



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 2PLV / pdb_00002plv
Title : STRUCTURAL FACTORS THAT CONTROL CONFORMATIONAL
TRANSITIONS AND SEROTYPE SPECIFICITY IN TYPE 3 POLIOVIRUS
Authors : Filman, D.J.; Hogle, J.M.
Deposited on : 1989-10-17
Resolution : 2.88 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

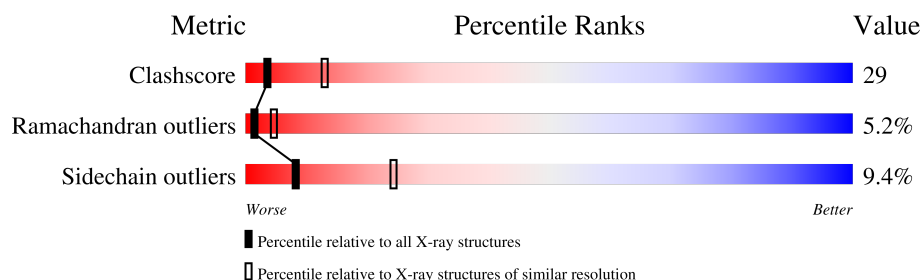
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)

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	302	
2	2	272	
3	3	238	
4	4	68	

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
5	SPH	1	0	X	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7162 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 HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	288	Total	C	N	O	S	0	0	0
			2251	1431	383	432	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	8	SER	ARG	conflict	UNP P03300
1	9	SER	GLU	conflict	UNP P03300

- Molecule 2 is a protein called HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	268	Total	C	N	O	S	0	0	0
			2085	1317	358	396	14			

- Molecule 3 is a protein called HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	235	Total	C	N	O	S	0	0	0
			1834	1169	299	349	17			

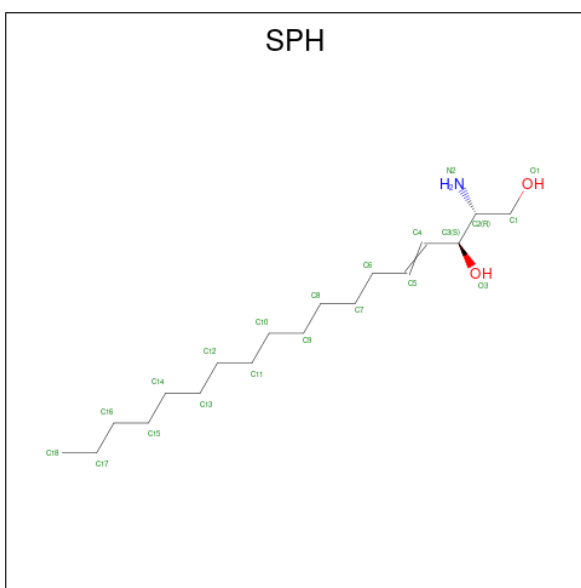
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	123	SER	PHE	conflict	UNP P03300

- Molecule 4 is a protein called HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP4).

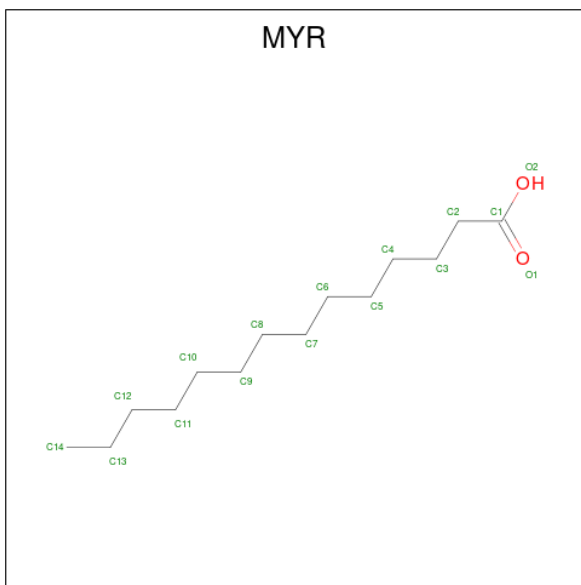
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	63	Total	C	N	O	S	0	0	1
			477	293	82	101	1			

- Molecule 5 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 7 is water.

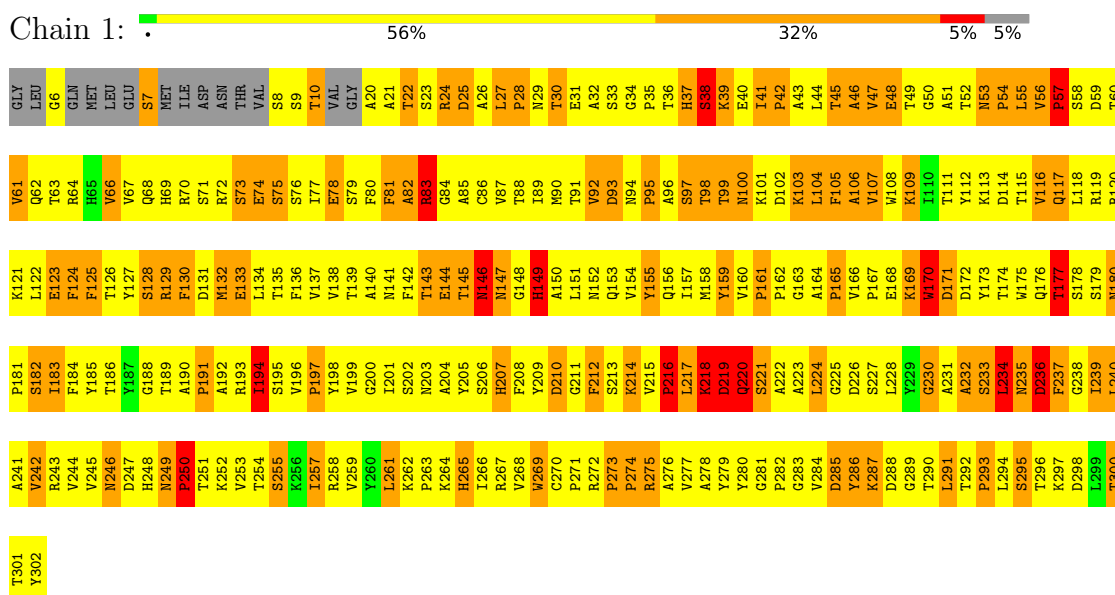
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	159	Total 159	O 159	0	0
7	2	149	Total 149	O 149	0	0
7	3	129	Total 129	O 129	0	0
7	4	42	Total 42	O 42	0	0

3 Residue-property plots

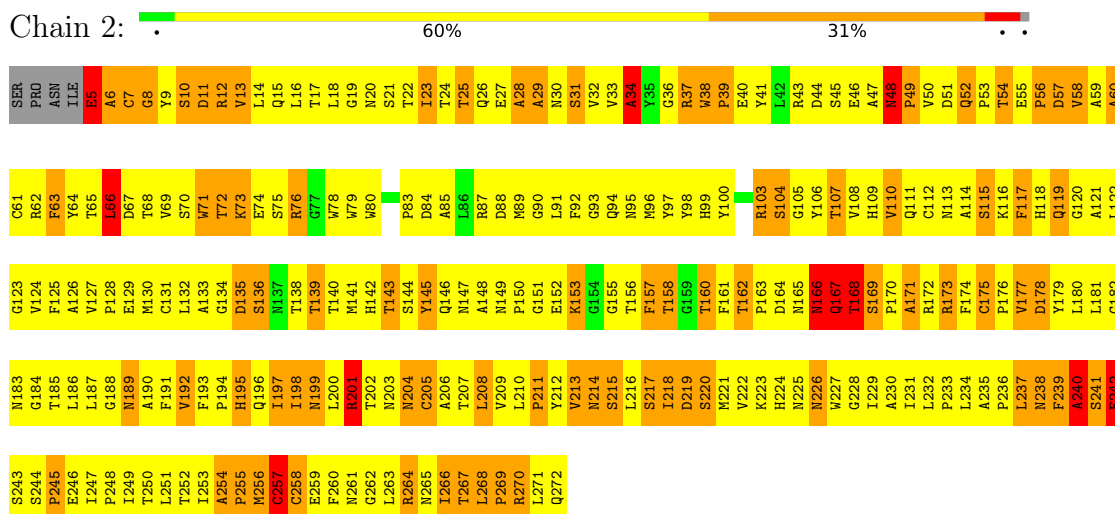
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP1)



• Molecule 2: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP2)



• Molecule 3: HUMAN POLIOVIRUS TYPE 1 (SUBUNIT VP3)

D181	D182	D183	D184	D185	D186	D187	D188	D189	D190	D191	D192	D193	D194	D195	D196	D197	D198	D199	D200	D201	D202	D203	D204	D205	D206	D207	D208	D209	D210	D211	D212	D213	D214	D215	D216	D217	D218	D219	D220	D221	D222	D223	D224	D225	D226	D227	D228	D229	D230	D231	D232	D233	D234	D235	D236	D237	D238	D239	D240	D241	D242	D243	D244	D245	D246	D247	D248	D249	D250
C121	C122	C123	C124	C125	C126	C127	C128	C129	C130	C131	C132	C133	C134	C135	C136	C137	C138	C139	C140	C141	C142	C143	C144	C145	C146	C147	C148	C149	C150	C151	C152	C153	C154	C155	C156	C157	C158	C159	C160	C161	C162	C163	C164	C165	C166	C167	C168	C169	C170	C171	C172	C173	C174	C175	C176	C177	C178	C179	C180										
G1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24	G25	G26	G27	G28	G29	G30	G31	G32	G33	G34	G35	G36	G37	G38	G39	G40	G41	G42	G43	G44	G45	G46	G47	G48	G49	G50	G51	G52	G53	G54	G55	G56	G57	G58	G59	G60										

Chain 4: 6% 43% 31% 13% 7%

I62	K63	K64	K65	K66	K67	K68	K69	G72	A3	Q4	V5	S6	S7	Q8	Q9	V10	G11	A12	H13	E14	M15	S16	N17	ARG	ALA	T19	GLY	GLY	S23	T24	T25	M26	Y27	T28	T29	T30	T31	G32	Y33	R34	R35	S36	A37	S38	N39	A40	A41	S42	K43	Q44	D45	F46	S47	Q48	D49	P50	S51	K52	F53	T54	E55	P56	S57	K58	D59	V60	S61
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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	322.94Å 358.04Å 380.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.88	Depositor
% Data completeness (in resolution range)	72.6 ((Not available)-2.88)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7162	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: MYR, SPH

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	3.05	373/2313 (16.1%)	2.84	287/3160 (9.1%)
2	2	3.02	320/2142 (14.9%)	2.88	291/2928 (9.9%)
3	3	3.00	270/1881 (14.4%)	2.79	224/2562 (8.7%)
4	4	3.02	83/484 (17.1%)	2.92	68/653 (10.4%)
All	All	3.02	1046/6820 (15.3%)	2.85	870/9303 (9.4%)

All (1046) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	151	GLY	N-CA	11.43	1.53	1.44
1	1	6	GLY	N-CA	10.07	1.61	1.45
1	1	196	VAL	N-CA	9.69	1.53	1.45
2	2	245	PRO	C-N	-9.34	1.22	1.33
3	3	159	GLY	N-CA	9.13	1.53	1.45
3	3	1	GLY	N-CA	8.83	1.59	1.45
3	3	196	THR	CA-C	8.82	1.60	1.52
4	4	14	GLU	N-CA	8.64	1.56	1.46
1	1	283	GLY	N-CA	8.62	1.52	1.44
1	1	20	ALA	N-CA	8.34	1.62	1.46
1	1	93	ASP	C-N	-8.28	1.22	1.33
2	2	237	LEU	C-N	-8.25	1.22	1.33
4	4	23	SER	N-CA	8.17	1.61	1.46
1	1	195	SER	C-N	-7.98	1.25	1.33
1	1	273	PRO	CA-C	7.97	1.59	1.52
2	2	30	ASN	C-N	-7.97	1.22	1.33
4	4	47	SER	C-N	-7.97	1.21	1.33
3	3	196	THR	N-CA	7.93	1.54	1.46
3	3	53	ILE	N-CA	7.89	1.52	1.46
2	2	246	GLU	C-N	-7.86	1.24	1.33
1	1	80	PHE	N-CA	7.83	1.55	1.46
3	3	141	PRO	CA-C	7.81	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	146	ASN	C-N	-7.77	1.22	1.33
2	2	235	ALA	N-CA	7.75	1.54	1.46
1	1	124	PHE	C-O	-7.71	1.14	1.24
1	1	272	ARG	CA-C	7.63	1.60	1.52
3	3	136	PRO	CA-C	7.62	1.59	1.52
3	3	231	ILE	C-N	-7.53	1.23	1.33
2	2	263	LEU	C-N	-7.53	1.25	1.33
1	1	124	PHE	N-CA	7.48	1.56	1.46
2	2	217	SER	N-CA	7.48	1.55	1.46
2	2	6	ALA	N-CA	7.47	1.55	1.46
1	1	149	HIS	C-N	-7.41	1.24	1.33
1	1	202	SER	N-CA	7.39	1.54	1.45
3	3	195	GLN	N-CA	7.38	1.55	1.46
1	1	163	GLY	CA-C	7.37	1.59	1.52
1	1	161	PRO	CA-C	7.36	1.59	1.52
1	1	8	SER	CA-C	7.33	1.62	1.52
1	1	292	THR	N-CA	7.31	1.53	1.46
3	3	204	THR	CA-C	7.31	1.59	1.52
2	2	127	VAL	N-CA	7.30	1.52	1.46
2	2	169	SER	N-CA	7.27	1.54	1.46
2	2	162	THR	N-CA	7.26	1.54	1.46
2	2	59	ALA	N-CA	7.24	1.55	1.46
2	2	92	PHE	N-CA	7.24	1.55	1.46
2	2	118	HIS	C-N	-7.24	1.23	1.33
1	1	115	THR	N-CA	7.21	1.54	1.45
3	3	70	VAL	CA-C	7.20	1.59	1.53
1	1	163	GLY	N-CA	7.19	1.53	1.45
1	1	72	ARG	N-CA	7.16	1.54	1.46
2	2	175	CYS	N-CA	7.14	1.53	1.46
3	3	148	ALA	N-CA	7.13	1.54	1.46
1	1	79	SER	N-CA	7.09	1.54	1.46
3	3	28	PHE	N-CA	7.08	1.55	1.46
3	3	47	ALA	N-CA	7.08	1.55	1.46
3	3	32	PRO	CA-C	7.07	1.58	1.52
4	4	13	HIS	C-N	-7.07	1.24	1.33
2	2	235	ALA	CA-C	7.06	1.60	1.52
1	1	7	SER	C-N	-7.04	1.23	1.33
1	1	73	SER	N-CA	7.02	1.54	1.46
3	3	51	THR	N-CA	7.02	1.54	1.46
1	1	76	SER	N-CA	7.01	1.54	1.45
2	2	94	GLN	N-CA	7.01	1.54	1.46
2	2	218	ILE	C-N	-7.01	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	184	PHE	N-CA	7.01	1.54	1.46
2	2	117	PHE	N-CA	7.00	1.55	1.46
4	4	37	ALA	N-CA	6.99	1.54	1.46
2	2	235	ALA	C-N	-6.98	1.24	1.33
3	3	98	THR	N-CA	6.97	1.55	1.45
1	1	96	ALA	N-CA	6.97	1.54	1.46
1	1	125	PHE	N-CA	6.96	1.54	1.46
2	2	240	ALA	N-CA	6.96	1.55	1.46
1	1	43	ALA	N-CA	6.96	1.55	1.46
1	1	171	ASP	N-CA	6.95	1.53	1.46
1	1	212	PHE	N-CA	6.94	1.54	1.45
1	1	237	PHE	N-CA	6.94	1.54	1.46
1	1	114	ASP	N-CA	6.94	1.54	1.46
1	1	99	THR	C-N	-6.93	1.24	1.34
2	2	248	PRO	C-N	-6.92	1.23	1.33
1	1	9	SER	N-CA	6.92	1.54	1.45
1	1	295	SER	N-CA	6.92	1.53	1.45
2	2	185	THR	N-CA	6.90	1.54	1.45
2	2	148	ALA	N-CA	6.89	1.55	1.46
1	1	232	ALA	N-CA	6.88	1.55	1.46
1	1	148	GLY	CA-C	6.88	1.59	1.52
2	2	238	ASN	C-N	-6.87	1.24	1.33
2	2	105	GLY	N-CA	6.87	1.53	1.45
2	2	133	ALA	N-CA	6.87	1.54	1.46
2	2	105	GLY	C-N	-6.86	1.24	1.33
2	2	177	VAL	N-CA	6.86	1.53	1.46
1	1	243	ARG	C-N	-6.84	1.26	1.33
3	3	183	SER	N-CA	6.84	1.54	1.46
3	3	120	PHE	N-CA	6.83	1.55	1.46
2	2	45	SER	N-CA	6.83	1.54	1.46
2	2	146	GLN	N-CA	6.82	1.54	1.46
2	2	270	ARG	CA-C	6.82	1.60	1.53
3	3	177	ARG	N-CA	6.82	1.53	1.45
1	1	82	ALA	N-CA	6.82	1.54	1.46
1	1	196	VAL	CA-C	6.81	1.58	1.52
2	2	60	ALA	CA-C	6.81	1.60	1.52
1	1	105	PHE	N-CA	6.80	1.54	1.46
3	3	64	THR	N-CA	6.80	1.54	1.45
2	2	29	ALA	N-CA	6.78	1.55	1.46
1	1	119	ARG	N-CA	6.77	1.54	1.46
1	1	78	GLU	CA-C	6.76	1.61	1.52
1	1	207	HIS	N-CA	6.76	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	175	THR	N-CA	6.76	1.54	1.46
1	1	202	SER	CA-C	6.75	1.60	1.52
2	2	93	GLY	CA-C	6.75	1.59	1.52
1	1	284	VAL	N-CA	6.74	1.53	1.46
2	2	138	THR	N-CA	6.74	1.55	1.46
2	2	190	ALA	N-CA	6.74	1.54	1.46
3	3	206	ARG	N-CA	6.74	1.55	1.46
1	1	33	SER	N-CA	6.73	1.54	1.46
1	1	64	ARG	N-CA	6.73	1.53	1.45
1	1	85	ALA	N-CA	6.72	1.54	1.46
1	1	208	PHE	N-CA	6.71	1.54	1.46
1	1	96	ALA	CA-C	6.71	1.61	1.52
1	1	180	ASN	CA-C	6.71	1.60	1.53
3	3	127	THR	N-CA	6.71	1.53	1.45
3	3	45	GLU	N-CA	6.71	1.54	1.46
1	1	51	ALA	N-CA	6.70	1.53	1.45
2	2	242	GLU	CA-C	6.69	1.60	1.52
2	2	85	ALA	N-CA	6.69	1.54	1.46
2	2	139	THR	N-CA	6.69	1.54	1.45
2	2	171	ALA	N-CA	6.69	1.54	1.46
2	2	88	ASP	N-CA	6.69	1.54	1.46
2	2	168	THR	N-CA	6.68	1.54	1.46
2	2	252	THR	N-CA	6.67	1.54	1.46
1	1	300	THR	N-CA	6.66	1.53	1.46
2	2	196	GLN	C-N	-6.66	1.25	1.33
4	4	38	SER	N-CA	6.66	1.54	1.46
4	4	53	PHE	N-CA	6.65	1.54	1.46
1	1	81	PHE	N-CA	6.65	1.54	1.46
2	2	211	PRO	N-CA	6.64	1.54	1.46
1	1	126	THR	N-CA	6.63	1.54	1.46
3	3	84	CYS	N-CA	6.63	1.54	1.46
1	1	97	SER	N-CA	6.63	1.54	1.46
1	1	117	GLN	N-CA	6.63	1.53	1.46
3	3	122	GLY	N-CA	6.62	1.53	1.45
2	2	172	ARG	C-N	-6.62	1.25	1.33
2	2	6	ALA	C-O	-6.60	1.15	1.24
4	4	12	ALA	CA-C	6.59	1.61	1.52
1	1	213	SER	N-CA	6.58	1.54	1.46
3	3	132	VAL	N-CA	6.58	1.53	1.46
3	3	101	GLY	CA-C	6.58	1.59	1.51
3	3	15	THR	N-CA	6.57	1.54	1.46
3	3	86	SER	N-CA	6.56	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	58	SER	N-CA	6.56	1.54	1.46
1	1	222	ALA	N-CA	6.56	1.54	1.46
2	2	191	PHE	N-CA	6.56	1.54	1.46
1	1	223	ALA	N-CA	6.56	1.54	1.46
1	1	227	SER	N-CA	6.55	1.54	1.46
1	1	281	GLY	C-N	-6.54	1.26	1.34
2	2	239	PHE	N-CA	6.54	1.54	1.46
3	3	217	CYS	N-CA	6.53	1.54	1.45
1	1	23	SER	N-CA	6.53	1.54	1.46
2	2	126	ALA	N-CA	6.53	1.54	1.46
3	3	20	GLN	C-N	-6.53	1.24	1.34
1	1	78	GLU	N-CA	6.52	1.54	1.46
4	4	40	ALA	C-N	-6.52	1.24	1.33
3	3	232	GLU	C-N	-6.51	1.24	1.33
2	2	234	LEU	N-CA	6.50	1.54	1.46
4	4	12	ALA	N-CA	6.50	1.55	1.46
1	1	178	SER	N-CA	6.50	1.54	1.46
2	2	11	ASP	N-CA	6.50	1.54	1.46
1	1	179	SER	N-CA	6.49	1.54	1.46
1	1	251	THR	N-CA	6.49	1.54	1.46
4	4	54	THR	N-CA	6.48	1.54	1.46
2	2	93	GLY	N-CA	6.48	1.53	1.45
3	3	24	ALA	N-CA	6.48	1.54	1.46
3	3	147	GLU	N-CA	6.46	1.54	1.46
4	4	36	SER	N-CA	6.46	1.54	1.46
4	4	8	GLN	CA-C	6.46	1.61	1.52
3	3	186	GLU	N-CA	6.46	1.53	1.46
1	1	233	SER	N-CA	6.45	1.54	1.46
1	1	172	ASP	N-CA	6.45	1.54	1.45
1	1	142	PHE	N-CA	6.44	1.53	1.46
3	3	102	GLU	N-CA	6.43	1.54	1.46
2	2	60	ALA	N-CA	6.42	1.54	1.46
2	2	128	PRO	N-CA	6.42	1.54	1.47
3	3	123	SER	N-CA	6.41	1.54	1.45
3	3	207	GLU	C-N	-6.40	1.25	1.33
3	3	219	ASP	N-CA	6.40	1.54	1.46
2	2	44	ASP	N-CA	6.40	1.54	1.46
3	3	16	ALA	N-CA	6.40	1.54	1.46
2	2	39	PRO	C-N	-6.39	1.25	1.33
4	4	62	ILE	N-CA	6.39	1.53	1.46
2	2	119	GLN	N-CA	6.39	1.53	1.45
2	2	198	ILE	CA-C	6.39	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	204	ALA	N-CA	6.38	1.54	1.46
3	3	151	GLY	CA-C	6.38	1.59	1.52
3	3	207	GLU	CA-C	6.38	1.60	1.52
3	3	101	GLY	N-CA	6.38	1.53	1.45
1	1	148	GLY	N-CA	6.38	1.53	1.45
1	1	22	THR	N-CA	6.38	1.53	1.46
1	1	120	ARG	N-CA	6.37	1.54	1.46
1	1	301	THR	N-CA	6.37	1.53	1.46
3	3	180	ILE	N-CA	6.37	1.53	1.46
3	3	161	GLN	N-CA	6.37	1.54	1.46
2	2	215	SER	N-CA	6.37	1.54	1.46
3	3	220	PHE	N-CA	6.37	1.54	1.46
1	1	32	ALA	N-CA	6.36	1.54	1.46
1	1	267	ARG	CA-C	6.36	1.60	1.52
1	1	244	VAL	CA-C	6.36	1.59	1.53
3	3	118	PHE	N-CA	6.36	1.53	1.46
3	3	90	ALA	N-CA	6.35	1.54	1.46
1	1	290	THR	N-CA	6.35	1.54	1.46
2	2	24	THR	C-N	-6.35	1.25	1.33
3	3	55	PHE	N-CA	6.34	1.54	1.46
1	1	219	ASP	N-CA	6.33	1.54	1.46
2	2	119	GLN	CA-C	6.32	1.60	1.52
2	2	115	SER	N-CA	6.32	1.53	1.46
1	1	40	GLU	C-N	-6.32	1.26	1.33
2	2	243	SER	N-CA	6.32	1.54	1.46
3	3	59	ALA	N-CA	6.32	1.54	1.46
3	3	185	THR	N-CA	6.32	1.53	1.46
1	1	220	GLN	N-CA	6.31	1.53	1.46
3	3	10	SER	N-CA	6.31	1.54	1.46
3	3	176	TYR	CA-C	6.31	1.60	1.52
3	3	94	ARG	N-CA	6.31	1.54	1.46
1	1	176	GLN	N-CA	6.31	1.54	1.46
1	1	189	THR	N-CA	6.31	1.53	1.45
2	2	34	ALA	N-CA	6.31	1.54	1.46
3	3	88	SER	N-CA	6.31	1.55	1.46
1	1	21	ALA	N-CA	6.30	1.54	1.46
3	3	53	ILE	CA-C	6.29	1.58	1.53
1	1	128	SER	C-N	-6.28	1.25	1.33
1	1	56	VAL	CA-C	6.26	1.59	1.52
1	1	140	ALA	N-CA	6.26	1.53	1.45
1	1	192	ALA	N-CA	6.26	1.54	1.46
3	3	182	ASP	N-CA	6.25	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	135	ALA	N-CA	6.24	1.53	1.46
2	2	129	GLU	CA-C	6.23	1.61	1.53
3	3	73	SER	N-CA	6.23	1.53	1.46
3	3	48	GLU	N-CA	6.22	1.54	1.46
3	3	179	THR	N-CA	6.22	1.54	1.46
4	4	64	THR	N-CA	6.22	1.54	1.46
3	3	64	THR	CA-C	6.21	1.60	1.52
4	4	48	GLN	N-CA	6.20	1.53	1.45
1	1	83	ARG	N-CA	6.20	1.53	1.46
2	2	157	PHE	C-N	-6.20	1.25	1.33
2	2	5	GLU	N-CA	6.19	1.58	1.46
3	3	103	ILE	N-CA	6.19	1.53	1.46
1	1	276	ALA	N-CA	6.19	1.54	1.46
2	2	206	ALA	N-CA	6.19	1.53	1.46
2	2	255	PRO	N-CA	6.19	1.54	1.47
2	2	257	CYS	N-CA	6.19	1.54	1.46
1	1	150	ALA	N-CA	6.18	1.53	1.46
1	1	168	GLU	N-CA	6.18	1.54	1.46
2	2	43	ARG	N-CA	6.18	1.53	1.46
1	1	40	GLU	N-CA	6.18	1.53	1.46
3	3	188	GLY	CA-C	6.18	1.58	1.52
2	2	247	ILE	C-N	-6.18	1.25	1.33
3	3	213	PHE	N-CA	6.17	1.53	1.46
3	3	164	CYS	N-CA	6.17	1.53	1.46
4	4	34	ARG	N-CA	6.17	1.54	1.46
1	1	71	SER	N-CA	6.17	1.53	1.45
3	3	214	VAL	C-N	-6.17	1.26	1.33
2	2	61	CYS	N-CA	6.17	1.54	1.46
2	2	167	GLN	N-CA	6.17	1.54	1.46
2	2	222	VAL	N-CA	6.16	1.53	1.46
1	1	75	SER	N-CA	6.16	1.54	1.46
1	1	26	ALA	N-CA	6.16	1.54	1.46
2	2	144	SER	N-CA	6.16	1.53	1.46
3	3	229	THR	N-CA	6.15	1.54	1.46
1	1	58	SER	N-CA	6.15	1.54	1.46
1	1	61	VAL	N-CA	6.15	1.52	1.46
1	1	127	TYR	CA-C	6.14	1.60	1.52
4	4	3	ALA	N-CA	6.14	1.53	1.46
1	1	247	ASP	N-CA	6.13	1.53	1.46
1	1	267	ARG	N-CA	6.13	1.53	1.46
3	3	172	SER	N-CA	6.13	1.53	1.45
3	3	178	GLN	N-CA	6.12	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	6	ALA	CA-C	6.12	1.61	1.52
1	1	195	SER	N-CA	6.12	1.53	1.46
1	1	281	GLY	N-CA	6.12	1.53	1.44
1	1	48	GLU	N-CA	6.12	1.54	1.46
2	2	230	ALA	N-CA	6.12	1.53	1.46
2	2	206	ALA	CA-C	6.11	1.59	1.52
3	3	108	THR	N-CA	6.11	1.54	1.46
2	2	40	GLU	N-CA	6.11	1.53	1.45
1	1	277	VAL	N-CA	6.11	1.53	1.46
4	4	41	ALA	N-CA	6.11	1.53	1.46
1	1	201	ILE	N-CA	6.10	1.53	1.46
3	3	215	SER	N-CA	6.10	1.53	1.45
2	2	196	GLN	N-CA	6.10	1.53	1.45
3	3	91	SER	N-CA	6.09	1.54	1.46
2	2	201	ARG	N-CA	6.09	1.54	1.46
2	2	114	ALA	N-CA	6.08	1.54	1.46
1	1	59	ASP	N-CA	6.08	1.54	1.46
1	1	233	SER	CA-C	6.08	1.60	1.52
3	3	9	GLY	CA-C	6.08	1.59	1.51
1	1	115	THR	CA-C	6.08	1.60	1.52
1	1	215	VAL	CA-C	6.08	1.59	1.52
1	1	52	THR	N-CA	6.07	1.53	1.46
3	3	111	ALA	N-CA	6.07	1.53	1.45
3	3	181	ASP	N-CA	6.07	1.54	1.46
1	1	92	VAL	N-CA	6.06	1.53	1.46
2	2	76	ARG	N-CA	6.06	1.54	1.46
2	2	209	VAL	CA-C	6.06	1.59	1.53
1	1	92	VAL	C-N	-6.06	1.25	1.33
3	3	174	THR	N-CA	6.06	1.54	1.46
2	2	31	SER	N-CA	6.05	1.53	1.46
3	3	168	VAL	CA-C	6.05	1.59	1.52
3	3	147	GLU	CA-C	6.04	1.60	1.52
2	2	140	THR	N-CA	6.04	1.53	1.45
3	3	164	CYS	CA-C	6.04	1.59	1.52
1	1	131	ASP	N-CA	6.03	1.53	1.46
4	4	42	SER	N-CA	6.03	1.53	1.46
1	1	275	ARG	N-CA	6.03	1.53	1.46
2	2	26	GLN	N-CA	6.03	1.54	1.46
1	1	111	THR	N-CA	6.03	1.53	1.46
2	2	57	ASP	CA-C	6.03	1.58	1.53
2	2	113	ASN	C-N	-6.03	1.25	1.33
2	2	158	THR	N-CA	6.03	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	191	SER	N-CA	6.02	1.53	1.45
2	2	157	PHE	N-CA	6.02	1.53	1.45
2	2	240	ALA	CA-C	6.02	1.60	1.52
3	3	19	PHE	N-CA	6.02	1.53	1.45
3	3	45	GLU	CA-C	6.01	1.60	1.52
3	3	60	THR	N-CA	6.01	1.53	1.46
3	3	222	VAL	N-CA	6.01	1.52	1.46
2	2	174	PHE	N-CA	6.01	1.53	1.46
3	3	82	ILE	N-CA	6.01	1.54	1.46
2	2	21	SER	N-CA	6.00	1.53	1.46
2	2	114	ALA	C-N	-6.00	1.26	1.33
2	2	131	CYS	N-CA	6.00	1.53	1.46
4	4	11	GLY	N-CA	6.00	1.54	1.45
2	2	47	ALA	N-CA	6.00	1.53	1.46
3	3	163	SER	N-CA	6.00	1.52	1.45
1	1	241	ALA	N-CA	6.00	1.54	1.46
2	2	12	ARG	N-CA	6.00	1.53	1.46
1	1	7	SER	CA-C	6.00	1.60	1.52
1	1	25	ASP	N-CA	6.00	1.53	1.46
1	1	164	ALA	CA-C	5.99	1.59	1.53
1	1	166	VAL	CA-C	5.99	1.59	1.52
2	2	260	PHE	N-CA	5.99	1.53	1.46
2	2	72	THR	N-CA	5.99	1.53	1.45
3	3	157	ASP	N-CA	5.99	1.53	1.46
2	2	87	ARG	N-CA	5.99	1.53	1.46
2	2	7	CYS	N-CA	5.98	1.54	1.46
2	2	110	VAL	N-CA	5.98	1.53	1.46
3	3	234	LYS	N-CA	5.98	1.53	1.46
1	1	129	ARG	N-CA	5.98	1.53	1.46
4	4	35	ASP	N-CA	5.97	1.53	1.46
1	1	121	LYS	N-CA	5.97	1.53	1.46
2	2	152	GLU	N-CA	5.97	1.53	1.46
3	3	96	SER	N-CA	5.97	1.53	1.46
3	3	12	GLN	N-CA	5.97	1.53	1.45
4	4	24	THR	N-CA	5.97	1.53	1.46
1	1	211	GLY	CA-C	5.96	1.58	1.51
1	1	251	THR	CA-C	5.96	1.60	1.52
3	3	177	ARG	CA-C	5.96	1.60	1.52
2	2	188	GLY	CA-C	5.96	1.59	1.51
2	2	62	ARG	N-CA	5.95	1.54	1.46
2	2	244	SER	N-CA	5.95	1.53	1.46
1	1	231	ALA	N-CA	5.95	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	78	THR	N-CA	5.94	1.53	1.46
1	1	190	ALA	N-CA	5.94	1.54	1.46
4	4	9	LYS	N-CA	5.94	1.53	1.46
4	4	44	GLN	N-CA	5.94	1.54	1.46
2	2	40	GLU	CA-C	5.93	1.59	1.52
3	3	74	ASP	N-CA	5.93	1.53	1.46
2	2	134	GLY	N-CA	5.93	1.52	1.45
2	2	196	GLN	CA-C	5.93	1.59	1.52
1	1	162	PRO	C-N	-5.92	1.28	1.34
2	2	46	GLU	N-CA	5.92	1.53	1.46
1	1	24	ARG	N-CA	5.92	1.53	1.46
3	3	145	ARG	N-CA	5.92	1.53	1.46
3	3	146	LYS	N-CA	5.92	1.53	1.46
2	2	10	SER	N-CA	5.91	1.53	1.45
1	1	40	GLU	CA-C	5.91	1.60	1.52
2	2	255	PRO	CA-C	5.91	1.59	1.52
1	1	60	THR	N-CA	5.90	1.54	1.45
1	1	221	SER	N-CA	5.90	1.53	1.46
2	2	125	PHE	N-CA	5.90	1.53	1.46
3	3	169	PRO	N-CA	5.90	1.53	1.47
1	1	190	ALA	CA-C	5.90	1.60	1.52
3	3	134	TYR	CA-C	5.90	1.59	1.52
3	3	33	PRO	C-N	-5.89	1.25	1.33
3	3	201	PRO	C-N	-5.89	1.26	1.33
3	3	21	SER	CA-C	5.89	1.58	1.52
2	2	111	GLN	N-CA	5.88	1.53	1.46
4	4	53	PHE	CA-C	5.88	1.59	1.52
1	1	133	GLU	CA-C	5.88	1.60	1.53
3	3	194	TYR	CA-C	5.88	1.60	1.52
1	1	250	PRO	N-CA	5.88	1.54	1.47
2	2	52	GLN	CA-C	5.88	1.60	1.52
3	3	186	GLU	CA-C	5.88	1.60	1.52
2	2	143	THR	N-CA	5.88	1.53	1.46
1	1	49	THR	N-CA	5.87	1.54	1.46
1	1	135	THR	N-CA	5.87	1.53	1.46
1	1	184	PHE	N-CA	5.87	1.54	1.46
3	3	39	GLU	CA-C	5.87	1.60	1.52
2	2	180	LEU	N-CA	5.87	1.52	1.46
1	1	50	GLY	N-CA	5.86	1.53	1.45
2	2	135	ASP	N-CA	5.86	1.53	1.46
2	2	19	GLY	N-CA	5.86	1.54	1.45
1	1	25	ASP	CA-C	5.85	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	60	VAL	N-CA	5.85	1.53	1.46
1	1	101	LYS	N-CA	5.85	1.53	1.46
4	4	51	SER	N-CA	5.85	1.53	1.46
1	1	176	GLN	CA-C	5.85	1.60	1.52
2	2	121	ALA	N-CA	5.84	1.53	1.46
2	2	43	ARG	CA-C	5.84	1.60	1.52
3	3	162	SER	N-CA	5.84	1.53	1.46
1	1	255	SER	N-CA	5.84	1.53	1.45
1	1	283	GLY	CA-C	5.84	1.58	1.52
3	3	26	PRO	N-CA	5.84	1.54	1.47
1	1	174	THR	N-CA	5.83	1.53	1.46
4	4	39	ASN	C-N	-5.83	1.25	1.33
2	2	116	LYS	N-CA	5.83	1.53	1.46
1	1	211	GLY	N-CA	5.83	1.52	1.45
2	2	52	GLN	N-CA	5.83	1.54	1.46
3	3	227	ASP	N-CA	5.83	1.53	1.46
4	4	40	ALA	N-CA	5.82	1.53	1.45
1	1	198	TYR	CA-C	5.82	1.60	1.52
2	2	242	GLU	N-CA	5.82	1.53	1.46
1	1	34	GLY	N-CA	5.82	1.52	1.44
1	1	205	TYR	CA-C	5.82	1.60	1.52
2	2	15	GLN	CA-C	5.82	1.60	1.53
3	3	226	ARG	N-CA	5.82	1.53	1.45
3	3	100	LEU	N-CA	5.81	1.53	1.46
2	2	65	THR	N-CA	5.81	1.53	1.46
4	4	15	ASN	CA-C	5.81	1.60	1.52
1	1	26	ALA	CA-C	5.81	1.60	1.52
1	1	279	TYR	CA-C	5.81	1.59	1.52
1	1	258	ARG	N-CA	5.80	1.53	1.46
1	1	186	THR	N-CA	5.80	1.53	1.46
2	2	18	LEU	N-CA	5.80	1.53	1.46
2	2	103	ARG	N-CA	5.80	1.53	1.46
2	2	267	THR	N-CA	5.79	1.53	1.46
2	2	195	HIS	C-N	-5.79	1.26	1.33
1	1	204	ALA	CA-C	5.79	1.60	1.52
2	2	100	TYR	N-CA	5.79	1.53	1.46
3	3	148	ALA	CA-C	5.79	1.60	1.52
2	2	192	VAL	N-CA	5.78	1.54	1.46
2	2	62	ARG	CA-C	5.78	1.60	1.52
2	2	151	GLY	C-N	-5.78	1.26	1.33
3	3	88	SER	CA-C	5.78	1.60	1.52
2	2	84	ASP	N-CA	5.78	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	139	ALA	N-CA	5.78	1.54	1.46
4	4	58	LYS	N-CA	5.78	1.53	1.46
1	1	120	ARG	CA-C	5.77	1.60	1.52
1	1	70	ARG	N-CA	5.77	1.53	1.46
2	2	211	PRO	CA-C	5.77	1.59	1.52
1	1	35	PRO	N-CA	5.76	1.53	1.47
1	1	193	ARG	N-CA	5.76	1.53	1.46
2	2	126	ALA	CA-C	5.76	1.60	1.52
4	4	14	GLU	CA-C	5.76	1.60	1.52
2	2	70	SER	N-CA	5.76	1.53	1.46
1	1	182	SER	N-CA	5.75	1.53	1.46
2	2	49	PRO	N-CA	5.75	1.54	1.47
3	3	126	ALA	N-CA	5.75	1.53	1.46
1	1	8	SER	N-CA	5.75	1.53	1.46
1	1	139	THR	N-CA	5.75	1.53	1.46
1	1	164	ALA	N-CA	5.75	1.54	1.45
3	3	98	THR	CA-C	5.75	1.60	1.52
3	3	17	ASP	N-CA	5.75	1.53	1.45
2	2	118	HIS	CA-C	5.74	1.60	1.52
3	3	4	VAL	N-CA	5.74	1.52	1.46
1	1	48	GLU	CA-C	5.73	1.60	1.52
3	3	193	PHE	N-CA	5.73	1.53	1.45
3	3	197	ARG	N-CA	5.73	1.53	1.46
2	2	242	GLU	C-N	-5.72	1.26	1.34
2	2	69	VAL	CA-C	5.72	1.59	1.52
2	2	128	PRO	CA-C	5.72	1.59	1.52
2	2	24	THR	N-CA	5.71	1.52	1.46
2	2	25	THR	N-CA	5.71	1.53	1.46
3	3	92	ASP	N-CA	5.71	1.54	1.46
1	1	130	PHE	N-CA	5.70	1.52	1.46
2	2	75	SER	N-CA	5.70	1.53	1.46
1	1	127	TYR	C-N	-5.70	1.26	1.33
1	1	129	ARG	CA-C	5.70	1.59	1.52
4	4	65	ALA	N-CA	5.69	1.54	1.45
3	3	152	THR	N-CA	5.69	1.53	1.46
1	1	83	ARG	CA-C	5.69	1.59	1.52
3	3	102	GLU	CA-C	5.69	1.60	1.52
1	1	115	THR	C-N	-5.68	1.26	1.33
2	2	64	TYR	CA-C	5.68	1.59	1.52
1	1	227	SER	CA-C	5.68	1.59	1.52
1	1	274	PRO	N-CA	5.68	1.54	1.47
1	1	236	ASP	N-CA	5.68	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	249	ASN	CA-C	5.68	1.58	1.52
1	1	234	LEU	N-CA	5.68	1.53	1.46
2	2	139	THR	CA-C	5.68	1.59	1.52
3	3	36	ILE	CA-C	5.68	1.58	1.52
1	1	179	SER	CA-C	5.67	1.59	1.52
3	3	158	ILE	N-CA	5.67	1.52	1.46
1	1	99	THR	CA-C	5.67	1.60	1.52
1	1	208	PHE	CA-C	5.67	1.59	1.52
2	2	59	ALA	CA-C	5.67	1.60	1.52
2	2	169	SER	CA-C	5.67	1.59	1.52
4	4	5	VAL	N-CA	5.67	1.53	1.46
2	2	218	ILE	N-CA	5.67	1.53	1.46
3	3	116	PHE	N-CA	5.67	1.53	1.46
4	4	29	THR	N-CA	5.67	1.52	1.46
2	2	220	SER	N-CA	5.67	1.53	1.46
3	3	47	ALA	CA-C	5.67	1.60	1.52
1	1	85	ALA	CA-C	5.66	1.59	1.52
3	3	66	GLU	N-CA	5.66	1.53	1.46
4	4	55	GLU	CA-C	5.66	1.59	1.52
2	2	160	THR	N-CA	5.66	1.53	1.46
3	3	78	THR	CA-C	5.66	1.59	1.52
3	3	160	LEU	N-CA	5.66	1.53	1.46
3	3	27	GLU	N-CA	5.65	1.53	1.46
1	1	140	ALA	C-N	-5.65	1.26	1.33
1	1	264	LYS	N-CA	5.65	1.52	1.45
1	1	103	LYS	N-CA	5.65	1.53	1.46
2	2	218	ILE	CA-C	5.64	1.59	1.52
3	3	180	ILE	CA-C	5.64	1.59	1.52
2	2	173	ARG	N-CA	5.64	1.53	1.45
3	3	20	GLN	N-CA	5.64	1.53	1.45
1	1	9	SER	CA-C	5.64	1.60	1.53
1	1	283	GLY	C-N	-5.64	1.28	1.34
3	3	112	GLY	N-CA	5.64	1.51	1.45
3	3	168	VAL	N-CA	5.64	1.53	1.46
1	1	56	VAL	N-CA	5.64	1.53	1.46
1	1	143	THR	N-CA	5.64	1.53	1.46
3	3	195	GLN	CA-C	5.63	1.60	1.52
1	1	284	VAL	CA-C	5.63	1.58	1.52
1	1	67	VAL	N-CA	5.63	1.53	1.46
2	2	175	CYS	CA-C	5.63	1.59	1.53
3	3	41	LYS	N-CA	5.63	1.53	1.45
1	1	47	VAL	N-CA	5.63	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	102	ASP	N-CA	5.63	1.52	1.46
3	3	204	THR	N-CA	5.63	1.54	1.45
1	1	69	HIS	N-CA	5.62	1.53	1.46
1	1	91	THR	C-N	-5.62	1.26	1.33
2	2	73	LYS	N-CA	5.62	1.53	1.46
3	3	29	ASP	N-CA	5.61	1.53	1.46
3	3	112	GLY	CA-C	5.61	1.57	1.52
2	2	264	ARG	CA-C	5.61	1.60	1.53
3	3	97	HIS	N-CA	5.61	1.53	1.46
3	3	143	LYS	N-CA	5.61	1.53	1.45
1	1	63	THR	N-CA	5.61	1.52	1.45
3	3	8	PRO	N-CA	5.61	1.54	1.47
2	2	202	THR	N-CA	5.61	1.53	1.46
3	3	201	PRO	N-CA	5.61	1.54	1.47
2	2	217	SER	C-N	-5.61	1.27	1.33
3	3	34	ILE	N-CA	5.61	1.52	1.46
2	2	71	TRP	N-CA	5.60	1.53	1.46
3	3	85	LEU	N-CA	5.60	1.53	1.46
1	1	23	SER	CA-C	5.60	1.60	1.52
1	1	146	ASN	CA-C	5.60	1.60	1.52
3	3	25	LEU	N-CA	5.60	1.52	1.46
3	3	32	PRO	C-N	-5.60	1.26	1.33
1	1	278	ALA	N-CA	5.60	1.53	1.46
1	1	27	LEU	C-N	-5.59	1.26	1.33
3	3	144	LYS	N-CA	5.59	1.52	1.46
1	1	128	SER	N-CA	5.59	1.53	1.45
1	1	275	ARG	CA-C	5.59	1.60	1.52
3	3	161	GLN	CA-C	5.58	1.60	1.52
4	4	55	GLU	N-CA	5.58	1.54	1.46
1	1	167	PRO	N-CA	5.58	1.53	1.47
3	3	230	HIS	C-N	-5.58	1.27	1.33
1	1	62	GLN	N-CA	5.58	1.53	1.46
3	3	37	PRO	N-CA	5.58	1.53	1.47
3	3	133	SER	N-CA	5.58	1.52	1.45
2	2	249	ILE	CA-C	5.58	1.59	1.52
1	1	245	VAL	N-CA	5.57	1.53	1.46
2	2	126	ALA	C-N	-5.57	1.28	1.33
3	3	176	TYR	C-N	-5.57	1.25	1.33
2	2	209	VAL	N-CA	5.57	1.53	1.46
1	1	28	PRO	N-CA	5.57	1.53	1.47
1	1	265	HIS	N-CA	5.57	1.55	1.46
2	2	148	ALA	CA-C	5.57	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	174	THR	CA-C	5.57	1.59	1.52
2	2	151	GLY	CA-C	5.56	1.59	1.52
3	3	203	SER	N-CA	5.56	1.54	1.46
1	1	244	VAL	N-CA	5.56	1.53	1.46
2	2	22	THR	N-CA	5.56	1.53	1.46
2	2	108	VAL	N-CA	5.56	1.52	1.46
2	2	194	PRO	N-CA	5.56	1.54	1.47
3	3	107	TYR	CA-C	5.56	1.59	1.52
4	4	48	GLN	CA-C	5.56	1.59	1.52
1	1	268	VAL	N-CA	5.56	1.52	1.46
2	2	36	GLY	N-CA	5.56	1.53	1.45
2	2	67	ASP	N-CA	5.55	1.53	1.46
4	4	37	ALA	CA-C	5.55	1.60	1.52
1	1	288	ASP	N-CA	5.55	1.53	1.46
3	3	9	GLY	N-CA	5.55	1.53	1.44
3	3	216	ALA	N-CA	5.55	1.53	1.46
1	1	79	SER	CA-C	5.55	1.59	1.52
2	2	234	LEU	C-N	-5.55	1.27	1.33
2	2	174	PHE	C-N	-5.55	1.26	1.33
3	3	84	CYS	CA-C	5.55	1.59	1.52
1	1	36	THR	N-CA	5.54	1.52	1.46
1	1	86	CYS	N-CA	5.54	1.53	1.46
1	1	98	THR	N-CA	5.54	1.53	1.46
2	2	99	HIS	N-CA	5.54	1.52	1.46
4	4	46	PHE	N-CA	5.54	1.52	1.46
1	1	76	SER	CA-C	5.53	1.60	1.52
2	2	24	THR	CA-C	5.53	1.59	1.52
4	4	7	SER	N-CA	5.53	1.53	1.46
4	4	41	ALA	CA-C	5.53	1.60	1.52
2	2	164	ASP	N-CA	5.53	1.53	1.46
2	2	188	GLY	N-CA	5.53	1.53	1.45
2	2	193	PHE	N-CA	5.53	1.54	1.46
3	3	23	CYS	N-CA	5.53	1.53	1.46
1	1	254	THR	N-CA	5.53	1.53	1.46
2	2	212	TYR	CA-C	5.52	1.60	1.52
1	1	156	GLN	CA-C	5.52	1.60	1.53
4	4	6	SER	N-CA	5.52	1.53	1.45
1	1	125	PHE	CA-C	5.51	1.59	1.52
2	2	118	HIS	N-CA	5.51	1.52	1.45
1	1	248	HIS	N-CA	5.51	1.52	1.46
2	2	33	VAL	N-CA	5.51	1.53	1.46
3	3	51	THR	CA-C	5.51	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	76	PRO	N-CA	5.51	1.53	1.47
2	2	136	SER	N-CA	5.50	1.52	1.46
3	3	228	THR	N-CA	5.50	1.52	1.45
2	2	270	ARG	N-CA	5.50	1.53	1.46
2	2	68	THR	N-CA	5.50	1.53	1.46
1	1	137	VAL	CA-C	5.50	1.58	1.53
3	3	221	SER	N-CA	5.50	1.53	1.45
1	1	97	SER	CA-C	5.50	1.60	1.52
4	4	4	GLN	N-CA	5.50	1.54	1.46
2	2	217	SER	CA-C	5.49	1.59	1.52
3	3	77	HIS	C-N	-5.49	1.26	1.33
2	2	121	ALA	CA-C	5.49	1.59	1.52
3	3	46	LEU	N-CA	5.49	1.53	1.46
3	3	42	ASN	CA-C	5.48	1.58	1.52
1	1	30	THR	N-CA	5.48	1.53	1.46
1	1	32	ALA	C-N	-5.48	1.26	1.33
1	1	100	ASN	N-CA	5.48	1.53	1.46
3	3	33	PRO	N-CA	5.48	1.53	1.47
3	3	26	PRO	CA-C	5.48	1.58	1.52
1	1	36	THR	C-N	-5.47	1.26	1.33
2	2	21	SER	CA-C	5.47	1.59	1.52
1	1	35	PRO	CA-C	5.47	1.59	1.52
1	1	137	VAL	N-CA	5.47	1.53	1.46
1	1	210	ASP	N-CA	5.47	1.53	1.46
1	1	220	GLN	CA-C	5.47	1.59	1.52
1	1	150	ALA	CA-C	5.47	1.59	1.52
1	1	248	HIS	CA-C	5.47	1.59	1.52
1	1	74	GLU	N-CA	5.46	1.53	1.46
2	2	146	GLN	CA-C	5.46	1.59	1.52
1	1	192	ALA	CA-C	5.46	1.59	1.52
1	1	139	THR	CA-C	5.45	1.59	1.52
1	1	289	GLY	N-CA	5.45	1.53	1.45
2	2	74	GLU	N-CA	5.45	1.53	1.46
1	1	119	ARG	CA-C	5.45	1.60	1.52
4	4	50	PRO	N-CA	5.45	1.54	1.47
2	2	133	ALA	CA-C	5.45	1.59	1.52
2	2	264	ARG	N-CA	5.45	1.54	1.46
2	2	94	GLN	CA-C	5.44	1.59	1.52
4	4	60	VAL	CA-C	5.44	1.59	1.52
3	3	62	LYS	N-CA	5.44	1.52	1.46
2	2	107	THR	CA-C	5.44	1.60	1.53
1	1	166	VAL	N-CA	5.44	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	195	SER	CA-C	5.44	1.59	1.52
1	1	197	PRO	N-CA	5.44	1.54	1.47
2	2	55	GLU	N-CA	5.44	1.53	1.46
2	2	30	ASN	CA-C	5.43	1.60	1.52
1	1	33	SER	CA-C	5.43	1.58	1.52
1	1	274	PRO	CA-C	5.43	1.58	1.52
1	1	107	VAL	CA-C	5.43	1.59	1.52
1	1	57	PRO	N-CA	5.43	1.54	1.47
1	1	122	LEU	N-CA	5.43	1.52	1.46
1	1	131	ASP	C-N	-5.42	1.25	1.33
3	3	40	VAL	N-CA	5.42	1.53	1.46
1	1	162	PRO	N-CA	5.42	1.54	1.47
1	1	188	GLY	N-CA	5.42	1.53	1.45
1	1	77	ILE	N-CA	5.42	1.53	1.46
1	1	271	PRO	N-CA	5.42	1.53	1.47
4	4	52	LYS	N-CA	5.42	1.53	1.46
1	1	32	ALA	CA-C	5.42	1.60	1.52
1	1	87	VAL	N-CA	5.42	1.53	1.46
1	1	168	GLU	CA-C	5.41	1.59	1.52
3	3	230	HIS	N-CA	5.41	1.53	1.46
1	1	259	VAL	N-CA	5.41	1.52	1.46
2	2	265	ASN	C-N	-5.41	1.27	1.33
4	4	9	LYS	CA-C	5.40	1.60	1.52
4	4	44	GLN	CA-C	5.40	1.59	1.53
1	1	178	SER	CA-C	5.40	1.60	1.52
1	1	200	GLY	CA-C	5.40	1.58	1.52
3	3	106	TYR	CA-C	5.40	1.60	1.52
2	2	49	PRO	C-N	-5.40	1.28	1.34
2	2	119	GLN	C-N	-5.40	1.26	1.33
1	1	118	LEU	N-CA	5.40	1.52	1.46
2	2	51	ASP	N-CA	5.39	1.52	1.46
4	4	13	HIS	N-CA	5.39	1.52	1.46
2	2	58	VAL	N-CA	5.39	1.53	1.46
1	1	216	PRO	N-CA	5.39	1.54	1.47
3	3	34	ILE	CA-C	5.39	1.58	1.52
3	3	215	SER	CA-C	5.39	1.59	1.52
1	1	111	THR	CA-C	5.38	1.59	1.52
1	1	157	ILE	N-CA	5.38	1.53	1.46
2	2	28	ALA	N-CA	5.38	1.53	1.46
2	2	141	MET	N-CA	5.38	1.53	1.46
3	3	223	ARG	N-CA	5.38	1.53	1.46
1	1	286	TYR	C-N	-5.38	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	68	GLN	N-CA	5.37	1.52	1.46
1	1	241	ALA	CA-C	5.37	1.59	1.52
2	2	25	THR	CA-C	5.37	1.58	1.52
2	2	29	ALA	CA-C	5.37	1.60	1.53
2	2	182	GLY	N-CA	5.37	1.53	1.45
3	3	140	ASP	CA-C	5.37	1.59	1.52
1	1	54	PRO	N-CA	5.37	1.54	1.47
3	3	50	ASP	N-CA	5.37	1.53	1.46
4	4	36	SER	CA-C	5.37	1.59	1.52
1	1	170	TRP	N-CA	5.37	1.53	1.46
3	3	54	PRO	N-CA	5.36	1.54	1.47
3	3	72	LEU	N-CA	5.36	1.52	1.45
2	2	163	PRO	N-CA	5.36	1.53	1.47
3	3	202	LEU	N-CA	5.36	1.53	1.45
1	1	153	GLN	N-CA	5.36	1.52	1.46
3	3	10	SER	CA-C	5.36	1.59	1.52
2	2	96	MET	N-CA	5.36	1.52	1.46
2	2	185	THR	CA-C	5.36	1.59	1.52
4	4	65	ALA	CA-C	5.36	1.59	1.52
4	4	66	PRO	N-CA	5.36	1.54	1.47
1	1	218	LYS	N-CA	5.35	1.53	1.46
1	1	269	TRP	N-CA	5.35	1.52	1.45
2	2	37	ARG	N-CA	5.35	1.53	1.46
1	1	145	THR	N-CA	5.35	1.53	1.46
1	1	226	ASP	N-CA	5.35	1.52	1.46
3	3	192	VAL	C-N	-5.35	1.26	1.33
2	2	127	VAL	CA-C	5.35	1.57	1.53
3	3	37	PRO	CA-C	5.35	1.59	1.52
1	1	106	ALA	N-CA	5.34	1.52	1.46
4	4	8	GLN	N-CA	5.34	1.52	1.46
3	3	93	PRO	N-CA	5.34	1.54	1.47
4	4	41	ALA	C-N	-5.34	1.26	1.34
4	4	56	PRO	N-CA	5.34	1.54	1.47
2	2	76	ARG	CA-C	5.34	1.59	1.52
2	2	177	VAL	CA-C	5.34	1.59	1.52
3	3	111	ALA	CA-C	5.34	1.59	1.52
3	3	222	VAL	C-N	-5.33	1.26	1.33
2	2	171	ALA	CA-C	5.33	1.60	1.52
1	1	140	ALA	CA-C	5.33	1.59	1.52
3	3	217	CYS	CA-C	5.33	1.59	1.52
1	1	232	ALA	CA-C	5.33	1.59	1.52
3	3	114	LEU	C-N	-5.33	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	43	ALA	CA-C	5.33	1.59	1.52
1	1	301	THR	CA-C	5.33	1.59	1.52
1	1	267	ARG	C-N	-5.32	1.25	1.33
3	3	33	PRO	CA-C	5.32	1.59	1.52
1	1	144	GLU	N-CA	5.32	1.52	1.46
2	2	63	PHE	N-CA	5.32	1.53	1.46
2	2	132	LEU	N-CA	5.32	1.52	1.45
2	2	161	PHE	C-N	-5.32	1.25	1.33
1	1	129	ARG	C-N	-5.31	1.27	1.33
1	1	231	ALA	CA-C	5.31	1.59	1.52
2	2	201	ARG	CA-C	5.31	1.60	1.52
1	1	38	SER	N-CA	5.31	1.52	1.45
3	3	12	GLN	CA-C	5.31	1.59	1.52
1	1	281	GLY	CA-C	5.31	1.59	1.51
2	2	184	GLY	N-CA	5.31	1.53	1.45
4	4	10	VAL	N-CA	5.31	1.52	1.46
2	2	259	GLU	N-CA	5.30	1.52	1.46
1	1	270	CYS	N-CA	5.30	1.53	1.46
2	2	258	CYS	N-CA	5.30	1.52	1.46
4	4	43	LYS	N-CA	5.30	1.53	1.46
1	1	160	VAL	N-CA	5.30	1.53	1.46
2	2	53	PRO	N-CA	5.30	1.53	1.47
2	2	74	GLU	CA-C	5.30	1.59	1.52
4	4	59	ASP	N-CA	5.30	1.53	1.46
1	1	282	PRO	N-CA	5.29	1.54	1.47
2	2	19	GLY	CA-C	5.29	1.60	1.52
1	1	89	ILE	CA-C	5.29	1.58	1.52
2	2	31	SER	CA-C	5.28	1.58	1.52
3	3	145	ARG	CA-C	5.28	1.60	1.52
3	3	205	PRO	N-CA	5.28	1.54	1.47
1	1	206	SER	CA-C	5.28	1.59	1.53
2	2	250	THR	N-CA	5.28	1.52	1.46
1	1	222	ALA	CA-C	5.28	1.59	1.52
2	2	124	VAL	CA-C	5.28	1.58	1.53
2	2	252	THR	CA-C	5.28	1.59	1.52
3	3	59	ALA	CA-C	5.28	1.59	1.52
3	3	113	SER	N-CA	5.28	1.52	1.46
1	1	88	THR	N-CA	5.28	1.52	1.46
2	2	103	ARG	C-N	-5.28	1.26	1.33
2	2	259	GLU	CA-C	5.27	1.58	1.52
2	2	192	VAL	C-O	-5.27	1.17	1.24
3	3	89	PRO	N-CA	5.27	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	64	THR	CA-C	5.27	1.59	1.52
3	3	86	SER	CA-C	5.27	1.59	1.52
4	4	8	GLN	C-N	-5.27	1.26	1.33
1	1	31	GLU	N-CA	5.27	1.52	1.46
2	2	56	PRO	N-CA	5.27	1.54	1.47
1	1	230	GLY	CA-C	5.27	1.59	1.51
2	2	224	HIS	N-CA	5.27	1.52	1.46
2	2	123	GLY	N-CA	5.26	1.53	1.45
2	2	124	VAL	N-CA	5.26	1.52	1.46
3	3	165	THR	N-CA	5.26	1.52	1.46
3	3	171	ILE	N-CA	5.26	1.52	1.46
1	1	93	ASP	N-CA	5.26	1.52	1.46
1	1	218	LYS	CA-C	5.26	1.59	1.52
1	1	296	THR	C-N	-5.26	1.27	1.33
2	2	152	GLU	CA-C	5.26	1.59	1.52
2	2	183	ASN	N-CA	5.26	1.51	1.46
3	3	72	LEU	C-N	-5.26	1.26	1.33
4	4	25	ILE	CA-C	5.26	1.59	1.52
1	1	142	PHE	C-N	-5.26	1.25	1.33
2	2	230	ALA	CA-C	5.26	1.59	1.52
3	3	4	VAL	C-N	-5.26	1.26	1.33
1	1	208	PHE	C-N	-5.25	1.26	1.33
2	2	17	THR	N-CA	5.25	1.52	1.46
2	2	36	GLY	CA-C	5.25	1.59	1.51
3	3	16	ALA	CA-C	5.25	1.60	1.52
3	3	137	PRO	N-CA	5.25	1.54	1.47
2	2	85	ALA	CA-C	5.25	1.59	1.52
2	2	262	GLY	N-CA	5.25	1.52	1.45
3	3	39	GLU	N-CA	5.25	1.52	1.46
1	1	239	ILE	N-CA	5.25	1.51	1.46
2	2	193	PHE	CA-C	5.25	1.59	1.53
1	1	95	PRO	N-CA	5.25	1.54	1.47
1	1	298	ASP	N-CA	5.25	1.52	1.46
2	2	229	ILE	CA-C	5.25	1.58	1.53
3	3	200	VAL	CA-C	5.25	1.58	1.52
4	4	11	GLY	CA-C	5.25	1.59	1.51
2	2	171	ALA	C-O	-5.24	1.17	1.24
2	2	213	VAL	N-CA	5.24	1.52	1.46
3	3	58	SER	CA-C	5.24	1.59	1.52
3	3	109	HIS	N-CA	5.24	1.52	1.46
4	4	62	ILE	CA-C	5.24	1.59	1.52
1	1	293	PRO	N-CA	5.24	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	216	LEU	N-CA	5.24	1.52	1.45
1	1	296	THR	N-CA	5.24	1.52	1.46
2	2	164	ASP	CA-C	5.24	1.59	1.52
1	1	177	THR	N-CA	5.24	1.52	1.46
1	1	243	ARG	CA-C	5.24	1.59	1.52
1	1	271	PRO	C-N	-5.24	1.26	1.33
3	3	190	ILE	N-CA	5.24	1.52	1.46
1	1	44	LEU	C-N	-5.23	1.26	1.33
1	1	151	LEU	N-CA	5.23	1.52	1.46
1	1	182	SER	CA-C	5.23	1.59	1.52
4	4	3	ALA	CA-C	5.23	1.59	1.52
2	2	69	VAL	N-CA	5.23	1.53	1.46
3	3	45	GLU	C-O	-5.23	1.18	1.24
3	3	114	LEU	N-CA	5.23	1.51	1.45
4	4	15	ASN	N-CA	5.23	1.52	1.46
3	3	7	THR	N-CA	5.22	1.53	1.45
3	3	61	LYS	N-CA	5.22	1.52	1.46
2	2	45	SER	CA-C	5.22	1.59	1.52
2	2	156	THR	N-CA	5.22	1.52	1.45
2	2	150	PRO	N-CA	5.22	1.54	1.47
4	4	24	THR	CA-C	5.22	1.59	1.52
2	2	92	PHE	CA-C	5.21	1.59	1.52
2	2	170	PRO	N-CA	5.21	1.53	1.47
3	3	95	LEU	N-CA	5.21	1.52	1.46
1	1	123	GLU	N-CA	5.21	1.53	1.46
2	2	228	GLY	N-CA	5.21	1.52	1.45
3	3	35	ASP	N-CA	5.21	1.52	1.46
1	1	64	ARG	CA-C	5.21	1.60	1.53
1	1	37	HIS	N-CA	5.21	1.54	1.46
1	1	230	GLY	N-CA	5.21	1.53	1.45
3	3	110	TRP	NE1-CE2	-5.21	1.31	1.37
1	1	25	ASP	C-N	-5.21	1.26	1.33
1	1	141	ASN	C-N	-5.21	1.26	1.33
4	4	25	ILE	C-N	-5.21	1.26	1.33
1	1	135	THR	CA-C	5.21	1.59	1.52
2	2	10	SER	CA-C	5.21	1.59	1.52
2	2	220	SER	CA-C	5.20	1.59	1.52
1	1	263	PRO	N-CA	5.20	1.53	1.47
2	2	120	GLY	N-CA	5.20	1.51	1.45
2	2	219	ASP	N-CA	5.20	1.54	1.46
1	1	84	GLY	N-CA	5.20	1.52	1.45
2	2	123	GLY	CA-C	5.20	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	223	LYS	N-CA	5.20	1.53	1.46
2	2	228	GLY	CA-C	5.20	1.59	1.51
1	1	223	ALA	CA-C	5.20	1.59	1.52
2	2	236	PRO	N-CA	5.20	1.53	1.47
3	3	22	PRO	N-CA	5.20	1.53	1.47
1	1	150	ALA	C-N	-5.20	1.26	1.33
1	1	39	LYS	N-CA	5.20	1.52	1.46
2	2	207	THR	N-CA	5.20	1.52	1.46
2	2	253	ILE	N-CA	5.20	1.52	1.46
3	3	23	CYS	CA-C	5.20	1.59	1.52
2	2	265	ASN	CA-C	5.19	1.59	1.52
3	3	190	ILE	CA-C	5.19	1.59	1.52
1	1	82	ALA	CA-C	5.19	1.59	1.52
1	1	246	ASN	CA-C	5.19	1.59	1.52
2	2	138	THR	CA-C	5.19	1.59	1.52
4	4	38	SER	CA-C	5.19	1.59	1.52
1	1	45	THR	N-CA	5.19	1.53	1.46
3	3	80	ASP	C-N	-5.19	1.27	1.33
2	2	257	CYS	CA-C	5.19	1.59	1.52
1	1	272	ARG	N-CA	5.18	1.52	1.45
2	2	149	ASN	N-CA	5.18	1.52	1.46
1	1	21	ALA	CA-C	5.18	1.59	1.52
1	1	213	SER	CA-C	5.18	1.59	1.52
3	3	220	PHE	C-N	-5.18	1.26	1.33
2	2	155	GLY	N-CA	5.18	1.52	1.45
2	2	80	TRP	NE1-CE2	-5.18	1.31	1.37
2	2	178	ASP	N-CA	5.18	1.52	1.46
1	1	181	PRO	N-CA	5.17	1.53	1.47
1	1	71	SER	CA-C	5.17	1.58	1.52
1	1	61	VAL	CA-C	5.17	1.59	1.52
2	2	103	ARG	CA-C	5.17	1.58	1.52
3	3	27	GLU	CA-C	5.17	1.59	1.52
3	3	49	ILE	N-CA	5.17	1.52	1.46
3	3	140	ASP	N-CA	5.17	1.53	1.46
4	4	57	ILE	N-CA	5.17	1.52	1.46
3	3	123	SER	CA-C	5.16	1.59	1.52
3	3	126	ALA	CA-C	5.16	1.59	1.52
3	3	156	TRP	NE1-CE2	-5.16	1.31	1.37
1	1	42	PRO	N-CA	5.16	1.54	1.47
2	2	269	PRO	N-CA	5.16	1.53	1.47
3	3	44	MET	N-CA	5.16	1.52	1.46
2	2	267	THR	CA-C	5.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	4	47	SER	CA-C	5.16	1.59	1.52
2	2	38	TRP	NE1-CE2	-5.15	1.31	1.37
2	2	168	THR	CA-C	5.15	1.59	1.52
2	2	149	ASN	CA-C	5.15	1.58	1.53
1	1	74	GLU	CA-C	5.15	1.59	1.52
2	2	115	SER	CA-C	5.15	1.59	1.52
3	3	172	SER	CA-C	5.15	1.58	1.52
3	3	209	ASP	N-CA	5.15	1.52	1.46
1	1	125	PHE	C-N	-5.15	1.27	1.33
2	2	104	SER	N-CA	5.15	1.52	1.46
1	1	175	TRP	N-CA	5.14	1.53	1.46
3	3	202	LEU	C-N	-5.14	1.26	1.33
4	4	7	SER	CA-C	5.14	1.59	1.52
1	1	124	PHE	CA-C	5.14	1.59	1.52
1	1	224	LEU	N-CA	5.14	1.52	1.46
3	3	66	GLU	CA-C	5.14	1.59	1.52
3	3	103	ILE	CA-C	5.14	1.59	1.52
1	1	169	LYS	N-CA	5.13	1.52	1.46
1	1	218	LYS	C-O	-5.13	1.17	1.24
1	1	30	THR	CA-C	5.13	1.59	1.52
1	1	81	PHE	CA-C	5.13	1.59	1.52
1	1	50	GLY	CA-C	5.13	1.58	1.51
2	2	47	ALA	CA-C	5.13	1.59	1.52
2	2	54	THR	N-CA	5.13	1.52	1.46
3	3	177	ARG	C-N	-5.13	1.26	1.33
4	4	29	THR	CA-C	5.13	1.58	1.52
2	2	173	ARG	CA-C	5.13	1.58	1.52
3	3	207	GLU	N-CA	5.13	1.52	1.46
4	4	49	ASP	CA-C	5.13	1.58	1.52
1	1	131	ASP	CA-C	5.12	1.59	1.52
1	1	35	PRO	C-N	-5.12	1.26	1.33
1	1	290	THR	CA-C	5.12	1.59	1.52
3	3	104	LEU	N-CA	5.12	1.52	1.46
1	1	258	ARG	CA-C	5.12	1.59	1.52
1	1	199	VAL	N-CA	5.12	1.52	1.46
2	2	155	GLY	C-N	-5.12	1.26	1.33
3	3	20	GLN	CA-C	5.12	1.60	1.53
1	1	271	PRO	CA-C	5.12	1.58	1.52
1	1	200	GLY	N-CA	5.12	1.52	1.45
2	2	49	PRO	CA-C	5.12	1.59	1.52
2	2	216	LEU	CA-C	5.12	1.58	1.52
1	1	273	PRO	C-N	-5.11	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	28	ALA	C-N	-5.11	1.27	1.33
2	2	54	THR	CA-C	5.11	1.59	1.52
2	2	153	LYS	N-CA	5.11	1.53	1.46
3	3	216	ALA	CA-C	5.11	1.59	1.52
3	3	229	THR	CA-C	5.11	1.59	1.52
4	4	47	SER	N-CA	5.11	1.52	1.45
2	2	245	PRO	CA-C	5.11	1.58	1.52
4	4	34	ARG	CA-C	5.11	1.59	1.52
3	3	8	PRO	CA-C	5.11	1.59	1.52
1	1	55	LEU	C-N	-5.11	1.27	1.33
2	2	39	PRO	N-CA	5.11	1.53	1.47
3	3	38	GLY	N-CA	5.11	1.52	1.45
3	3	81	PRO	N-CA	5.11	1.53	1.47
3	3	225	LEU	C-N	-5.10	1.27	1.33
1	1	84	GLY	CA-C	5.10	1.59	1.51
2	2	182	GLY	CA-C	5.10	1.59	1.51
2	2	190	ALA	CA-C	5.10	1.60	1.52
1	1	154	VAL	CA-C	5.10	1.59	1.52
1	1	167	PRO	CA-C	5.09	1.58	1.52
3	3	106	TYR	N-CA	5.09	1.52	1.46
2	2	78	TRP	NE1-CE2	-5.09	1.31	1.37
1	1	108	TRP	NE1-CE2	-5.09	1.31	1.37
3	3	188	GLY	N-CA	5.09	1.52	1.45
1	1	28	PRO	CA-C	5.09	1.58	1.52
4	4	42	SER	CA-C	5.09	1.59	1.52
1	1	269	TRP	NE1-CE2	-5.08	1.31	1.37
3	3	170	TRP	NE1-CE2	-5.08	1.31	1.37
1	1	170	TRP	NE1-CE2	-5.08	1.31	1.37
2	2	192	VAL	CA-C	5.08	1.60	1.52
2	2	215	SER	CA-C	5.08	1.59	1.52
3	3	117	THR	N-CA	5.08	1.52	1.46
3	3	156	TRP	N-CA	5.08	1.52	1.46
1	1	277	VAL	CA-C	5.08	1.58	1.52
1	1	165	PRO	N-CA	5.08	1.53	1.47
1	1	297	LYS	N-CA	5.08	1.52	1.46
2	2	136	SER	CA-C	5.07	1.58	1.52
3	3	24	ALA	CA-C	5.07	1.59	1.52
4	4	35	ASP	CA-C	5.07	1.59	1.52
2	2	8	GLY	N-CA	5.07	1.52	1.45
3	3	121	CYS	N-CA	5.07	1.53	1.46
1	1	105	PHE	CA-C	5.07	1.58	1.52
1	1	203	ASN	N-CA	5.06	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	13	VAL	N-CA	5.06	1.52	1.46
3	3	173	ASN	CA-C	5.06	1.59	1.52
1	1	51	ALA	CA-C	5.06	1.59	1.52
4	4	45	ASP	N-CA	5.06	1.51	1.45
1	1	160	VAL	CA-C	5.06	1.58	1.52
3	3	173	ASN	N-CA	5.06	1.52	1.46
1	1	212	PHE	CA-C	5.05	1.58	1.52
2	2	225	ASN	CA-C	5.05	1.59	1.53
4	4	29	THR	C-N	-5.05	1.27	1.33
2	2	99	HIS	CA-C	5.05	1.58	1.52
2	2	227	TRP	NE1-CE2	-5.05	1.31	1.37
3	3	49	ILE	CA-C	5.05	1.59	1.52
3	3	50	ASP	C-N	-5.05	1.26	1.33
1	1	52	THR	CA-C	5.05	1.59	1.52
1	1	128	SER	CA-C	5.05	1.58	1.52
1	1	243	ARG	N-CA	5.05	1.52	1.45
3	3	4	VAL	CA-C	5.05	1.58	1.52
1	1	255	SER	CA-C	5.04	1.58	1.52
3	3	91	SER	CA-C	5.04	1.59	1.52
3	3	130	LEU	N-CA	5.04	1.51	1.45
2	2	71	TRP	NE1-CE2	-5.04	1.31	1.37
2	2	78	TRP	N-CA	5.04	1.52	1.45
3	3	31	THR	CA-C	5.04	1.59	1.52
3	3	222	VAL	CA-C	5.03	1.58	1.52
1	1	136	PHE	N-CA	5.03	1.53	1.46
3	3	72	LEU	CA-C	5.03	1.59	1.52
4	4	40	ALA	CA-C	5.03	1.60	1.53
2	2	80	TRP	N-CA	5.03	1.52	1.45
1	1	101	LYS	C-N	-5.03	1.26	1.33
1	1	144	GLU	CA-C	5.03	1.58	1.52
2	2	161	PHE	N-CA	5.03	1.52	1.46
2	2	245	PRO	N-CA	5.03	1.53	1.47
2	2	226	ASN	N-CA	5.02	1.52	1.46
4	4	67	MET	N-CA	5.02	1.52	1.46
2	2	79	TRP	NE1-CE2	-5.02	1.31	1.37
2	2	202	THR	CA-C	5.02	1.58	1.52
3	3	138	GLY	N-CA	5.02	1.52	1.44
3	3	155	ILE	N-CA	5.02	1.52	1.46
2	2	22	THR	CA-C	5.02	1.58	1.52
2	2	155	GLY	CA-C	5.02	1.58	1.51
1	1	191	PRO	N-CA	5.02	1.53	1.47
2	2	90	GLY	N-CA	5.02	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	62	GLN	CA-C	5.02	1.59	1.52
1	1	225	GLY	N-CA	5.02	1.53	1.45
3	3	67	MET	N-CA	5.01	1.52	1.46
3	3	226	ARG	CA-C	5.01	1.58	1.52
1	1	175	TRP	NE1-CE2	-5.01	1.31	1.37
2	2	131	CYS	CA-C	5.01	1.59	1.52
3	3	92	ASP	CA-C	5.01	1.59	1.52
1	1	29	ASN	CA-C	5.01	1.59	1.52
2	2	23	ILE	CA-C	5.01	1.58	1.52
3	3	71	ARG	N-CA	5.01	1.52	1.46
1	1	278	ALA	CA-C	5.00	1.59	1.52
2	2	7	CYS	CA-C	5.00	1.59	1.52
2	2	110	VAL	CA-C	5.00	1.58	1.53
1	1	94	ASN	CA-C	5.00	1.58	1.52
1	1	194	ILE	N-CA	5.00	1.51	1.46
3	3	56	ASP	N-CA	5.00	1.53	1.46

All (870) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	127	VAL	N-CA-C	14.52	121.93	107.55
1	1	130	PHE	N-CA-C	13.49	128.84	108.46
1	1	272	ARG	O-C-N	13.01	131.12	121.88
2	2	125	PHE	N-CA-C	11.72	127.93	109.07
2	2	127	VAL	O-C-N	11.70	128.74	121.37
4	4	10	VAL	N-CA-C	11.16	123.08	108.12
2	2	63	PHE	N-CA-C	11.05	127.24	108.23
2	2	260	PHE	N-CA-C	11.03	127.39	109.40
3	3	21	SER	O-C-N	10.69	130.18	121.84
1	1	237	PHE	N-CA-C	10.66	126.90	111.87
1	1	116	VAL	N-CA-C	10.59	122.80	111.58
3	3	193	PHE	N-CA-C	10.59	124.91	109.14
3	3	53	ILE	N-CA-C	10.54	118.41	107.76
1	1	136	PHE	N-CA-C	10.47	127.23	107.75
2	2	174	PHE	N-CA-C	10.42	125.34	110.23
2	2	244	SER	O-C-N	10.38	129.92	121.20
3	3	19	PHE	N-CA-C	10.23	125.18	110.14
2	2	203	ASN	N-CA-C	10.16	126.13	108.75
2	2	226	ASN	N-CA-C	10.16	122.36	111.28
3	3	184	PHE	N-CA-C	10.08	122.27	111.28
4	4	46	PHE	N-CA-C	9.81	125.85	109.76
3	3	220	PHE	N-CA-C	9.75	125.26	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	239	PHE	N-CA-C	9.72	125.19	108.76
2	2	169	SER	O-C-N	9.58	129.87	121.34
3	3	118	PHE	N-CA-C	9.57	124.33	108.73
2	2	27	GLU	N-CA-C	9.55	121.91	110.44
1	1	94	ASN	O-C-N	9.49	129.24	121.17
1	1	106	ALA	N-CA-C	9.47	124.16	109.96
2	2	198	ILE	N-CA-C	9.42	116.29	106.21
3	3	213	PHE	N-CA-C	9.29	124.04	108.90
3	3	31	THR	O-C-N	9.15	129.44	121.20
2	2	205	CYS	N-CA-C	9.14	120.72	108.38
3	3	116	PHE	N-CA-C	9.13	124.06	107.99
1	1	196	VAL	O-C-N	9.10	129.51	120.59
1	1	266	ILE	N-CA-C	8.93	122.44	108.87
2	2	232	LEU	O-C-N	8.86	129.99	121.66
2	2	247	ILE	O-C-N	8.80	131.13	121.10
1	1	212	PHE	N-CA-C	8.79	123.74	109.85
2	2	193	PHE	N-CA-C	8.79	121.15	110.07
4	4	26	ASN	N-CA-C	8.75	123.70	110.14
2	2	165	ASN	N-CA-C	8.70	123.90	113.28
3	3	135	ALA	O-C-N	8.61	129.96	120.83
1	1	138	VAL	N-CA-C	8.60	120.55	107.99
1	1	180	ASN	O-C-N	8.59	130.15	121.30
3	3	66	GLU	N-CA-C	8.54	121.72	111.82
2	2	152	GLU	N-CA-C	8.48	121.59	111.33
1	1	144	GLU	N-CA-C	8.46	123.03	109.24
3	3	232	GLU	N-CA-C	8.44	120.39	108.74
2	2	191	PHE	N-CA-C	8.43	122.67	112.38
1	1	104	LEU	N-CA-C	8.36	122.00	108.63
1	1	235	ASN	N-CA-C	8.31	120.93	109.54
2	2	183	ASN	N-CA-C	8.30	125.07	112.54
2	2	193	PHE	CB-CA-C	-8.23	97.26	108.87
2	2	195	HIS	N-CA-C	8.19	120.55	108.60
2	2	161	PHE	N-CA-C	8.17	122.28	108.23
1	1	184	PHE	N-CA-C	8.16	122.72	108.52
4	4	39	ASN	N-CA-C	8.16	121.45	110.35
1	1	78	GLU	O-C-N	8.14	130.45	122.07
2	2	32	VAL	N-CA-C	8.13	119.98	108.36
1	1	208	PHE	N-CA-C	8.10	123.07	108.48
2	2	38	TRP	O-C-N	8.09	128.71	121.18
2	2	13	VAL	N-CA-C	8.08	118.32	106.85
2	2	157	PHE	N-CA-C	8.06	122.41	110.48
2	2	10	SER	N-CA-C	8.06	121.64	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	31	ASN	N-CA-C	8.05	121.16	108.67
3	3	133	SER	N-CA-C	8.02	122.71	109.95
1	1	125	PHE	N-CA-C	8.02	122.69	109.06
3	3	53	ILE	O-C-N	8.00	128.53	121.57
3	3	147	GLU	O-C-N	8.00	130.31	122.07
1	1	31	GLU	N-CA-C	7.99	122.46	109.76
2	2	57	ASP	CB-CA-C	-7.98	107.37	116.54
2	2	210	LEU	O-C-N	7.94	128.65	121.35
3	3	2	LEU	O-C-N	7.92	128.20	121.31
4	4	25	ILE	O-C-N	7.91	131.97	122.95
2	2	241	SER	O-C-N	7.88	130.46	122.10
3	3	200	VAL	O-C-N	7.84	130.04	121.10
2	2	176	PRO	CA-N-CD	-7.81	101.06	112.00
2	2	92	PHE	N-CA-C	7.81	119.79	111.28
2	2	198	ILE	O-C-N	7.78	128.49	121.96
2	2	204	ASN	N-CA-C	7.77	120.65	111.71
3	3	6	ASN	N-CA-C	7.77	121.67	110.10
1	1	245	VAL	O-C-N	7.77	129.74	121.90
4	4	8	GLN	O-C-N	7.74	132.54	123.02
2	2	149	ASN	O-C-N	7.71	128.43	121.42
2	2	210	LEU	N-CA-C	7.70	119.95	109.24
3	3	204	THR	O-C-N	7.68	129.25	121.72
3	3	189	TYR	N-CA-C	7.67	121.41	108.90
1	1	38	SER	N-CA-C	7.65	121.52	109.81
1	1	141	ASN	N-CA-C	7.65	120.85	108.76
1	1	163	GLY	O-C-N	7.65	128.83	122.71
1	1	45	THR	N-CA-C	7.64	118.32	108.24
1	1	56	VAL	O-C-N	7.63	129.79	121.10
1	1	215	VAL	O-C-N	7.60	129.76	121.10
4	4	49	ASP	O-C-N	7.59	127.76	121.31
1	1	298	ASP	N-CA-C	7.58	121.22	110.23
3	3	192	VAL	N-CA-C	7.57	118.71	108.11
2	2	124	VAL	N-CA-C	7.54	118.68	107.15
1	1	259	VAL	N-CA-C	7.53	119.48	107.73
3	3	71	ARG	N-CA-C	7.53	121.25	109.96
2	2	246	GLU	N-CA-C	7.52	120.65	108.32
3	3	158	ILE	N-CA-C	7.51	118.76	108.84
3	3	36	ILE	O-C-N	7.48	129.63	121.10
3	3	7	THR	O-C-N	7.48	130.26	121.21
4	4	5	VAL	N-CA-C	7.48	119.67	108.23
3	3	140	ASP	O-C-N	7.43	129.86	121.32
2	2	259	GLU	N-CA-C	7.42	121.67	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	80	PHE	N-CA-C	7.42	120.31	111.33
1	1	249	ASN	N-CA-C	7.42	120.31	109.04
1	1	242	VAL	N-CA-C	7.40	119.74	108.71
2	2	52	GLN	O-C-N	7.40	129.83	121.32
2	2	93	GLY	O-C-N	7.40	129.37	122.19
1	1	105	PHE	N-CA-C	7.40	121.30	109.24
1	1	79	SER	O-C-N	7.38	129.67	122.07
4	4	47	SER	O-C-N	7.37	131.32	123.06
1	1	190	ALA	O-C-N	7.37	129.79	121.32
3	3	167	VAL	N-CA-C	7.36	119.10	107.98
3	3	223	ARG	N-CA-C	7.36	118.90	108.74
3	3	232	GLU	O-C-N	7.36	131.53	122.92
3	3	153	HIS	N-CA-C	7.36	119.92	108.96
3	3	199	VAL	N-CA-C	7.34	118.86	108.36
2	2	104	SER	N-CA-C	7.33	120.42	108.55
3	3	196	THR	O-C-N	7.32	128.96	121.79
4	4	10	VAL	CB-CA-C	-7.31	103.39	111.35
2	2	175	CYS	O-C-N	7.30	128.53	121.31
3	3	30	VAL	N-CA-C	7.29	119.21	109.37
2	2	136	SER	N-CA-C	7.26	120.76	109.07
2	2	254	ALA	O-C-N	7.25	130.77	121.12
3	3	25	LEU	O-C-N	7.25	128.49	121.31
1	1	164	ALA	N-CA-C	7.25	119.03	109.83
2	2	219	ASP	N-CA-C	7.24	117.83	108.34
3	3	167	VAL	CB-CA-C	-7.24	103.41	111.23
3	3	70	VAL	CB-CA-C	-7.24	104.43	112.68
2	2	174	PHE	CB-CA-C	-7.23	97.72	109.72
1	1	7	SER	O-C-N	7.22	131.60	122.93
3	3	101	GLY	O-C-N	7.22	129.28	122.13
1	1	68	GLN	N-CA-C	7.22	120.20	109.59
1	1	93	ASP	N-CA-C	7.22	119.14	108.60
1	1	119	ARG	O-C-N	7.21	129.59	122.09
1	1	141	ASN	O-C-N	7.21	131.55	123.48
2	2	50	VAL	N-CA-C	7.19	122.25	111.89
3	3	42	ASN	N-CA-C	7.19	120.50	108.13
2	2	261	ASN	N-CA-C	7.18	120.80	109.81
1	1	166	VAL	O-C-N	7.18	129.29	121.10
1	1	34	GLY	O-C-N	7.18	128.95	121.77
2	2	74	GLU	N-CA-C	7.17	121.27	112.23
1	1	268	VAL	N-CA-C	7.17	119.15	108.46
1	1	142	PHE	N-CA-C	7.16	120.70	109.96
3	3	126	ALA	N-CA-C	7.15	119.93	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	66	VAL	N-CA-C	7.15	119.25	107.24
1	1	161	PRO	O-C-N	7.14	129.89	121.46
2	2	94	GLN	O-C-N	7.14	129.43	122.07
3	3	45	GLU	O-C-N	7.13	129.68	122.12
3	3	69	ARG	N-CA-C	7.12	120.37	108.20
3	3	32	PRO	O-C-N	7.11	129.85	121.46
1	1	123	GLU	N-CA-C	7.08	121.51	113.01
3	3	214	VAL	N-CA-C	7.08	118.80	108.53
2	2	224	HIS	N-CA-C	7.08	120.72	108.76
1	1	122	LEU	O-C-N	7.04	129.59	122.12
4	4	63	LYS	N-CA-C	7.04	119.85	111.33
2	2	40	GLU	N-CA-C	7.04	120.04	108.99
1	1	164	ALA	O-C-N	7.02	129.29	121.43
3	3	39	GLU	N-CA-C	7.02	120.49	109.96
2	2	113	ASN	N-CA-C	7.01	120.89	110.52
1	1	237	PHE	CB-CA-C	-7.01	100.21	111.28
1	1	249	ASN	O-C-N	7.01	129.14	121.36
1	1	281	GLY	O-C-N	7.00	128.77	121.77
1	1	257	ILE	N-CA-C	6.98	117.48	106.88
3	3	18	ASN	N-CA-C	6.97	122.39	109.56
2	2	108	VAL	N-CA-C	6.95	118.47	107.98
1	1	98	THR	N-CA-C	6.95	118.85	111.28
3	3	102	GLU	N-CA-C	6.94	118.84	111.28
1	1	120	ARG	O-C-N	6.93	129.47	122.12
3	3	19	PHE	CB-CA-C	-6.92	98.04	110.36
3	3	55	PHE	N-CA-C	6.92	125.54	110.80
4	4	46	PHE	CA-CB-CG	-6.92	106.88	113.80
2	2	70	SER	N-CA-C	6.91	120.00	108.73
1	1	160	VAL	O-C-N	6.90	128.97	121.10
4	4	37	ALA	O-C-N	6.90	129.44	122.12
2	2	55	GLU	O-C-N	6.90	129.26	121.32
1	1	292	THR	O-C-N	6.90	128.14	121.31
1	1	273	PRO	O-C-N	6.89	129.59	121.46
2	2	266	ILE	N-CA-C	6.89	118.33	109.30
2	2	204	ASN	CB-CA-C	-6.88	97.90	110.63
4	4	40	ALA	O-C-N	6.88	131.04	122.65
4	4	57	ILE	N-CA-C	6.87	118.44	109.58
3	3	103	ILE	O-C-N	6.86	128.90	121.83
3	3	102	GLU	O-C-N	6.86	129.39	122.12
2	2	127	VAL	CB-CA-C	-6.85	102.95	111.04
1	1	55	LEU	N-CA-C	6.85	119.66	110.35
3	3	163	SER	N-CA-C	6.84	120.75	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	65	ALA	O-C-N	6.83	129.48	121.21
1	1	180	ASN	N-CA-C	6.83	118.31	109.64
1	1	146	ASN	CB-CA-C	-6.80	96.88	110.42
2	2	47	ALA	N-CA-C	6.79	119.58	110.35
1	1	98	THR	O-C-N	6.78	129.30	122.12
2	2	48	ASN	O-C-N	6.77	129.10	121.32
2	2	117	PHE	N-CA-C	6.75	121.68	113.17
1	1	246	ASN	N-CA-C	6.75	120.02	110.23
3	3	73	SER	N-CA-C	6.73	119.39	108.76
3	3	168	VAL	O-C-N	6.73	128.77	121.10
1	1	231	ALA	N-CA-C	6.72	119.69	108.20
1	1	130	PHE	CB-CA-C	-6.71	98.92	109.72
3	3	231	ILE	O-C-N	6.70	129.63	123.19
2	2	204	ASN	O-C-N	6.70	130.06	122.22
2	2	230	ALA	N-CA-C	6.70	119.64	108.73
1	1	74	GLU	N-CA-C	6.69	120.70	112.54
4	4	53	PHE	N-CA-C	6.69	121.98	113.55
1	1	117	GLN	N-CA-C	6.67	119.16	111.02
3	3	195	GLN	O-C-N	6.67	129.03	122.09
2	2	146	GLN	O-C-N	6.67	128.94	122.07
1	1	153	GLN	N-CA-C	6.66	120.13	110.28
2	2	213	VAL	N-CA-C	6.66	117.88	108.36
1	1	85	ALA	N-CA-C	6.66	119.79	109.07
1	1	64	ARG	O-C-N	6.65	130.39	122.94
3	3	165	THR	N-CA-C	6.65	119.56	108.73
2	2	245	PRO	O-C-N	6.64	130.69	122.71
2	2	58	VAL	O-C-N	6.64	128.60	121.90
4	4	14	GLU	CA-C-O	-6.64	114.52	121.55
2	2	246	GLU	O-C-N	6.63	130.98	123.42
3	3	32	PRO	N-CA-C	6.62	118.78	110.70
3	3	139	ALA	N-CA-C	6.61	118.56	109.18
4	4	6	SER	N-CA-C	6.61	119.45	109.41
2	2	253	ILE	N-CA-C	6.60	118.30	108.46
1	1	243	ARG	O-C-N	6.60	130.77	123.25
1	1	249	ASN	CB-CA-C	-6.59	102.33	109.85
2	2	162	THR	O-C-N	6.59	127.81	120.83
1	1	253	VAL	N-CA-C	6.58	117.75	107.28
3	3	145	ARG	O-C-N	6.58	129.68	122.11
3	3	156	TRP	N-CA-C	6.58	118.63	109.15
1	1	92	VAL	O-C-N	6.58	129.88	122.97
2	2	92	PHE	O-C-N	6.56	129.08	122.12
1	1	185	TYR	N-CA-C	6.56	119.80	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	111	ALA	N-CA-C	6.55	119.28	108.99
3	3	148	ALA	O-C-N	6.55	129.06	122.12
1	1	276	ALA	N-CA-C	6.55	120.53	112.54
3	3	183	SER	O-C-N	6.55	129.64	122.11
3	3	116	PHE	CB-CA-C	-6.55	100.17	111.30
1	1	137	VAL	N-CA-C	6.54	117.16	107.15
1	1	239	ILE	N-CA-C	6.53	119.74	108.90
2	2	140	THR	N-CA-C	6.53	119.34	109.41
3	3	216	ALA	N-CA-C	6.52	120.28	109.46
2	2	168	THR	O-C-N	6.51	128.78	122.07
1	1	108	TRP	N-CA-C	6.51	119.13	108.52
1	1	133	GLU	N-CA-C	6.51	119.86	107.75
2	2	63	PHE	CB-CA-C	-6.51	100.05	111.05
2	2	149	ASN	N-CA-C	6.49	120.78	108.97
1	1	51	ALA	N-CA-C	6.48	120.61	110.17
1	1	136	PHE	CB-CA-C	-6.48	100.42	111.31
3	3	233	GLN	N-CA-C	6.48	118.71	110.61
1	1	42	PRO	O-C-N	6.48	129.18	122.18
2	2	264	ARG	O-C-N	6.48	130.33	122.88
1	1	48	GLU	O-C-N	6.47	129.58	122.20
1	1	46	ALA	N-CA-C	6.46	119.42	107.60
1	1	118	LEU	O-C-N	6.46	128.97	122.12
3	3	186	GLU	N-CA-C	6.45	119.59	110.23
1	1	29	ASN	N-CA-C	6.45	119.70	110.10
1	1	144	GLU	O-C-N	6.42	130.53	123.27
3	3	34	ILE	O-C-N	6.42	129.69	123.14
4	4	65	ALA	N-CA-C	6.42	118.81	110.40
3	3	154	VAL	N-CA-C	6.41	117.26	107.77
2	2	110	VAL	N-CA-C	6.41	117.66	107.98
1	1	66	VAL	O-C-N	6.41	129.25	123.03
3	3	184	PHE	CB-CA-C	-6.40	100.16	110.79
2	2	110	VAL	CB-CA-C	-6.40	104.32	111.23
3	3	117	THR	N-CA-C	6.40	119.14	108.96
2	2	121	ALA	N-CA-C	6.40	119.41	108.02
2	2	125	PHE	CB-CA-C	-6.40	98.65	109.72
1	1	126	THR	N-CA-C	6.39	117.91	111.07
3	3	141	PRO	O-C-N	6.39	129.00	121.46
4	4	55	GLU	O-C-N	6.38	128.66	121.32
1	1	61	VAL	O-C-N	6.38	129.78	122.82
1	1	121	LYS	O-C-N	6.38	128.65	122.07
3	3	88	SER	O-C-N	6.38	128.66	121.32
2	2	120	GLY	O-C-N	6.36	128.88	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	102	ASP	N-CA-C	6.36	119.45	110.23
2	2	92	PHE	CB-CA-C	-6.36	100.24	110.79
1	1	107	VAL	CB-CA-C	-6.35	104.04	111.09
1	1	270	CYS	O-C-N	6.35	128.62	121.32
3	3	30	VAL	O-C-N	6.35	129.15	122.67
3	3	160	LEU	O-C-N	6.34	129.41	122.11
4	4	46	PHE	O-C-N	6.34	130.61	123.19
3	3	184	PHE	O-C-N	6.34	128.84	122.12
1	1	25	ASP	O-C-N	6.34	130.49	123.01
3	3	11	ASN	O-C-N	6.34	128.52	121.87
2	2	9	TYR	N-CA-C	6.32	119.20	110.35
4	4	53	PHE	CB-CA-C	-6.28	99.60	109.34
4	4	25	ILE	CB-CA-C	-6.28	103.12	110.91
4	4	3	ALA	N-CA-C	6.27	119.44	110.10
2	2	17	THR	N-CA-C	6.27	119.18	108.02
2	2	108	VAL	CB-CA-C	-6.27	104.46	111.23
2	2	231	ILE	N-CA-C	6.26	116.67	106.72
2	2	268	LEU	O-C-N	6.26	128.52	121.32
2	2	144	SER	N-CA-C	6.26	119.30	110.23
3	3	220	PHE	CB-CA-C	-6.26	99.64	109.84
2	2	171	ALA	O-C-N	6.24	130.44	122.33
1	1	81	PHE	N-CA-C	6.23	121.04	113.38
3	3	147	GLU	N-CA-C	6.23	117.74	111.07
3	3	47	ALA	O-C-N	6.23	129.51	122.22
4	4	44	GLN	O-C-N	6.23	130.72	122.56
2	2	44	ASP	O-C-N	6.23	128.72	122.12
1	1	132	MET	N-CA-C	6.22	118.88	108.73
2	2	192	VAL	O-C-N	6.22	129.15	122.06
3	3	154	VAL	O-C-N	6.22	129.65	123.18
1	1	161	PRO	N-CA-C	6.22	118.29	110.70
3	3	81	PRO	N-CA-C	6.21	120.59	111.03
2	2	199	ASN	N-CA-C	6.20	119.65	108.17
2	2	190	ALA	O-C-N	6.20	130.38	122.33
2	2	28	ALA	N-CA-C	6.19	120.37	109.96
2	2	225	ASN	N-CA-C	6.19	119.26	107.75
2	2	145	TYR	O-C-N	6.19	128.68	122.12
2	2	160	THR	N-CA-C	6.19	119.64	108.69
1	1	41	ILE	O-C-N	6.18	128.14	121.10
2	2	37	ARG	N-CA-C	6.18	118.92	107.99
3	3	207	GLU	N-CA-C	6.17	119.19	108.76
1	1	36	THR	N-CA-C	6.16	119.57	108.48
4	4	30	ILE	N-CA-C	6.16	116.89	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	170	PRO	O-C-N	6.16	130.36	122.85
4	4	61	LEU	N-CA-C	6.15	119.27	109.24
1	1	87	VAL	O-C-N	6.15	128.35	122.20
2	2	161	PHE	CB-CA-C	-6.14	100.67	111.05
1	1	107	VAL	O-C-N	6.14	128.67	122.71
2	2	266	ILE	O-C-N	6.13	128.74	122.79
3	3	49	ILE	CB-CA-C	-6.13	103.55	110.96
2	2	21	SER	N-CA-C	6.12	118.87	108.90
2	2	229	ILE	N-CA-C	6.12	116.51	107.15
3	3	100	LEU	O-C-N	6.12	128.37	122.07
1	1	31	GLU	O-C-N	6.12	130.19	123.04
2	2	211	PRO	CA-C-O	-6.12	114.54	122.12
2	2	111	GLN	N-CA-C	6.11	118.68	108.96
1	1	91	THR	N-CA-C	6.10	118.79	107.99
2	2	188	GLY	O-C-N	6.10	128.47	122.19
3	3	222	VAL	O-C-N	6.10	129.52	123.00
1	1	80	PHE	O-C-N	6.09	128.58	122.12
1	1	252	LYS	N-CA-C	6.09	119.10	109.96
1	1	262	LYS	O-C-N	6.09	129.22	121.12
1	1	286	TYR	O-C-N	6.09	129.91	123.03
1	1	134	LEU	N-CA-C	6.09	118.22	108.41
3	3	172	SER	N-CA-C	6.09	118.67	109.23
2	2	198	ILE	CB-CA-C	-6.09	106.40	113.22
3	3	221	SER	N-CA-C	6.08	118.42	109.24
3	3	207	GLU	O-C-N	6.06	130.40	123.31
2	2	197	ILE	N-CA-C	6.06	116.58	107.80
2	2	238	ASN	N-CA-C	6.05	119.38	108.48
2	2	100	TYR	O-C-N	6.05	128.30	122.07
3	3	53	ILE	CB-CA-C	-6.05	104.23	110.71
3	3	113	SER	N-CA-C	6.04	119.49	109.46
1	1	196	VAL	CB-CA-C	-6.04	104.06	110.16
1	1	66	VAL	CB-CA-C	-6.02	103.57	110.73
3	3	119	LEU	N-CA-C	6.02	118.49	108.20
1	1	189	THR	O-C-N	6.02	129.80	123.06
2	2	156	THR	N-CA-C	6.02	118.56	109.23
2	2	152	GLU	O-C-N	6.02	128.50	122.12
1	1	76	SER	O-C-N	6.01	129.96	122.86
2	2	218	ILE	O-C-N	6.01	128.97	123.19
2	2	222	VAL	CB-CA-C	-6.01	104.18	112.24
4	4	40	ALA	CA-C-O	-6.01	115.14	121.99
3	3	177	ARG	O-C-N	6.01	130.01	123.10
2	2	112	CYS	N-CA-C	6.01	118.60	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	98	THR	O-C-N	6.01	129.75	122.96
1	1	192	ALA	N-CA-C	6.01	118.71	110.24
3	3	20	GLN	O-C-N	6.00	129.63	122.79
3	3	77	HIS	N-CA-C	6.00	119.06	110.24
2	2	193	PHE	CA-C-O	-5.99	115.16	120.19
3	3	180	ILE	O-C-N	5.99	129.78	123.02
1	1	29	ASN	CB-CA-C	-5.99	100.56	109.90
1	1	96	ALA	O-C-N	5.99	130.04	123.04
1	1	253	VAL	CB-CA-C	-5.98	103.22	110.99
3	3	28	PHE	N-CA-C	5.97	123.51	110.80
3	3	135	ALA	CB-CA-C	-5.96	104.25	110.33
1	1	53	ASN	O-C-N	5.96	128.18	121.32
1	1	199	VAL	N-CA-C	5.96	121.73	109.34
3	3	92	ASP	O-C-N	5.96	128.17	121.32
2	2	79	TRP	N-CA-C	5.95	119.17	109.06
2	2	129	GLU	CB-CA-C	-5.95	103.44	111.89
3	3	202	LEU	CA-C-O	-5.95	115.77	122.01
2	2	164	ASP	O-C-N	5.94	130.49	122.59
1	1	231	ALA	O-C-N	5.94	130.12	123.05
1	1	27	LEU	O-C-N	5.94	128.43	121.66
1	1	116	VAL	CB-CA-C	-5.93	104.46	111.94
1	1	99	THR	O-C-N	5.93	130.48	122.59
1	1	285	ASP	N-CA-C	5.93	118.95	110.24
2	2	235	ALA	O-C-N	5.92	129.70	121.47
1	1	80	PHE	CB-CA-C	-5.92	100.61	110.68
3	3	167	VAL	O-C-N	5.92	129.13	122.68
3	3	233	GLN	O-C-N	5.92	129.33	121.99
2	2	128	PRO	O-C-N	5.92	129.81	123.01
3	3	115	LYS	N-CA-C	5.91	118.04	108.34
3	3	226	ARG	N-CA-C	5.91	118.05	109.07
1	1	220	GLN	N-CA-C	5.91	118.53	108.90
1	1	241	ALA	N-CA-C	5.91	118.38	107.99
3	3	70	VAL	O-C-N	5.89	128.90	122.36
2	2	11	ASP	O-C-N	5.89	128.37	122.12
4	4	45	ASP	N-CA-C	5.89	119.66	110.17
1	1	193	ARG	N-CA-C	5.89	119.08	108.48
2	2	173	ARG	N-CA-C	5.89	118.13	109.24
4	4	5	VAL	CB-CA-C	-5.89	103.83	110.96
4	4	46	PHE	CB-CA-C	-5.88	99.60	109.48
1	1	244	VAL	O-C-N	5.88	129.50	122.62
1	1	194	ILE	O-C-N	5.87	129.69	123.00
3	3	228	THR	N-CA-C	5.87	118.48	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	196	GLN	O-C-N	5.87	129.96	123.33
2	2	238	ASN	O-C-N	5.87	130.66	123.44
1	1	151	LEU	O-C-N	5.87	130.02	122.81
1	1	180	ASN	CB-CA-C	-5.87	100.25	109.52
1	1	183	ILE	O-C-N	5.86	130.56	122.88
2	2	244	SER	N-CA-C	5.86	118.03	109.30
3	3	46	LEU	O-C-N	5.85	128.82	122.15
2	2	236	PRO	O-C-N	5.85	130.32	122.89
2	2	23	ILE	O-C-N	5.85	129.32	123.18
2	2	248	PRO	O-C-N	5.84	130.11	123.10
2	2	189	ASN	N-CA-C	5.84	120.41	113.28
1	1	61	VAL	N-CA-C	5.84	117.49	108.44
1	1	208	PHE	CB-CA-C	-5.83	99.89	109.80
2	2	249	ILE	O-C-N	5.83	129.78	122.66
4	4	13	HIS	N-CA-C	5.83	118.71	109.96
2	2	142	HIS	N-CA-C	5.82	120.39	113.28
2	2	236	PRO	N-CA-C	5.82	120.34	111.15
3	3	136	PRO	O-C-N	5.82	128.32	121.46
3	3	96	SER	O-C-N	5.81	128.83	122.20
3	3	114	LEU	O-C-N	5.81	129.60	123.03
2	2	157	PHE	O-C-N	5.81	129.53	122.96
3	3	173	ASN	O-C-N	5.81	128.77	122.15
3	3	210	ILE	O-C-N	5.81	129.90	123.10
1	1	291	LEU	N-CA-C	5.81	120.06	113.15
3	3	98	THR	CA-C-O	-5.81	114.79	121.47
3	3	151	GLY	O-C-N	5.81	129.32	123.11
2	2	45	SER	O-C-N	5.81	129.01	122.22
2	2	124	VAL	CB-CA-C	-5.80	104.39	111.88
2	2	43	ARG	O-C-N	5.80	129.95	122.81
3	3	40	VAL	N-CA-C	5.80	117.35	108.71
2	2	68	THR	N-CA-C	5.79	118.59	109.96
2	2	156	THR	O-C-N	5.79	129.99	123.27
4	4	7	SER	N-CA-C	5.79	119.08	109.46
4	4	39	ASN	O-C-N	5.79	129.94	122.81
1	1	73	SER	O-C-N	5.79	129.21	122.20
2	2	163	PRO	N-CA-C	5.79	120.69	111.26
2	2	239	PHE	O-C-N	5.79	130.08	123.31
3	3	75	LYS	O-C-N	5.79	128.26	121.66
1	1	140	ALA	N-CA-C	5.79	118.99	109.85
1	1	173	TYR	N-CA-C	5.78	119.15	111.75
2	2	133	ALA	N-CA-C	5.78	118.84	110.28
1	1	70	ARG	N-CA-C	5.78	118.61	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	186	LEU	N-CA-C	5.78	118.57	109.96
1	1	253	VAL	O-C-N	5.78	129.17	122.99
4	4	38	SER	O-C-N	5.77	128.98	122.22
3	3	136	PRO	N-CA-C	5.77	117.74	110.70
1	1	63	THR	N-CA-C	5.77	119.45	110.17
3	3	70	VAL	N-CA-C	5.77	114.91	106.55
1	1	40	GLU	N-CA-C	5.77	118.07	109.25
2	2	151	GLY	O-C-N	5.77	129.01	122.67
1	1	7	SER	CB-CA-C	-5.76	101.30	110.81
1	1	130	PHE	O-C-N	5.76	129.86	123.52
1	1	206	SER	O-C-N	5.76	129.66	122.63
3	3	120	PHE	N-CA-C	5.76	123.07	110.80
3	3	135	ALA	N-CA-C	5.76	120.93	109.01
3	3	226	ARG	O-C-N	5.76	129.82	123.25
2	2	206	ALA	N-CA-C	5.76	117.78	108.34
3	3	132	VAL	N-CA-C	5.75	116.66	107.98
1	1	111	THR	N-CA-C	5.73	117.25	108.42
2	2	106	TYR	N-CA-C	5.73	118.55	108.75
1	1	128	SER	N-CA-C	5.73	117.89	109.24
1	1	29	ASN	O-C-N	5.73	130.05	122.95
1	1	183	ILE	CB-CA-C	-5.72	103.23	111.19
2	2	103	ARG	O-C-N	5.72	130.25	123.27
1	1	150	ALA	O-C-N	5.71	130.46	123.44
4	4	28	THR	N-CA-C	5.71	118.93	109.46
2	2	23	ILE	N-CA-C	5.71	116.16	108.17
4	4	12	ALA	N-CA-C	5.71	117.76	108.63
3	3	196	THR	CB-CA-C	-5.70	103.58	112.31
3	3	112	GLY	O-C-N	5.70	128.77	123.35
3	3	215	SER	O-C-N	5.70	129.75	123.25
1	1	117	GLN	O-C-N	5.70	128.18	122.08
2	2	217	SER	O-C-N	5.70	128.16	122.12
2	2	161	PHE	O-C-N	5.70	130.20	122.57
3	3	4	VAL	O-C-N	5.70	129.01	123.03
3	3	213	PHE	CB-CA-C	-5.69	99.30	109.71
1	1	124	PHE	CA-C-O	5.69	126.27	119.10
1	1	174	THR	O-C-N	5.69	128.69	122.20
2	2	46	GLU	O-C-N	5.68	129.45	122.34
2	2	207	THR	N-CA-C	5.68	118.05	107.99
3	3	16	ALA	O-C-N	5.68	129.44	122.34
1	1	33	SER	N-CA-C	5.68	117.67	108.41
3	3	127	THR	O-C-N	5.68	129.43	122.84
2	2	27	GLU	O-C-N	5.67	129.38	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	168	THR	CB-CA-C	-5.67	101.97	110.88
2	2	243	SER	O-C-N	5.67	129.25	122.27
2	2	258	CYS	N-CA-C	5.67	118.78	109.76
3	3	214	VAL	O-C-N	5.66	128.92	123.14
3	3	9	GLY	O-C-N	5.66	129.05	122.65
3	3	193	PHE	CB-CA-C	-5.66	98.04	110.67
1	1	43	ALA	O-C-N	5.66	128.84	122.22
2	2	234	LEU	O-C-N	5.66	128.11	122.12
2	2	59	ALA	O-C-N	5.65	128.83	122.22
3	3	182	ASP	N-CA-C	5.65	117.58	107.80
1	1	217	LEU	N-CA-C	5.65	117.42	108.67
2	2	254	ALA	CA-C-N	-5.65	114.14	119.90
2	2	254	ALA	C-N-CA	-5.65	114.14	119.90
1	1	137	VAL	CB-CA-C	-5.64	104.60	111.88
2	2	197	ILE	CA-C-N	-5.64	116.34	121.65
2	2	197	ILE	C-N-CA	-5.64	116.34	121.65
4	4	58	LYS	O-C-N	5.64	128.12	122.08
1	1	183	ILE	N-CA-C	5.63	115.71	107.37
2	2	87	ARG	O-C-N	5.63	128.62	122.20
3	3	118	PHE	CB-CA-C	-5.62	101.08	110.19
2	2	64	TYR	O-C-N	5.62	129.59	123.13
1	1	283	GLY	O-C-N	5.62	128.82	122.86
2	2	206	ALA	O-C-N	5.62	129.84	123.27
1	1	214	LYS	N-CA-C	5.62	117.94	109.23
1	1	277	VAL	O-C-N	5.62	129.01	123.00
4	4	30	ILE	O-C-N	5.62	129.02	123.18
3	3	146	LYS	O-C-N	5.61	128.99	122.20
3	3	82	ILE	O-C-N	5.61	128.14	121.80
3	3	173	ASN	N-CA-C	5.61	117.47	111.36
2	2	163	PRO	O-C-N	5.61	129.69	122.85
1	1	205	TYR	O-C-N	5.60	129.78	123.06
2	2	14	LEU	N-CA-C	5.60	118.69	109.85
4	4	41	ALA	O-C-N	5.59	129.90	123.02
2	2	29	ALA	O-C-N	5.59	130.24	122.08
1	1	223	ALA	O-C-N	5.59	128.57	122.20
3	3	97	HIS	CA-CB-CG	-5.58	108.22	113.80
2	2	211	PRO	O-C-N	5.58	129.95	123.14
2	2	265	ASN	CA-C-O	-5.58	115.48	121.56
4	4	14	GLU	N-CA-C	5.58	117.93	110.35
2	2	72	THR	N-CA-C	5.57	118.15	109.52
1	1	295	SER	O-C-N	5.56	129.31	123.03
1	1	200	GLY	O-C-N	5.55	128.56	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	214	ASN	N-CA-C	5.55	122.63	110.80
1	1	147	ASN	O-C-N	5.55	129.98	122.59
2	2	13	VAL	CB-CA-C	-5.55	104.31	111.53
1	1	7	SER	N-CA-C	5.54	117.34	108.41
2	2	75	SER	N-CA-C	5.54	118.61	110.30
2	2	89	MET	N-CA-C	5.54	117.75	107.99
2	2	237	LEU	O-C-N	5.54	129.71	123.06
2	2	240	ALA	O-C-N	5.54	129.96	122.59
2	2	32	VAL	CB-CA-C	-5.54	103.31	110.84
2	2	271	LEU	N-CA-C	5.54	119.78	113.19
2	2	106	TYR	O-C-N	5.53	129.88	123.41
1	1	41	ILE	N-CA-C	5.53	120.82	108.88
2	2	107	THR	O-C-N	5.53	129.47	122.84
3	3	7	THR	N-CA-C	5.52	117.63	110.40
2	2	118	HIS	O-C-N	5.52	129.24	123.06
2	2	12	ARG	O-C-N	5.52	129.06	122.27
2	2	170	PRO	N-CA-C	5.52	120.25	111.26
3	3	44	MET	O-C-N	5.52	128.67	122.22
1	1	95	PRO	O-C-N	5.51	130.08	122.64
2	2	253	ILE	O-C-N	5.51	129.00	123.10
1	1	277	VAL	N-CA-C	5.51	117.85	108.86
1	1	202	SER	O-C-N	5.51	130.21	123.10
3	3	197	ARG	NE-CZ-NH2	5.51	124.16	119.20
3	3	52	MET	N-CA-C	5.51	118.31	110.10
2	2	265	ASN	O-C-N	5.50	129.35	122.86
4	4	48	GLN	O-C-N	5.50	130.01	123.24
3	3	96	SER	N-CA-C	5.50	118.79	111.75
2	2	91	LEU	N-CA-C	5.50	118.03	111.71
2	2	108	VAL	O-C-N	5.50	128.67	122.68
2	2	6	ALA	O-C-N	5.50	129.48	122.33
3	3	121	CYS	N-CA-C	5.50	119.53	113.21
2	2	113	ASN	O-C-N	5.49	129.09	122.94
3	3	66	GLU	O-C-N	5.49	129.03	122.27
3	3	169	PRO	N-CA-C	5.49	119.83	111.15
3	3	194	TYR	O-C-N	5.49	129.93	122.57
3	3	76	PRO	N-CA-C	5.49	119.71	111.14
2	2	115	SER	O-C-N	5.49	129.63	123.48
2	2	99	HIS	N-CA-C	5.49	118.42	109.59
1	1	102	ASP	O-C-N	5.49	129.62	122.87
1	1	261	LEU	N-CA-C	5.49	117.67	108.73
2	2	264	ARG	NE-CZ-NH2	5.48	124.14	119.20
1	1	71	SER	N-CA-C	5.48	118.16	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	104	LEU	O-C-N	5.48	128.63	122.22
3	3	132	VAL	CB-CA-C	-5.48	105.31	111.23
1	1	40	GLU	O-C-N	5.48	129.76	123.02
3	3	105	ASN	N-CA-C	5.48	119.71	113.19
3	3	188	GLY	O-C-N	5.48	128.05	122.85
1	1	154	VAL	CB-CA-C	-5.47	103.87	110.99
3	3	216	ALA	O-C-N	5.47	129.46	123.22
2	2	60	ALA	O-C-N	5.47	129.43	122.10
3	3	228	THR	O-C-N	5.47	129.09	122.85
1	1	267	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	2	65	THR	N-CA-C	5.47	117.21	108.41
2	2	177	VAL	N-CA-C	5.46	116.63	108.54
1	1	22	THR	N-CA-C	5.46	118.36	110.28
1	1	64	ARG	CA-C-O	-5.46	115.28	121.72
2	2	205	CYS	O-C-N	5.46	128.83	122.99
2	2	226	ASN	O-C-N	5.45	127.90	122.12
2	2	177	VAL	CB-CA-C	-5.45	104.70	111.08
3	3	154	VAL	CB-CA-C	-5.45	103.06	110.42
2	2	46	GLU	N-CA-C	5.44	120.03	113.17
3	3	109	HIS	N-CA-C	5.44	118.33	109.24
2	2	119	GLN	O-C-N	5.44	130.40	123.11
2	2	40	GLU	O-C-N	5.43	129.47	123.33
3	3	141	PRO	N-CA-C	5.43	117.33	110.70
1	1	92	VAL	CB-CA-C	-5.43	103.75	111.19
3	3	39	GLU	O-C-N	5.43	129.61	122.93
2	2	54	THR	O-C-N	5.42	129.50	123.05
3	3	223	ARG	NE-CZ-NH2	5.42	124.08	119.20
2	2	269	PRO	O-C-N	5.42	129.74	123.01
1	1	26	ALA	O-C-N	5.42	129.57	123.06
4	4	45	ASP	O-C-N	5.42	129.33	123.10
3	3	69	ARG	NE-CZ-NH2	5.42	124.08	119.20
4	4	64	THR	O-C-N	5.42	128.93	122.27
3	3	63	ASN	N-CA-C	5.41	119.05	111.90
3	3	199	VAL	CB-CA-C	-5.41	103.48	110.84
2	2	229	ILE	O-C-N	5.41	128.94	122.62
2	2	36	GLY	O-C-N	5.40	128.47	122.31
3	3	217	CYS	O-C-N	5.40	129.23	122.86
1	1	64	ARG	NE-CZ-NH2	5.40	124.06	119.20
2	2	20	ASN	N-CA-C	5.40	119.57	113.15
1	1	267	ARG	O-C-N	5.40	129.85	123.27
1	1	224	LEU	O-C-N	5.39	127.91	122.09
2	2	201	ARG	NE-CZ-NH2	5.39	124.05	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	144	LYS	O-C-N	5.39	129.72	123.41
2	2	103	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	1	154	VAL	N-CA-C	5.39	115.84	107.28
1	1	206	SER	N-CA-C	5.39	118.02	107.57
2	2	43	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	2	269	PRO	N-CA-C	5.38	119.77	111.21
1	1	72	ARG	O-C-N	5.38	128.97	122.35
1	1	129	ARG	NE-CZ-NH2	5.38	124.05	119.20
2	2	110	VAL	O-C-N	5.38	128.54	122.68
2	2	250	THR	O-C-N	5.38	129.35	123.22
1	1	296	THR	N-CA-C	5.38	117.97	109.96
2	2	69	VAL	N-CA-C	5.38	116.92	109.45
3	3	132	VAL	O-C-N	5.38	128.54	122.68
4	4	36	SER	O-C-N	5.38	129.74	122.59
1	1	81	PHE	CB-CA-C	-5.37	100.31	109.65
4	4	43	LYS	O-C-N	5.37	129.73	122.59
1	1	275	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	1	138	VAL	CB-CA-C	-5.37	103.63	110.98
1	1	193	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	1	120	ARG	NE-CZ-NH2	5.37	124.03	119.20
2	2	22	THR	N-CA-C	5.37	117.83	108.76
2	2	28	ALA	O-C-N	5.37	129.38	123.16
2	2	147	ASN	N-CA-C	5.37	118.99	112.23
1	1	89	ILE	CB-CA-C	-5.36	104.83	111.32
2	2	85	ALA	O-C-N	5.36	128.31	122.20
4	4	34	ARG	NE-CZ-NH2	5.36	124.03	119.20
3	3	145	ARG	NE-CZ-NH2	5.36	124.02	119.20
3	3	201	PRO	O-C-N	5.36	129.87	122.64
1	1	176	GLN	O-C-N	5.36	129.35	122.39
2	2	225	ASN	CB-CA-C	-5.36	102.31	111.31
3	3	38	GLY	O-C-N	5.36	128.60	122.33
1	1	243	ARG	NE-CZ-NH2	5.35	124.02	119.20
2	2	222	VAL	N-CA-C	5.35	116.83	111.00
1	1	76	SER	CA-C-O	-5.35	115.73	121.56
3	3	206	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	1	259	VAL	CB-CA-C	-5.35	104.46	111.25
3	3	177	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	1	92	VAL	CA-C-O	-5.34	116.01	121.67
1	1	24	ARG	O-C-N	5.34	128.75	122.34
2	2	91	LEU	O-C-N	5.34	128.47	122.22
2	2	209	VAL	N-CA-C	5.34	115.32	107.15
1	1	272	ARG	NE-CZ-NH2	5.34	124.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	12	ARG	NE-CZ-NH2	5.34	124.00	119.20
2	2	53	PRO	O-C-N	5.34	129.63	123.01
1	1	129	ARG	O-C-N	5.33	130.11	123.28
1	1	72	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	1	212	PHE	CB-CA-C	-5.33	99.31	109.66
2	2	197	ILE	O-C-N	5.33	129.34	123.10
2	2	62	ARG	NE-CZ-NH2	5.33	124.00	119.20
2	2	76	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	3	226	ARG	NE-CZ-NH2	5.33	124.00	119.20
3	3	176	TYR	O-C-N	5.33	129.35	123.33
3	3	185	THR	O-C-N	5.32	128.90	122.35
1	1	218	LYS	O-C-N	5.32	129.67	122.59
1	1	70	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	1	255	SER	N-CA-C	5.32	118.23	109.72
1	1	119	ARG	NE-CZ-NH2	5.32	123.98	119.20
3	3	71	ARG	NE-CZ-NH2	5.32	123.98	119.20
4	4	42	SER	O-C-N	5.32	128.26	122.20
2	2	62	ARG	O-C-N	5.31	129.85	122.78
2	2	69	VAL	CB-CA-C	-5.31	104.16	111.49
1	1	300	THR	N-CA-C	5.31	118.77	112.72
1	1	63	THR	O-C-N	5.31	129.21	123.10
2	2	270	ARG	NE-CZ-NH2	5.31	123.97	119.20
2	2	41	TYR	O-C-N	5.30	129.12	122.86
3	3	126	ALA	O-C-N	5.30	129.29	122.93
1	1	254	THR	O-C-N	5.30	129.26	123.22
2	2	172	ARG	NE-CZ-NH2	5.30	123.97	119.20
2	2	254	ALA	N-CA-C	5.30	120.40	109.11
2	2	256	MET	N-CA-C	5.30	117.87	109.50
3	3	78	THR	O-C-N	5.30	129.82	123.36
3	3	117	THR	O-C-N	5.30	129.22	123.13
4	4	67	MET	O-C-N	5.30	128.21	122.11
1	1	184	PHE	CB-CA-C	-5.30	103.36	111.83
3	3	12	GLN	O-C-N	5.29	128.94	122.96
2	2	104	SER	O-C-N	5.29	129.51	123.48
2	2	212	TYR	O-C-N	5.29	129.63	122.59
4	4	27	TYR	O-C-N	5.29	129.50	123.31
2	2	74	GLU	O-C-N	5.29	129.41	122.33
3	3	231	ILE	N-CA-C	5.29	114.83	108.06
1	1	114	ASP	O-C-N	5.29	128.40	122.22
1	1	123	GLU	O-C-N	5.29	129.75	122.46
1	1	24	ARG	NE-CZ-NH2	5.28	123.96	119.20
1	1	258	ARG	NE-CZ-NH2	5.28	123.95	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	287	LYS	N-CA-C	5.28	118.01	109.40
2	2	37	ARG	NE-CZ-NH2	5.28	123.96	119.20
2	2	95	ASN	O-C-N	5.28	128.76	122.27
3	3	94	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	1	294	LEU	N-CA-C	5.28	117.88	110.23
3	3	55	PHE	CB-CA-C	-5.28	99.92	110.42
1	1	107	VAL	N-CA-C	5.28	116.00	106.61
2	2	173	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	4	4	GLN	N-CA-C	5.27	117.80	107.57
3	3	33	PRO	O-C-N	5.27	129.70	123.06
2	2	87	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	1	202	SER	CA-C-O	-5.27	115.19	121.56
2	2	30	ASN	O-C-N	5.27	129.59	122.59
2	2	32	VAL	O-C-N	5.27	128.88	123.03
3	3	164	CYS	O-C-N	5.27	129.43	123.27
3	3	191	SER	N-CA-C	5.26	118.14	109.72
1	1	247	ASP	O-C-N	5.26	129.28	122.81
2	2	259	GLU	O-C-N	5.26	129.69	123.33
4	4	35	ASP	O-C-N	5.26	129.18	123.13
2	2	25	THR	N-CA-C	5.26	117.17	108.13
2	2	128	PRO	CA-C-O	-5.26	115.61	121.23
2	2	109	HIS	N-CA-C	5.25	118.02	107.41
3	3	23	CYS	N-CA-C	5.25	116.80	108.67
1	1	126	THR	O-C-N	5.25	127.47	122.07
3	3	199	VAL	O-C-N	5.25	128.85	123.03
2	2	51	ASP	O-C-N	5.24	129.19	123.01
3	3	209	ASP	O-C-N	5.24	129.32	123.19
1	1	99	THR	CB-CA-C	-5.24	100.00	110.42
1	1	192	ALA	O-C-N	5.24	129.36	122.97
1	1	173	TYR	O-C-N	5.24	128.17	122.20
3	3	197	ARG	O-C-N	5.23	129.55	122.59
1	1	83	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	2	157	PHE	CB-CA-C	-5.23	99.84	109.46
2	2	85	ALA	N-CA-C	5.23	118.44	111.75
1	1	52	THR	N-CA-C	5.22	117.24	108.73
1	1	53	ASN	N-CA-C	5.22	121.36	109.81
4	4	25	ILE	N-CA-C	5.22	116.10	108.58
3	3	111	ALA	O-C-N	5.22	129.23	123.33
3	3	152	THR	O-C-N	5.21	129.52	122.59
3	3	178	GLN	O-C-N	5.21	129.14	123.04
1	1	37	HIS	O-C-N	5.21	129.05	122.28
1	1	78	GLU	CB-CA-C	-5.21	102.70	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	135	THR	O-C-N	5.21	129.41	123.27
3	3	64	THR	O-C-N	5.21	129.21	123.33
2	2	166	ASN	N-CA-C	5.20	121.88	110.80
3	3	42	ASN	CB-CA-C	-5.20	102.64	110.24
3	3	76	PRO	O-C-N	5.20	129.33	123.03
1	1	137	VAL	O-C-N	5.20	128.71	122.62
3	3	49	ILE	O-C-N	5.20	129.28	122.94
3	3	174	THR	O-C-N	5.20	129.19	123.16
3	3	198	ILE	O-C-N	5.20	129.07	122.57
4	4	39	ASN	CB-CA-C	-5.20	100.31	109.62
3	3	58	SER	O-C-N	5.19	129.20	122.81
3	3	192	VAL	O-C-N	5.19	128.87	123.26
2	2	233	PRO	O-C-N	5.19	129.65	122.64
4	4	29	THR	N-CA-C	5.19	117.36	108.90
1	1	35	PRO	O-C-N	5.19	129.19	122.91
1	1	218	LYS	CB-CA-C	-5.19	100.09	110.42
2	2	158	THR	N-CA-C	5.19	117.42	109.07
2	2	58	VAL	N-CA-C	5.19	118.33	111.17
1	1	89	ILE	N-CA-C	5.18	114.96	106.72
3	3	213	PHE	O-C-N	5.18	129.47	123.30
2	2	256	MET	O-C-N	5.18	129.61	123.24
1	1	148	GLY	O-C-N	5.18	129.71	122.82
3	3	116	PHE	O-C-N	5.18	129.26	122.68
1	1	47	VAL	O-C-N	5.18	129.04	122.57
1	1	232	ALA	O-C-N	5.18	129.48	122.59
1	1	78	GLU	N-CA-C	5.17	116.61	111.07
1	1	154	VAL	O-C-N	5.17	128.53	122.99
3	3	40	VAL	O-C-N	5.17	128.41	122.93
3	3	81	PRO	O-C-N	5.17	128.96	123.01
1	1	152	ASN	N-CA-C	5.17	121.81	110.80
4	4	7	SER	O-C-N	5.17	129.11	123.22
4	4	59	ASP	N-CA-C	5.17	117.09	107.99
1	1	274	PRO	O-C-N	5.17	129.55	122.99
3	3	80	ASP	N-CA-C	5.17	116.34	109.93
4	4	35	ASP	N-CA-C	5.17	117.17	108.96
2	2	66	LEU	O-C-N	5.16	128.95	122.65
4	4	60	VAL	CB-CA-C	-5.16	102.82	111.29
3	3	4	VAL	N-CA-C	5.16	116.80	108.85
1	1	28	PRO	N-CA-C	5.16	119.67	111.26
4	4	33	TYR	N-CA-C	5.16	118.48	110.17
1	1	131	ASP	O-C-N	5.16	129.34	122.95
1	1	22	THR	O-C-N	5.16	129.18	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	95	ASN	N-CA-C	5.16	117.80	111.82
2	2	31	SER	O-C-N	5.15	129.57	123.33
2	2	242	GLU	O-C-N	5.15	129.28	122.89
1	1	227	SER	N-CA-C	5.15	116.67	108.79
2	2	87	ARG	N-CA-C	5.15	118.34	111.75
3	3	90	ALA	N-CA-C	5.15	119.64	112.90
3	3	110	TRP	N-CA-C	5.15	117.84	109.24
4	4	63	LYS	O-C-N	5.15	127.58	122.12
1	1	226	ASP	N-CA-C	5.15	118.33	110.20
2	2	209	VAL	CB-CA-C	-5.14	105.24	111.88
1	1	244	VAL	CB-CA-C	-5.14	105.25	111.88
3	3	77	HIS	CA-CB-CG	-5.14	108.66	113.80
2	2	208	LEU	N-CA-C	5.14	117.09	107.99
2	2	50	VAL	O-C-N	5.14	127.92	122.06
3	3	231	ILE	CB-CA-C	-5.14	103.89	111.80
1	1	246	ASN	O-C-N	5.13	129.18	122.87
1	1	28	PRO	O-C-N	5.13	129.11	122.85
2	2	129	GLU	O-C-N	5.13	128.91	122.55
3	3	123	SER	N-CA-C	5.13	117.73	110.50
1	1	242	VAL	CB-CA-C	-5.13	103.75	110.98
1	1	182	SER	N-CA-C	5.12	117.75	109.40
1	1	195	SER	O-C-N	5.12	129.18	123.19
2	2	264	ARG	CA-C-O	-5.12	115.59	120.56
1	1	113	LYS	N-CA-C	5.12	119.68	113.38
1	1	139	THR	O-C-N	5.12	129.39	123.30
1	1	23	SER	O-C-N	5.12	129.40	122.59
1	1	240	LEU	O-C-N	5.12	129.16	122.87
1	1	197	PRO	O-C-N	5.11	129.54	122.64
2	2	33	VAL	O-C-N	5.11	128.96	122.57
2	2	147	ASN	O-C-N	5.11	129.18	122.33
3	3	13	TYR	N-CA-C	5.11	117.73	107.41
1	1	133	GLU	O-C-N	5.11	129.15	122.87
1	1	227	SER	O-C-N	5.11	128.88	123.42
2	2	258	CYS	O-C-N	5.11	129.01	123.04
1	1	186	THR	N-CA-C	5.10	116.93	108.20
2	2	53	PRO	N-CA-C	5.10	119.33	111.21
2	2	149	ASN	CB-CA-C	-5.10	102.81	110.87
1	1	148	GLY	CA-C-O	-5.10	115.61	122.24
1	1	224	LEU	N-CA-C	5.10	116.64	111.14
4	4	57	ILE	O-C-N	5.10	128.17	122.61
4	4	15	ASN	O-C-N	5.10	129.37	122.59
3	3	227	ASP	O-C-N	5.09	129.19	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	173	ARG	O-C-N	5.09	129.33	123.17
3	3	172	SER	O-C-N	5.09	129.17	123.27
3	3	220	PHE	O-C-N	5.09	128.99	123.04
4	4	59	ASP	O-C-N	5.09	129.14	122.68
4	4	34	ARG	O-C-N	5.08	128.53	122.27
1	1	142	PHE	O-C-N	5.08	129.18	122.93
1	1	71	SER	O-C-N	5.08	129.49	123.24
1	1	177	THR	O-C-N	5.08	129.34	122.59
1	1	167	PRO	N-CA-C	5.07	119.53	111.26
1	1	223	ALA	N-CA-C	5.07	118.24	111.75
1	1	269	TRP	N-CA-C	5.07	117.86	109.85
3	3	61	LYS	O-C-N	5.07	128.82	122.23
2	2	115	SER	N-CA-C	5.07	116.77	108.76
2	2	124	VAL	O-C-N	5.07	128.55	122.62
1	1	50	GLY	O-C-N	5.06	128.62	122.60
3	3	27	GLU	O-C-N	5.06	129.32	122.59
3	3	103	ILE	CB-CA-C	-5.06	105.24	112.22
1	1	258	ARG	O-C-N	5.05	129.39	122.82
1	1	238	GLY	O-C-N	5.05	128.75	122.95
2	2	71	TRP	N-CA-C	5.04	116.98	108.96
2	2	168	THR	N-CA-C	5.04	116.47	111.07
1	1	241	ALA	O-C-N	5.04	129.08	122.68
3	3	80	ASP	O-C-N	5.04	128.49	121.64
1	1	273	PRO	N-CA-C	5.04	116.85	110.70
2	2	194	PRO	O-C-N	5.04	129.44	122.64
1	1	51	ALA	O-C-N	5.04	128.89	123.10
1	1	228	LEU	N-CA-C	5.04	117.60	110.10
4	4	28	THR	O-C-N	5.04	128.96	123.22
2	2	195	HIS	CA-CB-CG	-5.03	108.77	113.80
2	2	126	ALA	N-CA-C	5.03	116.84	107.99
1	1	181	PRO	O-C-N	5.02	129.42	122.64
1	1	251	THR	O-C-N	5.02	128.95	123.22
2	2	191	PHE	O-C-N	5.02	128.92	122.39
2	2	199	ASN	CB-CA-C	-5.02	103.12	111.41
1	1	135	THR	N-CA-C	5.02	116.70	108.52
2	2	16	LEU	O-C-N	5.02	128.94	123.22
2	2	213	VAL	O-C-N	5.02	128.60	123.03
2	2	267	THR	N-CA-C	5.02	116.45	108.67
3	3	69	ARG	O-C-N	5.02	129.02	123.05
1	1	155	TYR	O-C-N	5.01	128.93	123.01
1	1	159	TYR	O-C-N	5.01	128.95	122.93
2	2	12	ARG	N-CA-C	5.01	117.64	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	209	VAL	O-C-N	5.01	128.49	122.62
3	3	30	VAL	CB-CA-C	-5.01	103.42	111.59
3	3	134	TYR	O-C-N	5.01	129.74	123.12
1	1	82	ALA	O-C-N	5.01	129.26	122.59
2	2	257	CYS	O-C-N	5.01	129.25	122.59
2	2	51	ASP	N-CA-C	5.01	118.11	110.20
1	1	97	SER	O-C-N	5.01	129.25	122.59
3	3	40	VAL	CB-CA-C	-5.00	103.93	110.98

There are no chirality outliers.

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	2251	0	2197	139	0
2	2	2085	0	2000	119	0
3	3	1834	0	1816	127	0
4	4	477	0	457	44	0
5	1	21	0	36	29	0
6	4	15	0	27	1	0
7	1	159	0	0	7	0
7	2	149	0	0	4	0
7	3	129	0	0	12	0
7	4	42	0	0	6	0
All	All	7162	0	6533	388	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (388) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:5:GLU:CG	2:2:7:CYS:HB3	1.58	1.32
3:3:124:MET:HG3	7:3:320:HOH:O	1.32	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:132:MET:CE	5:1:0:SPH:H81	1.69	1.23
1:1:177:THR:HG21	1:1:182:SER:OG	1.40	1.21
2:2:187:LEU:HD22	3:3:65:MET:HE1	1.23	1.20
3:3:124:MET:CG	7:3:320:HOH:O	1.83	1.17
1:1:132:MET:HE1	5:1:0:SPH:H81	1.16	1.16
2:2:5:GLU:CG	2:2:7:CYS:CB	2.25	1.14
1:1:237:PHE:CE2	5:1:0:SPH:H71	1.82	1.14
2:2:5:GLU:HG2	2:2:7:CYS:HB3	1.19	1.11
1:1:149:HIS:HE1	7:1:303:HOH:O	1.35	1.08
2:2:48:ASN:HB3	2:2:49:PRO:HD3	1.18	1.08
3:3:167:VAL:O	3:3:169:PRO:HD3	1.56	1.05
2:2:48:ASN:HB3	2:2:49:PRO:CD	1.85	1.04
2:2:179:TYR:HA	3:3:65:MET:CE	1.90	1.02
2:2:5:GLU:HG3	2:2:7:CYS:CB	1.90	0.99
2:2:37:ARG:O	2:2:211:PRO:HG3	1.64	0.97
2:2:5:GLU:CD	2:2:7:CYS:H	1.72	0.96
2:2:187:LEU:CD2	3:3:65:MET:HE1	1.95	0.96
2:2:179:TYR:HA	3:3:65:MET:HE2	1.48	0.96
2:2:187:LEU:HD22	3:3:65:MET:CE	1.96	0.94
2:2:5:GLU:HG3	2:2:7:CYS:HB3	1.41	0.94
2:2:5:GLU:OE2	2:2:7:CYS:HB2	1.66	0.94
1:1:149:HIS:CE1	7:1:303:HOH:O	2.15	0.93
2:2:5:GLU:HG3	2:2:7:CYS:CA	1.99	0.93
3:3:83:LEU:HD12	3:3:83:LEU:O	1.69	0.93
1:1:22:THR:HG22	1:1:24:ARG:H	1.32	0.92
1:1:56:VAL:HB	1:1:57:PRO:HD2	1.52	0.91
1:1:112:TYR:HE2	5:1:0:SPH:HO3	0.92	0.90
1:1:132:MET:HE1	5:1:0:SPH:C8	2.01	0.89
1:1:144:GLU:C	1:1:146:ASN:H	1.79	0.88
2:2:168:THR:CG2	2:2:169:SER:N	2.36	0.88
3:3:71:ARG:NH1	3:3:209:ASP:OD2	2.07	0.87
2:2:267:THR:O	2:2:269:PRO:HD3	1.75	0.86
2:2:270:ARG:O	2:2:270:ARG:HG2	1.73	0.86
2:2:168:THR:HG22	2:2:169:SER:N	1.90	0.86
3:3:149:MET:HE2	3:3:150:LEU:CD2	2.06	0.85
1:1:144:GLU:O	1:1:146:ASN:N	2.09	0.84
1:1:237:PHE:CE2	5:1:0:SPH:C7	2.61	0.83
3:3:232:GLU:OE1	3:3:234:LYS:HG2	1.78	0.83
2:2:166:ASN:O	2:2:166:ASN:OD1	1.97	0.83
1:1:132:MET:HE2	5:1:0:SPH:H81	1.61	0.82
2:2:34:ALA:HB3	2:2:211:PRO:HD2	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:191:PRO:HG2	3:3:13:TYR:HB2	1.61	0.82
2:2:5:GLU:HG3	2:2:7:CYS:N	1.93	0.81
4:4:14:GLU:HG2	4:4:16:SER:HB2	1.63	0.81
1:1:132:MET:CE	5:1:0:SPH:C8	2.58	0.80
1:1:158:MET:SD	1:1:177:THR:HG23	2.22	0.80
3:3:149:MET:HE2	3:3:150:LEU:HG	1.63	0.79
2:2:5:GLU:HG2	2:2:7:CYS:CB	2.04	0.79
1:1:218:LYS:HD2	7:2:417:HOH:O	1.82	0.79
3:3:149:MET:HE2	3:3:150:LEU:CG	2.13	0.79
1:1:27:LEU:HB3	1:1:28:PRO:HD2	1.66	0.78
1:1:219:ASP:O	1:1:219:ASP:OD2	2.01	0.78
4:4:14:GLU:HG2	4:4:16:SER:H	1.50	0.77
1:1:237:PHE:CZ	5:1:0:SPH:H71	2.20	0.77
4:4:14:GLU:HG3	7:4:84:HOH:O	1.85	0.76
4:4:14:GLU:C	4:4:16:SER:H	1.94	0.75
3:3:7:THR:HB	3:3:8:PRO:HD2	1.67	0.75
2:2:242:GLU:OE2	2:2:242:GLU:N	2.19	0.74
3:3:71:ARG:HH12	3:3:209:ASP:CG	1.95	0.74
3:3:149:MET:CE	3:3:150:LEU:CD2	2.65	0.74
1:1:22:THR:HG22	1:1:24:ARG:N	2.03	0.74
3:3:149:MET:HE2	3:3:150:LEU:HD23	1.70	0.73
4:4:14:GLU:HG2	4:4:16:SER:N	2.03	0.73
2:2:5:GLU:CG	2:2:7:CYS:H	2.02	0.73
1:1:45:THR:OG1	4:4:67:MET:HE2	1.90	0.72
2:2:5:GLU:OE1	2:2:5:GLU:CA	2.38	0.72
3:3:210:ILE:O	3:3:210:ILE:HG13	1.89	0.72
1:1:112:TYR:HE2	5:1:0:SPH:O3	1.71	0.72
4:4:14:GLU:CG	4:4:16:SER:HB2	2.19	0.72
3:3:74:ASP:HA	3:3:198:ILE:O	1.89	0.71
1:1:109:LYS:HA	1:1:239:ILE:HG22	1.71	0.71
3:3:232:GLU:OE1	3:3:234:LYS:CG	2.39	0.71
2:2:38:TRP:CD1	2:2:39:PRO:HD2	2.26	0.71
4:4:14:GLU:CD	4:4:16:SER:HB2	2.15	0.70
2:2:168:THR:HG22	2:2:169:SER:H	1.54	0.70
2:2:179:TYR:HA	3:3:65:MET:HE3	1.70	0.70
2:2:34:ALA:HB3	2:2:211:PRO:CD	2.22	0.70
3:3:71:ARG:HB2	3:3:71:ARG:CZ	2.19	0.70
3:3:97:HIS:CE1	7:3:246:HOH:O	2.45	0.70
3:3:97:HIS:CE1	3:3:230:HIS:ND1	2.60	0.70
4:4:10:VAL:HG12	4:4:13:HIS:CE1	2.27	0.70
3:3:234:LYS:O	3:3:235:ALA:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:42:SER:OG	4:4:44:GLN:HB2	1.92	0.69
2:2:5:GLU:OE1	2:2:5:GLU:HA	1.91	0.69
2:2:12:ARG:HA	2:2:28:ALA:O	1.93	0.69
3:3:196:THR:O	3:3:197:ARG:HB3	1.93	0.69
4:4:10:VAL:CG2	4:4:25:ILE:HD12	2.22	0.69
3:3:97:HIS:ND1	7:3:246:HOH:O	2.25	0.69
3:3:234:LYS:O	3:3:235:ALA:CB	2.40	0.69
4:4:65:ALA:HB1	4:4:66:PRO:HD2	1.73	0.69
1:1:132:MET:HE1	5:1:0:SPH:H101	1.75	0.69
3:3:149:MET:CE	3:3:150:LEU:HD23	2.24	0.68
1:1:103:LYS:HD3	1:1:170:TRP:CD2	2.27	0.68
4:4:61:LEU:O	4:4:61:LEU:HG	1.93	0.68
2:2:5:GLU:OE1	2:2:6:ALA:N	2.27	0.68
3:3:195:GLN:OE1	3:3:195:GLN:HA	1.92	0.68
2:2:110:VAL:HG22	2:2:251:LEU:HD12	1.77	0.67
2:2:5:GLU:CG	2:2:7:CYS:N	2.58	0.67
3:3:124:MET:HG2	7:3:320:HOH:O	1.64	0.67
3:3:97:HIS:CE1	3:3:230:HIS:CE1	2.83	0.67
1:1:233:SER:HB2	7:1:410:HOH:O	1.95	0.66
1:1:47:VAL:HG22	3:3:119:LEU:HD13	1.78	0.65
2:2:48:ASN:CB	2:2:49:PRO:CD	2.65	0.65
1:1:159:TYR:HB2	5:1:0:SPH:H162	1.79	0.65
2:2:5:GLU:CD	2:2:7:CYS:N	2.53	0.65
1:1:249:ASN:CG	1:1:250:PRO:HD2	2.22	0.64
1:1:22:THR:HB	1:1:25:ASP:OD1	1.97	0.64
2:2:5:GLU:CD	2:2:7:CYS:CB	2.71	0.64
2:2:38:TRP:CG	2:2:39:PRO:HD2	2.32	0.64
1:1:90:MET:CE	1:1:240:LEU:O	2.46	0.64
1:1:132:MET:HE1	5:1:0:SPH:C10	2.27	0.64
1:1:159:TYR:O	1:1:161:PRO:HD3	1.98	0.64
2:2:5:GLU:CD	2:2:7:CYS:HB2	2.22	0.64
2:2:143:THR:HG23	2:2:173:ARG:HA	1.79	0.64
1:1:237:PHE:CZ	5:1:0:SPH:H4	2.33	0.64
3:3:83:LEU:HD12	3:3:83:LEU:C	2.22	0.64
2:2:179:TYR:CA	3:3:65:MET:HE2	2.27	0.63
2:2:187:LEU:HD22	3:3:65:MET:SD	2.39	0.63
4:4:42:SER:C	4:4:44:GLN:H	2.07	0.63
4:4:60:VAL:HG12	4:4:60:VAL:O	1.98	0.63
3:3:85:LEU:HD22	3:3:86:SER:N	2.13	0.62
1:1:177:THR:CG2	1:1:182:SER:OG	2.33	0.62
7:3:366:HOH:O	4:4:46:PHE:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:90:MET:HE1	1:1:240:LEU:O	2.00	0.62
1:1:103:LYS:HD3	1:1:170:TRP:CG	2.34	0.62
1:1:218:LYS:C	1:1:220:GLN:H	2.08	0.62
3:3:85:LEU:CD2	3:3:86:SER:N	2.62	0.62
1:1:237:PHE:CE2	5:1:0:SPH:C4	2.83	0.61
3:3:77:HIS:HE1	3:3:194:TYR:O	1.83	0.61
4:4:55:GLU:N	4:4:56:PRO:HD3	2.15	0.61
3:3:74:ASP:HB2	7:3:296:HOH:O	2.01	0.61
1:1:92:VAL:HG12	1:1:106:ALA:H	1.66	0.61
3:3:75:LYS:HB2	3:3:76:PRO:HD2	1.81	0.61
1:1:218:LYS:O	1:1:220:GLN:N	2.34	0.61
1:1:133:GLU:O	1:1:133:GLU:HG2	2.01	0.61
2:2:63:PHE:CD1	2:2:254:ALA:HB2	2.36	0.61
4:4:57:ILE:HD11	4:4:61:LEU:HB3	1.81	0.61
1:1:128:SER:HB3	1:1:207:HIS:CE1	2.35	0.60
4:4:10:VAL:HG21	4:4:25:ILE:HD12	1.82	0.60
2:2:5:GLU:C	2:2:7:CYS:N	2.57	0.60
2:2:179:TYR:CA	3:3:65:MET:CE	2.75	0.60
5:1:0:SPH:H3	7:1:361:HOH:O	2.02	0.60
1:1:104:LEU:O	1:1:104:LEU:HG	2.02	0.59
2:2:267:THR:HG22	2:2:269:PRO:HD3	1.84	0.59
3:3:208:MET:HE2	3:3:208:MET:H	1.67	0.58
2:2:239:PHE:CD2	2:2:240:ALA:N	2.71	0.58
3:3:87:LEU:HD13	3:3:190:ILE:HD11	1.86	0.58
2:2:25:THR:HG23	2:2:25:THR:O	2.04	0.58
3:3:77:HIS:CE1	3:3:194:TYR:O	2.57	0.58
2:2:187:LEU:CB	3:3:65:MET:HE1	2.34	0.58
4:4:15:ASN:N	7:4:84:HOH:O	2.21	0.58
2:2:178:ASP:C	3:3:65:MET:HE3	2.28	0.57
2:2:195:HIS:HA	2:2:208:LEU:HD21	1.87	0.57
4:4:10:VAL:CG1	4:4:13:HIS:CE1	2.87	0.57
2:2:192:VAL:HG11	3:3:99:MET:HE2	1.85	0.57
1:1:45:THR:OG1	1:1:46:ALA:N	2.38	0.57
3:3:88:SER:HB3	3:3:91:SER:OG	2.03	0.57
1:1:300:THR:HA	3:3:84:CYS:H	1.70	0.56
3:3:178:GLN:C	3:3:180:ILE:H	2.14	0.56
3:3:218:ASN:HD22	3:3:219:ASP:N	2.04	0.56
2:2:166:ASN:OD1	2:2:168:THR:HG22	2.06	0.56
1:1:47:VAL:CG2	3:3:119:LEU:HD13	2.36	0.56
1:1:216:PRO:HG2	2:2:145:TYR:CD1	2.41	0.55
3:3:204:THR:CG2	3:3:205:PRO:HD2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:144:GLU:C	1:1:146:ASN:N	2.50	0.55
1:1:237:PHE:CD2	5:1:0:SPH:H71	2.40	0.55
4:4:14:GLU:HG2	4:4:16:SER:CB	2.36	0.54
1:1:83:ARG:HG2	7:3:258:HOH:O	2.06	0.54
1:1:261:LEU:C	1:1:261:LEU:HD23	2.31	0.54
1:1:218:LYS:C	1:1:220:GLN:N	2.65	0.54
2:2:219:ASP:CG	2:2:220:SER:H	2.15	0.54
3:3:34:ILE:O	3:3:36:ILE:N	2.39	0.54
1:1:237:PHE:CD2	5:1:0:SPH:C7	2.91	0.54
3:3:13:TYR:C	3:3:13:TYR:CD2	2.86	0.54
2:2:60:ALA:O	2:2:255:PRO:HG2	2.08	0.53
1:1:38:SER:OG	1:1:39:LYS:N	2.41	0.53
1:1:105:PHE:CD1	1:1:105:PHE:O	2.62	0.53
3:3:55:PHE:HE1	3:3:212:GLY:HA3	1.73	0.53
2:2:110:VAL:HG22	2:2:251:LEU:CD1	2.39	0.53
3:3:73:SER:HA	3:3:208:MET:CE	2.38	0.53
4:4:10:VAL:HG11	4:4:13:HIS:ND1	2.23	0.53
4:4:14:GLU:C	4:4:16:SER:N	2.64	0.53
3:3:85:LEU:CD2	3:3:85:LEU:C	2.82	0.53
2:2:187:LEU:CG	3:3:65:MET:HE1	2.38	0.53
2:2:256:MET:O	2:2:258:CYS:N	2.41	0.53
3:3:104:LEU:O	3:3:179:THR:HG21	2.08	0.53
1:1:112:TYR:CD2	5:1:0:SPH:H5	2.43	0.53
1:1:99:THR:CG2	7:1:352:HOH:O	2.56	0.52
1:1:218:LYS:HD3	2:2:268:LEU:HB3	1.91	0.52
1:1:74:GLU:OE1	3:3:224:LEU:N	2.39	0.52
1:1:280:TYR:HB3	1:1:285:ASP:O	2.09	0.52
2:2:267:THR:C	2:2:269:PRO:HD3	2.33	0.52
1:1:133:GLU:HG2	7:1:369:HOH:O	2.08	0.52
2:2:136:SER:OG	2:2:139:THR:HG22	2.10	0.52
3:3:107:TYR:O	3:3:179:THR:HG21	2.08	0.52
1:1:183:ILE:HD11	1:1:194:ILE:HG12	1.91	0.52
1:1:209:TYR:O	1:1:230:GLY:HA2	2.10	0.52
2:2:98:TYR:CE1	2:2:266:ILE:HD12	2.45	0.52
2:2:122:LEU:HB2	2:2:198:ILE:HB	1.90	0.52
2:2:13:VAL:HA	2:2:25:THR:O	2.10	0.51
1:1:291:LEU:C	1:1:293:PRO:HD3	2.35	0.51
1:1:158:MET:SD	1:1:177:THR:CG2	2.96	0.51
1:1:302:TYR:CE2	3:3:189:TYR:HB3	2.46	0.51
2:2:5:GLU:C	2:2:7:CYS:H	2.18	0.51
1:1:48:GLU:OE2	3:3:162:SER:OG	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:112:TYR:HD2	5:1:0:SPH:H5	1.76	0.51
3:3:83:LEU:O	3:3:83:LEU:CD1	2.50	0.51
1:1:149:HIS:HB3	7:1:309:HOH:O	2.11	0.51
3:3:51:THR:HB	7:3:277:HOH:O	2.11	0.51
1:1:169:LYS:C	1:1:171:ASP:H	2.19	0.51
3:3:73:SER:C	3:3:75:LYS:H	2.18	0.51
1:1:22:THR:CG2	1:1:24:ARG:H	2.16	0.51
4:4:13:HIS:CD2	4:4:13:HIS:H	2.27	0.50
1:1:95:PRO:HD2	1:1:103:LYS:HG3	1.93	0.50
3:3:156:TRP:CD1	3:3:156:TRP:C	2.89	0.50
4:4:10:VAL:CG1	4:4:13:HIS:ND1	2.74	0.50
4:4:24:THR:HG23	4:4:24:THR:O	2.10	0.50
1:1:169:LYS:C	1:1:171:ASP:N	2.69	0.50
3:3:14:LEU:O	3:3:16:ALA:N	2.44	0.50
3:3:85:LEU:HD22	3:3:85:LEU:C	2.36	0.50
1:1:45:THR:HG1	4:4:67:MET:HE2	1.76	0.50
4:4:55:GLU:N	4:4:56:PRO:CD	2.74	0.50
1:1:75:SER:HA	3:3:107:TYR:OH	2.11	0.49
3:3:89:PRO:HB2	3:3:104:LEU:CD2	2.41	0.49
1:1:237:PHE:HZ	5:1:0:SPH:H4	1.77	0.49
2:2:256:MET:O	2:2:257:CYS:C	2.55	0.49
1:1:27:LEU:HB3	1:1:28:PRO:CD	2.40	0.49
1:1:81:PHE:C	1:1:83:ARG:H	2.17	0.49
1:1:130:PHE:O	1:1:130:PHE:CD1	2.66	0.49
2:2:198:ILE:HG22	2:2:198:ILE:O	2.11	0.49
3:3:87:LEU:HD13	3:3:190:ILE:CD1	2.43	0.49
3:3:155:ILE:O	3:3:155:ILE:HG22	2.13	0.49
3:3:129:LYS:O	3:3:195:GLN:HB3	2.11	0.49
1:1:81:PHE:O	1:1:83:ARG:N	2.34	0.49
1:1:233:SER:C	1:1:235:ASN:N	2.69	0.49
2:2:71:TRP:CD1	2:2:71:TRP:C	2.88	0.49
2:2:239:PHE:O	2:2:240:ALA:C	2.55	0.49
3:3:89:PRO:HB2	3:3:104:LEU:HD23	1.95	0.49
1:1:237:PHE:CZ	5:1:0:SPH:C4	2.96	0.49
2:2:110:VAL:O	2:2:205:CYS:HB2	2.13	0.49
2:2:213:VAL:O	2:2:214:ASN:HB2	2.12	0.49
3:3:149:MET:O	3:3:149:MET:HG2	2.02	0.49
1:1:159:TYR:CB	5:1:0:SPH:H162	2.42	0.48
3:3:14:LEU:O	3:3:14:LEU:HG	2.13	0.48
1:1:48:GLU:HA	2:2:197:ILE:HB	1.94	0.48
2:2:66:LEU:N	2:2:66:LEU:HD23	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:10:VAL:HG22	4:4:25:ILE:HD12	1.93	0.48
1:1:105:PHE:CD1	1:1:105:PHE:C	2.91	0.48
3:3:109:HIS:HB2	3:3:223:ARG:HG2	1.95	0.48
3:3:166:MET:HE3	3:3:168:VAL:CG2	2.43	0.48
1:1:78:GLU:OE1	1:1:265:HIS:N	2.47	0.48
2:2:5:GLU:OE1	2:2:5:GLU:C	2.55	0.48
1:1:56:VAL:HB	1:1:57:PRO:CD	2.36	0.48
2:2:76:ARG:HB2	2:2:157:PHE:O	2.14	0.48
2:2:256:MET:C	2:2:258:CYS:N	2.71	0.48
3:3:183:SER:O	3:3:186:GLU:HG2	2.13	0.48
1:1:103:LYS:NZ	1:1:246:ASN:O	2.47	0.48
3:3:56:ASP:OD1	3:3:61:LYS:HE3	2.14	0.48
2:2:213:VAL:HG22	3:3:37:PRO:HG2	1.95	0.47
3:3:156:TRP:CD1	3:3:164:CYS:HB2	2.49	0.47
4:4:27:TYR:OH	7:4:86:HOH:O	2.20	0.47
1:1:83:ARG:CG	7:3:258:HOH:O	2.62	0.47
1:1:169:LYS:O	1:1:171:ASP:N	2.46	0.47
1:1:30:THR:HB	1:1:66:VAL:HB	1.95	0.47
1:1:105:PHE:O	1:1:105:PHE:CG	2.67	0.47
2:2:97:TYR:CE1	2:2:269:PRO:HG3	2.50	0.47
1:1:53:ASN:C	1:1:55:LEU:H	2.22	0.47
1:1:237:PHE:HE2	5:1:0:SPH:C4	2.26	0.47
2:2:204:ASN:ND2	7:2:381:HOH:O	2.30	0.47
1:1:93:ASP:OD2	1:1:93:ASP:C	2.58	0.46
3:3:231:ILE:HG13	3:3:232:GLU:N	2.30	0.46
1:1:233:SER:O	1:1:235:ASN:N	2.48	0.46
3:3:233:GLN:O	3:3:235:ALA:N	2.47	0.46
4:4:42:SER:C	4:4:44:GLN:N	2.72	0.46
1:1:10:THR:OG1	4:4:4:GLN:OE1	2.33	0.46
1:1:124:PHE:CE1	1:1:274:PRO:HG3	2.50	0.46
2:2:71:TRP:CD1	2:2:72:THR:N	2.84	0.46
2:2:214:ASN:OD1	2:2:215:SER:N	2.48	0.46
1:1:123:GLU:C	1:1:125:PHE:H	2.22	0.46
1:1:197:PRO:HD3	3:3:23:CYS:SG	2.56	0.46
1:1:90:MET:CE	1:1:242:VAL:HG23	2.45	0.46
2:2:83:PRO:HG3	2:2:221:MET:HE2	1.97	0.46
3:3:98:THR:O	3:3:99:MET:C	2.59	0.46
1:1:217:LEU:O	1:1:218:LYS:C	2.59	0.46
2:2:54:THR:O	2:2:56:PRO:HD3	2.16	0.46
2:2:166:ASN:O	2:2:166:ASN:CG	2.55	0.46
3:3:166:MET:HE3	3:3:168:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:9:LYS:N	7:4:70:HOH:O	2.49	0.46
1:1:128:SER:HB3	1:1:207:HIS:NE2	2.31	0.46
2:2:168:THR:HG23	2:2:169:SER:N	2.26	0.46
3:3:233:GLN:O	3:3:234:LYS:C	2.59	0.46
4:4:14:GLU:O	4:4:16:SER:N	2.48	0.46
2:2:107:THR:O	2:2:107:THR:HG22	2.16	0.45
1:1:159:TYR:CG	5:1:0:SPH:H142	2.51	0.45
3:3:85:LEU:HD23	3:3:86:SER:N	2.31	0.45
4:4:65:ALA:HB1	4:4:66:PRO:CD	2.45	0.45
2:2:179:TYR:CA	3:3:65:MET:HE3	2.40	0.45
1:1:107:VAL:O	1:1:107:VAL:HG12	2.17	0.45
3:3:74:ASP:CG	3:3:206:ARG:HE	2.22	0.45
4:4:49:ASP:OD1	4:4:51:SER:HB2	2.17	0.45
1:1:22:THR:HB	1:1:25:ASP:CG	2.41	0.45
3:3:62:LYS:O	3:3:64:THR:HG23	2.17	0.45
1:1:235:ASN:O	1:1:236:ASP:C	2.60	0.45
3:3:196:THR:O	3:3:197:ARG:CB	2.63	0.45
1:1:116:VAL:H	3:3:233:GLN:NE2	2.16	0.44
4:4:61:LEU:HA	7:4:108:HOH:O	2.16	0.44
1:1:218:LYS:HB2	1:1:219:ASP:H	1.49	0.44
2:2:267:THR:O	2:2:269:PRO:CD	2.58	0.44
3:3:170:TRP:O	3:3:170:TRP:CG	2.71	0.44
2:2:158:THR:O	2:2:177:VAL:HA	2.18	0.44
2:2:226:ASN:ND2	7:2:342:HOH:O	2.48	0.44
3:3:51:THR:HG21	3:3:99:MET:H	1.82	0.44
3:3:87:LEU:HG	3:3:87:LEU:O	2.17	0.44
1:1:155:TYR:N	1:1:155:TYR:CD2	2.87	0.43
3:3:195:GLN:OE1	3:3:195:GLN:CA	2.64	0.43
1:1:274:PRO:HG2	3:3:102:GLU:HG3	2.00	0.43
2:2:219:ASP:OD1	2:2:220:SER:N	2.37	0.43
3:3:190:ILE:O	3:3:190:ILE:HG22	2.18	0.43
1:1:233:SER:O	1:1:234:LEU:C	2.62	0.43
3:3:233:GLN:O	3:3:233:GLN:HG2	2.19	0.43
3:3:14:LEU:C	3:3:16:ALA:N	2.76	0.43
2:2:219:ASP:CG	2:2:220:SER:N	2.76	0.43
4:4:55:GLU:C	4:4:57:ILE:H	2.26	0.43
1:1:212:PHE:CD1	1:1:212:PHE:N	2.87	0.43
2:2:29:ALA:HA	4:4:68:LEU:HD21	2.00	0.43
6:4:1:MYR:H101	6:4:1:MYR:H71	1.66	0.43
1:1:177:THR:HG22	1:1:180:ASN:HB2	2.01	0.42
1:1:219:ASP:OD2	1:1:219:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:166:ASN:O	2:2:168:THR:N	2.51	0.42
1:1:116:VAL:CG2	3:3:233:GLN:HB2	2.49	0.42
2:2:12:ARG:NH1	7:2:278:HOH:O	2.51	0.42
2:2:135:ASP:OD2	2:2:171:ALA:HB3	2.19	0.42
1:1:56:VAL:O	1:1:57:PRO:C	2.62	0.42
2:2:179:TYR:N	3:3:65:MET:HE3	2.35	0.42
3:3:204:THR:HG23	3:3:205:PRO:HD2	2.00	0.42
2:2:199:ASN:O	2:2:201:ARG:N	2.52	0.42
1:1:249:ASN:O	1:1:250:PRO:C	2.63	0.42
1:1:273:PRO:HB3	2:2:189:ASN:HB2	2.01	0.42
1:1:286:TYR:OH	2:2:175:CYS:O	2.33	0.42
1:1:98:THR:O	1:1:99:THR:C	2.62	0.42
3:3:10:SER:O	3:3:11:ASN:HB2	2.19	0.42
1:1:123:GLU:C	1:1:125:PHE:N	2.77	0.42
1:1:37:HIS:CD2	1:1:37:HIS:O	2.73	0.42
1:1:237:PHE:CG	5:1:0:SPH:H92	2.55	0.42
2:2:5:GLU:HG3	2:2:7:CYS:C	2.44	0.42
2:2:71:TRP:CE2	2:2:237:LEU:HB2	2.55	0.42
2:2:104:SER:HB3	2:2:221:MET:HE1	2.01	0.42
3:3:196:THR:OG1	3:3:197:ARG:N	2.50	0.42
1:1:24:ARG:O	1:1:24:ARG:HG3	2.20	0.42
2:2:198:ILE:HD13	2:2:205:CYS:HA	2.01	0.42
3:3:142:PRO:HD3	7:3:325:HOH:O	2.19	0.42
2:2:5:GLU:HG3	2:2:8:GLY:N	2.34	0.41
2:2:5:GLU:CD	2:2:5:GLU:C	2.87	0.41
2:2:104:SER:HB2	2:2:258:CYS:HB2	2.03	0.41
2:2:117:PHE:CE1	3:3:125:MET:HG3	2.55	0.41
1:1:57:PRO:HA	3:3:167:VAL:HG11	2.03	0.41
2:2:5:GLU:O	2:2:7:CYS:N	2.53	0.41
3:3:7:THR:HB	3:3:8:PRO:CD	2.45	0.41
3:3:14:LEU:HB3	3:3:17:ASP:HB3	2.02	0.41
3:3:64:THR:C	3:3:66:GLU:N	2.79	0.41
4:4:11:GLY:HA3	7:4:78:HOH:O	2.19	0.41
3:3:78:THR:C	3:3:80:ASP:H	2.29	0.41
3:3:113:SER:O	3:3:217:CYS:HB2	2.19	0.41
3:3:108:THR:HB	3:3:224:LEU:HB3	2.02	0.41
4:4:59:ASP:O	4:4:60:VAL:C	2.63	0.41
1:1:132:MET:HE1	5:1:0:SPH:C9	2.51	0.41
2:2:57:ASP:CG	2:2:58:VAL:H	2.28	0.41
1:1:257:ILE:HD12	1:1:257:ILE:N	2.36	0.41
1:1:116:VAL:HG22	3:3:233:GLN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:23:ILE:HD12	2:2:63:PHE:CZ	2.56	0.41
2:2:181:LEU:HG	2:2:181:LEU:O	2.21	0.41
3:3:232:GLU:HG2	7:3:363:HOH:O	2.21	0.41
1:1:116:VAL:HG23	1:1:117:GLN:N	2.36	0.40
1:1:132:MET:CE	5:1:0:SPH:C10	2.98	0.40
2:2:71:TRP:HD1	2:2:72:THR:N	2.19	0.40
2:2:103:ARG:HB3	2:2:218:ILE:HG13	2.03	0.40
3:3:71:ARG:HG3	3:3:72:LEU:N	2.36	0.40
1:1:57:PRO:O	1:1:61:VAL:HG22	2.21	0.40
1:1:269:TRP:CD1	3:3:39:GLU:HB2	2.57	0.40
2:2:242:GLU:O	2:2:245:PRO:HD3	2.21	0.40
4:4:68:LEU:HD23	4:4:68:LEU:HA	1.91	0.40
1:1:56:VAL:CB	1:1:57:PRO:HD2	2.33	0.40
1:1:237:PHE:CG	5:1:0:SPH:C9	3.04	0.40
3:3:34:ILE:HD13	3:3:34:ILE:HG21	1.86	0.40
1:1:42:PRO:HA	4:4:63:LYS:O	2.22	0.40
2:2:119:GLN:HG2	3:3:123:SER:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	284/302 (94%)	225 (79%)	43 (15%)	16 (6%)	1	4
2	2	266/272 (98%)	222 (84%)	36 (14%)	8 (3%)	3	12
3	3	233/238 (98%)	180 (77%)	38 (16%)	15 (6%)	1	3
4	4	59/68 (87%)	47 (80%)	7 (12%)	5 (8%)	0	1
All	All	842/880 (96%)	674 (80%)	124 (15%)	44 (5%)	1	5

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	82	ALA
1	1	145	THR
1	1	219	ASP
2	2	200	LEU
2	2	257	CYS
3	3	15	THR
3	3	29	ASP
3	3	35	ASP
3	3	137	PRO
3	3	197	ARG
1	1	146	ASN
1	1	170	TRP
1	1	234	LEU
1	1	236	ASP
2	2	130	MET
2	2	167	GLN
3	3	170	TRP
3	3	179	THR
3	3	234	LYS
4	4	15	ASN
1	1	210	ASP
1	1	232	ALA
2	2	240	ALA
3	3	168	VAL
1	1	54	PRO
1	1	57	PRO
1	1	165	PRO
1	1	218	LYS
1	1	275	ARG
2	2	48	ASN
2	2	166	ASN
3	3	65	MET
4	4	60	VAL
1	1	216	PRO
2	2	34	ALA
3	3	59	ALA
3	3	74	ASP
3	3	89	PRO
3	3	161	GLN
4	4	9	LYS
4	4	56	PRO
1	1	250	PRO
3	3	93	PRO

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Mol	Chain	Res	Type
4	4	11	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	249/261 (95%)	226 (91%)	23 (9%)	8	25
2	2	228/232 (98%)	207 (91%)	21 (9%)	8	25
3	3	210/212 (99%)	194 (92%)	16 (8%)	12	33
4	4	54/57 (95%)	44 (82%)	10 (18%)	1	5
All	All	741/762 (97%)	671 (91%)	70 (9%)	8	24

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	7	SER
1	1	10	THR
1	1	38	SER
1	1	41	ILE
1	1	73	SER
1	1	83	ARG
1	1	97	SER
1	1	100	ASN
1	1	109	LYS
1	1	129	ARG
1	1	143	THR
1	1	146	ASN
1	1	147	ASN
1	1	149	HIS
1	1	177	THR
1	1	194	ILE
1	1	214	LYS
1	1	220	GLN
1	1	221	SER
1	1	224	LEU

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Mol	Chain	Res	Type
1	1	255	SER
1	1	287	LYS
1	1	295	SER
2	2	5	GLU
2	2	10	SER
2	2	11	ASP
2	2	31	SER
2	2	48	ASN
2	2	52	GLN
2	2	66	LEU
2	2	73	LYS
2	2	115	SER
2	2	153	LYS
2	2	160	THR
2	2	162	THR
2	2	167	GLN
2	2	168	THR
2	2	201	ARG
2	2	217	SER
2	2	238	ASN
2	2	241	SER
2	2	242	GLU
2	2	264	ARG
2	2	272	GLN
3	3	51	THR
3	3	52	MET
3	3	61	LYS
3	3	71	ARG
3	3	85	LEU
3	3	103	ILE
3	3	104	LEU
3	3	143	LYS
3	3	146	LYS
3	3	149	MET
3	3	163	SER
3	3	190	ILE
3	3	197	ARG
3	3	208	MET
3	3	218	ASN
3	3	224	LEU
4	4	6	SER
4	4	7	SER

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Mol	Chain	Res	Type
4	4	13	HIS
4	4	36	SER
4	4	42	SER
4	4	49	ASP
4	4	52	LYS
4	4	60	VAL
4	4	61	LEU
4	4	64	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	69	HIS
1	1	149	HIS
1	1	152	ASN
1	1	180	ASN
1	1	220	GLN
2	2	48	ASN
2	2	94	GLN
2	2	95	ASN
2	2	165	ASN
2	2	238	ASN
2	2	261	ASN
3	3	6	ASN
3	3	218	ASN
3	3	233	GLN
4	4	26	ASN
4	4	31	ASN
4	4	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	SPH	1	0	-	19,20,20	1.44	2 (10%)	18,21,21	1.72	2 (11%)
6	MYR	4	1	4	13,14,15	0.50	0	12,13,15	1.06	0

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
5	SPH	1	0	-	2/2/2/4	12/21/21/21	-
6	MYR	4	1	4	-	8/12/12/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	0	SPH	C4-C5	5.41	1.53	1.31
5	1	0	SPH	C3-C4	2.10	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	0	SPH	C3-C4-C5	-5.88	112.51	124.69
5	1	0	SPH	C6-C5-C4	-2.71	113.37	125.47

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	1	0	SPH	C2
5	1	0	SPH	C3

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	0	SPH	O1-C1-C2-N2
5	1	0	SPH	O1-C1-C2-C3
5	1	0	SPH	C1-C2-C3-O3
5	1	0	SPH	N2-C2-C3-C4
5	1	0	SPH	C2-C3-C4-C5
5	1	0	SPH	O3-C3-C4-C5
6	4	1	MYR	O1-C1-C2-C3
6	4	1	MYR	C7-C8-C9-C10
6	4	1	MYR	C10-C11-C12-C13
6	4	1	MYR	C5-C6-C7-C8
6	4	1	MYR	C6-C7-C8-C9
5	1	0	SPH	C11-C12-C13-C14
6	4	1	MYR	C11-C12-C13-C14
5	1	0	SPH	C4-C5-C6-C7
5	1	0	SPH	C1-C2-C3-C4
6	4	1	MYR	C9-C10-C11-C12
5	1	0	SPH	C7-C8-C9-C10
5	1	0	SPH	N2-C2-C3-O3
5	1	0	SPH	C10-C11-C12-C13
6	4	1	MYR	C1-C2-C3-C4

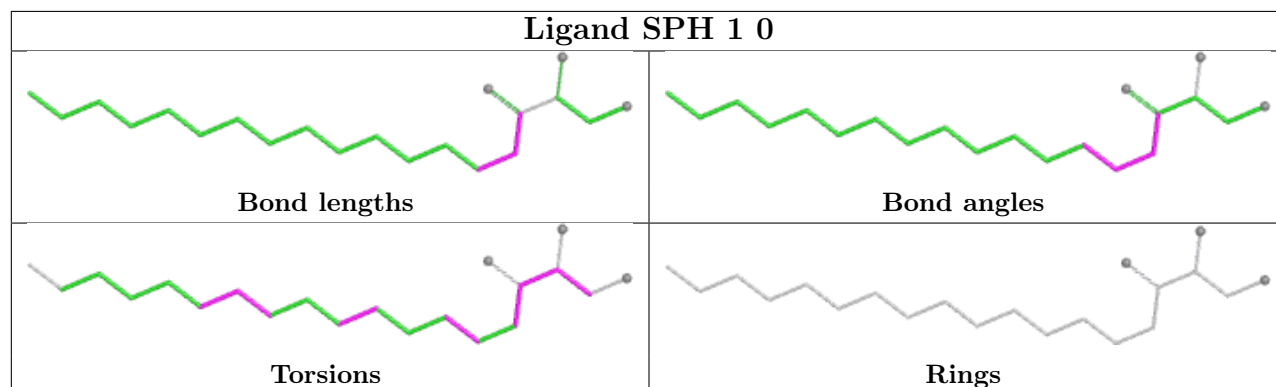
There are no ring outliers.

2 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	0	SPH	29	0
6	4	1	MYR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.