



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:24 AM UTC

PDB ID : 1DCU / pdb_00001dcu
Title : REDOX SIGNALING IN THE CHLOROPLAST: STRUCTURE OF OXIDIZED PEA FRUCTOSE-1,6-BISPHOSPHATE PHOSPHATASE
Authors : Chiadmi, M.; Navaza, A.; Miginiac-Maslow, M.; Jacquot, J.P.; Cherfils, J.
Deposited on : 1999-11-05
Resolution : 2.20 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

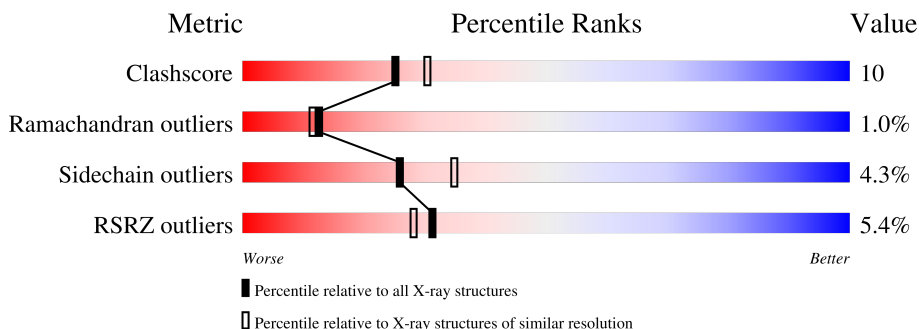
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	357	6% 52% 30% 10% • 8%
1	B	357	3% 54% 32% • • 10%
1	C	357	5% 54% 29% 7% • 8%
1	D	357	6% 54% 31% 6% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10102 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 FRUCTOSE-1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2507	1590	408	499	10			
1	B	323	Total	C	N	O	S	0	0	0
			2449	1558	401	480	10			
1	C	328	Total	C	N	O	S	0	0	0
			2497	1586	411	490	10			
1	D	325	Total	C	N	O	S	0	0	0
			2454	1561	402	481	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	ILE	engineered mutation	UNP P46275
B	103	ALA	ILE	engineered mutation	UNP P46275
C	103	ALA	ILE	engineered mutation	UNP P46275
D	103	ALA	ILE	engineered mutation	UNP P46275
A	232	LYS	GLU	engineered mutation	UNP P46275
B	232	LYS	GLU	engineered mutation	UNP P46275
C	232	LYS	GLU	engineered mutation	UNP P46275
D	232	LYS	GLU	engineered mutation	UNP P46275

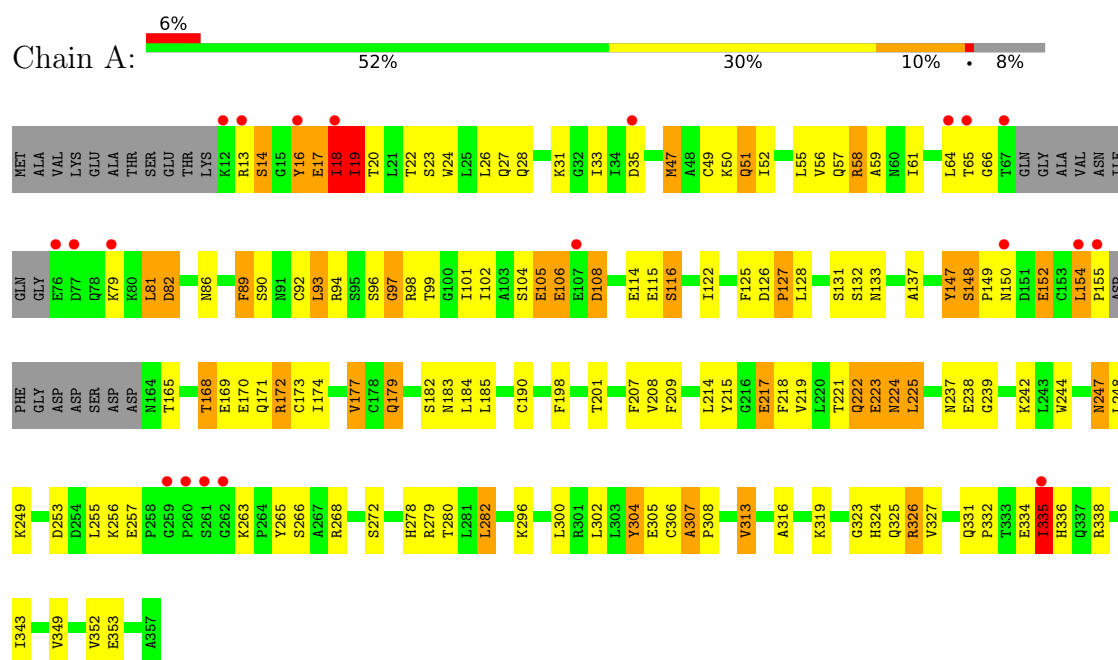
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	56	Total	O	0	0
			56	56		
2	C	47	Total	O	0	0
			47	47		
2	D	52	Total	O	0	0
			52	52		

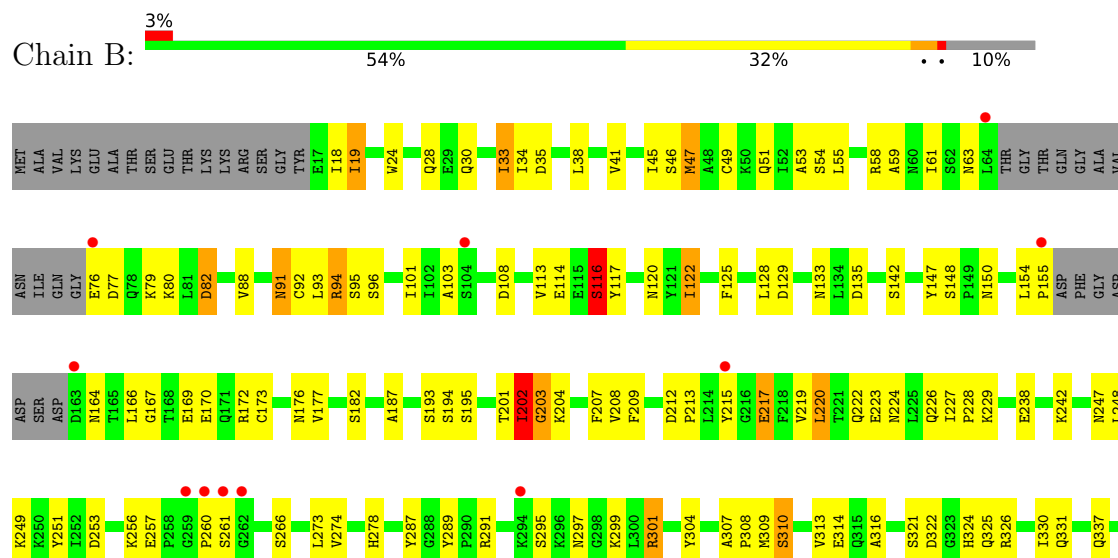
3 Residue-property plots [i](#)

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: FRUCTOSE-1,6-BISPHOSPHATASE

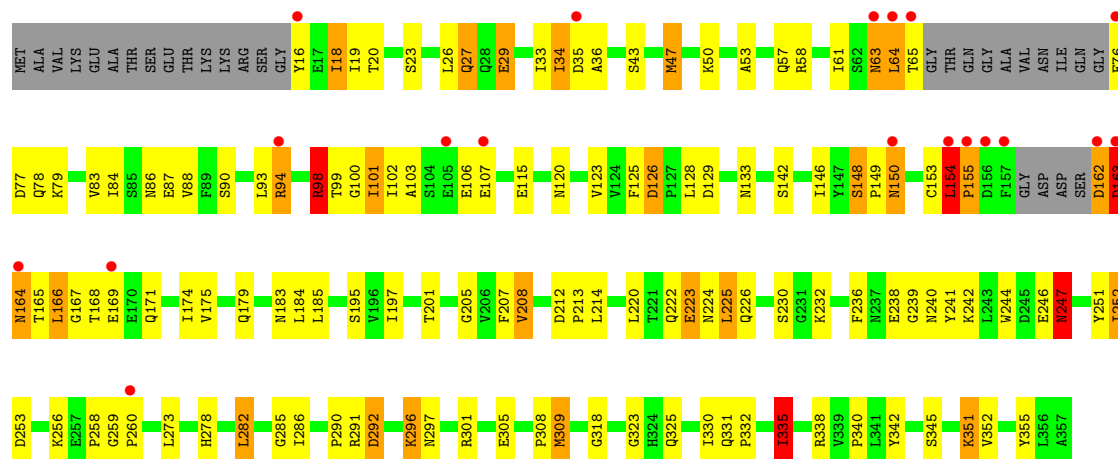


• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE

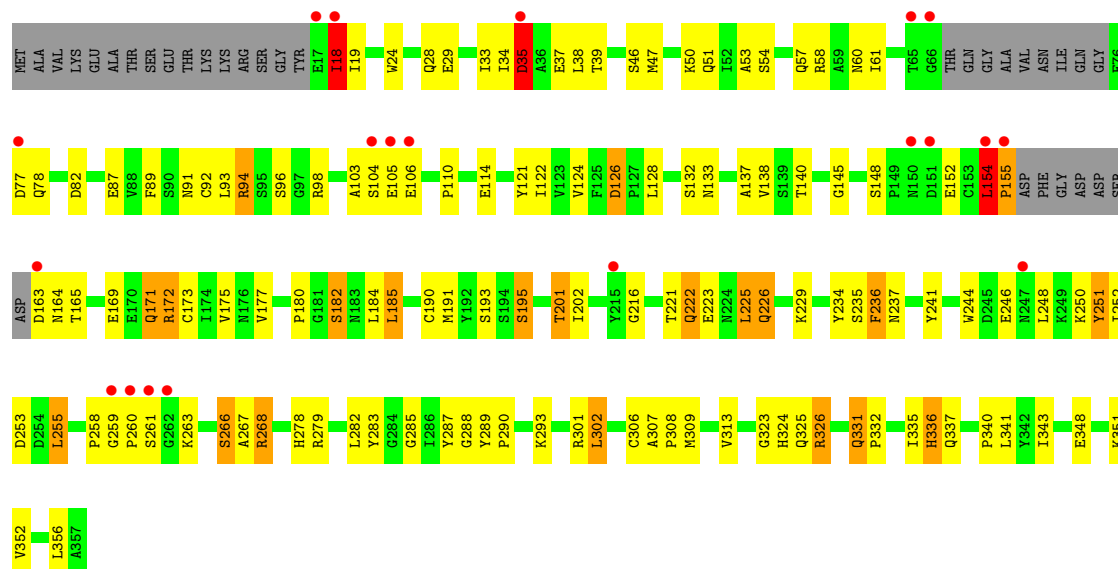




• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



• Molecule 1: FRUCTOSE-1,6-BISPHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.60Å 126.32Å 78.02Å 90.00° 97.73° 90.00°	Depositor
Resolution (Å)	23.80 – 2.20 23.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (23.80-2.20) 99.5 (23.80-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.247 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10102	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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

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	1.13	2/2553 (0.1%)	2.30	131/3463 (3.8%)
1	B	1.33	6/2493 (0.2%)	2.42	126/3383 (3.7%)
1	C	1.20	2/2541 (0.1%)	2.39	132/3444 (3.8%)
1	D	1.19	4/2499 (0.2%)	2.27	128/3393 (3.8%)
All	All	1.21	14/10086 (0.1%)	2.35	517/13683 (3.8%)

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	5
1	B	0	3
1	C	0	1
1	D	0	2
All	All	0	11

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ILE	C-O	11.04	1.37	1.24
1	B	202	ILE	CA-C	-8.43	1.42	1.52
1	B	278	HIS	CE1-NE2	-6.48	1.26	1.32
1	B	219	VAL	N-CA	-5.99	1.39	1.46
1	A	57	GLN	N-CA	-5.78	1.39	1.46
1	C	47	MET	C-N	5.70	1.41	1.33
1	D	190	CYS	CA-CB	-5.61	1.44	1.53
1	C	259	GLY	N-CA	5.34	1.52	1.44
1	B	208	VAL	N-CA	-5.29	1.39	1.46
1	A	219	VAL	CA-CB	5.15	1.60	1.54
1	D	35	ASP	CA-CB	5.14	1.60	1.53
1	B	193	SER	CA-C	-5.10	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	259	GLY	N-CA	5.10	1.51	1.44
1	D	37	GLU	N-CA	-5.01	1.40	1.46

All (517) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ILE	CA-C-O	-32.56	80.08	120.78
1	C	162	ASP	CA-C-N	27.90	174.83	121.54
1	C	162	ASP	C-N-CA	27.90	174.83	121.54
1	A	108	ASP	CA-CB-CG	16.77	129.37	112.60
1	B	120	ASN	CA-CB-CG	-13.63	98.97	112.60
1	B	202	ILE	CA-C-N	12.93	147.01	121.53
1	B	202	ILE	C-N-CA	12.93	147.01	121.53
1	C	247	ASN	CA-CB-CG	12.92	125.52	112.60
1	B	202	ILE	N-CA-C	-12.18	84.00	109.34
1	B	117	TYR	CA-C-N	11.33	137.53	120.31
1	B	117	TYR	C-N-CA	11.33	137.53	120.31
1	B	35	ASP	N-CA-CB	-11.12	94.53	110.44
1	A	325	GLN	OE1-CD-NE2	10.95	133.55	122.60
1	C	297	ASN	OD1-CG-ND2	10.87	133.47	122.60
1	A	82	ASP	CA-CB-CG	10.29	122.89	112.60
1	B	182	SER	CB-CA-C	10.17	122.28	109.16
1	C	98	ARG	CD-NE-CZ	10.00	138.41	124.40
1	D	236	PHE	CA-CB-CG	9.99	123.79	113.80
1	A	51	GLN	OE1-CD-NE2	-9.91	112.69	122.60
1	D	94	ARG	NE-CZ-NH2	9.73	127.96	119.20
1	D	164	ASN	CA-CB-CG	-9.65	102.95	112.60
1	D	268	ARG	NE-CZ-NH2	9.63	127.87	119.20
1	B	224	ASN	CA-CB-CG	-9.62	102.98	112.60
1	B	223	GLU	CA-C-O	-9.45	110.13	121.28
1	B	222	GLN	CB-CG-CD	9.37	128.52	112.60
1	C	278	HIS	CA-C-O	-9.30	111.05	120.82
1	D	248	LEU	CA-C-O	-9.30	111.11	120.70
1	B	82	ASP	CA-CB-CG	9.28	121.88	112.60
1	C	225	LEU	O-C-N	-9.26	111.67	122.97
1	C	162	ASP	O-C-N	-9.19	108.30	123.00
1	C	325	GLN	OE1-CD-NE2	9.05	131.65	122.60
1	C	29	GLU	CA-CB-CG	9.01	132.13	114.10
1	C	99	THR	CA-C-N	-8.99	114.27	121.82
1	C	99	THR	C-N-CA	-8.99	114.27	121.82
1	C	126	ASP	CA-C-O	-8.91	113.50	119.29
1	D	82	ASP	CA-CB-CG	8.90	121.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	LYS	CA-C-O	8.85	130.27	119.38
1	C	205	GLY	N-CA-C	-8.79	103.61	111.95
1	B	325	GLN	OE1-CD-NE2	8.70	131.29	122.60
1	C	205	GLY	CA-C-N	8.60	133.91	122.90
1	C	205	GLY	C-N-CA	8.60	133.91	122.90
1	B	94	ARG	NE-CZ-NH2	8.59	126.93	119.20
1	C	162	ASP	CA-C-O	8.59	135.39	120.80
1	D	237	ASN	OD1-CG-ND2	-8.53	114.07	122.60
1	B	94	ARG	NE-CZ-NH1	-8.51	112.99	121.50
1	D	195	SER	CA-CB-OG	-8.46	94.19	111.10
1	B	212	ASP	CA-C-O	8.44	124.78	119.29
1	A	225	LEU	O-C-N	-8.41	112.53	122.87
1	C	20	THR	CA-CB-OG1	-8.40	97.00	109.60
1	A	152	GLU	N-CA-CB	-8.40	97.59	111.20
1	D	184	LEU	CA-C-O	-8.29	112.02	120.98
1	D	260	PRO	CA-C-N	8.28	135.62	121.14
1	D	260	PRO	C-N-CA	8.28	135.62	121.14
1	D	287	TYR	CA-C-N	-8.24	115.27	121.61
1	D	287	TYR	C-N-CA	-8.24	115.27	121.61
1	C	223	GLU	CA-C-O	-8.18	112.04	120.71
1	A	57	GLN	O-C-N	8.12	131.73	122.22
1	B	222	GLN	OE1-CD-NE2	-8.12	114.48	122.60
1	C	163	ASP	N-CA-C	-8.10	93.54	110.80
1	B	92	CYS	CA-C-N	-8.06	110.03	122.60
1	B	92	CYS	C-N-CA	-8.06	110.03	122.60
1	C	35	ASP	N-CA-CB	-8.03	98.25	110.45
1	D	104	SER	N-CA-CB	8.02	123.94	110.87
1	A	326	ARG	CD-NE-CZ	8.01	135.61	124.40
1	A	237	ASN	CA-CB-CG	-8.00	104.60	112.60
1	A	147	TYR	CB-CG-CD1	7.96	132.74	120.80
1	B	53	ALA	CA-C-N	7.94	130.92	120.28
1	B	53	ALA	C-N-CA	7.94	130.92	120.28
1	B	194	SER	CA-C-O	7.92	128.96	119.61
1	A	253	ASP	CA-CB-CG	7.88	120.48	112.60
1	C	155	PRO	N-CA-CB	7.86	111.51	103.25
1	C	58	ARG	NH1-CZ-NH2	7.81	129.46	119.30
1	A	266	SER	CA-C-O	-7.81	111.94	120.92
1	C	323	GLY	O-C-N	7.81	130.11	122.77
1	A	28	GLN	O-C-N	7.80	131.04	122.15
1	B	203	GLY	N-CA-C	7.79	126.13	115.30
1	D	195	SER	CA-C-O	-7.77	112.33	121.11
1	B	91	ASN	CA-CB-CG	-7.77	104.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	58	ARG	NE-CZ-NH2	-7.76	112.22	119.20
1	D	126	ASP	N-CA-CB	-7.71	100.38	110.17
1	D	87	GLU	CB-CG-CD	7.68	125.67	112.60
1	C	183	ASN	CA-CB-CG	-7.68	104.92	112.60
1	A	99	THR	CA-C-N	-7.66	115.65	122.47
1	A	99	THR	C-N-CA	-7.66	115.65	122.47
1	C	27	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	A	279	ARG	CD-NE-CZ	7.65	135.10	124.40
1	D	258	PRO	CA-C-O	-7.61	113.09	121.23
1	C	58	ARG	CD-NE-CZ	-7.54	113.84	124.40
1	D	337	GLN	O-C-N	-7.52	113.63	122.95
1	D	103	ALA	N-CA-CB	-7.51	98.84	110.56
1	A	326	ARG	NE-CZ-NH1	7.48	128.98	121.50
1	D	348	GLU	O-C-N	7.47	130.67	122.15
1	C	223	GLU	CB-CG-CD	-7.45	99.94	112.60
1	D	61	ILE	CA-C-N	7.42	130.55	120.38
1	D	61	ILE	C-N-CA	7.42	130.55	120.38
1	B	301	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	A	28	GLN	N-CA-CB	7.39	121.09	110.16
1	C	154	LEU	O-C-N	7.36	129.78	121.32
1	B	182	SER	CA-C-O	-7.31	110.13	118.47
1	D	326	ARG	CD-NE-CZ	-7.29	114.19	124.40
1	A	338	ARG	NH1-CZ-NH2	7.29	128.77	119.30
1	B	228	PRO	N-CA-CB	7.26	109.42	103.32
1	A	23	SER	CA-CB-OG	-7.24	96.63	111.10
1	A	334	GLU	CA-C-N	7.22	134.97	121.97
1	A	334	GLU	C-N-CA	7.22	134.97	121.97
1	A	57	GLN	CA-C-O	-7.21	111.96	120.10
1	B	217	GLU	CA-C-N	7.21	132.17	121.72
1	B	217	GLU	C-N-CA	7.21	132.17	121.72
1	D	182	SER	CA-C-N	-7.19	111.19	122.49
1	D	182	SER	C-N-CA	-7.19	111.19	122.49
1	A	27	GLN	CB-CG-CD	7.19	124.82	112.60
1	A	98	ARG	CA-C-N	-7.17	112.87	122.99
1	A	98	ARG	C-N-CA	-7.17	112.87	122.99
1	B	61	ILE	CA-C-N	7.17	129.88	120.28
1	B	61	ILE	C-N-CA	7.17	129.88	120.28
1	B	209	PHE	O-C-N	-7.16	114.78	123.30
1	A	207	PHE	CA-CB-CG	-7.16	106.64	113.80
1	B	260	PRO	N-CA-CB	7.12	110.35	103.51
1	A	24	TRP	CA-C-O	-7.11	112.06	120.10
1	C	77	ASP	CA-CB-CG	7.11	119.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ILE	O-C-N	7.09	129.13	121.83
1	C	179	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	C	148	SER	CA-C-O	-7.05	114.00	119.71
1	A	126	ASP	CA-CB-CG	7.03	119.62	112.60
1	A	50	LYS	N-CA-CB	7.02	120.54	110.16
1	A	300	LEU	CA-C-O	-6.98	113.51	121.19
1	C	34	ILE	CA-C-N	6.93	135.87	121.32
1	C	34	ILE	C-N-CA	6.93	135.87	121.32
1	B	46	SER	CA-C-O	-6.93	112.00	119.97
1	A	16	TYR	O-C-N	-6.92	116.61	123.46
1	B	223	GLU	O-C-N	6.92	131.06	123.10
1	C	278	HIS	O-C-N	6.88	129.15	122.07
1	D	331	GLN	CA-C-O	6.86	127.30	119.61
1	C	86	ASN	CA-CB-CG	-6.85	105.75	112.60
1	C	212	ASP	CA-CB-CG	-6.85	105.75	112.60
1	C	260	PRO	N-CA-C	-6.85	104.60	113.57
1	C	224	ASN	CA-CB-CG	-6.84	105.75	112.60
1	B	202	ILE	CB-CA-C	6.84	122.51	111.29
1	B	58	ARG	CD-NE-CZ	-6.83	114.84	124.40
1	D	251	TYR	CA-C-O	-6.83	113.26	120.63
1	A	28	GLN	CA-C-O	-6.82	113.19	120.42
1	C	239	GLY	N-CA-C	-6.80	105.93	114.16
1	D	133	ASN	CA-CB-CG	6.79	119.39	112.60
1	C	50	LYS	N-CA-CB	6.76	119.81	110.01
1	D	325	GLN	N-CA-CB	-6.75	99.94	111.69
1	D	39	THR	CA-C-O	-6.72	113.29	120.42
1	C	225	LEU	CA-C-O	6.72	128.54	121.15
1	C	58	ARG	N-CA-C	-6.71	104.72	113.17
1	C	207	PHE	CA-CB-CG	-6.71	107.09	113.80
1	A	263	LYS	CA-C-O	6.70	126.82	119.32
1	D	180	PRO	CA-C-N	6.65	128.66	120.22
1	D	180	PRO	C-N-CA	6.65	128.66	120.22
1	C	225	LEU	CA-C-N	6.64	132.14	122.77
1	C	225	LEU	C-N-CA	6.64	132.14	122.77
1	B	41	VAL	N-CA-CB	6.64	118.32	110.55
1	D	279	ARG	NE-CZ-NH2	-6.63	113.23	119.20
1	A	296	LYS	CA-C-O	6.62	127.52	119.38
1	D	140	THR	CA-C-O	-6.60	114.12	121.05
1	A	137	ALA	CA-C-O	-6.59	113.85	120.90
1	A	172	ARG	NE-CZ-NH1	-6.59	114.91	121.50
1	D	173	CYS	O-C-N	-6.57	115.31	122.07
1	C	301	ARG	NE-CZ-NH1	-6.56	114.94	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	SER	N-CA-C	-6.55	97.83	108.52
1	D	216	GLY	CA-C-O	-6.55	111.14	119.13
1	D	337	GLN	CA-C-O	6.54	128.38	120.92
1	B	30	GLN	CA-C-O	-6.53	112.99	120.24
1	C	29	GLU	CB-CG-CD	6.52	123.69	112.60
1	B	330	ILE	O-C-N	-6.52	115.57	122.68
1	B	260	PRO	CA-C-O	6.51	128.11	119.00
1	A	280	THR	CA-C-O	6.49	127.43	120.55
1	A	223	GLU	CA-C-N	-6.46	113.19	122.36
1	A	223	GLU	C-N-CA	-6.46	113.19	122.36
1	B	260	PRO	CA-C-N	6.46	131.50	120.72
1	B	260	PRO	C-N-CA	6.46	131.50	120.72
1	B	117	TYR	O-C-N	-6.45	114.68	122.22
1	A	89	PHE	CA-C-O	-6.43	114.06	120.82
1	A	116	SER	O-C-N	-6.43	114.96	122.87
1	C	258	PRO	CA-C-N	-6.43	111.77	121.87
1	C	258	PRO	C-N-CA	-6.43	111.77	121.87
1	B	260	PRO	N-CA-C	-6.43	105.83	113.86
1	A	22	THR	CA-CB-OG1	-6.42	99.96	109.60
1	C	253	ASP	CA-CB-CG	-6.42	106.18	112.60
1	A	305	GLU	CA-CB-CG	-6.41	101.28	114.10
1	A	17	GLU	O-C-N	-6.40	115.72	123.27
1	C	246	GLU	CA-C-O	-6.40	114.05	120.90
1	B	207	PHE	CA-CB-CG	-6.39	107.41	113.80
1	A	35	ASP	O-C-N	-6.38	115.79	122.94
1	B	34	ILE	CA-C-O	6.37	128.03	121.28
1	C	285	GLY	CA-C-N	-6.37	112.14	122.33
1	C	285	GLY	C-N-CA	-6.37	112.14	122.33
1	A	35	ASP	N-CA-CB	-6.36	100.28	110.46
1	D	278	HIS	CA-C-O	-6.36	114.14	120.82
1	C	53	ALA	CA-C-N	6.36	128.80	120.28
1	C	53	ALA	C-N-CA	6.36	128.80	120.28
1	C	103	ALA	CA-C-N	6.35	129.77	120.82
1	C	103	ALA	C-N-CA	6.35	129.77	120.82
1	D	163	ASP	CA-C-N	6.35	132.95	122.73
1	D	163	ASP	C-N-CA	6.35	132.95	122.73
1	A	326	ARG	NH1-CZ-NH2	-6.35	111.05	119.30
1	A	23	SER	CA-C-O	-6.33	113.84	120.55
1	D	165	THR	CA-CB-OG1	-6.33	100.11	109.60
1	C	47	MET	CA-C-N	-6.33	111.80	120.28
1	C	47	MET	C-N-CA	-6.33	111.80	120.28
1	B	92	CYS	CA-C-O	-6.33	111.60	119.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	SER	N-CA-CB	-6.32	101.92	111.15
1	A	147	TYR	CB-CG-CD2	-6.32	111.32	120.80
1	C	83	VAL	N-CA-C	6.32	117.10	110.72
1	A	182	SER	CA-C-N	-6.31	112.58	122.49
1	A	182	SER	C-N-CA	-6.31	112.58	122.49
1	D	340	PRO	CA-C-O	-6.31	113.97	121.67
1	A	201	THR	CA-CB-CG2	6.31	121.22	110.50
1	D	175	VAL	CA-C-O	-6.30	113.83	120.57
1	B	187	ALA	O-C-N	6.28	130.55	123.27
1	D	98	ARG	CA-C-O	6.27	128.13	120.92
1	C	292	ASP	CA-CB-CG	-6.26	106.34	112.60
1	A	247	ASN	OD1-CG-ND2	6.24	128.84	122.60
1	C	100	GLY	O-C-N	-6.23	118.18	123.60
1	D	77	ASP	CA-C-O	6.22	127.79	120.20
1	A	239	GLY	CA-C-N	6.21	133.24	122.56
1	A	239	GLY	C-N-CA	6.21	133.24	122.56
1	C	155	PRO	N-CA-C	-6.21	99.68	112.47
1	D	236	PHE	CG-CD1-CE1	6.20	131.23	120.70
1	D	225	LEU	CA-C-O	-6.19	114.99	121.55
1	A	221	THR	N-CA-C	-6.19	105.42	114.39
1	D	331	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	D	289	TYR	O-C-N	6.17	126.92	121.37
1	D	323	GLY	N-CA-C	-6.15	106.62	114.37
1	C	351	LYS	O-C-N	-6.15	115.74	122.07
1	C	345	SER	CA-C-O	6.14	127.65	120.96
1	B	35	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	49	CYS	CA-C-N	6.13	129.00	120.29
1	A	49	CYS	C-N-CA	6.13	129.00	120.29
1	B	108	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	208	VAL	CA-C-O	6.12	127.21	120.48
1	D	287	TYR	CA-C-O	-6.12	114.10	120.70
1	B	325	GLN	N-CA-CB	-6.11	100.92	111.55
1	D	285	GLY	CA-C-N	-6.11	113.54	122.58
1	D	285	GLY	C-N-CA	-6.11	113.54	122.58
1	C	77	ASP	CA-C-O	6.11	127.93	120.60
1	A	352	VAL	CA-C-O	6.10	127.29	120.95
1	D	202	ILE	CA-C-N	-6.09	112.94	122.51
1	D	202	ILE	C-N-CA	-6.09	112.94	122.51
1	C	155	PRO	O-C-N	6.06	130.82	122.64
1	D	222	GLN	CA-C-O	6.05	127.52	120.14
1	C	345	SER	O-C-N	-6.03	115.82	123.06
1	B	337	GLN	CA-C-O	6.03	127.56	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	145	GLY	N-CA-C	-6.02	100.92	111.46
1	B	287	TYR	O-C-N	6.02	130.62	123.27
1	B	195	SER	O-C-N	-6.00	115.91	123.17
1	C	148	SER	CA-C-N	6.00	126.19	120.31
1	C	148	SER	C-N-CA	6.00	126.19	120.31
1	C	87	GLU	CA-C-N	-6.00	111.90	120.42
1	C	87	GLU	C-N-CA	-6.00	111.90	120.42
1	B	54	SER	CA-C-O	-5.99	114.20	120.55
1	D	78	GLN	O-C-N	-5.99	115.77	122.12
1	B	247	ASN	CA-CB-CG	5.99	118.59	112.60
1	C	338	ARG	CD-NE-CZ	5.98	132.77	124.40
1	A	278	HIS	CA-CB-CG	-5.97	107.83	113.80
1	C	282	LEU	CA-C-O	-5.97	114.17	120.55
1	B	215	TYR	CA-C-O	5.96	125.60	119.05
1	A	59	ALA	CA-C-O	-5.95	114.53	120.90
1	D	309	MET	CA-C-N	5.95	128.73	120.29
1	D	309	MET	C-N-CA	5.95	128.73	120.29
1	B	80	LYS	CA-C-O	5.94	126.72	120.42
1	B	226	GLN	CA-CB-CG	-5.94	102.22	114.10
1	C	286	ILE	CA-C-O	-5.94	114.28	120.64
1	B	177	VAL	O-C-N	-5.94	113.68	121.82
1	A	323	GLY	N-CA-C	-5.94	107.20	114.92
1	B	253	ASP	CA-C-O	-5.93	114.26	120.55
1	D	290	PRO	CB-CA-C	-5.93	102.27	111.22
1	B	101	ILE	N-CA-C	5.92	116.39	107.80
1	A	126	ASP	CA-C-N	5.92	125.12	118.97
1	A	126	ASP	C-N-CA	5.92	125.12	118.97
1	C	184	LEU	CA-C-O	-5.92	114.59	120.98
1	A	86	ASN	CA-CB-CG	-5.91	106.69	112.60
1	B	193	SER	O-C-N	-5.91	118.68	123.11
1	D	103	ALA	CA-C-N	5.89	131.43	122.95
1	D	103	ALA	C-N-CA	5.89	131.43	122.95
1	D	266	SER	CA-C-O	-5.89	114.01	120.43
1	A	24	TRP	O-C-N	5.89	129.11	122.22
1	D	94	ARG	CA-C-O	5.88	126.75	120.10
1	B	253	ASP	O-C-N	5.88	128.36	122.12
1	B	349	VAL	CA-C-O	5.88	127.08	120.85
1	D	34	ILE	CA-C-O	-5.88	115.05	121.28
1	D	60	ASN	CA-CB-CG	5.88	118.48	112.60
1	D	325	GLN	OE1-CD-NE2	5.87	128.47	122.60
1	D	331	GLN	CB-CA-C	5.87	116.53	109.31
1	B	129	ASP	O-C-N	5.87	129.38	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	GLU	N-CA-C	-5.85	105.45	112.59
1	B	59	ALA	CA-C-O	-5.84	114.32	120.63
1	D	35	ASP	N-CA-CB	-5.84	102.34	110.29
1	B	177	VAL	N-CA-CB	-5.83	99.93	110.95
1	C	125	PHE	CA-CB-CG	5.83	119.63	113.80
1	C	166	LEU	CA-C-N	-5.82	114.96	121.83
1	C	166	LEU	C-N-CA	-5.82	114.96	121.83
1	B	322	ASP	CA-C-O	-5.82	112.75	119.56
1	D	96	SER	CB-CA-C	-5.82	99.11	110.11
1	C	260	PRO	O-C-N	5.81	130.12	122.27
1	B	77	ASP	CA-C-O	5.81	127.43	120.28
1	D	201	THR	CA-CB-OG1	-5.81	100.89	109.60
1	D	290	PRO	CA-C-O	-5.80	114.14	122.31
1	A	319	LYS	CA-C-N	5.79	132.77	121.41
1	A	319	LYS	C-N-CA	5.79	132.77	121.41
1	C	345	SER	CA-C-N	5.79	129.51	120.82
1	C	345	SER	C-N-CA	5.79	129.51	120.82
1	C	195	SER	CA-CB-OG	-5.78	99.53	111.10
1	B	203	GLY	CA-C-O	5.78	126.18	119.13
1	B	18	ILE	CB-CA-C	5.77	117.95	110.96
1	B	91	ASN	CA-C-N	-5.77	111.08	120.72
1	B	91	ASN	C-N-CA	-5.77	111.08	120.72
1	C	33	ILE	O-C-N	-5.77	115.28	121.80
1	B	324	HIS	CA-CB-CG	-5.76	108.04	113.80
1	C	201	THR	CA-C-O	5.76	127.23	120.20
1	A	97	GLY	CA-C-O	-5.75	115.34	121.38
1	B	142	SER	CA-CB-OG	5.74	122.57	111.10
1	B	49	CYS	N-CA-CB	5.73	119.16	110.28
1	A	325	GLN	N-CA-CB	-5.72	101.93	111.20
1	D	124	VAL	N-CA-C	-5.72	99.40	107.75
1	A	304	TYR	CA-CB-CG	-5.72	103.61	113.90
1	A	249	LYS	N-CA-CB	5.71	118.62	110.06
1	B	55	LEU	CA-C-N	5.71	128.28	120.46
1	B	55	LEU	C-N-CA	5.71	128.28	120.46
1	B	103	ALA	CA-C-O	5.71	127.78	121.56
1	C	236	PHE	CA-CB-CG	5.70	119.50	113.80
1	D	46	SER	CA-C-O	-5.70	113.66	120.10
1	A	338	ARG	CG-CD-NE	-5.70	99.47	112.00
1	D	138	VAL	CA-C-O	5.69	124.84	118.98
1	D	182	SER	CA-C-O	-5.68	112.38	120.51
1	D	234	TYR	CA-C-N	-5.68	114.76	122.95
1	D	234	TYR	C-N-CA	-5.68	114.76	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	LYS	O-C-N	-5.67	116.27	123.24
1	D	343	ILE	O-C-N	5.67	129.00	122.82
1	D	137	ALA	CA-C-O	-5.66	114.52	120.63
1	B	116	SER	CA-CB-OG	-5.66	99.79	111.10
1	C	242	LYS	O-C-N	-5.64	114.92	122.43
1	D	35	ASP	CB-CA-C	-5.64	97.05	110.02
1	A	58	ARG	NH1-CZ-NH2	5.63	126.63	119.30
1	C	148	SER	O-C-N	5.63	126.54	120.85
1	C	297	ASN	CA-C-O	-5.63	113.14	119.95
1	D	226	GLN	CA-C-O	-5.62	114.08	120.32
1	C	323	GLY	CA-C-O	-5.62	114.67	119.56
1	A	334	GLU	N-CA-C	5.61	119.51	107.67
1	C	90	SER	N-CA-CB	5.61	118.15	110.01
1	C	232	LYS	CG-CD-CE	5.61	124.20	111.30
1	B	301	ARG	NH1-CZ-NH2	5.60	126.58	119.30
1	A	335	ILE	N-CA-C	5.59	120.97	109.34
1	D	34	ILE	CA-C-N	5.59	130.90	120.95
1	D	34	ILE	C-N-CA	5.59	130.90	120.95
1	B	34	ILE	O-C-N	-5.57	116.65	123.00
1	B	129	ASP	CA-C-O	-5.57	113.04	119.56
1	A	280	THR	O-C-N	-5.57	116.21	122.12
1	D	94	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	17	GLU	N-CA-CB	-5.56	101.82	110.55
1	A	92	CYS	CA-C-O	-5.56	112.54	119.38
1	B	227	ILE	CA-C-N	5.56	125.56	119.89
1	B	227	ILE	C-N-CA	5.56	125.56	119.89
1	A	125	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	335	ILE	CB-CG1-CD1	5.56	125.48	113.80
1	D	126	ASP	CA-C-N	5.56	125.22	119.05
1	D	126	ASP	C-N-CA	5.56	125.22	119.05
1	C	167	GLY	CA-C-O	-5.56	114.69	122.36
1	C	240	ASN	CB-CG-ND2	5.55	124.73	116.40
1	A	307	ALA	CA-C-O	-5.54	114.03	119.13
1	C	166	LEU	O-C-N	5.54	129.59	123.16
1	D	128	LEU	CA-C-O	-5.54	115.14	121.40
1	C	335	ILE	CA-CB-CG1	5.53	119.81	110.40
1	D	82	ASP	CA-C-O	5.52	126.40	120.55
1	D	121	TYR	CA-C-N	-5.51	115.33	122.99
1	D	121	TYR	C-N-CA	-5.51	115.33	122.99
1	D	253	ASP	CA-C-O	-5.51	113.87	120.10
1	A	182	SER	N-CA-C	5.51	120.51	113.18
1	A	56	VAL	O-C-N	-5.50	116.52	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	GLU	CA-C-N	-5.50	115.25	123.00
1	B	114	GLU	C-N-CA	-5.50	115.25	123.00
1	D	324	HIS	CA-CB-CG	-5.50	108.30	113.80
1	A	94	ARG	CD-NE-CZ	-5.49	116.71	124.40
1	C	201	THR	O-C-N	-5.49	116.25	123.28
1	A	28	GLN	OE1-CD-NE2	-5.48	117.12	122.60
1	C	150	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	C	340	PRO	CA-C-N	-5.47	114.31	122.74
1	C	340	PRO	C-N-CA	-5.47	114.31	122.74
1	A	127	PRO	O-C-N	5.47	128.35	122.17
1	A	19	ILE	CA-CB-CG2	-5.47	101.21	110.50
1	D	336	HIS	CA-CB-CG	-5.46	108.33	113.80
1	C	142	SER	O-C-N	-5.46	116.82	123.10
1	B	331	GLN	OE1-CD-NE2	5.45	128.05	122.60
1	B	125	PHE	N-CA-C	5.45	117.55	108.02
1	C	179	GLN	CB-CG-CD	5.44	121.85	112.60
1	C	36	ALA	CB-CA-C	-5.44	100.22	110.67
1	A	47	MET	O-C-N	-5.44	115.95	122.15
1	C	78	GLN	CA-C-N	5.44	127.51	120.44
1	C	78	GLN	C-N-CA	5.44	127.51	120.44
1	D	19	ILE	N-CA-CB	5.43	117.57	111.21
1	A	33	ILE	CA-C-O	5.43	126.34	120.47
1	B	120	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	C	167	GLY	O-C-N	5.42	129.99	122.84
1	D	105	GLU	CA-C-N	5.42	131.89	121.54
1	D	105	GLU	C-N-CA	5.42	131.89	121.54
1	B	133	ASN	CA-C-N	5.41	127.47	120.44
1	B	133	ASN	C-N-CA	5.41	127.47	120.44
1	C	128	LEU	CA-C-O	-5.40	115.46	121.51
1	B	148	SER	CA-C-N	5.39	125.59	120.31
1	B	148	SER	C-N-CA	5.39	125.59	120.31
1	A	168	THR	OG1-CB-CG2	-5.38	98.54	109.30
1	B	220	LEU	CA-C-O	-5.36	112.85	120.51
1	C	330	ILE	O-C-N	-5.36	116.86	122.81
1	A	20	THR	O-C-N	-5.35	116.75	122.85
1	A	224	ASN	CA-CB-CG	-5.34	107.26	112.60
1	B	113	VAL	N-CA-CB	5.34	118.58	111.64
1	B	326	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
1	A	18	ILE	N-CA-CB	5.34	118.40	111.67
1	A	324	HIS	CA-CB-CG	-5.34	108.46	113.80
1	A	81	LEU	CA-C-N	5.33	127.74	120.54
1	A	81	LEU	C-N-CA	5.33	127.74	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	SER	CA-C-N	5.33	128.17	120.38
1	B	295	SER	C-N-CA	5.33	128.17	120.38
1	D	324	HIS	CB-CA-C	-5.32	102.20	109.28
1	D	263	LYS	CA-C-O	5.32	123.74	119.59
1	A	179	GLN	CA-C-N	5.32	125.39	119.32
1	A	179	GLN	C-N-CA	5.32	125.39	119.32
1	A	23	SER	O-C-N	5.32	127.76	122.12
1	B	38	LEU	N-CA-C	-5.32	105.56	111.36
1	B	249	LYS	CA-C-O	5.32	126.37	120.63
1	A	101	ILE	O-C-N	-5.30	117.53	123.26
1	D	54	SER	CA-CB-OG	-5.30	100.49	111.10
1	A	33	ILE	O-C-N	-5.30	115.81	121.80
1	C	258	PRO	CA-C-O	-5.30	115.30	121.34
1	B	164	ASN	N-CA-C	-5.30	106.59	113.16
1	A	302	LEU	N-CA-C	5.29	116.74	110.97
1	B	310	SER	CA-C-O	-5.29	114.81	120.42
1	A	268	ARG	CD-NE-CZ	-5.29	117.00	124.40
1	A	282	LEU	CA-C-N	-5.28	113.86	122.26
1	A	282	LEU	C-N-CA	-5.28	113.86	122.26
1	C	252	ILE	CB-CG1-CD1	5.28	124.89	113.80
1	C	87	GLU	CB-CA-C	-5.28	100.53	110.67
1	C	79	LYS	CA-C-N	5.27	127.34	120.28
1	C	79	LYS	C-N-CA	5.27	127.34	120.28
1	D	246	GLU	O-C-N	5.27	127.70	122.12
1	A	58	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	D	172	ARG	N-CA-CB	5.25	117.83	110.12
1	B	201	THR	CA-C-O	-5.24	113.80	120.20
1	A	169	GLU	O-C-N	5.24	127.75	122.09
1	D	96	SER	O-C-N	-5.24	114.58	122.28
1	A	190	CYS	N-CA-C	-5.24	99.75	108.34
1	D	191	MET	CA-C-N	5.23	130.88	123.14
1	D	191	MET	C-N-CA	5.23	130.88	123.14
1	C	208	VAL	CA-C-O	-5.23	114.94	120.53
1	D	154	LEU	CA-C-O	5.23	126.02	120.64
1	C	197	ILE	N-CA-C	5.22	115.38	107.75
1	C	57	GLN	CG-CD-NE2	5.22	124.23	116.40
1	A	152	GLU	CB-CA-C	5.22	119.78	109.66
1	A	17	GLU	CA-C-O	5.22	126.06	120.32
1	A	316	ALA	CA-C-O	5.22	125.45	119.35
1	C	26	LEU	CA-C-O	-5.21	114.21	120.10
1	D	96	SER	CA-CB-OG	5.21	121.52	111.10
1	D	341	LEU	CA-C-N	5.21	130.25	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	341	LEU	C-N-CA	5.21	130.25	122.86
1	B	47	MET	CA-C-O	-5.21	114.90	120.42
1	A	132	SER	CA-CB-OG	-5.20	100.69	111.10
1	D	152	GLU	CA-C-O	-5.20	114.94	120.92
1	D	246	GLU	CA-C-O	-5.20	115.04	120.55
1	A	133	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	C	101	ILE	N-CA-C	5.19	115.37	108.11
1	D	351	LYS	O-C-N	-5.18	116.63	122.12
1	D	164	ASN	N-CA-CB	-5.18	102.99	110.70
1	C	129	ASP	CA-C-O	-5.17	113.51	119.56
1	A	52	ILE	N-CA-C	-5.17	105.50	110.72
1	B	295	SER	CB-CA-C	-5.17	104.20	112.05
1	D	193	SER	CA-CB-OG	-5.16	100.78	111.10
1	C	57	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	B	173	CYS	O-C-N	-5.15	116.73	122.09
1	A	282	LEU	CB-CA-C	-5.15	102.13	110.79
1	B	164	ASN	CA-C-O	5.14	125.50	119.28
1	D	255	LEU	O-C-N	-5.14	115.70	122.39
1	B	128	LEU	CA-C-O	-5.14	115.59	121.40
1	B	45	ILE	N-CA-CB	5.13	118.28	110.58
1	A	172	ARG	CA-C-N	-5.12	113.47	120.44
1	A	172	ARG	C-N-CA	-5.12	113.47	120.44
1	D	114	GLU	CA-C-N	-5.12	115.77	123.00
1	D	114	GLU	C-N-CA	-5.12	115.77	123.00
1	B	274	VAL	CA-C-O	5.12	126.73	121.05
1	D	154	LEU	N-CA-C	5.12	117.71	110.24
1	D	250	LYS	CA-C-O	-5.12	115.00	120.42
1	B	128	LEU	CA-C-N	-5.11	114.47	122.65
1	B	128	LEU	C-N-CA	-5.11	114.47	122.65
1	C	179	GLN	CG-CD-OE1	5.11	131.02	120.80
1	A	198	PHE	N-CA-CB	-5.11	102.00	110.47
1	B	350	GLU	O-C-N	-5.11	116.71	122.12
1	C	78	GLN	CG-CD-OE1	-5.11	110.59	120.80
1	B	301	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	D	132	SER	O-C-N	-5.10	117.51	123.27
1	A	31	LYS	N-CA-C	-5.09	107.12	113.38
1	C	325	GLN	N-CA-CB	-5.09	102.83	111.69
1	C	106	GLU	CA-C-O	5.09	127.78	120.51
1	A	165	THR	CA-CB-OG1	-5.08	101.97	109.60
1	A	338	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	B	35	ASP	O-C-N	-5.08	116.41	122.65
1	A	316	ALA	N-CA-C	-5.07	106.78	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	29	GLU	CA-C-O	5.07	125.87	120.24
1	D	223	GLU	CA-C-O	-5.07	115.34	120.71
1	A	306	CYS	N-CA-C	5.06	117.69	111.82
1	C	296	LYS	CA-C-N	-5.05	114.56	122.49
1	C	296	LYS	C-N-CA	-5.05	114.56	122.49
1	C	252	ILE	O-C-N	-5.05	116.89	121.94
1	A	93	LEU	CA-C-N	5.05	127.75	120.38
1	A	93	LEU	C-N-CA	5.05	127.75	120.38
1	B	297	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	A	96	SER	CB-CA-C	-5.04	100.42	109.24
1	D	268	ARG	CA-C-O	-5.04	114.34	120.54
1	C	63	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	B	94	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	B	135	ASP	CA-C-N	5.02	130.81	122.73
1	B	135	ASP	C-N-CA	5.02	130.81	122.73
1	A	131	SER	O-C-N	5.01	128.26	122.19
1	B	266	SER	CB-CA-C	-5.01	101.06	109.48
1	D	110	PRO	N-CA-C	-5.00	103.42	111.38
1	D	171	GLN	CG-CD-OE1	-5.00	110.79	120.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	SER	Mainchain
1	A	170	GLU	Mainchain
1	A	217	GLU	Mainchain
1	A	224	ASN	Mainchain
1	A	26	LEU	Mainchain
1	B	314	GLU	Mainchain
1	B	316	ALA	Mainchain
1	B	91	ASN	Mainchain
1	C	318	GLY	Mainchain
1	D	185	LEU	Mainchain
1	D	35	ASP	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	2507	0	2420	61	0
1	B	2449	0	2375	34	3
1	C	2497	0	2428	60	0
1	D	2454	0	2376	51	0
2	A	40	0	0	0	3
2	B	56	0	0	2	0
2	C	47	0	0	2	0
2	D	52	0	0	2	0
All	All	10102	0	9599	189	3

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 10.

All (189) 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:B:309:MET:HG2	2:B:409:HOH:O	1.51	1.10
1:A:105:GLU:HG2	1:A:106:GLU:HG3	1.31	1.06
1:A:154:LEU:H	1:A:155:PRO:CD	1.71	1.04
1:C:115:GLU:HB2	1:C:154:LEU:HD13	1.55	0.89
1:C:154:LEU:HD12	1:C:154:LEU:H	1.37	0.88
1:D:154:LEU:HD13	1:D:155:PRO:HD2	1.55	0.88
1:D:331:GLN:NE2	1:D:332:PRO:HD2	1.88	0.87
1:D:331:GLN:HE21	1:D:332:PRO:HD2	1.41	0.85
1:D:47:MET:HE2	1:D:51:GLN:HE21	1.42	0.85
1:A:154:LEU:H	1:A:155:PRO:HD3	1.43	0.83
1:C:148:SER:HB2	1:C:185:LEU:HD11	1.58	0.82
1:A:152:GLU:CB	1:A:155:PRO:HG2	2.14	0.78
1:C:115:GLU:HB2	1:C:154:LEU:CD1	2.15	0.77
1:C:101:ILE:HD12	1:C:164:ASN:HB3	1.67	0.77
1:B:238:GLU:OE1	1:B:256:LYS:NZ	2.18	0.76
1:C:115:GLU:CB	1:C:154:LEU:HD13	2.18	0.74
1:B:19:ILE:HG23	1:B:220:LEU:HB3	1.70	0.73
1:A:214:LEU:HD22	1:C:214:LEU:HD22	1.71	0.72
1:A:215:TYR:CG	1:D:47:MET:HE1	2.25	0.71
1:B:33:ILE:HD12	1:B:204:LYS:HD2	1.71	0.70
1:C:309:MET:HG2	2:C:402:HOH:O	1.92	0.70
1:D:47:MET:HE2	1:D:51:GLN:NE2	2.06	0.69
1:A:154:LEU:H	1:A:155:PRO:HD2	1.58	0.68
1:A:154:LEU:N	1:A:155:PRO:HD3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLN:HG2	1:A:331:GLN:HE22	1.59	0.67
1:D:302:LEU:HD12	1:D:332:PRO:HG3	1.77	0.67
1:C:94:ARG:HH11	1:C:94:ARG:HG3	1.59	0.66
1:B:172:ARG:HH21	1:B:176:ASN:HD21	1.43	0.66
1:C:64:LEU:O	1:C:65:THR:C	2.39	0.65
1:A:102:ILE:HD13	1:A:335:ILE:HD11	1.78	0.65
1:A:16:TYR:HE1	1:A:18:ILE:HG23	1.61	0.65
1:D:236:PHE:CD2	1:D:252:ILE:HD11	2.32	0.64
1:C:163:ASP:O	1:C:165:THR:N	2.30	0.64
1:A:18:ILE:HD11	1:D:92:CYS:SG	2.38	0.64
1:C:273:LEU:HD11	1:C:309:MET:HE1	1.80	0.63
1:D:154:LEU:CD1	1:D:155:PRO:HD2	2.28	0.63
1:A:215:TYR:CB	1:D:47:MET:HE1	2.29	0.63
1:A:105:GLU:HB3	1:A:108:ASP:OD2	1.99	0.63
1:A:115:GLU:OE1	1:A:155:PRO:HG3	1.98	0.62
1:C:61:ILE:HG23	1:C:65:THR:CB	2.30	0.62
1:C:305:GLU:O	1:C:309:MET:HG3	1.99	0.62
1:A:238:GLU:O	1:B:256:LYS:HE2	2.00	0.61
1:B:47:MET:HE3	1:C:18:ILE:HD11	1.82	0.61
1:B:291:ARG:HD3	2:B:388:HOH:O	1.99	0.61
1:D:307:ALA:HB3	1:D:308:PRO:HD3	1.82	0.61
1:B:169:GLU:HG2	1:B:170:GLU:N	2.16	0.61
1:D:171:GLN:HE21	1:D:335:ILE:HG21	1.65	0.61
1:C:225:LEU:HD23	1:C:226:GLN:N	2.16	0.60
1:C:61:ILE:HA	1:C:65:THR:HA	1.84	0.60
1:B:122:ILE:HG23	1:B:147:TYR:HB2	1.84	0.60
1:A:149:PRO:HB3	1:A:177:VAL:HG13	1.84	0.59
1:D:89:PHE:CZ	1:D:93:LEU:HD22	2.37	0.59
1:D:225:LEU:HD23	1:D:226:GLN:N	2.17	0.58
1:A:16:TYR:CE1	1:A:18:ILE:HG23	2.37	0.58
1:D:47:MET:O	1:D:47:MET:HE3	2.03	0.58
1:B:63:ASN:ND2	1:B:76:GLU:HA	2.19	0.58
1:D:251:TYR:CE1	1:D:255:LEU:HD11	2.37	0.58
1:C:238:GLU:OE1	1:C:256:LYS:NZ	2.26	0.57
1:B:79:LYS:O	1:B:82:ASP:HB2	2.04	0.57
1:B:289:TYR:OH	1:B:299:LYS:HD3	2.05	0.57
1:C:98:ARG:NH1	1:C:115:GLU:OE1	2.38	0.57
1:A:331:GLN:HE21	1:A:332:PRO:HD2	1.69	0.57
1:A:238:GLU:OE1	1:A:256:LYS:NZ	2.34	0.57
1:A:335:ILE:HG23	1:A:336:HIS:H	1.69	0.57
1:B:273:LEU:HD11	1:B:309:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ALA:HB3	1:B:308:PRO:HD3	1.87	0.56
1:A:58:ARG:HG2	1:B:213:PRO:HD2	1.86	0.56
1:C:16:TYR:CB	1:C:19:ILE:HD11	2.35	0.56
1:D:288:GLY:HA3	2:D:401:HOH:O	2.06	0.56
1:A:79:LYS:O	1:A:82:ASP:HB2	2.06	0.56
1:A:209:PHE:HB3	1:A:218:PHE:HB3	1.89	0.55
1:A:331:GLN:NE2	1:A:332:PRO:HD2	2.22	0.55
1:D:225:LEU:HD11	1:D:282:LEU:HD23	1.89	0.55
1:C:225:LEU:HD11	1:C:282:LEU:HD23	1.88	0.54
1:D:169:GLU:OE1	1:D:172:ARG:NH2	2.40	0.54
1:C:102:ILE:HG23	1:C:171:GLN:NE2	2.23	0.54
1:D:236:PHE:CE2	1:D:252:ILE:HD11	2.43	0.54
1:B:94:ARG:HG2	1:C:16:TYR:N	2.23	0.53
1:C:290:PRO:HB3	1:C:342:TYR:OH	2.09	0.53
1:C:43:SER:O	1:C:47:MET:HG3	2.09	0.52
1:D:267:ALA:O	1:D:268:ARG:HD3	2.10	0.52
1:D:47:MET:CE	1:D:51:GLN:HG3	2.39	0.52
1:C:23:SER:O	1:C:27:GLN:HG3	2.10	0.51
1:C:154:LEU:HD12	1:C:154:LEU:N	2.16	0.51
1:A:257:GLU:OE2	1:B:242:LYS:HE3	2.11	0.51
1:C:331:GLN:NE2	1:C:332:PRO:HD2	2.26	0.51
1:A:222:GLN:HG3	1:A:223:GLU:N	2.26	0.50
1:A:307:ALA:HB3	1:A:308:PRO:HD3	1.93	0.50
1:D:336:HIS:HE1	2:D:408:HOH:O	1.94	0.50
1:A:127:PRO:HG2	1:A:128:LEU:H	1.77	0.50
1:B:169:GLU:HG2	1:B:170:GLU:H	1.76	0.49
1:A:149:PRO:HB3	1:A:177:VAL:CG1	2.43	0.49
1:A:215:TYR:HB3	1:D:47:MET:HE1	1.95	0.49
1:D:244:TRP:CZ3	1:D:252:ILE:HG13	2.48	0.48
1:C:175:VAL:HG21	1:C:335:ILE:HA	1.94	0.48
1:B:24:TRP:O	1:B:28:GLN:HG2	2.14	0.48
1:A:215:TYR:CZ	1:D:51:GLN:HG2	2.49	0.48
1:D:302:LEU:CD1	1:D:332:PRO:HG3	2.44	0.48
1:D:28:GLN:OE1	1:D:33:ILE:HD12	2.13	0.48
1:A:115:GLU:OE1	1:A:155:PRO:CG	2.62	0.48
1:A:168:THR:HG21	1:A:172:ARG:NH2	2.29	0.48
1:B:172:ARG:HH21	1:B:176:ASN:ND2	2.11	0.47
1:C:84:ILE:O	1:C:88:VAL:HG23	2.13	0.47
1:D:148:SER:HB2	1:D:185:LEU:HD11	1.94	0.47
1:A:147:TYR:CZ	1:A:184:LEU:HD13	2.49	0.47
1:D:35:ASP:HB3	1:D:38:LEU:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:C	1:A:225:LEU:HD23	2.39	0.47
1:A:168:THR:HG22	1:A:172:ARG:CZ	2.44	0.47
1:C:123:VAL:HG22	1:C:146:ILE:HG12	1.97	0.47
1:C:162:ASP:HA	1:C:164:ASN:HB2	1.97	0.47
1:B:167:GLY:N	1:B:170:GLU:OE2	2.48	0.46
1:A:115:GLU:OE1	1:A:155:PRO:HD3	2.14	0.46
1:C:101:ILE:CD1	1:C:164:ASN:HB3	2.40	0.46
1:D:331:GLN:NE2	1:D:332:PRO:CD	2.72	0.46
1:C:29:GLU:HA	1:C:34:ILE:O	2.16	0.46
1:A:17:GLU:OE2	1:A:19:ILE:HD11	2.17	0.45
1:C:65:THR:CB	1:D:18:ILE:HG13	2.46	0.45
1:C:241:TYR:HA	1:C:244:TRP:CE3	2.52	0.45
1:C:291:ARG:HD2	1:C:296:LYS:O	2.17	0.45
1:A:349:VAL:O	1:A:353:GLU:HG3	2.17	0.45
1:C:115:GLU:OE1	1:C:154:LEU:HD12	2.16	0.45
1:A:148:SER:HB2	1:A:185:LEU:HD11	1.98	0.45
1:B:248:LEU:O	1:B:251:TYR:HB3	2.17	0.45
1:C:309:MET:CG	2:C:402:HOH:O	2.60	0.45
1:A:152:GLU:CB	1:A:155:PRO:CG	2.93	0.44
1:D:302:LEU:HA	1:D:306:CYS:HB2	1.98	0.44
1:A:217:GLU:OE2	1:D:50:LYS:NZ	2.50	0.44
1:A:244:TRP:CG	1:A:248:LEU:HD23	2.52	0.44
1:D:24:TRP:O	1:D:28:GLN:HG2	2.17	0.44
1:A:16:TYR:HE1	1:A:18:ILE:CG2	2.30	0.44
1:C:115:GLU:OE1	1:C:154:LEU:CD1	2.66	0.44
1:A:61:ILE:O	1:A:64:LEU:HB2	2.17	0.44
1:B:310:SER:O	1:B:313:VAL:HG12	2.18	0.44
1:A:225:LEU:HD11	1:A:282:LEU:HD23	1.99	0.43
1:C:305:GLU:O	1:C:308:PRO:HD2	2.18	0.43
1:D:331:GLN:HA	1:D:332:PRO:HD3	1.75	0.43
1:B:301:ARG:HD2	1:B:304:TYR:HD2	1.83	0.43
1:C:63:ASN:ND2	1:C:76:GLU:HA	2.34	0.43
1:D:244:TRP:HZ3	1:D:252:ILE:HG13	1.82	0.43
1:C:208:VAL:HB	1:C:222:GLN:HB3	2.00	0.43
1:A:51:GLN:O	1:A:55:LEU:HG	2.19	0.43
1:B:51:GLN:OE1	1:B:88:VAL:HG13	2.19	0.43
1:C:133:ASN:HB3	1:D:283:TYR:OH	2.19	0.43
1:D:326:ARG:HH11	1:D:326:ARG:HD3	1.50	0.43
1:A:104:SER:HB2	1:A:108:ASP:O	2.19	0.43
1:A:173:CYS:O	1:A:174:ILE:C	2.61	0.43
1:C:115:GLU:CD	1:C:154:LEU:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:VAL:O	1:D:356:LEU:HG	2.19	0.43
1:B:96:SER:O	1:B:116:SER:HA	2.19	0.43
1:C:154:LEU:H	1:C:154:LEU:CD1	2.07	0.43
1:A:89:PHE:CE1	1:A:93:LEU:HD13	2.53	0.42
1:A:304:TYR:OH	1:A:335:ILE:HD12	2.18	0.42
1:C:166:LEU:HD13	1:C:174:ILE:HD12	2.01	0.42
1:D:91:ASN:HA	1:D:94:ARG:NH1	2.34	0.42
1:B:19:ILE:HG21	1:B:220:LEU:HD23	2.01	0.42
1:A:171:GLN:HB3	1:A:335:ILE:HD13	2.01	0.42
1:C:163:ASP:O	1:C:164:ASN:C	2.62	0.42
1:B:155:PRO:HD3	1:B:170:GLU:HG2	2.01	0.42
1:C:220:LEU:HD21	1:C:223:GLU:CG	2.49	0.42
1:C:120:ASN:O	1:C:149:PRO:HD2	2.19	0.42
1:A:326:ARG:O	1:A:327:VAL:C	2.62	0.42
1:D:301:ARG:HH11	1:D:336:HIS:HD2	1.68	0.42
1:C:256:LYS:HD3	1:D:241:TYR:HB3	2.02	0.42
1:A:13:ARG:O	1:A:14:SER:C	2.63	0.41
1:D:122:ILE:HD13	1:D:122:ILE:HG21	1.89	0.41
1:C:292:ASP:OD2	1:C:292:ASP:C	2.63	0.41
1:D:53:ALA:O	1:D:57:GLN:HG3	2.20	0.41
1:A:242:LYS:HE3	1:B:257:GLU:OE2	2.20	0.41
1:C:251:TYR:O	1:C:252:ILE:C	2.61	0.41
1:D:331:GLN:HE21	1:D:332:PRO:CD	2.23	0.41
1:A:313:VAL:HG11	1:A:343:ILE:HG13	2.02	0.41
1:C:94:ARG:HH11	1:C:94:ARG:CG	2.31	0.41
1:C:213:PRO:HD2	1:D:58:ARG:HG2	2.02	0.41
1:A:148:SER:O	1:A:183:ASN:ND2	2.52	0.41
1:A:255:LEU:HD22	1:A:265:TYR:CE2	2.56	0.41
1:C:273:LEU:HD21	1:C:309:MET:SD	2.61	0.41
1:D:221:THR:O	1:D:222:GLN:HB2	2.20	0.41
1:C:153:CYS:O	1:C:154:LEU:C	2.64	0.41
1:D:47:MET:HE2	1:D:51:GLN:HG3	2.02	0.41
1:A:122:ILE:HD12	1:A:149:PRO:HB3	2.03	0.40
1:B:154:LEU:HA	1:B:155:PRO:HD3	1.99	0.40
1:B:238:GLU:CD	1:B:256:LYS:HZ1	2.17	0.40
1:C:168:THR:HG22	1:C:169:GLU:OE1	2.21	0.40
1:C:247:ASN:HB3	1:C:355:TYR:O	2.22	0.40
1:A:97:GLY:HA3	1:A:114:GLU:OE2	2.22	0.40
1:B:166:LEU:HD23	1:B:166:LEU:HA	1.83	0.40
1:B:229:LYS:C	1:B:345:SER:HB3	2.46	0.40
1:C:351:LYS:O	1:C:352:VAL:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:SER:C	1:D:236:PHE:HD1	2.30	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:O	2:A:382:HOH:O[2_656]	1.50	0.70
1:B:202:ILE:C	2:A:382:HOH:O[2_656]	2.07	0.13
1:B:203:GLY:N	2:A:382:HOH:O[2_656]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/357 (91%)	305 (94%)	12 (4%)	7 (2%)	5	3
1	B	317/357 (89%)	306 (96%)	10 (3%)	1 (0%)	36	42
1	C	322/357 (90%)	306 (95%)	13 (4%)	3 (1%)	14	14
1	D	319/357 (89%)	304 (95%)	13 (4%)	2 (1%)	21	23
All	All	1282/1428 (90%)	1221 (95%)	48 (4%)	13 (1%)	12	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	154	LEU
1	A	335	ILE
1	C	155	PRO
1	C	163	ASP
1	C	164	ASN
1	D	18	ILE

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Mol	Chain	Res	Type
1	D	106	GLU
1	A	105	GLU
1	A	14	SER
1	A	66	GLY
1	A	106	GLU
1	B	202	ILE

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	272/307 (89%)	261 (96%)	11 (4%)	28	38
1	B	264/307 (86%)	254 (96%)	10 (4%)	29	40
1	C	270/307 (88%)	258 (96%)	12 (4%)	25	34
1	D	264/307 (86%)	251 (95%)	13 (5%)	22	29
All	All	1070/1228 (87%)	1024 (96%)	46 (4%)	26	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ILE
1	A	19	ILE
1	A	47	MET
1	A	81	LEU
1	A	90	SER
1	A	116	SER
1	A	150	ASN
1	A	177	VAL
1	A	222	GLN
1	A	247	ASN
1	A	313	VAL
1	B	19	ILE
1	B	33	ILE
1	B	93	LEU
1	B	95	SER

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Mol	Chain	Res	Type
1	B	116	SER
1	B	122	ILE
1	B	150	ASN
1	B	217	GLU
1	B	261	SER
1	B	321	SER
1	C	18	ILE
1	C	64	LEU
1	C	93	LEU
1	C	94	ARG
1	C	98	ARG
1	C	126	ASP
1	C	150	ASN
1	C	154	LEU
1	C	230	SER
1	C	247	ASN
1	C	309	MET
1	C	335	ILE
1	D	18	ILE
1	D	126	ASP
1	D	154	LEU
1	D	155	PRO
1	D	177	VAL
1	D	182	SER
1	D	195	SER
1	D	201	THR
1	D	261	SER
1	D	266	SER
1	D	293	LYS
1	D	302	LEU
1	D	313	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	78	GLN
1	A	150	ASN
1	A	164	ASN
1	A	171	GLN
1	A	176	ASN
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	240	ASN
1	A	331	GLN
1	B	57	GLN
1	B	78	GLN
1	B	176	ASN
1	B	240	ASN
1	B	331	GLN
1	B	336	HIS
1	C	63	ASN
1	C	78	GLN
1	C	164	ASN
1	C	171	GLN
1	C	176	ASN
1	C	240	ASN
1	C	325	GLN
1	C	331	GLN
1	D	51	GLN
1	D	78	GLN
1	D	164	ASN
1	D	171	GLN
1	D	176	ASN
1	D	240	ASN
1	D	331	GLN
1	D	336	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	330/357 (92%)	0.30	20 (6%) 27 24	21, 40, 74, 93	0
1	B	323/357 (90%)	0.07	11 (3%) 48 45	21, 34, 70, 96	0
1	C	328/357 (91%)	0.19	19 (5%) 29 25	23, 39, 71, 90	0
1	D	325/357 (91%)	0.26	20 (6%) 26 23	23, 38, 68, 97	0
All	All	1306/1428 (91%)	0.20	70 (5%) 31 28	21, 38, 72, 97	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	65	THR	7.7
1	C	64	LEU	6.0
1	D	105	GLU	5.1
1	D	261	SER	4.9
1	A	260	PRO	4.7
1	A	67	THR	4.6
1	A	155	PRO	4.5
1	C	157	PHE	4.5
1	D	259	GLY	4.4
1	B	259	GLY	4.3
1	D	260	PRO	4.2
1	D	154	LEU	4.2
1	C	163	ASP	4.2
1	D	163	ASP	4.2
1	C	76	GLU	4.2
1	A	259	GLY	4.1
1	D	65	THR	3.9
1	C	16	TYR	3.9
1	D	17	GLU	3.9
1	D	35	ASP	3.6
1	B	260	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	162	ASP	3.4
1	D	106	GLU	3.3
1	A	16	TYR	3.2
1	B	262	GLY	3.2
1	D	247	ASN	3.2
1	C	164	ASN	3.0
1	A	150	ASN	2.9
1	D	155	PRO	2.9
1	A	35	ASP	2.9
1	C	63	ASN	2.9
1	A	13	ARG	2.9
1	A	261	SER	2.8
1	B	76	GLU	2.8
1	D	66	GLY	2.7
1	A	76	GLU	2.7
1	D	18	ILE	2.7
1	A	12	LYS	2.7
1	C	169	GLU	2.7
1	B	163	ASP	2.7
1	C	260	PRO	2.7
1	A	18	ILE	2.6
1	A	154	LEU	2.6
1	C	105	GLU	2.6
1	D	151	ASP	2.6
1	B	64	LEU	2.5
1	B	261	SER	2.5
1	D	77	ASP	2.5
1	C	94	ARG	2.5
1	D	150	ASN	2.5
1	B	104	SER	2.4
1	A	64	LEU	2.4
1	A	335	ILE	2.3
1	A	77	ASP	2.3
1	C	155	PRO	2.3
1	C	150	ASN	2.2
1	B	215	TYR	2.2
1	C	154	LEU	2.2
1	C	35	ASP	2.2
1	B	155	PRO	2.2
1	D	262	GLY	2.2
1	B	294	LYS	2.2
1	D	104	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	79	LYS	2.1
1	A	262	GLY	2.1
1	A	65	THR	2.1
1	C	107	GLU	2.0
1	D	215	TYR	2.0
1	A	107	GLU	2.0
1	C	156	ASP	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.