



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:36 AM GMT

PDB ID : 3PGA
Title : STRUCTURAL CHARACTERIZATION OF PSEUDOMONAS 7A GLUTAMINASE-ASPARAGINASE
Authors : Lubkowski, J.; Wlodawer, A.; Ammon, H.L.; Copeland, T.D.; Swain, A.L.
Deposited on : 1994-07-19
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

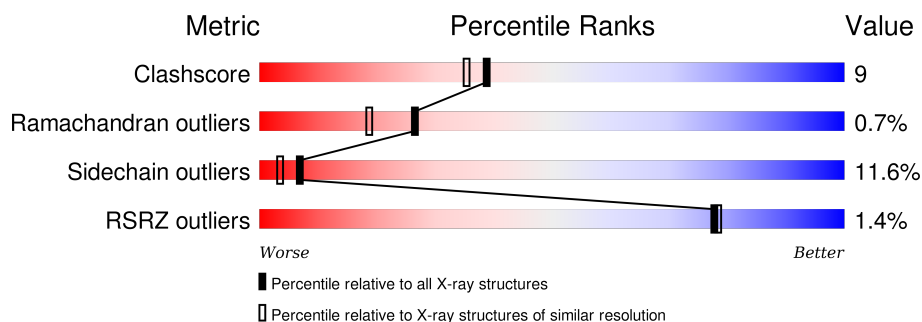
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1	337	<div> <div>2%</div> <div>57% 27% 12% . .</div> </div>
1	2	337	<div> <div>2%</div> <div>56% 29% 10% . .</div> </div>
1	3	337	<div> <div>57% 30% 8% . .</div> </div>
1	4	337	<div> <div>%</div> <div>56% 30% 9% . .</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10854 atoms, of which 0 are hydrogens and 0 are deuteriums.

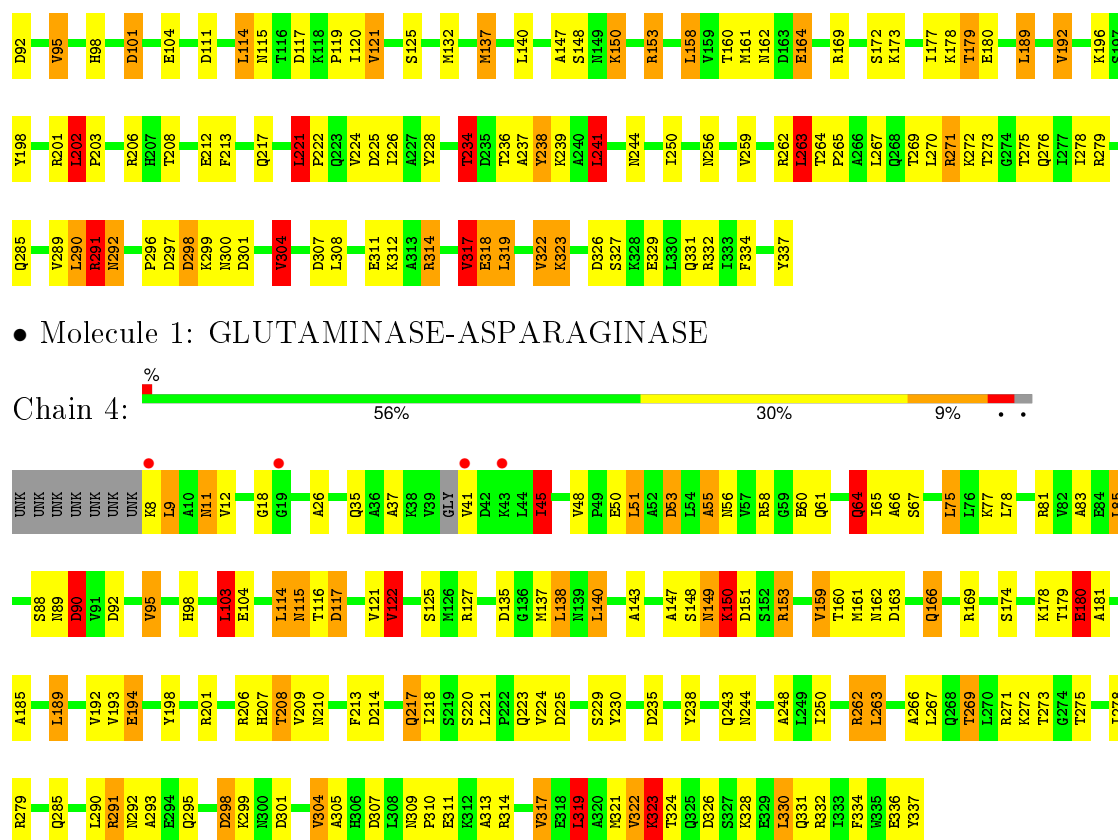
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called GLUTAMINASE-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	330	Total	C	N	O	S	253	20	0
			2611	1627	459	518	7			
1	2	330	Total	C	N	O	S	126	20	0
			2611	1627	459	518	7			
1	3	329	Total	C	N	O	S	253	20	0
			2607	1625	458	517	7			
1	4	329	Total	C	N	O	S	253	20	0
			2607	1625	458	517	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	113	Total	O	0	0
			113	113		
2	2	87	Total	O	0	0
			87	87		
2	3	112	Total	O	0	0
			112	112		
2	4	106	Total	O	0	0
			106	106		



• Molecule 1: GLUTAMINASE-ASPARAGINASE

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.26 Å 130.75 Å 85.09 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	86.0 (10.00-2.00) 39.0 (10.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROFFT, X-PLOR	Depositor
R, R_{free}	0.165 , (Not available) 0.140 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 71.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 43603 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10854	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1	1.05	1/2391 (0.0%)	2.58	162/3238 (5.0%)
1	2	1.05	1/2391 (0.0%)	2.55	163/3238 (5.0%)
1	3	1.08	2/2387 (0.1%)	2.40	148/3233 (4.6%)
1	4	1.07	2/2387 (0.1%)	2.54	151/3233 (4.7%)
All	All	1.06	6/9556 (0.1%)	2.52	624/12942 (4.8%)

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	1	0	3
1	2	0	1
1	3	0	3
1	4	0	3
All	All	0	10

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	318	GLU	CD-OE1	-6.43	1.18	1.25
1	3	104	GLU	CD-OE2	-6.12	1.19	1.25
1	1	318	GLU	CD-OE1	-5.83	1.19	1.25
1	4	336	GLU	CD-OE1	-5.75	1.19	1.25
1	4	269	THR	CB-OG1	5.36	1.53	1.43
1	2	104	GLU	CD-OE2	-5.11	1.20	1.25

All (624) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	262	ARG	NE-CZ-NH2	-29.86	105.37	120.30
1	4	332	ARG	NE-CZ-NH2	-26.29	107.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	314	ARG	NE-CZ-NH2	20.89	130.74	120.30
1	2	81	ARG	CD-NE-CZ	19.94	151.52	123.60
1	2	206	ARG	NE-CZ-NH1	19.41	130.01	120.30
1	4	271	ARG	NE-CZ-NH2	19.41	130.00	120.30
1	4	262	ARG	NE-CZ-NH2	-19.30	110.65	120.30
1	1	262	ARG	NE-CZ-NH1	19.04	129.82	120.30
1	1	206	ARG	NE-CZ-NH2	-18.85	110.87	120.30
1	2	262	ARG	NE-CZ-NH2	-18.42	111.09	120.30
1	2	72	ASN	CB-CA-C	18.23	146.85	110.40
1	4	262	ARG	NE-CZ-NH1	18.16	129.38	120.30
1	3	114	LEU	CB-CG-CD1	18.14	141.84	111.00
1	3	153	ARG	NE-CZ-NH2	-16.47	112.06	120.30
1	4	114	LEU	CB-CG-CD2	16.06	138.30	111.00
1	1	87	ASP	CB-CG-OD2	-15.80	104.08	118.30
1	1	153	ARG	NE-CZ-NH2	-15.47	112.57	120.30
1	2	101	ASP	CB-CG-OD1	15.21	131.99	118.30
1	2	271	ARG	NE-CZ-NH1	14.92	127.76	120.30
1	1	332	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	1	271	ARG	NE-CZ-NH1	14.37	127.49	120.30
1	1	114	LEU	CB-CG-CD2	14.30	135.31	111.00
1	4	127	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	3	201	ARG	NE-CZ-NH2	-14.15	113.23	120.30
1	4	214	ASP	CB-CG-OD1	14.12	131.01	118.30
1	4	214	ASP	CB-CG-OD2	-13.91	105.78	118.30
1	4	206	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	1	206	ARG	NE-CZ-NH1	13.45	127.03	120.30
1	1	153	ARG	NE-CZ-NH1	13.41	127.00	120.30
1	4	206	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	2	153	ARG	NE-CZ-NH2	-13.30	113.65	120.30
1	3	169	ARG	NE-CZ-NH2	13.27	126.94	120.30
1	1	214	ASP	CB-CG-OD1	13.20	130.18	118.30
1	2	318	GLU	OE1-CD-OE2	13.13	139.06	123.30
1	3	81	ARG	NE-CZ-NH2	13.08	126.84	120.30
1	2	114	LEU	CB-CG-CD2	13.02	133.12	111.00
1	3	323	LYS	CA-CB-CG	12.88	141.75	113.40
1	3	114	LEU	CB-CA-C	12.83	134.58	110.20
1	3	58	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	3	234	THR	CA-CB-CG2	12.74	130.23	112.40
1	2	201	ARG	NE-CZ-NH1	12.63	126.61	120.30
1	1	58	ARG	CD-NE-CZ	12.60	141.24	123.60
1	2	314	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	4	81	ARG	CD-NE-CZ	12.20	140.69	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	153	ARG	NE-CZ-NH2	-12.13	114.24	120.30
1	4	81	ARG	NE-CZ-NH2	12.10	126.35	120.30
1	1	298	ASP	CB-CG-OD2	-12.06	107.44	118.30
1	1	262	ARG	CA-CB-CG	11.97	139.74	113.40
1	1	272	LYS	CA-CB-CG	11.82	139.42	113.40
1	2	291	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	2	291	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	2	326	ASP	CB-CG-OD1	11.67	128.80	118.30
1	2	114	LEU	CB-CA-C	11.41	131.88	110.20
1	1	263	LEU	CB-CG-CD2	-11.29	91.82	111.00
1	1	114	LEU	CB-CA-C	11.07	131.23	110.20
1	4	150	LYS	CB-CG-CD	10.95	140.07	111.60
1	1	301	ASP	CB-CG-OD2	10.85	128.06	118.30
1	1	254	THR	N-CA-CB	-10.80	89.77	110.30
1	3	225	ASP	CB-CG-OD1	10.76	127.98	118.30
1	3	298	ASP	CB-CG-OD1	10.74	127.97	118.30
1	1	254	THR	CA-CB-CG2	10.70	127.38	112.40
1	1	141	TYR	CB-CG-CD1	10.66	127.40	121.00
1	2	279	ARG	NE-CZ-NH1	-10.66	114.97	120.30
1	4	332	ARG	NE-CZ-NH1	10.46	125.53	120.30
1	2	73	ASP	CB-CG-OD2	-10.41	108.93	118.30
1	2	60	GLU	N-CA-CB	10.39	129.31	110.60
1	3	81	ARG	NE-CZ-NH1	-10.39	115.11	120.30
1	1	298	ASP	CB-CG-OD1	10.37	127.63	118.30
1	4	291	ARG	NE-CZ-NH2	10.33	125.47	120.30
1	3	153	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	4	114	LEU	CB-CA-C	10.22	129.62	110.20
1	1	214	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	4	271	ARG	NH1-CZ-NH2	-10.16	108.22	119.40
1	2	74	ASP	CB-CG-OD1	10.16	127.44	118.30
1	2	169	ARG	CD-NE-CZ	10.12	137.78	123.60
1	4	201	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	3	206	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	1	58	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	3	111	ASP	CB-CG-OD2	9.81	127.13	118.30
1	2	271	ARG	CD-NE-CZ	9.72	137.21	123.60
1	4	122	VAL	CB-CA-C	9.68	129.78	111.40
1	3	50	GLU	CG-CD-OE1	9.59	137.47	118.30
1	3	314	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	4	290	LEU	CA-CB-CG	9.57	137.31	115.30
1	4	262	ARG	CA-CB-CG	9.54	134.39	113.40
1	2	101	ASP	CB-CG-OD2	-9.52	109.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	58	ARG	NH1-CZ-NH2	9.52	129.87	119.40
1	4	221	LEU	N-CA-CB	-9.47	91.47	110.40
1	3	311	GLU	CG-CD-OE1	9.45	137.20	118.30
1	1	263	LEU	CD1-CG-CD2	9.44	138.83	110.50
1	4	9	LEU	CB-CA-C	9.37	128.01	110.20
1	1	103	LEU	CA-CB-CG	9.36	136.82	115.30
1	2	121	VAL	CA-CB-CG1	9.35	124.93	110.90
1	3	332	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	2	206	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	2	337	TYR	CB-CG-CD1	-9.30	115.42	121.00
1	2	72	ASN	CB-CG-ND2	9.25	138.91	116.70
1	4	201	ARG	NE-CZ-NH2	-9.25	115.68	120.30
1	4	194	GLU	CA-CB-CG	9.06	133.33	113.40
1	3	262	ARG	NE-CZ-NH2	9.03	124.82	120.30
1	2	103	LEU	CB-CG-CD1	9.02	126.33	111.00
1	4	299	LYS	CB-CG-CD	8.99	134.98	111.60
1	4	8	LYS	CA-CB-CG	8.98	133.16	113.40
1	1	241	LEU	CB-CG-CD1	8.97	126.25	111.00
1	3	291	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	3	326	ASP	CB-CG-OD1	8.95	126.36	118.30
1	3	271	ARG	CD-NE-CZ	8.94	136.12	123.60
1	2	117	ASP	CB-CG-OD1	8.90	126.31	118.30
1	2	108	TYR	CB-CG-CD1	8.88	126.33	121.00
1	1	273	THR	OG1-CB-CG2	-8.88	89.59	110.00
1	1	71	THR	CA-CB-CG2	8.84	124.77	112.40
1	1	53	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	2	325	GLN	CB-CG-CD	8.72	134.27	111.60
1	1	84	GLU	CA-CB-CG	8.72	132.58	113.40
1	1	123	VAL	CG1-CB-CG2	8.72	124.85	110.90
1	3	289	VAL	CA-CB-CG1	8.65	123.88	110.90
1	4	163	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	2	314	ARG	CD-NE-CZ	8.61	135.66	123.60
1	3	201	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	3	311	GLU	OE1-CD-OE2	-8.58	113.01	123.30
1	3	291	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	4	285	GLN	CA-CB-CG	8.56	132.23	113.40
1	2	60	GLU	OE1-CD-OE2	8.52	133.52	123.30
1	1	263	LEU	CA-CB-CG	-8.49	95.78	115.30
1	2	269	THR	CA-CB-CG2	8.48	124.27	112.40
1	3	239	LYS	CD-CE-NZ	8.46	131.15	111.70
1	2	304	VAL	CG1-CB-CG2	8.46	124.43	110.90
1	1	304	VAL	CG1-CB-CG2	8.42	124.37	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	180	GLU	CA-CB-CG	8.40	131.89	113.40
1	2	72	ASN	CB-CG-OD1	-8.40	104.80	121.60
1	2	233	VAL	CG1-CB-CG2	8.38	124.30	110.90
1	3	73	ASP	CB-CG-OD1	8.37	125.84	118.30
1	1	307	ASP	CB-CG-OD1	8.36	125.82	118.30
1	1	123	VAL	CB-CA-C	-8.29	95.66	111.40
1	4	285	GLN	CB-CA-C	8.29	126.98	110.40
1	2	53	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	1	10	ALA	N-CA-CB	8.24	121.64	110.10
1	3	53	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	2	233	VAL	CB-CA-C	-8.23	95.77	111.40
1	4	221	LEU	CA-CB-CG	8.21	134.18	115.30
1	2	48	VAL	CB-CA-C	8.20	126.98	111.40
1	1	58	ARG	CA-CB-CG	8.19	131.41	113.40
1	3	241	LEU	CB-CG-CD1	8.16	124.87	111.00
1	2	135	ASP	CB-CG-OD1	8.16	125.64	118.30
1	3	58	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	1	250	ILE	CB-CG1-CD1	-8.12	91.15	113.90
1	4	103	LEU	CA-CB-CG	8.04	133.78	115.30
1	2	318	GLU	CG-CD-OE2	-8.03	102.24	118.30
1	2	81	ARG	CG-CD-NE	7.99	128.59	111.80
1	3	202	LEU	CB-CG-CD1	7.99	124.57	111.00
1	4	161	MET	CA-CB-CG	-7.97	99.75	113.30
1	4	201	ARG	CD-NE-CZ	7.96	134.74	123.60
1	1	279	ARG	NE-CZ-NH2	7.91	124.26	120.30
1	3	263	LEU	CD1-CG-CD2	7.86	134.09	110.50
1	4	115	ASN	CA-CB-CG	7.79	130.54	113.40
1	1	273	THR	O-C-N	-7.78	109.97	123.20
1	4	122	VAL	CA-CB-CG1	7.77	122.56	110.90
1	2	108	TYR	CB-CG-CD2	-7.75	116.35	121.00
1	4	114	LEU	CD1-CG-CD2	-7.73	87.31	110.50
1	2	115	ASN	O-C-N	-7.73	110.33	122.70
1	3	50	GLU	CG-CD-OE2	-7.72	102.86	118.30
1	1	131	ALA	N-CA-CB	7.71	120.89	110.10
1	1	262	ARG	CB-CA-C	7.71	125.81	110.40
1	1	194	GLU	CA-CB-CG	7.69	130.32	113.40
1	2	81	ARG	CB-CG-CD	7.69	131.59	111.60
1	3	73	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	2	235	ASP	CB-CG-OD1	7.66	125.20	118.30
1	1	201	ARG	CD-NE-CZ	7.64	134.30	123.60
1	1	225	ASP	CB-CG-OD1	7.64	125.17	118.30
1	2	60	GLU	CG-CD-OE2	-7.63	103.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	228	TYR	CB-CG-CD1	-7.63	116.42	121.00
1	1	327	SER	CA-CB-OG	-7.60	90.69	111.20
1	4	169	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	3	234	THR	N-CA-CB	-7.55	95.96	110.30
1	1	318	GLU	CG-CD-OE2	-7.52	103.27	118.30
1	4	95	VAL	CA-CB-CG1	7.50	122.15	110.90
1	3	319	LEU	CB-CG-CD1	-7.49	98.26	111.00
1	4	263	LEU	N-CA-CB	-7.48	95.44	110.40
1	1	259	VAL	CA-CB-CG2	7.44	122.06	110.90
1	1	117	ASP	CB-CA-C	-7.43	95.53	110.40
1	2	103	LEU	CA-CB-CG	7.42	132.38	115.30
1	3	271	ARG	CG-CD-NE	7.42	127.39	111.80
1	2	221	LEU	CA-CB-CG	7.40	132.33	115.30
1	1	269	THR	CA-CB-CG2	7.38	122.73	112.40
1	4	116	THR	CA-CB-CG2	7.36	122.71	112.40
1	1	273	THR	CA-CB-OG1	7.34	124.41	109.00
1	1	244	ASN	CB-CA-C	7.32	125.05	110.40
1	1	320	ALA	N-CA-CB	7.31	120.33	110.10
1	3	95	VAL	CA-CB-CG2	7.30	121.86	110.90
1	3	92	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	4	304	VAL	CG1-CB-CG2	7.29	122.56	110.90
1	4	244	ASN	OD1-CG-ND2	7.29	138.66	121.90
1	2	301	ASP	CB-CG-OD1	7.27	124.84	118.30
1	3	318	GLU	CG-CD-OE2	-7.25	103.79	118.30
1	2	202	LEU	CB-CG-CD1	7.24	123.30	111.00
1	2	116	THR	CA-CB-CG2	7.23	122.52	112.40
1	2	290	LEU	CB-CG-CD1	-7.22	98.72	111.00
1	3	279	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	4	314	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	4	179	THR	CA-CB-OG1	-7.17	93.94	109.00
1	4	332	ARG	NH1-CZ-NH2	7.15	127.26	119.40
1	3	64	GLN	CB-CA-C	7.15	124.70	110.40
1	4	217	GLN	CA-CB-CG	7.15	129.13	113.40
1	4	210	ASN	CB-CA-C	7.14	124.68	110.40
1	3	337	TYR	CZ-CE2-CD2	-7.13	113.39	119.80
1	3	319	LEU	CA-CB-CG	-7.12	98.93	115.30
1	2	275	THR	CA-CB-CG2	7.11	122.36	112.40
1	4	299	LYS	CA-CB-CG	7.11	129.04	113.40
1	2	159	VAL	CA-CB-CG1	7.11	121.56	110.90
1	1	58	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	2	92	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	2	279	ARG	CD-NE-CZ	7.08	133.52	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	90	ASP	N-CA-CB	-7.08	97.85	110.60
1	1	114	LEU	CD1-CG-CD2	-7.07	89.29	110.50
1	3	319	LEU	N-CA-CB	-7.04	96.32	110.40
1	1	330	LEU	CB-CG-CD2	-7.04	99.04	111.00
1	1	273	THR	CB-CA-C	7.02	130.54	111.60
1	1	71	THR	N-CA-CB	-7.00	97.01	110.30
1	1	326	ASP	CB-CG-OD1	6.99	124.59	118.30
1	2	151	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	4	115	ASN	CB-CG-OD1	6.96	135.52	121.60
1	1	196	LYS	N-CA-CB	6.96	123.13	110.60
1	3	111	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	1	319	LEU	CB-CG-CD2	-6.93	99.23	111.00
1	2	323	LYS	CD-CE-NZ	6.92	127.62	111.70
1	4	293	ALA	CB-CA-C	6.92	120.48	110.10
1	4	337	TYR	CD1-CE1-CZ	-6.91	113.58	119.80
1	2	214	ASP	CB-CG-OD1	6.91	124.52	118.30
1	2	80	LYS	CB-CG-CD	6.89	129.51	111.60
1	3	271	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	3	244	ASN	OD1-CG-ND2	6.87	137.70	121.90
1	2	230	TYR	CB-CG-CD1	6.86	125.11	121.00
1	1	293	ALA	N-CA-CB	6.85	119.69	110.10
1	3	202	LEU	CB-CG-CD2	-6.84	99.38	111.00
1	4	64	GLN	N-CA-CB	6.83	122.89	110.60
1	1	141	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	4	147	ALA	C-N-CA	6.83	138.77	121.70
1	3	114	LEU	CD1-CG-CD2	-6.81	90.08	110.50
1	4	159	VAL	CA-CB-CG2	6.81	121.11	110.90
1	3	263	LEU	CB-CG-CD1	-6.80	99.44	111.00
1	3	271	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	3	263	LEU	CB-CG-CD2	-6.77	99.48	111.00
1	4	85	LEU	CB-CG-CD1	6.77	122.52	111.00
1	4	55	ALA	N-CA-CB	-6.77	100.62	110.10
1	1	245	GLY	CA-C-O	-6.77	108.42	120.60
1	1	115	ASN	CB-CG-OD1	-6.76	108.08	121.60
1	1	263	LEU	N-CA-CB	-6.76	96.88	110.40
1	4	235	ASP	CB-CG-OD1	6.76	124.38	118.30
1	4	12	VAL	CA-CB-CG1	6.75	121.03	110.90
1	3	189	LEU	CB-CG-CD1	6.73	122.44	111.00
1	1	314	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	2	114	LEU	CA-CB-CG	6.72	130.76	115.30
1	3	332	ARG	CB-CG-CD	6.72	129.06	111.60
1	3	323	LYS	CG-CD-CE	6.71	132.04	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	238	TYR	CB-CG-CD1	6.71	125.03	121.00
1	3	169	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
1	4	53	ASP	CB-CG-OD1	6.71	124.34	118.30
1	3	238	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	3	148	SER	CB-CA-C	-6.68	97.40	110.10
1	3	150	LYS	CB-CG-CD	6.68	128.97	111.60
1	1	98	HIS	CA-CB-CG	6.68	124.95	113.60
1	4	77	LYS	CB-CG-CD	6.67	128.94	111.60
1	1	201	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	1	263	LEU	CB-CG-CD1	-6.64	99.71	111.00
1	2	279	ARG	CG-CD-NE	6.64	125.74	111.80
1	2	13	VAL	CA-CB-CG2	-6.63	100.96	110.90
1	4	140	LEU	CB-CG-CD2	6.63	122.26	111.00
1	2	72	ASN	N-CA-CB	-6.62	98.68	110.60
1	3	115	ASN	CB-CG-OD1	6.62	134.83	121.60
1	4	50	GLU	OE1-CD-OE2	-6.62	115.36	123.30
1	4	174	SER	O-C-N	6.58	133.23	122.70
1	4	117	ASP	CB-CG-OD2	6.56	124.21	118.30
1	4	125	SER	CB-CA-C	-6.54	97.68	110.10
1	4	328	LYS	CB-CG-CD	6.54	128.59	111.60
1	2	194	GLU	CA-CB-CG	6.53	127.77	113.40
1	2	81	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	2	149	ASN	CB-CA-C	6.53	123.45	110.40
1	1	244	ASN	CB-CG-ND2	-6.52	101.04	116.70
1	4	319	LEU	CD1-CG-CD2	6.52	130.05	110.50
1	3	301	ASP	CB-CG-OD1	6.51	124.16	118.30
1	1	294	GLU	OE1-CD-OE2	-6.51	115.48	123.30
1	1	64	GLN	CB-CG-CD	6.51	128.53	111.60
1	1	140	LEU	CB-CG-CD2	6.50	122.05	111.00
1	2	151	ASP	CB-CG-OD1	6.49	124.14	118.30
1	2	262	ARG	NH1-CZ-NH2	6.49	126.54	119.40
1	3	228	TYR	CB-CG-CD1	-6.49	117.11	121.00
1	2	332	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	3	114	LEU	O-C-N	-6.48	112.34	122.70
1	1	336	GLU	CB-CA-C	-6.47	97.45	110.40
1	3	162	ASN	CB-CG-OD1	-6.47	108.65	121.60
1	3	317	VAL	CB-CA-C	6.46	123.67	111.40
1	4	263	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	1	137	MET	CA-CB-CG	-6.41	102.40	113.30
1	2	209	VAL	N-CA-CB	-6.39	97.44	111.50
1	1	304	VAL	N-CA-CB	-6.39	97.44	111.50
1	4	65	ILE	O-C-N	6.37	132.89	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	318	GLU	CB-CA-C	-6.36	97.68	110.40
1	4	148	SER	CB-CA-C	-6.36	98.01	110.10
1	3	304	VAL	CG1-CB-CG2	6.36	121.07	110.90
1	3	58	ARG	CB-CA-C	6.34	123.09	110.40
1	1	325	GLN	CG-CD-OE1	6.34	134.28	121.60
1	1	176	ASN	OD1-CG-ND2	6.34	136.48	121.90
1	1	73	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	1	87	ASP	CB-CG-OD1	6.32	123.98	118.30
1	1	206	ARG	CB-CG-CD	-6.30	95.23	111.60
1	4	8	LYS	N-CA-CB	6.29	121.93	110.60
1	1	304	VAL	CB-CA-C	6.29	123.35	111.40
1	3	206	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	1	159	VAL	CG1-CB-CG2	6.28	120.95	110.90
1	2	53	ASP	CB-CG-OD1	6.28	123.95	118.30
1	3	318	GLU	CA-C-O	6.27	133.27	120.10
1	4	337	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	2	78	LEU	CB-CG-CD2	-6.25	100.37	111.00
1	4	198	TYR	CB-CG-CD1	6.25	124.75	121.00
1	2	160	THR	CA-CB-CG2	6.24	121.14	112.40
1	3	307	ASP	CB-CG-OD2	6.24	123.92	118.30
1	3	66	ALA	N-CA-C	-6.24	94.15	111.00
1	1	293	ALA	CA-C-O	-6.23	107.01	120.10
1	1	189	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	3	271	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
1	4	298	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	2	319	LEU	CB-CG-CD1	-6.23	100.42	111.00
1	1	318	GLU	CG-CD-OE1	6.22	130.75	118.30
1	1	196	LYS	CB-CA-C	-6.22	97.96	110.40
1	4	220	SER	CA-CB-OG	-6.22	94.42	111.20
1	1	193	VAL	CB-CA-C	6.21	123.21	111.40
1	2	72	ASN	CA-CB-CG	6.21	127.07	113.40
1	1	244	ASN	CB-CG-OD1	6.21	134.03	121.60
1	1	201	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	2	74	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	3	89	ASN	CA-CB-CG	-6.21	99.74	113.40
1	3	329	GLU	CG-CD-OE1	6.21	130.71	118.30
1	3	92	ASP	CB-CG-OD2	6.20	123.88	118.30
1	4	291	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	4	319	LEU	CB-CG-CD2	-6.17	100.50	111.00
1	3	289	VAL	CA-CB-CG2	6.17	120.15	110.90
1	3	322	VAL	CG1-CB-CG2	6.16	120.76	110.90
1	3	290	LEU	CA-CB-CG	6.15	129.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	263	LEU	CB-CA-C	-6.14	98.53	110.20
1	2	204	ALA	CA-C-N	6.13	130.69	117.20
1	2	233	VAL	CA-CB-CG2	6.12	120.09	110.90
1	3	158	LEU	CB-CG-CD1	6.12	121.40	111.00
1	4	290	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	4	314	ARG	CD-NE-CZ	6.11	132.15	123.60
1	4	323	LYS	CB-CG-CD	6.11	127.47	111.60
1	4	311	GLU	CA-CB-CG	6.10	126.83	113.40
1	1	271	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	2	100	THR	CA-CB-CG2	6.09	120.93	112.40
1	2	262	ARG	CB-CG-CD	6.09	127.43	111.60
1	2	161	MET	CA-CB-CG	-6.09	102.95	113.30
1	2	318	GLU	N-CA-CB	6.07	121.53	110.60
1	1	239	LYS	CB-CA-C	-6.07	98.27	110.40
1	2	263	LEU	CA-CB-CG	6.06	129.23	115.30
1	4	90	ASP	CB-CA-C	-6.06	98.29	110.40
1	2	96	ILE	CA-C-O	-6.05	107.39	120.10
1	3	121	VAL	CA-CB-CG1	6.05	119.98	110.90
1	4	229	SER	N-CA-CB	-6.04	101.44	110.50
1	1	125	SER	N-CA-CB	6.04	119.56	110.50
1	2	115	ASN	CB-CG-OD1	6.04	133.68	121.60
1	1	294	GLU	CG-CD-OE2	6.02	130.35	118.30
1	4	115	ASN	OD1-CG-ND2	-6.02	108.05	121.90
1	1	291	ARG	CD-NE-CZ	6.02	132.02	123.60
1	2	304	VAL	N-CA-CB	-6.02	98.27	111.50
1	4	336	GLU	CG-CD-OE2	-6.01	106.27	118.30
1	2	115	ASN	CA-CB-CG	6.01	126.62	113.40
1	2	319	LEU	CD1-CG-CD2	6.01	128.52	110.50
1	4	66	ALA	CB-CA-C	6.00	119.11	110.10
1	1	263	LEU	N-CA-C	6.00	127.21	111.00
1	2	44	LEU	CA-CB-CG	6.00	129.11	115.30
1	3	150	LYS	CA-CB-CG	6.00	126.60	113.40
1	2	262	ARG	CA-CB-CG	-5.98	100.25	113.40
1	3	308	LEU	O-C-N	5.97	132.25	122.70
1	3	104	GLU	CG-CD-OE2	5.97	130.23	118.30
1	3	17	THR	CA-CB-CG2	5.96	120.74	112.40
1	2	80	LYS	CA-CB-CG	-5.95	100.31	113.40
1	3	319	LEU	CD1-CG-CD2	5.95	128.35	110.50
1	4	307	ASP	CB-CG-OD2	5.95	123.66	118.30
1	1	127	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	2	42	ASP	CB-CG-OD1	5.93	123.64	118.30
1	3	263	LEU	CA-CB-CG	-5.93	101.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	262	ARG	CD-NE-CZ	5.92	131.88	123.60
1	3	101	ASP	O-C-N	5.92	132.17	122.70
1	3	275	THR	O-C-N	5.92	132.16	122.70
1	4	95	VAL	CB-CA-C	5.91	122.63	111.40
1	4	180	GLU	CG-CD-OE1	5.90	130.10	118.30
1	4	221	LEU	CB-CA-C	5.90	121.41	110.20
1	1	58	ARG	N-CA-CB	5.89	121.20	110.60
1	1	143	ALA	N-CA-CB	5.87	118.32	110.10
1	4	223	GLN	CG-CD-OE1	-5.86	109.88	121.60
1	2	90	ASP	CB-CG-OD1	5.86	123.58	118.30
1	2	73	ASP	OD1-CG-OD2	5.85	134.41	123.30
1	1	73	ASP	CB-CG-OD1	5.85	123.56	118.30
1	3	121	VAL	CA-CB-CG2	5.84	119.66	110.90
1	1	292	ASN	CB-CG-OD1	5.83	133.26	121.60
1	4	121	VAL	O-C-N	5.83	132.03	122.70
1	3	192	VAL	CB-CA-C	5.83	122.47	111.40
1	2	164	GLU	CG-CD-OE2	-5.82	106.66	118.30
1	1	115	ASN	CB-CG-ND2	5.82	130.67	116.70
1	4	147	ALA	N-CA-CB	5.81	118.24	110.10
1	3	98	HIS	CA-CB-CG	5.81	123.47	113.60
1	3	89	ASN	CB-CG-OD1	-5.80	110.00	121.60
1	3	312	LYS	CB-CG-CD	5.80	126.68	111.60
1	3	290	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	2	9	LEU	CB-CA-C	5.79	121.20	110.20
1	3	221	LEU	CA-CB-CG	5.79	128.62	115.30
1	4	98	HIS	N-CA-CB	-5.78	100.19	110.60
1	2	279	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	2	331	GLN	N-CA-CB	5.77	120.98	110.60
1	3	179	THR	CA-CB-CG2	5.75	120.45	112.40
1	4	9	LEU	N-CA-CB	-5.75	98.90	110.40
1	2	192	VAL	CB-CA-C	5.74	122.31	111.40
1	3	115	ASN	CA-CB-CG	5.73	126.00	113.40
1	3	290	LEU	N-CA-CB	-5.72	98.95	110.40
1	2	169	ARG	NE-CZ-NH1	-5.71	117.45	120.30
1	3	101	ASP	CB-CG-OD1	5.71	123.44	118.30
1	4	279	ARG	NE-CZ-NH1	-5.69	117.45	120.30
1	1	57	VAL	CA-CB-CG2	5.69	119.44	110.90
1	3	292	ASN	CB-CG-ND2	5.68	130.34	116.70
1	2	60	GLU	CA-CB-CG	5.68	125.90	113.40
1	2	308	LEU	CA-CB-CG	5.68	128.36	115.30
1	4	301	ASP	CB-CG-OD1	5.67	123.41	118.30
1	1	78	LEU	CA-CB-CG	5.67	128.34	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	112	LEU	CA-CB-CG	5.67	128.33	115.30
1	1	159	VAL	CB-CA-C	5.66	122.16	111.40
1	2	209	VAL	CG1-CB-CG2	5.66	119.96	110.90
1	4	150	LYS	CG-CD-CE	5.66	128.88	111.90
1	2	304	VAL	CB-CA-C	5.66	122.15	111.40
1	3	180	GLU	CG-CD-OE2	-5.66	106.99	118.30
1	2	300	ASN	CA-CB-CG	5.64	125.81	113.40
1	4	311	GLU	CG-CD-OE2	5.64	129.58	118.30
1	4	310	PRO	O-C-N	-5.64	113.68	122.70
1	4	51	LEU	CA-CB-CG	5.63	128.26	115.30
1	1	279	ARG	NH1-CZ-NH2	-5.62	113.21	119.40
1	3	276	GLN	CG-CD-OE1	5.62	132.84	121.60
1	3	289	VAL	CB-CA-C	5.62	122.08	111.40
1	4	266	ALA	N-CA-CB	5.62	117.97	110.10
1	4	273	THR	OG1-CB-CG2	-5.62	97.08	110.00
1	1	192	VAL	N-CA-CB	5.61	123.84	111.50
1	4	230	TYR	CG-CD1-CE1	5.61	125.79	121.30
1	3	78	LEU	CB-CG-CD2	5.61	120.53	111.00
1	2	337	TYR	CD1-CE1-CZ	-5.60	114.76	119.80
1	2	114	LEU	CD1-CG-CD2	-5.60	93.71	110.50
1	4	326	ASP	CB-CG-OD2	5.59	123.33	118.30
1	4	332	ARG	O-C-N	5.58	131.63	122.70
1	4	160	THR	CA-CB-OG1	-5.58	97.28	109.00
1	2	294	GLU	CG-CD-OE1	5.57	129.44	118.30
1	3	161	MET	CA-CB-CG	-5.57	103.83	113.30
1	2	104	GLU	OE1-CD-OE2	5.57	129.98	123.30
1	4	273	THR	O-C-N	-5.57	113.74	123.20
1	1	313	ALA	CB-CA-C	5.56	118.44	110.10
1	2	55	ALA	O-C-N	5.56	131.60	122.70
1	1	274	GLY	N-CA-C	5.56	126.99	113.10
1	4	244	ASN	CA-CB-CG	-5.55	101.18	113.40
1	2	327	SER	CA-CB-OG	-5.55	96.21	111.20
1	1	117	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	4	83	ALA	N-CA-CB	5.54	117.85	110.10
1	2	291	ARG	CD-NE-CZ	5.53	131.34	123.60
1	2	191	MET	O-C-N	5.53	131.55	122.70
1	3	84	GLU	N-CA-CB	5.53	120.55	110.60
1	3	172	SER	N-CA-CB	-5.53	102.21	110.50
1	3	323	LYS	CB-CG-CD	5.53	125.97	111.60
1	4	323	LYS	CA-CB-CG	5.53	125.56	113.40
1	1	113	THR	CA-CB-CG2	5.52	120.13	112.40
1	2	330	LEU	N-CA-CB	-5.52	99.35	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	104	GLU	OE1-CD-OE2	5.52	129.92	123.30
1	3	179	THR	N-CA-CB	-5.51	99.83	110.30
1	3	164	GLU	O-C-N	5.51	131.51	122.70
1	4	322	VAL	CA-CB-CG2	5.51	119.16	110.90
1	2	225	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	4	189	LEU	CA-CB-CG	5.51	127.97	115.30
1	2	12	VAL	CB-CA-C	5.50	121.84	111.40
1	2	48	VAL	CA-CB-CG1	5.49	119.14	110.90
1	1	270	LEU	CB-CA-C	5.49	120.63	110.20
1	3	80	LYS	CB-CA-C	-5.49	99.43	110.40
1	4	45	ILE	CB-CA-C	5.49	122.57	111.60
1	1	180	GLU	CB-CG-CD	5.48	129.01	114.20
1	3	259	VAL	O-C-N	5.48	131.46	122.70
1	3	213	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	3	169	ARG	CD-NE-CZ	5.47	131.25	123.60
1	1	254	THR	CA-C-N	5.46	127.13	116.20
1	3	71	THR	CA-CB-CG2	5.46	120.05	112.40
1	3	125	SER	N-CA-CB	5.46	118.69	110.50
1	2	54	LEU	CA-CB-CG	5.45	127.84	115.30
1	2	327	SER	O-C-N	5.45	131.42	122.70
1	4	291	ARG	CD-NE-CZ	5.44	131.22	123.60
1	4	311	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	1	244	ASN	C-N-CA	-5.44	110.88	122.30
1	4	75	LEU	CA-CB-CG	5.44	127.80	115.30
1	4	243	GLN	CA-CB-CG	5.43	125.34	113.40
1	1	206	ARG	CG-CD-NE	-5.42	100.41	111.80
1	4	64	GLN	O-C-N	5.42	131.37	122.70
1	1	76	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	4	185	ALA	CB-CA-C	-5.41	101.98	110.10
1	2	96	ILE	O-C-N	5.41	131.35	122.70
1	3	120	ILE	CA-C-O	-5.40	108.75	120.10
1	4	11	ASN	O-C-N	5.40	131.34	122.70
1	4	78	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	2	330	LEU	CB-CA-C	5.39	120.44	110.20
1	3	304	VAL	N-CA-CB	-5.39	99.64	111.50
1	1	273	THR	CA-C-O	5.38	131.41	120.10
1	3	317	VAL	CA-C-O	-5.38	108.79	120.10
1	4	181	ALA	O-C-N	5.38	131.32	122.70
1	4	275	THR	CA-CB-OG1	-5.38	97.70	109.00
1	4	138	LEU	CB-CG-CD2	5.38	120.14	111.00
1	3	273	THR	O-C-N	-5.37	114.07	123.20
1	4	244	ASN	CB-CG-OD1	-5.37	110.86	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	89	ASN	C-N-CA	5.37	135.12	121.70
1	3	147	ALA	C-N-CA	5.36	135.11	121.70
1	1	44	LEU	CA-CB-CG	5.36	127.63	115.30
1	2	135	ASP	OD1-CG-OD2	-5.36	113.12	123.30
1	3	137	MET	CA-CB-CG	-5.35	104.20	113.30
1	2	72	ASN	O-C-N	-5.35	114.14	122.70
1	2	159	VAL	CB-CA-C	5.35	121.56	111.40
1	1	167	SER	N-CA-CB	-5.35	102.48	110.50
1	2	263	LEU	N-CA-CB	-5.34	99.72	110.40
1	4	114	LEU	CA-CB-CG	5.34	127.58	115.30
1	2	323	LYS	CG-CD-CE	5.34	127.91	111.90
1	1	329	GLU	N-CA-CB	5.33	120.20	110.60
1	1	319	LEU	N-CA-CB	-5.33	99.74	110.40
1	3	61	GLN	N-CA-CB	5.33	120.19	110.60
1	2	298	ASP	CB-CG-OD2	5.33	123.10	118.30
1	1	194	GLU	CG-CD-OE1	5.33	128.95	118.30
1	1	311	GLU	CB-CG-CD	5.32	128.57	114.20
1	4	115	ASN	O-C-N	-5.32	114.19	122.70
1	1	68	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	1	64	GLN	CB-CA-C	5.32	121.03	110.40
1	1	192	VAL	CA-CB-CG2	5.30	118.86	110.90
1	1	243	GLN	N-CA-CB	5.30	120.15	110.60
1	1	53	ASP	CA-CB-CG	5.30	125.06	113.40
1	2	58	ARG	CA-CB-CG	5.30	125.06	113.40
1	2	97	THR	CA-CB-OG1	-5.30	97.87	109.00
1	2	317	VAL	CG1-CB-CG2	-5.30	102.42	110.90
1	4	147	ALA	CA-C-N	5.29	128.83	117.20
1	1	99	GLY	CA-C-O	-5.27	111.11	120.60
1	3	104	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	1	115	ASN	N-CA-CB	5.24	120.04	110.60
1	1	194	GLU	CB-CG-CD	5.24	128.34	114.20
1	3	327	SER	CB-CA-C	5.23	120.04	110.10
1	2	121	VAL	CB-CA-C	5.22	121.32	111.40
1	2	226	ILE	C-N-CA	5.22	134.75	121.70
1	4	58	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	4	321	MET	CA-CB-CG	-5.22	104.43	113.30
1	1	54	LEU	CA-CB-CG	5.21	127.28	115.30
1	2	235	ASP	OD1-CG-OD2	-5.21	113.40	123.30
1	1	117	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	1	272	LYS	CB-CA-C	5.21	120.81	110.40
1	1	152	SER	CB-CA-C	-5.20	100.22	110.10
1	2	319	LEU	N-CA-CB	-5.20	100.00	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	132	MET	N-CA-CB	-5.20	101.25	110.60
1	3	137	MET	CB-CA-C	5.19	120.78	110.40
1	2	89	ASN	O-C-N	5.19	131.00	122.70
1	3	55	ALA	O-C-N	5.18	130.99	122.70
1	3	337	TYR	CG-CD2-CE2	5.18	125.45	121.30
1	3	318	GLU	CB-CA-C	-5.18	100.04	110.40
1	4	225	ASP	CB-CG-OD2	5.18	122.96	118.30
1	3	307	ASP	OD1-CG-OD2	-5.18	113.46	123.30
1	1	115	ASN	CA-CB-CG	5.17	124.77	113.40
1	1	285	GLN	CA-C-N	5.17	126.53	116.20
1	3	262	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	2	65	ILE	CA-C-N	-5.16	105.85	117.20
1	2	269	THR	N-CA-CB	5.16	120.10	110.30
1	2	329	GLU	CG-CD-OE1	-5.16	107.98	118.30
1	4	92	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	3	60	GLU	CA-CB-CG	5.15	124.73	113.40
1	3	236	THR	CA-CB-CG2	5.15	119.61	112.40
1	3	15	LEU	O-C-N	5.15	130.94	122.70
1	2	12	VAL	CA-CB-CG1	5.15	118.62	110.90
1	2	273	THR	CB-CA-C	5.15	125.49	111.60
1	3	161	MET	O-C-N	5.15	130.93	122.70
1	4	248	ALA	N-CA-CB	5.15	117.31	110.10
1	1	267	LEU	CB-CG-CD1	5.14	119.75	111.00
1	1	117	ASP	OD1-CG-OD2	5.14	133.07	123.30
1	2	204	ALA	N-CA-CB	5.14	117.30	110.10
1	4	298	ASP	CB-CG-OD1	5.14	122.93	118.30
1	2	223	GLN	CB-CG-CD	5.14	124.95	111.60
1	2	168	GLY	O-C-N	-5.13	114.49	122.70
1	4	143	ALA	CB-CA-C	5.13	117.80	110.10
1	3	64	GLN	CA-CB-CG	5.13	124.69	113.40
1	1	67	SER	CB-CA-C	5.13	119.84	110.10
1	2	58	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	2	230	TYR	CD1-CE1-CZ	-5.13	115.19	119.80
1	3	269	THR	CA-CB-CG2	5.12	119.56	112.40
1	2	329	GLU	CB-CA-C	-5.11	100.17	110.40
1	4	317	VAL	CB-CA-C	-5.11	101.69	111.40
1	4	67	SER	CB-CA-C	5.10	119.80	110.10
1	1	280	SER	O-C-N	-5.10	114.54	122.70
1	2	264	THR	CB-CA-C	5.10	125.36	111.60
1	3	117	ASP	CB-CG-OD1	5.09	122.88	118.30
1	4	309	ASN	CB-CA-C	5.09	120.59	110.40
1	1	74	ASP	CB-CG-OD2	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	58	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	3	217	GLN	O-C-N	5.09	130.84	122.70
1	2	262	ARG	CD-NE-CZ	-5.08	116.48	123.60
1	1	132	MET	CB-CA-C	5.08	120.55	110.40
1	1	210	ASN	O-C-N	-5.08	114.58	122.70
1	2	301	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	2	184	SER	N-CA-CB	5.07	118.10	110.50
1	2	9	LEU	N-CA-CB	-5.07	100.27	110.40
1	1	270	LEU	CA-CB-CG	5.06	126.94	115.30
1	3	304	VAL	CB-CA-C	5.06	121.02	111.40
1	2	274	GLY	N-CA-C	5.06	125.75	113.10
1	3	263	LEU	N-CA-CB	-5.06	100.28	110.40
1	2	312	LYS	CA-CB-CG	5.06	124.53	113.40
1	4	77	LYS	CG-CD-CE	5.05	127.05	111.90
1	4	213	PHE	O-C-N	5.05	130.78	122.70
1	1	75	LEU	CB-CA-C	5.05	119.79	110.20
1	1	230	TYR	CB-CG-CD2	5.05	124.03	121.00
1	1	317	VAL	CA-C-O	-5.05	109.50	120.10
1	4	60	GLU	CA-CB-CG	5.04	124.49	113.40
1	2	125	SER	N-CA-CB	-5.04	102.94	110.50
1	4	319	LEU	O-C-N	5.03	130.75	122.70
1	2	201	ARG	CD-NE-CZ	5.03	130.64	123.60
1	2	76	LEU	CB-CG-CD1	5.03	119.55	111.00
1	3	51	LEU	CA-CB-CG	5.02	126.86	115.30
1	4	135	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	1	323	LYS	CA-C-N	5.02	128.25	117.20
1	3	17	THR	CA-CB-OG1	-5.02	98.46	109.00
1	3	224	VAL	O-C-N	5.02	130.73	122.70
1	1	239	LYS	CB-CG-CD	-5.01	98.56	111.60
1	1	250	ILE	CA-CB-CG1	-5.01	101.48	111.00
1	1	77	LYS	O-C-N	-5.00	114.69	122.70
1	2	230	TYR	CA-C-N	5.00	126.21	116.20
1	1	332	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	4	319	LEU	N-CA-CB	-5.00	100.40	110.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	332	ARG	Sidechain
1	1	35[C]	GLN	Mainchain
1	1	39[C]	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	2	332	ARG	Sidechain
1	3	291	ARG	Sidechain
1	3	34[C]	TYR	Mainchain
1	3	35[C]	GLN	Mainchain
1	4	153	ARG	Sidechain
1	4	262	ARG	Sidechain
1	4	35[C]	GLN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2611	0	2621	52	5
1	2	2611	0	2624	41	0
1	3	2607	0	2618	50	0
1	4	2607	0	2617	40	0
2	1	113	0	0	1	0
2	2	87	0	0	0	0
2	3	112	0	0	2	0
2	4	106	0	0	2	5
All	All	10854	0	10480	173	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (173) 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)
1:3:291:ARG:HH11	1:3:331:GLN:HE21	1.08	0.96
1:3:299:LYS:NZ	1:3:300:ASN:HD21	1.68	0.92
1:1:291:ARG:HH11	1:1:331:GLN:HE21	1.19	0.90
1:3:256:ASN:HD21	1:3:290:LEU:H	1.26	0.84
1:4:291:ARG:HH11	1:4:331:GLN:HE21	1.24	0.82
1:3:299:LYS:HZ1	1:3:300:ASN:HD21	1.30	0.78
1:4:149:ASN:ND2	1:4:151:ASP:H	1.80	0.78
1:4:149:ASN:HD22	1:4:151:ASP:H	1.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:291:ARG:NH1	1:3:331:GLN:HE21	1.83	0.76
1:3:291:ARG:HH11	1:3:331:GLN:NE2	1.83	0.74
1:1:72:ASN:HD21	1:1:314:ARG:HH22	1.35	0.73
1:4:291:ARG:NH1	1:4:331:GLN:HE21	1.85	0.73
1:3:292:ASN:HD21	1:3:298:ASP:H	1.36	0.72
1:1:304:VAL:H	1:1:331:GLN:HE22	1.39	0.70
1:2:313:ALA:O	1:2:317:VAL:HG23	1.91	0.69
1:4:48:VAL:HG13	1:4:51:LEU:HD22	1.75	0.69
1:4:319:LEU:O	1:4:322:VAL:HG22	1.92	0.69
1:3:72:ASN:HD21	1:3:314:ARG:HH22	1.41	0.68
1:4:149:ASN:HD22	1:4:150:LYS:N	1.93	0.67
1:1:254:THR:HG23	1:3:101:ASP:HB3	1.78	0.66
1:2:250:ILE:HD11	1:2:317:VAL:HG21	1.76	0.66
1:2:113:THR:HG22	1:2:319:LEU:HD11	1.80	0.64
1:1:256:ASN:HD21	1:1:290:LEU:H	1.46	0.63
1:1:82:VAL:HG13	1:1:94:ILE:HD13	1.80	0.62
1:3:11:ASN:HD22	1:3:56:ASN:HB2	1.64	0.62
1:2:278:ILE:HD13	1:2:317:VAL:HG21	1.82	0.62
1:2:193:VAL:HG12	1:2:194:GLU:HG2	1.82	0.62
1:3:292:ASN:ND2	1:3:298:ASP:H	1.99	0.61
1:4:117:ASP:HB3	1:4:209:VAL:HG11	1.83	0.61
1:4:61:GLN:HE22	1:4:64:GLN:NE2	1.98	0.60
1:3:264:THR:HB	1:3:265:PRO:HD3	1.81	0.60
1:1:250:ILE:HD11	1:1:314:ARG:HA	1.83	0.60
1:3:278:ILE:CD1	1:3:317:VAL:HG21	2.32	0.60
1:1:113:THR:HG22	1:1:319:LEU:HD11	1.84	0.59
1:3:299:LYS:HZ3	1:3:300:ASN:HD21	1.50	0.59
1:1:71:THR:HG22	1:1:74:ASP:H	1.68	0.59
1:4:291:ARG:HH11	1:4:331:GLN:NE2	1.96	0.58
1:2:319:LEU:O	1:2:322:VAL:HG22	2.03	0.58
1:2:259:VAL:HG12	1:2:264:THR:HG22	1.86	0.58
1:4:18:GLY:HA2	1:4:64:GLN:NE2	2.19	0.57
1:2:48:VAL:HG22	1:2:51:LEU:HD13	1.86	0.57
1:1:72:ASN:HD21	1:1:314:ARG:NH2	2.03	0.57
1:4:103:LEU:HD13	1:4:122:VAL:HG22	1.87	0.56
1:2:28[O]:ALA:HB1	1:2:47:GLY:O	2.05	0.56
1:4:64:GLN:HE21	1:4:64:GLN:HA	1.71	0.55
1:1:9:LEU:HB3	1:1:55:ALA:HA	1.88	0.55
1:4:322:VAL:HG23	1:4:323:LYS:NZ	2.22	0.55
1:4:218:ILE:HG12	1:4:322:VAL:HG21	1.88	0.54
1:1:178:LYS:HZ1	1:2:162:ASN:ND2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:324:THR:HG23	1:4:330:LEU:HD13	1.89	0.54
1:4:11:ASN:HD22	1:4:56:ASN:HB2	1.73	0.54
1:2:37[O]:ALA:HB3	1:2:43:LYS:HD3	1.89	0.54
1:4:41:VAL:O	1:4:45:ILE:HG23	2.08	0.54
1:3:299:LYS:NZ	1:3:300:ASN:ND2	2.48	0.53
1:1:254:THR:HG23	1:3:101:ASP:OD2	2.08	0.53
1:4:292:ASN:HD21	1:4:298:ASP:H	1.57	0.52
1:1:72:ASN:ND2	1:1:314:ARG:HH22	2.04	0.52
1:2:113:THR:CG2	1:2:319:LEU:HD11	2.39	0.52
1:3:196:LYS:HE3	1:3:198:TYR:OH	2.09	0.52
1:3:278:ILE:HD13	1:3:317:VAL:HG21	1.91	0.52
1:4:61:GLN:NE2	1:4:64:GLN:NE2	2.58	0.52
1:3:9:LEU:HG	1:3:55:ALA:HA	1.92	0.51
1:1:264:THR:HB	1:1:265:PRO:HD3	1.93	0.51
1:3:317:VAL:HG23	1:3:334:PHE:HE2	1.76	0.51
1:1:15:LEU:HD21	1:1:85:LEU:HD21	1.92	0.51
1:3:256:ASN:ND2	1:3:290:LEU:H	2.02	0.51
1:1:207:HIS:HD2	1:1:208:THR:OG1	1.94	0.51
1:1:285:GLN:NE2	1:3:285:GLN:HG3	2.26	0.51
1:1:264:THR:N	1:1:265:PRO:HD2	2.26	0.51
1:3:178:LYS:NZ	1:4:162:ASN:O	2.44	0.50
1:1:313:ALA:O	1:1:317:VAL:HG22	2.11	0.50
1:1:98:HIS:HD2	1:1:99:GLY:O	1.94	0.50
1:4:278:ILE:CD1	1:4:317:VAL:HG11	2.42	0.50
1:3:48:VAL:HG22	1:3:137:MET:HG3	1.94	0.50
1:1:278:ILE:CD1	1:1:317:VAL:HG11	2.41	0.49
1:3:314:ARG:O	1:3:318:GLU:HG3	2.11	0.49
1:1:178:LYS:NZ	1:2:162:ASN:ND2	2.59	0.49
1:3:82:VAL:HG12	1:3:114:LEU:HD22	1.93	0.49
1:3:65:ILE:HD11	1:3:70:ILE:HD12	1.93	0.49
1:3:76:LEU:HD13	1:3:221:LEU:HD22	1.94	0.49
1:2:278:ILE:HD13	1:2:317:VAL:CG2	2.43	0.49
1:2:226:ILE:HG12	1:2:250:ILE:HB	1.94	0.49
1:2:15:LEU:HD21	1:2:85:LEU:HD11	1.95	0.49
1:3:238:TYR:CE2	1:3:263:LEU:HD21	2.48	0.49
1:1:81:ARG:HH11	1:1:84:GLU:HG3	1.78	0.48
1:1:304:VAL:H	1:1:331:GLN:NE2	2.09	0.48
1:1:255:GLY:HA2	1:3:173:LYS:HE2	1.95	0.48
1:1:137:MET:HB2	2:1:785:HOH:O	2.13	0.48
1:2:248:ALA:HB2	1:2:276:GLN:HB2	1.95	0.48
1:4:166:GLN:NE2	2:4:438:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:225:ASP:HB3	1:2:241:LEU:HD13	1.94	0.48
1:3:79:GLY:O	1:3:114:LEU:HD11	2.13	0.48
1:4:193:VAL:O	1:4:194:GLU:HB2	2.13	0.48
1:1:260:SER:HB3	1:1:263:LEU:HD13	1.95	0.47
1:4:292:ASN:HA	1:4:295:GLN:O	2.14	0.47
1:3:114:LEU:HD23	2:3:742:HOH:O	2.15	0.47
1:4:305:ALA:HA	1:4:334:PHE:CD2	2.49	0.47
1:1:106:THR:HG22	1:1:110:LEU:HD22	1.97	0.47
1:2:155:LYS:HD3	1:2:199:TRP:CZ3	2.48	0.47
1:4:9:LEU:HG	1:4:55:ALA:HA	1.97	0.47
1:2:223:GLN:HG2	1:2:246:ALA:HA	1.97	0.47
1:2:259:VAL:CG1	1:2:264:THR:HG22	2.45	0.47
1:4:48:VAL:O	1:4:51:LEU:HB2	2.15	0.46
1:2:324:THR:HG21	1:2:329:GLU:HB3	1.97	0.46
1:3:160:THR:HA	1:3:164:GLU:O	2.16	0.46
1:3:61:GLN:NE2	1:3:63:MET:O	2.48	0.46
1:3:304:VAL:H	1:3:331:GLN:HE22	1.63	0.46
1:1:224:VAL:HG11	1:1:317:VAL:CG2	2.46	0.46
1:1:237:ALA:O	1:1:241:LEU:HD22	2.16	0.46
1:3:278:ILE:HD11	1:3:317:VAL:HG21	1.98	0.46
1:3:119:PRO:HD3	1:3:153:ARG:HG2	1.97	0.46
1:4:313:ALA:O	1:4:317:VAL:HG22	2.16	0.46
1:2:80:LYS:NZ	1:2:218:ILE:O	2.45	0.46
1:2:121:VAL:HG13	1:2:147:ALA:HB2	1.97	0.45
1:3:234:THR:HB	2:3:504:HOH:O	2.16	0.45
1:4:224:VAL:HG11	1:4:317:VAL:CG2	2.46	0.45
1:4:207:HIS:HD2	1:4:208:THR:OG1	1.99	0.45
1:4:88:SER:OG	1:4:90:ASP:HB2	2.16	0.45
1:3:62:VAL:HG11	1:3:78:LEU:HD23	1.99	0.45
1:1:224:VAL:HG11	1:1:317:VAL:HG23	1.98	0.45
1:2:250:ILE:HD13	1:2:278:ILE:HB	1.98	0.45
1:1:314:ARG:O	1:1:318:GLU:HG3	2.16	0.45
1:1:16:ALA:HA	1:1:97:THR:OG1	2.17	0.45
1:3:271:ARG:HA	1:3:271:ARG:HD2	1.84	0.45
1:3:237:ALA:O	1:3:241:LEU:HB2	2.17	0.45
1:1:160:THR:HA	1:1:164:GLU:O	2.17	0.44
1:1:319:LEU:O	1:1:322:VAL:HB	2.17	0.44
1:2:264:THR:N	1:2:265:PRO:CD	2.81	0.44
1:1:178:LYS:NZ	1:1:178:LYS:HB3	2.32	0.44
1:1:264:THR:N	1:1:265:PRO:CD	2.80	0.44
1:3:212:GLU:O	1:3:323:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:292:ASN:HD22	1:3:297:ASP:N	2.15	0.44
1:4:278:ILE:HD13	1:4:317:VAL:HG11	1.98	0.44
1:2:321:MET:HA	1:2:324:THR:O	2.18	0.44
1:1:113:THR:CG2	1:1:319:LEU:HD11	2.48	0.43
1:1:223:GLN:NE2	1:1:225:ASP:OD2	2.50	0.43
1:1:238:TYR:OH	1:1:251:HIS:HD2	2.01	0.43
1:1:166:GLN:HE22	1:1:184:SER:HB3	1.83	0.43
1:3:226:ILE:HG12	1:3:250:ILE:HB	2.01	0.43
1:2:314:ARG:O	1:2:318:GLU:HG3	2.18	0.43
1:3:299:LYS:HZ3	1:3:300:ASN:ND2	2.15	0.43
1:1:81:ARG:NH1	1:1:84:GLU:HG3	2.33	0.43
1:1:8:LYS:HE3	1:1:9:LEU:HG	2.00	0.43
1:1:259:VAL:HG23	1:1:263:LEU:HB3	1.99	0.43
1:2:289:VAL:HG12	1:2:304:VAL:HG22	2.01	0.43
1:2:60:GLU:OE2	1:2:81:ARG:NH1	2.52	0.42
1:2:230:TYR:CE1	1:2:233:VAL:HG13	2.54	0.42
1:3:132:MET:HG2	1:4:137:MET:SD	2.59	0.42
1:4:149:ASN:C	1:4:149:ASN:HD22	2.22	0.42
1:4:178:LYS:HE3	1:4:180:GLU:OE2	2.20	0.42
1:2:214:ASP:OD1	1:2:216:LYS:HB2	2.19	0.42
1:1:132:MET:HE2	1:1:132:MET:HB3	1.88	0.42
1:1:230:TYR:CG	1:3:226:ILE:HD12	2.55	0.42
1:2:24[O]:ALA:CB	1:2:29[O]:ALA:HB2	2.51	0.41
1:4:250:ILE:HD11	1:4:317:VAL:HG21	2.01	0.41
1:2:15:LEU:HD21	1:2:85:LEU:CD1	2.50	0.41
1:4:194:GLU:N	2:4:699:HOH:O	2.52	0.41
1:2:47:GLY:O	1:2:49:PRO:HD3	2.21	0.41
1:3:221:LEU:HA	1:3:222:PRO:HD3	1.86	0.41
1:1:137:MET:SD	1:2:132:MET:HG2	2.61	0.41
1:2:238:TYR:CE1	1:2:263:LEU:HD11	2.55	0.41
1:1:8:LYS:NZ	1:1:9:LEU:HG	2.35	0.41
1:3:76:LEU:HD13	1:3:221:LEU:CD2	2.49	0.40
1:2:115:ASN:ND2	1:2:213:PHE:O	2.54	0.40
1:4:224:VAL:HG11	1:4:317:VAL:HG21	2.02	0.40
1:1:238:TYR:CE1	1:1:263:LEU:HD21	2.56	0.40
1:2:292:ASN:HA	1:2:295:GLN:O	2.22	0.40
1:4:48:VAL:HG23	1:4:137:MET:HE2	2.03	0.40
1:2:47:GLY:C	1:2:49:PRO:HD3	2.42	0.40
1:1:239:LYS:O	1:1:243:GLN:HG3	2.22	0.40
1:3:202:LEU:HA	1:3:203:PRO:HD3	1.95	0.40
1:1:213:PHE:HZ	1:1:333:ILE:HD13	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:103:LEU:HD21	1:2:161:MET:CE	2.52	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:21[C]:ILE:CD1	2:4:834:HOH:O[3_645]	0.53	1.67
1:1:21[O]:ILE:CG1	2:4:834:HOH:O[3_645]	0.86	1.34
1:1:21[O]:ILE:CD1	2:4:834:HOH:O[3_645]	0.87	1.33
1:1:21[C]:ILE:CG1	2:4:834:HOH:O[3_645]	1.07	1.13
1:1:21[O]:ILE:CB	2:4:834:HOH:O[3_645]	1.73	0.47

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	348/337 (103%)	328 (94%)	17 (5%)	3 (1%)	21	13
1	2	348/337 (103%)	326 (94%)	19 (6%)	3 (1%)	21	13
1	3	344/337 (102%)	326 (95%)	16 (5%)	2 (1%)	30	22
1	4	344/337 (102%)	325 (94%)	14 (4%)	5 (2%)	13	5
All	All	1384/1348 (103%)	1305 (94%)	66 (5%)	13 (1%)	26	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	26[C]	ALA
1	1	26[O]	ALA
1	2	26[C]	ALA
1	2	26[O]	ALA
1	4	26[C]	ALA

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Mol	Chain	Res	Type
1	4	26[O]	ALA
1	2	208	THR
1	3	208	THR
1	4	208	THR
1	1	208	THR
1	4	37[C]	ALA
1	4	37[O]	ALA
1	3	177	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	1	256/266 (96%)	226 (88%)	30 (12%)	7	3
1	2	256/266 (96%)	222 (87%)	34 (13%)	5	2
1	3	256/266 (96%)	230 (90%)	26 (10%)	9	5
1	4	256/266 (96%)	227 (89%)	29 (11%)	7	4
All	All	1024/1064 (96%)	905 (88%)	119 (12%)	7	3

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	LYS
1	1	44	LEU
1	1	54	LEU
1	1	58	ARG
1	1	64	GLN
1	1	71	THR
1	1	78	LEU
1	1	85	LEU
1	1	89	ASN
1	1	101	ASP
1	1	103	LEU
1	1	110	LEU
1	1	114	LEU

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Mol	Chain	Res	Type
1	1	123	VAL
1	1	140	LEU
1	1	193	VAL
1	1	223	GLN
1	1	241	LEU
1	1	254	THR
1	1	263	LEU
1	1	267	LEU
1	1	272	LYS
1	1	273	THR
1	1	304	VAL
1	1	317	VAL
1	1	319	LEU
1	1	322	VAL
1	1	323	LYS
1	1	330	LEU
1	1	332	ARG
1	2	12	VAL
1	2	44	LEU
1	2	48	VAL
1	2	51	LEU
1	2	54	LEU
1	2	58	ARG
1	2	62	VAL
1	2	72	ASN
1	2	75	LEU
1	2	76	LEU
1	2	90	ASP
1	2	101	ASP
1	2	103	LEU
1	2	159	VAL
1	2	202	LEU
1	2	209	VAL
1	2	210	ASN
1	2	219	SER
1	2	221	LEU
1	2	222	PRO
1	2	233	VAL
1	2	243	GLN
1	2	263	LEU
1	2	264	THR
1	2	265	PRO

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Mol	Chain	Res	Type
1	2	267	LEU
1	2	269	THR
1	2	272	LYS
1	2	299	LYS
1	2	304	VAL
1	2	308	LEU
1	2	319	LEU
1	2	323	LYS
1	2	325	GLN
1	3	51	LEU
1	3	64	GLN
1	3	76	LEU
1	3	78	LEU
1	3	85	LEU
1	3	95	VAL
1	3	121	VAL
1	3	140	LEU
1	3	150	LYS
1	3	158	LEU
1	3	179	THR
1	3	189	LEU
1	3	192	VAL
1	3	202	LEU
1	3	221	LEU
1	3	234	THR
1	3	241	LEU
1	3	263	LEU
1	3	267	LEU
1	3	270	LEU
1	3	272	LYS
1	3	296	PRO
1	3	304	VAL
1	3	317	VAL
1	3	319	LEU
1	3	322	VAL
1	4	45	ILE
1	4	53	ASP
1	4	64	GLN
1	4	75	LEU
1	4	85	LEU
1	4	90	ASP
1	4	95	VAL

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Mol	Chain	Res	Type
1	4	103	LEU
1	4	114	LEU
1	4	115	ASN
1	4	122	VAL
1	4	138	LEU
1	4	140	LEU
1	4	149	ASN
1	4	150	LYS
1	4	159	VAL
1	4	166	GLN
1	4	180	GLU
1	4	189	LEU
1	4	192	VAL
1	4	217	GLN
1	4	263	LEU
1	4	267	LEU
1	4	269	THR
1	4	272	LYS
1	4	304	VAL
1	4	319	LEU
1	4	323	LYS
1	4	330	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	GLN
1	1	72	ASN
1	1	89	ASN
1	1	98	HIS
1	1	166	GLN
1	1	207	HIS
1	1	223	GLN
1	1	251	HIS
1	1	256	ASN
1	1	285	GLN
1	1	331	GLN
1	2	11	ASN
1	2	162	ASN
1	2	207	HIS
1	2	276	GLN
1	2	284	ASN

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Mol	Chain	Res	Type
1	2	306	HIS
1	3	11	ASN
1	3	61	GLN
1	3	72	ASN
1	3	162	ASN
1	3	166	GLN
1	3	256	ASN
1	3	285	GLN
1	3	292	ASN
1	3	300	ASN
1	3	306	HIS
1	3	331	GLN
1	4	11	ASN
1	4	64	GLN
1	4	149	ASN
1	4	162	ASN
1	4	166	GLN
1	4	207	HIS
1	4	223	GLN
1	4	284	ASN
1	4	292	ASN
1	4	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	1	310/337 (91%)	-1.04	6 (1%) 70 70	17, 27, 55, 103	0
1	2	330/337 (97%)	-0.95	7 (2%) 67 67	19, 29, 71, 103	0
1	3	309/337 (91%)	-1.16	1 (0%) 94 94	17, 25, 44, 68	0
1	4	309/337 (91%)	-1.06	4 (1%) 79 80	16, 26, 50, 92	0
All	All	1258/1348 (93%)	-1.05	18 (1%) 78 78	16, 27, 53, 103	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	39[C]	VAL	4.1
1	1	43	LYS	4.0
1	4	19	GLY	3.4
1	1	40	GLY	3.0
1	4	43	LYS	2.9
1	2	30[C]	ASN	2.8
1	2	29[C]	ALA	2.7
1	1	18	GLY	2.6
1	2	26[C]	ALA	2.5
1	2	27[C]	SER	2.4
1	2	35[C]	GLN	2.4
1	4	41	VAL	2.4
1	4	8	LYS	2.3
1	1	19	GLY	2.2
1	2	31[C]	SER	2.2
1	1	64	GLN	2.2
1	3	8	LYS	2.1
1	1	41	VAL	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 carbohydrates 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.