



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:07 PM UTC

PDB ID : 6PFK / pdb_00006pfk
Title : PHOSPHOFRUCTOKINASE, INHIBITED T-STATE
Authors : Evans, P.R.; Schirmer, T.; Auer, M.
Deposited on : 1996-01-04
Resolution : 2.60 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) : 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

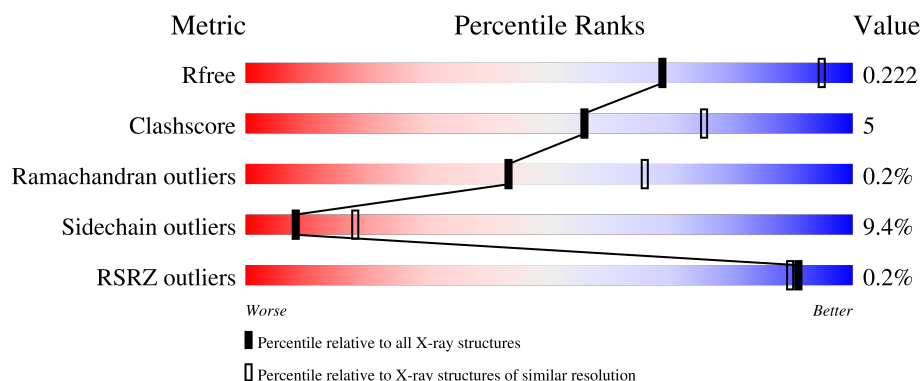
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	319	54% 36% 9% .
1	B	319	57% 35% 6% .
1	C	319	58% 35% 7% .
1	D	319	55% 35% 8% .

2 Entry composition [i](#)

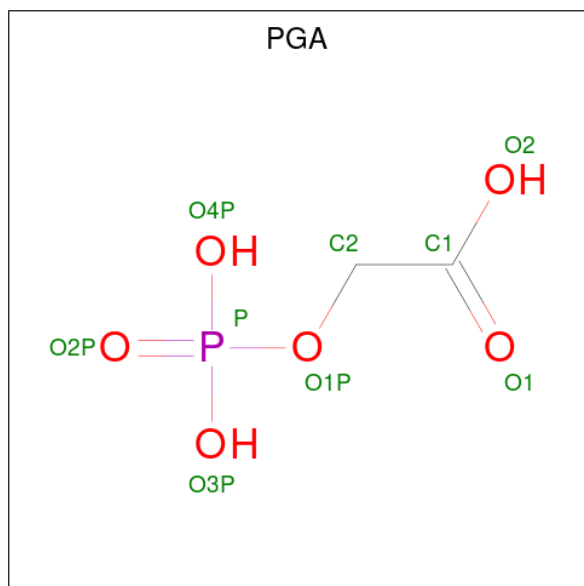
There are 3 unique types of molecules in this entry. The entry contains 9681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOFRUCTOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	1	0
			2341	1466	420	447	8			
1	B	319	Total	C	N	O	S	0	1	0
			2349	1470	422	449	8			
1	C	319	Total	C	N	O	S	0	1	0
			2355	1473	420	454	8			
1	D	319	Total	C	N	O	S	0	1	0
			2374	1486	425	455	8			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (CCD ID: PGA) (formula: C₂H₅O₆P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			9	2	6	1		
2	D	1	Total	C	O	P	0	0
			9	2	6	1		

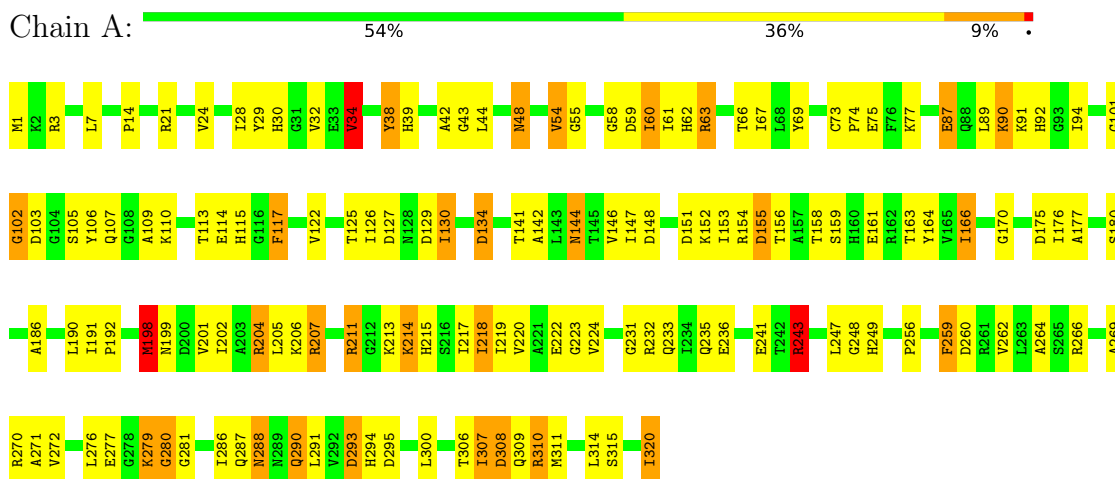
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	59	Total	O	0	0
			59	59		
3	C	50	Total	O	0	0
			50	50		
3	D	64	Total	O	0	0
			64	64		

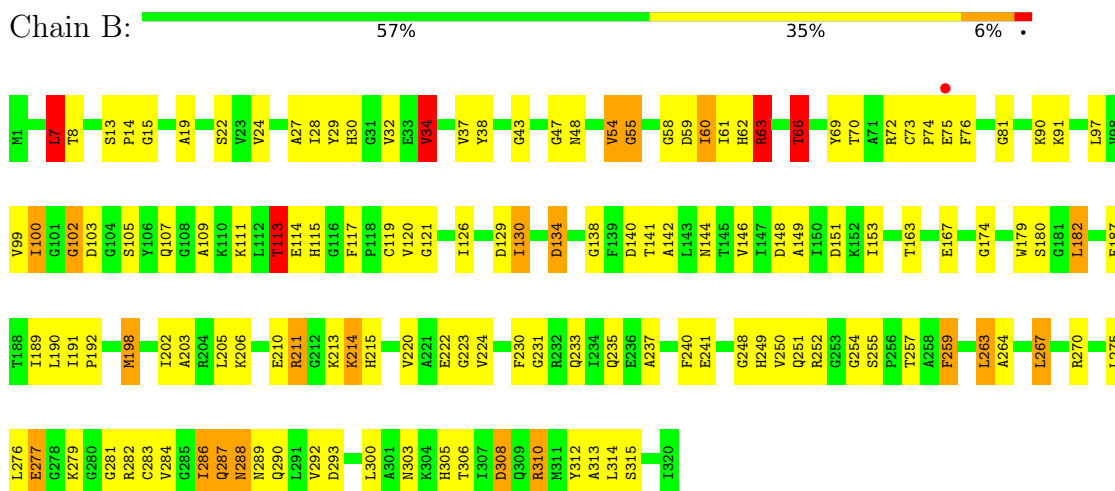
3 Residue-property plots

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: PHOSPHOFRUCTOKINASE

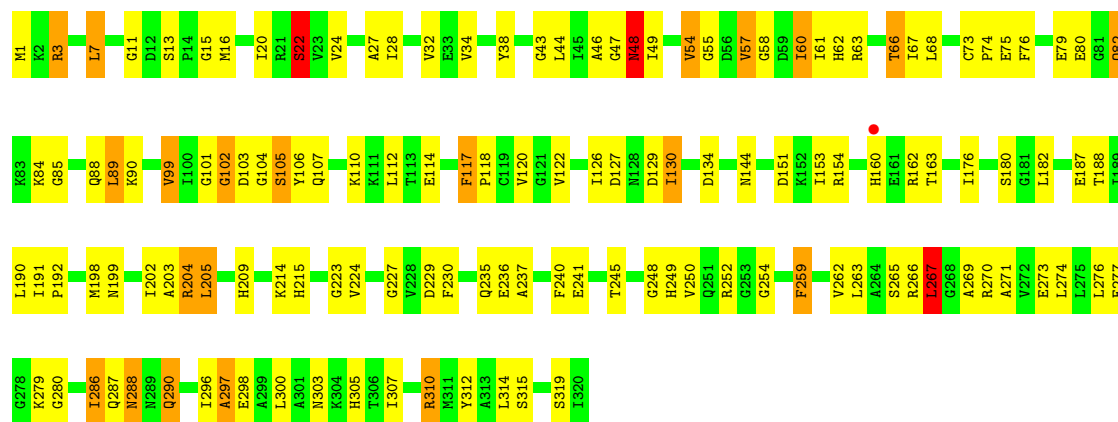


• Molecule 1: PHOSPHOFRUCTOKINASE



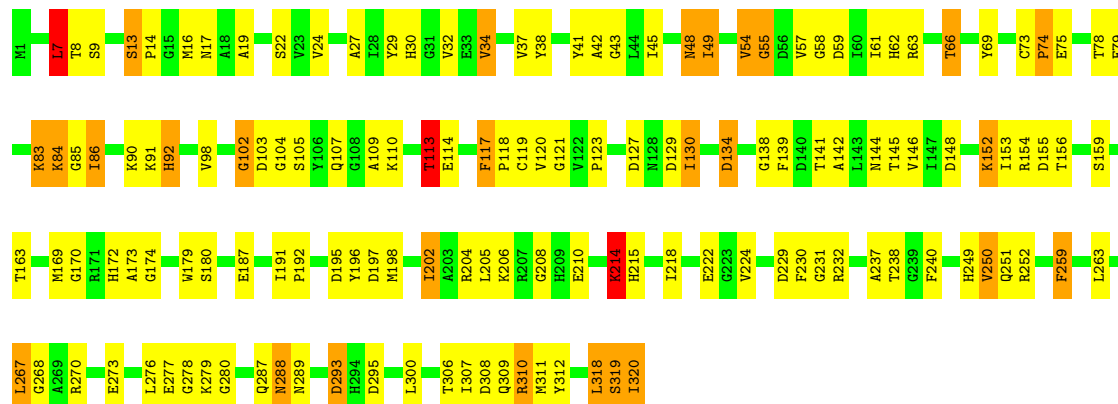
• Molecule 1: PHOSPHOFRUCTOKINASE





• Molecule 1: PHOSPHOFRUCTOKINASE

Chain D: 55% 35% 8% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.00Å 115.20Å 96.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 15.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.60) 96.4 (15.00-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.255 0.160 , 0.222	Depositor DCC
R_{free} test set	2242 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGA

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	0.86	0/2383	2.55	200/3226 (6.2%)
1	B	0.85	1/2391 (0.0%)	2.50	184/3235 (5.7%)
1	C	0.83	0/2397	2.61	203/3242 (6.3%)
1	D	0.89	0/2416	2.59	206/3263 (6.3%)
All	All	0.86	1/9587 (0.0%)	2.56	793/12966 (6.1%)

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	8
1	B	0	8
1	C	0	1
1	D	0	9
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	ILE	CA-CB	-5.25	1.50	1.54

All (793) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	ARG	CD-NE-CZ	26.86	162.01	124.40
1	C	122	VAL	CA-C-O	14.83	128.70	119.51
1	B	211	ARG	CD-NE-CZ	14.21	144.29	124.40
1	A	211	ARG	CD-NE-CZ	13.98	143.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	HIS	CA-C-N	13.57	137.66	120.56
1	C	249	HIS	C-N-CA	13.57	137.66	120.56
1	A	163	THR	CA-C-O	13.15	134.21	120.40
1	D	120	VAL	CA-C-N	12.75	134.31	122.20
1	D	120	VAL	C-N-CA	12.75	134.31	122.20
1	C	254	GLY	CA-C-O	12.72	131.00	122.23
1	C	300	LEU	CA-C-N	12.50	139.31	120.31
1	C	300	LEU	C-N-CA	12.50	139.31	120.31
1	A	249	HIS	CA-C-N	12.15	137.11	120.46
1	A	249	HIS	C-N-CA	12.15	137.11	120.46
1	C	198	MET	CA-C-N	11.69	137.11	120.28
1	C	198	MET	C-N-CA	11.69	137.11	120.28
1	B	103	ASP	CA-CB-CG	-11.35	101.25	112.60
1	A	198	MET	CA-C-N	11.20	135.73	120.38
1	A	198	MET	C-N-CA	11.20	135.73	120.38
1	B	153	ILE	O-C-N	-11.05	111.16	121.87
1	D	249	HIS	CA-C-N	10.91	135.92	120.42
1	D	249	HIS	C-N-CA	10.91	135.92	120.42
1	A	61	ILE	CA-C-N	10.86	141.23	122.56
1	A	61	ILE	C-N-CA	10.86	141.23	122.56
1	D	192	PRO	CA-C-N	10.66	134.94	120.54
1	D	192	PRO	C-N-CA	10.66	134.94	120.54
1	D	251	GLN	OE1-CD-NE2	-10.55	112.05	122.60
1	C	126	ILE	CA-C-N	10.26	134.44	120.38
1	C	126	ILE	C-N-CA	10.26	134.44	120.38
1	B	54	VAL	CB-CA-C	-10.16	98.42	112.14
1	D	287	GLN	N-CA-CB	10.14	127.85	110.81
1	C	79	GLU	CA-C-N	10.10	133.82	120.28
1	C	79	GLU	C-N-CA	10.10	133.82	120.28
1	C	28	ILE	O-C-N	-10.05	112.12	121.87
1	C	223	GLY	CA-C-N	9.88	134.45	120.42
1	C	223	GLY	C-N-CA	9.88	134.45	120.42
1	B	249	HIS	CA-C-N	9.84	133.94	120.46
1	B	249	HIS	C-N-CA	9.84	133.94	120.46
1	D	61	ILE	CA-C-N	9.77	139.37	122.56
1	D	61	ILE	C-N-CA	9.77	139.37	122.56
1	A	48	ASN	OD1-CG-ND2	9.70	132.30	122.60
1	C	120	VAL	CA-C-N	9.63	131.35	122.20
1	C	120	VAL	C-N-CA	9.63	131.35	122.20
1	C	267	LEU	O-C-N	-9.61	111.93	122.12
1	C	287	GLN	OE1-CD-NE2	9.59	132.19	122.60
1	B	254	GLY	CA-C-O	9.50	128.39	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	120	VAL	CA-C-N	9.44	130.68	121.62
1	B	120	VAL	C-N-CA	9.44	130.68	121.62
1	A	54	VAL	CB-CA-C	-9.43	99.90	111.97
1	A	61	ILE	O-C-N	-9.39	112.68	121.89
1	C	300	LEU	O-C-N	-9.39	109.94	122.43
1	B	114	GLU	CA-C-N	9.29	137.45	122.67
1	B	114	GLU	C-N-CA	9.29	137.45	122.67
1	D	54	VAL	CB-CA-C	-9.27	100.11	111.97
1	A	48	ASN	CA-C-N	9.25	135.82	123.06
1	A	48	ASN	C-N-CA	9.25	135.82	123.06
1	D	138	GLY	O-C-N	-9.10	115.43	122.71
1	D	129	ASP	CA-C-O	9.06	133.46	120.51
1	C	61	ILE	CA-C-N	9.05	137.47	122.54
1	C	61	ILE	C-N-CA	9.05	137.47	122.54
1	C	288	ASN	O-C-N	-8.89	111.53	122.55
1	A	192	PRO	CA-C-N	8.87	138.88	121.58
1	A	192	PRO	C-N-CA	8.87	138.88	121.58
1	B	61	ILE	CA-C-N	8.85	138.40	122.38
1	B	61	ILE	C-N-CA	8.85	138.40	122.38
1	B	250	VAL	CA-C-N	8.73	132.85	120.28
1	B	250	VAL	C-N-CA	8.73	132.85	120.28
1	A	134	ASP	O-C-N	-8.71	112.22	122.15
1	B	288	ASN	CA-C-N	8.70	134.73	122.46
1	B	288	ASN	C-N-CA	8.70	134.73	122.46
1	D	114	GLU	CA-C-N	8.70	136.17	122.60
1	D	114	GLU	C-N-CA	8.70	136.17	122.60
1	B	61	ILE	N-CA-C	8.59	119.38	110.62
1	C	271	ALA	O-C-N	-8.59	113.16	122.09
1	D	229	ASP	CA-CB-CG	-8.58	104.02	112.60
1	C	28	ILE	CA-C-N	8.57	131.76	120.28
1	C	28	ILE	C-N-CA	8.57	131.76	120.28
1	D	250	VAL	CA-C-N	8.44	131.95	120.38
1	D	250	VAL	C-N-CA	8.44	131.95	120.38
1	C	144	ASN	O-C-N	-8.43	113.18	122.12
1	D	252	ARG	NE-CZ-NH2	-8.40	111.64	119.20
1	C	280	GLY	O-C-N	-8.39	116.44	123.23
1	B	250	VAL	O-C-N	-8.28	113.84	121.87
1	A	243	ARG	CD-NE-CZ	8.25	135.95	124.40
1	D	179	TRP	CA-C-N	8.24	131.99	120.29
1	D	179	TRP	C-N-CA	8.24	131.99	120.29
1	D	55	GLY	O-C-N	-8.24	113.37	122.68
1	B	61	ILE	O-C-N	-8.23	113.89	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASP	O-C-N	-8.23	113.78	123.41
1	D	214	LYS	O-C-N	-8.21	113.61	122.07
1	A	277	GLU	O-C-N	-8.18	112.52	122.34
1	D	289	ASN	CA-C-N	8.17	136.06	122.33
1	D	289	ASN	C-N-CA	8.17	136.06	122.33
1	A	243	ARG	CG-CD-NE	8.13	129.89	112.00
1	D	145	THR	CA-CB-OG1	-8.12	97.41	109.60
1	C	310	ARG	CD-NE-CZ	8.10	135.75	124.40
1	A	155	ASP	CA-C-O	-8.07	110.99	120.10
1	C	127	ASP	N-CA-C	8.05	121.07	111.33
1	B	129	ASP	CA-C-O	8.04	135.49	121.09
1	A	117	PHE	CA-CB-CG	-8.04	105.76	113.80
1	D	129	ASP	O-C-N	-8.04	111.89	122.59
1	B	58	GLY	O-C-N	-8.04	114.56	122.84
1	A	122	VAL	CA-C-O	8.02	124.48	119.51
1	A	74	PRO	CA-C-N	7.94	131.72	120.28
1	A	74	PRO	C-N-CA	7.94	131.72	120.28
1	A	264	ALA	CA-C-N	7.94	130.76	120.44
1	A	264	ALA	C-N-CA	7.94	130.76	120.44
1	A	279	LYS	O-C-N	-7.94	113.74	122.79
1	A	207	ARG	CA-C-N	7.93	128.78	119.98
1	A	207	ARG	C-N-CA	7.93	128.78	119.98
1	C	252	ARG	NE-CZ-NH2	-7.92	112.07	119.20
1	D	117	PHE	CA-C-O	7.92	129.11	120.08
1	A	94	ILE	CA-C-O	-7.91	111.39	120.65
1	A	214	LYS	O-C-N	-7.88	113.95	122.07
1	B	48	ASN	CA-C-N	7.87	133.45	123.14
1	B	48	ASN	C-N-CA	7.87	133.45	123.14
1	C	16	MET	CA-C-O	-7.85	112.23	120.55
1	B	134	ASP	O-C-N	-7.83	113.23	122.15
1	D	78	THR	CA-C-O	7.83	130.95	121.87
1	C	198	MET	O-C-N	-7.80	113.85	122.12
1	B	47	GLY	O-C-N	-7.76	114.62	122.54
1	C	105	SER	CA-C-N	7.75	131.30	120.29
1	C	105	SER	C-N-CA	7.75	131.30	120.29
1	C	240	PHE	CA-CB-CG	7.75	121.55	113.80
1	B	117	PHE	CA-CB-CG	-7.74	106.06	113.80
1	C	180	SER	CB-CA-C	-7.74	98.73	110.88
1	B	55	GLY	O-C-N	-7.72	113.88	122.84
1	D	59	ASP	CA-CB-CG	-7.71	104.89	112.60
1	D	48	ASN	OD1-CG-ND2	7.66	130.26	122.60
1	A	288	ASN	CA-C-N	7.66	133.02	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASN	C-N-CA	7.66	133.02	122.07
1	B	310	ARG	NE-CZ-NH1	7.63	129.13	121.50
1	B	114	GLU	O-C-N	-7.61	112.31	122.43
1	C	117	PHE	CA-CB-CG	-7.59	106.21	113.80
1	B	129	ASP	O-C-N	-7.58	112.97	122.82
1	D	224	VAL	CB-CA-C	-7.55	102.13	112.24
1	A	28	ILE	O-C-N	-7.54	114.56	121.87
1	A	77	LYS	CA-C-N	7.53	134.63	122.81
1	A	77	LYS	C-N-CA	7.53	134.63	122.81
1	A	134	ASP	CA-C-N	7.52	134.22	122.94
1	A	134	ASP	C-N-CA	7.52	134.22	122.94
1	C	54	VAL	CB-CA-C	-7.51	102.26	111.88
1	C	191	ILE	CA-C-N	7.50	127.53	119.28
1	C	191	ILE	C-N-CA	7.50	127.53	119.28
1	D	34	VAL	CA-C-O	7.50	128.26	120.39
1	B	240	PHE	CA-CB-CG	7.50	121.30	113.80
1	C	248	GLY	O-C-N	-7.49	114.59	122.60
1	C	286	ILE	O-C-N	-7.49	115.26	123.20
1	B	151	ASP	CA-C-N	7.48	130.17	120.44
1	B	151	ASP	C-N-CA	7.48	130.17	120.44
1	C	55	GLY	CA-C-N	7.48	131.05	120.28
1	C	55	GLY	C-N-CA	7.48	131.05	120.28
1	D	232	ARG	NE-CZ-NH1	7.48	128.98	121.50
1	A	29	TYR	CA-C-N	7.46	135.40	122.56
1	A	29	TYR	C-N-CA	7.46	135.40	122.56
1	B	310	ARG	CD-NE-CZ	7.46	134.84	124.40
1	D	86	ILE	CA-C-N	7.46	130.27	120.28
1	D	86	ILE	C-N-CA	7.46	130.27	120.28
1	B	275	LEU	CA-C-N	7.44	130.26	120.28
1	B	275	LEU	C-N-CA	7.44	130.26	120.28
1	C	106	TYR	CA-C-N	7.41	130.08	120.44
1	C	106	TYR	C-N-CA	7.41	130.08	120.44
1	B	192	PRO	CA-C-N	7.41	136.02	121.58
1	B	192	PRO	C-N-CA	7.41	136.02	121.58
1	D	222	GLU	O-C-N	-7.41	114.27	122.12
1	D	138	GLY	CA-C-O	7.38	126.11	119.83
1	C	127	ASP	CB-CA-C	-7.37	98.15	110.68
1	C	204	ARG	CA-C-O	7.35	128.27	120.70
1	B	22	SER	CA-C-O	-7.35	112.76	120.55
1	B	277	GLU	O-C-N	-7.34	112.98	122.37
1	D	61	ILE	O-C-N	-7.32	114.72	121.89
1	B	148	ASP	CA-CB-CG	7.28	119.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	ALA	CA-C-O	-7.27	111.88	120.10
1	C	57	VAL	CA-C-N	7.26	127.72	120.31
1	C	57	VAL	C-N-CA	7.26	127.72	120.31
1	D	127	ASP	CB-CA-C	-7.26	96.73	110.67
1	B	63	ARG	CB-CG-CD	7.26	128.00	111.30
1	B	224	VAL	CB-CA-C	-7.26	102.52	112.24
1	D	22	SER	CA-C-O	-7.25	112.86	120.55
1	C	58	GLY	O-C-N	-7.25	115.38	122.84
1	B	308	ASP	CA-CB-CG	7.22	119.82	112.60
1	A	218	ILE	CB-CG1-CD1	7.21	128.93	113.80
1	A	29	TYR	O-C-N	-7.19	114.50	122.12
1	A	288	ASN	O-C-N	-7.18	113.64	122.55
1	B	252	ARG	NE-CZ-NH2	-7.17	112.75	119.20
1	B	277	GLU	N-CA-CB	-7.15	100.69	110.56
1	D	153	ILE	CA-C-N	7.15	130.57	120.28
1	D	153	ILE	C-N-CA	7.15	130.57	120.28
1	D	121	GLY	CA-C-N	7.11	133.31	123.28
1	D	121	GLY	C-N-CA	7.11	133.31	123.28
1	D	113	THR	O-C-N	-7.10	114.06	122.15
1	C	245	THR	O-C-N	-7.09	114.86	123.30
1	B	115	HIS	CA-CB-CG	7.09	120.89	113.80
1	B	277	GLU	CA-C-N	7.09	134.52	120.77
1	B	277	GLU	C-N-CA	7.09	134.52	120.77
1	B	100	ILE	CB-CG1-CD1	7.08	128.67	113.80
1	D	240	PHE	CA-CB-CG	7.08	120.88	113.80
1	C	274	LEU	O-C-N	-7.07	114.73	122.09
1	B	230	PHE	CA-C-N	7.06	127.97	119.99
1	B	230	PHE	C-N-CA	7.06	127.97	119.99
1	D	54	VAL	N-CA-CB	7.06	118.81	110.55
1	C	48	ASN	CA-C-N	7.04	132.37	123.14
1	C	48	ASN	C-N-CA	7.04	132.37	123.14
1	B	270	ARG	O-C-N	-7.03	114.14	122.15
1	D	73	CYS	CA-C-N	7.03	126.66	119.56
1	D	73	CYS	C-N-CA	7.03	126.66	119.56
1	D	130	ILE	CB-CA-C	7.02	117.25	110.16
1	C	296	ILE	N-CA-CB	7.02	118.76	110.55
1	C	54	VAL	N-CA-CB	7.01	118.29	110.51
1	C	129	ASP	CA-C-O	7.00	133.63	121.09
1	C	11	GLY	N-CA-C	-6.99	103.18	111.36
1	D	145	THR	CA-C-O	-6.99	113.48	120.82
1	A	153	ILE	O-C-N	-6.98	115.10	121.87
1	A	92	HIS	CA-C-O	6.97	127.10	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	VAL	N-CA-CB	6.97	118.70	110.55
1	C	61	ILE	O-C-N	-6.95	114.85	121.87
1	D	309	GLN	CA-C-N	6.95	130.16	120.29
1	D	309	GLN	C-N-CA	6.95	130.16	120.29
1	D	17	ASN	OD1-CG-ND2	6.94	129.54	122.60
1	A	231	GLY	CA-C-N	6.94	130.43	120.79
1	A	231	GLY	C-N-CA	6.94	130.43	120.79
1	B	289	ASN	O-C-N	-6.93	113.91	122.57
1	A	90	LYS	O-C-N	-6.92	114.78	122.12
1	C	13	SER	CA-C-O	6.92	126.97	119.91
1	D	288	ASN	O-C-N	-6.91	113.98	122.55
1	B	75	GLU	O-C-N	-6.90	114.15	122.22
1	C	73	CYS	CA-C-O	6.90	127.94	120.08
1	A	109	ALA	CA-C-N	6.89	130.37	120.79
1	A	109	ALA	C-N-CA	6.89	130.37	120.79
1	D	41	TYR	CA-C-N	6.88	129.50	120.28
1	D	41	TYR	C-N-CA	6.88	129.50	120.28
1	D	142	ALA	O-C-N	-6.88	114.83	122.12
1	D	202	ILE	CA-C-N	6.87	129.81	120.54
1	D	202	ILE	C-N-CA	6.87	129.81	120.54
1	D	232	ARG	NE-CZ-NH2	-6.86	113.03	119.20
1	A	114	GLU	O-C-N	-6.83	114.88	122.12
1	D	102	GLY	CA-C-N	6.83	129.75	120.54
1	D	102	GLY	C-N-CA	6.83	129.75	120.54
1	B	248	GLY	O-C-N	-6.82	115.30	122.60
1	C	47	GLY	CA-C-N	6.81	134.55	121.54
1	C	47	GLY	C-N-CA	6.81	134.55	121.54
1	B	303	ASN	CA-CB-CG	-6.80	105.80	112.60
1	B	103	ASP	CB-CA-C	-6.78	99.96	110.81
1	C	305	HIS	CA-CB-CG	-6.78	107.02	113.80
1	D	222	GLU	CA-C-N	6.78	132.40	120.74
1	D	222	GLU	C-N-CA	6.78	132.40	120.74
1	D	277	GLU	O-C-N	-6.76	113.47	122.19
1	D	214	LYS	CA-C-N	6.75	133.67	122.73
1	D	214	LYS	C-N-CA	6.75	133.67	122.73
1	A	199	ASN	CA-CB-CG	6.75	119.35	112.60
1	D	191	ILE	CA-C-N	6.74	125.98	118.97
1	D	191	ILE	C-N-CA	6.74	125.98	118.97
1	B	54	VAL	N-CA-CB	6.73	119.70	110.54
1	B	233	GLN	N-CA-C	6.71	118.59	111.28
1	B	191	ILE	CA-C-N	6.71	126.66	119.28
1	B	191	ILE	C-N-CA	6.71	126.66	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	GLY	O-C-N	-6.70	115.04	122.61
1	A	272	VAL	CA-C-N	6.69	129.14	120.44
1	A	272	VAL	C-N-CA	6.69	129.14	120.44
1	D	198	MET	O-C-N	-6.68	115.03	122.12
1	B	308	ASP	O-C-N	-6.68	114.13	122.82
1	D	61	ILE	N-CA-C	6.67	118.23	110.62
1	D	7	LEU	CA-CB-CG	6.65	139.58	116.30
1	A	233	GLN	OE1-CD-NE2	6.65	129.25	122.60
1	C	249	HIS	O-C-N	-6.64	113.75	122.59
1	D	172	HIS	CA-CB-CG	-6.64	107.16	113.80
1	B	107	GLN	O-C-N	-6.61	115.22	122.09
1	C	297	ALA	O-C-N	-6.61	115.11	122.12
1	B	30	HIS	O-C-N	-6.61	113.91	122.37
1	A	224	VAL	CB-CA-C	-6.60	103.39	112.24
1	C	153	ILE	O-C-N	-6.60	115.20	121.87
1	D	259[A]	PHE	O-C-N	-6.59	115.13	122.12
1	D	259[B]	PHE	O-C-N	-6.59	115.13	122.12
1	A	130	ILE	N-CA-CB	6.59	120.43	111.21
1	D	295	ASP	CA-C-O	-6.57	113.96	121.19
1	B	167	GLU	CA-C-O	6.56	127.38	120.36
1	D	180	SER	CB-CA-C	-6.56	99.70	110.85
1	B	134	ASP	CA-C-N	6.56	132.84	122.74
1	B	134	ASP	C-N-CA	6.56	132.84	122.74
1	B	73	CYS	CA-C-N	6.56	126.14	119.19
1	B	73	CYS	C-N-CA	6.56	126.14	119.19
1	C	101	GLY	CA-C-O	-6.55	115.16	121.05
1	A	154	ARG	CA-C-O	-6.54	112.72	120.10
1	C	290	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	A	310	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	C	48	ASN	O-C-N	-6.53	113.91	122.59
1	B	130	ILE	O-C-N	6.52	126.98	120.59
1	C	90	LYS	O-C-N	-6.52	115.21	122.12
1	B	310	ARG	CA-C-N	6.51	129.01	120.28
1	B	310	ARG	C-N-CA	6.51	129.01	120.28
1	A	42	ALA	O-C-N	-6.51	115.32	122.09
1	D	123	PRO	O-C-N	-6.51	118.11	122.73
1	C	267	LEU	CA-C-N	6.51	127.16	120.00
1	C	267	LEU	C-N-CA	6.51	127.16	120.00
1	A	180	SER	CB-CA-C	-6.51	100.67	110.88
1	D	141	THR	O-C-N	-6.51	115.37	122.07
1	A	163	THR	O-C-N	-6.50	114.53	123.12
1	D	278	GLY	N-CA-C	6.50	123.98	115.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	ALA	O-C-N	-6.50	115.23	122.12
1	C	314	LEU	CA-C-N	6.50	128.99	120.28
1	C	314	LEU	C-N-CA	6.50	128.99	120.28
1	C	129	ASP	O-C-N	-6.49	114.38	122.82
1	D	142	ALA	CA-C-N	6.49	129.50	120.29
1	D	142	ALA	C-N-CA	6.49	129.50	120.29
1	A	141	THR	O-C-N	-6.48	115.39	122.07
1	D	34	VAL	O-C-N	-6.48	116.27	123.26
1	A	73	CYS	CA-C-N	6.47	126.05	119.19
1	A	73	CYS	C-N-CA	6.47	126.05	119.19
1	B	315	SER	CA-C-O	-6.47	113.69	120.55
1	C	271	ALA	CA-C-N	6.46	129.60	120.42
1	C	271	ALA	C-N-CA	6.46	129.60	120.42
1	D	9	SER	CA-CB-OG	6.46	124.03	111.10
1	D	58	GLY	O-C-N	-6.46	117.08	122.77
1	D	230	PHE	CA-CB-CG	-6.46	107.34	113.80
1	B	105	SER	CA-C-N	6.45	128.93	120.28
1	B	105	SER	C-N-CA	6.45	128.93	120.28
1	C	269	ALA	CA-C-N	6.45	128.83	120.44
1	C	269	ALA	C-N-CA	6.45	128.83	120.44
1	A	314	LEU	N-CA-C	6.44	119.13	111.33
1	C	303	ASN	CA-CB-CG	-6.44	106.16	112.60
1	A	218	ILE	CA-CB-CG1	6.43	121.33	110.40
1	C	224	VAL	CB-CA-C	-6.43	103.35	112.22
1	A	295	ASP	CA-C-O	-6.41	113.99	121.16
1	C	57	VAL	O-C-N	-6.41	116.33	122.09
1	A	215	HIS	CB-CG-ND1	-6.39	113.11	122.70
1	D	103	ASP	CB-CA-C	-6.37	100.62	110.81
1	B	121	GLY	CA-C-O	6.37	125.92	120.76
1	D	198	MET	CA-C-N	6.35	128.79	120.28
1	D	198	MET	C-N-CA	6.35	128.79	120.28
1	A	290	GLN	CA-C-O	-6.35	112.73	120.54
1	D	293	ASP	O-C-N	-6.35	115.98	123.41
1	D	192	PRO	O-C-N	-6.34	115.00	122.17
1	D	27	ALA	O-C-N	-6.34	115.54	122.07
1	D	146	VAL	O-C-N	-6.34	115.72	121.87
1	A	198	MET	O-C-N	-6.33	115.41	122.12
1	A	270	ARG	CD-NE-CZ	6.33	133.26	124.40
1	B	19	ALA	CA-C-N	6.33	128.54	120.56
1	B	19	ALA	C-N-CA	6.33	128.54	120.56
1	B	313	ALA	CA-C-N	6.33	129.05	120.38
1	B	313	ALA	C-N-CA	6.33	129.05	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	GLY	O-C-N	-6.33	115.30	122.64
1	A	271	ALA	CA-C-N	6.30	129.37	120.42
1	A	271	ALA	C-N-CA	6.30	129.37	120.42
1	A	320	ILE	CB-CG1-CD1	6.30	127.04	113.80
1	C	102	GLY	CA-C-N	6.30	131.22	121.19
1	C	102	GLY	C-N-CA	6.30	131.22	121.19
1	B	47	GLY	CA-C-N	6.30	131.38	122.05
1	B	47	GLY	C-N-CA	6.30	131.38	122.05
1	A	21	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	D	320	ILE	CB-CG1-CD1	6.30	127.03	113.80
1	D	229	ASP	CA-C-O	-6.30	113.88	120.55
1	B	81	GLY	CA-C-N	6.29	129.04	120.54
1	B	81	GLY	C-N-CA	6.29	129.04	120.54
1	C	22	SER	CA-C-O	-6.29	112.73	119.97
1	C	237	ALA	CA-C-O	-6.29	114.17	120.90
1	A	202	ILE	CA-C-N	6.29	128.70	120.28
1	A	202	ILE	C-N-CA	6.29	128.70	120.28
1	A	163	THR	CA-C-N	6.28	131.86	123.00
1	A	163	THR	C-N-CA	6.28	131.86	123.00
1	B	215	HIS	CA-CB-CG	-6.28	107.52	113.80
1	D	75	GLU	CA-C-N	6.28	133.62	121.18
1	D	75	GLU	C-N-CA	6.28	133.62	121.18
1	C	250	VAL	CA-C-N	6.28	129.55	120.38
1	C	250	VAL	C-N-CA	6.28	129.55	120.38
1	A	146	VAL	O-C-N	-6.27	115.78	121.87
1	D	114	GLU	O-C-N	-6.26	114.10	122.43
1	C	310	ARG	NE-CZ-NH2	-6.25	113.57	119.20
1	A	231	GLY	O-C-N	-6.25	116.18	122.18
1	D	85	GLY	CA-C-N	6.24	129.01	120.46
1	D	85	GLY	C-N-CA	6.24	129.01	120.46
1	C	176	ILE	N-CA-CB	6.24	117.17	110.62
1	B	34	VAL	N-CA-CB	6.23	120.01	111.41
1	D	30	HIS	O-C-N	-6.23	113.71	122.06
1	B	114	GLU	N-CA-C	6.22	120.34	112.87
1	A	191	ILE	CA-C-N	6.22	125.84	119.56
1	A	191	ILE	C-N-CA	6.22	125.84	119.56
1	C	259[A]	PHE	O-C-N	-6.22	115.67	122.07
1	C	259[B]	PHE	O-C-N	-6.22	115.67	122.07
1	A	38	TYR	O-C-N	-6.22	116.10	123.06
1	A	102	GLY	CA-C-N	6.21	128.93	120.54
1	A	102	GLY	C-N-CA	6.21	128.93	120.54
1	D	134	ASP	O-C-N	-6.21	115.07	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	LEU	N-CA-C	6.21	119.95	112.38
1	B	59	ASP	N-CA-C	6.21	120.43	112.86
1	A	107	GLN	CA-C-N	6.20	126.82	120.00
1	A	107	GLN	C-N-CA	6.20	126.82	120.00
1	A	134	ASP	CA-C-O	6.20	126.99	120.42
1	A	300	LEU	CA-C-N	6.19	131.21	120.68
1	A	300	LEU	C-N-CA	6.19	131.21	120.68
1	A	34	VAL	CB-CA-C	-6.17	102.00	110.77
1	B	163	THR	N-CA-C	6.17	118.76	108.20
1	D	73	CYS	CA-C-O	6.17	127.05	121.06
1	A	142	ALA	CA-C-N	6.16	129.04	120.29
1	A	142	ALA	C-N-CA	6.16	129.04	120.29
1	D	92	HIS	CA-CB-CG	-6.16	107.64	113.80
1	D	279	LYS	CA-C-N	6.15	127.69	121.35
1	D	279	LYS	C-N-CA	6.15	127.69	121.35
1	B	102	GLY	CA-C-N	6.14	128.83	120.54
1	B	102	GLY	C-N-CA	6.14	128.83	120.54
1	A	266	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	A	204	ARG	CA-C-N	6.12	128.80	120.54
1	A	204	ARG	C-N-CA	6.12	128.80	120.54
1	B	59	ASP	CA-CB-CG	-6.11	106.49	112.60
1	D	308	ASP	CA-CB-CG	6.11	118.71	112.60
1	C	199	ASN	O-C-N	-6.11	115.08	122.22
1	D	90	LYS	CA-C-N	6.11	129.07	120.28
1	D	90	LYS	C-N-CA	6.11	129.07	120.28
1	B	29	TYR	CA-C-N	6.09	132.77	122.65
1	B	29	TYR	C-N-CA	6.09	132.77	122.65
1	C	202	ILE	O-C-N	-6.09	115.85	121.94
1	A	307	ILE	N-CA-CB	6.09	119.02	112.07
1	C	277	GLU	CA-CB-CG	6.09	126.28	114.10
1	A	129	ASP	CA-C-O	6.09	131.99	121.09
1	C	315	SER	CA-C-N	6.09	128.93	120.29
1	C	315	SER	C-N-CA	6.09	128.93	120.29
1	C	15	GLY	N-CA-C	-6.08	107.24	114.48
1	C	229	ASP	CA-C-O	-6.08	114.39	120.90
1	D	300	LEU	CA-C-N	6.08	131.78	121.14
1	D	300	LEU	C-N-CA	6.08	131.78	121.14
1	A	147	ILE	CA-C-N	6.07	128.33	120.44
1	A	147	ILE	C-N-CA	6.07	128.33	120.44
1	A	60	ILE	N-CA-C	-6.07	107.58	113.53
1	A	91	LYS	O-C-N	-6.07	115.12	122.22
1	D	288	ASN	OD1-CG-ND2	-6.07	116.53	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	154	ARG	CA-C-N	6.06	129.51	120.31
1	C	154	ARG	C-N-CA	6.06	129.51	120.31
1	A	151	ASP	CA-C-N	6.04	128.30	120.44
1	A	151	ASP	C-N-CA	6.04	128.30	120.44
1	B	222	GLU	O-C-N	-6.04	115.72	122.12
1	A	249	HIS	O-C-N	-6.02	112.77	122.41
1	C	151	ASP	CA-C-O	-6.02	114.50	120.82
1	C	192	PRO	CA-C-N	6.02	133.32	121.58
1	C	192	PRO	C-N-CA	6.02	133.32	121.58
1	D	173	ALA	O-C-N	-6.02	115.56	123.21
1	B	91	LYS	N-CA-C	6.01	118.61	111.33
1	B	180	SER	CB-CA-C	-6.01	100.62	110.85
1	D	59	ASP	N-CA-C	6.01	119.92	112.58
1	C	75	GLU	CA-C-N	6.01	133.08	121.18
1	C	75	GLU	C-N-CA	6.01	133.08	121.18
1	C	160	HIS	CA-CB-CG	6.01	119.81	113.80
1	C	103	ASP	CA-C-N	6.00	126.77	119.99
1	C	103	ASP	C-N-CA	6.00	126.77	119.99
1	D	300	LEU	N-CA-C	5.99	119.85	112.54
1	B	198	MET	O-C-N	-5.99	114.91	122.27
1	A	223	GLY	CA-C-N	5.98	130.12	120.55
1	A	223	GLY	C-N-CA	5.98	130.12	120.55
1	B	121	GLY	O-C-N	-5.97	118.93	123.35
1	A	154	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	A	222	GLU	N-CA-C	5.96	118.56	111.71
1	C	129	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	80	GLU	CA-C-N	5.95	126.43	119.94
1	C	80	GLU	C-N-CA	5.95	126.43	119.94
1	A	144	ASN	CB-CA-C	5.95	120.97	110.85
1	C	73	CYS	CA-C-N	5.95	125.33	118.85
1	C	73	CYS	C-N-CA	5.95	125.33	118.85
1	B	314	LEU	CA-C-N	5.94	128.24	120.28
1	B	314	LEU	C-N-CA	5.94	128.24	120.28
1	A	287	GLN	OE1-CD-NE2	5.93	128.53	122.60
1	B	249	HIS	O-C-N	-5.93	114.70	122.59
1	C	288	ASN	CA-C-N	5.93	130.82	122.46
1	C	288	ASN	C-N-CA	5.93	130.82	122.46
1	D	75	GLU	O-C-N	-5.91	114.70	122.39
1	A	270	ARG	O-C-N	-5.91	115.86	122.12
1	D	288	ASN	CA-C-N	5.89	130.49	122.07
1	D	288	ASN	C-N-CA	5.89	130.49	122.07
1	C	203	ALA	N-CA-C	5.88	117.69	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASP	O-C-N	-5.88	115.98	122.09
1	C	190	LEU	CA-C-O	5.87	126.75	120.46
1	C	236	GLU	O-C-N	-5.87	115.80	122.08
1	D	134	ASP	CA-C-N	5.87	131.26	122.99
1	D	134	ASP	C-N-CA	5.87	131.26	122.99
1	B	276	LEU	CA-C-O	5.87	126.77	120.55
1	A	256	PRO	N-CA-CB	5.86	108.52	103.31
1	D	49	ILE	CA-C-O	-5.85	114.25	120.39
1	B	66	THR	O-C-N	-5.85	116.13	123.27
1	C	227	GLY	CA-C-N	5.85	128.43	120.77
1	C	227	GLY	C-N-CA	5.85	128.43	120.77
1	B	179	TRP	CA-C-N	5.83	128.57	120.29
1	B	179	TRP	C-N-CA	5.83	128.57	120.29
1	C	252	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	D	30	HIS	CA-C-N	5.83	132.08	120.77
1	D	30	HIS	C-N-CA	5.83	132.08	120.77
1	C	209	HIS	O-C-N	-5.82	116.03	122.09
1	D	318	LEU	CA-C-N	5.82	132.31	122.65
1	D	318	LEU	C-N-CA	5.82	132.31	122.65
1	C	74	PRO	CA-C-N	5.82	132.65	121.54
1	C	74	PRO	C-N-CA	5.82	132.65	121.54
1	D	86	ILE	N-CA-C	5.81	116.55	110.62
1	B	189	ILE	O-C-N	-5.80	117.05	123.20
1	D	237	ALA	CA-C-O	-5.80	113.55	120.10
1	A	269	ALA	CA-C-N	5.80	128.05	120.28
1	A	269	ALA	C-N-CA	5.80	128.05	120.28
1	C	76	PHE	CA-C-N	5.80	130.53	120.68
1	C	76	PHE	C-N-CA	5.80	130.53	120.68
1	C	270	ARG	O-C-N	-5.79	116.11	122.07
1	C	245	THR	CA-C-N	5.79	130.97	123.10
1	C	245	THR	C-N-CA	5.79	130.97	123.10
1	A	106	TYR	CA-C-N	5.78	128.30	120.38
1	A	106	TYR	C-N-CA	5.78	128.30	120.38
1	D	319	SER	N-CA-C	5.78	119.41	112.93
1	C	265	SER	CA-C-O	-5.77	114.76	120.82
1	B	312	TYR	O-C-N	-5.77	116.13	122.07
1	C	134	ASP	O-C-N	-5.76	114.74	122.23
1	D	208	GLY	CA-C-N	5.76	127.93	120.44
1	D	208	GLY	C-N-CA	5.76	127.93	120.44
1	B	214	LYS	O-C-N	-5.76	116.14	122.07
1	B	192	PRO	O-C-N	-5.75	114.80	122.22
1	C	130	ILE	N-CA-CB	5.75	119.26	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114	GLU	N-CA-C	5.74	119.10	111.75
1	D	66	THR	O-C-N	-5.74	116.38	123.44
1	A	295	ASP	N-CA-C	-5.73	101.80	110.28
1	A	34	VAL	N-CA-CB	5.73	119.08	111.64
1	A	129	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	215	HIS	CB-CG-CD2	5.73	138.64	131.20
1	B	48	ASN	N-CA-CB	-5.73	103.54	110.53
1	D	54	VAL	CA-C-N	5.72	130.98	120.79
1	D	54	VAL	C-N-CA	5.72	130.98	120.79
1	D	98	VAL	O-C-N	-5.72	115.42	122.97
1	C	48	ASN	N-CA-CB	-5.71	100.83	110.49
1	D	138	GLY	CA-C-N	5.71	127.87	120.44
1	D	138	GLY	C-N-CA	5.71	127.87	120.44
1	A	39	HIS	CA-C-N	5.71	129.30	120.00
1	A	39	HIS	C-N-CA	5.71	129.30	120.00
1	A	300	LEU	O-C-N	-5.71	114.84	122.43
1	B	276	LEU	O-C-N	-5.70	116.07	122.12
1	D	252	ARG	CA-C-O	-5.69	112.38	119.38
1	B	223	GLY	CA-C-N	5.69	129.66	120.55
1	B	223	GLY	C-N-CA	5.69	129.66	120.55
1	C	310	ARG	CA-C-N	5.69	128.37	120.29
1	C	310	ARG	C-N-CA	5.69	128.37	120.29
1	B	149	ALA	O-C-N	-5.69	115.67	122.15
1	C	310	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	B	103	ASP	N-CA-C	5.69	117.93	111.11
1	C	88	GLN	N-CA-C	5.68	118.24	111.71
1	A	94	ILE	O-C-N	5.66	129.85	122.94
1	A	55	GLY	O-C-N	-5.66	116.29	122.68
1	A	91	LYS	N-CA-C	5.65	118.21	111.71
1	B	263	LEU	CA-C-N	5.65	128.32	120.29
1	B	263	LEU	C-N-CA	5.65	128.32	120.29
1	B	113	THR	O-C-N	-5.65	116.13	122.12
1	A	14	PRO	N-CA-CB	5.64	108.19	103.17
1	B	60	ILE	O-C-N	-5.63	116.56	122.25
1	B	198	MET	CA-C-N	5.63	127.83	120.28
1	B	198	MET	C-N-CA	5.63	127.83	120.28
1	A	314	LEU	O-C-N	-5.63	116.16	122.12
1	B	277	GLU	CB-CA-C	5.62	120.53	110.81
1	D	154	ARG	CA-C-O	-5.62	113.75	120.10
1	D	197	ASP	CA-CB-CG	-5.62	106.98	112.60
1	B	109	ALA	CA-C-O	-5.61	114.47	120.42
1	B	28	ILE	CA-C-N	5.61	128.06	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	ILE	C-N-CA	5.61	128.06	120.38
1	B	259[A]	PHE	O-C-N	-5.59	116.19	122.12
1	B	259[B]	PHE	O-C-N	-5.59	116.19	122.12
1	B	140	ASP	CA-C-N	5.59	127.70	120.44
1	B	140	ASP	C-N-CA	5.59	127.70	120.44
1	C	68	LEU	CA-C-N	5.58	132.19	121.54
1	C	68	LEU	C-N-CA	5.58	132.19	121.54
1	D	251	GLN	O-C-N	-5.58	116.21	122.12
1	A	58	GLY	O-C-N	-5.58	117.27	122.96
1	B	310	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	A	192	PRO	O-C-N	-5.55	114.75	122.30
1	B	182	LEU	O-C-N	-5.55	116.23	122.12
1	A	175	ASP	N-CA-CB	5.55	118.05	110.01
1	C	103	ASP	CB-CA-C	-5.54	101.64	110.84
1	C	182	LEU	CA-C-N	5.54	128.73	120.31
1	C	182	LEU	C-N-CA	5.54	128.73	120.31
1	C	162	ARG	CB-CG-CD	5.53	124.03	111.30
1	A	211	ARG	CA-CB-CG	5.53	125.16	114.10
1	D	218	ILE	O-C-N	-5.53	117.37	123.18
1	D	153	ILE	O-C-N	-5.53	115.55	121.80
1	C	68	LEU	O-C-N	-5.53	115.18	122.42
1	D	273	GLU	CA-C-O	-5.53	115.02	120.82
1	A	30	HIS	CA-C-N	5.51	130.94	121.07
1	A	30	HIS	C-N-CA	5.51	130.94	121.07
1	B	90	LYS	O-C-N	-5.51	116.39	122.07
1	A	3	ARG	CB-CA-C	-5.51	99.73	109.70
1	B	130	ILE	N-CA-CB	5.50	119.76	112.27
1	B	48	ASN	CA-CB-CG	5.50	118.10	112.60
1	C	85	GLY	O-C-N	-5.50	116.69	122.13
1	D	42	ALA	O-C-N	-5.49	116.30	122.12
1	A	236	GLU	N-CA-C	5.49	117.70	111.11
1	A	164	TYR	CA-C-O	5.49	126.17	120.30
1	B	287	GLN	N-CA-CB	5.48	120.27	110.80
1	B	202	ILE	O-C-N	-5.47	116.55	121.91
1	B	255	SER	N-CA-CB	-5.46	99.68	109.68
1	C	74	PRO	O-C-N	-5.46	115.40	122.23
1	C	254	GLY	CA-C-N	5.46	127.98	120.67
1	C	254	GLY	C-N-CA	5.46	127.98	120.67
1	D	45	ILE	O-C-N	-5.45	116.57	121.91
1	A	34	VAL	CA-C-O	5.45	126.06	120.39
1	C	58	GLY	CA-C-O	5.45	126.48	121.58
1	D	84	LYS	CA-C-N	5.44	125.98	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	LYS	C-N-CA	5.44	125.98	119.94
1	C	209	HIS	CA-C-N	5.44	127.84	120.38
1	C	209	HIS	C-N-CA	5.44	127.84	120.38
1	A	115	HIS	N-CA-C	5.44	119.62	113.15
1	A	186	ALA	N-CA-CB	5.44	117.97	109.97
1	A	310	ARG	CD-NE-CZ	5.44	132.02	124.40
1	D	144	ASN	CB-CA-C	5.44	120.10	110.85
1	D	174	GLY	CA-C-N	5.43	127.50	120.44
1	D	174	GLY	C-N-CA	5.43	127.50	120.44
1	B	142	ALA	CA-C-N	5.43	127.56	120.28
1	B	142	ALA	C-N-CA	5.43	127.56	120.28
1	D	215	HIS	CB-CG-CD2	5.43	138.26	131.20
1	C	267	LEU	N-CA-C	5.43	117.20	111.28
1	A	87	GLU	CA-C-N	5.43	128.00	120.29
1	A	87	GLU	C-N-CA	5.43	128.00	120.29
1	D	130	ILE	N-CA-CB	5.43	119.65	112.27
1	D	148	ASP	CA-C-N	5.43	127.50	120.44
1	D	148	ASP	C-N-CA	5.43	127.50	120.44
1	C	112	LEU	CA-C-N	5.42	127.48	120.44
1	C	112	LEU	C-N-CA	5.42	127.48	120.44
1	B	74	PRO	CA-C-N	5.41	128.07	120.28
1	B	74	PRO	C-N-CA	5.41	128.07	120.28
1	B	130	ILE	N-CA-C	-5.41	96.46	107.92
1	D	139	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	74	PRO	N-CA-CB	5.40	109.25	103.52
1	B	144	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	B	251	GLN	CA-C-O	-5.40	114.00	120.10
1	B	174	GLY	CA-C-N	5.39	127.45	120.44
1	B	174	GLY	C-N-CA	5.39	127.45	120.44
1	C	20	ILE	CA-C-N	5.39	127.82	120.54
1	C	20	ILE	C-N-CA	5.39	127.82	120.54
1	A	259[A]	PHE	O-C-N	-5.39	116.52	122.07
1	A	259[B]	PHE	O-C-N	-5.39	116.52	122.07
1	A	300	LEU	N-CA-C	5.38	119.33	112.87
1	A	233	GLN	CA-C-O	-5.38	114.85	120.55
1	A	310	ARG	CA-C-O	-5.38	115.17	120.82
1	B	142	ALA	O-C-N	-5.38	116.42	122.12
1	D	74	PRO	CA-C-N	5.38	129.20	120.60
1	D	74	PRO	C-N-CA	5.38	129.20	120.60
1	D	114	GLU	N-CA-C	5.37	119.31	112.87
1	D	268	GLY	CA-C-N	5.37	128.47	120.31
1	D	268	GLY	C-N-CA	5.37	128.47	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	84	LYS	CA-C-N	5.37	126.06	119.99
1	C	84	LYS	C-N-CA	5.37	126.06	119.99
1	B	107	GLN	CA-C-N	5.36	126.84	120.14
1	B	107	GLN	C-N-CA	5.36	126.84	120.14
1	A	75	GLU	O-C-N	-5.36	115.95	122.22
1	A	151	ASP	O-C-N	-5.36	116.44	122.12
1	C	27	ALA	O-C-N	-5.35	116.31	122.09
1	B	312	TYR	CA-C-N	5.35	127.39	120.44
1	B	312	TYR	C-N-CA	5.35	127.39	120.44
1	C	312	TYR	O-C-N	-5.35	116.56	122.07
1	C	163	THR	CA-C-O	5.34	126.18	120.46
1	D	16	MET	CA-C-O	-5.34	114.88	120.55
1	B	305	HIS	CA-CB-CG	-5.34	108.46	113.80
1	C	287	GLN	N-CA-CB	5.34	120.04	110.80
1	D	19	ALA	O-C-N	-5.34	116.06	122.15
1	A	260	ASP	CA-C-N	5.34	127.87	120.29
1	A	260	ASP	C-N-CA	5.34	127.87	120.29
1	D	78	THR	CA-C-N	5.34	127.87	120.29
1	D	78	THR	C-N-CA	5.34	127.87	120.29
1	B	75	GLU	CA-C-N	5.34	132.99	122.31
1	B	75	GLU	C-N-CA	5.34	132.99	122.31
1	A	61	ILE	N-CA-C	5.33	116.70	110.62
1	D	250	VAL	O-C-N	-5.33	116.34	121.83
1	C	214	LYS	O-C-N	-5.31	116.60	122.07
1	C	249	HIS	N-CA-C	5.31	122.10	110.80
1	D	231	GLY	O-C-N	-5.31	117.09	122.19
1	B	257	THR	CA-CB-CG2	5.30	119.51	110.50
1	C	118	PRO	N-CA-CB	5.29	107.88	103.17
1	C	198	MET	CA-C-O	5.29	126.16	120.55
1	D	152	LYS	CB-CG-CD	-5.29	99.13	111.30
1	D	57	VAL	N-CA-C	-5.29	107.15	112.17
1	D	118	PRO	N-CA-CB	5.28	108.03	103.27
1	A	177	ALA	CA-C-O	-5.28	114.95	120.55
1	C	68	LEU	CA-C-O	5.28	125.17	119.15
1	C	89	LEU	CA-C-N	5.27	127.34	120.28
1	C	89	LEU	C-N-CA	5.27	127.34	120.28
1	A	175	ASP	CA-C-O	-5.27	115.29	120.82
1	C	267	LEU	CA-C-O	5.26	126.13	120.55
1	A	103	ASP	CA-C-N	5.26	126.71	120.14
1	A	103	ASP	C-N-CA	5.26	126.71	120.14
1	C	199	ASN	N-CA-CB	-5.25	102.13	110.22
1	D	169	MET	CA-CB-CG	-5.25	103.61	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	PHE	CA-C-N	5.25	125.80	119.98
1	D	230	PHE	C-N-CA	5.25	125.80	119.98
1	C	107	GLN	CA-C-N	5.24	125.76	119.94
1	C	107	GLN	C-N-CA	5.24	125.76	119.94
1	A	54	VAL	CA-C-O	5.24	126.72	121.17
1	C	66	THR	O-C-N	-5.24	117.00	123.44
1	D	252	ARG	CG-CD-NE	-5.24	100.47	112.00
1	A	291	LEU	CA-C-O	-5.24	114.79	120.81
1	C	104	GLY	O-C-N	-5.24	116.95	122.13
1	A	222	GLU	CA-C-O	-5.23	114.19	120.10
1	B	148	ASP	CA-C-N	5.23	127.72	120.29
1	B	148	ASP	C-N-CA	5.23	127.72	120.29
1	C	163	THR	N-CA-C	5.23	117.25	107.99
1	D	215	HIS	CB-CG-ND1	-5.23	114.86	122.70
1	D	74	PRO	N-CA-CB	5.23	108.53	103.51
1	A	176	ILE	CA-C-O	-5.22	115.63	121.17
1	A	117	PHE	CA-C-O	5.22	124.53	119.62
1	B	282	ARG	CA-CB-CG	5.22	124.53	114.10
1	A	101	GLY	N-CA-C	5.21	118.09	110.63
1	B	206	LYS	O-C-N	-5.21	116.21	122.15
1	A	186	ALA	CA-C-N	5.20	129.48	120.58
1	A	186	ALA	C-N-CA	5.20	129.48	120.58
1	B	69	TYR	N-CA-CB	5.20	119.28	110.49
1	D	312	TYR	O-C-N	-5.20	116.72	122.07
1	A	247	LEU	N-CA-C	5.20	117.03	111.36
1	A	148	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	283	CYS	CA-C-O	-5.20	114.69	120.66
1	C	273	GLU	CA-C-O	-5.19	115.36	121.07
1	C	230	PHE	CA-C-N	5.19	125.74	119.98
1	C	230	PHE	C-N-CA	5.19	125.74	119.98
1	A	144	ASN	O-C-N	-5.18	116.24	122.15
1	C	192	PRO	N-CA-CB	5.18	108.99	103.39
1	D	163	THR	O-C-N	-5.17	116.28	123.01
1	D	280	GLY	O-C-N	-5.17	118.76	123.57
1	A	127	ASP	CB-CA-C	-5.17	102.06	110.85
1	A	280	GLY	N-CA-C	-5.17	100.92	113.18
1	A	294	HIS	CB-CA-C	-5.17	99.19	109.79
1	A	59	ASP	N-CA-C	5.17	118.85	112.24
1	A	94	ILE	N-CA-C	-5.16	100.33	108.23
1	B	223	GLY	O-C-N	-5.16	116.86	122.54
1	D	144	ASN	CA-C-O	-5.16	114.95	120.42
1	D	58	GLY	CA-C-O	5.15	125.82	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ILE	CA-C-N	5.15	129.88	123.14
1	A	219	ILE	C-N-CA	5.15	129.88	123.14
1	D	159	SER	N-CA-C	5.14	121.76	110.80
1	C	249	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	129	ASP	O-C-N	-5.13	116.16	122.82
1	A	279	LYS	N-CA-C	-5.13	103.76	110.53
1	B	264	ALA	CA-C-N	5.12	127.41	120.44
1	B	264	ALA	C-N-CA	5.12	127.41	120.44
1	D	69	TYR	N-CA-CB	5.12	119.15	110.49
1	A	206	LYS	CA-C-N	5.12	127.45	120.54
1	A	206	LYS	C-N-CA	5.12	127.45	120.54
1	A	315	SER	CA-C-O	-5.12	114.32	120.10
1	C	3	ARG	CB-CA-C	-5.12	100.69	109.65
1	D	210	GLU	N-CA-CB	5.12	117.64	110.12
1	D	249	HIS	N-CA-C	5.12	120.43	113.37
1	D	310	ARG	CD-NE-CZ	5.12	131.56	124.40
1	D	107	GLN	O-C-N	-5.11	116.70	122.12
1	D	289	ASN	O-C-N	-5.11	115.70	122.40
1	D	130	ILE	N-CA-C	-5.11	97.08	107.92
1	B	28	ILE	O-C-N	-5.11	116.92	121.87
1	B	15	GLY	O-C-N	-5.10	116.60	122.42
1	D	195	ASP	N-CA-C	-5.10	101.96	110.17
1	D	59	ASP	CA-C-N	5.10	127.92	121.85
1	D	59	ASP	C-N-CA	5.10	127.92	121.85
1	A	105	SER	CA-C-N	5.10	127.11	120.28
1	A	105	SER	C-N-CA	5.10	127.11	120.28
1	D	104	GLY	CA-C-N	5.10	127.53	120.29
1	D	104	GLY	C-N-CA	5.10	127.53	120.29
1	B	288	ASN	O-C-N	-5.09	116.59	122.86
1	C	205	LEU	CA-C-N	5.09	127.41	120.54
1	C	205	LEU	C-N-CA	5.09	127.41	120.54
1	B	138	GLY	CA-C-O	5.09	124.46	119.37
1	C	199	ASN	CA-CB-CG	5.09	117.69	112.60
1	D	13	SER	CA-C-O	5.08	125.09	120.26
1	D	163	THR	N-CA-C	5.08	117.62	107.62
1	D	110	LYS	O-C-N	-5.07	116.85	122.07
1	A	309	GLN	O-C-N	-5.07	116.75	122.12
1	B	214	LYS	CA-C-N	5.07	131.32	122.81
1	B	214	LYS	C-N-CA	5.07	131.32	122.81
1	A	67	ILE	CA-C-N	5.06	131.54	122.38
1	A	67	ILE	C-N-CA	5.06	131.54	122.38
1	C	61	ILE	N-CA-C	5.06	117.38	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	286	ILE	CA-C-O	5.06	125.27	120.31
1	C	79	GLU	CA-C-O	5.06	125.79	119.97
1	D	105	SER	CA-C-N	5.06	128.00	120.31
1	D	105	SER	C-N-CA	5.06	128.00	120.31
1	C	67	ILE	CA-C-N	5.06	131.02	122.26
1	C	67	ILE	C-N-CA	5.06	131.02	122.26
1	A	170	GLY	CA-C-O	5.05	129.36	120.57
1	B	231	GLY	CA-C-O	-5.04	115.86	121.05
1	B	192	PRO	N-CA-CB	5.04	108.83	103.39
1	D	206	LYS	CA-C-N	5.04	126.99	120.44
1	D	206	LYS	C-N-CA	5.04	126.99	120.44
1	A	166	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	C	60	ILE	N-CA-C	-5.04	108.38	113.47
1	B	76	PHE	N-CA-C	5.03	119.14	113.15
1	A	125	THR	CA-C-O	-5.03	115.57	121.10
1	A	73	CYS	CA-C-O	5.03	126.07	120.34
1	B	7	LEU	CA-CB-CG	5.03	133.90	116.30
1	C	144	ASN	CA-C-N	5.03	127.27	120.38
1	C	144	ASN	C-N-CA	5.03	127.27	120.38
1	D	196	TYR	CA-C-N	-5.03	115.90	122.99
1	D	196	TYR	C-N-CA	-5.03	115.90	122.99
1	A	126	ILE	CA-C-N	5.02	127.42	120.29
1	A	126	ILE	C-N-CA	5.02	127.42	120.29
1	C	300	LEU	N-CA-C	5.02	118.89	112.87
1	B	237	ALA	N-CA-C	5.02	116.75	111.28
1	C	82	GLN	CA-C-N	5.02	127.00	120.28
1	C	82	GLN	C-N-CA	5.02	127.00	120.28
1	B	58	GLY	CA-C-O	5.01	126.09	121.58
1	B	117	PHE	CA-C-O	5.01	125.00	120.09
1	B	146	VAL	O-C-N	-5.01	116.14	121.80
1	B	286	ILE	O-C-N	-5.01	118.17	123.03
1	D	29	TYR	CA-C-O	-5.00	115.55	120.90

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ASP	Mainchain
1	A	144	ASN	Mainchain
1	A	214	LYS	Mainchain
1	A	280	GLY	Mainchain

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Mol	Chain	Res	Type	Group
1	A	288	ASN	Mainchain
1	A	293	ASP	Mainchain
1	A	308	ASP	Mainchain
1	A	90	LYS	Mainchain
1	B	113	THR	Mainchain
1	B	134	ASP	Mainchain
1	B	214	LYS	Mainchain
1	B	288	ASN	Mainchain
1	B	293	ASP	Mainchain
1	B	308	ASP	Mainchain
1	B	55	GLY	Mainchain
1	B	66	THR	Mainchain
1	C	288	ASN	Mainchain
1	D	113	THR	Mainchain
1	D	134	ASP	Mainchain
1	D	152	LYS	Mainchain
1	D	214	LYS	Mainchain
1	D	238	THR	Mainchain
1	D	288	ASN	Mainchain
1	D	293	ASP	Mainchain
1	D	55	GLY	Mainchain
1	D	74	PRO	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2341	0	2284	27	0
1	B	2349	0	2302	29	0
1	C	2355	0	2305	24	0
1	D	2374	0	2349	28	0
2	A	9	0	2	0	0
2	B	9	0	2	0	0
2	C	9	0	2	0	0
2	D	9	0	2	0	0
3	A	53	0	0	0	0
3	B	59	0	0	0	0
3	C	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	64	0	0	1	0
All	All	9681	0	9248	88	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 5.

All (88) 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:A:259[B]:PHE:CD2	1:B:259[B]:PHE:CD2	2.62	0.88
1:A:259[B]:PHE:HD2	1:B:259[B]:PHE:CE2	1.93	0.85
1:A:259[B]:PHE:CD2	1:B:259[B]:PHE:HD2	1.95	0.84
1:C:259[B]:PHE:CE2	1:D:259[B]:PHE:HD2	1.97	0.83
1:A:259[B]:PHE:CE2	1:B:259[B]:PHE:HD2	1.97	0.82
1:A:259[B]:PHE:HD2	1:B:259[B]:PHE:CD2	1.97	0.81
1:B:102:GLY:HA2	1:B:130:ILE:HD11	1.63	0.80
1:C:259[B]:PHE:CD2	1:D:259[B]:PHE:CD2	2.70	0.80
1:C:259[B]:PHE:HD2	1:D:259[B]:PHE:CE2	2.01	0.79
1:C:24:VAL:HA	1:C:34:VAL:HG21	1.65	0.79
1:A:102:GLY:HA2	1:A:130:ILE:HD11	1.71	0.71
1:C:259[B]:PHE:CE2	1:D:259[B]:PHE:CD2	2.81	0.69
1:D:102:GLY:HA2	1:D:130:ILE:HD11	1.75	0.69
1:C:235:GLN:HE21	1:C:241:GLU:HA	1.56	0.68
1:B:190:LEU:HD12	1:B:220:VAL:HG22	1.76	0.67
1:C:102:GLY:HA2	1:C:130:ILE:HD11	1.77	0.66
1:C:259[B]:PHE:HD2	1:D:259[B]:PHE:CD2	2.14	0.65
1:C:262:VAL:HG13	1:D:311:MET:HE1	1.78	0.64
1:B:287:GLN:HG3	1:B:292:VAL:HG21	1.78	0.64
1:D:24:VAL:HA	1:D:34:VAL:HG21	1.81	0.62
1:A:24:VAL:HA	1:A:34:VAL:HG21	1.82	0.62
1:C:259[B]:PHE:HE2	1:D:259[B]:PHE:HD2	1.45	0.61
1:C:187:GLU:HG2	1:C:204:ARG:HD2	1.83	0.61
1:B:7:LEU:HD22	1:B:99:VAL:HG22	1.86	0.58
1:C:259[B]:PHE:CD2	1:D:259[B]:PHE:CE2	2.86	0.56
1:B:24:VAL:HA	1:B:34:VAL:HG21	1.87	0.55
1:A:259[B]:PHE:CE2	1:B:259[B]:PHE:CD2	2.85	0.55
1:A:262:VAL:HG13	1:B:182:LEU:HD23	1.89	0.55
1:D:187:GLU:HG2	1:D:204:ARG:HD2	1.89	0.54
1:A:259[B]:PHE:CD2	1:B:259[B]:PHE:CE2	2.83	0.54
1:B:113:THR:HG21	1:B:281:GLY:HA2	1.91	0.53
1:A:259[B]:PHE:HD2	1:B:259[B]:PHE:HE2	1.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:LEU:HD12	1:A:220:VAL:HG22	1.91	0.51
1:B:60:ILE:HA	1:B:63:ARG:HG3	1.92	0.51
1:C:7:LEU:HD22	1:C:99:VAL:HG22	1.92	0.51
1:B:14:PRO:HG2	1:B:141:THR:HB	1.92	0.51
1:D:79:GLU:HG3	1:D:83:LYS:HE3	1.92	0.51
1:C:22:SER:HA	1:D:318:LEU:HD22	1.92	0.51
1:C:263:LEU:HG	1:C:267:LEU:HD22	1.93	0.51
1:A:198:MET:HE2	1:A:201:VAL:HG11	1.92	0.50
1:C:235:GLN:NE2	1:C:241:GLU:HA	2.26	0.49
1:A:32:VAL:HG21	1:A:276:LEU:HD21	1.94	0.49
1:B:8:THR:HG22	1:B:100:ILE:HB	1.94	0.48
1:B:7:LEU:HB2	1:B:37:VAL:HB	1.94	0.48
1:A:44:LEU:HD11	1:A:89:LEU:HG	1.95	0.48
1:A:235:GLN:HE21	1:A:241:GLU:HA	1.79	0.48
1:C:44:LEU:HD11	1:C:89:LEU:HG	1.96	0.48
1:A:60:ILE:HA	1:A:63:ARG:HG3	1.95	0.48
1:C:32:VAL:HG21	1:C:276:LEU:HD21	1.97	0.46
1:A:113:THR:HG21	1:A:281:GLY:HA2	1.96	0.46
1:D:49:ILE:HD12	1:D:92:HIS:ND1	2.30	0.46
1:D:113:THR:HG22	1:D:119:CYS:H	1.79	0.46
1:A:243:ARG:HA	1:A:243:ARG:HD3	1.89	0.46
1:D:86:ILE:HG23	1:D:117:PHE:CE2	2.51	0.46
1:A:62:HIS:CD2	1:A:62:HIS:H	2.34	0.45
1:D:204:ARG:HD3	3:D:371:HOH:O	2.15	0.45
1:D:13:SER:HB2	1:D:14:PRO:HD2	1.98	0.45
1:D:109:ALA:O	1:D:113:THR:HG23	2.16	0.45
1:C:266:ARG:HD2	1:D:311:MET:HE3	1.99	0.45
1:D:32:VAL:HG21	1:D:276:LEU:HD21	1.97	0.45
1:A:235:GLN:NE2	1:A:241:GLU:HA	2.32	0.45
1:C:110:LYS:HD2	1:C:297:ALA:HB2	1.99	0.45
1:D:79:GLU:O	1:D:83:LYS:HG2	2.16	0.45
1:B:38:TYR:O	1:B:43:GLY:HA3	2.17	0.44
1:B:267:LEU:HG	1:B:284:VAL:HG23	1.99	0.44
1:C:204:ARG:HD3	3:C:361:HOH:O	2.16	0.44
1:D:62:HIS:CD2	1:D:62:HIS:H	2.35	0.44
1:B:97:LEU:HB3	1:B:119:CYS:SG	2.58	0.44
1:A:158:THR:HG22	1:A:161:GLU:H	1.83	0.43
1:A:38:TYR:O	1:A:43:GLY:HA3	2.18	0.43
1:D:7:LEU:HB2	1:D:37:VAL:HB	2.01	0.43
1:C:38:TYR:O	1:C:43:GLY:HA3	2.19	0.43
1:C:62:HIS:CD2	1:C:62:HIS:H	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ALA:HB1	1:B:32:VAL:HB	2.00	0.43
1:B:62:HIS:CD2	1:B:62:HIS:H	2.36	0.43
1:A:308:ASP:HB3	1:A:311:MET:HB2	2.01	0.42
1:A:155:ASP:O	1:A:156:THR:C	2.62	0.42
1:A:152:LYS:HD2	1:D:250:VAL:HG13	2.02	0.42
1:B:235:GLN:NE2	1:B:241:GLU:HA	2.34	0.42
1:D:155:ASP:O	1:D:156:THR:C	2.63	0.42
1:B:13:SER:HB2	1:B:126:ILE:HG23	2.01	0.42
1:D:263:LEU:HG	1:D:267:LEU:HD22	2.02	0.41
1:D:38:TYR:O	1:D:43:GLY:HA3	2.20	0.41
1:A:166:ILE:HD13	1:A:217:ILE:HG23	2.02	0.41
1:B:263:LEU:HG	1:B:267:LEU:HD22	2.03	0.41
1:C:57:VAL:O	1:C:60:ILE:HG12	2.20	0.41
1:B:113:THR:HG21	1:B:281:GLY:CA	2.51	0.41
1:B:187:GLU:HB2	1:B:213:LYS:NZ	2.36	0.41

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	318/319 (100%)	307 (96%)	10 (3%)	1 (0%)	36	58
1	B	318/319 (100%)	308 (97%)	10 (3%)	0	100	100
1	C	318/319 (100%)	300 (94%)	17 (5%)	1 (0%)	36	58
1	D	318/319 (100%)	306 (96%)	11 (4%)	1 (0%)	36	58
All	All	1272/1276 (100%)	1221 (96%)	48 (4%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ASN
1	A	69	TYR
1	D	170	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	A	231/247 (94%)	205 (89%)	26 (11%)	5	12
1	B	234/247 (95%)	215 (92%)	19 (8%)	11	24
1	C	236/247 (96%)	212 (90%)	24 (10%)	7	15
1	D	240/247 (97%)	221 (92%)	19 (8%)	11	26
All	All	941/988 (95%)	853 (91%)	88 (9%)	8	18

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LEU
1	A	34	VAL
1	A	48	ASN
1	A	54	VAL
1	A	63	ARG
1	A	66	THR
1	A	87	GLU
1	A	110	LYS
1	A	117	PHE
1	A	159	SER
1	A	198	MET
1	A	204	ARG
1	A	205	LEU
1	A	207	ARG
1	A	211	ARG
1	A	213	LYS
1	A	218	ILE
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	243	ARG
1	A	279	LYS
1	A	290	GLN
1	A	306	THR
1	A	307	ILE
1	A	310	ARG
1	A	320	ILE
1	B	7	LEU
1	B	34	VAL
1	B	54	VAL
1	B	63	ARG
1	B	66	THR
1	B	70	THR
1	B	72	ARG
1	B	111	LYS
1	B	198	MET
1	B	205	LEU
1	B	210	GLU
1	B	211	ARG
1	B	267	LEU
1	B	277	GLU
1	B	279	LYS
1	B	286	ILE
1	B	290	GLN
1	B	306	THR
1	B	310	ARG
1	C	1	MET
1	C	3	ARG
1	C	7	LEU
1	C	22	SER
1	C	48	ASN
1	C	49	ILE
1	C	54	VAL
1	C	63	ARG
1	C	66	THR
1	C	82	GLN
1	C	99	VAL
1	C	105	SER
1	C	117	PHE
1	C	188	THR
1	C	205	LEU
1	C	215	HIS

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Mol	Chain	Res	Type
1	C	267	LEU
1	C	279	LYS
1	C	286	ILE
1	C	290	GLN
1	C	298	GLU
1	C	307	ILE
1	C	310	ARG
1	C	319	SER
1	D	7	LEU
1	D	8	THR
1	D	48	ASN
1	D	54	VAL
1	D	63	ARG
1	D	66	THR
1	D	83	LYS
1	D	84	LYS
1	D	91	LYS
1	D	202	ILE
1	D	205	LEU
1	D	214	LYS
1	D	267	LEU
1	D	270	ARG
1	D	306	THR
1	D	307	ILE
1	D	310	ARG
1	D	319	SER
1	D	320	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	235	GLN
1	B	62	HIS
1	B	88	GLN
1	B	92	HIS
1	B	235	GLN
1	B	287	GLN
1	B	294	HIS
1	C	82	GLN
1	C	235	GLN
1	C	287	GLN

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Mol	Chain	Res	Type
1	C	288	ASN
1	D	62	HIS
1	D	288	ASN
1	D	294	HIS

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 ⓘ

4 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	$\# Z > 2$
2	PGA	B	325	-	8,8,8	1.93	1 (12%)	10,11,11	1.29	0
2	PGA	C	325	-	8,8,8	1.83	1 (12%)	10,11,11	2.01	2 (20%)
2	PGA	A	325	-	8,8,8	1.84	1 (12%)	10,11,11	1.60	1 (10%)
2	PGA	D	325	-	8,8,8	1.89	1 (12%)	10,11,11	1.46	1 (10%)

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
2	PGA	B	325	-	-	0/6/6/6	-
2	PGA	C	325	-	-	3/6/6/6	-
2	PGA	A	325	-	-	0/6/6/6	-
2	PGA	D	325	-	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	325	PGA	O1-C1	4.53	1.36	1.22
2	A	325	PGA	O1-C1	4.53	1.36	1.22
2	B	325	PGA	O1-C1	4.38	1.36	1.22
2	C	325	PGA	O1-C1	4.36	1.36	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	325	PGA	O1P-C2-C1	-5.07	102.89	110.54
2	A	325	PGA	O1P-C2-C1	-4.27	104.11	110.54
2	D	325	PGA	O1P-C2-C1	-3.35	105.48	110.54
2	C	325	PGA	O3P-P-O1P	2.87	114.17	106.67

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	325	PGA	C2-O1P-P-O3P
2	C	325	PGA	C2-O1P-P-O4P
2	C	325	PGA	C2-O1P-P-O2P

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	319/319 (100%)	-0.65	0 100 100	8, 29, 58, 71	1 (0%)
1	B	319/319 (100%)	-0.66	1 (0%) 90 88	10, 29, 61, 72	1 (0%)
1	C	319/319 (100%)	-0.63	1 (0%) 90 88	9, 31, 63, 83	1 (0%)
1	D	319/319 (100%)	-0.82	0 100 100	9, 26, 45, 63	1 (0%)
All	All	1276/1276 (100%)	-0.69	2 (0%) 91 90	8, 28, 59, 83	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	GLU	2.4
1	C	160	HIS	2.1

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($\text{\AA}^2$)	Q<0.9
2	PGA	A	325	9/9	0.97	0.07	33,34,37,37	0
2	PGA	B	325	9/9	0.98	0.05	28,30,39,40	0
2	PGA	C	325	9/9	0.98	0.05	31,33,38,39	0
2	PGA	D	325	9/9	0.98	0.05	33,34,39,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.