



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:53 PM UTC

PDB ID : 2MCG / pdb_00002mcg
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

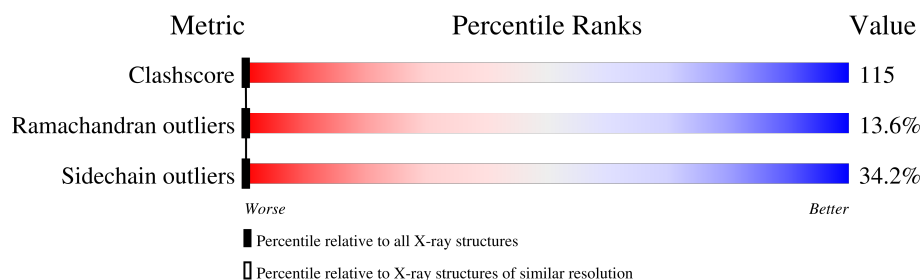
1 Overall quality at a glance

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	9% 30% 41% 20%
1	2	216	8% 26% 44% 22%

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
1	PCA	1	1	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3530 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	UNP P01709
1	23	THR	SER	conflict	UNP P01709
1	29	VAL	ILE	conflict	UNP P01709
1	31	GLY	ASN	conflict	UNP P01709
1	39	GLN	ARG	conflict	UNP P01709
1	42	ALA	PRO	conflict	UNP P01709
1	48	VAL	LEU	conflict	UNP P01709
1	49	ILE	MET	conflict	UNP P01709
1	54	ASN	THR	conflict	UNP P01709
1	62	ASP	ASN	conflict	UNP P01709
1	94	GLU	ALA	conflict	UNP P01709
1	97	ASP	ASN	conflict	UNP P01709
1	98	ASN	SER	conflict	UNP P01709
1	99	PHE	LEU	conflict	UNP P01709
1	100	VAL	ILE	conflict	UNP P01709
1	103	THR	GLY	conflict	UNP P01709
1	106	LYS	ARG	conflict	UNP P01709
1	107	VAL	LEU	conflict	UNP P01709
1	116	ASN	ALA	conflict	UNP P01709
1	118	THR	SER	conflict	UNP P01709
1	156	GLY	SER	conflict	UNP P01709
1	167	LYS	THR	conflict	UNP P01709
2	20	ILE	PHE	conflict	UNP P01709
2	23	THR	SER	conflict	UNP P01709

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Chain	Residue	Modelled	Actual	Comment	Reference
2	29	VAL	ILE	conflict	UNP P01709
2	31	GLY	ASN	conflict	UNP P01709
2	39	GLN	ARG	conflict	UNP P01709
2	42	ALA	PRO	conflict	UNP P01709
2	48	VAL	LEU	conflict	UNP P01709
2	49	ILE	MET	conflict	UNP P01709
2	54	ASN	THR	conflict	UNP P01709
2	62	ASP	ASN	conflict	UNP P01709
2	94	GLU	ALA	conflict	UNP P01709
2	97	ASP	ASN	conflict	UNP P01709
2	98	ASN	SER	conflict	UNP P01709
2	99	PHE	LEU	conflict	UNP P01709
2	100	VAL	ILE	conflict	UNP P01709
2	103	THR	GLY	conflict	UNP P01709
2	106	LYS	ARG	conflict	UNP P01709
2	107	VAL	LEU	conflict	UNP P01709
2	116	ASN	ALA	conflict	UNP P01709
2	118	THR	SER	conflict	UNP P01709
2	156	GLY	SER	conflict	UNP P01709
2	167	LYS	THR	conflict	UNP P01709

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	133	Total O 133 133	0	0
2	2	185	Total O 185 185	0	0

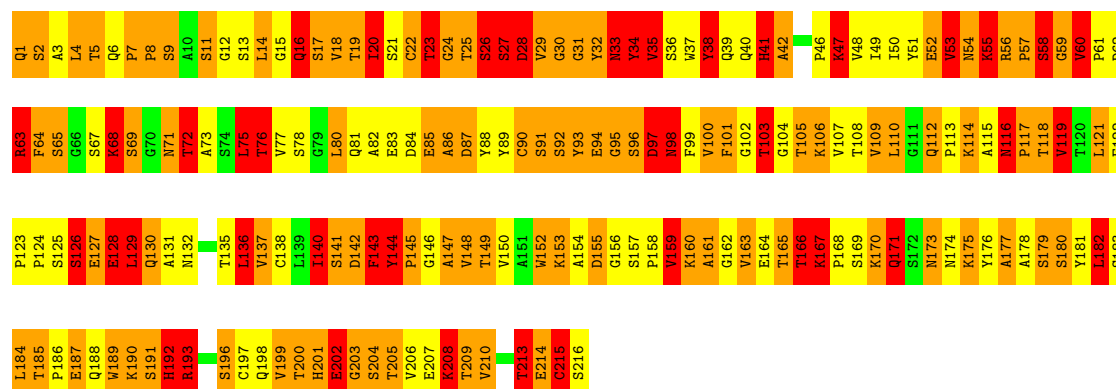
3 Residue-property plots

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.

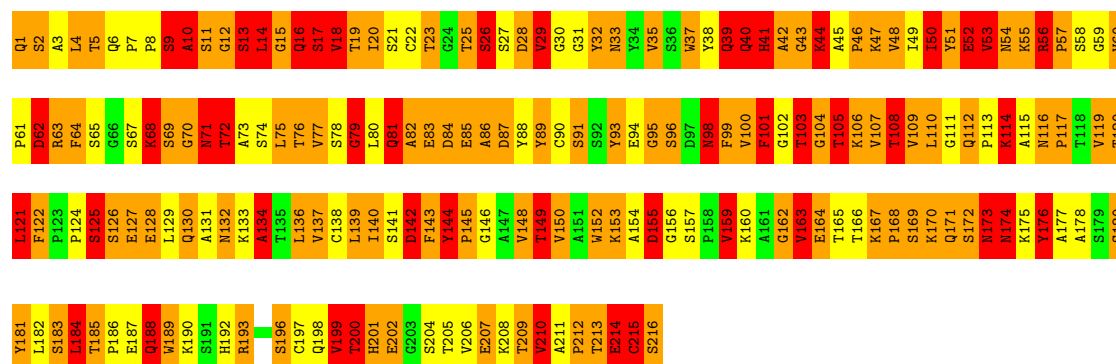
• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)

Chain 1: 



• Molecule 1: IMMUNOGLOBULIN LAMBDA DIMER MCG (LIGHT CHAIN)

Chain 2: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.30 Å 72.30 Å 185.90 Å 90.00° 90.00° 120.00°	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}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3530	wwPDB-VP
Average B, all atoms (Å ²)	8.0	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	26/1637 (1.6%)	3.16	233/2233 (10.4%)
1	2	1.85	27/1637 (1.6%)	3.15	224/2233 (10.0%)
All	All	1.84	53/3274 (1.6%)	3.16	457/4466 (10.2%)

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	0	2
1	2	0	1
All	All	0	3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	116	ASN	CA-CB	-9.98	1.41	1.54
1	2	171	GLN	C-O	8.68	1.31	1.24
1	1	58	SER	C-O	8.59	1.34	1.24
1	2	116	ASN	N-CA	8.45	1.55	1.45
1	1	4	LEU	CA-CB	-8.44	1.40	1.53
1	2	90	CYS	N-CA	8.04	1.55	1.45
1	1	202	GLU	N-CA	7.97	1.56	1.46
1	1	128	GLU	N-CA	7.52	1.55	1.46
1	2	60	VAL	CA-C	7.41	1.58	1.52
1	2	213	THR	CA-CB	7.24	1.63	1.52
1	2	137	VAL	N-CA	7.09	1.55	1.46
1	1	201	HIS	CA-C	-6.96	1.47	1.53
1	1	4	LEU	CA-C	6.56	1.60	1.52
1	2	98	ASN	N-CA	6.49	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	163	VAL	C-O	6.30	1.31	1.24
1	2	105	THR	CB-OG1	6.23	1.53	1.43
1	2	121	LEU	N-CA	6.19	1.53	1.45
1	1	62	ASP	C-O	6.15	1.32	1.24
1	1	25	THR	CB-OG1	6.11	1.53	1.43
1	2	69	SER	CA-CB	-6.07	1.46	1.54
1	2	103	THR	CA-CB	5.90	1.63	1.53
1	1	47	LYS	N-CA	5.89	1.53	1.45
1	1	63	ARG	NE-CZ	-5.89	1.26	1.33
1	1	63	ARG	CD-NE	-5.87	1.38	1.46
1	1	208	LYS	N-CA	5.77	1.52	1.45
1	2	21	SER	N-CA	5.76	1.52	1.45
1	1	215	CYS	N-CA	5.75	1.54	1.46
1	1	41	HIS	CA-CB	5.74	1.61	1.53
1	2	29	VAL	C-O	5.63	1.30	1.24
1	1	59	GLY	N-CA	5.61	1.54	1.45
1	2	163	VAL	CA-C	-5.60	1.45	1.52
1	1	213	THR	CA-CB	5.57	1.62	1.53
1	1	103	THR	CA-CB	5.55	1.63	1.53
1	1	92	SER	CA-CB	-5.46	1.46	1.53
1	2	188	GLN	N-CA	5.46	1.53	1.46
1	1	191	SER	C-O	5.45	1.29	1.23
1	1	166	THR	CA-CB	5.40	1.59	1.53
1	1	31	GLY	N-CA	5.38	1.53	1.45
1	2	85	GLU	N-CA	5.37	1.52	1.46
1	2	165	THR	CA-CB	5.32	1.60	1.52
1	2	81	GLN	C-N	-5.32	1.26	1.33
1	2	159	VAL	N-CA	5.32	1.52	1.46
1	2	208	LYS	N-CA	5.29	1.52	1.46
1	2	30	GLY	N-CA	5.19	1.52	1.45
1	1	8	PRO	C-O	5.17	1.29	1.23
1	2	106	LYS	C-N	-5.15	1.26	1.33
1	2	37	TRP	CA-CB	-5.14	1.45	1.53
1	1	158	PRO	C-N	-5.09	1.26	1.33
1	2	64	PHE	N-CA	5.09	1.52	1.45
1	1	26	SER	N-CA	-5.08	1.39	1.46
1	1	47	LYS	CA-CB	-5.08	1.45	1.53
1	2	39	GLN	C-N	-5.05	1.26	1.33
1	1	183	SER	N-CA	5.03	1.52	1.46

All (457) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	142	ASP	CA-CB-CG	28.93	141.53	112.60
1	1	130	GLN	CB-CG-CD	25.47	155.90	112.60
1	1	63	ARG	CD-NE-CZ	22.71	156.19	124.40
1	2	41	HIS	CA-CB-CG	-18.10	95.70	113.80
1	2	116	ASN	CA-CB-CG	17.70	130.31	112.60
1	1	55	LYS	CA-CB-CG	17.41	148.91	114.10
1	1	25	THR	CA-C-O	15.50	138.37	120.70
1	1	97	ASP	CA-CB-CG	15.01	127.61	112.60
1	1	116	ASN	OD1-CG-ND2	14.84	137.44	122.60
1	2	62	ASP	CA-CB-CG	-14.46	98.14	112.60
1	1	215	CYS	N-CA-C	-13.70	96.14	112.86
1	2	77	VAL	N-CA-CB	-12.88	99.77	112.65
1	2	60	VAL	O-C-N	12.87	133.02	121.57
1	1	4	LEU	CA-CB-CG	12.82	161.17	116.30
1	1	192	HIS	CA-CB-CG	-12.47	101.33	113.80
1	1	187	GLU	CB-CG-CD	12.39	133.67	112.60
1	1	190	LYS	CA-CB-CG	12.09	138.29	114.10
1	2	124	PRO	CA-C-N	12.09	140.52	121.66
1	2	124	PRO	C-N-CA	12.09	140.52	121.66
1	1	58	SER	CA-C-O	-12.00	103.35	120.51
1	2	171	GLN	N-CA-C	11.68	124.19	110.41
1	1	46	PRO	CA-C-O	-11.59	108.69	121.32
1	2	171	GLN	N-CA-CB	-11.24	98.30	111.79
1	1	130	GLN	OE1-CD-NE2	-11.17	111.43	122.60
1	2	174	ASN	CA-CB-CG	10.67	123.27	112.60
1	2	60	VAL	N-CA-C	-10.47	95.89	108.45
1	1	8	PRO	CA-C-O	-10.46	109.10	121.03
1	2	105	THR	CA-CB-OG1	-10.42	93.96	109.60
1	1	148	VAL	CA-C-O	-10.23	111.22	121.45
1	1	208	LYS	CA-CB-CG	10.03	134.17	114.10
1	1	161	ALA	CA-C-O	-9.94	107.97	119.60
1	2	130	GLN	CB-CG-CD	-9.90	95.77	112.60
1	2	109	VAL	N-CA-C	-9.89	95.90	109.55
1	1	69	SER	N-CA-CB	9.74	124.91	110.49
1	1	25	THR	CA-C-N	9.67	140.02	121.54
1	1	25	THR	C-N-CA	9.67	140.02	121.54
1	1	173	ASN	CA-CB-CG	-9.53	103.07	112.60
1	2	213	THR	N-CA-C	9.47	123.29	107.20
1	2	201	HIS	CA-CB-CG	9.39	123.19	113.80
1	1	103	THR	N-CA-C	9.35	124.49	112.34
1	2	4	LEU	CA-C-O	-9.30	111.64	121.87
1	1	4	LEU	N-CA-CB	9.12	125.09	110.77
1	2	81	GLN	CA-C-O	-9.09	107.51	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	145	PRO	CB-CA-C	9.07	126.53	111.56
1	2	197	CYS	CA-C-O	-9.05	111.51	120.92
1	2	155	ASP	N-CA-CB	-9.04	95.21	110.49
1	2	207	GLU	O-C-N	9.03	134.38	123.36
1	1	34	TYR	N-CA-CB	9.02	125.32	109.18
1	2	164	GLU	CB-CG-CD	8.96	127.83	112.60
1	1	32	TYR	CA-CB-CG	-8.95	97.80	113.90
1	1	201	HIS	N-CA-C	8.95	122.94	107.28
1	2	26	SER	N-CA-C	-8.94	101.43	111.71
1	2	19	THR	CA-C-O	8.88	132.28	120.11
1	1	40	GLN	CA-C-N	8.87	135.21	122.09
1	1	40	GLN	C-N-CA	8.87	135.21	122.09
1	2	121	LEU	CB-CA-C	8.84	125.30	109.83
1	2	105	THR	CA-CB-CG2	8.79	125.44	110.50
1	2	145	PRO	CB-CA-C	8.75	126.00	111.56
1	2	202	GLU	CA-C-O	-8.72	111.72	121.84
1	2	199	VAL	CB-CA-C	8.68	123.00	110.33
1	1	116	ASN	O-C-N	8.64	130.75	121.60
1	1	22	CYS	CA-C-O	-8.63	111.37	120.09
1	2	124	PRO	CA-C-O	8.57	132.32	121.86
1	2	192	HIS	CA-CB-CG	8.57	122.37	113.80
1	2	29	VAL	CA-C-O	-8.51	110.14	120.78
1	2	43	GLY	O-C-N	8.51	130.31	122.57
1	2	202	GLU	CB-CA-C	-8.49	99.84	111.89
1	1	140	ILE	CB-CA-C	8.44	120.78	110.73
1	1	41	HIS	CA-CB-CG	-8.44	105.36	113.80
1	2	116	ASN	O-C-N	8.39	128.48	121.35
1	1	34	TYR	N-CA-C	-8.38	97.14	109.63
1	1	35	VAL	O-C-N	8.33	132.98	122.57
1	1	141	SER	N-CA-C	8.32	121.71	109.07
1	1	5	THR	CB-CA-C	8.29	124.30	109.38
1	1	160	LYS	O-C-N	8.24	133.17	122.04
1	2	60	VAL	N-CA-CB	8.21	118.65	111.67
1	2	54	ASN	CA-C-O	8.18	130.19	120.53
1	2	70	GLY	CA-C-O	-8.17	113.14	121.64
1	2	157	SER	N-CA-C	-8.15	100.88	108.22
1	2	188	GLN	CB-CA-C	8.09	126.88	110.38
1	2	134	ALA	CA-C-O	-8.07	108.97	120.51
1	1	128	GLU	CB-CA-C	8.06	124.38	110.68
1	2	162	GLY	O-C-N	8.05	131.76	122.34
1	1	28	ASP	CA-CB-CG	8.05	120.65	112.60
1	2	85	GLU	N-CA-C	-8.04	97.78	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	25	THR	N-CA-CB	8.03	124.03	110.46
1	2	116	ASN	N-CA-C	-7.94	96.47	109.82
1	1	3	ALA	N-CA-C	7.94	122.10	111.30
1	2	98	ASN	CB-CA-C	7.91	125.33	110.62
1	1	87	ASP	CA-C-O	-7.90	111.96	121.28
1	1	140	ILE	CA-CB-CG2	7.89	123.91	110.50
1	1	130	GLN	CG-CD-OE1	7.88	136.57	120.80
1	1	112	GLN	O-C-N	7.85	130.35	121.32
1	1	58	SER	N-CA-C	7.84	127.50	110.80
1	1	175	LYS	CA-C-O	-7.81	112.75	121.89
1	1	15	GLY	N-CA-C	-7.81	105.19	114.48
1	2	163	VAL	CA-C-O	-7.79	111.04	120.78
1	2	180	SER	CA-C-O	-7.79	111.89	120.38
1	2	113	PRO	CA-C-O	-7.77	112.19	121.67
1	2	189	TRP	CA-CB-CG	7.73	128.29	113.60
1	1	202	GLU	CA-CB-CG	7.66	129.43	114.10
1	2	157	SER	CA-C-O	-7.64	113.00	120.26
1	2	55	LYS	CA-CB-CG	7.64	129.38	114.10
1	1	193	ARG	NE-CZ-NH2	-7.63	112.33	119.20
1	2	189	TRP	CB-CA-C	7.62	122.85	110.88
1	2	116	ASN	CB-CA-C	7.56	120.65	109.08
1	2	9	SER	CA-CB-OG	7.53	126.17	111.10
1	2	28	ASP	CA-C-O	-7.52	110.07	120.52
1	1	128	GLU	N-CA-C	-7.50	102.26	111.33
1	1	155	ASP	CA-C-O	-7.49	111.72	121.08
1	1	147	ALA	CA-C-O	-7.47	111.09	120.28
1	2	208	LYS	CB-CA-C	7.46	123.62	109.37
1	1	127	GLU	O-C-N	7.45	130.05	122.08
1	2	119	VAL	CB-CA-C	7.45	123.46	111.32
1	1	62	ASP	N-CA-C	7.40	121.22	112.93
1	1	198	GLN	CB-CA-C	7.39	121.89	109.48
1	2	188	GLN	CA-CB-CG	7.37	128.84	114.10
1	2	200	THR	CA-CB-OG1	-7.36	98.56	109.60
1	1	182	LEU	CA-C-O	-7.36	112.42	120.36
1	1	152	TRP	O-C-N	7.35	132.78	123.23
1	2	12	GLY	CA-C-O	-7.33	113.91	121.61
1	1	107	VAL	N-CA-CB	7.31	118.69	110.72
1	1	137	VAL	CA-C-O	7.29	128.08	120.36
1	2	171	GLN	OE1-CD-NE2	7.24	129.84	122.60
1	1	92	SER	N-CA-CB	7.22	122.63	111.22
1	1	166	THR	CA-C-O	-7.21	112.86	120.58
1	2	157	SER	O-C-N	7.21	128.27	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	180	SER	N-CA-CB	7.20	121.85	111.05
1	2	139	LEU	O-C-N	7.19	131.40	123.13
1	1	82	ALA	CB-CA-C	7.19	123.07	110.85
1	2	122	PHE	O-C-N	7.17	129.56	121.32
1	1	200	THR	CA-C-O	-7.15	112.98	120.70
1	2	210	VAL	O-C-N	7.13	130.73	123.10
1	1	71	ASN	N-CA-C	-7.12	103.76	113.30
1	2	162	GLY	N-CA-C	-7.11	101.59	114.46
1	2	159	VAL	CB-CA-C	7.08	119.76	110.12
1	2	202	GLU	O-C-N	7.08	131.34	122.55
1	1	72	THR	CA-CB-OG1	-7.08	98.98	109.60
1	2	64	PHE	CA-C-O	-7.08	113.33	121.47
1	1	203	GLY	N-CA-C	7.07	129.94	113.18
1	2	18	VAL	CB-CA-C	7.06	121.36	111.40
1	2	105	THR	CB-CA-C	7.04	124.44	110.42
1	2	101	PHE	CA-CB-CG	-7.03	106.77	113.80
1	1	14	LEU	N-CA-CB	7.03	122.37	110.49
1	1	118	THR	CA-C-O	-7.02	113.03	120.40
1	1	167	LYS	N-CA-CB	7.02	122.87	110.37
1	2	170	LYS	CA-C-O	-7.01	114.16	121.87
1	2	140	ILE	CA-C-O	-7.01	112.95	120.59
1	2	89	TYR	CA-C-N	-6.99	110.77	122.64
1	2	89	TYR	C-N-CA	-6.99	110.77	122.64
1	2	210	VAL	N-CA-CB	6.97	122.88	111.44
1	2	176	TYR	CA-CB-CG	6.96	126.43	113.90
1	1	16	GLN	CB-CG-CD	-6.96	100.77	112.60
1	1	187	GLU	CA-CB-CG	6.96	128.01	114.10
1	2	207	GLU	CA-C-N	-6.96	112.50	122.94
1	2	207	GLU	C-N-CA	-6.96	112.50	122.94
1	2	136	LEU	O-C-N	6.94	131.48	123.29
1	2	28	ASP	CA-CB-CG	6.93	119.53	112.60
1	1	208	LYS	N-CA-CB	6.91	122.39	111.20
1	2	63	ARG	CD-NE-CZ	6.89	134.05	124.40
1	1	204	SER	N-CA-C	6.89	120.77	109.06
1	2	130	GLN	OE1-CD-NE2	6.87	129.47	122.60
1	2	145	PRO	N-CA-C	-6.86	98.33	112.47
1	1	122	PHE	O-C-N	6.85	127.96	121.38
1	1	93	TYR	N-CA-CB	-6.83	100.05	110.77
1	1	16	GLN	CB-CA-C	6.82	123.41	110.51
1	1	135	THR	CA-CB-OG1	-6.82	99.37	109.60
1	1	85	GLU	CB-CG-CD	6.81	124.18	112.60
1	2	60	VAL	CA-C-O	-6.81	111.69	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	159	VAL	N-CA-C	-6.81	97.63	107.78
1	2	68	LYS	CA-C-O	-6.77	113.54	121.46
1	1	201	HIS	CA-C-O	-6.74	113.56	120.63
1	1	63	ARG	N-CA-CB	6.72	120.65	110.30
1	1	48	VAL	CA-C-O	-6.72	112.80	120.66
1	1	33	ASN	N-CA-CB	-6.71	99.14	110.49
1	2	189	TRP	N-CA-C	-6.71	103.89	111.07
1	2	136	LEU	CA-C-N	-6.70	112.80	122.45
1	2	136	LEU	C-N-CA	-6.70	112.80	122.45
1	2	215	CYS	CA-C-O	-6.69	110.94	120.51
1	1	127	GLU	CA-C-N	-6.68	111.23	120.38
1	1	127	GLU	C-N-CA	-6.68	111.23	120.38
1	1	201	HIS	CA-CB-CG	6.68	120.48	113.80
1	1	102	GLY	CA-C-N	6.67	131.36	120.63
1	1	102	GLY	C-N-CA	6.67	131.36	120.63
1	1	126	SER	O-C-N	6.66	129.18	122.12
1	1	59	GLY	N-CA-C	-6.64	107.03	114.40
1	2	54	ASN	N-CA-CB	-6.63	101.93	111.54
1	2	63	ARG	N-CA-C	6.60	121.50	113.38
1	2	74	SER	CA-CB-OG	-6.60	97.90	111.10
1	2	196	SER	CA-CB-OG	6.57	124.24	111.10
1	2	188	GLN	OE1-CD-NE2	6.56	129.16	122.60
1	1	34	TYR	CA-C-O	-6.55	113.61	120.89
1	2	168	PRO	CB-CA-C	6.54	122.34	111.56
1	1	171	GLN	N-CA-C	-6.51	99.92	109.63
1	1	157	SER	CA-CB-OG	6.51	124.12	111.10
1	1	214	GLU	O-C-N	6.51	129.02	122.12
1	1	175	LYS	N-CA-C	-6.50	101.16	110.59
1	2	144	TYR	O-C-N	6.50	128.80	121.32
1	1	53	VAL	CA-C-O	-6.48	112.67	120.78
1	1	214	GLU	CB-CA-C	-6.47	100.05	110.79
1	1	68	LYS	CG-CD-CE	6.46	126.17	111.30
1	2	150	VAL	N-CA-C	6.45	119.61	108.90
1	2	178	ALA	CA-C-O	-6.45	111.29	120.51
1	2	128	GLU	N-CA-C	-6.44	104.18	111.07
1	1	215	CYS	N-CA-CB	-6.42	102.46	112.41
1	2	68	LYS	CA-C-N	-6.41	113.94	121.64
1	2	68	LYS	C-N-CA	-6.41	113.94	121.64
1	1	25	THR	O-C-N	-6.41	114.68	123.01
1	1	205	THR	CA-C-N	6.38	131.28	121.71
1	1	205	THR	C-N-CA	6.38	131.28	121.71
1	2	109	VAL	CB-CA-C	6.35	120.40	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	59	GLY	CA-C-N	6.35	132.23	121.88
1	2	59	GLY	C-N-CA	6.35	132.23	121.88
1	2	10	ALA	CA-C-N	6.35	130.90	120.94
1	2	10	ALA	C-N-CA	6.35	130.90	120.94
1	2	63	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	2	86	ALA	CA-C-O	-6.32	111.48	120.51
1	2	70	GLY	N-CA-C	-6.31	101.78	112.77
1	2	113	PRO	CB-CA-C	6.31	119.25	110.98
1	1	159	VAL	O-C-N	6.30	129.88	123.07
1	1	170	LYS	N-CA-C	-6.30	101.09	110.23
1	1	114	LYS	CA-CB-CG	6.29	126.69	114.10
1	1	152	TRP	CA-C-O	-6.29	113.91	120.70
1	2	33	ASN	CB-CA-C	6.29	121.75	112.07
1	1	69	SER	O-C-N	6.28	130.19	122.34
1	2	108	THR	CB-CA-C	6.27	119.12	110.34
1	2	137	VAL	CB-CA-C	6.27	120.16	111.19
1	2	149	THR	N-CA-CB	6.27	121.09	110.49
1	2	43	GLY	N-CA-C	-6.26	102.48	113.76
1	1	71	ASN	N-CA-CB	-6.25	101.16	110.61
1	1	199	VAL	CA-C-O	-6.25	113.36	120.67
1	1	170	LYS	N-CA-CB	6.24	119.25	109.83
1	1	196	SER	O-C-N	6.24	130.61	123.31
1	2	173	ASN	CA-CB-CG	6.23	118.83	112.60
1	2	98	ASN	N-CA-CB	-6.22	101.92	111.56
1	2	206	VAL	O-C-N	6.22	130.34	122.57
1	2	197	CYS	O-C-N	6.22	130.58	122.68
1	2	56	ARG	NE-CZ-NH1	6.21	127.72	121.50
1	1	85	GLU	N-CA-CB	6.21	119.19	109.69
1	2	67	SER	O-C-N	6.20	130.42	123.48
1	2	115	ALA	CA-C-O	-6.19	114.08	121.56
1	1	193	ARG	CG-CD-NE	-6.18	98.41	112.00
1	1	25	THR	CA-CB-CG2	6.16	120.97	110.50
1	2	84	ASP	CA-CB-CG	-6.16	106.44	112.60
1	2	181	TYR	CB-CA-C	6.15	121.53	109.35
1	1	170	LYS	O-C-N	6.12	130.40	122.87
1	1	126	SER	N-CA-C	-6.12	104.61	111.28
1	1	159	VAL	CA-C-O	-6.12	113.77	120.43
1	2	74	SER	N-CA-CB	-6.11	100.15	111.52
1	1	108	THR	CA-C-N	-6.11	114.93	122.93
1	1	108	THR	C-N-CA	-6.11	114.93	122.93
1	2	23	THR	CB-CA-C	6.10	119.65	109.89
1	1	64	PHE	CB-CA-C	6.10	119.84	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	111	GLY	O-C-N	6.08	130.61	122.70
1	1	47	LYS	CA-C-O	-6.07	113.53	121.73
1	1	153	LYS	O-C-N	6.05	130.66	123.27
1	2	112	GLN	N-CA-C	-6.05	102.43	109.93
1	1	121	LEU	CB-CA-C	6.03	120.24	109.38
1	2	104	GLY	CA-C-O	-6.03	115.96	122.47
1	1	136	LEU	O-C-N	6.02	130.03	123.10
1	1	75	LEU	CA-C-O	-6.02	113.70	120.32
1	2	91	SER	O-C-N	6.02	130.84	123.44
1	1	24	GLY	CA-C-N	6.01	132.04	123.14
1	1	24	GLY	C-N-CA	6.01	132.04	123.14
1	2	150	VAL	N-CA-CB	-6.00	101.25	112.36
1	2	163	VAL	N-CA-C	6.00	121.82	109.34
1	1	119	VAL	N-CA-CB	5.99	120.45	110.86
1	1	209	THR	CA-CB-OG1	-5.98	100.62	109.60
1	2	72	THR	O-C-N	5.97	130.41	123.30
1	1	118	THR	N-CA-CB	5.96	120.07	110.65
1	1	179	SER	N-CA-CB	5.96	122.60	111.52
1	1	16	GLN	OE1-CD-NE2	5.95	128.55	122.60
1	1	214	GLU	CA-C-N	-5.95	113.71	123.05
1	1	214	GLU	C-N-CA	-5.95	113.71	123.05
1	1	173	ASN	OD1-CG-ND2	5.93	128.53	122.60
1	2	121	LEU	CA-CB-CG	5.93	137.06	116.30
1	1	32	TYR	CA-C-O	-5.92	112.04	120.51
1	1	170	LYS	CA-C-O	-5.92	114.67	121.19
1	2	13	SER	CA-C-O	-5.92	113.49	120.60
1	1	94	GLU	CA-CB-CG	5.91	125.92	114.10
1	1	56	ARG	CA-CB-CG	5.90	125.91	114.10
1	2	117	PRO	CB-CA-C	-5.90	103.84	111.39
1	1	214	GLU	CB-CG-CD	-5.88	102.59	112.60
1	2	188	GLN	N-CA-C	-5.88	104.81	112.23
1	2	103	THR	N-CA-C	5.87	123.31	110.80
1	1	127	GLU	N-CA-C	-5.86	103.87	111.02
1	1	143	PHE	O-C-N	5.86	129.95	123.33
1	1	71	ASN	OD1-CG-ND2	5.86	128.46	122.60
1	2	150	VAL	CA-C-O	5.85	127.42	121.63
1	1	180	SER	O-C-N	5.81	131.24	122.94
1	2	112	GLN	CB-CA-C	5.81	117.80	109.26
1	1	52	GLU	CB-CG-CD	-5.79	102.76	112.60
1	2	98	ASN	N-CA-C	5.78	117.63	108.79
1	2	112	GLN	O-C-N	5.78	129.49	121.64
1	2	119	VAL	CA-C-O	5.77	127.71	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	16	GLN	CB-CG-CD	5.77	122.41	112.60
1	1	69	SER	N-CA-C	-5.76	105.91	113.17
1	2	157	SER	CB-CA-C	5.76	117.83	110.22
1	2	116	ASN	N-CA-CB	5.76	120.70	110.39
1	1	109	VAL	N-CA-CB	5.76	118.61	111.41
1	1	171	GLN	CA-C-O	-5.75	114.50	120.89
1	1	109	VAL	CA-C-O	-5.74	114.08	120.74
1	2	184	LEU	CA-C-O	5.73	128.15	121.44
1	1	144	TYR	O-C-N	5.72	127.90	121.32
1	1	5	THR	N-CA-CB	-5.71	101.49	110.69
1	2	19	THR	CA-CB-OG1	-5.71	101.04	109.60
1	1	184	LEU	O-C-N	5.70	130.60	122.74
1	2	200	THR	CA-C-N	5.69	130.82	122.39
1	2	200	THR	C-N-CA	5.69	130.82	122.39
1	2	87	ASP	CB-CA-C	5.69	119.77	109.37
1	2	185	THR	N-CA-C	-5.69	102.88	109.93
1	1	202	GLU	N-CA-C	-5.68	98.69	110.80
1	1	200	THR	O-C-N	5.68	130.61	123.23
1	2	87	ASP	N-CA-C	-5.67	100.94	109.95
1	1	31	GLY	N-CA-C	-5.67	99.75	113.18
1	1	105	THR	CA-CB-OG1	-5.66	101.11	109.60
1	2	44	LYS	N-CA-C	5.66	115.50	108.19
1	2	60	VAL	CA-CB-CG1	5.66	120.03	110.40
1	2	98	ASN	CA-CB-CG	5.65	118.25	112.60
1	2	143	PHE	CB-CA-C	5.65	120.62	109.66
1	1	71	ASN	CB-CA-C	5.65	119.72	110.17
1	2	213	THR	CA-CB-OG1	-5.65	101.13	109.60
1	2	120	THR	CA-C-O	-5.64	113.14	120.25
1	1	179	SER	O-C-N	5.64	129.70	123.33
1	2	124	PRO	CB-CA-C	5.64	118.69	110.63
1	2	162	GLY	CA-C-O	-5.64	113.28	119.88
1	1	143	PHE	CA-CB-CG	5.63	119.44	113.80
1	1	202	GLU	CA-C-N	5.62	132.44	121.41
1	1	202	GLU	C-N-CA	5.62	132.44	121.41
1	2	19	THR	CA-C-N	5.60	130.13	123.19
1	2	19	THR	C-N-CA	5.60	130.13	123.19
1	1	65	SER	CA-C-O	-5.59	114.73	120.99
1	2	71	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	2	101	PHE	CA-C-O	-5.59	111.72	121.62
1	1	193	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	1	98	ASN	CA-C-O	-5.58	112.54	120.51
1	2	167	LYS	O-C-N	5.58	126.59	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	117	PRO	N-CD-CG	-5.57	94.84	103.20
1	1	121	LEU	CA-C-O	5.56	126.61	120.71
1	2	87	ASP	CA-C-O	-5.56	114.88	121.16
1	1	63	ARG	NH1-CZ-NH2	-5.55	112.08	119.30
1	2	62	ASP	CB-CG-OD2	-5.55	105.63	118.40
1	1	56	ARG	CB-CA-C	5.55	117.44	109.11
1	1	73	ALA	CA-C-O	-5.54	114.71	121.36
1	2	165	THR	CB-CA-C	-5.54	103.36	111.23
1	2	99	PHE	CA-C-O	5.54	127.66	121.40
1	1	159	VAL	N-CA-C	-5.53	100.09	108.17
1	1	89	TYR	O-C-N	5.50	129.85	123.30
1	1	117	PRO	CB-CA-C	5.49	119.86	111.40
1	1	163	VAL	N-CA-CB	-5.49	101.84	111.39
1	2	53	VAL	N-CA-C	5.49	120.75	109.34
1	1	89	TYR	N-CA-C	5.49	117.84	108.90
1	1	163	VAL	N-CA-C	5.48	116.38	108.48
1	2	115	ALA	CA-C-N	-5.48	112.70	123.56
1	2	115	ALA	C-N-CA	-5.48	112.70	123.56
1	2	16	GLN	N-CA-CB	5.48	119.76	110.49
1	2	138	CYS	CA-C-O	-5.47	113.09	120.47
1	1	183	SER	CA-CB-OG	-5.47	100.17	111.10
1	2	100	VAL	N-CA-CB	-5.46	103.30	112.47
1	2	103	THR	CA-C-O	5.46	128.32	120.51
1	1	165	THR	CA-CB-CG2	5.46	119.78	110.50
1	2	79	GLY	CA-C-N	5.45	129.93	121.26
1	2	79	GLY	C-N-CA	5.45	129.93	121.26
1	1	50	ILE	CA-C-O	-5.45	115.58	121.19
1	2	214	GLU	CA-C-O	5.45	128.30	120.51
1	1	57	PRO	CB-CA-C	5.44	115.91	109.92
1	1	179	SER	CA-CB-OG	5.44	121.98	111.10
1	2	18	VAL	CA-CB-CG1	5.42	119.61	110.40
1	2	183	SER	N-CA-C	5.41	117.55	108.73
1	1	122	PHE	CA-CB-CG	5.41	119.21	113.80
1	1	165	THR	CA-C-O	5.40	126.44	120.71
1	2	40	GLN	N-CA-CB	5.38	119.59	110.49
1	1	60	VAL	N-CA-CB	-5.38	103.68	111.21
1	2	120	THR	O-C-N	5.38	130.13	123.14
1	2	114	LYS	CA-C-N	5.37	132.38	122.92
1	2	114	LYS	C-N-CA	5.37	132.38	122.92
1	1	101	PHE	CA-C-O	-5.37	114.62	120.36
1	1	118	THR	O-C-N	5.37	130.20	123.12
1	2	121	LEU	N-CA-C	-5.36	102.58	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	23	THR	CA-CB-OG1	-5.36	101.56	109.60
1	1	80	LEU	N-CA-CB	5.36	118.21	109.69
1	1	130	GLN	N-CA-C	-5.36	105.36	111.14
1	1	156	GLY	O-C-N	5.35	128.70	122.65
1	2	52	GLU	CB-CG-CD	-5.35	103.51	112.60
1	1	107	VAL	N-CA-C	-5.34	100.89	108.58
1	1	63	ARG	O-C-N	5.34	129.49	122.33
1	2	20	ILE	N-CA-CB	-5.34	103.99	111.25
1	2	72	THR	CA-C-O	-5.34	114.59	120.36
1	2	45	ALA	O-C-N	5.33	127.40	121.43
1	1	136	LEU	CB-CA-C	5.33	118.51	109.50
1	2	174	ASN	N-CA-CB	5.33	121.81	111.53
1	2	70	GLY	O-C-N	5.32	129.24	122.85
1	1	184	LEU	CA-C-O	-5.31	115.33	121.49
1	2	64	PHE	N-CA-C	-5.30	102.64	110.48
1	2	40	GLN	O-C-N	5.30	129.64	122.59
1	1	38	TYR	N-CA-CB	5.29	119.95	110.80
1	1	76	THR	N-CA-C	5.29	118.07	109.24
1	1	114	LYS	CA-C-N	5.29	130.22	122.39
1	1	114	LYS	C-N-CA	5.29	130.22	122.39
1	2	71	ASN	CB-CA-C	5.27	120.91	110.42
1	1	189	TRP	CB-CA-C	5.26	120.33	110.70
1	2	107	VAL	N-CA-CB	-5.25	102.56	111.23
1	1	153	LYS	CA-C-O	-5.25	114.63	120.66
1	1	177	ALA	O-C-N	5.24	129.35	123.48
1	2	110	LEU	O-C-N	5.23	129.66	123.33
1	2	114	LYS	CA-C-O	5.22	126.59	120.80
1	1	160	LYS	N-CA-C	-5.21	104.96	113.19
1	2	152	TRP	N-CA-C	-5.20	102.77	110.46
1	1	160	LYS	CA-C-N	-5.19	111.97	121.52
1	1	160	LYS	C-N-CA	-5.19	111.97	121.52
1	1	128	GLU	CA-CB-CG	5.18	124.47	114.10
1	1	200	THR	CA-C-N	-5.18	113.54	121.26
1	1	200	THR	C-N-CA	-5.18	113.54	121.26
1	2	116	ASN	CA-C-O	-5.17	115.33	120.66
1	1	109	VAL	O-C-N	5.17	130.36	122.76
1	1	130	GLN	N-CA-CB	5.16	117.56	110.07
1	1	82	ALA	CA-C-O	-5.16	114.95	120.42
1	1	63	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	1	7	PRO	O-C-N	5.16	127.54	121.46
1	2	144	TYR	N-CA-CB	5.16	119.55	110.37
1	2	193	ARG	NE-CZ-NH2	-5.15	114.56	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	23	THR	CA-C-O	-5.15	114.78	121.73
1	2	85	GLU	CA-CB-CG	5.15	124.39	114.10
1	2	93	TYR	N-CA-C	-5.15	103.35	110.35
1	1	80	LEU	CA-C-O	5.14	126.81	121.15
1	1	116	ASN	CB-CG-OD1	-5.14	110.51	120.80
1	1	4	LEU	O-C-N	5.14	129.29	123.27
1	1	20	ILE	CA-C-O	-5.14	114.91	120.67
1	1	33	ASN	N-CA-C	5.13	121.74	110.80
1	2	51	TYR	O-C-N	5.13	129.38	123.17
1	1	214	GLU	OE1-CD-OE2	5.13	135.21	122.90
1	2	84	ASP	N-CA-C	-5.13	107.08	113.19
1	1	210	VAL	N-CA-C	-5.13	100.95	108.85
1	2	41	HIS	CA-C-O	-5.13	113.56	119.61
1	2	122	PHE	N-CA-CB	5.13	119.49	110.37
1	1	22	CYS	O-C-N	5.12	128.84	123.62
1	1	30	GLY	O-C-N	5.12	128.93	122.54
1	1	157	SER	CB-CA-C	5.11	116.42	108.61
1	1	54	ASN	CA-CB-CG	-5.10	107.50	112.60
1	1	118	THR	CA-C-N	-5.10	115.62	122.91
1	1	118	THR	C-N-CA	-5.10	115.62	122.91
1	2	76	THR	CA-C-O	5.09	125.97	120.32
1	2	50	ILE	O-C-N	5.09	128.93	122.57
1	2	108	THR	N-CA-CB	5.08	118.70	110.32
1	2	193	ARG	NH1-CZ-NH2	5.08	125.90	119.30
1	1	53	VAL	N-CA-C	5.07	119.89	109.34
1	2	142	ASP	O-C-N	5.07	129.33	122.59
1	1	26	SER	N-CA-C	5.06	121.58	110.80
1	2	44	LYS	CB-CA-C	-5.06	103.42	114.10
1	1	40	GLN	OE1-CD-NE2	5.06	127.66	122.60
1	1	190	LYS	N-CA-CB	5.05	118.78	110.39
1	1	129	LEU	CB-CA-C	5.04	119.16	110.79
1	1	207	GLU	CA-C-N	-5.03	114.36	122.81
1	1	207	GLU	C-N-CA	-5.03	114.36	122.81
1	2	125	SER	CA-C-O	5.03	126.61	120.62
1	2	25	THR	N-CA-CB	5.01	119.74	111.62
1	2	130	GLN	N-CA-C	-5.00	105.83	112.34

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	193	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	1	58	SER	Mainchain
1	2	163	VAL	Mainchain

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	1538	374	4
1	2	1606	0	1537	363	1
2	1	133	0	0	35	2
2	2	185	0	0	44	1
All	All	3530	0	3075	725	5

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 115.

All (725) 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)
1:1:177:ALA:HB3	2:1:347:HOH:O	1.32	1.26
1:1:19:THR:HG23	1:1:76:THR:CG2	1.66	1.26
2:1:314:HOH:O	1:2:141:SER:HB2	1.33	1.25
1:1:52:GLU:O	1:1:53:VAL:HG22	1.34	1.23
1:1:117:PRO:HB3	1:1:140:ILE:CD1	1.70	1.20
1:1:9:SER:HB2	1:1:147:ALA:HB3	1.18	1.16
1:1:24:GLY:C	1:1:29:VAL:HG21	1.71	1.15
1:2:25:THR:HG22	1:2:26:SER:H	1.14	1.12
1:2:196:SER:HB3	1:2:209:THR:HG23	1.20	1.12
1:2:27:SER:O	2:2:250:HOH:O	1.66	1.11
1:1:23:THR:HG23	1:1:72:THR:HG22	1.28	1.11
1:1:97:ASP:O	1:1:98:ASN:HB2	1.48	1.09
1:2:201:HIS:O	2:2:389:HOH:O	1.68	1.09
1:1:4:LEU:HD13	1:1:22:CYS:SG	1.92	1.09
1:2:4:LEU:HD13	1:2:100:VAL:HG22	1.35	1.06
1:1:94:GLU:HB3	1:1:98:ASN:HB3	1.36	1.06
1:2:47:LYS:N	2:2:256:HOH:O	1.88	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:144:TYR:HB3	1:2:145:PRO:HD3	1.12	1.05
1:1:25:THR:N	1:1:29:VAL:HG21	1.71	1.05
1:2:7:PRO:HA	2:2:235:HOH:O	1.51	1.05
1:1:117:PRO:HB3	1:1:140:ILE:HD11	1.31	1.05
1:2:58:SER:HB3	2:2:269:HOH:O	1.56	1.04
1:1:112:GLN:HG3	1:1:113:PRO:N	1.72	1.03
1:2:23:THR:HG22	2:2:230:HOH:O	1.55	1.03
1:2:116:ASN:ND2	2:2:389:HOH:O	1.89	1.03
1:1:119:VAL:HG22	1:1:208:LYS:HD3	1.37	1.03
1:1:19:THR:CG2	1:1:76:THR:HG22	1.88	1.03
1:2:54:ASN:ND2	2:2:284:HOH:O	1.90	1.03
1:1:68:LYS:HE2	1:1:68:LYS:H	1.21	1.02
1:1:136:LEU:HD21	1:1:210:VAL:HG21	1.37	1.02
1:2:144:TYR:HB3	1:2:145:PRO:CD	1.85	1.02
1:1:9:SER:HB2	1:1:147:ALA:CB	1.90	1.02
1:2:171:GLN:HG2	1:2:173:ASN:HD21	1.22	1.01
1:2:25:THR:HG22	1:2:26:SER:N	1.73	1.01
1:2:112:GLN:HB2	1:2:144:TYR:CE1	1.95	1.01
1:2:134:ALA:HB3	1:2:184:LEU:O	1.61	1.00
1:1:114:LYS:NZ	1:1:202:GLU:HG3	1.76	0.99
1:1:117:PRO:CB	1:1:140:ILE:CD1	2.39	0.99
1:1:214:GLU:HB3	1:1:216:SER:C	1.88	0.99
1:1:25:THR:H	1:1:29:VAL:HG11	1.28	0.98
1:2:25:THR:CG2	1:2:26:SER:H	1.77	0.98
1:2:53:VAL:HG13	1:2:54:ASN:OD1	1.63	0.97
1:1:28:ASP:HA	1:1:32:TYR:HD1	1.28	0.97
1:2:112:GLN:HB2	1:2:144:TYR:HE1	1.27	0.96
1:1:19:THR:HG23	1:1:76:THR:HG22	0.96	0.96
1:1:114:LYS:HZ2	1:1:202:GLU:HG3	1.30	0.95
1:2:49:ILE:O	1:2:50:ILE:HB	1.64	0.95
1:2:52:GLU:O	1:2:53:VAL:HG12	1.67	0.95
1:2:14:LEU:H	1:2:14:LEU:CD1	1.79	0.94
1:1:110:LEU:HD12	1:1:144:TYR:CE1	2.03	0.94
1:1:143:PHE:CE2	1:1:176:TYR:HB2	2.02	0.94
1:1:167:LYS:HZ3	1:2:43:GLY:HA3	1.31	0.94
1:2:17:SER:HA	1:2:77:VAL:O	1.68	0.93
1:1:143:PHE:HE2	1:1:176:TYR:HB2	1.32	0.93
1:2:171:GLN:HG2	1:2:173:ASN:ND2	1.81	0.93
1:1:94:GLU:O	1:1:96:SER:N	2.01	0.93
1:2:18:VAL:HG12	1:2:77:VAL:CG1	1.98	0.93
1:2:121:LEU:HD13	1:2:210:VAL:HB	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:196:SER:HB3	1:2:209:THR:CG2	1.98	0.92
1:2:148:VAL:O	1:2:149:THR:HG23	1.69	0.92
1:1:171:GLN:HE21	1:1:173:ASN:HD21	1.13	0.92
1:1:204:SER:CB	2:1:265:HOH:O	2.18	0.91
1:1:26:SER:O	1:1:28:ASP:N	2.04	0.91
1:1:94:GLU:CG	1:1:95:GLY:H	1.79	0.91
1:1:38:TYR:HE2	1:1:91:SER:HB2	1.34	0.91
1:1:150:VAL:O	2:1:313:HOH:O	1.86	0.91
1:2:117:PRO:O	2:2:336:HOH:O	1.86	0.91
1:1:47:LYS:HZ3	1:1:47:LYS:HB2	1.35	0.90
1:1:167:LYS:NZ	1:2:43:GLY:HA3	1.84	0.90
1:1:1:PCA:O	1:1:2:SER:HB3	1.69	0.90
1:1:20:ILE:HG13	1:1:105:THR:HG21	1.54	0.90
1:2:28:ASP:O	1:2:28:ASP:OD1	1.90	0.90
1:2:144:TYR:CB	1:2:145:PRO:HD3	2.02	0.89
1:2:103:THR:OG1	1:2:104:GLY:N	2.05	0.89
1:1:34:TYR:O	1:1:35:VAL:HG23	1.70	0.89
1:2:148:VAL:HG22	1:2:149:THR:H	1.37	0.89
1:1:23:THR:CG2	1:1:72:THR:HG22	2.02	0.89
1:2:189:TRP:CZ2	1:2:212:PRO:HA	2.08	0.89
1:1:28:ASP:HA	1:1:32:TYR:CD1	2.07	0.89
1:1:68:LYS:HE2	1:1:68:LYS:N	1.87	0.88
1:2:40:GLN:HE21	1:2:40:GLN:HA	1.35	0.88
1:2:42:ALA:CB	2:2:310:HOH:O	2.21	0.88
1:2:16:GLN:NE2	2:2:328:HOH:O	2.05	0.88
1:1:68:LYS:HE3	1:1:68:LYS:O	1.73	0.88
1:1:127:GLU:HG3	2:2:397:HOH:O	1.72	0.87
1:2:133:LYS:O	1:2:186:PRO:HD3	1.74	0.87
1:2:185:THR:HG1	1:2:188:GLN:HB3	1.38	0.87
1:2:14:LEU:H	1:2:14:LEU:HD13	1.37	0.87
1:2:62:ASP:C	1:2:63:ARG:HD2	2.00	0.87
1:1:94:GLU:HB3	1:1:98:ASN:CB	2.05	0.86
1:1:214:GLU:CD	1:1:214:GLU:H	1.84	0.86
1:1:97:ASP:OD1	2:1:257:HOH:O	1.93	0.86
1:1:110:LEU:HD12	1:1:144:TYR:HE1	1.39	0.86
1:1:112:GLN:CG	1:1:113:PRO:N	2.37	0.85
1:2:98:ASN:HD22	1:2:99:PHE:N	1.74	0.85
1:1:52:GLU:O	1:1:53:VAL:CG2	2.21	0.85
1:2:56:ARG:HG2	1:2:60:VAL:HG21	1.57	0.85
1:2:128:GLU:O	1:2:131:ALA:HB3	1.77	0.84
1:1:9:SER:CB	1:1:147:ALA:HB3	2.03	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:30:GLY:C	1:1:32:TYR:N	2.31	0.83
1:2:171:GLN:O	1:2:172:SER:HB3	1.78	0.83
1:1:41:HIS:NE2	2:1:301:HOH:O	2.09	0.83
1:2:98:ASN:HD22	1:2:99:PHE:H	1.26	0.83
1:2:18:VAL:HG12	1:2:77:VAL:HG12	1.60	0.83
1:1:88:TYR:O	1:1:104:GLY:HA2	1.79	0.83
1:2:87:ASP:OD1	1:2:106:LYS:HB2	1.78	0.83
1:1:144:TYR:CD1	1:1:145:PRO:HD3	2.14	0.82
1:2:144:TYR:C	1:2:144:TYR:CD2	2.54	0.82
1:1:93:TYR:HE2	2:1:341:HOH:O	1.63	0.82
1:1:27:SER:OG	2:1:228:HOH:O	1.81	0.82
1:2:39:GLN:O	1:2:87:ASP:O	1.95	0.82
1:1:144:TYR:CG	1:1:145:PRO:HD3	2.15	0.82
1:2:39:GLN:HG2	1:2:88:TYR:CE2	2.14	0.82
1:1:32:TYR:O	1:1:34:TYR:N	2.12	0.81
1:1:28:ASP:CA	1:1:32:TYR:HD1	1.93	0.81
1:1:95:GLY:C	1:1:97:ASP:H	1.87	0.81
1:2:12:GLY:HA3	1:2:80:LEU:CD1	2.11	0.81
1:2:63:ARG:HD2	1:2:63:ARG:N	1.96	0.80
1:2:126:SER:OG	1:2:216:SER:HA	1.80	0.80
1:1:144:TYR:HB3	1:1:145:PRO:HD3	1.61	0.80
1:1:161:ALA:O	2:1:296:HOH:O	1.99	0.80
1:2:18:VAL:HG23	2:2:239:HOH:O	1.81	0.80
1:2:77:VAL:O	1:2:77:VAL:HG13	1.82	0.80
1:1:214:GLU:OE1	1:1:214:GLU:N	2.15	0.79
1:2:86:ALA:O	1:2:106:LYS:HA	1.82	0.79
1:2:149:THR:HB	2:2:352:HOH:O	1.81	0.79
1:2:18:VAL:HG12	1:2:77:VAL:HG11	1.66	0.78
1:1:144:TYR:CB	1:1:145:PRO:HD3	2.12	0.78
1:2:41:HIS:CE1	1:2:83:GLU:O	2.36	0.78
1:2:185:THR:OG1	1:2:188:GLN:HB3	1.84	0.78
1:1:214:GLU:C	1:1:216:SER:N	2.33	0.78
1:2:6:GLN:CG	1:2:7:PRO:HD3	2.13	0.78
1:1:166:THR:O	1:1:166:THR:HG22	1.85	0.77
1:1:123:PRO:O	2:1:271:HOH:O	2.02	0.77
1:1:144:TYR:HB3	1:1:145:PRO:CD	2.13	0.77
1:1:93:TYR:HB2	1:1:99:PHE:HE1	1.50	0.77
1:2:159:VAL:HG21	1:2:182:LEU:HD11	1.67	0.77
1:1:125:SER:O	1:1:129:LEU:HD22	1.84	0.76
1:2:81:GLN:HG3	1:2:84:ASP:CG	2.10	0.76
1:2:144:TYR:C	1:2:144:TYR:HD2	1.93	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:173:ASN:HD22	1:2:173:ASN:H	1.32	0.76
1:1:201:HIS:C	1:1:202:GLU:O	2.24	0.76
1:1:143:PHE:HE2	1:1:176:TYR:CB	1.98	0.76
1:1:47:LYS:HB2	1:1:47:LYS:NZ	1.99	0.76
1:2:4:LEU:CD1	1:2:100:VAL:HG22	2.16	0.76
1:2:98:ASN:ND2	2:2:317:HOH:O	2.18	0.76
1:2:116:ASN:HB3	1:2:117:PRO:HD2	1.68	0.76
1:1:68:LYS:O	1:1:68:LYS:CE	2.34	0.75
1:1:8:PRO:HG3	1:1:149:THR:HG23	1.69	0.75
1:1:81:GLN:HB2	1:1:84:ASP:OD2	1.86	0.75
1:1:214:GLU:CD	1:1:214:GLU:N	2.42	0.75
1:1:119:VAL:CG2	1:1:208:LYS:HD3	2.15	0.75
1:1:25:THR:N	1:1:29:VAL:CG2	2.48	0.75
1:1:25:THR:C	1:1:29:VAL:HG22	2.11	0.75
1:1:30:GLY:C	1:1:32:TYR:H	1.93	0.75
1:1:28:ASP:O	1:1:32:TYR:HB2	1.86	0.75
1:1:144:TYR:CB	1:1:145:PRO:CD	2.65	0.74
1:1:39:GLN:HB2	1:1:49:ILE:HD13	1.69	0.74
1:1:41:HIS:O	1:1:42:ALA:C	2.29	0.74
1:2:170:LYS:NZ	1:2:174:ASN:HB3	2.01	0.74
1:1:94:GLU:HB3	1:1:98:ASN:O	1.86	0.74
1:1:167:LYS:HB2	1:1:168:PRO:CD	2.17	0.74
1:2:170:LYS:HZ1	1:2:174:ASN:HB3	1.51	0.74
1:1:4:LEU:CD1	1:1:22:CYS:SG	2.76	0.74
1:2:14:LEU:CD1	1:2:14:LEU:N	2.50	0.73
1:1:106:LYS:HG3	1:1:147:ALA:HB2	1.70	0.73
1:1:130:GLN:O	1:1:132:ASN:N	2.21	0.73
1:2:17:SER:HA	1:2:78:SER:HA	1.71	0.73
1:1:31:GLY:O	2:1:229:HOH:O	2.06	0.73
1:2:63:ARG:N	1:2:63:ARG:CD	2.50	0.73
1:2:6:GLN:HG3	1:2:7:PRO:HD3	1.69	0.73
1:2:146:GLY:O	1:2:168:PRO:HG2	1.87	0.73
1:2:163:VAL:CG2	1:2:163:VAL:O	2.35	0.73
1:1:26:SER:HA	1:1:71:ASN:HD21	1.53	0.73
1:1:94:GLU:CB	1:1:98:ASN:HB3	2.15	0.73
1:1:170:LYS:CE	1:1:174:ASN:HA	2.18	0.73
1:1:127:GLU:OE2	2:1:273:HOH:O	2.06	0.73
1:2:15:GLY:HA2	1:2:79:GLY:HA2	1.71	0.72
1:2:32:TYR:CE1	2:2:250:HOH:O	2.41	0.72
1:2:37:TRP:CD1	1:2:50:ILE:HG21	2.24	0.72
1:1:28:ASP:CA	1:1:32:TYR:CD1	2.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:117:PRO:CB	1:1:140:ILE:HD13	2.17	0.72
1:1:32:TYR:HE2	1:1:93:TYR:HD1	1.35	0.72
1:2:200:THR:HG22	2:2:325:HOH:O	1.88	0.72
1:1:1:PCA:O	1:1:2:SER:CB	2.36	0.72
1:1:91:SER:OG	1:1:99:PHE:CE2	2.38	0.72
1:2:4:LEU:HD13	1:2:100:VAL:CG2	2.16	0.72
1:1:35:VAL:HA	1:1:91:SER:O	1.88	0.71
1:1:12:GLY:O	1:1:110:LEU:HD22	1.90	0.71
1:2:28:ASP:O	1:2:29:VAL:HB	1.90	0.71
1:2:163:VAL:O	1:2:163:VAL:HG22	1.90	0.71
1:1:136:LEU:HD11	1:1:189:TRP:CZ3	2.25	0.71
1:2:6:GLN:CG	1:2:7:PRO:CD	2.68	0.71
1:2:121:LEU:CD1	1:2:210:VAL:HB	2.20	0.71
1:2:62:ASP:HB3	1:2:63:ARG:HD2	1.72	0.71
1:2:81:GLN:HG3	1:2:84:ASP:OD1	1.91	0.70
1:1:38:TYR:CE2	1:1:91:SER:HB2	2.24	0.70
1:1:52:GLU:C	1:1:53:VAL:HG22	2.16	0.70
1:1:19:THR:C	1:1:20:ILE:HD13	2.17	0.70
1:1:137:VAL:HG23	1:2:122:PHE:CZ	2.27	0.70
1:2:19:THR:HA	1:2:75:LEU:O	1.91	0.70
1:2:143:PHE:CE2	1:2:176:TYR:O	2.44	0.70
1:2:148:VAL:HG22	1:2:149:THR:N	2.05	0.70
1:2:37:TRP:HB2	1:2:50:ILE:HG22	1.74	0.70
1:1:2:SER:H	1:1:100:VAL:HG12	1.57	0.70
1:2:85:GLU:HG3	1:2:108:THR:HA	1.74	0.70
1:2:174:ASN:ND2	2:2:302:HOH:O	2.24	0.70
1:1:23:THR:HG23	1:1:72:THR:CG2	2.15	0.70
1:1:1:PCA:H2	1:1:100:VAL:HG13	1.57	0.69
1:2:150:VAL:O	2:2:370:HOH:O	2.09	0.69
1:2:215:CYS:O	1:2:216:SER:C	2.34	0.69
1:1:26:SER:C	1:1:28:ASP:H	1.98	0.69
1:1:49:ILE:HD12	1:1:64:PHE:CD1	2.27	0.69
1:2:152:TRP:C	1:2:153:LYS:HG2	2.16	0.69
1:2:6:GLN:HG2	1:2:7:PRO:HD2	1.75	0.69
1:1:200:THR:HG23	1:1:205:THR:CG2	2.23	0.69
1:2:12:GLY:HA3	1:2:80:LEU:HD11	1.75	0.69
1:2:214:GLU:O	1:2:215:CYS:HB3	1.93	0.69
1:1:75:LEU:CD1	1:1:75:LEU:C	2.66	0.68
1:2:41:HIS:HE1	1:2:83:GLU:O	1.74	0.68
1:2:171:GLN:HB3	1:2:175:LYS:O	1.93	0.68
1:2:144:TYR:CB	1:2:145:PRO:CD	2.60	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:34:TYR:O	1:1:35:VAL:CG2	2.42	0.68
1:1:75:LEU:C	1:1:75:LEU:HD13	2.18	0.68
1:1:26:SER:N	1:1:29:VAL:HG22	2.09	0.68
1:1:51:TYR:CE2	1:1:57:PRO:HB3	2.28	0.68
1:1:121:LEU:HD12	1:1:137:VAL:O	1.93	0.68
1:1:170:LYS:HE2	1:1:174:ASN:HA	1.74	0.68
1:1:215:CYS:O	1:1:216:SER:CB	2.42	0.68
1:1:28:ASP:HB2	1:1:32:TYR:CE1	2.29	0.67
1:2:62:ASP:CB	1:2:63:ARG:HD2	2.24	0.67
1:1:49:ILE:HD12	1:1:64:PHE:CE1	2.29	0.67
1:2:37:TRP:HD1	1:2:50:ILE:HG21	1.59	0.67
1:1:165:THR:OG1	1:1:180:SER:HB3	1.93	0.67
1:2:37:TRP:HB2	1:2:50:ILE:CG2	2.25	0.67
1:2:70:GLY:C	1:2:72:THR:H	2.03	0.67
1:2:6:GLN:OE1	1:2:102:GLY:O	2.13	0.67
1:2:196:SER:CB	1:2:209:THR:HG23	2.12	0.67
1:1:166:THR:O	1:1:166:THR:CG2	2.42	0.67
1:1:137:VAL:CG2	1:2:122:PHE:CZ	2.78	0.67
1:1:94:GLU:HG2	1:1:95:GLY:H	1.60	0.66
1:1:121:LEU:HD22	1:1:197:CYS:HB3	1.75	0.66
1:2:47:LYS:HD3	1:2:49:ILE:HG23	1.77	0.66
1:2:77:VAL:O	1:2:77:VAL:CG1	2.43	0.66
1:2:95:GLY:O	1:2:96:SER:HB2	1.94	0.66
1:1:25:THR:H	1:1:29:VAL:CG1	2.04	0.66
1:1:130:GLN:C	1:1:132:ASN:H	2.04	0.66
1:2:40:GLN:HA	1:2:40:GLN:NE2	2.10	0.66
1:1:28:ASP:O	1:1:32:TYR:N	2.29	0.66
1:1:92:SER:C	1:1:100:VAL:HG23	2.20	0.66
1:1:30:GLY:O	1:1:32:TYR:N	2.28	0.66
1:1:201:HIS:O	1:1:202:GLU:HB2	1.96	0.66
1:2:6:GLN:HG2	1:2:7:PRO:CD	2.26	0.66
1:2:51:TYR:HD2	1:2:52:GLU:HB2	1.58	0.66
1:2:171:GLN:OE1	1:2:177:ALA:HB2	1.97	0.65
1:1:31:GLY:C	2:1:229:HOH:O	2.39	0.65
1:1:201:HIS:O	1:1:202:GLU:O	2.14	0.65
1:1:213:THR:HG22	1:1:213:THR:O	1.95	0.65
1:2:112:GLN:CB	1:2:144:TYR:CE1	2.77	0.65
1:1:29:VAL:HA	2:1:253:HOH:O	1.96	0.65
1:1:119:VAL:HG13	1:1:206:VAL:HG11	1.78	0.65
1:2:150:VAL:HG22	1:2:199:VAL:HB	1.79	0.65
1:2:164:GLU:HB2	1:2:181:TYR:CE1	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:11:SER:HG	1:1:202:GLU:CD	2.05	0.65
1:1:6:GLN:O	2:1:259:HOH:O	2.14	0.65
1:1:117:PRO:HB2	1:1:140:ILE:CD1	2.27	0.65
1:2:10:ALA:O	1:2:107:VAL:HB	1.97	0.65
1:1:94:GLU:CD	1:1:98:ASN:ND2	2.55	0.64
1:1:47:LYS:NZ	1:1:47:LYS:CB	2.58	0.64
1:2:80:LEU:HB3	1:2:109:VAL:HG12	1.80	0.64
1:2:125:SER:O	1:2:126:SER:C	2.39	0.64
1:2:42:ALA:HB2	2:2:310:HOH:O	1.93	0.64
1:2:32:TYR:CD1	1:2:32:TYR:N	2.65	0.64
1:1:32:TYR:CE2	1:1:93:TYR:HD1	2.14	0.64
1:1:51:TYR:CE1	1:1:55:LYS:HG2	2.32	0.64
1:2:4:LEU:CD1	1:2:100:VAL:CG2	2.75	0.64
1:1:53:VAL:HG23	1:1:54:ASN:H	1.63	0.64
1:1:94:GLU:HG3	1:1:95:GLY:H	1.59	0.64
1:1:204:SER:HB2	2:1:265:HOH:O	1.90	0.64
1:2:8:PRO:HD3	2:2:235:HOH:O	1.97	0.64
1:2:81:GLN:CG	1:2:84:ASP:OD2	2.45	0.64
1:1:1:PCA:N	1:1:98:ASN:HD21	1.95	0.63
1:1:24:GLY:HA3	1:1:29:VAL:HB	1.80	0.63
1:2:50:ILE:HA	1:2:55:LYS:O	1.99	0.63
1:2:56:ARG:HD3	1:2:64:PHE:O	1.97	0.63
1:2:57:PRO:HG2	1:2:60:VAL:HG13	1.79	0.63
1:1:1:PCA:H2	1:1:98:ASN:HD21	1.45	0.63
1:1:37:TRP:CE2	1:1:75:LEU:HB2	2.34	0.63
1:1:101:PHE:CE2	1:2:46:PRO:HG2	2.34	0.63
2:1:314:HOH:O	1:2:171:GLN:NE2	2.30	0.63
1:1:16:GLN:NE2	2:1:243:HOH:O	2.31	0.63
1:2:107:VAL:HG23	1:2:108:THR:N	2.13	0.63
1:1:28:ASP:CB	1:1:32:TYR:CD1	2.82	0.62
1:1:95:GLY:O	1:1:97:ASP:N	2.29	0.62
1:2:18:VAL:O	1:2:76:THR:HA	1.98	0.62
1:2:114:LYS:HB2	2:2:326:HOH:O	1.97	0.62
1:1:24:GLY:CA	1:1:29:VAL:HG21	2.29	0.62
1:1:137:VAL:HG21	1:2:122:PHE:CE2	2.34	0.62
1:1:166:THR:O	1:1:178:ALA:HB1	2.00	0.62
1:2:4:LEU:O	1:2:102:GLY:HA3	1.99	0.62
1:2:13:SER:O	1:2:14:LEU:C	2.41	0.62
1:1:20:ILE:HD13	1:1:20:ILE:N	2.15	0.62
1:2:171:GLN:O	1:2:171:GLN:CG	2.47	0.62
1:1:28:ASP:CB	1:1:32:TYR:CE1	2.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:114:LYS:HZ3	1:1:202:GLU:HG3	1.63	0.62
1:2:93:TYR:CE2	1:2:95:GLY:HA2	2.34	0.62
1:1:93:TYR:CD2	2:1:258:HOH:O	2.52	0.62
1:2:81:GLN:HG3	1:2:84:ASP:OD2	1.99	0.62
1:1:18:VAL:O	1:1:76:THR:HB	2.00	0.62
1:1:53:VAL:HG23	1:1:54:ASN:N	2.13	0.62
1:2:70:GLY:O	1:2:72:THR:N	2.31	0.62
1:1:85:GLU:O	1:1:86:ALA:HB2	2.00	0.61
1:1:140:ILE:O	1:1:177:ALA:HB1	1.99	0.61
1:1:16:GLN:CB	2:1:283:HOH:O	2.48	0.61
1:1:127:GLU:O	1:1:130:GLN:N	2.32	0.61
1:1:192:HIS:ND1	1:1:192:HIS:N	2.43	0.61
1:1:215:CYS:O	1:1:216:SER:OG	2.15	0.61
1:2:52:GLU:O	1:2:53:VAL:CG1	2.45	0.61
1:2:141:SER:O	1:2:142:ASP:CB	2.47	0.61
1:2:189:TRP:CH2	1:2:212:PRO:HA	2.36	0.61
1:1:114:LYS:NZ	1:1:202:GLU:CG	2.59	0.61
1:2:215:CYS:SG	1:2:216:SER:N	2.74	0.61
1:1:117:PRO:HB2	1:1:140:ILE:HD13	1.80	0.61
1:1:150:VAL:HG11	1:1:180:SER:OG	2.01	0.60
1:2:185:THR:HG23	1:2:188:GLN:OE1	2.01	0.60
1:1:94:GLU:CD	1:1:98:ASN:CG	2.70	0.60
1:1:28:ASP:OD2	1:1:32:TYR:CD1	2.54	0.60
1:1:136:LEU:HD21	1:1:210:VAL:CG2	2.22	0.60
1:1:57:PRO:HD2	1:1:60:VAL:HG11	1.83	0.60
1:2:125:SER:O	1:2:129:LEU:HD12	2.02	0.60
1:1:19:THR:HG23	1:1:76:THR:HG21	1.78	0.60
1:1:19:THR:CG2	1:1:76:THR:CG2	2.61	0.60
1:1:94:GLU:CG	1:1:95:GLY:N	2.56	0.60
1:2:88:TYR:O	1:2:104:GLY:C	2.45	0.60
1:1:201:HIS:O	1:1:202:GLU:CB	2.50	0.60
1:1:94:GLU:HB3	1:1:98:ASN:CG	2.27	0.60
1:1:114:LYS:HA	1:1:144:TYR:CB	2.31	0.59
1:2:125:SER:O	1:2:128:GLU:N	2.35	0.59
1:2:122:PHE:HB2	1:2:137:VAL:HG12	1.84	0.59
1:2:211:ALA:O	1:2:213:THR:N	2.35	0.59
1:1:29:VAL:HG23	1:1:29:VAL:O	2.02	0.59
1:2:88:TYR:H	1:2:105:THR:H	1.48	0.59
1:1:185:THR:HG23	1:1:188:GLN:HG3	1.83	0.59
1:2:129:LEU:C	1:2:131:ALA:N	2.58	0.59
1:1:162:GLY:O	1:1:182:LEU:HD23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:144:TYR:CG	1:1:145:PRO:CD	2.86	0.59
1:2:152:TRP:O	1:2:153:LYS:HG2	2.03	0.59
1:1:25:THR:O	1:1:29:VAL:HG13	2.03	0.58
1:2:17:SER:CA	1:2:78:SER:HA	2.31	0.58
1:2:46:PRO:O	1:2:47:LYS:HB3	2.02	0.58
1:2:81:GLN:N	1:2:84:ASP:OD2	2.36	0.58
1:1:36:SER:HB3	1:1:51:TYR:HA	1.85	0.58
1:2:169:SER:O	1:2:176:TYR:HA	2.03	0.58
1:1:97:ASP:HA	1:2:51:TYR:OH	2.04	0.58
1:1:127:GLU:O	1:1:128:GLU:C	2.46	0.58
1:1:141:SER:O	1:1:142:ASP:HB2	2.03	0.58
1:1:8:PRO:HG3	1:1:149:THR:CG2	2.33	0.58
1:1:41:HIS:O	1:1:42:ALA:O	2.21	0.58
1:1:140:ILE:HD11	1:1:143:PHE:CE1	2.39	0.58
1:1:143:PHE:CE2	1:1:176:TYR:C	2.82	0.58
1:2:53:VAL:CG1	2:2:262:HOH:O	2.51	0.58
1:1:200:THR:HA	1:1:205:THR:HG22	1.85	0.58
1:2:145:PRO:O	1:2:201:HIS:HE1	1.86	0.58
1:1:93:TYR:CE2	2:1:258:HOH:O	2.52	0.58
1:1:167:LYS:CB	1:1:168:PRO:HD3	2.33	0.58
1:1:213:THR:HG23	1:1:215:CYS:N	2.19	0.58
1:2:23:THR:C	2:2:230:HOH:O	2.47	0.58
1:2:57:PRO:HG2	1:2:60:VAL:CG1	2.34	0.58
1:2:148:VAL:CG2	1:2:149:THR:H	2.14	0.57
1:1:94:GLU:HB3	1:1:98:ASN:ND2	2.19	0.57
1:2:8:PRO:CD	2:2:235:HOH:O	2.52	0.57
1:2:87:ASP:OD1	1:2:106:LYS:CB	2.50	0.57
1:1:148:VAL:HG12	1:1:201:HIS:HB2	1.85	0.57
1:1:141:SER:HA	1:1:177:ALA:HB2	1.85	0.57
1:2:129:LEU:C	1:2:131:ALA:H	2.12	0.57
1:1:51:TYR:C	1:1:53:VAL:H	2.12	0.57
1:2:4:LEU:O	1:2:102:GLY:CA	2.52	0.57
1:1:28:ASP:CG	1:1:32:TYR:CD1	2.83	0.57
1:1:144:TYR:O	1:1:145:PRO:C	2.47	0.57
1:2:11:SER:HA	1:2:108:THR:O	2.04	0.57
1:2:61:PRO:C	1:2:63:ARG:H	2.12	0.57
1:1:28:ASP:HB2	1:1:32:TYR:HE1	1.70	0.57
1:2:38:TYR:CE2	1:2:101:PHE:CZ	2.93	0.57
1:1:1:PCA:H2	1:1:100:VAL:CG1	2.18	0.57
1:1:25:THR:C	1:1:29:VAL:CG2	2.78	0.57
1:2:4:LEU:HB2	1:2:102:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:94:GLU:CB	1:1:98:ASN:ND2	2.67	0.56
1:2:68:LYS:HA	1:2:73:ALA:HA	1.87	0.56
1:2:214:GLU:HG3	1:2:215:CYS:N	2.20	0.56
1:1:16:GLN:HB3	2:1:283:HOH:O	2.05	0.56
1:1:25:THR:C	2:1:225:HOH:O	2.48	0.56
1:1:149:THR:OG1	1:1:200:THR:HB	2.05	0.56
1:1:201:HIS:O	1:1:201:HIS:CD2	2.58	0.56
1:1:213:THR:O	1:1:213:THR:CG2	2.54	0.56
1:2:28:ASP:O	1:2:29:VAL:CB	2.53	0.56
1:2:32:TYR:HE1	2:2:250:HOH:O	1.83	0.56
1:2:47:LYS:HE2	1:2:49:ILE:CG2	2.34	0.56
1:1:51:TYR:HE2	1:1:57:PRO:HB3	1.71	0.56
1:2:7:PRO:CA	2:2:235:HOH:O	2.29	0.56
1:1:34:TYR:O	1:1:35:VAL:CB	2.53	0.56
1:1:214:GLU:HB3	1:1:216:SER:OXT	2.04	0.56
1:2:5:THR:HG21	2:2:244:HOH:O	2.05	0.56
1:2:20:ILE:HD13	1:2:105:THR:HG21	1.88	0.56
1:2:141:SER:O	1:2:142:ASP:HB2	2.03	0.56
1:2:25:THR:CG2	1:2:26:SER:N	2.42	0.56
1:2:85:GLU:OE2	1:2:108:THR:HG22	2.06	0.56
1:2:98:ASN:ND2	1:2:99:PHE:N	2.50	0.56
1:2:155:ASP:OD1	1:2:193:ARG:HB2	2.05	0.56
1:2:25:THR:N	1:2:28:ASP:O	2.25	0.55
1:2:53:VAL:HG11	2:2:262:HOH:O	2.04	0.55
1:1:94:GLU:CG	1:1:98:ASN:CG	2.80	0.55
1:2:133:LYS:CB	1:2:133:LYS:HZ3	2.20	0.55
1:1:6:GLN:HE22	1:1:104:GLY:HA2	1.70	0.55
1:1:30:GLY:O	1:1:33:ASN:N	2.37	0.55
1:1:94:GLU:C	1:1:96:SER:N	2.65	0.55
1:1:117:PRO:HB3	1:1:140:ILE:HD12	1.81	0.55
1:2:7:PRO:HD2	1:2:105:THR:OG1	2.07	0.55
1:2:65:SER:O	1:2:75:LEU:CD2	2.54	0.55
1:1:116:ASN:ND2	1:1:116:ASN:H	2.03	0.55
1:2:85:GLU:CD	1:2:108:THR:HG22	2.32	0.55
1:2:125:SER:C	1:2:129:LEU:HD12	2.32	0.55
1:2:20:ILE:CG1	1:2:105:THR:HG21	2.36	0.55
1:1:6:GLN:OE1	1:1:90:CYS:SG	2.65	0.55
1:1:1:PCA:N	1:1:100:VAL:CG1	2.70	0.54
1:2:167:LYS:HE3	2:2:307:HOH:O	2.07	0.54
1:1:164:GLU:HG3	1:2:171:GLN:HG3	1.89	0.54
1:2:94:GLU:HA	2:2:250:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:42:ALA:HB3	2:2:310:HOH:O	2.00	0.54
1:1:26:SER:C	1:1:28:ASP:N	2.56	0.54
1:1:97:ASP:HA	1:2:51:TYR:CE1	2.43	0.54
1:1:115:ALA:H	1:1:144:TYR:HB2	1.73	0.54
1:2:16:GLN:H	1:2:79:GLY:HA2	1.73	0.54
1:2:62:ASP:HB3	1:2:63:ARG:CD	2.35	0.54
1:1:28:ASP:O	1:1:32:TYR:CB	2.55	0.54
1:2:14:LEU:N	1:2:14:LEU:HD12	2.20	0.54
1:2:144:TYR:O	1:2:145:PRO:C	2.48	0.54
1:1:93:TYR:HB2	1:1:99:PHE:CE1	2.37	0.54
1:2:62:ASP:CA	1:2:63:ARG:HD2	2.37	0.54
1:2:140:ILE:HD11	1:2:150:VAL:HG21	1.90	0.54
1:1:30:GLY:O	1:1:31:GLY:C	2.50	0.54
1:2:143:PHE:O	1:2:175:LYS:HA	2.08	0.54
1:1:11:SER:OG	1:1:202:GLU:CD	2.51	0.53
1:1:25:THR:N	1:1:29:VAL:HG11	2.11	0.53
1:1:164:GLU:OE1	1:2:171:GLN:O	2.26	0.53
1:2:91:SER:HB2	1:2:101:PHE:CE1	2.43	0.53
1:2:159:VAL:O	1:2:160:LYS:HD2	2.09	0.53
1:1:28:ASP:O	1:1:30:GLY:N	2.42	0.53
1:2:37:TRP:H	1:2:50:ILE:HG22	1.72	0.53
1:1:12:GLY:C	1:1:110:LEU:HD22	2.34	0.53
1:2:6:GLN:OE1	1:2:103:THR:O	2.25	0.53
1:2:20:ILE:CD1	1:2:105:THR:HG21	2.39	0.53
1:1:143:PHE:CE1	1:1:148:VAL:HG11	2.44	0.53
1:2:20:ILE:HG12	1:2:105:THR:HG21	1.89	0.53
1:2:8:PRO:O	1:2:9:SER:HB2	2.09	0.52
1:1:91:SER:OG	1:1:99:PHE:CD2	2.59	0.52
1:1:170:LYS:HE3	1:1:174:ASN:HA	1.91	0.52
1:1:121:LEU:HD11	1:1:152:TRP:CH2	2.45	0.52
1:1:215:CYS:O	1:1:215:CYS:SG	2.67	0.52
1:1:6:GLN:HB2	1:1:103:THR:OG1	2.10	0.52
1:1:140:ILE:HD11	1:1:143:PHE:CD1	2.45	0.52
1:2:56:ARG:O	1:2:57:PRO:O	2.28	0.52
1:2:189:TRP:CH2	1:2:212:PRO:CA	2.93	0.52
1:2:32:TYR:CZ	2:2:250:HOH:O	2.62	0.52
1:2:38:TYR:CE2	1:2:101:PHE:HZ	2.28	0.52
1:2:89:TYR:CE2	1:2:104:GLY:HA2	2.45	0.52
1:2:140:ILE:CD1	1:2:150:VAL:HG21	2.39	0.52
1:2:148:VAL:O	1:2:149:THR:CG2	2.52	0.52
1:1:110:LEU:HD12	1:1:144:TYR:CD1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:62:ASP:O	1:2:62:ASP:CG	2.52	0.52
1:1:200:THR:HG23	1:1:205:THR:HG22	1.91	0.52
1:2:50:ILE:CG2	1:2:50:ILE:O	2.58	0.52
1:2:126:SER:OG	1:2:216:SER:HB2	2.10	0.52
1:2:143:PHE:CD2	1:2:176:TYR:O	2.62	0.51
1:1:166:THR:O	1:1:167:LYS:C	2.53	0.51
1:1:114:LYS:HZ3	1:1:202:GLU:CG	2.20	0.51
1:1:137:VAL:HG21	1:2:122:PHE:CZ	2.45	0.51
1:1:19:THR:C	1:1:20:ILE:CD1	2.83	0.51
1:1:38:TYR:HB3	1:1:47:LYS:O	2.10	0.51
1:1:75:LEU:HD13	1:1:76:THR:N	2.26	0.51
1:1:106:LYS:HG3	1:1:147:ALA:CB	2.41	0.51
1:1:140:ILE:HD13	1:1:199:VAL:HG11	1.93	0.51
1:1:214:GLU:C	1:1:216:SER:H	2.09	0.51
1:2:31:GLY:C	1:2:32:TYR:CD1	2.89	0.51
1:1:155:ASP:OD2	1:1:193:ARG:HB2	2.11	0.51
1:2:213:THR:O	1:2:213:THR:HG22	2.11	0.51
1:1:130:GLN:C	1:1:132:ASN:N	2.67	0.51
1:2:171:GLN:O	1:2:171:GLN:HG3	2.09	0.51
1:2:189:TRP:CZ2	1:2:212:PRO:CA	2.89	0.51
1:1:20:ILE:N	1:1:20:ILE:CD1	2.73	0.50
1:1:32:TYR:HE2	1:1:93:TYR:CD1	2.22	0.50
1:2:128:GLU:CG	1:2:133:LYS:HB2	2.41	0.50
1:1:123:PRO:CB	1:1:124:PRO:CD	2.89	0.50
1:1:126:SER:O	1:1:127:GLU:C	2.55	0.50
1:2:15:GLY:HA2	1:2:79:GLY:CA	2.40	0.50
1:1:26:SER:HA	1:1:71:ASN:ND2	2.25	0.50
1:2:51:TYR:O	1:2:55:LYS:HB2	2.11	0.50
1:1:97:ASP:HA	1:2:51:TYR:CZ	2.47	0.50
1:1:114:LYS:HA	1:1:144:TYR:HB2	1.93	0.50
1:2:1:PCA:O	2:2:226:HOH:O	2.20	0.50
1:2:43:GLY:HA2	2:2:309:HOH:O	2.12	0.50
1:1:21:SER:HB3	2:1:220:HOH:O	2.12	0.50
1:1:145:PRO:O	1:1:201:HIS:HE1	1.95	0.50
1:1:11:SER:HB2	1:1:110:LEU:HD11	1.94	0.50
1:1:116:ASN:HB3	1:1:117:PRO:HD3	1.93	0.50
1:1:167:LYS:CB	1:1:168:PRO:CD	2.81	0.50
1:2:182:LEU:HD23	1:2:183:SER:N	2.26	0.50
1:1:27:SER:O	1:1:28:ASP:CB	2.59	0.49
1:1:121:LEU:HD13	1:1:138:CYS:HB2	1.92	0.49
1:1:20:ILE:CG2	1:1:105:THR:OG1	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:116:ASN:HB3	1:1:117:PRO:CD	2.42	0.49
1:2:39:GLN:O	1:2:40:GLN:CB	2.61	0.49
1:2:13:SER:O	1:2:14:LEU:O	2.31	0.49
1:2:68:LYS:HB2	1:2:68:LYS:NZ	2.27	0.49
1:1:1:PCA:CD	1:1:94:GLU:OE1	2.61	0.49
1:1:121:LEU:HD13	1:1:138:CYS:CB	2.43	0.49
1:1:167:LYS:HE2	2:2:371:HOH:O	2.13	0.49
1:1:214:GLU:CB	1:1:216:SER:H	2.25	0.49
1:2:8:PRO:O	1:2:9:SER:CB	2.61	0.49
1:2:144:TYR:CG	1:2:145:PRO:N	2.78	0.49
1:1:95:GLY:O	1:1:96:SER:OG	2.30	0.49
1:2:133:LYS:HZ3	1:2:133:LYS:HB3	1.77	0.49
1:1:34:TYR:HB3	2:1:288:HOH:O	2.13	0.49
1:1:145:PRO:HB2	2:1:261:HOH:O	2.12	0.49
1:2:50:ILE:CD1	1:2:56:ARG:HG3	2.43	0.49
1:1:152:TRP:O	1:1:159:VAL:HG23	2.13	0.49
1:1:214:GLU:HB2	1:1:216:SER:H	1.77	0.49
1:2:51:TYR:CD2	1:2:52:GLU:HB2	2.44	0.49
1:2:95:GLY:O	1:2:96:SER:CB	2.61	0.49
1:2:145:PRO:HD2	1:2:201:HIS:CE1	2.48	0.49
1:1:56:ARG:HB2	1:1:60:VAL:CG1	2.42	0.49
1:1:112:GLN:HG3	1:1:113:PRO:CD	2.43	0.49
1:1:214:GLU:O	1:1:215:CYS:C	2.56	0.49
2:1:314:HOH:O	1:2:171:GLN:CD	2.55	0.49
1:2:88:TYR:H	1:2:105:THR:N	2.10	0.49
1:1:24:GLY:HA3	1:1:29:VAL:CB	2.41	0.48
1:1:81:GLN:HB2	1:1:84:ASP:CG	2.38	0.48
1:2:14:LEU:H	1:2:14:LEU:HD12	1.67	0.48
1:2:49:ILE:O	1:2:50:ILE:CB	2.46	0.48
1:2:61:PRO:HG2	1:2:64:PHE:CD1	2.48	0.48
1:2:159:VAL:C	1:2:160:LYS:HD2	2.39	0.48
1:1:117:PRO:CB	1:1:140:ILE:HD12	2.38	0.48
1:2:88:TYR:HB2	1:2:105:THR:HB	1.95	0.48
1:2:128:GLU:HG3	1:2:133:LYS:HB2	1.94	0.48
1:2:61:PRO:O	1:2:63:ARG:N	2.47	0.48
1:2:71:ASN:ND2	1:2:71:ASN:H	2.10	0.48
1:2:145:PRO:O	1:2:201:HIS:CE1	2.65	0.48
1:1:63:ARG:HH11	1:1:81:GLN:HB2	1.78	0.48
1:2:116:ASN:ND2	1:2:204:SER:HB2	2.29	0.48
1:2:14:LEU:O	1:2:15:GLY:O	2.32	0.48
1:2:50:ILE:HD13	1:2:56:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:134:ALA:HB3	1:2:184:LEU:C	2.33	0.48
1:1:214:GLU:CB	1:1:216:SER:C	2.76	0.47
1:2:2:SER:O	1:2:3:ALA:C	2.57	0.47
1:2:25:THR:HG22	1:2:27:SER:H	1.78	0.47
1:2:32:TYR:O	1:2:33:ASN:OD1	2.33	0.47
1:2:43:GLY:CA	2:2:309:HOH:O	2.62	0.47
1:2:131:ALA:O	1:2:132:ASN:CB	2.62	0.47
1:1:214:GLU:O	1:1:215:CYS:HB3	2.14	0.47
1:2:131:ALA:O	1:2:132:ASN:HB2	2.14	0.47
1:2:209:THR:O	2:2:401:HOH:O	2.20	0.47
1:2:202:GLU:HA	2:2:388:HOH:O	2.13	0.47
1:1:160:LYS:O	1:1:160:LYS:HG3	2.09	0.47
1:2:17:SER:CA	1:2:77:VAL:O	2.51	0.47
1:2:20:ILE:HD13	1:2:105:THR:CG2	2.44	0.47
1:1:201:HIS:O	1:1:201:HIS:CG	2.60	0.47
1:1:58:SER:C	1:1:60:VAL:H	2.21	0.47
1:1:124:PRO:HB2	1:1:129:LEU:CD2	2.45	0.47
1:1:141:SER:HA	1:1:177:ALA:CB	2.44	0.47
1:1:141:SER:CA	1:1:177:ALA:HB2	2.44	0.47
1:1:173:ASN:OD1	1:1:175:LYS:HG3	2.14	0.47
1:2:47:LYS:HD3	1:2:49:ILE:CG2	2.43	0.47
1:1:28:ASP:CG	1:1:32:TYR:CE1	2.92	0.47
1:1:95:GLY:C	1:1:97:ASP:N	2.59	0.47
1:2:65:SER:O	1:2:75:LEU:HD22	2.14	0.47
1:2:81:GLN:CB	1:2:84:ASP:OD2	2.63	0.47
1:2:28:ASP:C	1:2:29:VAL:HG23	2.39	0.47
1:2:40:GLN:NE2	1:2:46:PRO:HA	2.30	0.47
1:2:44:LYS:NZ	2:2:218:HOH:O	2.30	0.47
1:2:61:PRO:CG	1:2:64:PHE:CE1	2.98	0.47
1:1:63:ARG:NH1	1:1:81:GLN:HB2	2.30	0.46
1:1:143:PHE:O	1:1:144:TYR:O	2.33	0.46
1:1:182:LEU:HD23	1:1:182:LEU:HA	1.65	0.46
1:1:34:TYR:O	1:1:35:VAL:HB	2.16	0.46
1:2:9:SER:O	1:2:10:ALA:HB2	2.14	0.46
1:2:144:TYR:O	1:2:146:GLY:N	2.48	0.46
1:2:154:ALA:O	1:2:155:ASP:C	2.57	0.46
1:2:185:THR:CG2	1:2:188:GLN:OE1	2.62	0.46
1:1:144:TYR:HD2	1:1:144:TYR:HA	1.52	0.46
1:2:17:SER:CB	1:2:78:SER:HA	2.45	0.46
1:2:89:TYR:CD2	1:2:104:GLY:HA2	2.49	0.46
1:1:114:LYS:HZ3	1:1:202:GLU:CD	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:35:VAL:HG23	2:2:311:HOH:O	2.15	0.46
1:2:39:GLN:HB2	1:2:47:LYS:HD3	1.98	0.46
1:1:29:VAL:CG2	1:1:29:VAL:O	2.63	0.46
1:1:167:LYS:HB2	1:1:168:PRO:HD3	1.90	0.46
1:1:17:SER:CB	2:1:221:HOH:O	2.63	0.46
1:1:116:ASN:CB	1:1:117:PRO:CD	2.94	0.46
2:1:345:HOH:O	1:2:127:GLU:HG2	2.16	0.46
1:1:51:TYR:C	1:1:53:VAL:N	2.74	0.46
1:2:65:SER:O	1:2:75:LEU:HD23	2.16	0.45
1:2:120:THR:HG22	1:2:122:PHE:CE2	2.51	0.45
1:2:152:TRP:CD1	1:2:152:TRP:N	2.85	0.45
1:2:18:VAL:C	1:2:19:THR:OG1	2.59	0.45
1:2:126:SER:OG	1:2:216:SER:CA	2.59	0.45
1:2:56:ARG:HA	1:2:57:PRO:HD2	1.71	0.45
1:2:167:LYS:O	1:2:167:LYS:CG	2.64	0.45
1:2:133:LYS:O	1:2:134:ALA:CB	2.65	0.45
1:1:16:GLN:NE2	1:1:17:SER:H	2.14	0.45
1:1:93:TYR:HA	1:1:99:PHE:CD1	2.52	0.45
1:2:28:ASP:HB2	1:2:100:VAL:HG11	1.99	0.45
1:2:37:TRP:HD1	1:2:50:ILE:CG2	2.27	0.45
1:1:20:ILE:HG23	1:1:105:THR:OG1	2.17	0.45
1:1:94:GLU:OE2	1:1:98:ASN:OD1	2.35	0.45
1:1:60:VAL:HA	1:1:61:PRO:HD2	1.79	0.44
1:1:143:PHE:HE1	1:1:148:VAL:HG11	1.82	0.44
1:2:39:GLN:HG2	1:2:88:TYR:HE2	1.76	0.44
1:2:96:SER:O	1:2:98:ASN:HB3	2.17	0.44
1:1:25:THR:N	1:1:29:VAL:CG1	2.76	0.44
1:2:11:SER:HB3	1:2:110:LEU:CD1	2.48	0.44
1:2:12:GLY:CA	1:2:80:LEU:CD1	2.92	0.44
1:2:50:ILE:HD12	1:2:55:LYS:C	2.43	0.44
1:2:106:LYS:HB2	1:2:106:LYS:HE2	1.62	0.44
1:1:4:LEU:HD13	1:1:90:CYS:SG	2.57	0.44
1:1:34:TYR:CD2	1:1:52:GLU:HA	2.53	0.44
1:2:144:TYR:HD2	1:2:144:TYR:O	2.01	0.44
1:2:37:TRP:CD1	1:2:50:ILE:CG2	3.00	0.44
1:2:80:LEU:HD22	1:2:109:VAL:CG1	2.47	0.44
1:2:109:VAL:HG23	1:2:112:GLN:NE2	2.33	0.44
1:1:17:SER:HA	1:1:77:VAL:O	2.18	0.44
1:2:54:ASN:ND2	2:2:282:HOH:O	2.50	0.43
1:2:56:ARG:CG	1:2:60:VAL:HG21	2.38	0.43
1:2:129:LEU:O	1:2:131:ALA:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:109:VAL:C	1:2:110:LEU:HD12	2.43	0.43
1:1:7:PRO:HA	1:1:8:PRO:HD2	1.91	0.43
1:1:69:SER:CB	2:1:237:HOH:O	2.66	0.43
1:1:200:THR:CA	1:1:205:THR:HG22	2.48	0.43
1:2:17:SER:HA	1:2:77:VAL:C	2.41	0.43
1:1:94:GLU:OE1	1:1:98:ASN:ND2	2.51	0.43
1:1:97:ASP:O	1:1:98:ASN:CB	2.35	0.43
1:2:38:TYR:CE1	1:2:48:VAL:HG22	2.53	0.43
1:2:62:ASP:C	1:2:63:ARG:CD	2.79	0.43
1:2:82:ALA:HA	1:2:109:VAL:HG21	2.00	0.43
1:2:141:SER:O	1:2:142:ASP:HB3	2.16	0.43
1:1:125:SER:O	1:1:129:LEU:CD2	2.61	0.43
1:1:94:GLU:CB	1:1:98:ASN:CG	2.91	0.43
1:2:56:ARG:HG2	1:2:60:VAL:CG2	2.38	0.43
1:2:152:TRP:CD1	1:2:163:VAL:HG21	2.53	0.43
1:1:167:LYS:CE	2:2:371:HOH:O	2.67	0.43
1:2:154:ALA:O	1:2:156:GLY:N	2.51	0.43
1:1:202:GLU:O	1:1:204:SER:N	2.39	0.43
1:1:32:TYR:C	1:1:34:TYR:H	2.20	0.43
1:1:56:ARG:HB2	1:1:60:VAL:HG12	2.00	0.43
1:1:11:SER:OG	1:1:202:GLU:OE1	2.29	0.43
1:1:215:CYS:O	1:1:216:SER:HB2	2.15	0.43
1:2:167:LYS:O	1:2:167:LYS:HG2	2.18	0.43
1:1:41:HIS:CE1	2:1:301:HOH:O	2.64	0.42
1:2:11:SER:HB3	1:2:110:LEU:HD11	2.00	0.42
1:2:162:GLY:O	1:2:182:LEU:HA	2.18	0.42
1:2:164:GLU:HB2	1:2:181:TYR:CZ	2.54	0.42
1:1:92:SER:O	1:1:99:PHE:CE1	2.72	0.42
1:2:20:ILE:CG2	1:2:105:THR:HG21	2.49	0.42
1:2:91:SER:CB	1:2:101:PHE:CE1	3.01	0.42
1:2:80:LEU:HD22	1:2:109:VAL:HG12	2.00	0.42
1:1:125:SER:OG	1:1:128:GLU:HB2	2.20	0.42
1:1:186:PRO:O	1:1:187:GLU:C	2.63	0.42
1:1:196:SER:HA	1:1:208:LYS:O	2.19	0.42
1:2:133:LYS:HB3	1:2:133:LYS:HE2	1.82	0.42
1:2:91:SER:HB2	1:2:101:PHE:CD1	2.54	0.42
1:2:187:GLU:H	1:2:187:GLU:HG3	1.32	0.42
1:1:119:VAL:HG13	1:1:206:VAL:CG1	2.49	0.42
1:2:144:TYR:CD2	1:2:145:PRO:N	2.87	0.42
1:1:27:SER:O	1:1:28:ASP:HB3	2.18	0.42
1:1:51:TYR:CD2	1:1:57:PRO:HB3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:189:TRP:CH2	1:1:210:VAL:HG23	2.54	0.42
1:2:52:GLU:O	1:2:53:VAL:CB	2.67	0.42
1:1:6:GLN:NE2	1:1:104:GLY:HA2	2.34	0.42
1:2:46:PRO:O	1:2:47:LYS:CB	2.68	0.42
1:2:143:PHE:CE1	1:2:146:GLY:HA2	2.55	0.42
1:1:106:LYS:H	1:1:106:LYS:HG2	1.71	0.41
1:1:144:TYR:CG	1:1:145:PRO:N	2.87	0.41
1:2:16:GLN:N	1:2:79:GLY:HA2	2.34	0.41
1:2:28:ASP:O	1:2:28:ASP:CG	2.55	0.41
1:2:53:VAL:HG13	1:2:54:ASN:H	1.85	0.41
1:1:28:ASP:O	1:1:29:VAL:C	2.63	0.41
1:1:32:TYR:HB2	2:1:253:HOH:O	2.20	0.41
1:2:173:ASN:ND2	1:2:173:ASN:H	2.09	0.41
1:1:124:PRO:O	1:1:129:LEU:CD2	2.69	0.41
1:1:214:GLU:HB3	1:1:216:SER:CA	2.48	0.41
1:1:214:GLU:O	1:1:216:SER:N	2.54	0.41
1:2:7:PRO:HA	1:2:8:PRO:HD3	1.75	0.41
1:2:37:TRP:N	1:2:50:ILE:HG22	2.36	0.41
1:2:53:VAL:HG13	1:2:54:ASN:N	2.35	0.41
1:2:114:LYS:HZ3	1:2:114:LYS:HG3	1.57	0.41
1:1:87:ASP:CB	2:1:224:HOH:O	2.68	0.41
1:1:138:CYS:O	1:1:179:SER:HB2	2.20	0.41
1:1:154:ALA:HB2	1:1:159:VAL:HG11	2.03	0.41
1:2:196:SER:OG	1:2:207:GLU:CD	2.64	0.41
1:1:72:THR:O	1:1:72:THR:OG1	2.37	0.41
1:2:13:SER:HA	1:2:110:LEU:O	2.20	0.41
1:2:37:TRP:HB2	1:2:50:ILE:HG21	2.01	0.41
1:1:57:PRO:O	1:1:58:SER:HB2	2.21	0.41
1:2:17:SER:HA	1:2:78:SER:CA	2.45	0.41
1:2:87:ASP:HA	1:2:106:LYS:N	2.35	0.41
1:2:149:THR:C	2:2:352:HOH:O	2.64	0.41
1:1:32:TYR:HA	2:1:229:HOH:O	2.20	0.41
1:1:143:PHE:O	1:1:143:PHE:HD2	2.04	0.41
1:2:87:ASP:OD1	1:2:106:LYS:HE2	2.21	0.41
1:1:118:THR:HG21	2:1:266:HOH:O	2.21	0.40
1:1:152:TRP:C	1:1:159:VAL:HG23	2.46	0.40
1:2:71:ASN:ND2	1:2:71:ASN:N	2.67	0.40
1:2:196:SER:HB2	1:2:207:GLU:HG2	2.02	0.40
1:1:200:THR:HG23	1:1:205:THR:HG23	2.02	0.40
1:2:4:LEU:HB2	1:2:102:GLY:CA	2.51	0.40
1:2:25:THR:HB	1:2:28:ASP:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:133:LYS:HB3	1:2:133:LYS:NZ	2.30	0.40
1:1:28:ASP:C	1:1:32:TYR:HD1	2.28	0.40
1:1:37:TRP:CG	1:1:75:LEU:HD23	2.56	0.40
1:1:85:GLU:O	1:1:86:ALA:CB	2.67	0.40
1:1:143:PHE:N	1:1:175:LYS:HB3	2.36	0.40
1:2:41:HIS:CE1	1:2:85:GLU:O	2.74	0.40
1:2:71:ASN:N	1:2:71:ASN:HD22	2.17	0.40
1:2:152:TRP:HZ2	1:2:180:SER:C	2.29	0.40
1:1:91:SER:CB	1:1:99:PHE:CE2	3.04	0.40
1:1:92:SER:O	1:1:99:PHE:CD1	2.75	0.40
1:1:106:LYS:HE2	1:1:147:ALA:HB1	2.03	0.40

All (5) 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)
2:1:266:HOH:O	2:2:333:HOH:O[6_656]	1.54	0.66
1:1:81:GLN:NE2	2:1:242:HOH:O[4_646]	1.76	0.44
1:1:58:SER:O	1:1:215:CYS:CA[3_654]	2.11	0.09
1:1:32:TYR:OH	1:2:9:SER:CB[4_546]	2.14	0.06
1:1:59:GLY:O	1:1:216:SER:N[3_654]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	214/216 (99%)	163 (76%)	28 (13%)	23 (11%)	0	0
1	2	214/216 (99%)	140 (65%)	39 (18%)	35 (16%)	0	0
All	All	428/432 (99%)	303 (71%)	67 (16%)	58 (14%)	0	0

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	2	SER
1	1	9	SER
1	1	14	LEU
1	1	26	SER
1	1	27	SER
1	1	28	ASP
1	1	33	ASN
1	1	35	VAL
1	1	42	ALA
1	1	53	VAL
1	1	95	GLY
1	1	98	ASN
1	1	144	TYR
1	1	203	GLY
1	2	14	LEU
1	2	29	VAL
1	2	40	GLN
1	2	50	ILE
1	2	53	VAL
1	2	57	PRO
1	2	81	GLN
1	2	82	ALA
1	2	103	THR
1	2	134	ALA
1	2	144	TYR
1	2	155	ASP
1	2	166	THR
1	2	215	CYS
1	1	86	ALA
1	1	131	ALA
1	1	202	GLU
1	2	15	GLY
1	2	16	GLN
1	2	42	ALA
1	2	62	ASP
1	2	79	GLY
1	2	96	SER
1	2	214	GLU
1	1	192	HIS
1	2	9	SER
1	2	10	ALA
1	2	71	ASN
1	2	149	THR

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Mol	Chain	Res	Type
1	2	173	ASN
1	2	212	PRO
1	1	96	SER
1	1	142	ASP
1	2	39	GLN
1	2	126	SER
1	1	29	VAL
1	1	58	SER
1	2	17	SER
1	2	95	GLY
1	2	148	VAL
1	2	172	SER
1	2	142	ASP
1	1	146	GLY
1	2	46	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	1	180/180 (100%)	116 (64%)	64 (36%)	0	0
1	2	180/180 (100%)	121 (67%)	59 (33%)	0	0
All	All	360/360 (100%)	237 (66%)	123 (34%)	0	0

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	5	THR
1	1	11	SER
1	1	13	SER
1	1	16	GLN
1	1	17	SER
1	1	18	VAL
1	1	19	THR
1	1	20	ILE

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Mol	Chain	Res	Type
1	1	23	THR
1	1	27	SER
1	1	28	ASP
1	1	34	TYR
1	1	38	TYR
1	1	41	HIS
1	1	47	LYS
1	1	55	LYS
1	1	58	SER
1	1	60	VAL
1	1	63	ARG
1	1	65	SER
1	1	67	SER
1	1	68	LYS
1	1	72	THR
1	1	75	LEU
1	1	76	THR
1	1	78	SER
1	1	80	LEU
1	1	83	GLU
1	1	90	CYS
1	1	91	SER
1	1	97	ASP
1	1	98	ASN
1	1	100	VAL
1	1	103	THR
1	1	106	LYS
1	1	109	VAL
1	1	110	LEU
1	1	116	ASN
1	1	119	VAL
1	1	126	SER
1	1	128	GLU
1	1	129	LEU
1	1	136	LEU
1	1	140	ILE
1	1	143	PHE
1	1	149	THR
1	1	153	LYS
1	1	159	VAL
1	1	163	VAL
1	1	166	THR

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Mol	Chain	Res	Type
1	1	167	LYS
1	1	169	SER
1	1	171	GLN
1	1	181	TYR
1	1	182	LEU
1	1	184	LEU
1	1	185	THR
1	1	190	LYS
1	1	191	SER
1	1	202	GLU
1	1	208	LYS
1	1	209	THR
1	1	213	THR
1	1	215	CYS
1	2	2	SER
1	2	5	THR
1	2	11	SER
1	2	13	SER
1	2	14	LEU
1	2	16	GLN
1	2	17	SER
1	2	18	VAL
1	2	22	CYS
1	2	26	SER
1	2	32	TYR
1	2	35	VAL
1	2	40	GLN
1	2	41	HIS
1	2	44	LYS
1	2	47	LYS
1	2	48	VAL
1	2	50	ILE
1	2	52	GLU
1	2	56	ARG
1	2	68	LYS
1	2	69	SER
1	2	71	ASN
1	2	72	THR
1	2	75	LEU
1	2	81	GLN
1	2	83	GLU
1	2	98	ASN

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Mol	Chain	Res	Type
1	2	101	PHE
1	2	103	THR
1	2	105	THR
1	2	108	THR
1	2	114	LYS
1	2	119	VAL
1	2	121	LEU
1	2	125	SER
1	2	127	GLU
1	2	130	GLN
1	2	132	ASN
1	2	136	LEU
1	2	139	LEU
1	2	142	ASP
1	2	153	LYS
1	2	159	VAL
1	2	163	VAL
1	2	169	SER
1	2	173	ASN
1	2	174	ASN
1	2	176	TYR
1	2	184	LEU
1	2	188	GLN
1	2	190	LYS
1	2	198	GLN
1	2	199	VAL
1	2	200	THR
1	2	205	THR
1	2	209	THR
1	2	210	VAL
1	2	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	16	GLN
1	1	39	GLN
1	1	40	GLN
1	1	71	ASN
1	1	98	ASN
1	1	116	ASN
1	1	173	ASN

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Mol	Chain	Res	Type
1	1	201	HIS
1	2	16	GLN
1	2	33	ASN
1	2	40	GLN
1	2	41	HIS
1	2	98	ASN
1	2	112	GLN
1	2	116	ASN
1	2	173	ASN
1	2	198	GLN
1	2	201	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	2	1	1	7,8,9	3.31	3 (42%)	9,10,12	1.83	4 (44%)
1	PCA	1	1	1	7,8,9	3.79	2 (28%)	9,10,12	2.48	3 (33%)

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	2	1	1	-	0/0/11/13	0/1/1/1
1	PCA	1	1	1	-	0/0/11/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	PCA	CD-N	8.88	1.57	1.34
1	2	1	PCA	CD-N	7.47	1.53	1.34
1	2	1	PCA	CA-N	3.32	1.50	1.46
1	1	1	PCA	CA-N	3.25	1.50	1.46
1	2	1	PCA	CB-CG	2.55	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1	PCA	OE-CD-N	4.19	134.03	124.96
1	1	1	PCA	OE-CD-CG	-3.80	119.94	126.72
1	1	1	PCA	CA-N-CD	-3.49	101.62	113.58
1	2	1	PCA	CB-CA-N	2.88	111.18	103.24
1	2	1	PCA	CA-N-CD	-2.47	105.11	113.58
1	2	1	PCA	CB-CA-C	2.43	115.98	112.66
1	2	1	PCA	OE-CD-CG	-2.02	123.12	126.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1	PCA	1	0
1	1	1	PCA	8	0

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 ⓘ

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.