	THR	CA-CB-OG1	-7.61	98.18	109.60
1	1	49	ILE	O-C-N	7.60	130.18	122.04
1	1	198	GLN	O-C-N	7.60	132.24	123.27
1	2	140	ILE	N-CA-C	-7.55	97.70	108.58
1	2	46	PRO	CB-CA-C	7.54	121.13	111.56
1	1	81	GLN	CB-CA-C	7.53	123.76	111.26
1	1	83	GLU	CA-C-O	-7.52	109.76	120.51
1	2	78	SER	O-C-N	7.51	131.78	123.22
1	2	97	ASP	CA-CB-CG	-7.50	105.10	112.60
1	1	154	ALA	CA-C-N	7.49	135.85	121.54
1	1	154	ALA	C-N-CA	7.49	135.85	121.54
1	1	87	ASP	N-CA-CB	7.45	122.55	110.41
1	2	208	LYS	CA-CB-CG	7.44	128.98	114.10
1	2	197	CYS	N-CA-C	-7.42	97.58	109.76
1	2	136	LEU	CB-CA-C	7.42	121.97	109.80
1	1	216	SER	N-CA-C	7.41	131.75	111.00
1	2	196	SER	CA-C-O	-7.40	112.48	121.36
1	2	182	LEU	CA-C-O	-7.37	112.74	120.70
1	1	84	ASP	CA-CB-CG	7.36	119.96	112.60
1	2	141	SER	O-C-N	7.36	131.08	122.17
1	2	155	ASP	N-CA-CB	7.34	122.90	110.49
1	2	104	GLY	CA-C-O	7.33	133.32	120.57
1	2	130	GLN	CA-CB-CG	-7.33	99.45	114.10
1	1	149	THR	N-CA-C	-7.33	99.44	110.28
1	2	77	VAL	N-CA-CB	-7.32	102.23	111.46
1	1	174	ASN	CA-CB-CG	7.30	119.90	112.60
1	1	80	LEU	O-C-N	7.25	132.23	122.59
1	2	190	LYS	O-C-N	7.25	129.80	122.12
1	1	3	ALA	O-C-N	7.24	131.08	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	198	GLN	N-CA-CB	7.20	121.85	110.55
1	1	160	LYS	CA-CB-CG	7.19	128.48	114.10
1	2	9	SER	N-CA-C	7.19	120.11	108.32
1	1	34	TYR	CA-CB-CG	7.15	126.78	113.90
1	2	121	LEU	O-C-N	7.14	132.02	123.24
1	1	180	SER	CA-C-O	-7.12	110.35	120.11
1	2	60	VAL	O-C-N	7.12	129.22	121.10
1	2	188	GLN	N-CA-C	-7.09	103.55	111.71
1	2	116	ASN	N-CA-C	-7.08	99.53	110.58
1	2	118	THR	CB-CA-C	-7.06	99.37	111.23
1	1	71	ASN	CB-CG-OD1	7.04	134.87	120.80
1	2	142	ASP	CA-CB-CG	7.03	119.63	112.60
1	1	126	SER	N-CA-C	-7.02	104.87	113.50
1	1	142	ASP	N-CA-C	7.02	125.75	110.80
1	2	63	ARG	CG-CD-NE	7.02	127.44	112.00
1	1	159	VAL	CA-CB-CG1	7.01	122.32	110.40
1	1	151	ALA	CA-C-O	6.98	128.65	120.14
1	1	28	ASP	N-CA-C	-6.97	100.48	110.59
1	2	161	ALA	N-CA-C	-6.97	102.33	111.74
1	2	9	SER	CA-CB-OG	6.97	125.04	111.10
1	2	110	LEU	N-CA-CB	-6.97	98.71	110.49
1	2	49	ILE	CA-C-N	6.96	134.51	121.97
1	2	49	ILE	C-N-CA	6.96	134.51	121.97
1	1	152	TRP	O-C-N	6.94	131.91	123.16
1	1	167	LYS	N-CA-C	-6.93	101.63	109.60
1	2	106	LYS	N-CA-C	-6.92	96.05	110.80
1	2	63	ARG	CD-NE-CZ	6.92	134.09	124.40
1	1	171	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	1	81	GLN	N-CA-C	-6.90	102.87	112.12
1	2	19	THR	N-CA-CB	6.86	121.54	110.77
1	2	106	LYS	CA-C-O	-6.86	110.70	120.51
1	1	135	THR	CA-CB-OG1	-6.84	99.34	109.60
1	2	94	GLU	CA-CB-CG	6.83	127.76	114.10
1	1	29	VAL	CA-CB-CG1	6.83	122.01	110.40
1	1	94	GLU	CB-CA-C	6.81	121.87	110.43
1	1	10	ALA	CA-C-O	-6.80	113.02	120.43
1	2	129	LEU	CA-C-O	-6.80	113.70	120.70
1	1	45	ALA	O-C-N	6.80	128.03	120.83
1	2	139	LEU	CB-CA-C	-6.80	99.80	110.74
1	1	19	THR	CA-CB-CG2	6.79	122.04	110.50
1	1	135	THR	N-CA-C	6.79	119.58	108.52
1	1	108	THR	CB-CA-C	-6.78	96.92	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	153	LYS	CA-C-N	6.78	133.37	123.13
1	1	153	LYS	C-N-CA	6.78	133.37	123.13
1	2	101	PHE	CA-C-O	6.77	128.72	120.60
1	2	130	GLN	CB-CG-CD	-6.76	101.10	112.60
1	2	78	SER	CA-C-O	-6.74	113.15	120.36
1	2	48	VAL	CA-C-O	-6.74	112.36	120.78
1	1	13	SER	CB-CA-C	6.74	120.52	111.70
1	2	118	THR	N-CA-C	6.72	121.20	107.69
1	2	83	GLU	CA-CB-CG	6.71	127.51	114.10
1	2	121	LEU	CA-C-N	-6.65	116.43	122.28
1	2	121	LEU	C-N-CA	-6.65	116.43	122.28
1	1	194	SER	N-CA-C	6.64	118.61	108.52
1	1	193	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	2	152	TRP	CA-C-O	-6.58	112.70	120.60
1	2	153	LYS	CA-C-O	-6.57	113.03	120.32
1	2	71	ASN	CB-CA-C	6.57	123.49	110.42
1	1	110	LEU	CB-CA-C	6.55	123.45	110.42
1	1	12	GLY	CA-C-O	6.55	128.74	121.67
1	2	16	GLN	OE1-CD-NE2	6.54	129.14	122.60
1	1	210	VAL	CA-CB-CG2	6.54	121.52	110.40
1	2	167	LYS	O-C-N	6.54	128.84	121.32
1	2	19	THR	CB-CA-C	-6.53	99.70	110.14
1	1	134	ALA	N-CA-C	6.48	124.61	110.80
1	2	56	ARG	CD-NE-CZ	-6.48	115.33	124.40
1	2	10	ALA	CA-C-N	6.47	132.71	122.36
1	2	10	ALA	C-N-CA	6.47	132.71	122.36
1	2	23	THR	N-CA-C	6.46	119.98	109.59
1	1	79	GLY	N-CA-C	-6.45	97.90	113.18
1	1	122	PHE	O-C-N	6.44	127.36	120.85
1	2	86	ALA	CA-C-N	6.42	130.52	121.02
1	2	86	ALA	C-N-CA	6.42	130.52	121.02
1	2	138	CYS	CB-CA-C	6.41	121.60	109.37
1	1	6	GLN	CB-CG-CD	6.40	123.47	112.60
1	1	22	CYS	CA-C-O	6.39	126.55	120.09
1	2	169	SER	CA-C-N	6.39	133.75	121.54
1	2	169	SER	C-N-CA	6.39	133.75	121.54
1	2	209	THR	CB-CA-C	6.38	120.43	109.51
1	1	182	LEU	CA-C-O	6.38	127.99	120.66
1	2	94	GLU	CG-CD-OE1	6.37	133.05	118.40
1	2	158	PRO	CB-CA-C	6.36	119.65	111.64
1	1	92	SER	N-CA-CB	-6.35	100.07	110.42
1	2	145	PRO	N-CD-CG	-6.35	93.67	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	144	TYR	CA-C-N	6.33	125.56	118.97
1	2	144	TYR	C-N-CA	6.33	125.56	118.97
1	2	157	SER	O-C-N	6.33	127.92	121.72
1	2	66	GLY	N-CA-C	-6.32	101.13	110.87
1	2	71	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	1	6	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	2	39	GLN	CA-C-O	-6.28	114.39	120.92
1	2	98	ASN	CA-CB-CG	6.27	118.87	112.60
1	2	143	PHE	CA-CB-CG	-6.27	107.53	113.80
1	1	73	ALA	N-CA-C	-6.26	99.03	109.24
1	1	80	LEU	CA-C-N	-6.26	112.53	122.17
1	1	80	LEU	C-N-CA	-6.26	112.53	122.17
1	2	166	THR	N-CA-CB	6.26	121.07	110.49
1	1	21	SER	N-CA-CB	6.26	120.03	110.70
1	1	147	ALA	N-CA-C	6.24	119.56	107.71
1	1	113	PRO	CA-C-O	6.23	129.46	121.86
1	2	11	SER	CA-C-N	6.22	132.24	121.97
1	2	11	SER	C-N-CA	6.22	132.24	121.97
1	1	85	GLU	CB-CG-CD	6.22	123.17	112.60
1	1	191	SER	N-CA-C	-6.22	104.76	112.90
1	2	39	GLN	O-C-N	6.20	130.56	122.68
1	1	176	TYR	N-CA-CB	-6.20	100.54	111.39
1	1	34	TYR	CA-C-N	-6.19	113.40	122.68
1	1	34	TYR	C-N-CA	-6.19	113.40	122.68
1	1	140	ILE	N-CA-CB	-6.16	101.06	111.23
1	1	188	GLN	N-CA-C	-6.16	97.68	110.80
1	1	201	HIS	CB-CA-C	6.15	122.66	110.42
1	1	54	ASN	CA-CB-CG	6.14	118.74	112.60
1	2	141	SER	CA-C-N	-6.13	111.54	122.45
1	2	141	SER	C-N-CA	-6.13	111.54	122.45
1	2	98	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	2	107	VAL	CA-C-O	6.12	128.43	120.78
1	2	17	SER	N-CA-CB	-6.12	100.18	111.13
1	2	102	GLY	N-CA-C	-6.10	103.83	112.37
1	1	91	SER	CA-CB-OG	-6.10	98.91	111.10
1	2	149	THR	CA-CB-OG1	-6.07	100.49	109.60
1	1	27	SER	O-C-N	6.07	130.66	122.59
1	1	89	TYR	CA-C-O	6.07	126.67	120.24
1	2	34	TYR	CA-C-N	6.06	131.36	123.11
1	2	34	TYR	C-N-CA	6.06	131.36	123.11
1	1	26	SER	O-C-N	6.06	129.81	122.48
1	1	199	VAL	O-C-N	6.04	130.38	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	47	LYS	CA-C-O	-6.04	114.69	121.81
1	2	111	GLY	CA-C-O	6.04	131.07	120.57
1	1	101	PHE	N-CA-C	-6.03	100.32	109.85
1	2	37	TRP	O-C-N	6.01	130.63	123.24
1	2	151	ALA	N-CA-C	-6.01	100.28	109.41
1	1	132	ASN	N-CA-CB	-6.00	103.11	112.41
1	2	138	CYS	CA-C-N	6.00	131.83	123.07
1	2	138	CYS	C-N-CA	6.00	131.83	123.07
1	2	72	THR	CA-CB-CG2	6.00	120.69	110.50
1	2	135	THR	CA-CB-CG2	5.99	120.69	110.50
1	1	76	THR	O-C-N	5.98	131.02	123.12
1	1	77	VAL	N-CA-CB	5.98	118.81	110.56
1	1	144	TYR	O-C-N	5.98	128.20	121.32
1	1	128	GLU	O-C-N	5.97	129.04	122.11
1	2	165	THR	N-CA-CB	5.97	121.64	111.66
1	2	188	GLN	CA-C-O	5.96	126.83	120.10
1	1	23	THR	CA-CB-CG2	5.95	120.61	110.50
1	1	98	ASN	CB-CA-C	5.94	125.74	112.78
1	1	113	PRO	CA-C-N	5.94	132.30	122.62
1	1	113	PRO	C-N-CA	5.94	132.30	122.62
1	1	181	TYR	CA-CB-CG	5.93	124.58	113.90
1	2	135	THR	CB-CA-C	5.93	119.54	109.99
1	1	45	ALA	CB-CA-C	5.93	116.38	110.33
1	2	140	ILE	CA-CB-CG1	5.92	120.46	110.40
1	1	107	VAL	CA-C-N	5.92	132.84	121.54
1	1	107	VAL	C-N-CA	5.92	132.84	121.54
1	1	109	VAL	N-CA-C	-5.91	97.06	109.34
1	2	84	ASP	CA-CB-CG	5.90	118.50	112.60
1	2	160	LYS	N-CA-C	5.90	118.15	109.24
1	1	77	VAL	O-C-N	5.89	129.67	122.83
1	1	35	VAL	CA-C-O	-5.89	113.92	121.40
1	2	131	ALA	N-CA-C	5.88	121.12	113.88
1	1	175	LYS	N-CA-C	-5.88	99.29	108.00
1	2	12	GLY	N-CA-C	5.88	117.90	110.38
1	2	167	LYS	CA-CB-CG	5.88	125.85	114.10
1	1	191	SER	CB-CA-C	5.85	121.43	109.67
1	2	51	TYR	CA-CB-CG	5.85	124.43	113.90
1	1	3	ALA	N-CA-C	-5.85	107.95	114.62
1	1	188	GLN	CA-C-O	-5.84	112.16	120.51
1	1	33	ASN	CA-CB-CG	-5.84	106.76	112.60
1	1	139	LEU	O-C-N	5.83	130.77	123.19
1	2	181	TYR	CA-CB-CG	5.83	124.39	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	143	PHE	N-CA-CB	-5.83	100.64	110.49
1	1	120	THR	CB-CA-C	5.82	122.86	110.07
1	1	202	GLU	CA-C-O	5.81	128.82	120.16
1	2	16	GLN	CB-CG-CD	-5.81	102.72	112.60
1	2	109	VAL	O-C-N	5.81	129.20	122.99
1	2	123	PRO	CB-CA-C	5.81	118.00	110.92
1	2	169	SER	N-CA-CB	-5.79	100.70	110.49
1	1	167	LYS	O-C-N	5.78	126.88	121.27
1	2	35	VAL	CB-CA-C	5.78	119.22	111.19
1	1	73	ALA	O-C-N	5.78	129.80	123.27
1	1	192	HIS	O-C-N	-5.78	116.59	123.06
1	1	57	PRO	CA-C-N	5.77	130.45	120.58
1	1	57	PRO	C-N-CA	5.77	130.45	120.58
1	2	128	GLU	CA-C-N	5.77	128.29	120.44
1	2	128	GLU	C-N-CA	5.77	128.29	120.44
1	2	39	GLN	CA-C-N	-5.76	114.29	122.94
1	2	39	GLN	C-N-CA	-5.76	114.29	122.94
1	1	91	SER	CA-C-N	5.76	130.44	122.77
1	1	91	SER	C-N-CA	5.76	130.44	122.77
1	2	148	VAL	CA-C-O	5.76	127.98	120.78
1	2	107	VAL	CB-CA-C	-5.75	101.85	111.29
1	2	35	VAL	N-CA-CB	-5.75	104.42	111.67
1	1	192	HIS	CA-CB-CG	5.75	119.55	113.80
1	2	18	VAL	CB-CA-C	5.74	119.18	110.62
1	2	84	ASP	N-CA-C	-5.74	101.98	110.48
1	1	155	ASP	N-CA-CB	5.73	120.17	110.49
1	2	49	ILE	CA-CB-CG1	-5.72	100.68	110.40
1	1	164	GLU	CG-CD-OE1	5.69	131.48	118.40
1	2	6	GLN	O-C-N	5.67	127.84	121.32
1	1	52	GLU	N-CA-CB	5.67	120.06	110.49
1	1	201	HIS	N-CA-CB	5.67	120.07	110.49
1	1	202	GLU	CG-CD-OE1	5.67	131.43	118.40
1	2	36	SER	N-CA-C	-5.66	100.91	109.85
1	2	32	TYR	N-CA-CB	5.65	119.55	110.85
1	1	19	THR	O-C-N	5.63	129.80	123.27
1	2	194	SER	CA-C-N	-5.63	115.17	123.05
1	2	194	SER	C-N-CA	-5.63	115.17	123.05
1	1	184	LEU	O-C-N	5.62	129.01	122.99
1	2	176	TYR	CB-CA-C	-5.62	99.81	109.65
1	1	183	SER	CA-C-N	5.62	131.43	122.10
1	1	183	SER	C-N-CA	5.62	131.43	122.10
1	2	92	SER	CA-CB-OG	-5.61	99.87	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	187	GLU	CG-CD-OE1	5.60	131.28	118.40
1	2	14	LEU	CB-CA-C	5.59	122.18	110.45
1	2	99	PHE	N-CA-C	5.58	117.50	110.24
1	1	96	SER	O-C-N	5.58	129.48	121.95
1	2	139	LEU	O-C-N	5.58	130.48	123.12
1	2	190	LYS	CB-CG-CD	5.57	124.12	111.30
1	1	53	VAL	CA-C-N	5.55	130.29	121.18
1	1	53	VAL	C-N-CA	5.55	130.29	121.18
1	2	112	GLN	O-C-N	5.55	127.70	121.32
1	1	103	THR	CA-CB-CG2	5.55	119.93	110.50
1	2	85	GLU	CB-CG-CD	5.55	122.03	112.60
1	1	63	ARG	NH1-CZ-NH2	-5.54	112.09	119.30
1	1	176	TYR	CA-C-O	-5.54	114.79	120.89
1	1	33	ASN	CA-C-N	-5.54	114.69	123.23
1	1	33	ASN	C-N-CA	-5.54	114.69	123.23
1	2	186	PRO	N-CA-CB	-5.54	97.44	103.25
1	1	108	THR	CA-C-N	5.53	131.92	121.97
1	1	108	THR	C-N-CA	5.53	131.92	121.97
1	1	56	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	1	56	ARG	O-C-N	5.52	127.67	121.32
1	2	112	GLN	OE1-CD-NE2	-5.51	117.09	122.60
1	1	28	ASP	CA-C-O	-5.50	115.46	121.89
1	2	162	GLY	O-C-N	5.50	129.85	122.70
1	1	63	ARG	O-C-N	5.49	127.60	122.00
1	1	64	PHE	O-C-N	5.48	129.62	123.27
1	1	202	GLU	CG-CD-OE2	-5.48	105.81	118.40
1	1	121	LEU	N-CA-CB	-5.46	101.97	110.87
1	1	90	CYS	O-C-N	5.46	129.43	123.27
1	1	53	VAL	N-CA-CB	-5.45	102.24	111.23
1	1	80	LEU	CA-C-O	-5.43	112.75	120.51
1	2	107	VAL	N-CA-CB	5.42	120.18	111.23
1	2	39	GLN	CB-CG-CD	5.42	121.82	112.60
1	2	115	ALA	CA-C-O	-5.42	115.21	121.49
1	2	7	PRO	O-C-N	5.41	127.85	121.46
1	2	17	SER	N-CA-C	5.41	118.26	109.06
1	1	137	VAL	O-C-N	5.41	129.10	123.26
1	2	195	TYR	N-CA-CB	-5.40	102.07	110.55
1	1	26	SER	CA-CB-OG	5.39	121.88	111.10
1	2	83	GLU	N-CA-C	-5.39	101.51	109.86
1	1	76	THR	CB-CA-C	-5.38	102.07	110.74
1	2	164	GLU	N-CA-CB	5.38	119.64	110.71
1	2	142	ASP	CA-C-O	5.37	127.10	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	35	VAL	N-CA-C	-5.37	99.42	107.37
1	1	102	GLY	O-C-N	5.36	129.67	122.70
1	2	180	SER	O-C-N	5.34	129.07	123.03
1	1	16	GLN	CA-C-O	5.33	127.48	121.51
1	1	108	THR	CA-CB-CG2	5.33	119.56	110.50
1	2	94	GLU	CA-C-N	5.33	131.86	121.41
1	2	94	GLU	C-N-CA	5.33	131.86	121.41
1	2	75	LEU	N-CA-CB	5.32	118.92	110.57
1	2	99	PHE	CA-CB-CG	5.32	119.12	113.80
1	2	140	ILE	O-C-N	5.31	129.01	122.95
1	2	119	VAL	CB-CA-C	5.31	119.59	111.68
1	2	71	ASN	CA-C-N	5.31	130.23	122.85
1	2	71	ASN	C-N-CA	5.31	130.23	122.85
1	1	147	ALA	CB-CA-C	-5.30	103.97	111.76
1	1	60	VAL	O-C-N	5.29	127.14	121.10
1	1	84	ASP	CB-CA-C	5.29	120.82	110.67
1	1	25	THR	O-C-N	5.29	129.62	122.59
1	2	85	GLU	CA-CB-CG	5.28	124.67	114.10
1	2	36	SER	CA-CB-OG	-5.28	100.54	111.10
1	1	46	PRO	N-CA-C	-5.27	101.99	110.74
1	1	196	SER	O-C-N	5.27	129.57	123.30
1	1	104	GLY	N-CA-C	5.26	125.65	113.18
1	1	115	ALA	CA-C-N	5.26	132.21	121.48
1	1	115	ALA	C-N-CA	5.26	132.21	121.48
1	2	17	SER	CA-CB-OG	-5.26	100.58	111.10
1	2	110	LEU	CA-C-O	-5.25	113.00	120.51
1	1	198	GLN	CA-C-N	-5.25	114.02	121.85
1	1	198	GLN	C-N-CA	-5.25	114.02	121.85
1	1	132	ASN	CA-C-O	-5.25	114.13	120.32
1	2	205	THR	CA-CB-CG2	5.24	119.40	110.50
1	1	25	THR	N-CA-CB	5.23	119.33	110.49
1	2	143	PHE	CA-C-N	5.23	127.27	120.26
1	2	143	PHE	C-N-CA	5.23	127.27	120.26
1	1	14	LEU	N-CA-CB	5.22	119.31	110.49
1	2	173	ASN	N-CA-CB	5.22	119.31	110.49
1	1	193	ARG	CD-NE-CZ	5.22	131.71	124.40
1	2	105	THR	N-CA-CB	5.21	119.30	110.49
1	1	63	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	1	165	THR	CA-C-O	5.20	127.49	120.47
1	2	89	TYR	N-CA-C	5.20	117.91	109.06
1	1	43	GLY	CA-C-N	5.20	131.46	121.54
1	1	43	GLY	C-N-CA	5.20	131.46	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	157	SER	N-CA-C	5.17	117.62	110.07
1	2	67	SER	N-CA-C	-5.17	101.21	109.07
1	2	96	SER	N-CA-C	-5.17	99.78	110.80
1	1	135	THR	CA-C-N	-5.17	115.71	122.99
1	1	135	THR	C-N-CA	-5.17	115.71	122.99
1	2	165	THR	CB-CA-C	-5.16	99.35	110.45
1	1	63	ARG	CB-CG-CD	5.16	123.16	111.30
1	1	71	ASN	CB-CA-C	5.16	120.69	110.42
1	2	18	VAL	N-CA-C	5.16	115.90	108.48
1	2	52	GLU	N-CA-CB	5.14	119.18	110.49
1	2	134	ALA	CB-CA-C	-5.14	109.11	115.89
1	1	83	GLU	OE1-CD-OE2	5.13	135.22	122.90
1	2	30	GLY	N-CA-C	-5.13	101.02	113.18
1	1	16	GLN	CA-C-N	5.13	130.64	122.74
1	1	16	GLN	C-N-CA	5.13	130.64	122.74
1	1	10	ALA	N-CA-C	-5.12	100.89	109.24
1	2	138	CYS	N-CA-C	-5.12	101.05	109.40
1	2	78	SER	CA-C-N	-5.12	111.38	121.41
1	2	78	SER	C-N-CA	-5.12	111.38	121.41
1	1	34	TYR	CA-C-O	-5.11	110.82	120.69
1	2	30	GLY	O-C-N	5.10	129.33	122.70
1	2	196	SER	N-CA-C	-5.10	102.22	110.32
1	1	193	ARG	CA-C-O	-5.08	115.66	120.90
1	1	208	LYS	CA-C-O	5.08	126.43	120.43
1	1	113	PRO	O-C-N	-5.08	116.73	123.13
1	1	106	LYS	CA-C-O	5.08	126.44	120.80
1	1	174	ASN	N-CA-C	-5.08	99.99	110.80
1	2	113	PRO	N-CA-C	5.08	119.17	110.74
1	1	154	ALA	CA-C-O	5.07	126.96	120.57
1	1	184	LEU	CB-CA-C	-5.06	101.49	111.91
1	1	195	TYR	O-C-N	5.06	129.44	123.27
1	1	63	ARG	N-CA-CB	-5.05	106.57	114.45
1	2	103	THR	N-CA-CB	-5.05	103.07	110.85
1	2	67	SER	CA-C-O	-5.04	115.88	121.33
1	2	211	ALA	O-C-N	5.04	127.12	121.32
1	2	47	LYS	N-CA-C	5.04	116.73	108.52
1	2	78	SER	N-CA-C	-5.04	100.52	108.73
1	2	108	THR	CB-CA-C	5.04	119.43	111.77
1	2	210	VAL	O-C-N	5.04	128.64	123.05
1	2	156	GLY	N-CA-C	5.02	125.08	113.18
1	1	210	VAL	N-CA-C	-5.02	101.25	108.48
1	2	137	VAL	O-C-N	5.01	128.61	123.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	1	148	VAL	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1606	0	1537	467	8
1	2	1606	0	1537	628	8
2	1	123	0	0	49	5
2	2	143	0	0	73	6
All	All	3478	0	3074	1054	18

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 168.

All (1054) 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)
1:2:56:ARG:HB2	1:2:60:VAL:CG2	1.62	1.29
1:1:92:SER:OG	1:1:100:VAL:HB	1.31	1.29
1:2:56:ARG:CB	1:2:60:VAL:HG21	1.66	1.25
1:2:137:VAL:HG11	2:2:252:HOH:O	1.32	1.25
2:1:224:HOH:O	1:2:210:VAL:HG11	1.41	1.21
1:2:154:ALA:HA	2:2:308:HOH:O	1.39	1.21
1:1:134:ALA:HB3	1:1:184:LEU:O	1.39	1.20
1:2:196:SER:HB3	1:2:209:THR:HB	1.24	1.20
1:1:112:GLN:CB	1:1:113:PRO:HD3	1.71	1.19
1:2:168:PRO:HA	2:2:325:HOH:O	1.43	1.18
1:2:29:VAL:HG22	1:2:71:ASN:HA	1.20	1.18
1:2:60:VAL:HG13	1:2:64:PHE:HB3	1.27	1.17
1:2:210:VAL:HG12	2:2:222:HOH:O	1.45	1.16
1:1:63:ARG:HH11	1:1:81:GLN:NE2	1.42	1.16
1:1:112:GLN:HB3	1:1:113:PRO:CD	1.75	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:136:LEU:HD11	1:2:184:LEU:HB2	1.20	1.14
1:1:84:ASP:HB3	1:1:107:VAL:HG11	1.22	1.14
1:1:127:GLU:OE1	1:2:122:PHE:HE1	1.30	1.12
1:2:196:SER:HA	1:2:209:THR:HA	1.29	1.12
1:2:115:ALA:HB3	1:2:143:PHE:HA	1.31	1.11
1:1:77:VAL:HG11	1:1:84:ASP:OD2	1.49	1.10
1:1:65:SER:O	1:1:75:LEU:HD23	1.51	1.09
1:1:168:PRO:HB3	1:1:178:ALA:HB2	1.34	1.08
1:2:47:LYS:O	1:2:49:ILE:HG12	1.52	1.08
1:1:62:ASP:O	1:1:63:ARG:HB2	1.54	1.07
1:1:121:LEU:HG	1:1:210:VAL:HG22	1.13	1.06
1:1:127:GLU:OE1	1:2:122:PHE:CE1	2.07	1.06
1:1:45:ALA:HB2	2:1:263:HOH:O	1.54	1.05
1:2:117:PRO:HG2	2:2:260:HOH:O	1.53	1.05
1:2:198:GLN:HB2	2:2:341:HOH:O	1.54	1.05
1:1:192:HIS:O	1:1:212:PRO:HG3	1.55	1.04
1:2:142:ASP:O	1:2:143:PHE:HB3	1.52	1.04
1:2:86:ALA:HB3	2:2:273:HOH:O	1.54	1.04
1:2:4:LEU:HB3	1:2:102:GLY:CA	1.88	1.03
1:1:152:TRP:HA	1:1:196:SER:O	1.58	1.02
1:2:208:LYS:HB2	2:2:227:HOH:O	1.59	1.02
1:2:211:ALA:HB3	1:2:212:PRO:HD2	1.42	1.01
1:2:211:ALA:CB	1:2:212:PRO:CD	2.37	1.01
1:2:187:GLU:O	1:2:191:SER:HB3	1.58	1.01
1:1:143:PHE:HE2	1:1:148:VAL:HG21	1.26	1.01
1:2:194:SER:O	2:2:308:HOH:O	1.79	1.00
1:1:63:ARG:NH1	1:1:81:GLN:NE2	2.10	0.99
1:1:119:VAL:HG22	1:1:140:ILE:HG23	1.44	0.99
1:1:123:PRO:HB3	1:1:210:VAL:HG11	1.40	0.99
1:1:124:PRO:HD3	1:1:136:LEU:HB2	1.45	0.99
1:2:136:LEU:HB3	2:2:292:HOH:O	1.60	0.99
1:2:8:PRO:HD2	1:2:9:SER:H	1.24	0.98
1:2:26:SER:HA	1:2:30:GLY:HA3	1.43	0.98
1:2:38:TYR:CD2	2:2:240:HOH:O	2.17	0.98
1:1:152:TRP:CZ2	2:1:317:HOH:O	2.16	0.97
1:2:2:SER:O	1:2:100:VAL:HG21	1.63	0.97
1:2:39:GLN:HB2	1:2:49:ILE:HD13	1.46	0.97
1:1:121:LEU:HG	1:1:210:VAL:CG2	1.93	0.96
1:2:20:ILE:HD11	1:2:75:LEU:CD2	1.94	0.96
1:2:132:ASN:O	1:2:186:PRO:HD2	1.65	0.96
1:1:5:THR:HB	1:1:23:THR:OG1	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:138:CYS:CB	2:1:317:HOH:O	2.13	0.96
1:2:18:VAL:HG23	1:2:80:LEU:HD11	1.45	0.95
1:1:205:THR:O	2:1:337:HOH:O	1.84	0.95
1:1:124:PRO:O	1:2:216:SER:OG	1.83	0.95
1:2:185:THR:O	1:2:188:GLN:HB2	1.66	0.95
1:1:143:PHE:HD1	1:1:176:TYR:C	1.73	0.94
1:1:56:ARG:HH21	1:1:56:ARG:HG3	1.30	0.94
1:2:16:GLN:HG2	1:2:17:SER:N	1.79	0.94
1:2:2:SER:HB2	1:2:100:VAL:HG21	1.47	0.94
1:2:56:ARG:HB2	1:2:60:VAL:HG21	0.96	0.93
1:1:157:SER:HB2	1:1:158:PRO:CD	1.98	0.93
1:2:28:ASP:OD1	1:2:92:SER:HB3	1.68	0.93
1:2:8:PRO:CD	1:2:9:SER:H	1.81	0.93
1:1:7:PRO:HD3	2:1:250:HOH:O	1.69	0.92
1:1:86:ALA:HB3	1:1:88:TYR:CE2	2.03	0.92
1:2:183:SER:HB2	2:2:316:HOH:O	1.67	0.92
1:2:115:ALA:HB3	1:2:144:TYR:H	1.35	0.92
1:1:4:LEU:HD12	1:1:22:CYS:SG	2.08	0.92
1:2:46:PRO:HB2	2:2:240:HOH:O	1.67	0.92
1:2:189:TRP:HH2	2:2:222:HOH:O	1.51	0.92
1:2:153:LYS:HD2	1:2:156:GLY:C	1.95	0.92
1:1:80:LEU:HG	1:1:84:ASP:HB2	1.49	0.92
1:1:121:LEU:CG	1:1:210:VAL:HG22	2.00	0.92
1:1:214:GLU:HA	2:1:307:HOH:O	1.67	0.92
1:2:57:PRO:HG3	2:2:248:HOH:O	1.70	0.92
1:1:194:SER:HB3	2:1:335:HOH:O	1.69	0.92
1:1:70:GLY:O	1:1:71:ASN:HB2	1.68	0.91
1:1:143:PHE:O	1:1:175:LYS:HE2	1.69	0.91
1:2:211:ALA:HB1	1:2:212:PRO:HD3	1.50	0.91
1:2:29:VAL:HG22	1:2:29:VAL:O	1.66	0.91
1:1:42:ALA:HB3	2:1:261:HOH:O	1.69	0.91
1:1:68:LYS:HG2	2:1:260:HOH:O	1.70	0.91
1:1:28:ASP:HA	1:1:32:TYR:HB2	1.52	0.91
1:1:136:LEU:HD11	1:1:195:TYR:CD1	2.05	0.91
1:2:196:SER:CA	1:2:209:THR:HA	2.01	0.90
1:1:53:VAL:HG12	1:1:54:ASN:OD1	1.71	0.90
1:1:183:SER:O	1:1:184:LEU:HD22	1.72	0.90
1:2:56:ARG:HD2	1:2:60:VAL:HG11	1.51	0.90
1:2:38:TYR:C	1:2:49:ILE:HD11	1.97	0.90
1:1:143:PHE:HE2	1:1:148:VAL:CG2	1.85	0.89
1:2:60:VAL:CG1	1:2:64:PHE:HB3	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:157:SER:HB2	1:1:158:PRO:HD3	1.52	0.89
1:2:130:GLN:H	1:2:130:GLN:HE21	1.16	0.89
1:2:188:GLN:OE1	1:2:192:HIS:HE1	1.56	0.89
1:2:87:ASP:HB3	1:2:89:TYR:HE1	1.38	0.89
1:2:119:VAL:CG2	1:2:208:LYS:HG3	2.03	0.89
1:2:121:LEU:C	1:2:121:LEU:HD23	1.97	0.89
1:2:40:GLN:HB3	1:2:46:PRO:HG3	1.55	0.88
1:2:87:ASP:HB3	1:2:89:TYR:CE1	2.09	0.88
1:2:168:PRO:HG2	1:2:169:SER:H	1.37	0.88
1:2:38:TYR:HB3	2:2:240:HOH:O	1.74	0.87
1:2:50:ILE:HD13	1:2:75:LEU:CD1	2.05	0.87
1:2:77:VAL:HG11	2:2:267:HOH:O	1.72	0.87
1:1:125:SER:O	1:2:216:SER:HB3	1.75	0.87
1:1:128:GLU:OE1	1:1:189:TRP:CD1	2.27	0.87
1:2:211:ALA:HB3	1:2:212:PRO:CD	2.03	0.87
1:2:132:ASN:O	1:2:186:PRO:CD	2.22	0.87
1:1:34:TYR:HB3	1:1:93:TYR:HB3	1.56	0.87
1:1:68:LYS:O	1:1:68:LYS:HD3	1.73	0.87
1:2:170:LYS:HA	1:2:170:LYS:CE	2.03	0.87
1:2:210:VAL:CG1	2:2:345:HOH:O	2.21	0.87
1:1:63:ARG:NH1	1:1:81:GLN:HE21	1.71	0.86
1:2:86:ALA:C	1:2:106:LYS:HA	1.99	0.86
1:2:197:CYS:O	1:2:207:GLU:HB2	1.75	0.86
1:2:213:THR:HG22	2:2:345:HOH:O	1.74	0.86
1:2:115:ALA:CB	1:2:143:PHE:HA	2.06	0.86
1:1:57:PRO:HG2	1:1:60:VAL:HG11	1.56	0.86
1:1:163:VAL:HB	1:1:182:LEU:HD13	1.57	0.86
1:1:207:GLU:OE2	1:1:208:LYS:N	2.09	0.86
1:1:163:VAL:HG23	1:1:182:LEU:HB2	1.55	0.86
1:1:125:SER:HA	1:2:216:SER:HA	1.56	0.86
1:1:134:ALA:CB	1:1:184:LEU:O	2.24	0.86
1:2:196:SER:HA	1:2:209:THR:CA	2.06	0.86
1:2:148:VAL:HG23	1:2:149:THR:H	1.39	0.85
1:1:84:ASP:HB3	1:1:107:VAL:CG1	2.04	0.85
1:2:123:PRO:CD	1:2:124:PRO:HD3	2.06	0.85
1:2:167:LYS:HB2	1:2:168:PRO:HD2	1.58	0.85
1:2:4:LEU:HB3	1:2:102:GLY:N	1.92	0.85
1:2:129:LEU:HD11	1:2:189:TRP:HB3	1.57	0.85
1:2:121:LEU:HD23	1:2:121:LEU:O	1.77	0.85
1:1:40:GLN:HG2	2:1:269:HOH:O	1.77	0.85
1:1:84:ASP:O	1:1:86:ALA:N	2.10	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:119:VAL:HA	1:1:139:LEU:O	1.74	0.85
1:1:92:SER:OG	1:1:100:VAL:CB	2.20	0.84
1:2:63:ARG:HB2	1:2:78:SER:HB3	1.57	0.84
1:1:138:CYS:HB3	2:1:317:HOH:O	1.75	0.84
1:2:140:ILE:HG12	1:2:177:ALA:HB1	1.59	0.84
1:2:136:LEU:HD12	1:2:182:LEU:O	1.77	0.84
1:1:41:HIS:CE1	1:1:83:GLU:O	2.30	0.84
1:1:187:GLU:O	1:1:188:GLN:C	2.20	0.84
1:1:77:VAL:CG1	1:1:84:ASP:OD2	2.25	0.84
1:2:170:LYS:HA	1:2:170:LYS:HE2	1.58	0.84
1:2:34:TYR:O	1:2:92:SER:HA	1.77	0.84
1:1:106:LYS:H	1:1:106:LYS:HD2	1.42	0.84
1:2:109:VAL:HG13	1:2:109:VAL:O	1.77	0.84
1:2:189:TRP:CH2	2:2:222:HOH:O	2.24	0.84
1:1:119:VAL:HG21	1:1:199:VAL:HG11	1.58	0.84
1:2:188:GLN:HA	1:2:192:HIS:CE1	2.12	0.84
1:2:143:PHE:H	1:2:175:LYS:HD2	1.42	0.84
1:1:40:GLN:HG3	1:1:87:ASP:HB3	1.58	0.83
1:1:69:SER:O	1:1:71:ASN:N	2.11	0.83
1:1:63:ARG:HH11	1:1:81:GLN:HE22	1.25	0.83
1:1:143:PHE:CE2	1:1:148:VAL:HG21	2.14	0.83
1:1:112:GLN:HA	2:1:310:HOH:O	1.77	0.83
1:1:155:ASP:HB3	1:1:193:ARG:HB3	1.61	0.83
1:2:196:SER:HB3	1:2:209:THR:CB	2.06	0.83
1:1:113:PRO:O	1:1:144:TYR:CD2	2.31	0.83
1:2:136:LEU:CD1	1:2:184:LEU:HB2	2.06	0.83
1:2:39:GLN:NE2	1:2:88:TYR:CE2	2.47	0.83
1:1:37:TRP:O	1:1:49:ILE:HG12	1.79	0.83
1:1:104:GLY:O	1:1:106:LYS:HE2	1.79	0.82
1:2:85:GLU:HG2	1:2:106:LYS:NZ	1.95	0.82
1:2:136:LEU:HD13	1:2:184:LEU:HD23	1.59	0.82
1:1:17:SER:HA	1:1:77:VAL:O	1.80	0.82
1:1:124:PRO:HD3	1:1:136:LEU:CB	2.09	0.82
1:1:119:VAL:CG2	1:1:140:ILE:HG23	2.10	0.82
1:1:181:TYR:CE2	1:2:139:LEU:HD23	2.13	0.82
1:1:194:SER:CB	2:1:335:HOH:O	2.24	0.82
1:1:201:HIS:HB2	1:1:204:SER:CB	2.10	0.82
1:1:130:GLN:O	1:1:132:ASN:N	2.13	0.81
1:2:63:ARG:HD3	1:2:78:SER:OG	1.81	0.81
1:2:2:SER:O	1:2:100:VAL:CG2	2.28	0.81
2:1:232:HOH:O	1:2:101:PHE:CE2	2.34	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:77:VAL:HG21	2:2:267:HOH:O	1.80	0.80
1:2:143:PHE:N	1:2:175:LYS:HD2	1.97	0.80
1:2:29:VAL:O	1:2:29:VAL:CG2	2.29	0.80
1:2:109:VAL:C	1:2:110:LEU:O	2.20	0.80
1:1:38:TYR:CD1	1:1:48:VAL:HG22	2.17	0.80
1:2:28:ASP:OD2	1:2:92:SER:OG	1.98	0.80
1:1:135:THR:HG22	1:1:181:TYR:CD1	2.16	0.80
1:1:166:THR:CG2	1:2:167:LYS:HD3	2.10	0.80
1:2:152:TRP:CD2	1:2:182:LEU:HD13	2.18	0.80
2:1:232:HOH:O	1:2:101:PHE:HE2	1.65	0.79
1:2:56:ARG:CD	1:2:60:VAL:HG11	2.10	0.79
1:2:79:GLY:O	1:2:80:LEU:HB2	1.80	0.79
1:1:8:PRO:O	1:1:106:LYS:HD2	1.82	0.79
1:1:188:GLN:O	1:1:192:HIS:HB2	1.82	0.79
1:2:66:GLY:HA2	1:2:75:LEU:HA	1.64	0.79
1:2:201:HIS:HB3	2:2:260:HOH:O	1.82	0.79
1:1:47:LYS:HA	2:1:232:HOH:O	1.81	0.79
1:1:13:SER:O	1:1:16:GLN:HG3	1.82	0.79
1:1:192:HIS:O	1:1:212:PRO:CG	2.28	0.79
1:2:90:CYS:O	1:2:101:PHE:HA	1.81	0.79
1:2:86:ALA:O	1:2:106:LYS:HA	1.82	0.79
1:1:2:SER:HB3	1:1:100:VAL:HG11	1.62	0.79
1:1:77:VAL:HG21	1:1:84:ASP:OD1	1.83	0.78
1:2:117:PRO:HA	1:2:142:ASP:O	1.83	0.78
1:2:8:PRO:CD	1:2:9:SER:N	2.44	0.78
1:1:135:THR:HG22	1:1:181:TYR:HD1	1.47	0.78
1:1:5:THR:HG22	1:1:5:THR:O	1.83	0.78
1:1:111:GLY:HA3	1:1:144:TYR:HE2	1.49	0.78
1:1:32:TYR:HE2	1:1:93:TYR:HE1	1.30	0.78
1:1:125:SER:HB2	2:1:313:HOH:O	1.82	0.78
1:1:165:THR:HG23	1:1:179:SER:O	1.82	0.78
1:2:36:SER:OG	1:2:38:TYR:CE1	2.37	0.78
1:1:129:LEU:O	1:1:129:LEU:HD22	1.83	0.77
1:2:50:ILE:HD11	1:2:75:LEU:HB2	1.64	0.77
1:2:150:VAL:HB	2:2:315:HOH:O	1.84	0.77
1:1:110:LEU:HD21	2:1:262:HOH:O	1.83	0.77
1:1:112:GLN:HB3	1:1:113:PRO:HD3	0.84	0.77
1:1:56:ARG:HG3	1:1:56:ARG:NH2	1.96	0.77
1:2:142:ASP:HB2	1:2:175:LYS:HD2	1.65	0.77
1:2:107:VAL:HG13	1:2:108:THR:N	1.99	0.77
1:2:114:LYS:CE	1:2:202:GLU:OE2	2.33	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:51:TYR:CE1	1:1:55:LYS:HD3	2.20	0.77
1:2:143:PHE:CA	1:2:175:LYS:HD3	2.15	0.77
1:2:96:SER:O	1:2:98:ASN:N	2.18	0.77
1:2:4:LEU:HD23	1:2:90:CYS:SG	2.24	0.77
1:2:20:ILE:HD11	1:2:75:LEU:HD23	1.67	0.77
1:2:85:GLU:HG2	1:2:106:LYS:HZ3	1.50	0.77
1:2:119:VAL:HG21	1:2:208:LYS:HG3	1.67	0.77
1:1:97:ASP:O	1:2:57:PRO:CB	2.33	0.76
1:2:168:PRO:HG2	1:2:169:SER:N	1.98	0.76
1:1:194:SER:CA	2:1:335:HOH:O	2.32	0.76
1:2:188:GLN:OE1	1:2:188:GLN:HA	1.86	0.76
1:2:5:THR:HB	1:2:23:THR:HG22	1.68	0.76
1:2:51:TYR:CE1	1:2:57:PRO:HD3	2.21	0.76
1:2:106:LYS:HG3	1:2:107:VAL:H	1.50	0.76
1:2:94:GLU:OE1	1:2:100:VAL:HG11	1.85	0.76
1:2:118:THR:HG23	1:2:118:THR:O	1.84	0.76
1:1:113:PRO:HD2	1:1:144:TYR:CE2	2.21	0.76
1:1:52:GLU:C	1:1:53:VAL:HG23	2.10	0.76
1:1:92:SER:HG	1:1:100:VAL:HB	1.51	0.76
1:1:113:PRO:O	1:1:144:TYR:HB3	1.85	0.76
1:2:36:SER:HB3	2:2:238:HOH:O	1.85	0.76
1:1:38:TYR:HD1	1:1:48:VAL:HG22	1.51	0.75
1:2:125:SER:HB3	1:2:127:GLU:OE2	1.87	0.75
1:1:130:GLN:C	1:1:132:ASN:H	1.93	0.75
1:1:187:GLU:C	1:1:189:TRP:N	2.41	0.75
1:1:38:TYR:HB3	1:1:47:LYS:O	1.85	0.75
1:1:52:GLU:HB2	1:1:55:LYS:HD2	1.67	0.75
1:1:44:LYS:CG	1:1:45:ALA:H	1.98	0.75
1:2:61:PRO:HG2	1:2:62:ASP:H	1.48	0.75
1:2:211:ALA:CB	1:2:212:PRO:HD3	2.08	0.75
1:1:127:GLU:O	1:1:131:ALA:HB3	1.86	0.75
1:2:115:ALA:HB3	1:2:143:PHE:CA	2.15	0.75
1:2:115:ALA:HB3	1:2:144:TYR:N	2.02	0.74
1:1:109:VAL:HG23	2:1:272:HOH:O	1.86	0.74
1:2:86:ALA:HA	1:2:106:LYS:HB2	1.69	0.74
1:2:136:LEU:HD21	1:2:189:TRP:CD1	2.21	0.74
1:1:153:LYS:HG3	1:1:196:SER:OG	1.87	0.74
1:1:127:GLU:HA	1:1:131:ALA:HB3	1.68	0.74
1:2:186:PRO:HB2	1:2:187:GLU:HG3	1.69	0.74
1:2:123:PRO:N	1:2:124:PRO:CD	2.51	0.74
1:1:39:GLN:HG3	1:1:88:TYR:CZ	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:61:PRO:CG	1:2:62:ASP:H	2.01	0.74
1:2:127:GLU:HG2	1:2:128:GLU:N	2.02	0.74
1:2:136:LEU:CD2	1:2:189:TRP:NE1	2.51	0.74
1:1:173:ASN:O	1:1:174:ASN:HB2	1.87	0.73
1:2:69:SER:O	1:2:72:THR:OG1	2.05	0.73
1:2:136:LEU:HD21	1:2:189:TRP:NE1	2.02	0.73
1:2:68:LYS:HB2	1:2:73:ALA:HB2	1.69	0.73
1:1:32:TYR:HE2	1:1:93:TYR:CE1	2.06	0.73
1:1:80:LEU:CG	1:1:84:ASP:HB2	2.18	0.73
1:1:86:ALA:HB3	1:1:88:TYR:CZ	2.22	0.73
1:2:153:LYS:HB2	1:2:153:LYS:NZ	2.03	0.73
1:1:93:TYR:O	1:1:94:GLU:HB3	1.85	0.73
1:2:4:LEU:HB3	1:2:102:GLY:HA3	1.71	0.73
1:2:50:ILE:HD13	1:2:75:LEU:HD12	1.69	0.73
1:2:114:LYS:HE2	1:2:202:GLU:OE2	1.88	0.73
1:2:188:GLN:OE1	1:2:192:HIS:CE1	2.41	0.73
1:1:89:TYR:CE1	1:2:45:ALA:HB2	2.23	0.73
1:2:50:ILE:CD1	1:2:75:LEU:HB2	2.17	0.73
1:2:143:PHE:H	1:2:175:LYS:CD	2.01	0.73
1:2:26:SER:CA	1:2:30:GLY:HA3	2.19	0.73
1:1:68:LYS:HD3	1:1:68:LYS:C	2.14	0.73
1:2:214:GLU:OE2	2:2:355:HOH:O	2.07	0.73
1:1:181:TYR:CZ	1:2:139:LEU:HD23	2.24	0.72
1:1:213:THR:O	2:1:307:HOH:O	2.06	0.72
1:2:153:LYS:HB2	1:2:153:LYS:HZ2	1.52	0.72
1:2:56:ARG:HB2	1:2:60:VAL:HG23	1.71	0.72
1:1:201:HIS:HB2	1:1:204:SER:HB3	1.70	0.72
1:2:129:LEU:HD13	1:2:186:PRO:HA	1.70	0.72
1:2:29:VAL:CG2	1:2:71:ASN:HA	2.10	0.72
1:1:52:GLU:CB	1:1:55:LYS:HD2	2.19	0.72
1:1:57:PRO:HG2	1:1:60:VAL:CG1	2.20	0.72
1:1:170:LYS:HG2	1:1:174:ASN:O	1.88	0.72
1:2:16:GLN:HG2	1:2:17:SER:H	1.54	0.72
1:2:20:ILE:CG2	1:2:105:THR:HG21	2.19	0.72
1:2:40:GLN:CB	1:2:46:PRO:HG3	2.19	0.72
1:1:51:TYR:CE2	1:1:55:LYS:HB3	2.24	0.72
1:2:143:PHE:N	1:2:175:LYS:CD	2.53	0.72
1:2:186:PRO:O	1:2:189:TRP:HB3	1.89	0.72
1:1:183:SER:C	1:1:184:LEU:HD22	2.14	0.72
1:2:213:THR:OG1	1:2:216:SER:OXT	2.07	0.72
1:2:184:LEU:HG	1:2:195:TYR:OH	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:52:GLU:HB2	1:1:55:LYS:CD	2.20	0.72
1:1:104:GLY:O	1:1:106:LYS:CE	2.38	0.72
1:1:193:ARG:O	1:1:212:PRO:HD2	1.90	0.72
1:2:4:LEU:CB	1:2:102:GLY:N	2.53	0.72
1:2:85:GLU:HG3	1:2:107:VAL:O	1.89	0.71
1:2:162:GLY:HA2	2:2:314:HOH:O	1.89	0.71
1:1:84:ASP:O	1:1:88:TYR:HE2	1.73	0.71
1:1:137:VAL:HG11	1:2:122:PHE:CD2	2.25	0.71
1:2:126:SER:CB	2:2:355:HOH:O	2.38	0.71
1:2:144:TYR:HA	1:2:175:LYS:HG2	1.71	0.71
1:1:186:PRO:O	1:1:189:TRP:HB3	1.89	0.71
1:2:93:TYR:C	1:2:95:GLY:H	1.99	0.71
1:2:168:PRO:CG	1:2:169:SER:H	2.04	0.71
1:1:164:GLU:O	1:1:180:SER:HA	1.89	0.71
1:2:14:LEU:CD2	1:2:111:GLY:HA3	2.20	0.71
1:2:208:LYS:CB	2:2:227:HOH:O	2.24	0.71
1:1:152:TRP:HZ2	2:1:317:HOH:O	1.64	0.71
1:2:18:VAL:HB	1:2:80:LEU:HD21	1.73	0.71
1:2:86:ALA:HA	1:2:106:LYS:HE2	1.71	0.71
1:2:77:VAL:CB	2:2:267:HOH:O	2.38	0.71
1:2:133:LYS:HB3	1:2:185:THR:HG22	1.73	0.71
1:2:144:TYR:N	1:2:145:PRO:HD3	2.05	0.70
1:2:189:TRP:O	1:2:192:HIS:HB2	1.91	0.70
1:1:88:TYR:HB2	1:1:105:THR:O	1.92	0.70
1:2:143:PHE:CE2	1:2:176:TYR:O	2.44	0.70
1:1:13:SER:O	1:1:16:GLN:CG	2.40	0.70
1:2:46:PRO:CB	2:2:240:HOH:O	2.31	0.70
1:1:143:PHE:CE2	1:1:148:VAL:CG2	2.73	0.70
1:2:118:THR:HG22	1:2:142:ASP:H	1.55	0.70
1:2:34:TYR:HB3	2:2:236:HOH:O	1.91	0.69
1:2:190:LYS:HG3	1:2:191:SER:N	2.06	0.69
1:1:39:GLN:HG3	1:1:88:TYR:CE1	2.27	0.69
1:2:148:VAL:CG2	1:2:149:THR:N	2.56	0.69
1:2:77:VAL:CG1	2:2:267:HOH:O	2.35	0.69
1:2:93:TYR:O	1:2:95:GLY:N	2.25	0.69
1:2:129:LEU:HD11	1:2:189:TRP:CB	2.22	0.69
1:2:148:VAL:HG23	1:2:149:THR:N	2.05	0.69
1:2:206:VAL:O	1:2:207:GLU:HB3	1.91	0.69
1:1:124:PRO:HB3	1:1:128:GLU:CB	2.22	0.69
1:2:124:PRO:HG3	1:2:213:THR:HG21	1.74	0.69
1:2:153:LYS:HD2	1:2:156:GLY:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:10:ALA:CB	1:2:105:THR:HG23	2.22	0.69
1:2:123:PRO:HD2	1:2:124:PRO:HD3	1.73	0.69
1:1:143:PHE:CD1	1:1:176:TYR:C	2.65	0.69
1:2:41:HIS:HA	2:2:273:HOH:O	1.92	0.69
1:2:50:ILE:HD13	1:2:75:LEU:HD13	1.72	0.69
1:2:201:HIS:CB	2:2:260:HOH:O	2.40	0.69
1:1:49:ILE:HD12	1:1:64:PHE:CZ	2.27	0.69
1:2:38:TYR:HA	1:2:47:LYS:O	1.92	0.69
1:2:105:THR:HG22	1:2:106:LYS:O	1.92	0.69
1:1:40:GLN:O	1:1:42:ALA:N	2.25	0.68
1:2:109:VAL:O	1:2:109:VAL:CG1	2.41	0.68
1:2:190:LYS:C	1:2:192:HIS:N	2.43	0.68
1:1:135:THR:CG2	1:1:181:TYR:CE1	2.76	0.68
1:2:119:VAL:HG22	1:2:208:LYS:HD2	1.73	0.68
1:1:138:CYS:HB2	2:1:317:HOH:O	1.86	0.68
1:2:187:GLU:C	1:2:191:SER:HB3	2.19	0.68
1:1:36:SER:HB2	1:1:91:SER:OG	1.94	0.68
1:1:198:GLN:HB3	1:1:207:GLU:OE1	1.93	0.68
1:1:95:GLY:HA2	2:1:265:HOH:O	1.94	0.67
1:2:29:VAL:HG22	1:2:71:ASN:CA	2.13	0.67
1:2:39:GLN:N	1:2:49:ILE:HD11	2.08	0.67
1:2:49:ILE:O	1:2:50:ILE:CG2	2.42	0.67
1:1:97:ASP:O	1:2:57:PRO:HB2	1.94	0.67
1:2:38:TYR:CB	2:2:240:HOH:O	2.34	0.67
1:2:63:ARG:HB2	1:2:78:SER:CB	2.24	0.67
1:1:170:LYS:HG3	1:1:171:GLN:O	1.94	0.67
1:1:113:PRO:HD2	1:1:144:TYR:CD2	2.30	0.67
1:2:140:ILE:HG12	1:2:177:ALA:CB	2.24	0.67
1:1:41:HIS:O	1:1:42:ALA:HB3	1.92	0.67
1:1:113:PRO:O	1:1:144:TYR:CB	2.42	0.67
1:1:44:LYS:HG2	1:1:45:ALA:H	1.58	0.67
1:2:116:ASN:HB3	1:2:117:PRO:CD	2.24	0.67
1:1:172:SER:C	1:1:174:ASN:H	2.02	0.67
1:1:101:PHE:CE1	1:2:46:PRO:HB2	2.30	0.67
1:2:39:GLN:N	1:2:49:ILE:CD1	2.57	0.67
1:2:61:PRO:HG2	1:2:62:ASP:N	2.10	0.67
1:2:26:SER:HA	1:2:30:GLY:CA	2.21	0.66
1:1:124:PRO:CD	1:1:136:LEU:HB2	2.24	0.66
1:1:141:SER:HA	1:1:177:ALA:HB2	1.76	0.66
1:1:2:SER:HB3	1:1:100:VAL:CG1	2.26	0.66
1:2:36:SER:HA	1:2:50:ILE:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:39:GLN:CB	1:2:49:ILE:HD13	2.22	0.66
1:1:145:PRO:HB3	2:1:251:HOH:O	1.95	0.66
1:2:88:TYR:C	1:2:89:TYR:CD1	2.73	0.66
1:2:119:VAL:HG22	1:2:208:LYS:HG3	1.77	0.66
1:2:185:THR:O	1:2:187:GLU:OE1	2.13	0.66
1:2:85:GLU:CB	1:2:107:VAL:HG12	2.25	0.66
1:1:180:SER:O	2:1:317:HOH:O	2.14	0.66
1:2:85:GLU:HB3	1:2:107:VAL:HG12	1.77	0.66
1:1:57:PRO:O	1:1:60:VAL:CG1	2.44	0.66
1:1:89:TYR:HE1	1:2:45:ALA:HB2	1.59	0.66
1:1:152:TRP:CD1	2:1:292:HOH:O	2.49	0.66
1:2:198:GLN:CB	2:2:341:HOH:O	2.26	0.66
1:1:77:VAL:HG21	1:1:84:ASP:CG	2.21	0.66
1:1:160:LYS:O	1:1:160:LYS:HG3	1.96	0.66
1:2:39:GLN:NE2	1:2:88:TYR:HE2	1.91	0.66
1:2:54:ASN:HB3	1:2:66:GLY:O	1.96	0.66
1:1:41:HIS:CE1	1:1:85:GLU:C	2.74	0.65
1:1:14:LEU:O	1:1:16:GLN:N	2.29	0.65
1:2:168:PRO:CG	1:2:169:SER:N	2.60	0.65
1:2:151:ALA:HB3	1:2:198:GLN:HB3	1.77	0.65
1:1:4:LEU:CD1	1:1:22:CYS:SG	2.82	0.65
1:1:97:ASP:O	1:2:57:PRO:HB3	1.97	0.65
1:2:38:TYR:N	1:2:38:TYR:CD1	2.64	0.65
1:2:154:ALA:O	1:2:155:ASP:O	2.14	0.65
1:1:94:GLU:OE1	1:1:96:SER:HB2	1.96	0.65
1:2:2:SER:HB2	1:2:100:VAL:CG2	2.22	0.65
1:2:61:PRO:CG	1:2:62:ASP:N	2.60	0.65
1:2:93:TYR:C	1:2:95:GLY:N	2.49	0.65
1:2:130:GLN:H	1:2:130:GLN:NE2	1.91	0.65
1:2:8:PRO:HD2	1:2:9:SER:N	2.03	0.65
1:2:18:VAL:CG2	1:2:80:LEU:HD11	2.22	0.65
1:1:147:ALA:HB3	1:1:201:HIS:CE1	2.33	0.64
1:1:163:VAL:CG2	1:1:182:LEU:HB2	2.25	0.64
1:2:121:LEU:CD2	1:2:123:PRO:HD3	2.27	0.64
1:2:154:ALA:O	1:2:155:ASP:C	2.39	0.64
1:2:187:GLU:O	1:2:191:SER:CB	2.42	0.64
1:1:43:GLY:O	1:1:44:LYS:HG2	1.97	0.64
1:2:115:ALA:CB	1:2:144:TYR:H	2.10	0.64
1:1:51:TYR:CZ	1:1:55:LYS:HB3	2.32	0.64
1:1:85:GLU:CD	1:1:85:GLU:H	2.05	0.64
1:1:123:PRO:CB	1:1:210:VAL:HG11	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:THR:HA	1:1:182:LEU:O	1.97	0.64
1:1:157:SER:CB	1:1:158:PRO:CD	2.72	0.64
1:1:196:SER:HA	1:1:208:LYS:O	1.97	0.64
1:2:155:ASP:HB3	1:2:193:ARG:HG3	1.78	0.64
1:2:167:LYS:HB2	1:2:168:PRO:CD	2.28	0.64
1:1:123:PRO:HB3	1:1:210:VAL:CG1	2.24	0.64
1:1:216:SER:HB2	1:2:214:GLU:OE1	1.97	0.64
1:2:20:ILE:CD1	1:2:75:LEU:HD23	2.28	0.64
1:2:63:ARG:HD3	1:2:78:SER:O	1.97	0.64
1:2:186:PRO:O	1:2:189:TRP:CB	2.46	0.64
1:2:127:GLU:OE2	1:2:128:GLU:HB3	1.98	0.64
1:1:32:TYR:CE2	1:1:93:TYR:CE1	2.86	0.64
1:2:109:VAL:O	1:2:110:LEU:O	2.15	0.64
1:1:77:VAL:HG21	1:1:84:ASP:OD2	1.97	0.64
1:1:84:ASP:CB	1:1:107:VAL:HG11	2.15	0.64
1:1:163:VAL:HG23	1:1:182:LEU:CB	2.27	0.64
1:2:127:GLU:CG	1:2:128:GLU:N	2.61	0.64
1:2:141:SER:O	1:2:142:ASP:HB3	1.98	0.64
1:1:148:VAL:CG1	1:1:150:VAL:HG13	2.28	0.63
1:1:13:SER:C	1:1:16:GLN:HG3	2.23	0.63
1:1:207:GLU:OE2	1:1:207:GLU:CA	2.45	0.63
1:2:10:ALA:HB3	1:2:105:THR:HG23	1.80	0.63
1:2:119:VAL:HG22	1:2:208:LYS:CG	2.28	0.63
1:1:111:GLY:CA	1:1:144:TYR:HE2	2.11	0.63
1:2:33:ASN:ND2	1:2:52:GLU:HG2	2.14	0.63
1:2:199:VAL:HG23	1:2:206:VAL:O	1.97	0.63
1:1:122:PHE:HB2	1:1:137:VAL:HG13	1.80	0.63
1:1:212:PRO:O	1:1:213:THR:HB	1.98	0.63
1:2:38:TYR:HD2	2:2:240:HOH:O	1.64	0.63
1:2:185:THR:O	1:2:188:GLN:CB	2.44	0.63
1:2:16:GLN:CG	1:2:17:SER:N	2.50	0.63
1:1:194:SER:HA	2:1:335:HOH:O	1.93	0.63
1:2:198:GLN:N	2:2:341:HOH:O	2.31	0.63
1:1:139:LEU:C	1:1:140:ILE:HG12	2.22	0.62
1:2:20:ILE:CG1	1:2:75:LEU:HD23	2.29	0.62
1:2:63:ARG:HD3	1:2:78:SER:CB	2.29	0.62
1:1:20:ILE:O	1:1:74:SER:HA	1.99	0.62
1:2:20:ILE:HG21	1:2:105:THR:HG21	1.80	0.62
1:2:114:LYS:HE3	1:2:202:GLU:OE2	1.99	0.62
1:1:15:GLY:C	1:1:16:GLN:HG2	2.24	0.62
1:1:21:SER:HB2	1:1:72:THR:OG1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:127:GLU:CA	1:1:131:ALA:HB3	2.28	0.62
1:1:135:THR:CG2	1:1:181:TYR:CD1	2.82	0.62
1:2:211:ALA:CB	1:2:212:PRO:HD2	2.12	0.62
1:1:52:GLU:O	1:1:53:VAL:HG23	1.99	0.62
1:2:155:ASP:HB3	1:2:193:ARG:CB	2.28	0.62
1:1:62:ASP:OD2	1:1:62:ASP:N	2.25	0.62
1:2:77:VAL:CG2	2:2:267:HOH:O	2.43	0.62
1:2:14:LEU:HG	1:2:111:GLY:HA3	1.80	0.62
1:2:192:HIS:C	1:2:193:ARG:HG2	2.24	0.62
1:1:201:HIS:HB2	1:1:204:SER:HB2	1.80	0.61
1:2:126:SER:OG	1:2:214:GLU:HG2	1.99	0.61
1:2:192:HIS:O	1:2:193:ARG:HG2	1.99	0.61
1:1:148:VAL:HG13	1:1:149:THR:O	1.99	0.61
1:2:63:ARG:CD	1:2:78:SER:OG	2.46	0.61
1:1:171:GLN:HG2	1:1:172:SER:H	1.65	0.61
1:2:70:GLY:O	1:2:71:ASN:HB3	1.99	0.61
1:1:141:SER:HA	1:1:177:ALA:CB	2.30	0.61
1:1:166:THR:HG21	1:2:167:LYS:HD3	1.80	0.61
1:2:81:GLN:O	1:2:83:GLU:N	2.31	0.61
1:2:49:ILE:O	1:2:50:ILE:HG23	2.00	0.61
1:1:35:VAL:HG21	1:1:73:ALA:HB1	1.82	0.61
1:1:57:PRO:O	1:1:60:VAL:HG12	2.01	0.61
1:1:128:GLU:HG3	1:1:134:ALA:HA	1.82	0.61
1:1:37:TRP:HZ2	1:1:73:ALA:C	2.09	0.61
1:1:163:VAL:HA	1:1:181:TYR:O	2.00	0.61
1:2:64:PHE:CD1	1:2:77:VAL:HB	2.36	0.61
1:2:143:PHE:CE2	1:2:177:ALA:HB2	2.36	0.61
1:2:161:ALA:C	2:2:314:HOH:O	2.43	0.61
1:2:91:SER:HA	1:2:100:VAL:O	2.01	0.61
1:2:198:GLN:CA	2:2:341:HOH:O	2.48	0.61
1:1:124:PRO:HB3	1:1:128:GLU:HB3	1.83	0.60
1:1:130:GLN:OE1	2:1:217:HOH:O	2.16	0.60
1:1:164:GLU:HG3	1:1:165:THR:N	2.15	0.60
1:2:117:PRO:HG2	1:2:201:HIS:ND1	2.16	0.60
1:2:190:LYS:O	1:2:191:SER:C	2.44	0.60
1:2:107:VAL:CG1	1:2:108:THR:N	2.65	0.60
1:1:108:THR:HG22	1:1:109:VAL:H	1.66	0.60
1:1:207:GLU:OE2	1:1:207:GLU:HA	2.00	0.60
1:1:185:THR:CG2	1:1:186:PRO:HD2	2.32	0.60
1:1:189:TRP:HE3	1:1:195:TYR:HE1	1.48	0.60
1:2:196:SER:CB	1:2:209:THR:HB	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:39:GLN:HB2	1:1:49:ILE:HD13	1.83	0.60
1:1:106:LYS:HD2	1:1:106:LYS:N	2.13	0.60
1:2:143:PHE:C	1:2:175:LYS:HD3	2.27	0.60
1:1:8:PRO:O	1:1:106:LYS:CD	2.49	0.60
1:1:84:ASP:O	1:1:88:TYR:CE2	2.54	0.60
1:1:46:PRO:O	1:2:101:PHE:HZ	1.85	0.60
1:2:68:LYS:HA	1:2:73:ALA:HA	1.83	0.60
1:2:194:SER:C	2:2:308:HOH:O	2.34	0.60
1:1:6:GLN:OE1	1:1:90:CYS:HB3	2.02	0.60
1:2:136:LEU:CD1	1:2:184:LEU:HD23	2.32	0.60
1:1:26:SER:O	1:1:30:GLY:HA3	2.02	0.59
1:2:5:THR:HB	1:2:23:THR:CG2	2.32	0.59
1:1:125:SER:CA	1:2:216:SER:HA	2.31	0.59
1:2:56:ARG:HG3	1:2:60:VAL:HB	1.83	0.59
1:1:52:GLU:C	1:1:53:VAL:CG2	2.75	0.59
1:2:196:SER:HA	1:2:208:LYS:O	2.03	0.59
1:2:210:VAL:CG1	1:2:211:ALA:N	2.65	0.59
1:2:128:GLU:HG2	1:2:129:LEU:N	2.17	0.59
1:1:45:ALA:CB	2:1:263:HOH:O	2.28	0.59
1:1:52:GLU:OE1	1:1:55:LYS:HD3	2.03	0.59
1:1:145:PRO:HA	2:1:247:HOH:O	2.03	0.59
1:1:39:GLN:C	1:1:46:PRO:HA	2.27	0.59
1:1:205:THR:O	1:1:206:VAL:HG12	2.03	0.59
1:2:114:LYS:HA	1:2:144:TYR:HD1	1.66	0.59
1:1:125:SER:CB	2:1:313:HOH:O	2.47	0.59
1:2:66:GLY:HA2	1:2:74:SER:O	2.02	0.59
1:2:123:PRO:N	1:2:124:PRO:HD3	2.15	0.59
1:2:162:GLY:CA	2:2:314:HOH:O	2.47	0.58
1:1:109:VAL:O	1:1:110:LEU:HB3	2.02	0.58
1:1:52:GLU:OE1	1:1:55:LYS:CD	2.51	0.58
1:2:50:ILE:CD1	1:2:75:LEU:HD12	2.32	0.58
1:2:64:PHE:HE1	2:2:267:HOH:O	1.85	0.58
1:2:40:GLN:CG	1:2:46:PRO:HG3	2.33	0.58
1:2:61:PRO:O	1:2:62:ASP:HB2	2.02	0.58
1:1:3:ALA:O	1:1:4:LEU:C	2.46	0.58
1:1:41:HIS:HE1	1:1:83:GLU:O	1.82	0.58
1:1:149:THR:O	1:1:199:VAL:HA	2.03	0.58
1:2:88:TYR:C	1:2:89:TYR:HD1	2.11	0.58
1:2:144:TYR:N	1:2:175:LYS:HD3	2.19	0.58
1:1:135:THR:HG21	1:1:181:TYR:CE1	2.39	0.58
1:2:186:PRO:HB2	1:2:187:GLU:CG	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:49:ILE:HG13	1:1:50:ILE:HG12	1.85	0.58
1:1:143:PHE:O	1:1:175:LYS:HB3	2.04	0.58
1:1:46:PRO:O	1:2:101:PHE:CZ	2.57	0.58
1:1:113:PRO:O	1:1:144:TYR:CG	2.56	0.58
1:1:124:PRO:HD3	1:1:136:LEU:CA	2.34	0.58
1:1:5:THR:CB	1:1:23:THR:OG1	2.44	0.58
1:1:132:ASN:OD1	1:1:186:PRO:HG2	2.04	0.58
1:1:185:THR:HG22	1:1:186:PRO:HD2	1.84	0.58
1:2:133:LYS:HA	1:2:186:PRO:CD	2.34	0.58
1:1:128:GLU:HG3	1:1:134:ALA:CA	2.33	0.57
1:2:122:PHE:HE2	1:2:139:LEU:CD2	2.17	0.57
1:1:211:ALA:HB2	2:1:335:HOH:O	2.05	0.57
1:2:32:TYR:CE1	1:2:34:TYR:HE1	2.23	0.57
1:1:34:TYR:CB	1:1:93:TYR:HB3	2.32	0.57
1:1:135:THR:HG21	1:1:181:TYR:HE1	1.69	0.57
1:1:189:TRP:HE3	1:1:195:TYR:CE1	2.23	0.57
1:2:189:TRP:O	1:2:192:HIS:N	2.36	0.57
1:1:6:GLN:OE1	1:1:90:CYS:CB	2.53	0.57
1:2:29:VAL:O	1:2:71:ASN:HA	2.05	0.57
1:2:188:GLN:O	1:2:192:HIS:CG	2.58	0.57
1:2:14:LEU:HD23	1:2:111:GLY:O	2.04	0.57
1:2:186:PRO:HB2	1:2:187:GLU:CD	2.30	0.57
1:1:77:VAL:CB	1:1:84:ASP:OD2	2.52	0.57
1:2:136:LEU:HD23	1:2:189:TRP:NE1	2.18	0.57
1:2:111:GLY:O	1:2:112:GLN:HG2	2.03	0.57
1:1:39:GLN:O	1:1:46:PRO:HA	2.04	0.56
1:2:63:ARG:CG	1:2:78:SER:OG	2.53	0.56
1:1:89:TYR:CE1	1:2:45:ALA:CB	2.87	0.56
1:1:162:GLY:O	1:1:182:LEU:HD12	2.06	0.56
1:1:168:PRO:CB	1:1:178:ALA:HB2	2.21	0.56
1:2:90:CYS:O	1:2:101:PHE:CA	2.51	0.56
1:2:106:LYS:HE3	2:2:272:HOH:O	2.03	0.56
1:2:123:PRO:CD	1:2:124:PRO:CD	2.82	0.56
1:2:189:TRP:HE3	1:2:190:LYS:N	2.02	0.56
1:1:124:PRO:HD2	1:1:136:LEU:HG	1.86	0.56
1:1:154:ALA:HB2	1:1:159:VAL:HB	1.87	0.56
1:1:170:LYS:NZ	1:1:171:GLN:O	2.33	0.56
1:2:112:GLN:CD	2:2:321:HOH:O	2.48	0.56
1:1:166:THR:CG2	1:2:167:LYS:CD	2.82	0.56
1:2:119:VAL:HG22	1:2:208:LYS:CD	2.35	0.56
1:2:201:HIS:CD2	1:2:202:GLU:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:143:PHE:O	1:2:143:PHE:CD1	2.59	0.56
1:2:152:TRP:CE3	1:2:182:LEU:HD13	2.41	0.56
1:1:52:GLU:O	1:1:53:VAL:CG2	2.52	0.56
1:2:201:HIS:O	1:2:204:SER:O	2.23	0.56
1:1:124:PRO:HB3	1:1:128:GLU:HB2	1.88	0.55
1:2:14:LEU:CG	1:2:111:GLY:HA3	2.36	0.55
1:2:118:THR:CG2	1:2:141:SER:HB3	2.36	0.55
1:2:2:SER:C	1:2:100:VAL:HG21	2.29	0.55
1:2:137:VAL:HG21	2:2:252:HOH:O	2.05	0.55
1:2:165:THR:HG22	1:2:166:THR:N	2.20	0.55
1:1:98:ASN:CG	1:1:99:PHE:H	2.15	0.55
1:1:144:TYR:HB3	1:1:145:PRO:HD3	1.88	0.55
1:1:187:GLU:O	1:1:189:TRP:N	2.39	0.55
1:1:3:ALA:O	1:1:4:LEU:O	2.25	0.55
1:1:120:THR:HA	1:1:208:LYS:HE2	1.88	0.55
1:1:127:GLU:C	1:1:131:ALA:HB3	2.30	0.55
1:2:106:LYS:CE	2:2:272:HOH:O	2.54	0.55
1:1:124:PRO:HG2	1:1:128:GLU:OE2	2.06	0.55
1:2:118:THR:HG22	1:2:142:ASP:N	2.22	0.55
1:2:128:GLU:OE2	1:2:129:LEU:HB2	2.07	0.55
1:2:140:ILE:HD11	1:2:143:PHE:CE2	2.41	0.55
1:1:41:HIS:ND1	1:1:86:ALA:HB2	2.22	0.55
1:1:92:SER:HG	1:1:100:VAL:CB	2.14	0.55
1:1:93:TYR:HA	1:1:99:PHE:CD2	2.41	0.55
1:1:201:HIS:HB3	1:1:202:GLU:OE1	2.06	0.55
1:2:141:SER:O	1:2:142:ASP:CB	2.54	0.55
1:1:2:SER:OG	1:1:3:ALA:N	2.37	0.55
1:2:10:ALA:HB2	1:2:105:THR:HG23	1.88	0.55
1:2:68:LYS:HB2	1:2:73:ALA:CB	2.37	0.55
1:2:85:GLU:HG2	1:2:106:LYS:HZ1	1.71	0.55
1:2:125:SER:HA	2:2:351:HOH:O	2.05	0.55
1:1:134:ALA:HB3	1:1:184:LEU:C	2.27	0.55
1:1:154:ALA:HB2	1:1:159:VAL:CG1	2.36	0.55
1:2:125:SER:OG	1:2:127:GLU:OE1	2.22	0.55
1:2:18:VAL:HG23	1:2:80:LEU:CD1	2.28	0.55
1:2:129:LEU:HD11	1:2:189:TRP:CG	2.40	0.55
1:1:44:LYS:CG	1:1:45:ALA:N	2.70	0.55
1:1:201:HIS:CB	1:1:204:SER:HB2	2.36	0.54
1:2:114:LYS:HG3	1:2:145:PRO:HG2	1.89	0.54
1:2:126:SER:HB3	2:2:355:HOH:O	2.03	0.54
1:1:126:SER:HB3	1:2:216:SER:OXT	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:112:GLN:NE2	2:2:321:HOH:O	2.39	0.54
1:2:190:LYS:C	1:2:192:HIS:H	2.14	0.54
1:2:35:VAL:HG22	1:2:92:SER:HB2	1.89	0.54
1:2:155:ASP:HB3	1:2:193:ARG:CG	2.37	0.54
1:1:111:GLY:HA3	1:1:144:TYR:CE2	2.36	0.54
1:2:51:TYR:CD1	1:2:57:PRO:HD3	2.42	0.54
1:2:87:ASP:CB	1:2:89:TYR:HE1	2.17	0.54
1:2:192:HIS:O	1:2:193:ARG:CG	2.56	0.54
1:1:18:VAL:HG23	1:1:19:THR:N	2.23	0.54
1:1:136:LEU:HD11	1:1:195:TYR:CE1	2.42	0.54
1:2:144:TYR:N	1:2:145:PRO:CD	2.71	0.54
1:1:165:THR:CG2	1:1:179:SER:O	2.55	0.54
1:1:37:TRP:HB2	1:1:50:ILE:HG13	1.89	0.54
1:2:35:VAL:HA	1:2:91:SER:O	2.08	0.54
1:1:140:ILE:O	1:1:177:ALA:HA	2.08	0.54
1:1:87:ASP:OD1	1:1:106:LYS:NZ	2.41	0.53
1:2:16:GLN:CG	1:2:17:SER:H	2.16	0.53
1:2:114:LYS:HG3	1:2:145:PRO:CG	2.39	0.53
1:1:143:PHE:HD1	1:1:176:TYR:O	1.91	0.53
1:1:168:PRO:HB3	1:1:178:ALA:CB	2.22	0.53
1:2:13:SER:OG	1:2:14:LEU:N	2.35	0.53
1:2:32:TYR:CE1	1:2:34:TYR:CE1	2.96	0.53
1:2:144:TYR:C	1:2:144:TYR:CD2	2.85	0.53
1:1:202:GLU:CD	1:1:202:GLU:H	2.17	0.53
1:2:144:TYR:CD2	1:2:144:TYR:O	2.62	0.53
1:2:123:PRO:CG	1:2:124:PRO:HD3	2.38	0.53
1:2:139:LEU:N	1:2:139:LEU:HD12	2.24	0.53
1:1:117:PRO:CG	2:1:303:HOH:O	2.56	0.53
1:2:2:SER:CB	1:2:100:VAL:HG21	2.28	0.53
1:1:121:LEU:CG	1:1:210:VAL:CG2	2.74	0.53
1:1:130:GLN:C	1:1:132:ASN:N	2.49	0.53
1:1:135:THR:CG2	1:1:181:TYR:HE1	2.19	0.53
1:2:37:TRP:HA	1:2:89:TYR:O	2.08	0.53
1:1:49:ILE:CG1	1:1:50:ILE:HG12	2.38	0.53
1:1:116:ASN:HB3	1:1:117:PRO:HD2	1.91	0.53
1:1:128:GLU:CG	1:1:134:ALA:HA	2.39	0.53
1:2:37:TRP:C	1:2:38:TYR:CD1	2.87	0.53
1:2:106:LYS:HG3	1:2:107:VAL:N	2.23	0.53
1:1:40:GLN:HG2	1:1:46:PRO:HB3	1.91	0.52
1:1:91:SER:OG	1:1:91:SER:O	2.18	0.52
1:1:112:GLN:CB	1:1:113:PRO:CD	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:127:GLU:CG	1:1:128:GLU:N	2.73	0.52
1:2:4:LEU:CB	1:2:102:GLY:CA	2.75	0.52
1:1:41:HIS:O	1:1:42:ALA:CB	2.56	0.52
1:1:137:VAL:CG1	1:2:122:PHE:CD2	2.92	0.52
1:2:48:VAL:HB	2:2:248:HOH:O	2.09	0.52
1:2:96:SER:HA	2:2:277:HOH:O	2.09	0.52
1:2:121:LEU:HD21	1:2:123:PRO:HD3	1.91	0.52
1:2:125:SER:HB3	1:2:127:GLU:CD	2.34	0.52
1:1:195:TYR:O	1:1:209:THR:HA	2.10	0.52
1:2:113:PRO:C	1:2:114:LYS:O	2.51	0.52
1:1:133:LYS:HE2	1:2:120:THR:CG2	2.39	0.52
1:2:93:TYR:O	1:2:94:GLU:C	2.52	0.52
1:1:93:TYR:HB2	1:1:99:PHE:CZ	2.44	0.52
1:2:100:VAL:HG22	1:2:101:PHE:N	2.24	0.52
1:1:166:THR:HG22	1:2:167:LYS:HD3	1.90	0.52
1:2:121:LEU:HA	1:2:137:VAL:O	2.10	0.52
1:2:133:LYS:HG2	1:2:134:ALA:N	2.23	0.52
1:2:134:ALA:HB2	2:2:299:HOH:O	2.08	0.52
1:1:108:THR:HG22	1:1:109:VAL:N	2.25	0.52
1:1:144:TYR:HD1	1:1:175:LYS:HA	1.75	0.52
1:2:114:LYS:HA	1:2:144:TYR:CD1	2.45	0.52
1:2:121:LEU:C	1:2:121:LEU:CD2	2.71	0.52
1:2:155:ASP:HB3	1:2:193:ARG:HB2	1.91	0.52
1:1:157:SER:HB2	1:1:158:PRO:HD2	1.89	0.52
1:2:171:GLN:HG3	1:2:175:LYS:H	1.73	0.52
1:1:89:TYR:HE1	1:1:102:GLY:O	1.92	0.51
1:1:189:TRP:CE3	1:1:195:TYR:HE1	2.28	0.51
1:1:198:GLN:HB3	1:1:207:GLU:CD	2.35	0.51
1:2:28:ASP:CG	1:2:92:SER:OG	2.52	0.51
1:2:44:LYS:O	1:2:45:ALA:HB3	2.10	0.51
1:2:83:GLU:C	1:2:173:ASN:HD21	2.18	0.51
1:2:136:LEU:CD2	2:2:292:HOH:O	2.58	0.51
1:2:210:VAL:HG13	1:2:211:ALA:N	2.26	0.51
1:1:173:ASN:O	1:1:174:ASN:CB	2.57	0.51
1:2:28:ASP:OD1	1:2:92:SER:CB	2.50	0.51
1:2:195:TYR:HA	2:2:308:HOH:O	2.09	0.51
1:2:114:LYS:NZ	1:2:202:GLU:HG3	2.25	0.51
1:2:143:PHE:HE2	1:2:177:ALA:CB	2.24	0.51
1:1:29:VAL:HG22	1:1:35:VAL:CG1	2.39	0.51
1:2:28:ASP:CG	1:2:92:SER:HB3	2.36	0.51
1:2:56:ARG:HG2	1:2:56:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:122:PHE:CE2	1:2:139:LEU:CD1	2.93	0.51
1:1:106:LYS:NZ	1:1:106:LYS:HB3	2.25	0.51
1:2:19:THR:HG22	1:2:76:THR:HB	1.90	0.51
1:2:86:ALA:CB	2:2:241:HOH:O	2.58	0.51
1:1:41:HIS:CE1	1:1:85:GLU:O	2.63	0.51
1:2:61:PRO:CD	1:2:62:ASP:H	2.23	0.51
1:1:52:GLU:OE1	1:1:55:LYS:HE3	2.11	0.51
1:2:115:ALA:HB3	1:2:175:LYS:HD3	1.92	0.51
1:1:64:PHE:HE2	2:1:243:HOH:O	1.93	0.51
1:1:97:ASP:O	1:1:98:ASN:HB2	2.11	0.51
1:2:41:HIS:CE1	1:2:83:GLU:OE2	2.63	0.51
1:1:37:TRP:HB2	1:1:50:ILE:CG1	2.41	0.51
1:1:97:ASP:HB3	1:2:57:PRO:CB	2.41	0.51
1:2:190:LYS:O	1:2:192:HIS:N	2.44	0.51
1:1:19:THR:HA	1:1:75:LEU:O	2.11	0.51
1:1:101:PHE:CE1	1:2:46:PRO:HD2	2.46	0.51
1:1:172:SER:C	1:1:174:ASN:N	2.69	0.51
1:2:62:ASP:O	1:2:64:PHE:N	2.36	0.51
1:2:128:GLU:CG	1:2:129:LEU:H	2.23	0.51
1:2:135:THR:HB	1:2:183:SER:HA	1.92	0.51
1:1:119:VAL:O	1:1:120:THR:HG23	2.10	0.50
1:2:134:ALA:CB	2:2:299:HOH:O	2.59	0.50
1:1:164:GLU:CG	1:1:165:THR:N	2.74	0.50
1:2:170:LYS:HA	1:2:170:LYS:NZ	2.26	0.50
1:1:28:ASP:C	1:1:30:GLY:H	2.19	0.50
1:1:166:THR:HG22	1:2:167:LYS:CD	2.40	0.50
1:2:137:VAL:CG1	2:2:252:HOH:O	2.16	0.50
1:2:162:GLY:N	2:2:314:HOH:O	2.45	0.50
1:2:14:LEU:CD2	1:2:111:GLY:CA	2.88	0.50
1:2:114:LYS:CA	1:2:144:TYR:HD1	2.24	0.50
1:2:143:PHE:O	1:2:143:PHE:CG	2.65	0.50
1:1:127:GLU:HB2	1:1:133:LYS:HZ3	1.77	0.50
1:2:4:LEU:O	1:2:102:GLY:HA2	2.11	0.50
1:2:86:ALA:CA	1:2:106:LYS:HB2	2.39	0.50
1:2:155:ASP:CB	1:2:193:ARG:HB2	2.42	0.50
1:2:118:THR:HG23	1:2:141:SER:HB3	1.94	0.50
1:1:127:GLU:OE1	1:2:122:PHE:CZ	2.60	0.50
1:2:13:SER:O	1:2:109:VAL:HG23	2.12	0.50
1:2:50:ILE:CD1	1:2:75:LEU:CD1	2.86	0.50
1:2:63:ARG:CD	1:2:78:SER:O	2.60	0.50
1:2:128:GLU:HB2	1:2:134:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:215:CYS:O	1:2:215:CYS:SG	2.69	0.50
1:2:28:ASP:CG	1:2:92:SER:CB	2.85	0.49
1:1:8:PRO:HG2	1:1:9:SER:H	1.77	0.49
1:1:126:SER:N	1:2:216:SER:OXT	2.46	0.49
1:2:32:TYR:HE1	1:2:34:TYR:CE1	2.30	0.49
1:2:122:PHE:HE2	1:2:139:LEU:HD21	1.76	0.49
1:2:133:LYS:HA	1:2:186:PRO:HD2	1.94	0.49
1:1:14:LEU:O	1:1:16:GLN:CB	2.61	0.49
1:1:80:LEU:HD23	1:1:84:ASP:H	1.77	0.49
1:1:97:ASP:HB3	1:2:57:PRO:HB3	1.93	0.49
1:1:133:LYS:HE2	1:2:120:THR:HG22	1.92	0.49
1:1:168:PRO:C	1:1:169:SER:OG	2.55	0.49
1:2:14:LEU:CD2	1:2:111:GLY:O	2.61	0.49
1:2:92:SER:OG	1:2:93:TYR:N	2.40	0.49
1:2:122:PHE:C	1:2:124:PRO:HD2	2.38	0.49
1:2:127:GLU:CA	1:2:130:GLN:HE22	2.25	0.49
1:2:133:LYS:CB	1:2:185:THR:HA	2.43	0.49
1:2:192:HIS:O	1:2:193:ARG:CB	2.60	0.49
1:2:37:TRP:CD1	1:2:50:ILE:HG12	2.48	0.49
1:2:57:PRO:O	1:2:58:SER:C	2.55	0.49
1:2:155:ASP:CB	1:2:193:ARG:CB	2.90	0.49
1:2:94:GLU:OE1	1:2:100:VAL:CG1	2.57	0.49
1:2:113:PRO:O	1:2:114:LYS:O	2.31	0.49
1:2:128:GLU:CG	1:2:129:LEU:N	2.75	0.49
1:2:155:ASP:O	1:2:155:ASP:CG	2.54	0.49
1:1:184:LEU:HD21	2:1:291:HOH:O	2.12	0.48
1:2:20:ILE:HG13	1:2:37:TRP:CZ3	2.48	0.48
1:2:133:LYS:HB2	1:2:185:THR:HA	1.95	0.48
1:1:137:VAL:HA	1:1:181:TYR:HB2	1.94	0.48
1:2:32:TYR:HE1	1:2:34:TYR:HE1	1.59	0.48
1:2:111:GLY:O	1:2:112:GLN:CG	2.61	0.48
1:1:159:VAL:HG22	1:1:160:LYS:N	2.28	0.48
1:1:193:ARG:HG2	1:1:193:ARG:HH21	1.78	0.48
1:2:117:PRO:HG3	1:2:143:PHE:CB	2.43	0.48
1:1:49:ILE:HA	1:1:60:VAL:HG21	1.95	0.48
1:1:205:THR:HG22	2:1:337:HOH:O	2.12	0.48
1:2:152:TRP:CE2	1:2:182:LEU:HD13	2.48	0.48
1:1:186:PRO:O	1:1:189:TRP:CB	2.60	0.48
1:2:51:TYR:CD2	1:2:55:LYS:HB2	2.48	0.48
1:2:96:SER:O	1:2:97:ASP:C	2.57	0.48
1:1:96:SER:C	1:1:98:ASN:N	2.64	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:175:LYS:O	1:1:176:TYR:CG	2.67	0.48
1:1:186:PRO:O	1:1:189:TRP:CA	2.62	0.48
1:2:183:SER:CB	2:2:316:HOH:O	2.43	0.48
1:2:64:PHE:CE1	1:2:77:VAL:HB	2.48	0.48
1:2:115:ALA:CB	1:2:175:LYS:HD3	2.43	0.48
1:2:113:PRO:O	1:2:114:LYS:C	2.57	0.48
1:2:129:LEU:CD1	1:2:189:TRP:HB3	2.36	0.48
1:1:108:THR:O	1:1:109:VAL:HB	2.14	0.48
1:2:118:THR:CG2	1:2:142:ASP:H	2.26	0.47
1:1:116:ASN:OD1	1:1:116:ASN:N	2.47	0.47
1:2:140:ILE:CG1	1:2:143:PHE:CE2	2.97	0.47
1:1:124:PRO:HG3	1:1:135:THR:N	2.28	0.47
1:1:127:GLU:HG3	1:1:128:GLU:N	2.28	0.47
1:2:148:VAL:HB	1:2:201:HIS:HB2	1.96	0.47
1:2:187:GLU:HA	1:2:191:SER:H	1.79	0.47
1:2:188:GLN:O	1:2:192:HIS:ND1	2.47	0.47
1:1:38:TYR:CE1	1:1:48:VAL:HG22	2.50	0.47
1:1:42:ALA:CB	2:1:261:HOH:O	2.45	0.47
1:1:109:VAL:HA	2:1:272:HOH:O	2.14	0.47
1:1:155:ASP:HA	1:1:194:SER:OG	2.15	0.47
1:2:36:SER:O	1:2:90:CYS:HA	2.15	0.47
1:2:114:LYS:HA	1:2:144:TYR:HB3	1.96	0.47
1:1:80:LEU:C	1:1:80:LEU:CD2	2.87	0.47
1:2:18:VAL:N	1:2:80:LEU:HD11	2.29	0.47
1:2:100:VAL:HG22	1:2:101:PHE:H	1.78	0.47
1:2:136:LEU:HD23	2:2:292:HOH:O	2.15	0.47
1:2:187:GLU:CD	1:2:187:GLU:N	2.70	0.47
1:1:13:SER:O	1:1:14:LEU:C	2.58	0.47
1:1:18:VAL:O	1:1:76:THR:HA	2.14	0.47
1:1:40:GLN:HB2	1:1:43:GLY:HA2	1.97	0.47
1:1:157:SER:C	1:1:158:PRO:O	2.55	0.47
1:2:26:SER:CB	1:2:30:GLY:HA3	2.45	0.47
1:2:122:PHE:HE2	1:2:139:LEU:CD1	2.28	0.47
1:1:34:TYR:CD2	1:1:93:TYR:CG	3.03	0.46
1:2:4:LEU:HB2	1:2:101:PHE:C	2.40	0.46
1:2:65:SER:O	1:2:75:LEU:CG	2.63	0.46
1:2:117:PRO:HA	1:2:143:PHE:HB3	1.97	0.46
1:2:188:GLN:C	1:2:192:HIS:ND1	2.73	0.46
1:1:28:ASP:HA	1:1:32:TYR:CB	2.36	0.46
1:1:35:VAL:CG2	1:1:37:TRP:HE1	2.29	0.46
1:1:89:TYR:CE1	1:1:102:GLY:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:113:PRO:O	1:1:144:TYR:HD2	1.88	0.46
1:2:16:GLN:HG2	1:2:17:SER:CB	2.46	0.46
1:1:14:LEU:O	1:1:16:GLN:CG	2.63	0.46
1:1:77:VAL:CG2	1:1:84:ASP:OD2	2.61	0.46
1:1:189:TRP:CE3	1:1:195:TYR:CE1	3.01	0.46
1:2:45:ALA:HA	1:2:46:PRO:HD3	1.76	0.46
1:2:131:ALA:O	1:2:132:ASN:CG	2.59	0.46
1:2:147:ALA:C	1:2:148:VAL:HG12	2.40	0.46
1:1:93:TYR:HA	1:1:99:PHE:CG	2.50	0.46
1:1:94:GLU:OE1	1:1:96:SER:CB	2.63	0.46
1:2:121:LEU:CG	1:2:123:PRO:HD3	2.45	0.46
1:2:34:TYR:HA	1:2:52:GLU:HA	1.98	0.46
1:2:122:PHE:C	1:2:124:PRO:CD	2.89	0.46
1:2:143:PHE:HA	1:2:175:LYS:HD3	1.97	0.46
1:2:162:GLY:O	1:2:163:VAL:HB	2.15	0.46
1:2:186:PRO:O	1:2:189:TRP:N	2.48	0.46
1:2:197:CYS:C	2:2:341:HOH:O	2.58	0.46
1:1:28:ASP:C	1:1:30:GLY:N	2.73	0.46
1:1:163:VAL:CB	1:1:182:LEU:HB2	2.45	0.46
1:1:167:LYS:HG3	1:1:168:PRO:HD2	1.98	0.46
1:1:184:LEU:HD13	1:1:184:LEU:HA	1.51	0.46
1:1:84:ASP:HA	1:1:88:TYR:OH	2.16	0.46
1:1:98:ASN:O	1:1:99:PHE:HB2	2.16	0.46
1:1:113:PRO:HD2	1:1:144:TYR:CZ	2.51	0.46
1:1:136:LEU:HD23	1:1:210:VAL:HG23	1.97	0.46
1:1:144:TYR:CD1	1:1:175:LYS:HA	2.50	0.46
1:2:4:LEU:HA	1:2:4:LEU:HD12	1.51	0.46
1:2:162:GLY:C	1:2:163:VAL:HG12	2.39	0.46
1:1:41:HIS:ND1	1:1:85:GLU:O	2.49	0.46
1:2:49:ILE:O	1:2:50:ILE:HG22	2.15	0.46
1:2:125:SER:HB2	2:2:356:HOH:O	2.15	0.46
1:2:81:GLN:CD	1:2:81:GLN:N	2.75	0.46
1:2:122:PHE:CE2	1:2:139:LEU:HD11	2.51	0.46
1:2:136:LEU:HB3	1:2:152:TRP:HZ3	1.80	0.46
1:2:186:PRO:O	1:2:189:TRP:CA	2.64	0.46
1:2:56:ARG:CG	1:2:60:VAL:HG21	2.42	0.45
1:2:144:TYR:CA	1:2:175:LYS:HG2	2.43	0.45
1:2:153:LYS:HD2	1:2:156:GLY:CA	2.44	0.45
1:1:51:TYR:HE1	1:1:52:GLU:OE1	1.99	0.45
1:1:186:PRO:O	1:1:189:TRP:N	2.49	0.45
1:2:95:GLY:O	1:2:97:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:184:LEU:HG	1:2:195:TYR:CZ	2.50	0.45
1:1:4:LEU:HD22	1:1:24:GLY:HA2	1.98	0.45
1:1:68:LYS:CG	2:1:260:HOH:O	2.43	0.45
1:1:127:GLU:O	1:1:131:ALA:CB	2.59	0.45
1:1:181:TYR:CD2	1:2:139:LEU:HD23	2.51	0.45
1:2:201:HIS:CG	2:2:260:HOH:O	2.69	0.45
1:1:101:PHE:HE1	1:2:46:PRO:HB2	1.77	0.45
1:2:41:HIS:O	1:2:43:GLY:N	2.49	0.45
1:2:174:ASN:O	1:2:175:LYS:HG3	2.16	0.45
1:2:69:SER:O	1:2:71:ASN:N	2.50	0.45
1:2:90:CYS:O	1:2:101:PHE:CB	2.64	0.45
1:1:128:GLU:OE1	1:1:189:TRP:HD1	1.92	0.45
1:1:138:CYS:N	2:1:317:HOH:O	2.49	0.45
1:2:126:SER:HB2	1:2:215:CYS:CA	2.47	0.45
1:1:157:SER:CB	1:1:158:PRO:HD3	2.30	0.45
1:2:107:VAL:HG11	1:2:109:VAL:HB	1.98	0.45
1:1:49:ILE:HD12	1:1:64:PHE:CE1	2.51	0.45
1:1:56:ARG:HH21	1:1:56:ARG:CG	2.00	0.45
1:1:184:LEU:CD2	2:1:291:HOH:O	2.65	0.45
1:1:204:SER:O	1:1:205:THR:HB	2.17	0.45
1:2:14:LEU:HD21	1:2:111:GLY:CA	2.47	0.45
1:1:40:GLN:CD	1:1:46:PRO:HG3	2.42	0.45
1:1:123:PRO:O	1:1:123:PRO:HG2	2.15	0.45
1:1:37:TRP:CZ2	1:1:73:ALA:C	2.92	0.44
1:2:171:GLN:HG3	1:2:175:LYS:O	2.17	0.44
1:1:125:SER:C	1:2:216:SER:C	2.84	0.44
1:2:185:THR:O	1:2:188:GLN:N	2.50	0.44
1:2:50:ILE:HD12	1:2:50:ILE:HG21	1.71	0.44
1:2:136:LEU:O	1:2:181:TYR:HA	2.18	0.44
1:1:29:VAL:HG22	1:1:35:VAL:HG12	1.99	0.44
1:1:140:ILE:HG13	1:1:178:ALA:O	2.17	0.44
1:2:23:THR:HA	1:2:71:ASN:O	2.17	0.44
1:2:121:LEU:HG	1:2:123:PRO:HD3	1.98	0.44
1:1:143:PHE:CE1	1:1:177:ALA:HA	2.52	0.44
1:1:152:TRP:NE1	2:1:292:HOH:O	2.50	0.44
1:1:153:LYS:HG3	1:1:196:SER:HG	1.80	0.44
1:2:1:PCA:N	2:2:217:HOH:O	2.46	0.44
1:2:187:GLU:OE1	1:2:188:GLN:HB2	2.17	0.44
1:1:44:LYS:C	1:1:46:PRO:HD3	2.43	0.44
1:1:62:ASP:HB2	2:1:244:HOH:O	2.18	0.44
1:1:69:SER:HB3	1:1:72:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:202:GLU:CB	2:1:299:HOH:O	2.65	0.44
1:2:10:ALA:HB3	1:2:105:THR:CG2	2.47	0.44
1:2:32:TYR:CE1	1:2:93:TYR:HD2	2.36	0.44
1:1:143:PHE:HE2	1:1:148:VAL:HG23	1.78	0.44
1:1:154:ALA:HB2	1:1:159:VAL:CB	2.48	0.44
1:2:114:LYS:N	1:2:144:TYR:HD1	2.16	0.44
1:2:129:LEU:HD22	1:2:129:LEU:HA	1.74	0.44
1:1:29:VAL:HG22	1:1:35:VAL:HG11	2.00	0.44
1:1:52:GLU:OE1	1:1:55:LYS:CE	2.66	0.44
1:1:127:GLU:HB2	1:1:133:LYS:NZ	2.32	0.44
1:2:66:GLY:CA	1:2:75:LEU:HA	2.43	0.44
1:2:189:TRP:O	1:2:192:HIS:CB	2.61	0.44
1:1:14:LEU:O	1:1:16:GLN:HB2	2.17	0.43
1:1:35:VAL:HG23	1:1:37:TRP:NE1	2.33	0.43
1:1:80:LEU:CD2	1:1:84:ASP:HB2	2.47	0.43
1:2:41:HIS:O	1:2:42:ALA:C	2.61	0.43
1:1:136:LEU:HD23	1:1:210:VAL:CG2	2.48	0.43
1:1:159:VAL:CG2	1:1:160:LYS:N	2.80	0.43
1:2:8:PRO:CG	1:2:9:SER:N	2.81	0.43
1:2:192:HIS:HB2	1:2:195:TYR:HE1	1.83	0.43
1:2:19:THR:CG2	1:2:76:THR:HB	2.48	0.43
1:2:86:ALA:O	1:2:106:LYS:CA	2.59	0.43
1:2:181:TYR:C	1:2:182:LEU:HD12	2.43	0.43
1:2:65:SER:O	1:2:75:LEU:HD12	2.17	0.43
1:2:127:GLU:CA	1:2:130:GLN:NE2	2.80	0.43
1:2:20:ILE:CG2	1:2:105:THR:CG2	2.93	0.43
1:2:147:ALA:H	1:2:148:VAL:HG12	1.83	0.43
1:1:92:SER:HG	1:1:100:VAL:CA	2.31	0.43
1:2:187:GLU:OE1	1:2:187:GLU:N	2.52	0.43
1:1:22:CYS:HB3	1:1:73:ALA:HB3	2.00	0.43
1:2:62:ASP:C	1:2:64:PHE:H	2.26	0.43
1:2:131:ALA:O	1:2:132:ASN:ND2	2.51	0.43
1:2:189:TRP:HE3	1:2:189:TRP:C	2.26	0.43
1:1:101:PHE:CD1	1:2:46:PRO:HD2	2.53	0.43
1:1:137:VAL:O	1:1:137:VAL:HG22	2.13	0.43
1:2:20:ILE:HG22	1:2:105:THR:OG1	2.19	0.43
1:2:40:GLN:HB3	1:2:46:PRO:CG	2.37	0.43
1:2:175:LYS:HB3	1:2:176:TYR:H	1.51	0.43
1:2:196:SER:CB	1:2:209:THR:CA	2.96	0.43
1:2:210:VAL:HG13	1:2:211:ALA:H	1.84	0.43
1:1:157:SER:O	1:1:158:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:20:ILE:O	1:2:74:SER:HA	2.18	0.43
1:2:50:ILE:CD1	1:2:66:GLY:HA3	2.49	0.43
1:2:51:TYR:CE2	1:2:55:LYS:HB2	2.54	0.43
1:2:61:PRO:HD2	1:2:64:PHE:HB2	2.01	0.43
1:2:171:GLN:CG	1:2:175:LYS:O	2.66	0.43
1:1:124:PRO:CD	1:1:136:LEU:HG	2.49	0.43
1:1:125:SER:C	1:2:216:SER:HA	2.43	0.43
1:2:56:ARG:NE	1:2:60:VAL:HG11	2.33	0.43
1:2:89:TYR:CD1	1:2:89:TYR:N	2.87	0.43
1:2:101:PHE:CG	2:2:274:HOH:O	2.70	0.43
1:2:137:VAL:HA	1:2:180:SER:O	2.18	0.43
1:1:202:GLU:HB3	2:1:299:HOH:O	2.18	0.42
1:2:68:LYS:O	1:2:68:LYS:HG2	2.19	0.42
1:2:160:LYS:NZ	2:2:310:HOH:O	2.47	0.42
1:2:18:VAL:O	1:2:76:THR:HA	2.19	0.42
1:2:136:LEU:CB	1:2:152:TRP:HZ3	2.32	0.42
1:1:62:ASP:O	1:1:63:ARG:CB	2.39	0.42
1:1:122:PHE:CD2	1:2:122:PHE:O	2.73	0.42
1:1:148:VAL:HG12	1:1:150:VAL:HG13	1.98	0.42
1:2:81:GLN:CD	1:2:81:GLN:H	2.26	0.42
1:2:117:PRO:HG3	1:2:143:PHE:HB2	2.00	0.42
1:2:11:SER:HA	1:2:108:THR:O	2.19	0.42
1:2:20:ILE:HG12	1:2:75:LEU:HD23	2.01	0.42
1:2:110:LEU:HD23	1:2:110:LEU:HA	1.62	0.42
1:2:120:THR:O	1:2:139:LEU:HD13	2.19	0.42
1:2:152:TRP:HE1	1:2:180:SER:CB	2.32	0.42
1:2:202:GLU:C	1:2:204:SER:H	2.27	0.42
1:1:97:ASP:O	1:1:98:ASN:CB	2.67	0.42
1:1:185:THR:HG22	1:1:186:PRO:CD	2.47	0.42
1:2:56:ARG:NH2	1:2:56:ARG:CG	2.78	0.42
1:2:85:GLU:HB2	1:2:107:VAL:CB	2.50	0.42
1:2:116:ASN:O	1:2:142:ASP:O	2.38	0.42
1:2:127:GLU:HA	1:2:130:GLN:NE2	2.35	0.42
1:2:36:SER:OG	1:2:38:TYR:CZ	2.69	0.42
1:2:170:LYS:HD3	1:2:171:GLN:O	2.19	0.42
1:2:42:ALA:N	2:2:241:HOH:O	2.36	0.42
1:2:136:LEU:HD12	1:2:182:LEU:C	2.45	0.42
1:2:142:ASP:C	1:2:143:PHE:CD2	2.98	0.42
1:2:185:THR:O	1:2:186:PRO:C	2.63	0.42
1:2:77:VAL:HG11	2:2:265:HOH:O	2.20	0.42
1:2:136:LEU:CD2	1:2:189:TRP:CE2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:157:SER:O	1:1:158:PRO:O	2.38	0.41
1:2:4:LEU:HB2	1:2:102:GLY:N	2.31	0.41
1:2:14:LEU:C	1:2:14:LEU:HD12	2.44	0.41
1:2:50:ILE:HD11	1:2:66:GLY:HA3	2.02	0.41
1:2:37:TRP:O	1:2:49:ILE:HG13	2.20	0.41
1:2:196:SER:HB3	1:2:209:THR:CA	2.49	0.41
1:2:119:VAL:O	1:2:120:THR:CG2	2.68	0.41
1:2:132:ASN:O	1:2:186:PRO:CG	2.67	0.41
1:2:183:SER:O	1:2:184:LEU:C	2.63	0.41
1:1:127:GLU:O	1:1:131:ALA:C	2.63	0.41
1:1:128:GLU:CD	1:1:189:TRP:CD1	2.96	0.41
1:2:14:LEU:HD21	1:2:111:GLY:HA3	2.02	0.41
1:2:96:SER:C	1:2:97:ASP:OD1	2.63	0.41
1:1:40:GLN:CB	1:1:46:PRO:HB3	2.50	0.41
1:1:141:SER:HB2	2:1:318:HOH:O	2.20	0.41
1:1:167:LYS:CG	1:1:168:PRO:CD	2.98	0.41
1:1:52:GLU:HB2	1:1:55:LYS:HD3	1.98	0.41
1:1:125:SER:C	1:2:216:SER:CA	2.93	0.41
1:2:4:LEU:O	1:2:102:GLY:CA	2.68	0.41
1:2:136:LEU:CD1	1:2:184:LEU:CD2	2.98	0.41
1:1:3:ALA:O	1:1:103:THR:HG22	2.20	0.41
1:1:32:TYR:CE2	1:1:93:TYR:CD1	3.08	0.41
1:1:48:VAL:N	2:1:232:HOH:O	2.53	0.41
1:1:148:VAL:HG13	1:1:150:VAL:HG13	2.00	0.41
1:1:160:LYS:O	1:1:160:LYS:CG	2.60	0.41
1:2:56:ARG:HG2	1:2:56:ARG:HH21	1.85	0.41
1:2:132:ASN:C	1:2:186:PRO:CD	2.94	0.41
1:1:54:ASN:OD1	1:1:54:ASN:N	2.54	0.41
1:1:159:VAL:O	1:1:160:LYS:HB3	2.21	0.41
1:1:212:PRO:O	1:1:213:THR:CB	2.67	0.41
1:2:136:LEU:HB2	1:2:152:TRP:CZ3	2.55	0.41
1:2:165:THR:HG22	1:2:166:THR:H	1.84	0.41
1:2:32:TYR:CD1	1:2:34:TYR:CE1	3.09	0.41
1:2:185:THR:HG21	2:2:298:HOH:O	2.21	0.41
1:2:192:HIS:HB2	1:2:195:TYR:CE1	2.55	0.41
1:1:37:TRP:HA	1:1:89:TYR:O	2.21	0.40
1:2:20:ILE:HG12	1:2:20:ILE:H	1.53	0.40
1:1:40:GLN:HB2	1:1:43:GLY:CA	2.51	0.40
1:1:119:VAL:O	1:1:120:THR:CG2	2.70	0.40
1:2:6:GLN:HA	1:2:7:PRO:HD3	1.83	0.40
1:2:50:ILE:HD12	1:2:65:SER:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:50:ILE:HD12	1:2:66:GLY:N	2.37	0.40
1:2:152:TRP:CD2	1:2:182:LEU:CD1	2.98	0.40
1:1:124:PRO:CD	1:1:136:LEU:CB	2.90	0.40
1:1:125:SER:O	1:2:216:SER:CB	2.59	0.40
1:2:133:LYS:HG2	1:2:134:ALA:O	2.21	0.40
1:2:185:THR:OG1	1:2:188:GLN:HB2	2.20	0.40
1:1:154:ALA:HB2	1:1:159:VAL:HG11	2.04	0.40
1:2:6:GLN:HG2	1:2:103:THR:O	2.22	0.40
1:2:14:LEU:CD2	1:2:111:GLY:C	2.95	0.40
1:1:57:PRO:O	1:1:60:VAL:HG11	2.20	0.40
1:1:114:LYS:HA	1:1:145:PRO:HD3	2.03	0.40
1:2:119:VAL:CG2	1:2:208:LYS:CG	2.82	0.40
1:2:189:TRP:CZ2	2:2:222:HOH:O	2.62	0.40
1:2:210:VAL:HG13	2:2:345:HOH:O	2.08	0.40

All (18) 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)
1:1:34:TYR:OH	1:1:157:SER:OG[3_455]	1.40	0.80
1:1:51:TYR:OH	2:1:281:HOH:O[3_455]	1.45	0.75
2:1:221:HOH:O	2:1:334:HOH:O[3_455]	1.59	0.61
1:2:1:PCA:CG	2:1:234:HOH:O[2_555]	1.63	0.57
1:1:93:TYR:OH	1:1:156:GLY:CA[3_455]	1.66	0.54
1:2:17:SER:CB	1:2:19:THR:OG1[2_455]	1.80	0.40
2:1:226:HOH:O	2:2:289:HOH:O[4_546]	1.86	0.34
1:1:158:PRO:CD	2:2:237:HOH:O[3_445]	1.95	0.25
1:1:62:ASP:OD1	2:2:217:HOH:O[2_555]	2.02	0.18
1:1:16:GLN:NE2	1:1:96:SER:OG[4_545]	2.06	0.14
1:1:158:PRO:CG	2:2:237:HOH:O[3_445]	2.09	0.11
1:2:5:THR:OG1	2:2:334:HOH:O[3_456]	2.11	0.09
1:2:1:PCA:CB	2:1:234:HOH:O[2_555]	2.12	0.08
1:2:16:GLN:CD	1:2:19:THR:O[2_455]	2.12	0.08
1:2:63:ARG:N	1:2:69:SER:OG[2_455]	2.15	0.05
1:2:63:ARG:CG	1:2:69:SER:OG[2_455]	2.16	0.04
1:1:34:TYR:CZ	1:1:157:SER:OG[3_455]	2.18	0.02
1:2:5:THR:CA	2:2:334:HOH:O[3_456]	2.19	0.01

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	1	214/216 (99%)	138 (64%)	42 (20%)	34 (16%)	0	0
1	2	214/216 (99%)	135 (63%)	43 (20%)	36 (17%)	0	0
All	All	428/432 (99%)	273 (64%)	85 (20%)	70 (16%)	0	0

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	15	GLY
1	1	52	GLU
1	1	53	VAL
1	1	70	GLY
1	1	71	ASN
1	1	85	GLU
1	1	109	VAL
1	1	142	ASP
1	1	174	ASN
1	1	213	THR
1	2	42	ALA
1	2	62	ASP
1	2	94	GLU
1	2	97	ASP
1	2	106	LYS
1	2	114	LYS
1	2	126	SER
1	2	143	PHE
1	2	166	THR
1	2	186	PRO
1	2	211	ALA
1	1	4	LEU
1	1	29	VAL
1	1	42	ALA
1	1	110	LEU

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Mol	Chain	Res	Type
1	1	131	ALA
1	1	156	GLY
1	1	172	SER
1	1	205	THR
1	1	206	VAL
1	2	44	LYS
1	2	50	ILE
1	2	70	GLY
1	2	82	ALA
1	2	110	LEU
1	2	127	GLU
1	2	133	LYS
1	2	155	ASP
1	2	168	PRO
1	2	173	ASN
1	2	184	LEU
1	1	8	PRO
1	1	32	TYR
1	1	44	LYS
1	1	57	PRO
1	1	112	GLN
1	1	124	PRO
1	1	155	ASP
1	1	160	LYS
1	2	45	ALA
1	2	54	ASN
1	2	71	ASN
1	2	96	SER
1	2	124	PRO
1	2	169	SER
1	2	189	TRP
1	2	193	ARG
1	1	30	GLY
1	1	144	TYR
1	1	189	TRP
1	2	112	GLN
1	1	99	PHE
1	1	188	GLN
1	2	53	VAL
1	2	171	GLN
1	2	105	THR
1	2	132	ASN

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Mol	Chain	Res	Type
1	2	43	GLY
1	1	61	PRO
1	1	146	GLY

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	1	180/180 (100%)	121 (67%)	59 (33%)	0	0
1	2	180/180 (100%)	114 (63%)	66 (37%)	0	0
All	All	360/360 (100%)	235 (65%)	125 (35%)	0	0

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	9	SER
1	1	13	SER
1	1	14	LEU
1	1	18	VAL
1	1	19	THR
1	1	35	VAL
1	1	38	TYR
1	1	41	HIS
1	1	47	LYS
1	1	49	ILE
1	1	50	ILE
1	1	52	GLU
1	1	54	ASN
1	1	58	SER
1	1	63	ARG
1	1	64	PHE
1	1	65	SER
1	1	68	LYS
1	1	75	LEU
1	1	80	LEU

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Mol	Chain	Res	Type
1	1	81	GLN
1	1	85	GLU
1	1	94	GLU
1	1	97	ASP
1	1	100	VAL
1	1	106	LYS
1	1	123	PRO
1	1	124	PRO
1	1	129	LEU
1	1	132	ASN
1	1	133	LYS
1	1	135	THR
1	1	136	LEU
1	1	137	VAL
1	1	140	ILE
1	1	149	THR
1	1	155	ASP
1	1	160	LYS
1	1	167	LYS
1	1	169	SER
1	1	170	LYS
1	1	172	SER
1	1	176	TYR
1	1	182	LEU
1	1	184	LEU
1	1	185	THR
1	1	186	PRO
1	1	192	HIS
1	1	193	ARG
1	1	194	SER
1	1	199	VAL
1	1	201	HIS
1	1	202	GLU
1	1	204	SER
1	1	205	THR
1	1	206	VAL
1	1	210	VAL
1	1	215	CYS
1	1	216	SER
1	2	2	SER
1	2	6	GLN
1	2	8	PRO

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Mol	Chain	Res	Type
1	2	14	LEU
1	2	20	ILE
1	2	25	THR
1	2	27	SER
1	2	29	VAL
1	2	38	TYR
1	2	41	HIS
1	2	47	LYS
1	2	48	VAL
1	2	49	ILE
1	2	50	ILE
1	2	53	VAL
1	2	55	LYS
1	2	63	ARG
1	2	68	LYS
1	2	75	LEU
1	2	77	VAL
1	2	78	SER
1	2	81	GLN
1	2	83	GLU
1	2	89	TYR
1	2	92	SER
1	2	103	THR
1	2	106	LYS
1	2	107	VAL
1	2	110	LEU
1	2	119	VAL
1	2	121	LEU
1	2	124	PRO
1	2	127	GLU
1	2	128	GLU
1	2	129	LEU
1	2	130	GLN
1	2	133	LYS
1	2	135	THR
1	2	136	LEU
1	2	139	LEU
1	2	140	ILE
1	2	148	VAL
1	2	153	LYS
1	2	155	ASP
1	2	157	SER

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Mol	Chain	Res	Type
1	2	159	VAL
1	2	163	VAL
1	2	164	GLU
1	2	165	THR
1	2	167	LYS
1	2	170	LYS
1	2	171	GLN
1	2	180	SER
1	2	183	SER
1	2	184	LEU
1	2	187	GLU
1	2	188	GLN
1	2	189	TRP
1	2	190	LYS
1	2	197	CYS
1	2	199	VAL
1	2	200	THR
1	2	201	HIS
1	2	202	GLU
1	2	207	GLU
1	2	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	41	HIS
1	1	81	GLN
1	1	173	ASN
1	1	201	HIS
1	2	39	GLN
1	2	41	HIS
1	2	98	ASN
1	2	112	GLN
1	2	130	GLN
1	2	132	ASN
1	2	173	ASN
1	2	174	ASN
1	2	192	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PCA	1	1	1	7,8,9	3.86	4 (57%)	9,10,12	4.26	5 (55%)
1	PCA	2	1	1	7,8,9	3.38	3 (42%)	9,10,12	2.13	4 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	1	1	1	-	0/0/11/13	0/1/1/1
1	PCA	2	1	1	-	0/0/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	PCA	CD-N	9.06	1.57	1.34
1	2	1	PCA	CD-N	7.59	1.53	1.34
1	2	1	PCA	CA-N	3.43	1.50	1.46
1	1	1	PCA	OE-CD	2.93	1.29	1.23
1	1	1	PCA	CG-CD	2.50	1.57	1.50
1	2	1	PCA	CB-CG	2.47	1.58	1.53
1	1	1	PCA	CB-CG	2.05	1.57	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1	PCA	OE-CD-CG	-8.43	111.68	126.72
1	1	1	PCA	OE-CD-N	8.05	142.37	124.96
1	2	1	PCA	O-C-CA	-4.36	113.56	124.77
1	1	1	PCA	O-C-CA	-3.21	116.52	124.77
1	1	1	PCA	CG-CD-N	-2.35	102.64	108.39
1	2	1	PCA	OE-CD-CG	-2.33	122.55	126.72
1	1	1	PCA	CB-CG-CD	-2.12	101.14	104.41
1	2	1	PCA	CA-N-CD	-2.04	106.59	113.58
1	2	1	PCA	CB-CA-N	2.03	108.82	103.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1	PCA	1	2

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.