



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:29 AM UTC

PDB ID : 4SBV / pdb_00004sbv
Title : The REFINEMENT OF SOUTHERN BEAN MOSAIC VIRUS IN RECIPROCAL SPACE
Authors : Rossmann, M.G.
Deposited on : 1985-04-01
Resolution : 2.80 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

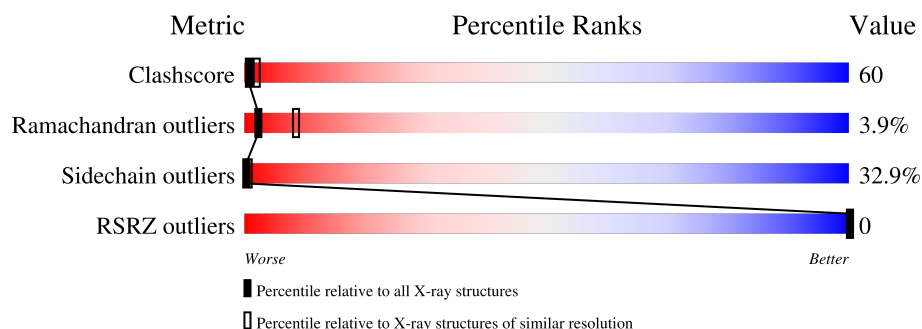
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

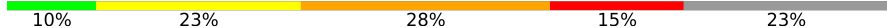
The reported resolution of this entry is 2.80 Å.

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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	260	
1	B	260	
1	C	260	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4723 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 SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1506	956	249	292	9			
1	B	199	Total	C	N	O	S	0	0	0
			1506	956	249	292	9			
1	C	222	Total	C	N	O	S	0	0	0
			1674	1062	281	319	12			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

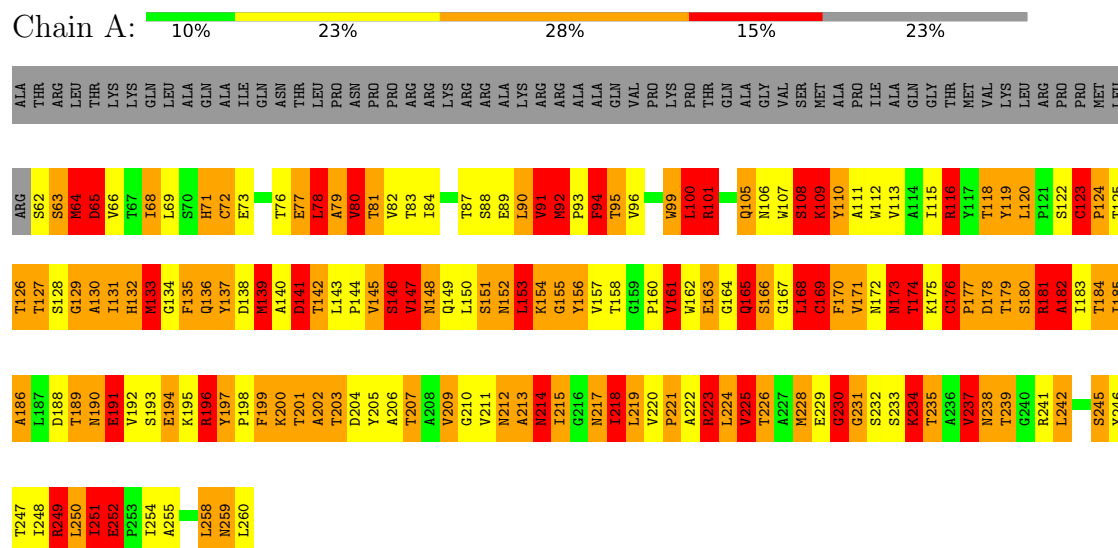
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		

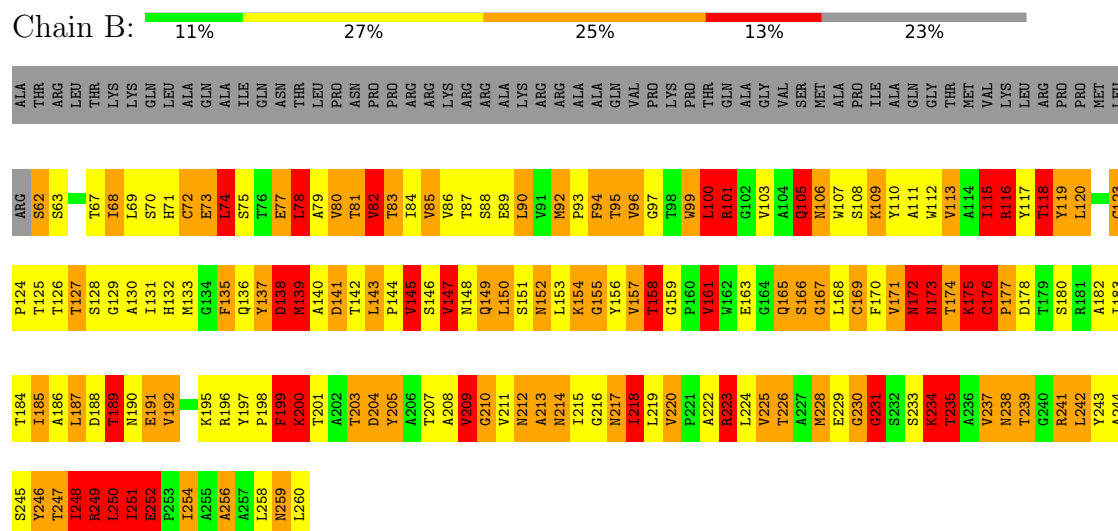
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

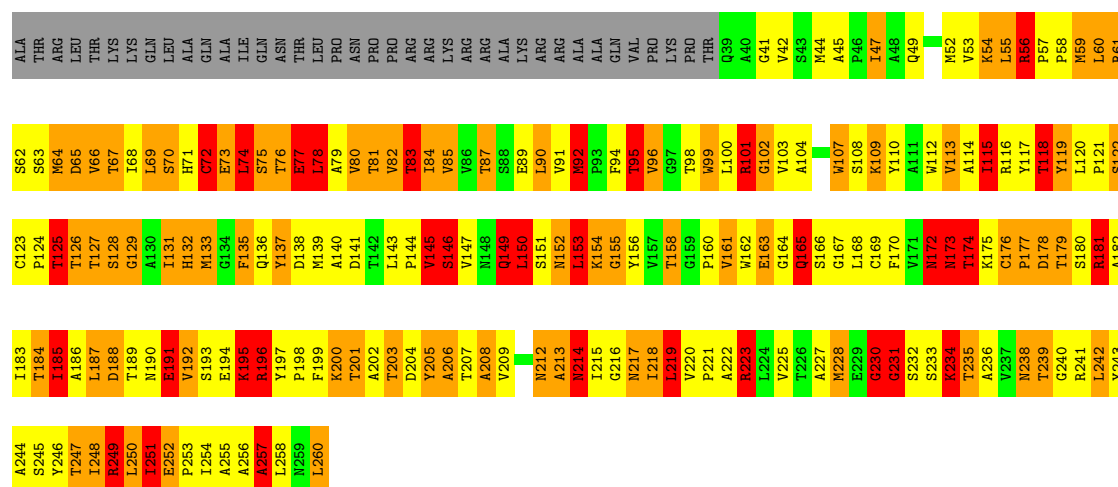
• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	334.30Å 334.30Å 757.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80 0.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 0.0 (0.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available) 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 100.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.00	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.99	40/1537 (2.6%)	3.30	239/2104 (11.4%)
1	B	1.92	23/1537 (1.5%)	3.16	222/2104 (10.6%)
1	C	2.01	31/1708 (1.8%)	3.14	243/2335 (10.4%)
All	All	1.97	94/4782 (2.0%)	3.20	704/6543 (10.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
All	All	0	10

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	GLU	N-CA	21.62	1.66	1.46
1	A	252	GLU	N-CA	14.62	1.60	1.46
1	C	251	ILE	C-N	-11.91	1.23	1.33
1	C	252	GLU	CA-CB	-10.56	1.42	1.53
1	C	251	ILE	C-O	10.15	1.36	1.24
1	B	251	ILE	C-O	9.90	1.35	1.24
1	C	155	GLY	N-CA	9.90	1.59	1.45
1	A	230	GLY	N-CA	9.06	1.58	1.45
1	A	168	LEU	C-O	8.83	1.34	1.23
1	B	231	GLY	N-CA	-8.68	1.32	1.45
1	C	231	GLY	N-CA	-8.61	1.32	1.45
1	C	160	PRO	C-N	-8.31	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	155	GLY	N-CA	8.23	1.57	1.45
1	A	109	LYS	N-CA	8.22	1.56	1.45
1	A	251	ILE	C-N	-8.21	1.27	1.33
1	B	252	GLU	N-CA	8.18	1.57	1.46
1	A	252	GLU	CA-CB	-8.13	1.44	1.53
1	B	138	ASP	N-CA	8.08	1.56	1.46
1	A	168	LEU	C-N	-7.90	1.22	1.33
1	B	97	GLY	N-CA	7.74	1.53	1.45
1	B	252	GLU	CA-CB	-7.63	1.41	1.53
1	C	231	GLY	CA-C	-7.58	1.41	1.51
1	C	133	MET	N-CA	7.15	1.55	1.45
1	C	214	ASN	N-CA	7.07	1.54	1.46
1	A	169	CYS	N-CA	7.03	1.55	1.46
1	A	218	ILE	N-CA	-6.98	1.37	1.46
1	C	231	GLY	C-O	6.96	1.33	1.23
1	A	251	ILE	C-O	6.87	1.32	1.24
1	A	109	LYS	CA-CB	-6.81	1.41	1.53
1	B	137	TYR	C-O	6.79	1.33	1.24
1	C	173	ASN	C-N	-6.71	1.23	1.33
1	B	74	LEU	CA-C	6.68	1.61	1.52
1	C	64	MET	CA-CB	-6.63	1.42	1.53
1	C	133	MET	CA-CB	-6.58	1.42	1.53
1	C	154	LYS	C-O	6.52	1.31	1.24
1	A	178	ASP	N-CA	6.46	1.54	1.46
1	B	128	SER	N-CA	6.44	1.53	1.46
1	C	92	MET	CA-CB	-6.42	1.45	1.53
1	C	182	ALA	N-CA	6.41	1.54	1.45
1	A	154	LYS	C-O	6.31	1.31	1.24
1	B	96	VAL	N-CA	6.23	1.54	1.46
1	C	173	ASN	CA-CB	-6.22	1.43	1.53
1	A	136	GLN	N-CA	6.21	1.53	1.45
1	B	109	LYS	N-CA	6.19	1.54	1.45
1	C	73	GLU	CA-CB	-6.17	1.43	1.54
1	A	91	VAL	N-CA	6.11	1.53	1.46
1	A	169	CYS	CA-CB	-6.07	1.43	1.53
1	C	183	ILE	N-CA	6.01	1.53	1.46
1	C	179	THR	N-CA	5.93	1.53	1.46
1	A	235	THR	CB-OG1	5.92	1.53	1.43
1	A	126	THR	CA-CB	5.81	1.62	1.53
1	A	181	ARG	C-N	-5.79	1.25	1.33
1	A	225	VAL	C-O	5.79	1.30	1.24
1	B	74	LEU	CA-CB	-5.75	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	245	SER	C-O	5.73	1.30	1.23
1	B	142	THR	CA-CB	5.72	1.62	1.53
1	C	73	GLU	N-CA	5.71	1.53	1.45
1	C	222	ALA	C-O	5.71	1.30	1.23
1	A	229	GLU	C-O	5.70	1.31	1.23
1	C	188	ASP	CA-CB	-5.69	1.44	1.53
1	B	84	ILE	CA-CB	5.57	1.60	1.54
1	B	73	GLU	N-CA	5.57	1.53	1.46
1	C	173	ASN	C-O	-5.55	1.17	1.24
1	A	95	THR	N-CA	-5.54	1.39	1.46
1	A	251	ILE	CA-C	-5.50	1.45	1.52
1	A	100	LEU	C-N	-5.50	1.25	1.33
1	A	142	THR	CA-CB	5.47	1.62	1.53
1	C	218	ILE	CA-C	5.43	1.59	1.52
1	A	65	ASP	CA-C	5.39	1.59	1.52
1	B	251	ILE	CA-C	-5.38	1.46	1.52
1	B	241	ARG	NE-CZ	5.34	1.39	1.33
1	C	63	SER	N-CA	5.34	1.53	1.46
1	A	231	GLY	CA-C	-5.33	1.44	1.51
1	A	94	PHE	N-CA	5.32	1.53	1.46
1	A	166	SER	N-CA	5.32	1.53	1.46
1	C	64	MET	N-CA	5.31	1.53	1.46
1	C	250	LEU	N-CA	5.31	1.52	1.45
1	B	73	GLU	C-O	5.28	1.30	1.23
1	A	95	THR	CA-CB	5.20	1.62	1.53
1	C	219	LEU	C-O	5.20	1.30	1.24
1	B	251	ILE	CA-CB	5.19	1.61	1.54
1	A	126	THR	N-CA	-5.16	1.40	1.46
1	A	128	SER	CA-C	-5.14	1.46	1.53
1	A	251	ILE	CA-CB	5.11	1.61	1.54
1	C	251	ILE	CA-C	-5.11	1.46	1.52
1	A	92	MET	CA-CB	-5.11	1.47	1.54
1	B	94	PHE	N-CA	5.09	1.52	1.46
1	A	168	LEU	N-CA	5.08	1.52	1.46
1	B	200	LYS	N-CA	5.08	1.51	1.45
1	A	161	VAL	C-O	5.06	1.30	1.24
1	A	226	THR	N-CA	5.04	1.52	1.46
1	A	126	THR	CA-C	-5.04	1.46	1.52
1	A	129	GLY	N-CA	5.01	1.51	1.45
1	B	138	ASP	CA-CB	-5.01	1.45	1.53

All (704) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	LYS	CA-CB-CG	27.96	170.01	114.10
1	A	125	THR	N-CA-CB	21.81	144.05	110.46
1	A	168	LEU	CA-C-O	-20.12	99.02	121.15
1	B	251	ILE	CA-C-O	-17.79	98.55	120.78
1	C	231	GLY	N-CA-C	17.59	154.88	113.18
1	C	252	GLU	CB-CA-C	16.64	131.94	110.81
1	C	252	GLU	CA-CB-CG	16.63	147.37	114.10
1	A	178	ASP	CA-C-N	15.86	147.18	121.18
1	A	178	ASP	C-N-CA	15.86	147.18	121.18
1	C	251	ILE	CA-C-O	-15.04	101.98	120.78
1	C	173	ASN	CA-C-N	14.92	152.04	123.09
1	C	173	ASN	C-N-CA	14.92	152.04	123.09
1	A	178	ASP	CA-CB-CG	14.75	127.35	112.60
1	C	154	LYS	CA-C-O	-14.60	105.01	121.07
1	B	138	ASP	CA-CB-CG	14.57	127.17	112.60
1	A	196	ARG	NE-CZ-NH1	14.43	135.93	121.50
1	C	173	ASN	CA-CB-CG	14.02	126.62	112.60
1	B	231	GLY	N-CA-C	13.61	145.43	113.18
1	A	218	ILE	CB-CA-C	-13.44	95.01	111.94
1	C	152	ASN	CA-CB-CG	13.23	125.83	112.60
1	B	74	LEU	N-CA-CB	13.18	131.90	110.16
1	A	223	ARG	CD-NE-CZ	-13.09	106.08	124.40
1	A	179	THR	CA-C-O	12.84	132.30	119.08
1	C	76	THR	CA-C-O	-12.58	107.98	121.45
1	B	74	LEU	O-C-N	12.56	137.54	123.22
1	C	188	ASP	CA-CB-CG	12.29	124.89	112.60
1	A	251	ILE	CA-C-O	-12.18	105.55	120.78
1	A	178	ASP	CB-CA-C	12.17	127.38	110.34
1	A	196	ARG	CD-NE-CZ	12.04	141.26	124.40
1	C	214	ASN	CB-CA-C	11.90	130.08	111.28
1	C	101	ARG	NE-CZ-NH1	11.83	133.33	121.50
1	C	217	ASN	CA-C-O	-11.78	105.71	119.61
1	A	178	ASP	CA-C-O	11.65	134.20	119.98
1	A	211	VAL	N-CA-C	-11.60	100.66	111.45
1	C	215	ILE	CA-C-O	11.56	132.96	120.47
1	A	232	SER	N-CA-C	-11.34	98.21	112.72
1	A	69	LEU	O-C-N	11.33	136.17	123.48
1	B	224	LEU	CA-C-O	-11.33	107.89	120.92
1	C	213	ALA	CA-C-N	-11.08	104.74	122.79
1	C	213	ALA	C-N-CA	-11.08	104.74	122.79
1	B	165	GLN	OE1-CD-NE2	11.07	133.67	122.60
1	C	152	ASN	OD1-CG-ND2	-11.01	111.59	122.60
1	C	188	ASP	N-CA-C	-10.93	94.29	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	ILE	N-CA-C	10.86	131.94	109.34
1	B	73	GLU	CA-C-O	-10.84	109.17	121.10
1	B	113	VAL	N-CA-C	-10.82	101.39	111.45
1	B	135	PHE	CA-CB-CG	10.76	124.56	113.80
1	C	95	THR	CA-CB-OG1	-10.74	93.48	109.60
1	B	138	ASP	O-C-N	10.61	136.94	123.14
1	B	204	ASP	CA-CB-CG	-10.57	102.03	112.60
1	A	191	GLU	CA-CB-CG	10.56	135.22	114.10
1	B	152	ASN	CA-CB-CG	10.55	123.16	112.60
1	B	158	THR	O-C-N	10.54	135.92	123.17
1	A	229	GLU	CA-C-O	-10.50	108.83	121.11
1	B	89	GLU	CB-CG-CD	10.45	130.36	112.60
1	C	254	ILE	CA-C-O	-10.40	110.47	121.19
1	B	238	ASN	CA-C-O	-10.32	109.16	120.92
1	A	212	ASN	CA-CB-CG	-10.15	102.45	112.60
1	A	80	VAL	CB-CA-C	-9.98	96.23	111.31
1	A	252	GLU	CB-CA-C	9.89	124.66	111.01
1	B	172	ASN	CA-CB-CG	-9.87	102.73	112.60
1	C	190	ASN	CA-CB-CG	-9.82	102.78	112.60
1	C	73	GLU	CA-CB-CG	9.78	133.65	114.10
1	C	217	ASN	OD1-CG-ND2	9.75	132.35	122.60
1	B	182	ALA	CA-C-N	-9.66	111.11	122.22
1	B	182	ALA	C-N-CA	-9.66	111.11	122.22
1	C	208	ALA	CA-C-O	9.62	130.92	120.82
1	B	138	ASP	CA-C-O	-9.57	108.19	120.25
1	A	133	MET	O-C-N	9.57	133.70	123.56
1	A	165	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	B	166	SER	O-C-N	9.54	133.78	122.24
1	C	215	ILE	N-CA-C	-9.53	99.18	111.09
1	A	65	ASP	N-CA-C	-9.53	100.88	114.12
1	A	142	THR	CA-C-O	-9.46	111.25	121.56
1	A	112	TRP	CA-C-O	-9.43	109.56	120.49
1	C	214	ASN	N-CA-CB	-9.43	96.69	111.39
1	C	193	SER	N-CA-C	9.40	121.61	111.36
1	B	158	THR	CA-C-O	-9.37	110.81	121.40
1	B	254	ILE	CA-C-O	-9.34	113.11	120.96
1	C	234	LYS	CA-C-N	9.30	135.86	122.09
1	C	234	LYS	C-N-CA	9.30	135.86	122.09
1	A	196	ARG	NE-CZ-NH2	-9.29	110.84	119.20
1	A	190	ASN	OD1-CG-ND2	9.28	131.88	122.60
1	B	252	GLU	CB-CG-CD	9.27	128.36	112.60
1	A	168	LEU	N-CA-C	-9.24	97.20	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	SER	N-CA-C	-9.21	100.95	113.30
1	C	251	ILE	CA-C-N	-9.16	112.11	122.00
1	C	251	ILE	C-N-CA	-9.16	112.11	122.00
1	A	258	LEU	N-CA-CB	-9.12	96.99	110.49
1	A	197	TYR	O-C-N	9.10	129.63	121.80
1	B	185	ILE	CB-CG1-CD1	9.10	132.90	113.80
1	A	249	ARG	CA-C-N	9.07	133.76	120.87
1	A	249	ARG	C-N-CA	9.07	133.76	120.87
1	B	230	GLY	CA-C-N	9.07	139.19	121.41
1	B	230	GLY	C-N-CA	9.07	139.19	121.41
1	B	152	ASN	CA-C-O	-9.05	108.76	119.35
1	C	214	ASN	OD1-CG-ND2	9.04	131.64	122.60
1	B	165	GLN	CA-CB-CG	-8.95	96.20	114.10
1	C	216	GLY	O-C-N	8.95	130.85	122.17
1	C	141	ASP	CA-CB-CG	8.91	121.51	112.60
1	C	204	ASP	CA-CB-CG	-8.84	103.76	112.60
1	A	170	PHE	N-CA-C	-8.83	100.18	112.45
1	A	235	THR	CA-CB-OG1	-8.81	96.38	109.60
1	B	101	ARG	CG-CD-NE	8.80	131.36	112.00
1	A	190	ASN	CB-CA-C	-8.80	94.78	109.03
1	A	238	ASN	CA-CB-CG	-8.74	103.86	112.60
1	B	68	ILE	O-C-N	8.71	132.66	123.26
1	B	145	VAL	CA-C-N	8.71	137.73	122.67
1	B	145	VAL	C-N-CA	8.71	137.73	122.67
1	B	229	GLU	CA-C-O	-8.70	111.04	121.66
1	C	248	ILE	N-CA-CB	-8.69	93.92	111.91
1	C	96	VAL	CA-C-O	-8.67	111.43	120.71
1	C	109	LYS	CA-C-O	-8.66	111.01	121.06
1	B	214	ASN	OD1-CG-ND2	-8.64	113.96	122.60
1	A	251	ILE	CA-C-N	-8.61	112.53	122.52
1	A	251	ILE	C-N-CA	-8.61	112.53	122.52
1	B	209	VAL	CB-CA-C	8.59	122.70	111.70
1	A	164	GLY	N-CA-C	8.57	124.68	114.48
1	B	100	LEU	O-C-N	8.57	131.21	122.12
1	C	249	ARG	CA-C-O	-8.55	110.85	120.43
1	B	234	LYS	N-CA-C	-8.53	102.86	113.18
1	B	241	ARG	NE-CZ-NH2	-8.50	111.55	119.20
1	A	251	ILE	N-CA-C	8.48	126.98	109.34
1	A	135	PHE	CA-CB-CG	8.47	122.27	113.80
1	A	217	ASN	CA-C-N	8.46	135.04	121.34
1	A	217	ASN	C-N-CA	8.46	135.04	121.34
1	B	259	ASN	N-CA-C	8.45	124.16	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	THR	CB-CA-C	-8.44	94.74	110.36
1	A	191	GLU	CB-CG-CD	8.44	126.94	112.60
1	C	236	ALA	N-CA-C	8.43	122.66	110.10
1	B	119	TYR	CA-C-O	-8.42	111.38	121.56
1	B	75	SER	N-CA-C	-8.41	100.77	112.45
1	A	115	ILE	O-C-N	8.40	131.25	123.19
1	B	172	ASN	OD1-CG-ND2	8.40	131.00	122.60
1	A	119	TYR	CA-C-O	-8.38	111.65	120.70
1	A	130	ALA	CA-C-O	-8.37	111.61	120.99
1	C	108	SER	N-CA-C	8.37	120.03	111.07
1	C	213	ALA	CA-C-O	-8.36	109.75	119.61
1	B	73	GLU	CA-C-N	-8.32	110.46	122.19
1	B	73	GLU	C-N-CA	-8.32	110.46	122.19
1	B	210	GLY	CA-C-N	8.31	131.02	120.88
1	B	210	GLY	C-N-CA	8.31	131.02	120.88
1	A	141	ASP	CA-C-N	8.30	133.97	120.94
1	A	141	ASP	C-N-CA	8.30	133.97	120.94
1	C	61	ARG	CA-C-N	8.18	133.35	122.30
1	C	61	ARG	C-N-CA	8.18	133.35	122.30
1	B	138	ASP	N-CA-C	-8.18	93.65	107.80
1	C	165	GLN	OE1-CD-NE2	8.15	130.75	122.60
1	A	214	ASN	O-C-N	8.14	130.56	121.93
1	A	106	ASN	CA-CB-CG	-8.13	104.47	112.60
1	C	45	ALA	O-C-N	8.12	128.50	121.20
1	C	59	MET	CA-CB-CG	-8.11	97.88	114.10
1	C	204	ASP	N-CA-CB	8.08	121.73	110.01
1	B	96	VAL	CB-CA-C	8.06	123.05	112.24
1	B	86	VAL	N-CA-CB	-8.05	101.52	111.67
1	C	119	TYR	CA-C-O	-8.06	111.77	121.28
1	A	174	THR	CA-CB-OG1	-8.04	97.54	109.60
1	A	175	LYS	N-CA-CB	8.04	123.68	110.17
1	C	99	TRP	O-C-N	8.02	131.55	122.32
1	A	152	ASN	CA-CB-CG	8.01	120.61	112.60
1	C	241	ARG	NE-CZ-NH1	-8.01	113.49	121.50
1	B	80	VAL	O-C-N	7.99	131.55	123.00
1	B	109	LYS	CG-CD-CE	7.99	129.67	111.30
1	A	123	CYS	CB-CA-C	-7.98	93.14	111.89
1	C	101	ARG	NE-CZ-NH2	-7.97	112.03	119.20
1	A	174	THR	CB-CA-C	7.92	123.87	109.37
1	C	252	GLU	CB-CG-CD	7.92	126.06	112.60
1	C	133	MET	CA-CB-CG	7.90	129.91	114.10
1	A	176	CYS	CA-CB-SG	7.88	132.52	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ASN	CA-CB-CG	-7.85	104.75	112.60
1	C	146	SER	CA-CB-OG	7.84	126.78	111.10
1	C	182	ALA	CA-C-O	-7.83	111.15	121.73
1	A	154	LYS	CA-C-O	-7.81	112.85	120.90
1	C	89	GLU	N-CA-C	7.81	121.97	108.76
1	B	72	CYS	CA-CB-SG	-7.81	96.44	114.40
1	B	120	LEU	CB-CA-C	7.81	120.54	110.16
1	B	137	TYR	CA-C-O	-7.81	110.83	119.34
1	B	252	GLU	N-CA-C	-7.80	92.56	109.81
1	C	196	ARG	N-CA-CB	7.80	125.26	111.69
1	A	163	GLU	CB-CG-CD	7.72	125.73	112.60
1	C	241	ARG	CA-C-O	-7.70	113.00	121.23
1	B	252	GLU	CA-CB-CG	7.69	129.48	114.10
1	C	68	ILE	CA-C-O	-7.66	112.35	120.39
1	A	251	ILE	N-CA-CB	-7.61	98.67	111.23
1	B	238	ASN	OD1-CG-ND2	7.61	130.21	122.60
1	C	63	SER	CA-C-O	-7.61	109.63	120.51
1	C	241	ARG	CA-C-N	-7.61	110.75	122.62
1	C	241	ARG	C-N-CA	-7.61	110.75	122.62
1	B	182	ALA	CA-C-O	-7.60	112.14	120.43
1	C	252	GLU	N-CA-C	-7.59	94.97	108.55
1	B	241	ARG	CD-NE-CZ	-7.57	113.80	124.40
1	A	169	CYS	CA-CB-SG	7.57	131.81	114.40
1	C	112	TRP	CA-C-O	-7.56	113.32	121.56
1	B	67	THR	CA-CB-OG1	-7.54	98.28	109.60
1	C	62	SER	CA-C-O	-7.54	111.98	120.43
1	A	145	VAL	N-CA-CB	-7.53	101.16	112.67
1	B	80	VAL	CA-C-N	-7.53	112.23	122.16
1	B	80	VAL	C-N-CA	-7.53	112.23	122.16
1	C	188	ASP	CB-CA-C	7.52	123.20	112.07
1	B	173	ASN	CA-C-O	7.50	131.24	120.51
1	A	113	VAL	N-CA-C	-7.50	101.78	112.35
1	B	178	ASP	CA-C-O	-7.49	111.22	122.38
1	A	188	ASP	CA-CB-CG	7.48	120.08	112.60
1	C	204	ASP	O-C-N	7.47	129.77	122.07
1	A	170	PHE	CB-CA-C	7.47	124.23	110.11
1	B	186	ALA	CA-C-N	7.47	131.32	120.71
1	B	186	ALA	C-N-CA	7.47	131.32	120.71
1	C	230	GLY	N-CA-C	7.47	130.88	113.18
1	A	214	ASN	N-CA-C	-7.46	103.30	114.64
1	C	235	THR	CA-CB-OG1	-7.44	98.44	109.60
1	B	174	THR	N-CA-C	-7.42	94.91	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	CYS	O-C-N	7.40	132.44	122.59
1	C	118	THR	CB-CA-C	7.38	124.37	109.38
1	C	196	ARG	CA-CB-CG	7.38	128.85	114.10
1	B	220	VAL	N-CA-CB	-7.35	100.92	111.21
1	A	78	LEU	O-C-N	7.35	132.70	123.15
1	A	95	THR	CA-C-N	-7.34	109.45	121.34
1	A	95	THR	C-N-CA	-7.34	109.45	121.34
1	A	127	THR	CA-CB-OG1	-7.33	98.61	109.60
1	C	241	ARG	NE-CZ-NH2	7.33	125.80	119.20
1	C	196	ARG	NE-CZ-NH2	-7.31	112.62	119.20
1	B	82	VAL	O-C-N	7.31	128.96	121.87
1	A	146	SER	N-CA-CB	-7.30	97.96	111.53
1	A	182	ALA	O-C-N	7.30	132.29	122.59
1	B	67	THR	CA-C-N	-7.29	113.58	123.14
1	B	67	THR	C-N-CA	-7.29	113.58	123.14
1	A	123	CYS	N-CA-C	7.29	120.56	109.41
1	A	186	ALA	CA-C-O	-7.28	112.69	121.28
1	C	61	ARG	CA-CB-CG	7.28	128.65	114.10
1	B	128	SER	CA-C-O	-7.26	112.74	120.80
1	B	209	VAL	N-CA-CB	-7.26	103.00	110.62
1	A	65	ASP	N-CA-CB	7.25	120.88	110.88
1	B	74	LEU	N-CA-C	-7.24	97.44	109.46
1	A	224	LEU	CA-C-O	-7.23	112.80	121.05
1	A	81	THR	CA-C-N	7.23	132.72	120.29
1	A	81	THR	C-N-CA	7.23	132.72	120.29
1	B	163	GLU	CG-CD-OE2	-7.21	101.81	118.40
1	B	254	ILE	O-C-N	7.21	129.25	122.97
1	B	115	ILE	CA-CB-CG1	-7.19	98.18	110.40
1	B	68	ILE	CA-C-O	-7.19	112.84	120.39
1	C	96	VAL	O-C-N	7.17	131.31	121.84
1	B	238	ASN	CA-CB-CG	-7.15	105.45	112.60
1	B	77	GLU	CA-C-O	-7.15	113.03	121.11
1	B	147	VAL	CA-C-O	7.14	128.39	120.46
1	A	185	ILE	CA-C-O	-7.14	113.18	120.25
1	C	214	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	215	ILE	N-CA-C	-7.09	103.28	111.00
1	A	108	SER	N-CA-C	7.08	119.08	111.36
1	A	135	PHE	O-C-N	7.08	131.03	123.03
1	B	182	ALA	O-C-N	7.07	131.26	123.27
1	B	239	THR	CA-CB-OG1	-7.05	99.02	109.60
1	C	143	LEU	O-C-N	7.03	129.26	121.53
1	B	256	ALA	CA-C-O	7.02	130.55	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	VAL	CA-C-N	7.01	131.34	120.82
1	A	171	VAL	C-N-CA	7.01	131.34	120.82
1	C	94	PHE	CA-C-O	7.00	128.01	120.24
1	A	213	ALA	CA-C-O	-6.99	109.46	120.37
1	A	169	CYS	N-CA-C	-6.97	95.96	110.80
1	C	119	TYR	N-CA-C	6.94	121.34	110.17
1	C	238	ASN	OD1-CG-ND2	6.93	129.53	122.60
1	B	259	ASN	CA-CB-CG	-6.92	105.67	112.60
1	A	105	GLN	O-C-N	6.92	131.39	122.39
1	C	251	ILE	N-CA-C	6.92	123.72	109.34
1	A	141	ASP	CA-CB-CG	6.90	119.50	112.60
1	A	118	THR	CA-C-O	-6.88	113.07	121.11
1	B	217	ASN	CA-C-O	-6.87	110.69	120.51
1	B	252	GLU	CG-CD-OE1	6.86	134.18	118.40
1	C	132	HIS	CA-C-N	-6.86	109.88	121.75
1	C	132	HIS	C-N-CA	-6.86	109.88	121.75
1	A	64	MET	CA-C-N	6.86	133.00	122.23
1	A	64	MET	C-N-CA	6.86	133.00	122.23
1	C	65	ASP	CA-C-N	-6.86	110.02	122.43
1	C	65	ASP	C-N-CA	-6.86	110.02	122.43
1	A	90	LEU	CA-C-O	-6.85	113.59	121.47
1	C	185	ILE	N-CA-C	-6.85	99.30	108.35
1	A	137	TYR	N-CA-CB	-6.85	101.09	110.95
1	C	85	VAL	CA-C-N	-6.84	113.97	122.93
1	C	85	VAL	C-N-CA	-6.84	113.97	122.93
1	B	105	GLN	CA-CB-CG	6.84	127.78	114.10
1	C	113	VAL	CA-C-O	6.84	129.33	120.78
1	B	141	ASP	N-CA-CB	-6.84	100.99	110.29
1	C	115	ILE	CA-C-O	6.82	127.93	120.64
1	A	111	ALA	O-C-N	6.81	131.11	123.48
1	B	223	ARG	NH1-CZ-NH2	6.79	128.13	119.30
1	A	173	ASN	CA-CB-CG	-6.78	105.82	112.60
1	B	217	ASN	CA-CB-CG	-6.78	105.82	112.60
1	C	78	LEU	N-CA-CB	-6.78	100.00	110.85
1	C	83	THR	N-CA-C	6.78	120.18	109.81
1	A	95	THR	CA-C-O	-6.75	110.86	120.51
1	C	251	ILE	CA-CB-CG1	-6.74	98.94	110.40
1	A	213	ALA	O-C-N	6.74	131.42	121.72
1	A	91	VAL	CB-CA-C	6.73	122.33	111.29
1	C	90	LEU	CA-C-O	-6.73	112.61	120.62
1	C	83	THR	CA-CB-OG1	-6.70	99.55	109.60
1	B	192	VAL	CA-C-O	-6.70	114.69	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	GLN	O-C-N	6.69	129.21	122.12
1	C	87	THR	N-CA-CB	-6.69	100.09	110.46
1	B	247	THR	CA-CB-OG1	-6.67	99.59	109.60
1	B	211	VAL	N-CA-C	-6.67	104.67	110.74
1	B	118	THR	CA-C-O	-6.64	113.90	121.40
1	A	151	SER	CA-C-N	-6.62	113.30	123.17
1	A	151	SER	C-N-CA	-6.62	113.30	123.17
1	B	251	ILE	CA-CB-CG1	-6.61	99.17	110.40
1	B	198	PRO	CA-C-O	-6.60	113.81	121.86
1	A	101	ARG	CD-NE-CZ	6.60	133.63	124.40
1	B	165	GLN	CB-CG-CD	-6.59	101.40	112.60
1	A	65	ASP	CA-CB-CG	6.57	119.17	112.60
1	A	238	ASN	CB-CA-C	6.57	120.12	110.26
1	A	180	SER	CA-C-N	6.56	133.83	121.69
1	A	180	SER	C-N-CA	6.56	133.83	121.69
1	A	110	TYR	CA-C-O	-6.55	114.30	121.31
1	B	95	THR	CA-C-N	-6.54	110.08	120.55
1	B	95	THR	C-N-CA	-6.54	110.08	120.55
1	C	230	GLY	O-C-N	-6.53	114.21	122.70
1	A	124	PRO	N-CA-C	-6.53	101.40	111.13
1	C	179	THR	N-CA-CB	-6.53	101.01	110.47
1	B	96	VAL	CA-C-O	-6.51	113.74	120.71
1	B	157	VAL	CA-C-O	-6.51	112.65	120.78
1	B	250	LEU	O-C-N	6.50	130.92	122.93
1	A	178	ASP	O-C-N	-6.49	115.21	123.26
1	C	252	GLU	CA-C-O	6.49	127.35	121.06
1	C	133	MET	CB-CA-C	6.46	124.35	110.45
1	C	138	ASP	CB-CA-C	6.46	121.12	110.78
1	B	176	CYS	CA-CB-SG	-6.46	99.54	114.40
1	B	85	VAL	N-CA-C	-6.45	99.43	108.27
1	C	126	THR	N-CA-C	-6.43	105.06	114.39
1	A	161	VAL	CA-C-O	-6.42	112.75	120.78
1	C	250	LEU	CB-CA-C	6.42	120.35	109.50
1	B	246	TYR	O-C-N	6.42	131.49	123.15
1	A	95	THR	CB-CA-C	-6.41	97.67	110.42
1	C	149	GLN	CA-C-O	6.41	128.12	121.07
1	B	250	LEU	CA-C-N	-6.40	110.45	121.97
1	B	250	LEU	C-N-CA	-6.40	110.45	121.97
1	B	175	LYS	CB-CA-C	6.40	120.65	111.82
1	B	139	MET	CA-CB-CG	-6.39	101.31	114.10
1	A	164	GLY	CA-C-N	6.39	129.13	120.38
1	A	164	GLY	C-N-CA	6.39	129.13	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	GLN	CB-CA-C	6.38	123.73	109.56
1	C	147	VAL	O-C-N	6.38	128.40	121.83
1	B	143	LEU	O-C-N	6.38	126.98	121.30
1	B	95	THR	CA-CB-OG1	-6.37	100.04	109.60
1	A	175	LYS	N-CA-C	-6.37	98.83	108.96
1	B	127	THR	CA-C-N	-6.36	113.17	122.65
1	B	127	THR	C-N-CA	-6.36	113.17	122.65
1	C	241	ARG	O-C-N	6.35	130.22	123.42
1	A	217	ASN	CB-CG-OD1	6.35	133.50	120.80
1	A	79	ALA	CA-C-N	6.35	132.86	122.64
1	A	79	ALA	C-N-CA	6.35	132.86	122.64
1	A	221	PRO	CA-C-O	-6.34	110.02	119.34
1	A	234	LYS	N-CA-C	-6.34	105.83	112.93
1	B	99	TRP	CB-CA-C	6.33	121.42	110.79
1	C	153	LEU	CA-CB-CG	6.32	138.43	116.30
1	C	223	ARG	O-C-N	6.32	130.98	123.27
1	A	127	THR	CA-C-N	-6.32	113.50	123.23
1	A	127	THR	C-N-CA	-6.32	113.50	123.23
1	B	249	ARG	CA-C-O	-6.31	113.34	121.11
1	A	132	HIS	CA-C-O	-6.31	114.27	121.40
1	B	176	CYS	O-C-N	6.31	128.58	121.32
1	A	179	THR	N-CA-C	-6.30	103.24	113.19
1	C	191	GLU	CA-C-O	6.30	127.38	119.95
1	C	77	GLU	N-CA-CB	6.29	121.78	110.83
1	C	132	HIS	O-C-N	6.29	130.94	123.33
1	C	56	ARG	CD-NE-CZ	6.29	133.20	124.40
1	B	165	GLN	CG-CD-NE2	-6.28	106.98	116.40
1	A	255	ALA	N-CA-C	-6.27	101.13	110.23
1	C	119	TYR	N-CA-CB	-6.27	100.41	110.63
1	B	127	THR	CA-CB-OG1	-6.27	100.19	109.60
1	B	141	ASP	CB-CA-C	6.27	124.44	110.02
1	C	72	CYS	CA-C-N	-6.27	112.29	122.82
1	C	72	CYS	C-N-CA	-6.27	112.29	122.82
1	B	149	GLN	O-C-N	6.26	129.55	122.22
1	A	80	VAL	N-CA-C	6.26	118.67	108.97
1	A	77	GLU	CA-C-N	-6.25	112.78	122.59
1	A	77	GLU	C-N-CA	-6.25	112.78	122.59
1	B	212	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	B	127	THR	CA-C-O	-6.25	113.52	120.70
1	C	242	LEU	CB-CA-C	6.24	122.41	109.38
1	B	234	LYS	CA-C-N	6.23	130.71	122.30
1	B	234	LYS	C-N-CA	6.23	130.71	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	CYS	N-CA-C	6.22	118.65	109.50
1	B	84	ILE	N-CA-C	6.22	117.60	109.58
1	B	123	CYS	CA-C-N	6.20	126.12	119.85
1	B	123	CYS	C-N-CA	6.20	126.12	119.85
1	A	258	LEU	N-CA-C	6.20	120.98	113.17
1	A	184	THR	CA-CB-OG1	-6.20	100.30	109.60
1	A	212	ASN	OD1-CG-ND2	6.18	128.78	122.60
1	B	81	THR	CA-CB-OG1	-6.17	100.34	109.60
1	B	90	LEU	CA-CB-CG	6.16	137.88	116.30
1	C	201	THR	CA-C-O	-6.15	114.47	121.72
1	A	68	ILE	CA-C-O	-6.14	113.48	120.67
1	C	160	PRO	CA-C-N	6.14	130.95	121.19
1	C	160	PRO	C-N-CA	6.14	130.95	121.19
1	C	136	GLN	CA-C-N	-6.13	112.69	122.08
1	C	136	GLN	C-N-CA	-6.13	112.69	122.08
1	C	81	THR	CA-C-N	6.13	133.01	121.97
1	C	81	THR	C-N-CA	6.13	133.01	121.97
1	A	175	LYS	O-C-N	6.13	130.18	123.13
1	B	220	VAL	N-CA-C	6.11	122.09	108.88
1	A	247	THR	N-CA-CB	6.10	120.42	110.90
1	C	110	TYR	O-C-N	6.10	131.47	122.81
1	A	247	THR	O-C-N	6.10	131.06	123.14
1	C	223	ARG	CA-C-O	-6.09	113.65	120.66
1	B	191	GLU	CB-CG-CD	6.08	122.94	112.60
1	A	174	THR	CA-CB-CG2	6.07	120.81	110.50
1	B	154	LYS	CA-C-O	-6.06	113.73	120.70
1	A	81	THR	CA-CB-OG1	-6.06	100.51	109.60
1	A	142	THR	N-CA-C	6.06	119.04	110.50
1	B	82	VAL	CB-CA-C	-6.04	103.98	112.14
1	C	183	ILE	CB-CA-C	6.03	121.18	111.29
1	B	173	ASN	CA-C-N	6.03	130.12	122.16
1	B	173	ASN	C-N-CA	6.03	130.12	122.16
1	B	226	THR	CA-CB-CG2	6.03	120.75	110.50
1	B	155	GLY	CA-C-N	6.03	129.40	120.90
1	B	155	GLY	C-N-CA	6.03	129.40	120.90
1	A	194	GLU	CB-CG-CD	-6.03	102.35	112.60
1	A	241	ARG	NE-CZ-NH1	-6.02	115.48	121.50
1	A	131	ILE	CB-CA-C	6.01	119.79	111.38
1	C	131	ILE	O-C-N	6.01	129.43	123.00
1	A	92	MET	O-C-N	6.01	126.23	121.55
1	B	96	VAL	CA-CB-CG1	6.00	120.60	110.40
1	C	75	SER	N-CA-C	6.00	120.91	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	A	241	ARG	CD-NE-CZ	-5.96	116.05	124.40
1	B	182	ALA	N-CA-C	-5.96	99.52	109.24
1	A	210	GLY	CA-C-N	-5.96	112.83	121.65
1	A	210	GLY	C-N-CA	-5.96	112.83	121.65
1	A	108	SER	CA-C-O	-5.95	114.12	120.42
1	B	243	TYR	CA-C-O	-5.94	114.27	121.28
1	C	145	VAL	O-C-N	5.94	127.94	122.06
1	A	242	LEU	CA-C-O	-5.93	113.96	120.43
1	C	62	SER	N-CA-CB	-5.93	100.20	110.17
1	B	128	SER	CB-CA-C	5.93	119.45	109.48
1	C	218	ILE	N-CA-CB	5.93	121.02	111.23
1	B	67	THR	CA-C-O	-5.92	113.85	120.66
1	C	251	ILE	CA-CB-CG2	5.92	120.56	110.50
1	A	128	SER	CA-C-O	-5.91	109.28	120.69
1	B	237	VAL	CA-C-O	-5.91	114.20	120.53
1	A	119	TYR	O-C-N	5.89	130.89	123.23
1	C	217	ASN	CA-CB-CG	-5.89	106.71	112.60
1	B	225	VAL	N-CA-CB	-5.89	103.99	111.64
1	C	47	ILE	O-C-N	5.89	128.09	122.20
1	C	120	LEU	CB-CA-C	5.88	117.97	109.45
1	A	217	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	C	255	ALA	CA-C-O	-5.87	115.16	121.56
1	C	166	SER	N-CA-C	-5.87	104.47	111.69
1	B	191	GLU	CG-CD-OE1	5.87	131.90	118.40
1	C	146	SER	N-CA-CB	-5.87	100.69	111.37
1	A	99	TRP	O-C-N	5.85	128.90	122.11
1	A	106	ASN	OD1-CG-ND2	5.84	128.44	122.60
1	A	90	LEU	CA-C-N	-5.84	111.45	121.97
1	A	90	LEU	C-N-CA	-5.84	111.45	121.97
1	C	73	GLU	CG-CD-OE1	5.84	131.83	118.40
1	A	73	GLU	N-CA-C	5.83	115.80	108.45
1	A	228	MET	CA-C-O	5.83	126.70	120.46
1	A	249	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	A	230	GLY	N-CA-C	-5.83	99.36	113.18
1	B	95	THR	CA-CB-CG2	5.83	120.41	110.50
1	A	252	GLU	CG-CD-OE1	5.83	131.80	118.40
1	B	199	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	182	ALA	CA-C-O	-5.79	112.23	120.51
1	C	219	LEU	CA-C-O	-5.79	112.23	120.51
1	C	172	ASN	CA-C-N	5.78	132.59	121.54
1	C	172	ASN	C-N-CA	5.78	132.59	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	LYS	CA-CB-CG	5.78	125.66	114.10
1	C	173	ASN	N-CA-CB	5.78	120.26	110.49
1	C	147	VAL	N-CA-C	-5.78	104.89	110.72
1	A	171	VAL	CA-C-O	5.77	127.99	120.78
1	C	129	GLY	CA-C-N	-5.76	111.92	123.09
1	C	129	GLY	C-N-CA	-5.76	111.92	123.09
1	B	73	GLU	CA-CB-CG	5.75	125.61	114.10
1	A	189	THR	CA-CB-OG1	-5.75	100.97	109.60
1	A	73	GLU	CB-CG-CD	5.75	122.38	112.60
1	C	174	THR	CA-CB-OG1	-5.75	100.98	109.60
1	C	42	VAL	CB-CA-C	5.75	117.94	110.12
1	C	76	THR	O-C-N	5.75	129.71	123.10
1	A	116	ARG	N-CA-CB	-5.74	101.24	110.77
1	A	84	ILE	O-C-N	5.74	129.40	123.03
1	A	157	VAL	CA-C-O	-5.74	115.57	120.96
1	A	76	THR	N-CA-C	5.74	116.97	107.73
1	C	174	THR	CA-C-O	-5.74	114.29	121.46
1	B	172	ASN	CB-CA-C	-5.74	102.27	111.39
1	C	219	LEU	N-CA-CB	-5.73	100.81	110.49
1	B	99	TRP	CA-CB-CG	5.72	124.47	113.60
1	A	130	ALA	O-C-N	5.71	129.78	123.33
1	C	65	ASP	O-C-N	5.70	130.27	122.46
1	B	81	THR	CA-C-N	5.69	128.26	120.46
1	B	81	THR	C-N-CA	5.69	128.26	120.46
1	C	201	THR	CA-CB-OG1	-5.69	101.07	109.60
1	A	174	THR	N-CA-CB	-5.68	101.76	110.85
1	C	122	SER	CA-CB-OG	-5.68	99.73	111.10
1	A	254	ILE	CA-C-O	-5.68	116.01	121.63
1	C	128	SER	O-C-N	5.68	129.63	123.10
1	A	72	CYS	O-C-N	5.68	131.12	123.34
1	B	73	GLU	N-CA-CB	-5.67	102.95	111.56
1	A	156	TYR	O-C-N	5.66	130.12	122.59
1	A	207	THR	O-C-N	5.66	127.90	122.07
1	C	204	ASP	N-CA-C	-5.66	105.02	111.07
1	C	77	GLU	CA-C-O	-5.65	114.59	120.70
1	C	149	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	C	235	THR	CA-C-O	-5.65	114.43	120.92
1	B	100	LEU	N-CA-C	-5.64	104.50	111.33
1	C	58	PRO	N-CA-CB	5.64	108.26	103.35
1	C	73	GLU	CG-CD-OE2	-5.64	105.44	118.40
1	A	122	SER	N-CA-C	-5.63	106.08	114.64
1	B	252	GLU	OE1-CD-OE2	-5.63	109.40	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ASN	O-C-N	5.62	129.90	122.36
1	A	245	SER	CA-CB-OG	-5.62	99.85	111.10
1	A	194	GLU	CG-CD-OE2	-5.61	105.49	118.40
1	B	172	ASN	CA-C-N	5.61	132.26	121.54
1	B	172	ASN	C-N-CA	5.61	132.26	121.54
1	C	107	TRP	CA-C-O	-5.61	114.21	120.66
1	C	95	THR	CA-CB-CG2	5.61	120.03	110.50
1	B	207	THR	CA-CB-OG1	-5.60	101.20	109.60
1	B	173	ASN	CA-CB-CG	-5.60	107.00	112.60
1	B	218	ILE	CA-C-N	-5.60	111.65	122.06
1	B	218	ILE	C-N-CA	-5.60	111.65	122.06
1	A	192	VAL	CB-CA-C	5.60	119.35	111.63
1	A	209	VAL	CA-C-N	-5.59	112.77	122.83
1	A	209	VAL	C-N-CA	-5.59	112.77	122.83
1	C	154	LYS	CA-C-N	-5.59	110.45	121.41
1	C	154	LYS	C-N-CA	-5.59	110.45	121.41
1	A	147	VAL	CA-C-O	-5.58	115.60	121.41
1	C	95	THR	CA-C-O	-5.57	113.22	119.79
1	A	210	GLY	O-C-N	5.57	128.62	122.27
1	A	182	ALA	CA-C-N	-5.56	111.96	121.97
1	A	182	ALA	C-N-CA	-5.56	111.96	121.97
1	A	252	GLU	N-CA-C	-5.56	96.52	108.64
1	C	58	PRO	O-C-N	5.55	129.89	123.01
1	A	83	THR	CA-CB-OG1	-5.55	101.28	109.60
1	C	61	ARG	CA-C-O	5.54	126.74	119.98
1	C	64	MET	CA-CB-CG	5.54	125.19	114.10
1	B	252	GLU	CB-CA-C	5.54	121.08	110.17
1	B	132	HIS	CA-C-O	-5.53	113.48	120.28
1	B	189	THR	CA-CB-OG1	-5.53	101.31	109.60
1	A	90	LEU	N-CA-C	-5.53	102.30	110.48
1	C	76	THR	CA-C-N	-5.53	114.65	122.94
1	C	76	THR	C-N-CA	-5.53	114.65	122.94
1	B	187	LEU	N-CA-C	5.52	118.23	110.23
1	C	89	GLU	CB-CA-C	-5.51	99.72	109.70
1	B	130	ALA	N-CA-C	5.51	117.44	109.07
1	B	226	THR	CB-CA-C	5.51	119.79	109.71
1	C	212	ASN	CA-CB-CG	-5.50	107.10	112.60
1	C	204	ASP	CA-C-O	-5.50	115.05	120.82
1	A	232	SER	O-C-N	5.49	128.84	122.09
1	C	173	ASN	CA-C-O	5.49	128.36	120.51
1	A	63	SER	CB-CA-C	5.48	117.96	110.94
1	A	145	VAL	CB-CA-C	5.48	116.13	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-C-N	-5.48	112.10	121.97
1	A	250	LEU	C-N-CA	-5.48	112.10	121.97
1	A	229	GLU	N-CA-C	-5.48	100.84	109.50
1	B	74	LEU	CA-C-O	-5.48	114.35	120.54
1	B	172	ASN	CA-C-O	5.47	126.64	120.89
1	C	174	THR	CA-CB-CG2	5.47	119.81	110.50
1	A	182	ALA	N-CA-C	-5.46	99.16	110.80
1	B	169	CYS	CA-CB-SG	-5.46	101.85	114.40
1	C	137	TYR	CA-C-O	-5.45	112.34	118.55
1	A	203	THR	CA-C-O	-5.44	114.75	120.63
1	B	112	TRP	CA-C-N	-5.44	113.60	121.65
1	B	112	TRP	C-N-CA	-5.44	113.60	121.65
1	C	104	ALA	CA-C-O	5.44	126.02	119.61
1	C	137	TYR	N-CA-C	5.44	121.46	114.56
1	A	190	ASN	N-CA-C	5.43	120.56	113.88
1	A	151	SER	CA-CB-OG	5.43	121.96	111.10
1	B	68	ILE	CB-CG1-CD1	-5.43	102.40	113.80
1	A	196	ARG	O-C-N	5.43	129.80	122.96
1	C	68	ILE	CB-CA-C	-5.42	102.60	110.63
1	A	225	VAL	CA-C-N	-5.42	114.39	122.74
1	A	225	VAL	C-N-CA	-5.42	114.39	122.74
1	B	92	MET	CA-CB-CG	5.42	124.93	114.10
1	C	56	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	B	228	MET	CA-C-N	5.42	132.59	122.74
1	B	228	MET	C-N-CA	5.42	132.59	122.74
1	C	203	THR	CA-C-N	-5.42	113.40	120.44
1	C	203	THR	C-N-CA	-5.42	113.40	120.44
1	A	64	MET	CA-C-O	5.41	128.25	120.51
1	C	72	CYS	O-C-N	5.41	130.10	123.44
1	C	141	ASP	CA-C-O	-5.41	114.70	120.92
1	C	166	SER	O-C-N	5.41	129.26	122.23
1	B	138	ASP	N-CA-CB	5.40	119.33	110.90
1	A	110	TYR	CA-CB-CG	-5.40	104.18	113.90
1	C	247	THR	O-C-N	5.39	130.36	123.24
1	B	158	THR	N-CA-CB	5.39	121.07	111.69
1	C	117	TYR	CB-CA-C	5.39	119.03	110.19
1	C	206	ALA	N-CA-CB	-5.39	101.38	110.49
1	C	199	PHE	O-C-N	5.39	129.34	123.04
1	C	160	PRO	N-CA-C	-5.38	102.65	111.21
1	C	222	ALA	N-CA-CB	-5.38	102.60	111.69
1	A	259	ASN	CA-C-O	-5.37	115.34	120.92
1	B	128	SER	N-CA-CB	-5.36	101.68	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LEU	N-CA-CB	-5.36	102.09	110.44
1	A	199	PHE	CA-C-O	-5.35	114.25	120.62
1	A	133	MET	N-CA-CB	5.35	119.74	111.24
1	C	132	HIS	CA-CB-CG	-5.34	108.46	113.80
1	B	82	VAL	N-CA-CB	5.33	117.79	110.54
1	C	63	SER	CA-C-N	-5.33	111.35	121.54
1	C	63	SER	C-N-CA	-5.33	111.35	121.54
1	C	195	LYS	CA-CB-CG	5.33	124.76	114.10
1	C	217	ASN	O-C-N	5.33	129.25	122.33
1	B	144	PRO	CA-C-N	5.32	128.35	120.74
1	B	144	PRO	C-N-CA	5.32	128.35	120.74
1	C	90	LEU	N-CA-C	5.31	116.80	109.15
1	A	235	THR	CA-C-O	-5.30	115.19	121.66
1	B	254	ILE	CA-C-N	5.30	129.89	121.99
1	B	254	ILE	C-N-CA	5.30	129.89	121.99
1	A	62	SER	CA-CB-OG	5.30	121.70	111.10
1	B	246	TYR	CA-C-N	-5.30	115.07	123.23
1	B	246	TYR	C-N-CA	-5.30	115.07	123.23
1	A	210	GLY	N-CA-C	-5.30	106.83	115.46
1	B	77	GLU	CA-CB-CG	5.30	124.69	114.10
1	A	90	LEU	O-C-N	5.29	128.94	122.96
1	B	63	SER	CA-CB-OG	5.29	121.69	111.10
1	A	153	LEU	CA-C-O	-5.29	115.90	121.88
1	B	86	VAL	CA-C-O	-5.29	114.47	120.66
1	A	166	SER	N-CA-CB	-5.28	101.57	110.49
1	A	189	THR	CA-C-N	5.26	131.41	122.36
1	A	189	THR	C-N-CA	5.26	131.41	122.36
1	A	259	ASN	N-CA-C	5.26	117.24	107.99
1	C	74	LEU	CA-C-O	-5.25	114.88	120.92
1	B	223	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	126	THR	N-CA-CB	-5.24	102.33	110.98
1	C	61	ARG	CB-CA-C	5.23	117.67	110.34
1	B	119	TYR	N-CA-CB	-5.23	102.80	110.85
1	B	174	THR	O-C-N	5.23	131.32	121.70
1	C	218	ILE	CB-CG1-CD1	-5.23	102.82	113.80
1	A	166	SER	CB-CA-C	5.23	120.82	110.42
1	C	222	ALA	N-CA-C	5.23	116.38	108.07
1	C	73	GLU	CB-CA-C	5.22	120.64	110.30
1	C	152	ASN	CB-CG-OD1	5.22	131.24	120.80
1	B	222	ALA	N-CA-CB	-5.22	102.80	111.57
1	C	198	PRO	O-C-N	5.22	129.51	123.14
1	C	65	ASP	CA-C-O	-5.22	113.17	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	LEU	O-C-N	5.22	128.32	122.22
1	C	235	THR	CA-CB-CG2	5.22	119.37	110.50
1	C	185	ILE	CB-CA-C	5.20	120.93	111.30
1	A	242	LEU	O-C-N	5.20	129.15	123.27
1	C	181	ARG	CA-C-O	-5.20	114.04	122.20
1	A	93	PRO	O-C-N	5.19	127.78	122.18
1	A	105	GLN	CA-C-O	-5.19	113.21	119.49
1	A	105	GLN	OE1-CD-NE2	5.18	127.78	122.60
1	C	163	GLU	CG-CD-OE2	-5.18	106.49	118.40
1	B	78	LEU	O-C-N	5.18	129.05	123.10
1	B	116	ARG	N-CA-C	5.18	117.80	108.48
1	B	197	TYR	CA-C-N	5.17	125.62	120.14
1	B	197	TYR	C-N-CA	5.17	125.62	120.14
1	C	239	THR	CA-CB-OG1	-5.17	101.85	109.60
1	C	249	ARG	CB-CA-C	-5.17	101.59	110.22
1	B	205	TYR	O-C-N	5.17	127.61	122.08
1	C	173	ASN	N-CA-C	-5.17	99.80	110.80
1	B	248	ILE	N-CA-CB	-5.16	101.46	110.49
1	C	56	ARG	CA-C-N	5.16	125.69	120.38
1	C	56	ARG	C-N-CA	5.16	125.69	120.38
1	C	135	PHE	CA-C-O	-5.16	115.32	121.56
1	C	132	HIS	CA-C-O	-5.16	114.41	120.60
1	A	229	GLU	CB-CA-C	5.15	120.15	109.38
1	C	158	THR	CA-C-O	-5.15	115.77	121.33
1	B	167	GLY	CA-C-N	-5.13	112.36	120.63
1	B	167	GLY	C-N-CA	-5.13	112.36	120.63
1	A	111	ALA	N-CA-CB	5.13	120.36	111.39
1	C	181	ARG	CA-C-N	-5.13	113.78	123.27
1	C	181	ARG	C-N-CA	-5.13	113.78	123.27
1	C	67	THR	N-CA-CB	5.12	119.75	110.83
1	C	247	THR	N-CA-CB	5.12	118.55	110.71
1	C	186	ALA	N-CA-CB	-5.12	101.97	111.13
1	A	239	THR	N-CA-CB	-5.12	104.10	110.90
1	A	147	VAL	O-C-N	5.11	127.48	121.96
1	C	41	GLY	O-C-N	5.11	127.75	122.54
1	C	257	ALA	CA-C-O	-5.11	113.21	120.51
1	B	247	THR	O-C-N	5.11	131.10	122.93
1	C	102	GLY	CA-C-O	-5.10	114.69	120.30
1	A	135	PHE	CA-C-O	-5.10	115.43	121.66
1	A	209	VAL	CA-C-O	5.10	126.20	120.03
1	A	201	THR	CA-CB-OG1	-5.10	101.95	109.60
1	C	255	ALA	O-C-N	5.10	128.87	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	HIS	O-C-N	5.09	129.57	123.36
1	B	95	THR	N-CA-CB	-5.08	102.66	110.44
1	C	222	ALA	O-C-N	-5.08	118.84	123.41
1	C	55	LEU	O-C-N	5.08	129.06	122.81
1	B	96	VAL	O-C-N	5.08	128.54	121.84
1	B	83	THR	N-CA-C	5.07	116.99	109.69
1	A	176	CYS	CA-C-N	5.07	126.17	119.84
1	A	176	CYS	C-N-CA	5.07	126.17	119.84
1	C	146	SER	O-C-N	5.07	129.47	123.24
1	C	179	THR	CB-CA-C	5.06	119.38	110.37
1	A	153	LEU	CB-CA-C	5.06	123.00	111.71
1	C	128	SER	CA-C-O	-5.05	115.32	121.28
1	B	249	ARG	O-C-N	5.05	128.90	122.84
1	C	53	VAL	CB-CA-C	-5.05	104.58	111.15
1	C	160	PRO	CB-CA-C	5.05	117.70	111.23
1	B	169	CYS	CA-C-O	-5.05	114.17	119.97
1	B	235	THR	CA-C-O	-5.04	114.78	120.43
1	C	218	ILE	CB-CA-C	-5.04	103.03	111.29
1	B	183	ILE	CA-C-O	-5.03	116.37	121.70
1	B	158	THR	CB-CA-C	-5.03	99.01	110.07
1	B	177	PRO	N-CA-C	-5.03	106.54	113.53
1	A	71	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	237	VAL	CA-C-O	5.02	125.90	120.53
1	B	161	VAL	CA-C-O	-5.02	114.50	120.78
1	A	193	SER	N-CA-C	5.02	116.44	111.07
1	B	92	MET	O-C-N	5.02	126.38	121.66
1	C	76	THR	N-CA-C	5.01	116.43	108.96
1	C	230	GLY	CA-C-N	5.00	131.22	121.41
1	C	230	GLY	C-N-CA	5.00	131.22	121.41
1	A	120	LEU	CB-CA-C	5.00	116.17	109.42
1	B	155	GLY	N-CA-C	5.00	122.48	115.43

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	249	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	241	ARG	Sidechain
1	B	249	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	101	ARG	Sidechain
1	C	181	ARG	Sidechain
1	C	196	ARG	Sidechain
1	C	223	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1506	0	1505	216	0
1	B	1506	0	1505	186	0
1	C	1674	0	1691	190	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	1	0
3	B	10	0	0	0	0
3	C	9	0	0	0	0
All	All	4723	0	4701	559	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 60.

All (559) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASN:ND2	1:C:214:ASN:H	1.42	1.14
1:C:145:VAL:H	1:C:149:GLN:NE2	1.46	1.12
1:C:161:VAL:HG22	1:C:239:THR:CG2	1.82	1.09
1:C:161:VAL:HG22	1:C:239:THR:HG21	1.09	1.08
1:C:187:LEU:HD22	1:C:188:ASP:H	1.19	1.05
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.21	1.04
1:A:168:LEU:O	1:A:169:CYS:HB2	1.57	1.01
1:A:201:THR:HG22	1:A:260:LEU:OXT	1.61	0.99
1:C:145:VAL:H	1:C:149:GLN:HE22	1.07	0.98
1:C:131:ILE:HG13	1:C:228:MET:HE2	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:LYS:HB3	1:C:195:LYS:HZ3	1.26	0.95
1:A:105:GLN:HA	1:A:199:PHE:CE1	2.01	0.95
1:C:54:LYS:H	1:C:172:ASN:HD21	0.99	0.94
1:A:78:LEU:HB2	1:A:228:MET:HE2	1.50	0.94
1:C:212:ASN:HD22	1:C:214:ASN:N	1.66	0.93
1:C:119:TYR:OH	1:C:239:THR:HG22	1.68	0.93
1:C:125:THR:HG22	1:C:162:TRP:CE3	2.04	0.91
1:C:161:VAL:CG2	1:C:239:THR:HG21	2.01	0.90
1:C:139:MET:H	1:C:217:ASN:HD21	0.94	0.89
1:C:187:LEU:HD22	1:C:188:ASP:N	1.87	0.89
1:B:248:ILE:HD12	1:B:250:LEU:HD13	1.52	0.89
1:A:251:ILE:HG23	1:A:252:GLU:HG2	1.52	0.89
1:A:178:ASP:HB2	1:A:180:SER:OG	1.72	0.89
1:A:205:TYR:CE2	1:A:209:VAL:HG21	2.08	0.88
1:C:187:LEU:CD2	1:C:188:ASP:H	1.86	0.88
1:A:137:TYR:CE1	1:B:252:GLU:HG3	2.10	0.87
1:B:150:LEU:HA	1:B:153:LEU:HD12	1.53	0.87
1:C:78:LEU:HG	1:C:228:MET:HE3	1.57	0.87
1:A:148:ASN:O	1:A:151:SER:HB3	1.74	0.87
1:A:133:MET:HE1	1:A:242:LEU:HD11	1.55	0.86
1:C:115:ILE:HG23	1:C:187:LEU:HB2	1.55	0.86
1:B:82:VAL:HG22	1:B:234:LYS:HA	1.57	0.86
1:C:195:LYS:HB3	1:C:195:LYS:NZ	1.90	0.86
1:C:90:LEU:HB2	1:C:95:THR:HG21	1.57	0.85
1:C:139:MET:H	1:C:217:ASN:ND2	1.74	0.85
1:C:129:GLY:O	1:C:161:VAL:HB	1.77	0.84
1:C:212:ASN:ND2	1:C:214:ASN:N	2.25	0.84
1:C:129:GLY:HA2	1:C:230:GLY:HA3	1.58	0.83
1:A:168:LEU:O	1:A:169:CYS:CB	2.20	0.83
1:B:103:VAL:O	1:B:106:ASN:ND2	2.11	0.82
1:B:78:LEU:HB2	1:B:228:MET:HE2	1.61	0.82
1:B:140:ALA:O	1:C:260:LEU:HD12	1.79	0.81
1:C:146:SER:H	1:C:149:GLN:HE21	1.28	0.81
1:A:136:GLN:HE21	1:A:223:ARG:HH11	1.25	0.81
1:B:78:LEU:HD22	1:B:228:MET:HE2	1.61	0.81
1:C:212:ASN:HD22	1:C:214:ASN:H	0.81	0.80
1:B:124:PRO:HD2	1:B:127:THR:OG1	1.82	0.80
1:A:165:GLN:HA	1:A:165:GLN:NE2	1.97	0.79
1:A:92:MET:O	1:A:96:VAL:HG23	1.83	0.79
1:B:131:ILE:O	1:B:158:THR:HG23	1.80	0.79
1:A:105:GLN:HA	1:A:199:PHE:HE1	1.42	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HG	1:B:246:TYR:CE2	2.17	0.78
1:B:139:MET:HE2	1:B:223:ARG:HB3	1.66	0.78
1:B:212:ASN:ND2	1:B:214:ASN:HB2	1.98	0.78
1:B:151:SER:HA	1:B:156:TYR:CD2	2.18	0.78
1:A:144:PRO:HA	1:B:258:LEU:HD11	1.66	0.78
1:B:120:LEU:HD11	1:B:171:VAL:HG21	1.64	0.78
1:C:145:VAL:N	1:C:149:GLN:NE2	2.29	0.78
1:C:119:TYR:OH	1:C:239:THR:CG2	2.32	0.77
1:A:143:LEU:N	1:A:143:LEU:HD12	2.00	0.77
1:B:214:ASN:HD21	1:C:200:LYS:NZ	1.82	0.77
1:C:163:GLU:HG3	1:C:164:GLY:N	1.99	0.77
1:A:105:GLN:CA	1:A:199:PHE:HE1	1.98	0.77
1:C:139:MET:N	1:C:217:ASN:HD21	1.77	0.77
1:A:123:CYS:HB3	1:A:124:PRO:HD2	1.67	0.77
1:C:49:GLN:NE2	1:C:165:GLN:HG2	2.00	0.76
1:B:117:TYR:HB3	1:B:242:LEU:HD21	1.65	0.76
1:A:181:ARG:HG2	1:A:181:ARG:O	1.84	0.76
1:A:90:LEU:HD13	1:A:92:MET:HE1	1.68	0.75
1:A:136:GLN:HE21	1:A:223:ARG:NH1	1.86	0.74
1:A:161:VAL:HB	1:A:239:THR:OG1	1.86	0.74
1:A:200:LYS:HE3	1:A:260:LEU:C	2.11	0.74
1:C:169:CYS:O	1:C:173:ASN:N	2.20	0.73
1:A:109:LYS:HE3	1:A:252:GLU:OE1	1.88	0.73
1:A:129:GLY:HA2	1:A:230:GLY:CA	2.18	0.73
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.24	0.73
1:C:150:LEU:HD13	1:C:150:LEU:O	1.89	0.73
1:C:60:LEU:HD12	1:C:69:LEU:HD13	1.70	0.72
1:A:79:ALA:HA	1:A:237:VAL:O	1.89	0.72
1:C:101:ARG:HG2	1:C:102:GLY:N	2.03	0.72
1:A:201:THR:HG22	1:A:260:LEU:C	2.14	0.72
1:C:54:LYS:H	1:C:172:ASN:ND2	1.81	0.72
1:C:66:VAL:HG12	1:C:251:ILE:HD11	1.70	0.71
1:A:129:GLY:HA2	1:A:230:GLY:HA2	1.72	0.71
1:A:148:ASN:C	1:A:148:ASN:HD22	1.98	0.71
1:B:146:SER:OG	1:B:148:ASN:HB2	1.89	0.71
1:A:78:LEU:CB	1:A:228:MET:HE2	2.18	0.71
1:C:125:THR:HG22	1:C:162:TRP:CD2	2.24	0.70
1:C:239:THR:HG22	1:C:240:GLY:N	2.06	0.70
1:A:105:GLN:HA	1:A:199:PHE:CD1	2.26	0.70
1:B:110:TYR:HB2	1:B:248:ILE:HD11	1.74	0.70
1:A:258:LEU:HD11	1:C:144:PRO:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:THR:HG23	1:C:83:THR:O	1.92	0.69
1:B:139:MET:H	1:B:217:ASN:HD21	1.40	0.69
1:C:205:TYR:O	1:C:209:VAL:HG23	1.93	0.69
1:B:118:THR:O	1:B:242:LEU:HD23	1.93	0.69
1:B:138:ASP:HA	1:B:217:ASN:HD21	1.58	0.69
1:C:116:ARG:HH21	1:C:184:THR:HG21	1.57	0.69
1:B:174:THR:HG22	1:B:175:LYS:H	1.58	0.68
1:A:155:GLY:HA3	1:A:185:ILE:HG13	1.74	0.68
1:C:163:GLU:HG3	1:C:164:GLY:H	1.58	0.68
1:C:234:LYS:HE3	1:C:234:LYS:H	1.58	0.68
1:A:155:GLY:O	1:A:156:TYR:C	2.36	0.68
1:B:94:PHE:CE1	1:B:101:ARG:HD2	2.29	0.68
1:B:125:THR:HG22	1:B:125:THR:O	1.95	0.67
1:C:195:LYS:NZ	1:C:195:LYS:CB	2.57	0.67
1:C:118:THR:HB	1:C:184:THR:OG1	1.94	0.67
1:A:218:ILE:HD11	1:B:218:ILE:HD12	1.77	0.67
1:B:175:LYS:O	1:B:177:PRO:HD3	1.94	0.67
1:B:218:ILE:HG12	1:B:219:LEU:CD1	2.25	0.67
1:A:94:PHE:HB2	1:A:199:PHE:HE2	1.59	0.66
1:A:116:ARG:NE	1:A:170:PHE:HD1	1.92	0.66
1:A:108:SER:HB2	1:A:252:GLU:O	1.96	0.66
1:B:195:LYS:HE3	1:C:195:LYS:HZ1	1.61	0.66
1:C:69:LEU:HD12	1:C:70:SER:N	2.10	0.66
1:B:73:GLU:OE1	1:B:99:TRP:HB3	1.96	0.66
1:B:137:TYR:CD1	1:C:252:GLU:HG3	2.31	0.66
1:C:92:MET:O	1:C:96:VAL:HG23	1.94	0.66
1:A:81:THR:O	1:A:231:GLY:HA2	1.95	0.66
1:B:166:SER:O	1:B:176:CYS:SG	2.54	0.66
1:A:160:PRO:HG2	1:A:163:GLU:HB2	1.78	0.65
1:A:110:TYR:CD1	1:A:248:ILE:HD11	2.31	0.65
1:B:119:TYR:O	1:B:120:LEU:HD23	1.96	0.65
1:A:71:HIS:HB3	1:A:246:TYR:CZ	2.31	0.65
1:B:71:HIS:HD2	1:B:99:TRP:CZ3	2.13	0.65
1:A:139:MET:HE2	1:A:220:VAL:HG21	1.78	0.65
1:B:136:GLN:HE22	1:B:143:LEU:HD23	1.61	0.65
1:A:66:VAL:HG21	1:A:249:ARG:HH21	1.61	0.65
1:A:139:MET:HE1	1:A:223:ARG:HB3	1.78	0.65
1:B:150:LEU:HA	1:B:153:LEU:CD1	2.25	0.65
1:A:129:GLY:C	1:A:161:VAL:HG13	2.22	0.65
1:C:139:MET:HA	1:C:139:MET:HE2	1.78	0.65
1:B:115:ILE:HG13	1:B:246:TYR:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PRO:O	1:C:127:THR:OG1	2.14	0.64
1:B:189:THR:HA	1:B:192:VAL:HG23	1.79	0.64
1:A:174:THR:HG22	1:A:176:CYS:SG	2.38	0.64
1:B:138:ASP:O	1:B:141:ASP:HB2	1.97	0.64
1:A:215:ILE:O	1:A:219:LEU:HD12	1.99	0.63
1:B:106:ASN:ND2	1:B:106:ASN:H	1.94	0.63
1:B:135:PHE:HE2	1:B:187:LEU:HA	1.64	0.63
1:A:133:MET:HE1	1:A:242:LEU:CD1	2.28	0.63
1:B:78:LEU:HB2	1:B:228:MET:CE	2.29	0.63
1:C:78:LEU:HG	1:C:228:MET:CE	2.29	0.63
1:B:248:ILE:HD13	1:B:249:ARG:H	1.63	0.62
1:C:169:CYS:O	1:C:173:ASN:HA	1.99	0.62
1:A:100:LEU:HG	1:A:246:TYR:CE2	2.34	0.62
1:A:179:THR:O	1:A:180:SER:C	2.43	0.62
1:C:144:PRO:CG	1:C:150:LEU:HD23	2.29	0.62
1:B:81:THR:O	1:B:231:GLY:HA3	2.00	0.62
1:C:155:GLY:HA3	1:C:185:ILE:HG13	1.82	0.62
1:C:169:CYS:O	1:C:173:ASN:CA	2.48	0.62
1:A:116:ARG:NE	1:A:170:PHE:CD1	2.68	0.62
1:B:78:LEU:N	1:B:78:LEU:HD12	2.15	0.61
1:B:79:ALA:HB1	1:B:237:VAL:O	2.00	0.61
1:A:144:PRO:CA	1:B:258:LEU:HD11	2.29	0.61
1:A:71:HIS:CG	1:A:72:CYS:H	2.18	0.61
1:A:109:LYS:CE	1:A:252:GLU:OE1	2.49	0.61
1:A:195:LYS:C	1:A:196:ARG:HD2	2.26	0.61
1:C:66:VAL:CG1	1:C:251:ILE:HD11	2.31	0.61
1:A:260:LEU:N	1:A:260:LEU:HD23	2.16	0.60
1:B:71:HIS:ND1	1:B:72:CYS:N	2.49	0.60
1:C:74:LEU:HD12	1:C:75:SER:N	2.16	0.60
1:B:139:MET:CE	1:B:223:ARG:HB3	2.31	0.60
1:C:49:GLN:CD	1:C:165:GLN:HG2	2.26	0.60
1:A:138:ASP:C	1:A:140:ALA:N	2.57	0.60
1:C:146:SER:H	1:C:149:GLN:NE2	1.97	0.60
1:C:192:VAL:HG13	1:C:197:TYR:OH	2.01	0.60
1:A:138:ASP:O	1:A:140:ALA:N	2.35	0.60
1:B:156:TYR:C	1:B:157:VAL:HG23	2.26	0.60
1:B:199:PHE:C	1:B:199:PHE:CD2	2.80	0.60
1:B:214:ASN:HD21	1:C:200:LYS:HZ2	1.46	0.60
1:A:137:TYR:CE2	1:B:252:GLU:OE1	2.55	0.60
1:B:212:ASN:HD21	1:B:214:ASN:HB2	1.67	0.60
1:C:145:VAL:N	1:C:149:GLN:HE22	1.88	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:C	1:A:260:LEU:HD23	2.27	0.60
1:B:199:PHE:C	1:B:199:PHE:HD2	2.10	0.60
1:A:135:PHE:HE1	1:A:185:ILE:HG12	1.67	0.59
1:B:94:PHE:O	1:B:101:ARG:NH1	2.35	0.59
1:C:187:LEU:CD2	1:C:188:ASP:N	2.56	0.59
1:C:256:ALA:O	1:C:257:ALA:C	2.43	0.59
1:C:115:ILE:CG2	1:C:187:LEU:HB2	2.27	0.59
1:B:74:LEU:HD12	1:B:74:LEU:H	1.67	0.59
1:B:195:LYS:HE3	1:C:195:LYS:CE	2.32	0.59
1:A:135:PHE:CE1	1:A:185:ILE:HG12	2.37	0.59
1:C:131:ILE:HD12	1:C:228:MET:HE1	1.85	0.59
1:A:196:ARG:HD2	1:A:196:ARG:N	2.18	0.59
1:B:218:ILE:HG12	1:B:219:LEU:HD12	1.85	0.59
1:A:129:GLY:HA2	1:A:230:GLY:HA3	1.85	0.59
1:B:158:THR:HG22	1:B:159:GLY:H	1.66	0.59
1:C:125:THR:CG2	1:C:162:TRP:CE3	2.81	0.59
1:C:133:MET:HA	1:C:225:VAL:O	2.03	0.59
1:A:138:ASP:C	1:A:140:ALA:H	2.09	0.58
1:A:248:ILE:HG23	1:A:250:LEU:HD13	1.85	0.58
1:B:139:MET:H	1:B:217:ASN:ND2	2.01	0.58
1:B:71:HIS:HB3	1:B:246:TYR:CZ	2.38	0.58
1:A:137:TYR:CD1	1:B:252:GLU:HG3	2.38	0.58
1:A:204:ASP:O	1:A:205:TYR:C	2.46	0.58
1:B:136:GLN:NE2	1:B:143:LEU:HD23	2.19	0.58
1:C:131:ILE:HG13	1:C:228:MET:CE	2.27	0.58
1:A:123:CYS:CB	1:A:124:PRO:CD	2.79	0.58
1:A:212:ASN:OD1	1:A:214:ASN:HB2	2.02	0.58
1:A:71:HIS:HD2	1:A:99:TRP:CE3	2.23	0.57
1:C:52:MET:SD	1:C:52:MET:N	2.76	0.57
1:A:200:LYS:CE	1:A:260:LEU:OXT	2.51	0.57
1:B:155:GLY:O	1:B:157:VAL:HG23	2.04	0.57
1:B:195:LYS:HE3	1:C:195:LYS:NZ	2.19	0.57
1:C:80:VAL:HG13	1:C:81:THR:N	2.19	0.57
1:A:92:MET:HE2	1:A:220:VAL:CG1	2.34	0.57
1:B:248:ILE:HD13	1:B:249:ARG:N	2.20	0.57
1:C:114:ALA:O	1:C:246:TYR:HA	2.04	0.57
1:A:123:CYS:CB	1:A:124:PRO:HD2	2.35	0.57
1:A:141:ASP:HB3	1:B:258:LEU:O	2.04	0.57
1:B:158:THR:HG22	1:B:159:GLY:N	2.20	0.57
1:C:139:MET:HE1	1:C:223:ARG:HG2	1.87	0.57
1:A:251:ILE:CG2	1:A:252:GLU:HG2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE1	1:B:99:TRP:N	2.30	0.57
1:A:123:CYS:HB3	1:A:124:PRO:CD	2.34	0.57
1:A:142:THR:HB	1:B:258:LEU:HD22	1.87	0.57
1:B:82:VAL:HG21	1:B:234:LYS:HG3	1.86	0.57
1:B:139:MET:N	1:B:217:ASN:HD21	2.03	0.57
1:B:145:VAL:N	1:B:149:GLN:OE1	2.33	0.57
1:B:246:TYR:CD1	1:B:246:TYR:N	2.72	0.57
1:B:135:PHE:CE2	1:B:187:LEU:HA	2.40	0.56
1:A:248:ILE:HG23	1:A:250:LEU:CD1	2.35	0.56
1:B:216:GLY:O	1:B:219:LEU:N	2.37	0.56
1:A:160:PRO:O	1:A:162:TRP:N	2.39	0.56
1:A:200:LYS:HE3	1:A:260:LEU:OXT	2.05	0.56
1:C:144:PRO:HG3	1:C:150:LEU:CD2	2.35	0.56
1:A:137:TYR:CZ	1:B:252:GLU:OE1	2.58	0.56
1:B:138:ASP:HA	1:B:217:ASN:ND2	2.21	0.56
1:C:135:PHE:O	1:C:153:LEU:HG	2.05	0.56
1:A:116:ARG:HG3	1:A:186:ALA:HB2	1.86	0.56
1:A:212:ASN:OD1	1:A:212:ASN:C	2.48	0.56
1:A:143:LEU:N	1:A:143:LEU:CD1	2.68	0.56
1:B:189:THR:HA	1:B:192:VAL:CG2	2.35	0.56
1:B:251:ILE:HG23	1:B:252:GLU:OE2	2.06	0.56
1:B:70:SER:OG	1:B:247:THR:HG23	2.06	0.56
1:B:82:VAL:CG2	1:B:234:LYS:HA	2.33	0.56
1:A:71:HIS:CG	1:A:72:CYS:N	2.74	0.55
1:A:119:TYR:O	1:A:120:LEU:HD23	2.06	0.55
1:C:218:ILE:O	1:C:219:LEU:C	2.49	0.55
1:A:251:ILE:HG23	1:A:252:GLU:CG	2.31	0.55
1:A:155:GLY:HA3	1:A:185:ILE:CG1	2.36	0.55
1:C:234:LYS:H	1:C:234:LYS:CE	2.19	0.55
1:A:199:PHE:O	1:A:200:LYS:HD2	2.05	0.55
1:A:223:ARG:O	1:A:223:ARG:HG2	2.07	0.55
1:B:124:PRO:HD2	1:B:127:THR:HG1	1.69	0.55
1:B:169:CYS:HA	1:B:172:ASN:HB2	1.89	0.55
1:C:90:LEU:HD11	1:C:205:TYR:CE1	2.41	0.55
1:C:234:LYS:H	1:C:234:LYS:CD	2.19	0.55
1:A:91:VAL:HG13	1:A:222:ALA:O	2.05	0.55
1:A:92:MET:HE2	1:A:220:VAL:HG12	1.89	0.55
1:A:200:LYS:HZ2	1:C:140:ALA:HB3	1.70	0.55
1:B:106:ASN:ND2	1:B:106:ASN:N	2.54	0.55
1:B:213:ALA:O	1:B:214:ASN:C	2.50	0.54
1:B:150:LEU:HD12	1:B:150:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:CYS:HB2	1:A:124:PRO:O	2.07	0.54
1:A:81:THR:O	1:A:231:GLY:CA	2.56	0.54
1:B:195:LYS:HE3	1:C:195:LYS:HE3	1.89	0.54
1:C:218:ILE:O	1:C:220:VAL:N	2.41	0.54
1:B:123:CYS:HB2	1:B:124:PRO:CD	2.38	0.54
1:C:60:LEU:CD1	1:C:69:LEU:HD13	2.36	0.54
1:C:146:SER:N	1:C:149:GLN:NE2	2.56	0.53
1:B:137:TYR:CE1	1:C:252:GLU:HG3	2.43	0.53
1:B:131:ILE:O	1:B:158:THR:CG2	2.52	0.53
1:C:144:PRO:HG3	1:C:150:LEU:HD23	1.89	0.53
1:C:167:GLY:O	1:C:168:LEU:C	2.51	0.53
1:C:178:ASP:OD1	1:C:180:SER:HB2	2.08	0.53
1:A:139:MET:N	1:A:217:ASN:OD1	2.40	0.53
1:C:205:TYR:CE1	1:C:209:VAL:HG21	2.43	0.53
1:C:90:LEU:O	1:C:95:THR:CG2	2.57	0.53
1:A:139:MET:HG3	1:A:205:TYR:OH	2.08	0.53
1:A:218:ILE:CD1	1:B:218:ILE:HD12	2.38	0.53
1:C:131:ILE:HG12	1:C:132:HIS:N	2.24	0.53
1:A:212:ASN:OD1	1:A:213:ALA:N	2.42	0.52
1:A:250:LEU:CD1	1:A:250:LEU:N	2.72	0.52
1:A:63:SER:HA	1:A:66:VAL:O	2.09	0.52
1:A:71:HIS:ND1	1:A:72:CYS:N	2.51	0.52
1:A:147:VAL:HG12	1:A:148:ASN:N	2.24	0.52
1:A:195:LYS:HB3	1:A:196:ARG:HD2	1.92	0.52
1:B:248:ILE:HG23	1:B:250:LEU:HD22	1.91	0.52
1:A:92:MET:CE	1:A:220:VAL:HG11	2.39	0.52
1:B:103:VAL:HG12	1:B:107:TRP:HZ3	1.74	0.52
1:B:161:VAL:HB	1:B:239:THR:HB	1.89	0.52
1:C:99:TRP:O	1:C:100:LEU:C	2.51	0.52
1:A:94:PHE:HB2	1:A:199:PHE:CE2	2.43	0.52
1:C:233:SER:HA	1:C:234:LYS:HE3	1.90	0.52
1:C:101:ARG:CG	1:C:102:GLY:N	2.69	0.52
1:C:107:TRP:CE3	1:C:250:LEU:HD23	2.45	0.52
1:B:73:GLU:OE1	1:B:99:TRP:CB	2.57	0.52
1:A:124:PRO:HB2	1:A:126:THR:HG22	1.90	0.52
1:A:200:LYS:CG	1:A:219:LEU:HD23	2.39	0.52
1:B:80:VAL:HG22	1:B:239:THR:CG2	2.39	0.52
1:A:134:GLY:HA3	1:A:153:LEU:HB3	1.91	0.52
1:B:175:LYS:O	1:B:177:PRO:CD	2.58	0.51
1:C:73:GLU:OE1	1:C:99:TRP:N	2.32	0.51
1:C:101:ARG:HG2	1:C:102:GLY:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:HB2	1:A:197:TYR:CZ	2.45	0.51
1:A:132:HIS:CE1	1:A:147:VAL:CG2	2.93	0.51
1:A:138:ASP:HB3	1:A:141:ASP:CG	2.35	0.51
1:A:201:THR:CG2	1:A:260:LEU:HA	2.41	0.51
1:C:84:ILE:HG23	1:C:85:VAL:N	2.24	0.51
1:C:90:LEU:CB	1:C:95:THR:HG21	2.35	0.51
1:A:165:GLN:O	1:A:167:GLY:N	2.38	0.51
1:A:200:LYS:HE3	1:A:260:LEU:O	2.10	0.51
1:C:133:MET:HG3	1:C:185:ILE:HG21	1.92	0.51
1:B:129:GLY:HA2	1:B:230:GLY:CA	2.40	0.51
1:A:201:THR:HG22	1:A:260:LEU:CA	2.41	0.51
1:A:218:ILE:HG22	1:A:218:ILE:O	2.09	0.51
1:B:138:ASP:CA	1:B:217:ASN:HD21	2.23	0.51
1:A:124:PRO:C	1:A:126:THR:H	2.18	0.51
1:C:116:ARG:NH2	1:C:184:THR:HG21	2.24	0.51
1:C:168:LEU:O	1:C:169:CYS:C	2.54	0.51
1:A:142:THR:HG22	1:A:143:LEU:O	2.11	0.51
1:B:118:THR:HG23	1:B:184:THR:HB	1.93	0.51
1:B:131:ILE:O	1:B:158:THR:HA	2.11	0.51
1:B:185:ILE:HG23	1:B:185:ILE:O	2.11	0.51
1:C:80:VAL:CG1	1:C:81:THR:N	2.70	0.51
1:C:131:ILE:CG1	1:C:228:MET:HE2	2.30	0.51
1:B:205:TYR:O	1:B:208:ALA:HB3	2.11	0.51
1:A:139:MET:N	1:A:139:MET:SD	2.80	0.50
1:B:106:ASN:H	1:B:106:ASN:HD22	1.57	0.50
1:C:119:TYR:CD1	1:C:119:TYR:C	2.88	0.50
1:B:62:SER:HA	1:B:68:ILE:CD1	2.41	0.50
1:B:138:ASP:OD2	1:B:140:ALA:HB3	2.11	0.50
1:B:214:ASN:HD22	1:C:219:LEU:HD11	1.76	0.50
1:A:129:GLY:CA	1:A:230:GLY:HA3	2.41	0.50
1:A:94:PHE:O	1:A:101:ARG:NH1	2.41	0.50
1:C:69:LEU:HD12	1:C:70:SER:H	1.77	0.50
1:C:131:ILE:O	1:C:158:THR:HA	2.11	0.50
1:A:124:PRO:HD2	1:A:127:THR:OG1	2.11	0.50
1:A:258:LEU:HD11	1:C:144:PRO:CA	2.40	0.50
1:B:72:CYS:HA	1:B:244:ALA:O	2.12	0.50
1:A:107:TRP:CZ3	1:A:250:LEU:HD23	2.47	0.49
1:B:110:TYR:C	1:B:110:TYR:CD1	2.90	0.49
1:C:113:VAL:HB	1:C:247:THR:O	2.12	0.49
1:C:116:ARG:NE	1:C:170:PHE:CE2	2.80	0.49
1:C:169:CYS:HB3	1:C:174:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:MET:HA	1:A:225:VAL:O	2.13	0.49
1:B:212:ASN:O	1:B:213:ALA:C	2.55	0.49
1:A:116:ARG:HE	1:A:170:PHE:HD1	1.59	0.49
1:A:200:LYS:HE2	1:A:260:LEU:OXT	2.12	0.49
1:C:201:THR:HG23	1:C:260:LEU:HA	1.94	0.49
1:C:146:SER:N	1:C:149:GLN:HE21	2.03	0.49
1:A:138:ASP:O	1:A:139:MET:C	2.56	0.49
1:B:105:GLN:HA	1:B:199:PHE:CE1	2.48	0.49
1:C:196:ARG:NH1	1:C:249:ARG:HH21	2.10	0.49
1:B:78:LEU:HD12	1:B:78:LEU:H	1.77	0.49
1:A:92:MET:HE1	1:A:220:VAL:HG11	1.95	0.49
1:A:200:LYS:HZ2	1:C:140:ALA:CB	2.26	0.49
1:A:238:ASN:N	1:A:238:ASN:HD22	2.11	0.49
1:B:74:LEU:HD12	1:B:74:LEU:N	2.28	0.49
1:B:78:LEU:CD2	1:B:228:MET:HE2	2.38	0.49
1:B:69:LEU:HB3	1:B:248:ILE:CG2	2.43	0.49
1:C:76:THR:CG2	1:C:77:GLU:N	2.75	0.49
1:A:199:PHE:HD2	1:A:200:LYS:N	2.10	0.49
1:A:249:ARG:NH2	1:C:191:GLU:OE1	2.45	0.49
1:A:124:PRO:HG2	1:A:126:THR:HG22	1.95	0.48
1:B:124:PRO:C	1:B:126:THR:H	2.22	0.48
1:B:156:TYR:C	1:B:157:VAL:CG2	2.86	0.48
1:C:194:GLU:HB2	1:C:197:TYR:CE2	2.48	0.48
1:C:206:ALA:O	1:C:207:THR:C	2.56	0.48
1:C:179:THR:O	1:C:180:SER:C	2.56	0.48
1:A:177:PRO:O	1:A:178:ASP:HB3	2.14	0.48
1:B:188:ASP:OD1	1:B:191:GLU:HB2	2.13	0.48
1:A:252:GLU:OE2	1:C:137:TYR:CZ	2.67	0.48
1:B:69:LEU:HB3	1:B:248:ILE:HG22	1.95	0.48
1:B:167:GLY:C	1:B:169:CYS:N	2.70	0.48
1:C:150:LEU:HD22	1:C:153:LEU:HD22	1.95	0.48
1:A:155:GLY:HA3	1:A:185:ILE:CD1	2.44	0.47
1:B:72:CYS:O	1:B:73:GLU:HB2	2.13	0.47
1:B:169:CYS:HB2	1:B:174:THR:HB	1.96	0.47
1:C:56:ARG:HG2	1:C:57:PRO:HD2	1.95	0.47
1:C:151:SER:HA	1:C:156:TYR:CD2	2.49	0.47
1:B:70:SER:HA	1:B:246:TYR:O	2.14	0.47
1:A:71:HIS:HB3	1:A:246:TYR:OH	2.15	0.47
1:A:215:ILE:HG22	1:A:219:LEU:HD11	1.95	0.47
1:B:62:SER:HA	1:B:68:ILE:HD12	1.95	0.47
1:B:212:ASN:HD22	1:B:214:ASN:HB2	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HG3	1:A:219:LEU:HD23	1.95	0.47
1:B:101:ARG:O	1:B:105:GLN:HB2	2.13	0.47
1:C:116:ARG:HE	1:C:184:THR:HG21	1.79	0.47
1:A:179:THR:C	1:A:181:ARG:N	2.70	0.47
1:C:155:GLY:O	1:C:156:TYR:C	2.55	0.47
1:A:82:VAL:HA	1:A:231:GLY:HA3	1.97	0.47
1:A:92:MET:CE	1:A:220:VAL:CG1	2.93	0.47
1:A:138:ASP:HB3	1:A:141:ASP:OD2	2.15	0.47
1:B:93:PRO:CB	1:B:100:LEU:HD13	2.45	0.47
1:C:84:ILE:O	1:C:85:VAL:HG23	2.14	0.47
1:C:227:ALA:C	1:C:228:MET:HG2	2.38	0.47
1:B:71:HIS:CD2	1:B:99:TRP:CZ3	3.00	0.47
1:C:116:ARG:CZ	1:C:170:PHE:CE2	2.97	0.47
1:C:116:ARG:HD3	1:C:170:PHE:CD2	2.50	0.47
1:A:129:GLY:O	1:A:160:PRO:HA	2.15	0.47
1:A:181:ARG:O	1:A:182:ALA:HB2	2.14	0.47
1:A:105:GLN:CA	1:A:199:PHE:CE1	2.78	0.47
1:C:145:VAL:CG2	1:C:149:GLN:HE22	2.28	0.47
1:C:197:TYR:CZ	1:C:221:PRO:HB3	2.50	0.47
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.14	0.46
1:A:142:THR:CG2	1:B:258:LEU:HD22	2.45	0.46
1:A:146:SER:HB3	1:A:149:GLN:HG3	1.97	0.46
1:A:169:CYS:N	1:A:172:ASN:HB2	2.30	0.46
1:A:133:MET:HB2	1:A:224:LEU:HD11	1.98	0.46
1:B:110:TYR:HB2	1:B:248:ILE:CD1	2.43	0.46
1:C:123:CYS:HB2	1:C:127:THR:OG1	2.15	0.46
1:A:66:VAL:CG2	1:A:249:ARG:HH21	2.27	0.46
1:B:145:VAL:HG12	1:B:146:SER:N	2.30	0.46
1:C:201:THR:CG2	1:C:260:LEU:HA	2.46	0.46
1:A:233:SER:C	1:A:235:THR:H	2.22	0.46
1:B:71:HIS:HD2	1:B:99:TRP:CH2	2.33	0.46
1:B:172:ASN:HD22	1:B:172:ASN:HA	1.20	0.46
1:B:219:LEU:C	1:B:220:VAL:HG23	2.41	0.46
1:A:132:HIS:CE1	1:A:147:VAL:HG22	2.51	0.46
1:A:167:GLY:O	1:A:168:LEU:C	2.59	0.46
1:B:219:LEU:O	1:B:220:VAL:HG23	2.16	0.46
1:C:223:ARG:HG3	1:C:223:ARG:O	2.16	0.46
1:A:66:VAL:HG21	1:A:249:ARG:NH2	2.28	0.46
1:A:82:VAL:HG13	1:A:233:SER:C	2.41	0.46
1:A:202:ALA:O	1:A:203:THR:C	2.58	0.46
1:C:251:ILE:O	1:C:252:GLU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:MET:HA	3:A:262:HOH:O	2.15	0.46
1:A:90:LEU:HD13	1:A:92:MET:CE	2.40	0.46
1:A:108:SER:N	1:A:252:GLU:O	2.42	0.46
1:A:203:THR:O	1:A:206:ALA:HB3	2.16	0.46
1:B:100:LEU:HG	1:B:246:TYR:CZ	2.51	0.46
1:C:90:LEU:O	1:C:95:THR:HG21	2.16	0.45
1:B:213:ALA:O	1:B:216:GLY:N	2.40	0.45
1:C:196:ARG:HH11	1:C:249:ARG:HH21	1.63	0.45
1:C:205:TYR:O	1:C:208:ALA:N	2.50	0.45
1:A:201:THR:HG21	1:A:260:LEU:HA	1.99	0.45
1:A:150:LEU:HD12	1:A:150:LEU:O	2.17	0.45
1:A:233:SER:HB3	1:A:235:THR:OG1	2.17	0.45
1:B:167:GLY:O	1:B:168:LEU:C	2.58	0.45
1:C:116:ARG:CD	1:C:170:PHE:CD2	3.00	0.45
1:B:146:SER:OG	1:B:147:VAL:N	2.49	0.45
1:B:151:SER:HA	1:B:156:TYR:CE2	2.52	0.45
1:C:91:VAL:HG12	1:C:91:VAL:O	2.16	0.45
1:B:248:ILE:HD12	1:B:250:LEU:CD1	2.37	0.44
1:C:82:VAL:HB	1:C:234:LYS:HA	1.99	0.44
1:A:160:PRO:C	1:A:162:TRP:N	2.75	0.44
1:A:233:SER:CB	1:A:235:THR:OG1	2.65	0.44
1:C:150:LEU:HD13	1:C:150:LEU:C	2.42	0.44
1:A:170:PHE:N	1:A:170:PHE:CD2	2.85	0.44
1:B:173:ASN:HD22	1:B:173:ASN:C	2.26	0.44
1:C:144:PRO:HG2	1:C:150:LEU:HD23	1.99	0.44
1:C:248:ILE:HG23	1:C:248:ILE:O	2.18	0.44
1:A:91:VAL:CG1	1:A:222:ALA:O	2.66	0.44
1:C:64:MET:HB3	1:C:64:MET:HE2	1.52	0.44
1:A:181:ARG:N	1:A:181:ARG:HD2	2.33	0.44
1:A:107:TRP:CE3	1:A:250:LEU:HD23	2.53	0.44
1:A:191:GLU:HG3	1:B:251:ILE:CD1	2.48	0.44
1:A:238:ASN:N	1:A:238:ASN:ND2	2.66	0.44
1:B:99:TRP:O	1:B:100:LEU:C	2.60	0.44
1:A:214:ASN:HD21	1:B:200:LYS:CE	2.31	0.44
1:B:92:MET:HA	1:B:93:PRO:HD2	1.86	0.44
1:B:140:ALA:HB2	1:B:214:ASN:OD1	2.18	0.44
1:A:90:LEU:HB3	1:A:92:MET:HE3	2.00	0.44
1:C:212:ASN:ND2	1:C:214:ASN:ND2	2.66	0.44
1:C:256:ALA:O	1:C:258:LEU:N	2.50	0.44
1:A:79:ALA:CA	1:A:237:VAL:O	2.61	0.43
1:C:116:ARG:O	1:C:244:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:PHE:HE1	1:B:184:THR:HG21	1.82	0.43
1:B:209:VAL:O	1:B:212:ASN:N	2.51	0.43
1:B:92:MET:HG2	1:B:94:PHE:H	1.82	0.43
1:C:116:ARG:NE	1:C:170:PHE:CD2	2.86	0.43
1:A:135:PHE:O	1:A:153:LEU:HG	2.18	0.43
1:B:69:LEU:HD21	1:B:99:TRP:HZ3	1.83	0.43
1:A:199:PHE:C	1:A:199:PHE:CD2	2.95	0.43
1:B:72:CYS:SG	1:B:171:VAL:HG13	2.59	0.43
1:A:80:VAL:HG11	1:A:129:GLY:HA3	2.01	0.43
1:A:165:GLN:C	1:A:167:GLY:H	2.24	0.43
1:B:110:TYR:CD1	1:B:111:ALA:N	2.86	0.43
1:A:64:MET:HB2	1:A:65:ASP:H	1.46	0.43
1:C:201:THR:HG23	1:C:260:LEU:CA	2.48	0.43
1:B:115:ILE:HG12	1:B:116:ARG:N	2.34	0.43
1:C:202:ALA:O	1:C:205:TYR:HB3	2.19	0.43
1:A:88:SER:HA	1:A:224:LEU:O	2.19	0.43
1:A:165:GLN:C	1:A:167:GLY:N	2.77	0.43
1:B:203:THR:O	1:B:204:ASP:C	2.62	0.43
1:B:259:ASN:OD1	1:B:260:LEU:N	2.52	0.43
1:C:80:VAL:CG1	1:C:231:GLY:HA2	2.49	0.43
1:C:82:VAL:HG12	1:C:83:THR:N	2.34	0.43
1:A:173:ASN:HD22	1:A:173:ASN:HA	1.27	0.42
1:C:205:TYR:O	1:C:208:ALA:HB3	2.19	0.42
1:A:153:LEU:HA	1:A:153:LEU:HD12	1.67	0.42
1:B:216:GLY:O	1:B:217:ASN:C	2.61	0.42
1:A:130:ALA:N	1:A:161:VAL:HG13	2.33	0.42
1:A:212:ASN:C	1:A:214:ASN:H	2.27	0.42
1:B:92:MET:HE3	1:B:200:LYS:HB2	2.00	0.42
1:B:129:GLY:HA2	1:B:230:GLY:HA3	2.00	0.42
1:B:200:LYS:HD2	1:B:260:LEU:O	2.19	0.42
1:C:79:ALA:CB	1:C:238:ASN:HA	2.50	0.42
1:C:194:GLU:HG3	1:C:218:ILE:HG23	2.01	0.42
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.19	0.42
1:A:200:LYS:HD2	1:A:200:LYS:HA	1.73	0.42
1:C:59:MET:HG2	1:C:60:LEU:N	2.31	0.42
1:A:146:SER:O	1:A:147:VAL:C	2.63	0.42
1:A:185:ILE:O	1:A:185:ILE:HG23	2.19	0.42
1:A:221:PRO:O	1:A:222:ALA:HB2	2.20	0.42
1:B:204:ASP:O	1:B:205:TYR:C	2.62	0.42
1:A:82:VAL:HG13	1:A:234:LYS:N	2.34	0.42
1:B:116:ARG:HH11	1:B:116:ARG:HD2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:PRO:C	1:C:126:THR:H	2.28	0.42
1:A:82:VAL:HG13	1:A:234:LYS:CA	2.49	0.42
1:A:132:HIS:CE1	1:A:147:VAL:HG21	2.54	0.42
1:B:123:CYS:HB2	1:B:124:PRO:HD2	2.02	0.42
1:C:78:LEU:CG	1:C:228:MET:HE3	2.40	0.42
1:C:212:ASN:C	1:C:214:ASN:N	2.76	0.42
1:C:231:GLY:O	1:C:232:SER:HB3	2.18	0.42
1:B:79:ALA:HB2	1:B:238:ASN:HA	2.00	0.42
1:B:195:LYS:CE	1:C:195:LYS:HE3	2.50	0.42
1:C:172:ASN:HD22	1:C:172:ASN:HA	1.62	0.42
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.20	0.42
1:A:170:PHE:N	1:A:170:PHE:HD2	2.18	0.42
1:C:116:ARG:CZ	1:C:170:PHE:HE2	2.32	0.42
1:A:219:LEU:HD21	1:C:214:ASN:OD1	2.20	0.41
1:B:125:THR:O	1:B:125:THR:CG2	2.63	0.41
1:B:218:ILE:HG12	1:B:219:LEU:HD13	2.00	0.41
1:A:140:ALA:O	1:B:260:LEU:HD12	2.20	0.41
1:B:82:VAL:HG21	1:B:234:LYS:CG	2.50	0.41
1:B:175:LYS:O	1:B:177:PRO:N	2.53	0.41
1:B:233:SER:HB3	1:B:235:THR:HB	2.01	0.41
1:C:55:LEU:HD23	1:C:55:LEU:HA	1.72	0.41
1:A:71:HIS:HB3	1:A:246:TYR:CE2	2.56	0.41
1:B:74:LEU:H	1:B:74:LEU:CD1	2.32	0.41
1:C:109:LYS:HB3	1:C:197:TYR:O	2.19	0.41
1:A:142:THR:HG22	1:B:258:LEU:HD22	2.02	0.41
1:A:250:LEU:N	1:A:250:LEU:HD12	2.35	0.41
1:C:181:ARG:H	1:C:181:ARG:HG2	1.63	0.41
1:A:92:MET:HE2	1:A:92:MET:HB3	1.54	0.41
1:A:246:TYR:CD1	1:A:246:TYR:N	2.89	0.41
1:B:133:MET:HA	1:B:225:VAL:O	2.20	0.41
1:A:139:MET:HE1	1:A:223:ARG:CB	2.48	0.41
1:C:69:LEU:O	1:C:248:ILE:HG22	2.20	0.41
1:C:76:THR:HG22	1:C:77:GLU:N	2.36	0.41
1:C:90:LEU:O	1:C:95:THR:HG22	2.21	0.41
1:A:167:GLY:C	1:A:168:LEU:O	2.59	0.41
1:B:79:ALA:HB2	1:B:238:ASN:HD22	1.86	0.41
1:A:201:THR:HG22	1:A:260:LEU:HA	2.03	0.41
1:B:113:VAL:HB	1:B:247:THR:O	2.20	0.41
1:B:200:LYS:HD2	1:B:200:LYS:HA	1.47	0.41
1:B:213:ALA:O	1:B:215:ILE:N	2.54	0.41
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:HIS:CG	1:C:72:CYS:H	2.38	0.41
1:C:74:LEU:HB2	1:C:243:TYR:CE2	2.55	0.41
1:C:219:LEU:H	1:C:219:LEU:HG	1.49	0.41
1:A:72:CYS:SG	1:A:171:VAL:HA	2.61	0.41
1:B:74:LEU:N	1:B:74:LEU:CD1	2.84	0.41
1:C:154:LYS:O	1:C:154:LYS:HD3	2.21	0.41
1:C:205:TYR:O	1:C:206:ALA:C	2.64	0.41
1:C:176:CYS:HA	1:C:177:PRO:HD3	1.83	0.40
1:B:136:GLN:NE2	1:B:143:LEU:CD2	2.84	0.40
1:B:161:VAL:H	1:B:161:VAL:HG22	1.59	0.40
1:B:201:THR:HG23	1:B:260:LEU:HA	2.04	0.40
1:C:212:ASN:O	1:C:213:ALA:C	2.63	0.40
1:C:252:GLU:HA	1:C:253:PRO:HD2	1.71	0.40
1:A:160:PRO:O	1:A:161:VAL:C	2.63	0.40
1:A:160:PRO:C	1:A:162:TRP:H	2.30	0.40
1:C:201:THR:HG23	1:C:260:LEU:OXT	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/260 (76%)	160 (81%)	27 (14%)	10 (5%)	1	5
1	B	197/260 (76%)	163 (83%)	29 (15%)	5 (2%)	4	16
1	C	220/260 (85%)	182 (83%)	29 (13%)	9 (4%)	2	8
All	All	614/780 (79%)	505 (82%)	85 (14%)	24 (4%)	2	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	THR

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Mol	Chain	Res	Type
1	B	231	GLY
1	C	219	LEU
1	C	230	GLY
1	C	231	GLY
1	A	161	VAL
1	A	166	SER
1	A	169	CYS
1	B	210	GLY
1	C	177	PRO
1	A	139	MET
1	A	202	ALA
1	B	173	ASN
1	A	94	PHE
1	A	182	ALA
1	B	213	ALA
1	B	256	ALA
1	C	125	THR
1	C	205	TYR
1	C	257	ALA
1	C	173	ASN
1	C	251	ILE
1	A	177	PRO
1	A	230	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	167/217 (77%)	114 (68%)	53 (32%)	0	1
1	B	167/217 (77%)	113 (68%)	54 (32%)	0	1
1	C	185/217 (85%)	121 (65%)	64 (35%)	0	0
All	All	519/651 (80%)	348 (67%)	171 (33%)	0	1

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	MET
1	A	65	ASP
1	A	68	ILE
1	A	77	GLU
1	A	78	LEU
1	A	80	VAL
1	A	87	THR
1	A	91	VAL
1	A	92	MET
1	A	95	THR
1	A	100	LEU
1	A	101	ARG
1	A	108	SER
1	A	109	LYS
1	A	116	ARG
1	A	118	THR
1	A	123	CYS
1	A	131	ILE
1	A	133	MET
1	A	139	MET
1	A	141	ASP
1	A	145	VAL
1	A	146	SER
1	A	147	VAL
1	A	148	ASN
1	A	152	ASN
1	A	153	LEU
1	A	154	LYS
1	A	158	THR
1	A	165	GLN
1	A	168	LEU
1	A	173	ASN
1	A	174	THR
1	A	176	CYS
1	A	181	ARG
1	A	183	ILE
1	A	184	THR
1	A	190	ASN
1	A	191	GLU
1	A	196	ARG
1	A	198	PRO
1	A	200	LYS
1	A	207	THR

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Mol	Chain	Res	Type
1	A	214	ASN
1	A	218	ILE
1	A	223	ARG
1	A	225	VAL
1	A	226	THR
1	A	234	LYS
1	A	237	VAL
1	A	245	SER
1	A	251	ILE
1	A	252	GLU
1	B	62	SER
1	B	74	LEU
1	B	77	GLU
1	B	78	LEU
1	B	82	VAL
1	B	83	THR
1	B	85	VAL
1	B	87	THR
1	B	88	SER
1	B	90	LEU
1	B	95	THR
1	B	96	VAL
1	B	100	LEU
1	B	105	GLN
1	B	106	ASN
1	B	108	SER
1	B	109	LYS
1	B	115	ILE
1	B	116	ARG
1	B	118	THR
1	B	138	ASP
1	B	139	MET
1	B	145	VAL
1	B	147	VAL
1	B	150	LEU
1	B	152	ASN
1	B	154	LYS
1	B	158	THR
1	B	161	VAL
1	B	165	GLN
1	B	171	VAL
1	B	172	ASN

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Mol	Chain	Res	Type
1	B	173	ASN
1	B	175	LYS
1	B	176	CYS
1	B	180	SER
1	B	189	THR
1	B	190	ASN
1	B	196	ARG
1	B	199	PHE
1	B	200	LYS
1	B	203	THR
1	B	209	VAL
1	B	218	ILE
1	B	223	ARG
1	B	226	THR
1	B	234	LYS
1	B	235	THR
1	B	242	LEU
1	B	248	ILE
1	B	250	LEU
1	B	251	ILE
1	B	252	GLU
1	B	254	ILE
1	C	44	MET
1	C	47	ILE
1	C	54	LYS
1	C	56	ARG
1	C	60	LEU
1	C	61	ARG
1	C	65	ASP
1	C	66	VAL
1	C	67	THR
1	C	69	LEU
1	C	70	SER
1	C	72	CYS
1	C	74	LEU
1	C	77	GLU
1	C	78	LEU
1	C	80	VAL
1	C	82	VAL
1	C	83	THR
1	C	84	ILE
1	C	87	THR

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Mol	Chain	Res	Type
1	C	92	MET
1	C	95	THR
1	C	98	THR
1	C	103	VAL
1	C	115	ILE
1	C	118	THR
1	C	121	PRO
1	C	122	SER
1	C	125	THR
1	C	127	THR
1	C	128	SER
1	C	145	VAL
1	C	146	SER
1	C	149	GLN
1	C	150	LEU
1	C	152	ASN
1	C	153	LEU
1	C	161	VAL
1	C	165	GLN
1	C	172	ASN
1	C	173	ASN
1	C	174	THR
1	C	175	LYS
1	C	178	ASP
1	C	181	ARG
1	C	184	THR
1	C	185	ILE
1	C	187	LEU
1	C	189	THR
1	C	191	GLU
1	C	192	VAL
1	C	195	LYS
1	C	196	ARG
1	C	200	LYS
1	C	203	THR
1	C	214	ASN
1	C	228	MET
1	C	234	LYS
1	C	235	THR
1	C	242	LEU
1	C	245	SER
1	C	249	ARG

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Mol	Chain	Res	Type
1	C	251	ILE
1	C	260	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	136	GLN
1	A	148	ASN
1	A	165	GLN
1	A	172	ASN
1	A	173	ASN
1	A	190	ASN
1	A	214	ASN
1	A	238	ASN
1	B	106	ASN
1	B	136	GLN
1	B	148	ASN
1	B	152	ASN
1	B	165	GLN
1	B	172	ASN
1	B	173	ASN
1	B	190	ASN
1	B	214	ASN
1	B	217	ASN
1	B	238	ASN
1	C	49	GLN
1	C	106	ASN
1	C	149	GLN
1	C	172	ASN
1	C	212	ASN
1	C	217	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	199/260 (76%)	-2.12	0 100 100	12, 22, 60, 83	0
1	B	199/260 (76%)	-2.12	0 100 100	10, 21, 50, 65	0
1	C	222/260 (85%)	-2.12	0 100 100	8, 21, 37, 60	0
All	All	620/780 (79%)	-2.12	0 100 100	8, 21, 46, 83	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	261	1/1	0.69	0.01	27,27,27,27	0
2	CA	B	261	1/1	0.69	0.01	16,16,16,16	0
2	CA	C	261	1/1	1.00	0.01	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.