



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:15 PM UTC

PDB ID : 1FLG / pdb_00001flg
Title : CRYSTAL STRUCTURE OF THE QUINOPROTEIN ETHANOL DEHYDROGENASE FROM PSEUDOMONAS AERUGINOSA
Authors : Keitel, T.; Diehl, A.; Knaute, T.; Stezowski, J.J.; Hohne, W.; Gorisch, H.
Deposited on : 2000-08-14
Resolution : 2.60 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

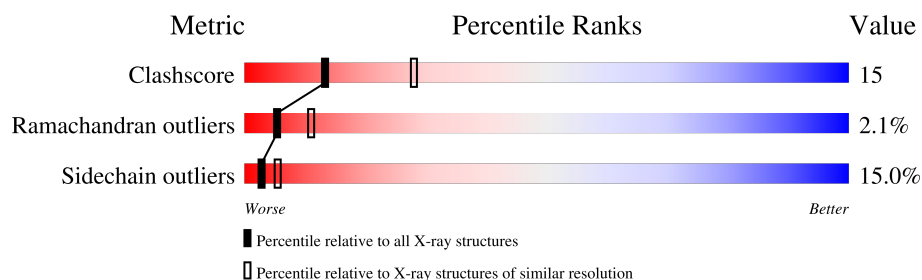
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	31% 45% 20% .
1	B	582	36% 41% 18% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9232 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.

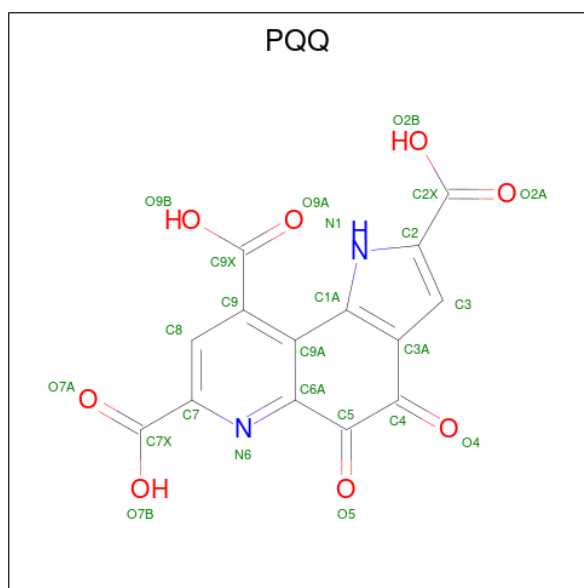
- Molecule 1 is a protein called PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4537	2891	783	852	11			
1	B	582	Total	C	N	O	S	0	0	0
			4537	2891	783	852	11			

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

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

- Molecule 3 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	14	2	8		
3	B	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 4 is water.

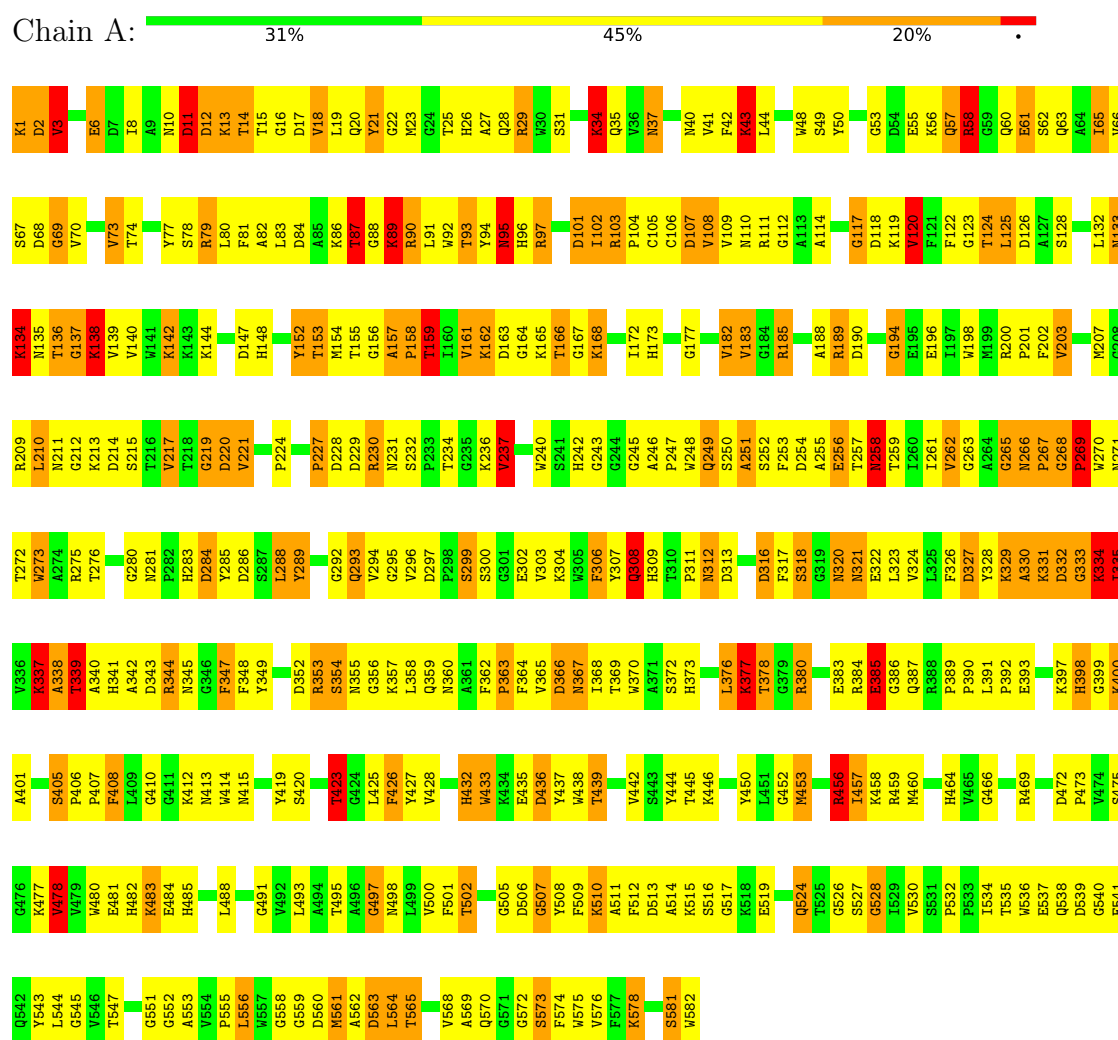
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	33	Total	O	0	0
			33	33		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE)



• Molecule 1: PROTEIN (QUINOPROTEIN ETHANOL DEHYDROGENASE)



L564	T565	R566	P567	G572	W575	W576	F577	K578	L579	W582	K1	D2	V3	T4	W5	E6	D7	I8	A9	N10	D11	T14	T15	G16	D17	V18	L19	G22	P23	G24	Q28	R29	X30	S31	P32	L33	K34	Q35	A38	D39	N40	N41	F42	V43	L44	T45	P46	A47	W48	S49	Y50	S51	F52	G53	D54	E55	K56	Q57	R58	G59	Q60	E61	S62	Q63	T64	A64	I65
											D68	I71	V72	T73	T74	Y77	S78	R79	L80	F81	A82	L83	K86	T87	G88	K89	R90	T93	Y94	N95	H96	R97	D101	I102	T103	R103	P104	C105	D106	D107	V108	V109	N110	R111	G112	A113	A114	I115	Y116	G117	D118	V120	F121	L125	D126	A127	S128	N133	K134	T135	T136	G137					
											K138	K143	K144	F145	A146	D147	H148	Y152	T153	M154	A157	P158	T159	I160	W161	X162	D163	G164	K165	T166	V169	I172	H173	S176	G177	D178	V182	R185	L186	F187	R189	D190	P191	E195	M199	R200	P201	F202	V203	H206	P207	G208	R209	L210	M211	G212	K213										
											D214	S215	T216	V217	T218	G219	D220	V221	K222	A223	P224	S225	W226	R230	N231	S232	P233	T234	G235	K236	V237	S241	H242	G243	G244	G245	A246	P247	W248	Q249	S250	A251	E252	F253	E256	T257	N258	T259	I260	D261	V262	G263	A264	G265	G268	P269	W270	N271	T272	W273	A274	A277	K278	G279	G280		
											N281	P282	H283	D284	Y285	D286	S287	L288	Y289	G292	Q293	V294	G295	S299	S300	G301	E302	F306	Y307	Q308	H309	P311	D312	A314	W315	D316	F317	S318	G319	N320	N321	E322	L323	V324	L325	F326	D327	Y328	K329	A330	D332	G333	K334	I335	V336	K337	A338	T339	A340	H341	A342	D343	R344	N345			
											G346	F347	F348	Y349	V350	V351	D352	R353	G356	K357	A361	P362	P363	D366	R367	I368	T369	W370	A371	S372	H373	I374	D375	L376	K377	T378	G379	R380	E383	R384	E385	G386	Q387	R388	P389	P390	L391	P392	E393	P394	G395	Q396	K397	H398	V402	S405	P406	P407	K412	N413	W414	N415	P416				
											Y419	S420	Q421	D422	Y427	V428	P429	A430	N431	H432	W433	K434	P435	D436	Y437	W438	T439	V442	T445	K446	A449	G452	M453	G454	F455	R456	T457	R458	R459	M460	V465	G466	S467	L468	R469	A470	W471	D472	G476	K477	V478	V479	W480	E481	H482	K483	E484	H485	L488	W489	A490						
											L493	A494	T495	A496	N498	L499	F501	T502	G503	T504	G507	Y508	F509	K510	A511	F512	D513	A514	G517	L520	W521	K522	F523	Q524	S527	S531	P532	P533	R536	D539	G540	E541	Q542	Y543	L544	T547	Y550	G551	G552	A553	V554	P555	L556	W557	D560	M561	A562	D563									

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	159.40Å 159.40Å 130.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.50 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (12.50-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9232	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.36	25/4679 (0.5%)	3.11	612/6366 (9.6%)
1	B	1.07	8/4679 (0.2%)	2.69	394/6366 (6.2%)
All	All	1.22	33/9358 (0.4%)	2.91	1006/12732 (7.9%)

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	36
1	B	0	21
All	All	0	57

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ASN	N-CA	16.12	1.69	1.46
1	A	312	ASN	N-CA	8.54	1.58	1.46
1	A	386	GLY	N-CA	8.51	1.57	1.45
1	A	414	TRP	CA-CB	7.37	1.65	1.53
1	A	295	GLY	CA-C	7.37	1.57	1.51
1	B	289	TYR	N-CA	-6.86	1.37	1.46
1	A	366	ASP	C-O	6.74	1.32	1.24
1	A	68	ASP	C-O	6.74	1.32	1.24
1	A	414	TRP	C-O	-6.61	1.16	1.24
1	A	366	ASP	CA-C	-6.46	1.43	1.52
1	A	385	GLU	C-O	6.44	1.32	1.24
1	A	410	GLY	N-CA	-6.32	1.38	1.45
1	A	88	GLY	N-CA	6.32	1.54	1.45
1	B	251	ALA	N-CA	6.23	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	ARG	C-N	-6.22	1.25	1.33
1	B	161	VAL	N-CA	6.00	1.53	1.46
1	B	288	LEU	C-O	-5.90	1.17	1.23
1	A	87	THR	C-O	5.80	1.30	1.23
1	A	111	ARG	C-O	-5.73	1.16	1.24
1	A	26	HIS	CE1-NE2	5.70	1.38	1.32
1	B	454	GLY	CA-C	5.55	1.57	1.52
1	A	385	GLU	N-CA	-5.45	1.39	1.46
1	B	252	SER	CA-C	5.40	1.59	1.52
1	A	106	CYS	CA-CB	5.28	1.60	1.53
1	A	69	GLY	N-CA	5.27	1.53	1.45
1	B	137	GLY	N-CA	5.27	1.51	1.45
1	B	554	VAL	CA-CB	-5.25	1.51	1.54
1	A	124	THR	N-CA	-5.21	1.39	1.45
1	A	289	TYR	N-CA	-5.17	1.36	1.46
1	A	285	TYR	N-CA	-5.16	1.40	1.47
1	A	426	PHE	CA-CB	5.13	1.60	1.53
1	A	414	TRP	CD2-CE3	5.07	1.48	1.40
1	A	384	ARG	C-O	-5.06	1.17	1.23

All (1006) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	LEU	CA-C-N	30.53	176.66	121.70
1	A	288	LEU	C-N-CA	30.53	176.66	121.70
1	A	29	ARG	CD-NE-CZ	26.56	161.58	124.40
1	B	288	LEU	CA-C-N	25.25	169.76	121.54
1	B	288	LEU	C-N-CA	25.25	169.76	121.54
1	A	288	LEU	CA-C-O	19.55	142.70	121.19
1	A	353	ARG	NE-CZ-NH2	-19.29	101.84	119.20
1	A	366	ASP	CA-C-O	18.56	140.99	119.27
1	A	367	ASN	CA-CB-CG	18.28	130.88	112.60
1	B	187	PHE	CA-CB-CG	17.95	131.75	113.80
1	A	366	ASP	O-C-N	-17.81	98.06	122.46
1	B	29	ARG	NE-CZ-NH2	17.71	135.14	119.20
1	A	283	HIS	CA-C-O	17.62	141.01	120.92
1	B	268	GLY	CA-C-O	-17.49	96.51	121.52
1	B	539	ASP	CA-CB-CG	15.52	128.12	112.60
1	A	312	ASN	CA-CB-CG	15.13	127.73	112.60
1	B	288	LEU	CA-C-O	14.13	136.69	121.15
1	A	136	THR	CA-CB-OG1	-13.89	88.76	109.60
1	A	103	ARG	CD-NE-CZ	13.83	143.76	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	ASN	CA-CB-CG	13.78	126.38	112.60
1	A	288	LEU	O-C-N	-13.72	106.00	122.87
1	A	68	ASP	CA-CB-CG	13.44	126.04	112.60
1	B	483	LYS	CA-CB-CG	12.91	139.92	114.10
1	B	252	SER	CA-CB-OG	12.89	136.88	111.10
1	A	14	THR	O-C-N	-12.88	105.31	122.57
1	B	97	ARG	CD-NE-CZ	12.86	142.40	124.40
1	A	469	ARG	NE-CZ-NH1	-12.83	108.67	121.50
1	A	385	GLU	O-C-N	-12.72	105.67	122.59
1	A	82	ALA	CA-C-O	12.66	133.85	120.30
1	A	87	THR	CA-C-O	-12.59	106.43	121.28
1	B	288	LEU	O-C-N	-12.46	107.76	122.97
1	A	271	ASN	OD1-CG-ND2	-12.30	110.30	122.60
1	B	209	ARG	CD-NE-CZ	12.04	141.26	124.40
1	A	311	PRO	O-C-N	-12.03	109.19	122.18
1	A	221	VAL	CB-CA-C	-11.94	96.03	112.14
1	A	284	ASP	CA-C-N	11.85	142.08	122.76
1	A	284	ASP	C-N-CA	11.85	142.08	122.76
1	A	268	GLY	CA-C-O	-11.80	104.64	121.52
1	A	385	GLU	CA-C-O	-11.79	103.64	120.51
1	A	366	ASP	N-CA-C	11.79	127.84	113.23
1	A	353	ARG	NH1-CZ-NH2	11.73	134.55	119.30
1	B	507	GLY	N-CA-C	11.67	131.53	115.30
1	A	68	ASP	CA-C-N	-11.61	98.65	121.41
1	A	68	ASP	C-N-CA	-11.61	98.65	121.41
1	B	153	THR	CA-CB-CG2	11.53	130.09	110.50
1	B	577	PHE	CA-CB-CG	11.36	125.16	113.80
1	A	321	ASN	OD1-CG-ND2	-11.30	111.30	122.60
1	A	433	TRP	CA-CB-CG	11.04	134.58	113.60
1	B	65	ILE	CA-CB-CG2	11.03	129.25	110.50
1	B	312	ASN	CA-CB-CG	11.01	123.61	112.60
1	A	182	VAL	N-CA-CB	-10.93	98.50	112.60
1	B	469	ARG	CD-NE-CZ	10.87	139.62	124.40
1	B	236	LYS	CA-C-O	-10.87	108.85	121.68
1	B	262	VAL	CB-CA-C	-10.71	94.01	110.50
1	A	87	THR	N-CA-CB	-10.69	93.21	110.63
1	A	110	ASN	CB-CG-ND2	10.63	132.34	116.40
1	B	110	ASN	CA-CB-CG	-10.62	101.97	112.60
1	A	283	HIS	O-C-N	-10.61	109.80	122.95
1	B	273	TRP	CA-CB-CG	-10.60	93.46	113.60
1	A	366	ASP	CB-CA-C	-10.56	88.11	109.55
1	A	60	GLN	OE1-CD-NE2	-10.48	112.12	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ARG	NE-CZ-NH1	-10.48	111.02	121.50
1	B	258	ASN	OD1-CG-ND2	-10.47	112.13	122.60
1	A	321	ASN	CB-CG-ND2	10.43	132.04	116.40
1	A	545	GLY	CA-C-O	10.41	132.76	121.63
1	B	87	THR	CA-C-O	-10.39	108.51	121.50
1	B	216	THR	N-CA-C	10.38	126.01	112.72
1	A	269	PRO	CA-N-CD	-10.36	96.99	111.50
1	A	142	LYS	O-C-N	-10.36	108.81	122.59
1	A	472	ASP	CA-C-O	10.34	126.01	119.29
1	A	155	THR	CA-C-N	10.30	130.13	120.34
1	A	155	THR	C-N-CA	10.30	130.13	120.34
1	B	284	ASP	CA-C-O	10.30	135.83	122.45
1	A	469	ARG	CD-NE-CZ	10.29	138.81	124.40
1	A	79	ARG	NE-CZ-NH2	10.28	128.45	119.20
1	A	348	PHE	CB-CG-CD1	10.25	138.12	120.70
1	A	190	ASP	CA-C-O	10.23	130.03	119.80
1	A	363	PRO	CA-C-O	-10.19	109.05	120.97
1	A	469	ARG	NE-CZ-NH2	10.15	128.34	119.20
1	A	87	THR	O-C-N	-10.13	111.45	123.10
1	A	341	HIS	CA-CB-CG	10.08	123.88	113.80
1	A	332	ASP	CA-CB-CG	-9.97	102.63	112.60
1	A	317	PHE	CA-CB-CG	9.94	123.73	113.80
1	B	109	VAL	CA-C-N	9.88	139.33	121.94
1	B	109	VAL	C-N-CA	9.88	139.33	121.94
1	B	269	PRO	CA-N-CD	-9.84	98.23	112.00
1	B	456	ARG	CD-NE-CZ	9.78	138.09	124.40
1	A	502	THR	CA-C-O	-9.71	110.92	121.31
1	A	13	LYS	N-CA-C	9.62	125.16	113.23
1	A	123	GLY	CA-C-N	9.61	139.84	122.92
1	A	123	GLY	C-N-CA	9.61	139.84	122.92
1	A	368	ILE	CB-CG1-CD1	9.60	133.95	113.80
1	A	73	VAL	O-C-N	-9.57	112.98	123.03
1	A	159	THR	N-CA-CB	-9.54	96.49	111.56
1	B	344	ARG	CD-NE-CZ	9.53	137.74	124.40
1	A	459	ARG	NE-CZ-NH2	-9.49	110.66	119.20
1	A	444	TYR	O-C-N	-9.48	112.16	123.16
1	A	376	LEU	CA-C-O	-9.48	109.07	119.97
1	B	110	ASN	OD1-CG-ND2	9.48	132.08	122.60
1	A	348	PHE	CB-CG-CD2	-9.47	104.59	120.70
1	B	494	ALA	CA-C-N	9.39	137.28	122.62
1	B	494	ALA	C-N-CA	9.39	137.28	122.62
1	B	253	PHE	CA-CB-CG	9.38	123.18	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	THR	CA-C-N	9.35	134.05	122.37
1	A	259	THR	C-N-CA	9.35	134.05	122.37
1	A	262	VAL	CA-C-O	9.32	130.86	121.63
1	A	537	GLU	OE1-CD-OE2	9.31	145.24	122.90
1	B	483	LYS	CB-CG-CD	9.29	132.66	111.30
1	A	366	ASP	CA-C-N	-9.28	106.63	123.34
1	A	366	ASP	C-N-CA	-9.28	106.63	123.34
1	A	56	LYS	CA-CB-CG	9.28	132.66	114.10
1	B	470	ALA	CA-C-N	9.28	135.52	122.72
1	B	470	ALA	C-N-CA	9.28	135.52	122.72
1	B	479	VAL	CA-C-O	-9.27	111.02	120.85
1	A	120	VAL	O-C-N	-9.21	113.40	122.98
1	A	501	PHE	CA-CB-CG	9.21	123.00	113.80
1	A	545	GLY	O-C-N	-9.20	115.02	123.57
1	B	121	PHE	CA-C-O	-9.17	110.11	120.66
1	B	271	ASN	CA-CB-CG	9.16	121.76	112.60
1	A	198	TRP	CA-CB-CG	9.14	130.97	113.60
1	A	368	ILE	O-C-N	9.12	132.61	122.67
1	B	472	ASP	CA-CB-CG	9.07	121.67	112.60
1	A	265	GLY	O-C-N	-9.03	115.67	122.71
1	A	558	GLY	N-CA-C	9.02	125.54	113.99
1	B	56	LYS	CB-CG-CD	8.98	131.95	111.30
1	A	528	GLY	O-C-N	-8.94	114.08	122.93
1	A	359	GLN	OE1-CD-NE2	-8.93	113.67	122.60
1	A	2	ASP	O-C-N	-8.92	111.90	122.87
1	A	284	ASP	O-C-N	-8.91	112.17	122.86
1	A	326	PHE	CA-CB-CG	8.91	122.71	113.80
1	A	568	VAL	CA-C-N	8.87	135.39	121.56
1	A	568	VAL	C-N-CA	8.87	135.39	121.56
1	B	62	SER	N-CA-C	8.87	123.26	109.96
1	A	185	ARG	CA-C-O	-8.85	110.48	120.66
1	B	286	ASP	CA-C-N	-8.84	109.95	122.41
1	B	286	ASP	C-N-CA	-8.84	109.95	122.41
1	B	416	PRO	CA-C-N	8.82	137.16	122.07
1	B	416	PRO	C-N-CA	8.82	137.16	122.07
1	A	26	HIS	CB-CG-CD2	-8.82	119.73	131.20
1	A	82	ALA	O-C-N	-8.79	113.08	123.27
1	A	34	LYS	CA-CB-CG	8.79	131.67	114.10
1	A	408	PHE	CA-C-O	-8.78	111.15	120.63
1	A	185	ARG	NE-CZ-NH2	8.77	127.09	119.20
1	B	232	SER	CA-C-N	8.74	129.61	119.47
1	B	232	SER	C-N-CA	8.74	129.61	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ASP	CA-CB-CG	-8.74	103.86	112.60
1	B	17	ASP	CA-CB-CG	8.73	121.33	112.60
1	A	106	CYS	N-CA-C	8.72	122.05	110.88
1	A	88	GLY	O-C-N	-8.71	111.38	122.70
1	B	428	VAL	N-CA-C	8.70	117.52	107.77
1	A	211	ASN	O-C-N	-8.69	110.77	122.41
1	A	231	ASN	N-CA-CB	8.67	122.77	114.10
1	A	79	ARG	CD-NE-CZ	8.65	136.51	124.40
1	A	380	ARG	N-CA-C	8.65	121.63	110.39
1	A	384	ARG	CA-C-N	8.59	137.94	121.54
1	A	384	ARG	C-N-CA	8.59	137.94	121.54
1	A	539	ASP	O-C-N	-8.58	111.85	122.57
1	A	384	ARG	NE-CZ-NH2	8.54	126.89	119.20
1	B	202	PHE	CA-CB-CG	8.52	122.32	113.80
1	B	31	SER	CA-C-O	8.51	128.52	119.50
1	A	362	PHE	O-C-N	-8.50	115.45	121.65
1	A	237	VAL	CA-C-N	8.46	131.97	120.38
1	A	237	VAL	C-N-CA	8.46	131.97	120.38
1	A	73	VAL	CB-CA-C	-8.42	97.85	110.82
1	A	15	THR	CA-C-O	8.40	129.68	119.10
1	A	299	SER	CA-CB-OG	8.39	127.89	111.10
1	A	262	VAL	CB-CA-C	-8.37	96.15	110.30
1	A	6	GLU	CB-CG-CD	8.36	126.82	112.60
1	B	32	PRO	CA-C-N	8.32	132.53	120.71
1	B	32	PRO	C-N-CA	8.32	132.53	120.71
1	B	316	ASP	O-C-N	-8.31	112.64	122.86
1	A	570	GLN	CA-C-N	8.27	133.99	120.51
1	A	570	GLN	C-N-CA	8.27	133.99	120.51
1	B	314	ALA	CA-C-N	8.27	137.34	122.38
1	B	314	ALA	C-N-CA	8.27	137.34	122.38
1	A	86	LYS	CA-C-O	8.26	130.08	120.00
1	A	438	TRP	CA-C-N	8.26	133.23	121.42
1	A	438	TRP	C-N-CA	8.26	133.23	121.42
1	A	306	PHE	O-C-N	-8.25	113.76	123.41
1	A	528	GLY	N-CA-C	8.25	121.01	111.36
1	A	110	ASN	OD1-CG-ND2	-8.25	114.35	122.60
1	B	252	SER	CA-C-O	-8.22	111.82	121.11
1	B	35	GLN	CA-C-O	8.22	129.13	120.42
1	B	311	PRO	CA-C-O	-8.19	105.69	120.60
1	B	187	PHE	CA-C-O	8.16	130.52	121.06
1	B	221	VAL	CB-CA-C	-8.14	100.99	112.22
1	A	453	MET	CA-C-N	8.14	131.67	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	MET	C-N-CA	8.14	131.67	122.15
1	A	11	ASP	CA-CB-CG	8.12	120.72	112.60
1	A	323	LEU	CA-C-N	-8.10	109.53	122.50
1	A	323	LEU	C-N-CA	-8.10	109.53	122.50
1	B	283	HIS	N-CA-CB	8.07	122.15	110.37
1	A	480	TRP	CA-CB-CG	8.04	128.89	113.60
1	B	284	ASP	O-C-N	-8.05	113.10	123.32
1	A	103	ARG	NE-CZ-NH2	-8.02	111.98	119.20
1	B	550	TYR	N-CA-C	8.02	121.86	110.23
1	B	560	ASP	CA-C-N	8.01	132.08	120.38
1	B	560	ASP	C-N-CA	8.01	132.08	120.38
1	A	478	VAL	CB-CA-C	8.00	121.42	111.25
1	B	483	LYS	CB-CA-C	8.00	124.01	109.37
1	A	221	VAL	N-CA-CB	7.99	121.40	110.54
1	A	119	LYS	N-CA-C	7.96	122.08	109.50
1	B	576	VAL	CA-C-O	7.96	128.75	120.39
1	A	534	ILE	CA-C-O	7.95	130.50	121.44
1	A	106	CYS	N-CA-CB	-7.95	99.75	111.51
1	A	144	LYS	CA-C-O	-7.95	111.53	120.43
1	B	282	PRO	CA-C-N	7.87	133.37	121.40
1	B	282	PRO	C-N-CA	7.87	133.37	121.40
1	A	237	VAL	O-C-N	-7.82	114.56	122.62
1	A	81	PHE	CA-CB-CG	7.81	121.61	113.80
1	A	273	TRP	CA-CB-CG	-7.80	98.78	113.60
1	A	345	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	A	329	LYS	CA-C-N	7.75	136.33	121.54
1	A	329	LYS	C-N-CA	7.75	136.33	121.54
1	B	114	ALA	O-C-N	-7.73	114.30	123.27
1	A	196	GLU	O-C-N	-7.73	112.31	122.59
1	A	400	LYS	CA-C-O	-7.73	113.36	121.55
1	B	106	CYS	N-CA-CB	-7.71	100.36	111.54
1	B	142	LYS	CA-CB-CG	7.70	129.49	114.10
1	A	348	PHE	CA-CB-CG	7.69	121.49	113.80
1	A	159	THR	O-C-N	-7.69	114.26	123.10
1	A	500	VAL	N-CA-CB	7.69	124.05	111.44
1	B	206	HIS	CA-C-N	7.69	132.87	121.72
1	B	206	HIS	C-N-CA	7.69	132.87	121.72
1	A	104	PRO	O-C-N	-7.68	113.48	123.01
1	B	308	GLN	CA-C-O	-7.68	112.09	120.92
1	A	242	HIS	CA-C-O	7.66	130.21	121.32
1	A	269	PRO	N-CD-CG	7.62	112.94	103.80
1	B	10	ASN	OD1-CG-ND2	7.60	130.20	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	GLY	CA-C-N	7.60	134.43	122.49
1	B	319	GLY	C-N-CA	7.60	134.43	122.49
1	B	563	ASP	N-CA-C	7.59	119.56	111.28
1	B	259	THR	N-CA-C	7.58	121.57	108.76
1	A	460	MET	CA-CB-CG	7.58	129.26	114.10
1	A	311	PRO	CA-C-N	-7.58	110.90	123.33
1	A	311	PRO	C-N-CA	-7.58	110.90	123.33
1	B	260	ILE	CA-C-O	-7.58	112.21	120.85
1	B	34	LYS	CA-CB-CG	7.57	129.24	114.10
1	B	11	ASP	O-C-N	-7.52	112.59	122.59
1	A	96	HIS	CA-C-O	-7.51	112.74	121.16
1	B	326	PHE	CA-CB-CG	7.47	121.27	113.80
1	A	27	ALA	N-CA-CB	-7.47	100.95	112.30
1	A	209	ARG	CD-NE-CZ	7.46	134.84	124.40
1	A	220	ASP	CA-C-N	7.45	130.67	120.46
1	A	220	ASP	C-N-CA	7.45	130.67	120.46
1	B	551	GLY	CA-C-O	-7.45	115.16	121.04
1	A	275	ARG	NE-CZ-NH2	7.44	125.90	119.20
1	A	485	HIS	CA-CB-CG	7.43	121.23	113.80
1	A	459	ARG	O-C-N	-7.42	114.33	122.79
1	A	60	GLN	CA-C-O	7.42	129.91	120.57
1	B	375	ASP	CA-CB-CG	-7.41	105.19	112.60
1	A	524	GLN	OE1-CD-NE2	-7.39	115.20	122.60
1	B	14	THR	CA-C-O	-7.39	113.11	121.39
1	A	17	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	484	GLU	CA-C-N	7.38	130.17	120.28
1	A	484	GLU	C-N-CA	7.38	130.17	120.28
1	A	330	ALA	CA-C-O	-7.38	109.95	120.51
1	A	309	HIS	CA-CB-CG	-7.36	106.44	113.80
1	A	95	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	A	284	ASP	CA-CB-CG	-7.34	105.26	112.60
1	B	261	ILE	CA-C-N	7.34	133.15	122.94
1	B	261	ILE	C-N-CA	7.34	133.15	122.94
1	B	343	ASP	N-CA-CB	-7.34	99.95	110.44
1	A	368	ILE	CA-C-N	-7.33	110.08	122.11
1	A	368	ILE	C-N-CA	-7.33	110.08	122.11
1	A	35	GLN	OE1-CD-NE2	-7.33	115.27	122.60
1	A	340	ALA	CA-C-O	-7.33	112.44	120.36
1	A	29	ARG	NE-CZ-NH2	-7.33	112.60	119.20
1	A	331	LYS	N-CA-C	-7.32	95.20	110.80
1	A	230	ARG	CA-C-O	-7.32	113.79	121.55
1	A	263	GLY	CA-C-O	-7.32	113.33	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	GLU	CA-C-O	7.31	128.14	120.25
1	B	338	ALA	CA-C-N	7.31	133.54	122.65
1	B	338	ALA	C-N-CA	7.31	133.54	122.65
1	B	243	GLY	N-CA-C	7.30	122.80	113.24
1	A	2	ASP	CA-CB-CG	-7.30	105.30	112.60
1	A	288	LEU	N-CA-CB	7.30	120.85	109.83
1	B	176	SER	CA-C-O	-7.30	112.82	120.99
1	B	496	ALA	CA-C-O	-7.30	110.08	120.51
1	B	187	PHE	O-C-N	-7.29	114.81	123.27
1	B	489	TRP	CA-C-O	-7.29	111.93	119.51
1	B	241	SER	O-C-N	-7.28	111.80	122.43
1	A	122	PHE	O-C-N	-7.28	115.63	123.42
1	B	108	VAL	O-C-N	-7.27	113.48	122.57
1	B	495	THR	CA-C-O	7.27	129.62	121.11
1	A	62	SER	N-CA-C	7.27	121.03	110.28
1	B	223	ALA	CA-C-O	7.26	130.10	120.16
1	A	556	LEU	O-C-N	-7.25	112.07	122.36
1	B	413	ASN	CA-C-O	-7.25	112.95	119.91
1	B	387	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	512	PHE	CA-CB-CG	-7.23	106.57	113.80
1	B	114	ALA	CA-C-N	7.23	132.61	123.14
1	B	114	ALA	C-N-CA	7.23	132.61	123.14
1	A	511	ALA	CA-C-N	7.23	134.50	122.87
1	A	511	ALA	C-N-CA	7.23	134.50	122.87
1	A	135	ASN	OD1-CG-ND2	7.22	129.82	122.60
1	A	340	ALA	N-CA-CB	7.22	122.81	110.68
1	A	555	PRO	CA-C-O	-7.22	108.86	119.18
1	A	231	ASN	CB-CA-C	-7.22	102.69	109.83
1	A	118	ASP	CB-CG-OD1	7.21	134.98	118.40
1	B	49	SER	CA-C-N	7.20	133.15	122.99
1	B	49	SER	C-N-CA	7.20	133.15	122.99
1	A	323	LEU	CA-C-O	-7.20	112.84	120.40
1	A	188	ALA	N-CA-CB	7.20	122.77	110.68
1	B	284	ASP	CB-CA-C	7.20	125.54	112.30
1	B	102	ILE	O-C-N	-7.19	114.88	122.57
1	A	183	VAL	CA-C-O	-7.19	112.40	120.74
1	A	26	HIS	ND1-CE1-NE2	7.18	115.58	108.40
1	B	271	ASN	CA-C-O	7.18	128.55	120.80
1	B	102	ILE	CA-CB-CG2	7.17	122.70	110.50
1	A	263	GLY	O-C-N	7.17	131.81	123.21
1	B	125	LEU	O-C-N	-7.17	112.56	122.46
1	A	44	LEU	CB-CA-C	7.16	121.89	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	252	SER	O-C-N	-7.16	113.89	123.19
1	A	539	ASP	CA-C-O	7.15	130.40	122.03
1	B	384	ARG	CA-C-O	7.15	128.29	120.71
1	A	334	LYS	CA-C-N	-7.14	113.40	123.11
1	A	334	LYS	C-N-CA	-7.14	113.40	123.11
1	A	387	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	B	72	TYR	CA-C-O	-7.14	112.47	120.32
1	B	324	VAL	N-CA-CB	7.14	119.56	110.99
1	A	137	GLY	CA-C-N	-7.13	110.75	120.87
1	A	137	GLY	C-N-CA	-7.13	110.75	120.87
1	B	82	ALA	CA-C-N	7.12	134.00	122.81
1	B	82	ALA	C-N-CA	7.12	134.00	122.81
1	B	11	ASP	CA-CB-CG	7.12	119.72	112.60
1	B	339	THR	CA-CB-CG2	7.11	122.58	110.50
1	A	153	THR	CB-CA-C	-7.10	96.29	110.42
1	A	92	TRP	CA-C-O	-7.10	113.66	121.33
1	A	209	ARG	NE-CZ-NH2	7.10	125.59	119.20
1	A	250	SER	N-CA-CB	-7.08	99.23	111.55
1	A	334	LYS	N-CA-C	7.08	120.50	110.23
1	B	539	ASP	CA-C-N	7.07	136.67	121.18
1	B	539	ASP	C-N-CA	7.07	136.67	121.18
1	A	469	ARG	N-CA-C	7.07	120.92	109.40
1	B	465	VAL	CA-C-N	7.06	127.51	120.31
1	B	465	VAL	C-N-CA	7.06	127.51	120.31
1	A	415	ASN	CB-CA-C	7.06	124.08	110.17
1	B	377	LYS	CA-CB-CG	7.06	128.21	114.10
1	A	28	GLN	CA-C-O	-7.05	111.86	119.97
1	B	498	ASN	CA-CB-CG	-7.05	105.55	112.60
1	B	343	ASP	N-CA-C	7.05	119.62	110.53
1	A	28	GLN	N-CA-C	7.05	120.00	111.82
1	B	29	ARG	NH1-CZ-NH2	-7.02	110.18	119.30
1	B	102	ILE	CA-C-N	6.99	128.87	122.37
1	B	102	ILE	C-N-CA	6.99	128.87	122.37
1	A	49	SER	N-CA-CB	-6.99	99.39	111.55
1	A	93	THR	CA-C-N	6.99	132.73	122.39
1	A	93	THR	C-N-CA	6.99	132.73	122.39
1	A	508	TYR	N-CA-C	6.99	121.06	109.46
1	A	284	ASP	CA-C-O	6.98	130.37	122.27
1	A	517	GLY	N-CA-C	6.97	124.63	115.36
1	A	156	GLY	CA-C-N	6.96	130.38	120.49
1	A	156	GLY	C-N-CA	6.96	130.38	120.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ARG	CG-CD-NE	6.96	127.32	112.00
1	A	293	GLN	OE1-CD-NE2	-6.96	115.64	122.60
1	A	482	HIS	CA-CB-CG	-6.94	106.86	113.80
1	B	477	LYS	N-CA-C	6.93	121.34	110.32
1	A	26	HIS	CB-CG-ND1	6.93	133.09	122.70
1	A	251	ALA	O-C-N	-6.92	114.90	122.79
1	A	330	ALA	O-C-N	6.91	131.78	122.59
1	A	530	VAL	O-C-N	-6.90	113.95	122.57
1	A	426	PHE	CA-CB-CG	-6.89	106.91	113.80
1	A	412	LYS	CG-CD-CE	6.89	127.15	111.30
1	B	185	ARG	NE-CZ-NH1	-6.89	114.61	121.50
1	B	237	VAL	CB-CA-C	6.88	122.57	111.29
1	A	266	ASN	CA-CB-CG	-6.86	105.74	112.60
1	B	55	GLU	CB-CG-CD	6.86	124.26	112.60
1	A	569	ALA	CB-CA-C	-6.86	100.18	109.71
1	B	315	TRP	N-CA-C	6.85	121.66	113.16
1	B	295	GLY	CA-C-O	-6.85	114.95	120.91
1	B	216	THR	CA-C-O	-6.85	111.80	119.81
1	A	569	ALA	N-CA-C	6.84	120.40	110.42
1	A	450	TYR	N-CA-CB	-6.84	100.77	111.23
1	B	513	ASP	CA-C-O	-6.84	112.95	120.81
1	A	534	ILE	O-C-N	-6.83	115.74	122.92
1	B	472	ASP	CB-CA-C	6.83	117.64	109.85
1	A	337	LYS	CD-CE-NZ	6.83	133.76	111.90
1	B	422	ASP	CA-C-O	-6.83	113.67	120.70
1	B	378	THR	CA-C-O	-6.82	111.55	119.05
1	A	270	TRP	O-C-N	6.82	130.19	122.22
1	B	29	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	B	60	GLN	O-C-N	-6.80	115.43	122.64
1	B	368	ILE	CA-C-N	6.78	132.89	122.24
1	B	368	ILE	C-N-CA	6.78	132.89	122.24
1	B	376	LEU	CA-C-O	-6.76	112.19	119.97
1	B	419	TYR	CA-C-N	6.76	131.41	122.42
1	B	419	TYR	C-N-CA	6.76	131.41	122.42
1	B	320	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	466	GLY	O-C-N	-6.75	115.89	122.84
1	B	7	ASP	N-CA-C	-6.75	103.84	111.07
1	B	488	LEU	CA-C-O	6.75	127.74	120.38
1	B	541	GLU	N-CA-CB	-6.75	99.34	110.68
1	A	249	GLN	OE1-CD-NE2	-6.75	115.85	122.60
1	A	385	GLU	CA-C-N	-6.72	108.23	121.41
1	A	385	GLU	C-N-CA	-6.72	108.23	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	LEU	CA-C-N	6.72	133.55	122.73
1	B	125	LEU	C-N-CA	6.72	133.55	122.73
1	A	221	VAL	CA-C-O	-6.72	113.97	120.95
1	B	185	ARG	CA-C-O	6.71	128.84	121.06
1	A	565	THR	CA-CB-CG2	6.71	121.90	110.50
1	A	126	ASP	CA-C-N	6.70	134.34	121.54
1	A	126	ASP	C-N-CA	6.70	134.34	121.54
1	A	353	ARG	CA-CB-CG	6.70	127.50	114.10
1	A	535	THR	O-C-N	-6.70	115.76	123.33
1	B	10	ASN	CA-CB-CG	-6.70	105.90	112.60
1	A	307	TYR	N-CA-CB	6.70	121.28	110.77
1	A	333	GLY	CA-C-N	6.70	130.22	120.71
1	A	333	GLY	C-N-CA	6.70	130.22	120.71
1	A	498	ASN	CA-CB-CG	-6.69	105.91	112.60
1	A	66	VAL	O-C-N	-6.69	115.84	123.00
1	B	363	PRO	CA-C-O	-6.68	113.52	121.67
1	B	138	LYS	CA-C-O	6.68	128.38	120.70
1	A	69	GLY	O-C-N	-6.68	114.02	122.70
1	A	330	ALA	N-CA-CB	6.65	121.73	110.49
1	A	67	SER	N-CA-CB	-6.64	100.68	111.24
1	A	258	ASN	OD1-CG-ND2	-6.64	115.96	122.60
1	A	560	ASP	N-CA-CB	6.63	120.56	110.28
1	A	67	SER	CA-C-O	-6.62	113.33	120.75
1	B	160	ILE	O-C-N	6.62	129.89	123.14
1	A	294	VAL	CA-C-O	-6.62	113.47	120.48
1	A	327	ASP	CA-C-N	-6.61	113.63	122.42
1	A	327	ASP	C-N-CA	-6.61	113.63	122.42
1	A	266	ASN	N-CA-CB	6.60	119.56	110.05
1	A	10	ASN	CA-CB-CG	-6.60	106.00	112.60
1	B	50	TYR	CA-CB-CG	-6.59	102.03	113.90
1	B	173	HIS	CA-CB-CG	6.57	120.37	113.80
1	B	484	GLU	CA-C-N	6.56	129.07	120.28
1	B	484	GLU	C-N-CA	6.56	129.07	120.28
1	A	152	TYR	CA-C-O	-6.55	113.58	121.05
1	A	114	ALA	CA-C-O	-6.54	113.90	121.49
1	A	405	SER	CA-C-O	6.54	126.44	119.50
1	A	423	THR	CA-C-O	-6.54	112.08	119.79
1	A	452	GLY	CA-C-O	-6.53	111.10	119.58
1	B	28	GLN	OE1-CD-NE2	6.52	129.12	122.60
1	A	316	ASP	O-C-N	-6.51	114.77	122.58
1	A	237	VAL	CB-CA-C	6.49	120.62	111.08
1	B	500	VAL	CB-CA-C	6.49	120.23	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	GLN	CG-CD-NE2	6.48	126.12	116.40
1	B	557	TRP	CA-CB-CG	6.47	125.90	113.60
1	B	421	GLN	CA-C-N	6.47	129.24	120.44
1	B	421	GLN	C-N-CA	6.47	129.24	120.44
1	A	273	TRP	CD2-CE3-CZ3	-6.47	110.19	118.60
1	A	87	THR	CA-C-N	-6.47	108.73	121.41
1	A	87	THR	C-N-CA	-6.47	108.73	121.41
1	A	295	GLY	O-C-N	-6.46	119.28	123.35
1	B	498	ASN	OD1-CG-ND2	6.46	129.06	122.60
1	B	73	VAL	CA-CB-CG2	6.46	121.38	110.40
1	B	241	SER	CA-C-O	6.46	127.37	119.11
1	A	484	GLU	O-C-N	-6.45	115.30	123.24
1	B	79	ARG	CD-NE-CZ	6.45	133.43	124.40
1	A	344	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	A	355	ASN	CA-C-O	-6.44	111.76	119.03
1	A	427	TYR	CA-C-N	6.42	128.95	123.04
1	A	427	TYR	C-N-CA	6.42	128.95	123.04
1	B	575	TRP	CA-CB-CG	6.42	125.79	113.60
1	A	444	TYR	CA-C-N	6.41	131.44	121.76
1	A	444	TYR	C-N-CA	6.41	131.44	121.76
1	B	202	PHE	CA-C-N	-6.41	114.85	122.93
1	B	202	PHE	C-N-CA	-6.41	114.85	122.93
1	B	258	ASN	CB-CG-OD1	6.41	133.62	120.80
1	A	400	LYS	N-CA-C	6.41	119.06	110.35
1	A	61	GLU	OE1-CD-OE2	-6.40	107.53	122.90
1	A	23	MET	CA-C-N	6.40	131.43	121.32
1	A	23	MET	C-N-CA	6.40	131.43	121.32
1	A	105	CYS	CA-C-O	6.39	127.33	119.79
1	B	538	GLN	CG-CD-NE2	6.39	125.99	116.40
1	A	183	VAL	O-C-N	6.38	132.14	122.76
1	A	258	ASN	CB-CG-ND2	6.38	125.97	116.40
1	A	253	PHE	CA-CB-CG	-6.38	107.42	113.80
1	B	309	HIS	O-C-N	-6.38	113.30	122.36
1	B	133	ASN	CA-CB-CG	6.37	118.97	112.60
1	B	469	ARG	N-CA-C	6.36	119.51	108.76
1	B	18	VAL	CA-C-O	-6.36	114.56	120.22
1	B	533	PRO	CA-C-N	6.35	132.72	122.68
1	B	533	PRO	C-N-CA	6.35	132.72	122.68
1	A	576	VAL	CA-C-N	6.35	132.52	122.62
1	A	576	VAL	C-N-CA	6.35	132.52	122.62
1	B	242	HIS	CA-CB-CG	-6.35	107.45	113.80
1	B	160	ILE	CA-C-N	-6.34	113.09	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ILE	C-N-CA	-6.34	113.09	122.23
1	B	540	GLY	N-CA-C	6.34	124.43	115.30
1	B	221	VAL	N-CA-C	6.34	117.12	110.72
1	B	68	ASP	CA-C-O	6.32	129.98	122.14
1	B	544	LEU	CA-CB-CG	6.32	138.43	116.30
1	A	335	ILE	CB-CA-C	6.32	119.98	111.19
1	B	133	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	A	251	ALA	CA-C-N	6.31	132.72	122.81
1	A	251	ALA	C-N-CA	6.31	132.72	122.81
1	A	101	ASP	OD1-CG-OD2	6.30	138.02	122.90
1	A	227	PRO	CB-CA-C	6.30	119.59	111.46
1	A	90	ARG	NE-CZ-NH2	-6.30	113.53	119.20
1	B	15	THR	CA-CB-OG1	-6.30	100.15	109.60
1	A	317	PHE	CA-C-O	-6.29	114.01	122.44
1	A	539	ASP	CA-C-N	6.29	134.96	121.18
1	A	539	ASP	C-N-CA	6.29	134.96	121.18
1	B	565	THR	N-CA-CB	-6.28	100.24	110.42
1	A	276	THR	O-C-N	-6.28	115.61	123.27
1	A	537	GLU	CG-CD-OE2	-6.25	104.02	118.40
1	A	539	ASP	OD1-CG-OD2	-6.25	107.89	122.90
1	A	478	VAL	N-CA-CB	6.24	118.98	111.31
1	A	564	LEU	CA-C-N	6.23	133.73	121.58
1	A	564	LEU	C-N-CA	6.23	133.73	121.58
1	A	472	ASP	CB-CG-OD1	6.23	132.73	118.40
1	B	49	SER	CA-C-O	-6.23	113.12	120.60
1	B	284	ASP	CA-C-N	6.21	132.92	123.04
1	B	284	ASP	C-N-CA	6.21	132.92	123.04
1	A	283	HIS	CB-CA-C	6.21	119.59	109.90
1	B	225	SER	O-C-N	-6.21	113.36	122.43
1	B	65	ILE	CA-CB-CG1	-6.20	99.87	110.40
1	A	140	VAL	CA-C-N	6.19	132.03	121.87
1	A	140	VAL	C-N-CA	6.19	132.03	121.87
1	B	65	ILE	O-C-N	-6.19	116.36	122.99
1	A	74	THR	CA-C-O	-6.19	114.17	121.16
1	A	540	GLY	CA-C-O	6.19	127.17	119.25
1	B	189	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	B	126	ASP	CA-C-N	6.19	132.19	122.78
1	B	126	ASP	C-N-CA	6.19	132.19	122.78
1	A	574	PHE	O-C-N	-6.19	115.35	123.21
1	A	133	ASN	CA-C-N	6.18	128.56	120.28
1	A	133	ASN	C-N-CA	6.18	128.56	120.28
1	B	237	VAL	CA-CB-CG1	6.18	120.90	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLN	N-CA-CB	-6.17	102.18	111.56
1	B	189	ARG	CD-NE-CZ	6.17	133.04	124.40
1	A	338	ALA	N-CA-CB	-6.17	101.56	110.87
1	A	285	TYR	CA-C-N	6.16	131.93	121.14
1	A	285	TYR	C-N-CA	6.16	131.93	121.14
1	A	437	TYR	CA-CB-CG	6.15	124.97	113.90
1	B	221	VAL	CA-C-N	6.15	129.35	120.38
1	B	221	VAL	C-N-CA	6.15	129.35	120.38
1	A	456	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	B	14	THR	O-C-N	-6.14	115.14	122.63
1	B	485	HIS	CA-CB-CG	6.14	119.94	113.80
1	A	561	MET	CA-C-N	6.13	129.00	120.29
1	A	561	MET	C-N-CA	6.13	129.00	120.29
1	B	279	GLY	N-CA-C	-6.13	98.64	113.18
1	B	539	ASP	N-CA-CB	-6.12	102.41	111.71
1	B	274	ALA	N-CA-C	-6.12	104.72	111.82
1	A	136	THR	CA-C-N	-6.11	109.43	121.41
1	A	136	THR	C-N-CA	-6.11	109.43	121.41
1	A	190	ASP	OD1-CG-OD2	-6.11	108.23	122.90
1	A	109	VAL	CA-C-O	6.11	129.07	121.92
1	A	428	VAL	CB-CA-C	-6.11	104.05	110.53
1	A	481	GLU	O-C-N	-6.11	115.82	123.27
1	A	79	ARG	CA-CB-CG	6.10	126.31	114.10
1	A	148	HIS	N-CA-C	6.10	118.72	111.71
1	A	425	LEU	CA-C-N	6.09	130.78	122.19
1	A	425	LEU	C-N-CA	6.09	130.78	122.19
1	A	303	VAL	CA-C-O	-6.08	113.56	120.74
1	A	308	GLN	N-CA-CB	6.08	120.09	110.23
1	A	322	GLU	CA-C-O	6.08	128.56	121.87
1	A	536	TRP	O-C-N	-6.08	117.44	123.46
1	B	327	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	185	ARG	CG-CD-NE	-6.07	98.65	112.00
1	A	117	GLY	O-C-N	-6.05	114.83	122.70
1	B	237	VAL	N-CA-CB	-6.04	101.26	111.23
1	A	65	ILE	CA-CB-CG2	6.03	120.75	110.50
1	B	375	ASP	CA-C-O	6.03	129.13	120.51
1	B	35	GLN	CB-CA-C	6.03	121.09	110.85
1	A	185	ARG	N-CA-C	6.02	119.30	109.24
1	B	324	VAL	CA-CB-CG2	6.02	120.64	110.40
1	A	15	THR	N-CA-C	6.02	120.09	112.87
1	A	210	LEU	CA-C-O	-6.02	112.67	120.25
1	A	29	ARG	NE-CZ-NH1	6.01	127.51	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	CA-C-O	-6.01	114.73	121.40
1	B	243	GLY	CA-C-O	-6.00	113.92	120.40
1	A	119	LYS	CA-C-O	6.00	128.13	121.11
1	B	324	VAL	CA-C-O	-6.00	114.15	120.57
1	A	313	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	412	LYS	CA-CB-CG	-5.99	102.12	114.10
1	A	562	ALA	N-CA-CB	5.99	119.02	110.16
1	A	211	ASN	CA-C-O	5.99	128.41	121.28
1	A	122	PHE	CA-CB-CG	5.99	119.78	113.80
1	B	95	ASN	CA-CB-CG	5.99	118.59	112.60
1	B	46	PRO	CA-C-O	-5.98	114.52	121.34
1	B	416	PRO	O-C-N	-5.98	114.56	122.64
1	A	58	ARG	CB-CG-CD	5.98	125.06	111.30
1	A	237	VAL	N-CA-CB	-5.98	98.03	110.64
1	A	565	THR	N-CA-CB	-5.97	100.38	110.41
1	A	3	VAL	CA-C-O	5.96	128.23	120.78
1	A	133	ASN	CA-CB-CG	-5.96	106.64	112.60
1	B	317	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	65	ILE	O-C-N	-5.95	116.64	123.00
1	B	346	GLY	N-CA-C	5.94	123.24	115.40
1	A	316	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	428	VAL	N-CA-C	5.93	115.05	108.05
1	A	255	ALA	CA-C-O	-5.93	113.15	119.97
1	B	264	ALA	CA-C-O	-5.93	114.22	120.80
1	B	428	VAL	CB-CA-C	-5.93	103.96	110.78
1	A	435	GLU	CA-C-N	5.93	130.90	122.72
1	A	435	GLU	C-N-CA	5.93	130.90	122.72
1	B	242	HIS	CA-C-O	5.93	127.52	120.53
1	A	347	PHE	O-C-N	-5.92	116.25	123.30
1	B	262	VAL	N-CA-C	5.92	117.29	108.46
1	A	29	ARG	CA-C-N	5.92	131.34	122.99
1	A	29	ARG	C-N-CA	5.92	131.34	122.99
1	B	384	ARG	CA-C-N	5.92	132.85	121.54
1	B	384	ARG	C-N-CA	5.92	132.85	121.54
1	A	89	LYS	CB-CA-C	5.92	119.77	109.65
1	A	272	THR	CA-C-N	5.92	130.60	120.72
1	A	272	THR	C-N-CA	5.92	130.60	120.72
1	A	363	PRO	O-C-N	-5.92	116.35	123.03
1	B	270	TRP	N-CA-CB	5.92	118.59	110.01
1	A	475	SER	CA-C-O	-5.91	112.55	119.05
1	A	281	ASN	CA-C-O	5.91	125.22	119.55
1	B	109	VAL	O-C-N	-5.91	114.73	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	N-CA-C	5.90	127.17	113.18
1	A	326	PHE	N-CA-CB	-5.90	101.36	111.21
1	B	335	ILE	N-CA-CB	5.89	117.36	110.82
1	A	445	THR	N-CA-CB	5.88	119.71	110.71
1	B	393	GLU	N-CA-C	-5.88	101.73	110.20
1	A	364	PHE	O-C-N	-5.88	114.25	122.37
1	A	506	ASP	O-C-N	-5.88	114.81	122.39
1	B	341	HIS	CB-CA-C	5.87	119.81	109.89
1	B	547	THR	CA-C-O	-5.86	113.91	120.54
1	A	211	ASN	CA-C-N	5.86	133.30	121.93
1	A	211	ASN	C-N-CA	5.86	133.30	121.93
1	A	144	LYS	N-CA-C	-5.86	99.65	108.96
1	A	189	ARG	CG-CD-NE	-5.86	99.11	112.00
1	B	166	THR	N-CA-CB	-5.86	101.26	110.46
1	A	308	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	A	578	LYS	CA-CB-CG	5.85	125.80	114.10
1	A	306	PHE	CA-C-N	5.84	131.01	122.77
1	A	306	PHE	C-N-CA	5.84	131.01	122.77
1	A	284	ASP	N-CA-C	5.84	119.40	111.17
1	A	294	VAL	N-CA-C	5.84	116.35	108.17
1	A	13	LYS	CA-C-O	-5.83	112.44	119.27
1	A	148	HIS	CA-C-O	5.83	126.69	120.10
1	B	112	GLY	N-CA-C	5.83	118.49	110.56
1	A	256	GLU	CA-C-O	-5.83	114.37	120.55
1	B	311	PRO	CB-CA-C	5.83	121.18	111.56
1	A	31	SER	CA-C-O	5.82	125.63	119.69
1	A	514	ALA	N-CA-C	5.81	119.63	112.54
1	A	307	TYR	CB-CG-CD1	5.81	129.51	120.80
1	B	422	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	40	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	A	194	GLY	CA-C-N	5.81	130.49	121.26
1	A	194	GLY	C-N-CA	5.81	130.49	121.26
1	B	432	HIS	CA-C-O	-5.81	114.30	120.40
1	A	356	GLY	CA-C-O	-5.80	111.90	119.44
1	A	125	LEU	N-CA-C	5.79	120.08	113.19
1	B	550	TYR	O-C-N	-5.79	115.74	122.87
1	A	254	ASP	CA-C-N	5.79	129.11	120.31
1	A	254	ASP	C-N-CA	5.79	129.11	120.31
1	A	198	TRP	O-C-N	-5.79	116.65	123.25
1	A	436	ASP	CA-CB-CG	-5.78	106.82	112.60
1	B	176	SER	O-C-N	5.78	129.86	123.33
1	B	416	PRO	N-CA-C	5.78	124.37	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ASN	O-C-N	-5.78	114.91	122.59
1	A	307	TYR	CA-CB-CG	-5.78	103.50	113.90
1	B	287	SER	CB-CA-C	5.78	120.83	112.05
1	A	493	LEU	CA-C-O	-5.77	114.13	120.36
1	A	304	LYS	CA-C-O	-5.77	113.10	120.31
1	B	504	THR	CA-C-N	5.77	127.54	120.22
1	B	504	THR	C-N-CA	5.77	127.54	120.22
1	A	390	PRO	N-CA-C	5.76	120.54	111.38
1	A	459	ARG	N-CA-C	5.76	118.13	110.53
1	B	28	GLN	CA-C-N	5.76	130.31	122.19
1	B	28	GLN	C-N-CA	5.76	130.31	122.19
1	A	157	ALA	N-CA-C	-5.75	102.53	109.83
1	B	51	SER	CA-CB-OG	5.75	122.59	111.10
1	B	434	LYS	N-CA-C	5.74	115.59	108.19
1	A	516	SER	CA-CB-OG	-5.73	99.64	111.10
1	B	210	LEU	O-C-N	-5.73	116.39	123.44
1	A	42	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	147	ASP	O-C-N	-5.72	116.06	122.93
1	A	412	LYS	CA-C-O	-5.72	113.22	120.20
1	B	289	TYR	CB-CA-C	5.72	121.80	110.42
1	A	286	ASP	N-CA-C	5.72	119.98	112.89
1	A	505	GLY	N-CA-C	5.72	121.08	114.16
1	B	322	GLU	N-CA-C	5.72	117.92	110.43
1	A	19	LEU	CA-C-O	5.71	126.12	119.32
1	A	376	LEU	N-CA-CB	5.71	119.12	110.28
1	A	365	VAL	CA-CB-CG1	-5.70	100.70	110.40
1	B	273	TRP	CE3-CZ3-CH2	5.70	128.51	121.10
1	B	111	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	A	563	ASP	CB-CA-C	5.70	122.00	110.38
1	A	182	VAL	O-C-N	-5.69	116.99	122.97
1	A	401	ALA	N-CA-C	5.69	119.52	109.96
1	B	309	HIS	CA-CB-CG	5.69	119.49	113.80
1	A	323	LEU	CD1-CG-CD2	5.69	123.31	110.80
1	B	564	LEU	CA-C-O	5.69	126.79	120.82
1	A	153	THR	CA-CB-CG2	5.67	120.14	110.50
1	B	250	SER	CA-C-N	-5.67	109.31	121.45
1	B	250	SER	C-N-CA	-5.67	109.31	121.45
1	A	118	ASP	OD1-CG-OD2	-5.67	109.29	122.90
1	A	308	GLN	CB-CG-CD	5.67	122.23	112.60
1	A	578	LYS	N-CA-C	5.66	116.87	108.60
1	A	242	HIS	N-CA-CB	-5.66	103.13	111.51
1	B	512	PHE	CA-CB-CG	-5.66	108.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	547	THR	CA-C-N	5.66	130.87	123.06
1	A	547	THR	C-N-CA	5.66	130.87	123.06
1	A	60	GLN	CA-CB-CG	5.66	125.41	114.10
1	B	102	ILE	N-CA-CB	-5.66	99.42	110.45
1	A	25	THR	CA-CB-CG2	5.65	120.10	110.50
1	A	383	GLU	CG-CD-OE1	5.64	131.38	118.40
1	B	65	ILE	N-CA-CB	-5.64	104.80	111.90
1	B	217	VAL	N-CA-CB	5.64	120.53	111.23
1	A	19	LEU	O-C-N	-5.64	115.42	122.24
1	B	87	THR	O-C-N	-5.64	114.62	121.83
1	A	27	ALA	N-CA-C	5.63	119.45	112.24
1	A	398	HIS	CA-C-O	-5.63	113.94	120.31
1	B	318	SER	CA-C-O	-5.63	112.46	120.51
1	A	252	SER	CA-CB-OG	5.63	122.36	111.10
1	A	91	LEU	N-CA-CB	5.63	118.91	110.19
1	A	312	ASN	N-CA-C	-5.62	95.36	107.49
1	A	568	VAL	O-C-N	-5.61	115.81	122.77
1	A	128	SER	CA-C-N	5.61	130.49	123.14
1	A	128	SER	C-N-CA	5.61	130.49	123.14
1	A	236	LYS	CA-CB-CG	5.61	125.32	114.10
1	B	120	VAL	CB-CA-C	5.61	119.45	110.82
1	B	524	GLN	CG-CD-NE2	5.59	124.79	116.40
1	A	575	TRP	CA-C-O	5.59	126.53	120.32
1	A	185	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	A	560	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	137	GLY	CA-C-N	5.58	129.28	121.02
1	B	137	GLY	C-N-CA	5.58	129.28	121.02
1	A	95	ASN	CA-C-O	-5.58	114.19	120.32
1	B	251	ALA	N-CA-CB	-5.58	102.47	110.44
1	A	367	ASN	N-CA-C	5.58	117.13	110.44
1	A	77	TYR	CB-CG-CD2	-5.57	112.45	120.80
1	A	414	TRP	CA-CB-CG	-5.56	103.04	113.60
1	A	509	PHE	CA-C-N	5.56	131.54	122.81
1	A	509	PHE	C-N-CA	5.56	131.54	122.81
1	B	274	ALA	CB-CA-C	5.56	121.34	110.67
1	B	38	ALA	N-CA-C	5.55	119.16	112.38
1	B	172	ILE	CA-C-O	5.55	126.64	120.59
1	B	374	ILE	N-CA-CB	5.55	118.86	112.15
1	B	433	TRP	CA-C-O	-5.54	115.35	121.28
1	B	490	ALA	N-CA-CB	5.54	120.18	111.20
1	A	464	HIS	CA-CB-CG	5.54	119.34	113.80
1	A	507	GLY	N-CA-C	5.54	122.96	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	VAL	CB-CA-C	5.54	118.89	111.19
1	A	353	ARG	CA-C-O	-5.53	110.06	118.91
1	A	355	ASN	O-C-N	5.53	128.26	122.23
1	B	142	LYS	N-CA-C	5.53	118.11	108.76
1	A	484	GLU	CA-CB-CG	5.53	125.16	114.10
1	B	63	GLN	N-CA-CB	5.53	119.44	110.43
1	A	12	ASP	CA-C-O	-5.53	114.01	120.20
1	A	365	VAL	CA-C-O	-5.52	114.03	121.32
1	A	2	ASP	CA-C-O	5.51	126.79	120.84
1	B	480	TRP	CA-CB-CG	5.51	124.07	113.60
1	A	35	GLN	N-CA-C	-5.51	105.18	111.07
1	A	256	GLU	CA-C-N	-5.50	113.96	122.49
1	A	256	GLU	C-N-CA	-5.50	113.96	122.49
1	A	153	THR	N-CA-CB	5.50	119.79	110.49
1	B	345	ASN	OD1-CG-ND2	-5.50	117.10	122.60
1	A	207	MET	N-CA-CB	-5.50	101.75	110.06
1	B	6	GLU	CA-CB-CG	5.50	125.10	114.10
1	A	243	GLY	N-CA-C	5.50	122.52	115.32
1	A	414	TRP	O-C-N	-5.50	115.09	122.23
1	B	449	ALA	CA-C-O	-5.50	115.57	121.56
1	A	21	TYR	OH-CZ-CE2	5.49	136.38	119.90
1	A	28	GLN	CG-CD-NE2	5.49	124.63	116.40
1	B	57	GLN	O-C-N	-5.49	118.03	122.03
1	A	108	VAL	N-CA-C	5.48	120.74	109.34
1	B	177	GLY	O-C-N	-5.48	115.58	122.70
1	B	286	ASP	CA-C-O	-5.48	115.59	121.56
1	A	331	LYS	N-CA-CB	5.47	119.74	110.49
1	A	553	ALA	CA-C-O	5.47	126.24	119.79
1	A	368	ILE	CA-C-O	-5.46	114.81	121.04
1	A	133	ASN	O-C-N	-5.46	116.18	122.95
1	A	581	SER	N-CA-C	5.45	117.22	111.28
1	A	509	PHE	O-C-N	-5.44	116.87	123.13
1	A	198	TRP	CA-C-N	5.44	130.46	121.86
1	A	198	TRP	C-N-CA	5.44	130.46	121.86
1	A	240	TRP	CA-C-O	5.44	126.07	119.38
1	A	267	PRO	CA-C-O	-5.44	115.22	121.86
1	A	156	GLY	O-C-N	-5.43	115.86	122.76
1	A	256	GLU	N-CA-CB	5.43	118.10	110.12
1	A	491	GLY	CA-C-N	5.43	130.55	123.06
1	A	491	GLY	C-N-CA	5.43	130.55	123.06
1	A	210	LEU	O-C-N	-5.42	116.09	123.14
1	A	342	ALA	CA-C-N	5.42	128.94	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ALA	C-N-CA	5.42	128.94	120.75
1	A	273	TRP	CE3-CZ3-CH2	5.42	128.15	121.10
1	B	249	GLN	CB-CA-C	5.42	121.21	110.42
1	A	16	GLY	O-C-N	-5.42	115.66	122.70
1	B	527	SER	O-C-N	-5.42	116.98	123.27
1	B	283	HIS	CA-C-N	-5.41	114.56	122.78
1	B	283	HIS	C-N-CA	-5.41	114.56	122.78
1	A	510	LYS	N-CA-C	5.41	118.38	109.72
1	A	161	VAL	CA-C-O	5.40	126.98	121.63
1	A	497	GLY	CA-C-O	-5.40	109.17	119.54
1	B	172	ILE	N-CA-C	5.40	115.87	107.99
1	B	458	LYS	CA-CB-CG	5.40	124.89	114.10
1	B	208	GLY	CA-C-O	-5.39	113.49	121.58
1	A	43	LYS	CA-CB-CG	5.39	124.88	114.10
1	B	316	ASP	CA-C-O	5.39	128.82	122.14
1	B	221	VAL	O-C-N	-5.38	116.28	121.83
1	B	14	THR	CA-C-N	5.38	131.81	121.54
1	B	14	THR	C-N-CA	5.38	131.81	121.54
1	A	302	GLU	CA-CB-CG	-5.38	103.35	114.10
1	A	158	PRO	O-C-N	-5.38	115.38	122.64
1	A	79	ARG	NH1-CZ-NH2	-5.37	112.32	119.30
1	B	280	GLY	N-CA-C	5.37	125.90	113.18
1	A	31	SER	N-CA-C	5.37	117.99	109.40
1	B	203	VAL	CA-C-N	5.37	128.72	121.05
1	B	203	VAL	C-N-CA	5.37	128.72	121.05
1	B	421	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	B	514	ALA	N-CA-C	5.36	119.44	113.01
1	A	219	GLY	CA-C-N	5.36	128.37	120.82
1	A	219	GLY	C-N-CA	5.36	128.37	120.82
1	B	496	ALA	CA-C-N	5.36	133.69	122.66
1	B	496	ALA	C-N-CA	5.36	133.69	122.66
1	A	338	ALA	N-CA-C	5.35	117.40	109.69
1	A	57	GLN	CB-CG-CD	5.35	121.70	112.60
1	A	537	GLU	CA-C-O	-5.35	115.04	120.71
1	B	101	ASP	CA-C-N	5.35	128.56	120.75
1	B	101	ASP	C-N-CA	5.35	128.56	120.75
1	A	165	LYS	CA-C-N	5.35	131.07	121.66
1	A	165	LYS	C-N-CA	5.35	131.07	121.66
1	B	68	ASP	CA-CB-CG	-5.34	107.26	112.60
1	A	377	LYS	CA-C-O	5.34	125.85	119.60
1	A	41	VAL	O-C-N	-5.34	116.51	121.90
1	A	147	ASP	N-CA-C	5.34	117.00	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ILE	O-C-N	-5.34	117.11	123.03
1	A	311	PRO	CA-C-O	-5.34	111.62	120.05
1	A	527	SER	N-CA-CB	-5.34	102.75	111.66
1	B	15	THR	OG1-CB-CG2	5.34	119.97	109.30
1	B	466	GLY	CA-C-N	-5.34	114.46	122.47
1	B	466	GLY	C-N-CA	-5.34	114.46	122.47
1	A	120	VAL	CA-C-O	5.33	128.18	121.40
1	B	270	TRP	CA-C-N	5.33	129.74	121.26
1	B	270	TRP	C-N-CA	5.33	129.74	121.26
1	B	234	THR	O-C-N	-5.33	114.84	122.41
1	B	560	ASP	CA-C-O	5.32	126.59	120.90
1	A	312	ASN	OD1-CG-ND2	-5.32	117.28	122.60
1	A	369	THR	CA-CB-OG1	5.32	117.58	109.60
1	B	112	GLY	CA-C-O	5.32	127.39	121.86
1	B	105	CYS	CB-CA-C	-5.32	101.81	110.85
1	A	108	VAL	O-C-N	-5.32	115.93	122.57
1	B	24	GLY	CA-C-N	5.32	128.39	120.31
1	B	24	GLY	C-N-CA	5.32	128.39	120.31
1	A	102	ILE	CA-C-O	-5.31	116.12	121.59
1	B	115	ILE	CA-C-N	5.31	130.24	121.86
1	B	115	ILE	C-N-CA	5.31	130.24	121.86
1	A	159	THR	CA-CB-CG2	5.30	119.52	110.50
1	A	387	GLN	N-CA-C	5.30	119.60	113.18
1	A	271	ASN	CA-C-N	5.30	127.64	120.38
1	A	271	ASN	C-N-CA	5.30	127.64	120.38
1	B	420	SER	N-CA-C	5.30	116.95	108.41
1	A	307	TYR	CB-CG-CD2	-5.30	112.85	120.80
1	B	556	LEU	CA-C-O	-5.30	113.31	119.14
1	A	107	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	18	VAL	N-CA-CB	5.29	119.22	112.34
1	B	64	ALA	N-CA-CB	-5.29	102.41	110.45
1	B	223	ALA	O-C-N	-5.29	115.24	121.32
1	B	250	SER	O-C-N	5.28	130.02	123.15
1	B	218	THR	CA-CB-OG1	5.28	117.52	109.60
1	A	139	VAL	N-CA-C	5.27	115.80	108.84
1	B	283	HIS	N-CA-C	-5.27	98.33	107.49
1	A	134	LYS	CA-CB-CG	5.26	124.63	114.10
1	A	354	SER	CA-CB-OG	-5.26	100.57	111.10
1	B	567	PRO	N-CA-C	5.26	120.93	114.35
1	B	494	ALA	O-C-N	-5.26	116.39	123.23
1	A	232	SER	CA-C-N	5.26	124.87	119.56
1	A	232	SER	C-N-CA	5.26	124.87	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	GLY	N-CA-C	-5.26	106.48	112.79
1	B	312	ASN	CB-CG-ND2	5.25	124.28	116.40
1	B	483	LYS	N-CA-CB	-5.25	102.44	110.85
1	A	551	GLY	CA-C-O	-5.25	111.43	120.57
1	A	576	VAL	O-C-N	-5.25	117.51	123.18
1	B	369	THR	N-CA-C	5.25	121.08	114.31
1	A	552	GLY	O-C-N	-5.25	115.88	122.70
1	A	390	PRO	O-C-N	-5.24	116.61	123.06
1	A	380	ARG	CA-C-O	5.24	126.03	120.63
1	B	306	PHE	O-C-N	-5.24	117.45	123.42
1	B	61	GLU	N-CA-C	5.24	119.66	113.16
1	A	570	GLN	N-CA-C	-5.24	103.97	110.41
1	A	250	SER	N-CA-C	5.22	117.62	109.52
1	A	308	GLN	CA-C-O	-5.22	114.92	120.92
1	A	138	LYS	CA-C-O	-5.22	115.31	121.16
1	A	165	LYS	CA-C-O	5.22	126.13	120.55
1	A	224	PRO	N-CA-CB	5.21	108.69	103.48
1	A	307	TYR	N-CA-C	-5.21	99.79	108.34
1	A	480	TRP	CA-C-N	5.21	131.17	122.73
1	A	480	TRP	C-N-CA	5.21	131.17	122.73
1	A	106	CYS	CA-C-N	5.21	131.49	121.54
1	A	106	CYS	C-N-CA	5.21	131.49	121.54
1	A	300	SER	CA-C-O	-5.21	113.17	118.90
1	B	65	ILE	CB-CA-C	5.20	117.75	110.99
1	A	538	GLN	CA-C-O	-5.20	114.14	120.54
1	B	281	ASN	CA-C-O	5.20	124.99	119.69
1	A	495	THR	N-CA-C	5.19	117.30	109.41
1	A	513	ASP	N-CA-CB	-5.19	102.12	109.85
1	B	436	ASP	CB-CG-OD1	5.19	130.34	118.40
1	B	437	TYR	CA-C-O	-5.19	114.69	120.66
1	B	334	LYS	N-CA-C	5.19	117.15	108.23
1	A	119	LYS	O-C-N	-5.19	116.86	123.24
1	B	214	ASP	CA-C-O	5.19	127.93	120.51
1	B	126	ASP	N-CA-C	-5.18	106.81	112.72
1	A	257	THR	CA-CB-OG1	-5.18	101.83	109.60
1	B	387	GLN	CG-CD-NE2	5.18	124.17	116.40
1	A	370	TRP	CA-CB-CG	-5.17	103.77	113.60
1	B	325	LEU	O-C-N	-5.17	116.66	123.02
1	A	292	GLY	CA-C-N	5.17	130.14	123.00
1	A	292	GLY	C-N-CA	5.17	130.14	123.00
1	B	416	PRO	CA-C-O	5.17	130.01	120.60
1	A	323	LEU	O-C-N	5.17	129.94	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	SER	CA-C-N	-5.17	113.48	122.37
1	B	252	SER	C-N-CA	-5.17	113.48	122.37
1	B	60	GLN	CA-C-O	5.17	127.98	121.58
1	B	200	ARG	CA-CB-CG	5.16	124.43	114.10
1	A	271	ASN	CA-CB-CG	5.16	117.76	112.60
1	B	29	ARG	CA-CB-CG	5.16	124.42	114.10
1	A	318	SER	CA-C-O	5.16	127.89	120.51
1	A	337	LYS	N-CA-C	-5.16	101.36	109.25
1	A	358	LEU	O-C-N	-5.16	116.46	122.96
1	A	215	SER	CA-C-O	5.16	122.69	119.55
1	A	563	ASP	N-CA-CB	-5.16	102.36	110.30
1	A	159	THR	CA-C-N	5.15	130.17	123.06
1	A	159	THR	C-N-CA	5.15	130.17	123.06
1	B	499	LEU	CA-C-N	-5.15	116.39	123.14
1	B	499	LEU	C-N-CA	-5.15	116.39	123.14
1	A	360	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	A	157	ALA	CB-CA-C	5.15	117.50	109.42
1	B	509	PHE	O-C-N	-5.15	117.35	123.22
1	A	62	SER	CA-CB-OG	5.14	121.39	111.10
1	B	524	GLN	N-CA-C	5.14	117.07	108.23
1	A	8	ILE	O-C-N	-5.14	116.56	121.90
1	A	126	ASP	CB-CG-OD1	5.14	130.21	118.40
1	B	455	PHE	N-CA-C	5.14	116.88	109.07
1	A	29	ARG	CA-C-O	5.13	127.39	121.28
1	A	228	ASP	CB-CA-C	-5.13	100.09	109.54
1	B	273	TRP	N-CA-C	5.13	118.80	112.54
1	B	495	THR	OG1-CB-CG2	-5.13	99.03	109.30
1	A	459	ARG	NH1-CZ-NH2	5.13	125.97	119.30
1	A	142	LYS	CA-C-N	5.13	130.00	122.77
1	A	142	LYS	C-N-CA	5.13	130.00	122.77
1	B	312	ASN	N-CA-CB	5.13	119.89	111.58
1	A	214	ASP	CA-CB-CG	-5.13	107.47	112.60
1	B	128	SER	CB-CA-C	-5.13	100.15	110.30
1	B	336	VAL	O-C-N	-5.13	117.80	123.18
1	A	101	ASP	N-CA-C	5.12	119.02	112.26
1	A	339	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	58	ARG	CG-CD-NE	-5.12	100.75	112.00
1	A	212	GLY	CA-C-N	-5.11	114.78	122.81
1	A	212	GLY	C-N-CA	-5.11	114.78	122.81
1	A	573	SER	CA-C-O	5.11	126.73	121.06
1	B	81	PHE	CA-CB-CG	5.11	118.91	113.80
1	B	517	GLY	O-C-N	-5.11	115.72	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ALA	CA-C-N	5.11	130.60	122.94
1	A	82	ALA	C-N-CA	5.11	130.60	122.94
1	A	110	ASN	CA-CB-CG	-5.11	107.49	112.60
1	B	8	ILE	CA-C-N	5.11	127.13	120.28
1	B	8	ILE	C-N-CA	5.11	127.13	120.28
1	B	185	ARG	O-C-N	-5.11	117.34	123.27
1	A	254	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	80	LEU	CA-C-O	5.10	125.98	120.32
1	A	40	ASN	CB-CG-OD1	5.10	131.00	120.80
1	A	172	ILE	N-CA-C	5.10	115.65	108.36
1	A	543	TYR	CA-C-O	5.10	126.11	120.71
1	B	220	ASP	CA-C-O	-5.10	115.45	121.16
1	B	235	GLY	CA-C-N	-5.10	113.91	123.03
1	B	235	GLY	C-N-CA	-5.10	113.91	123.03
1	A	213	LYS	CB-CA-C	5.09	119.36	109.33
1	B	35	GLN	N-CA-C	-5.08	105.82	111.36
1	B	524	GLN	CA-C-N	5.08	130.03	121.14
1	B	524	GLN	C-N-CA	5.08	130.03	121.14
1	B	562	ALA	N-CA-CB	5.08	117.44	110.07
1	A	48	TRP	CA-CB-CG	5.08	123.25	113.60
1	B	509	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	70	VAL	N-CA-C	5.08	115.79	108.48
1	B	147	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	313	ASP	CA-C-O	5.07	127.76	120.51
1	B	145	PHE	CA-C-O	-5.07	113.42	119.35
1	A	570	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	356	GLY	CA-C-O	-5.07	111.75	120.57
1	B	261	ILE	O-C-N	-5.07	117.57	122.99
1	B	34	LYS	CB-CA-C	-5.06	101.34	110.35
1	A	15	THR	OG1-CB-CG2	-5.05	99.19	109.30
1	A	564	LEU	CA-C-O	5.05	125.78	120.42
1	B	342	ALA	CA-C-O	-5.05	114.90	121.11
1	A	147	ASP	N-CA-CB	-5.05	102.18	110.21
1	A	256	GLU	CA-CB-CG	5.05	124.20	114.10
1	B	489	TRP	CB-CA-C	5.05	121.36	110.41
1	A	138	LYS	N-CA-CB	5.05	117.39	109.97
1	B	242	HIS	N-CA-CB	-5.05	104.22	111.54
1	A	144	LYS	CB-CA-C	5.04	118.64	110.22
1	A	534	ILE	CA-CB-CG1	-5.04	101.83	110.40
1	B	511	ALA	N-CA-CB	5.04	119.14	110.68
1	B	389	PRO	CB-CA-C	5.04	117.06	110.92
1	A	92	TRP	O-C-N	5.03	128.99	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	GLY	N-CA-C	5.03	125.11	113.18
1	A	243	GLY	O-C-N	5.02	129.76	122.68
1	A	284	ASP	CB-CG-OD1	-5.02	106.85	118.40
1	A	297	ASP	CA-C-O	5.02	123.33	119.46
1	A	513	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	515	LYS	N-CA-C	-5.02	107.29	113.41
1	B	582	TRP	CA-C-O	5.02	129.33	120.80
1	A	134	LYS	N-CA-CB	-5.02	102.74	110.12
1	A	426	PHE	CD1-CE1-CZ	-5.02	110.97	120.00
1	A	25	THR	CA-C-O	5.01	125.55	119.38
1	B	161	VAL	N-CA-CB	-5.01	102.09	111.62
1	B	366	ASP	CA-C-O	-5.01	113.34	120.51
1	A	473	PRO	CA-C-N	5.01	129.46	121.34
1	A	473	PRO	C-N-CA	5.01	129.46	121.34
1	B	369	THR	CB-CA-C	-5.01	100.60	109.02
1	A	317	PHE	CA-C-N	5.01	131.11	121.54
1	A	317	PHE	C-N-CA	5.01	131.11	121.54
1	B	288	LEU	N-CA-CB	5.01	117.66	109.69
1	A	105	CYS	O-C-N	-5.01	115.62	122.33
1	B	431	ASN	OD1-CG-ND2	-5.00	117.60	122.60
1	B	553	ALA	N-CA-C	5.00	117.62	111.82

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	ASP	Mainchain
1	A	120	VAL	Mainchain
1	A	13	LYS	Mainchain
1	A	14	THR	Mainchain
1	A	142	LYS	Mainchain
1	A	157	ALA	Mainchain
1	A	158	PRO	Mainchain
1	A	177	GLY	Mainchain
1	A	210	LEU	Mainchain
1	A	220	ASP	Mainchain
1	A	234	THR	Mainchain
1	A	248	TRP	Mainchain
1	A	251	ALA	Mainchain
1	A	268	GLY	Mainchain,Peptide
1	A	284	ASP	Mainchain,Peptide
1	A	288	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	A	316	ASP	Mainchain
1	A	328	TYR	Mainchain
1	A	331	LYS	Mainchain
1	A	338	ALA	Mainchain
1	A	347	PHE	Mainchain
1	A	353	ARG	Mainchain
1	A	363	PRO	Mainchain
1	A	385	GLU	Mainchain
1	A	413	ASN	Mainchain
1	A	423	THR	Mainchain
1	A	478	VAL	Mainchain
1	A	528	GLY	Mainchain
1	A	559	GLY	Mainchain
1	A	563	ASP	Mainchain
1	A	58	ARG	Mainchain
1	A	6	GLU	Mainchain
1	A	69	GLY	Mainchain
1	A	95	ASN	Mainchain
1	B	103	ARG	Mainchain
1	B	142	LYS	Mainchain
1	B	218	THR	Mainchain
1	B	234	THR	Mainchain
1	B	262	VAL	Mainchain
1	B	268	GLY	Mainchain,Peptide
1	B	284	ASP	Peptide
1	B	285	TYR	Mainchain
1	B	287	SER	Mainchain
1	B	288	LEU	Peptide
1	B	289	TYR	Mainchain
1	B	351	VAL	Mainchain
1	B	356	GLY	Mainchain
1	B	366	ASP	Mainchain
1	B	390	PRO	Mainchain
1	B	40	ASN	Mainchain
1	B	459	ARG	Mainchain
1	B	49	SER	Mainchain
1	B	496	ALA	Mainchain
1	B	65	ILE	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	4537	0	4312	125	6
1	B	4537	0	4312	149	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	24	0	3	1	0
3	B	24	0	3	0	0
4	A	73	0	0	4	0
4	B	33	0	0	1	0
All	All	9232	0	8630	263	6

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 15.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASN:N	1:A:367:ASN:CA	1.69	1.51
1:A:366:ASP:O	1:A:367:ASN:HA	1.37	1.21
1:A:293:GLN:HE22	1:A:339:THR:HG21	0.95	1.06
1:A:366:ASP:O	1:A:367:ASN:CA	2.02	1.02
1:A:293:GLN:NE2	1:A:339:THR:HG21	1.77	0.98
1:B:329:LYS:HE3	1:B:333:GLY:H	1.29	0.97
1:A:79:ARG:HG2	1:A:95:ASN:HD22	1.30	0.94
1:A:366:ASP:C	1:A:367:ASN:CA	2.43	0.92
1:A:29:ARG:HH22	1:A:63:GLN:HE21	1.13	0.92
1:A:366:ASP:H	1:A:432:HIS:HE1	1.19	0.91
1:A:456:ARG:HD2	1:A:458:LYS:HE3	1.50	0.90
1:A:183:VAL:HB	1:A:185:ARG:HH12	1.37	0.88
1:B:125:LEU:O	1:B:153:THR:HG22	1.74	0.88
1:B:391:LEU:HA	1:B:439:THR:HG21	1.57	0.87
1:B:442:VAL:HG22	1:B:452:GLY:HA3	1.58	0.85
1:A:392:PRO:HD3	1:A:439:THR:HG21	1.58	0.85
1:B:293:GLN:OE1	1:B:339:THR:HG21	1.78	0.84
1:B:339:THR:HG22	1:B:351:VAL:HB	1.62	0.82
1:B:65:ILE:HG22	1:B:72:TYR:HB2	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:HA	1:B:134:LYS:HD2	1.62	0.81
1:A:456:ARG:CD	1:A:458:LYS:HE3	2.10	0.79
1:A:87:THR:HG22	1:A:89:LYS:H	1.48	0.79
1:B:456:ARG:HH11	1:B:456:ARG:HB3	1.46	0.79
1:A:166:THR:HG23	1:A:168:LYS:HB2	1.63	0.78
1:A:22:GLY:H	1:A:63:GLN:HE22	1.31	0.77
1:B:199:MET:HE2	1:B:209:ARG:HH21	1.48	0.77
1:A:97:ARG:HG2	1:A:97:ARG:HH11	1.49	0.77
1:A:392:PRO:HD3	1:A:439:THR:CG2	2.14	0.77
1:A:366:ASP:H	1:A:432:HIS:CE1	2.03	0.76
1:A:183:VAL:HB	1:A:185:ARG:NH1	2.01	0.75
1:B:216:THR:O	1:B:217:VAL:HB	1.87	0.73
1:B:22:GLY:H	1:B:63:GLN:HE22	1.37	0.72
1:B:28:GLN:HG3	1:B:419:TYR:HB3	1.73	0.71
1:A:29:ARG:HH22	1:A:63:GLN:NE2	1.87	0.69
1:A:339:THR:HG22	4:A:775:HOH:O	1.92	0.69
1:A:334:LYS:HE3	1:A:334:LYS:HA	1.75	0.69
1:A:524:GLN:HE21	1:A:526:GLY:H	1.41	0.69
1:B:366:ASP:H	1:B:432:HIS:HE1	1.41	0.68
1:B:378:THR:HG23	1:B:380:ARG:HB2	1.76	0.68
1:A:436:ASP:OD2	1:A:458:LYS:NZ	2.28	0.67
1:B:325:LEU:HD22	1:B:353:ARG:HD2	1.76	0.66
1:B:102:ILE:HD11	1:B:126:ASP:HA	1.77	0.66
1:A:327:ASP:HB3	1:A:335:ILE:HD13	1.79	0.65
1:B:405:SER:HB2	1:B:434:LYS:HB3	1.79	0.65
1:B:249:GLN:HE22	1:B:321:ASN:HA	1.60	0.65
1:A:136:THR:OG1	1:A:137:GLY:N	2.28	0.65
1:A:133:ASN:O	1:A:136:THR:O	2.16	0.64
1:A:57:GLN:NE2	1:B:55:GLU:H	1.96	0.64
1:B:538:GLN:O	1:B:539:ASP:C	2.40	0.64
1:A:273:TRP:HZ3	1:A:389:PRO:O	1.80	0.64
1:A:266:ASN:HB2	1:A:267:PRO:HD2	1.78	0.64
1:A:378:THR:HG22	1:A:380:ARG:H	1.62	0.64
1:A:391:LEU:HA	1:A:439:THR:HG21	1.80	0.63
1:A:173:HIS:HE1	1:A:189:ARG:HE	1.46	0.63
1:B:392:PRO:HD3	1:B:439:THR:HG22	1.81	0.63
1:A:87:THR:CG2	1:A:89:LYS:HB3	2.28	0.63
1:B:273:TRP:HZ3	1:B:389:PRO:O	1.81	0.63
1:A:53:GLY:HA2	1:B:57:GLN:HE22	1.64	0.62
1:B:329:LYS:HE3	1:B:333:GLY:N	2.10	0.62
1:B:372:SER:OG	1:B:373:HIS:HD2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:GLU:OE2	1:B:578:LYS:HE3	1.99	0.61
1:B:133:ASN:HB3	1:B:136:THR:HG23	1.82	0.61
1:B:366:ASP:H	1:B:432:HIS:CE1	2.17	0.61
1:B:3:VAL:HG21	1:B:115:ILE:HG13	1.81	0.60
1:B:17:ASP:CG	1:B:19:LEU:HD11	2.26	0.60
1:A:162:LYS:HD2	1:A:167:GLY:O	2.01	0.60
1:B:34:LYS:HE3	1:B:497:GLY:HA2	1.83	0.60
1:A:408:PHE:CE1	1:A:457:ILE:HD11	2.38	0.59
1:B:468:LEU:HB3	1:B:482:HIS:HB3	1.84	0.59
1:A:152:TYR:OH	1:A:185:ARG:NH1	2.36	0.59
1:A:79:ARG:CG	1:A:95:ASN:HD22	2.11	0.59
1:A:457:ILE:HD13	4:A:807:HOH:O	2.02	0.58
1:A:582:TRP:H	1:A:582:TRP:CD1	2.20	0.58
1:B:281:ASN:OD1	1:B:283:HIS:HB2	2.02	0.58
1:B:328:TYR:CE2	1:B:330:ALA:HA	2.39	0.58
1:A:57:GLN:HE21	1:B:55:GLU:H	1.52	0.57
1:B:56:LYS:CB	1:B:56:LYS:NZ	2.66	0.57
1:B:434:LYS:NZ	1:B:458:LYS:HE2	2.19	0.57
1:A:183:VAL:HG13	1:A:203:VAL:CG1	2.34	0.57
1:A:329:LYS:HE2	1:A:333:GLY:O	2.04	0.57
1:A:166:THR:HG23	1:A:168:LYS:H	1.68	0.57
1:B:116:TYR:CZ	1:B:169:VAL:HG11	2.39	0.57
1:A:510:LYS:HE2	1:A:519:GLU:OE1	2.05	0.57
1:B:210:LEU:HD12	1:B:211:ASN:H	1.68	0.57
1:B:34:LYS:NZ	1:B:496:ALA:O	2.33	0.57
1:A:405:SER:HA	1:A:406:PRO:C	2.29	0.56
1:B:133:ASN:CG	1:B:136:THR:HG22	2.31	0.56
1:B:144:LYS:NZ	1:B:148:HIS:HD2	2.03	0.56
1:A:378:THR:HG22	1:A:380:ARG:HB2	1.88	0.55
1:A:582:TRP:CH2	1:B:43:LYS:HD2	2.41	0.55
1:A:245:GLY:HA2	1:A:265:GLY:O	2.06	0.55
1:A:329:LYS:HD2	1:A:335:ILE:HG22	1.88	0.55
1:A:136:THR:HG23	1:A:138:LYS:H	1.71	0.55
1:B:362:PHE:CZ	1:B:476:GLY:HA2	2.42	0.55
1:A:189:ARG:HD3	1:A:194:GLY:O	2.07	0.55
1:A:456:ARG:HB3	1:A:456:ARG:HH11	1.72	0.55
1:A:483:LYS:O	1:A:483:LYS:HD3	2.06	0.55
1:A:510:LYS:HE2	1:A:519:GLU:CD	2.31	0.54
1:B:59:GLY:CA	1:B:551:GLY:HA3	2.37	0.54
1:B:153:THR:HG23	4:B:795:HOH:O	2.07	0.54
1:B:490:ALA:HB1	1:B:531:SER:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:HIS:HE1	1:B:189:ARG:HE	1.54	0.54
1:B:456:ARG:HH11	1:B:456:ARG:CB	2.18	0.54
1:B:245:GLY:HA2	1:B:265:GLY:O	2.06	0.54
1:B:56:LYS:CB	1:B:56:LYS:HZ3	2.20	0.54
1:A:84:ASP:OD1	1:A:87:THR:HB	2.08	0.54
1:A:164:GLY:H	1:A:258:ASN:ND2	2.04	0.54
1:A:320:ASN:H	1:A:320:ASN:HD22	1.54	0.54
1:A:372:SER:OG	1:A:373:HIS:HD2	1.90	0.54
1:B:256:GLU:OE2	1:B:353:ARG:NH2	2.40	0.54
1:A:163:ASP:HB3	1:A:166:THR:HG22	1.90	0.54
1:B:392:PRO:HD3	1:B:439:THR:CG2	2.37	0.54
1:A:55:GLU:O	1:B:55:GLU:HG2	2.08	0.53
1:A:456:ARG:HD2	1:A:458:LYS:CE	2.30	0.53
1:A:524:GLN:NE2	1:A:526:GLY:H	2.05	0.53
1:A:57:GLN:HE22	1:B:53:GLY:HA2	1.74	0.53
1:A:524:GLN:HE21	1:A:526:GLY:N	2.05	0.52
1:B:133:ASN:OD1	1:B:136:THR:HG22	2.09	0.52
1:A:1:LYS:HE3	1:A:1:LYS:O	2.08	0.52
1:A:29:ARG:NH2	1:A:63:GLN:HE21	1.95	0.52
1:B:102:ILE:HD11	1:B:126:ASP:CA	2.40	0.52
1:B:456:ARG:HB3	1:B:456:ARG:NH1	2.20	0.51
1:B:56:LYS:HG2	1:B:77:TYR:CD2	2.45	0.51
1:A:93:THR:HG22	1:A:94:TYR:N	2.26	0.51
1:A:87:THR:HG22	1:A:89:LYS:HB3	1.93	0.51
1:A:327:ASP:HB3	1:A:335:ILE:CD1	2.41	0.51
1:B:286:ASP:CG	1:B:380:ARG:HH22	2.18	0.51
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.21	0.51
1:A:378:THR:CG2	1:A:380:ARG:HB2	2.41	0.51
1:B:210:LEU:O	1:B:211:ASN:C	2.54	0.51
1:A:43:LYS:HD2	1:B:582:TRP:CZ3	2.47	0.50
1:A:2:ASP:O	1:A:3:VAL:HB	2.11	0.50
1:A:164:GLY:H	1:A:258:ASN:HD21	1.58	0.50
1:A:200:ARG:HD3	1:A:201:PRO:HD2	1.93	0.50
1:A:256:GLU:OE1	1:A:337:LYS:HE2	2.11	0.50
1:B:283:HIS:O	1:B:284:ASP:C	2.54	0.50
1:B:3:VAL:HG21	1:B:115:ILE:CG1	2.42	0.50
1:A:159:THR:HG21	4:A:789:HOH:O	2.12	0.50
1:A:18:VAL:O	1:A:65:ILE:HB	2.11	0.49
1:A:34:LYS:HE3	1:A:37:ASN:HD22	1.76	0.49
1:B:226:TRP:O	1:B:236:LYS:NZ	2.30	0.49
1:A:456:ARG:HH11	1:A:456:ARG:CB	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:HD2	1:B:579:LEU:O	2.13	0.49
1:B:300:SER:OG	1:B:302:GLU:HG3	2.12	0.49
1:A:377:LYS:HG3	1:A:378:THR:N	2.28	0.49
1:B:337:LYS:HZ3	1:B:353:ARG:NH2	2.10	0.49
1:A:366:ASP:C	1:A:367:ASN:HA	2.20	0.48
1:B:17:ASP:OD1	1:B:19:LEU:HD11	2.13	0.48
1:B:164:GLY:H	1:B:258:ASN:ND2	2.11	0.48
1:B:405:SER:HA	1:B:406:PRO:C	2.38	0.48
1:A:217:VAL:HG12	1:A:219:GLY:O	2.14	0.48
1:B:111:ARG:HD3	1:B:414:TRP:CE3	2.48	0.48
1:B:133:ASN:HB3	1:B:136:THR:CG2	2.43	0.48
1:B:1:LYS:O	1:B:1:LYS:HE2	2.13	0.48
1:B:392:PRO:HB2	1:B:396:GLN:O	2.13	0.48
1:B:412:LYS:HD2	1:B:429:PRO:HG2	1.96	0.48
1:B:19:LEU:N	1:B:19:LEU:HD12	2.29	0.48
1:B:201:PRO:HD3	1:B:208:GLY:HA2	1.97	0.47
1:B:216:THR:O	1:B:217:VAL:CB	2.58	0.47
1:B:362:PHE:HB2	1:B:363:PRO:HD2	1.96	0.47
1:B:28:GLN:CG	1:B:419:TYR:HB3	2.43	0.47
1:B:200:ARG:NE	1:B:301:GLY:O	2.36	0.47
1:B:414:TRP:O	1:B:415:ASN:C	2.55	0.47
1:B:555:PRO:HB2	1:B:556:LEU:HD23	1.97	0.47
1:A:101:ASP:OD1	1:A:101:ASP:N	2.40	0.47
1:B:406:PRO:CB	1:B:407:PRO:HD2	2.44	0.47
1:B:56:LYS:HZ2	1:B:56:LYS:HB2	1.80	0.47
1:B:556:LEU:HD23	1:B:556:LEU:N	2.30	0.47
1:A:269:PRO:HG3	1:A:442:VAL:HG21	1.97	0.47
1:B:312:ASN:C	1:B:312:ASN:HD22	2.24	0.47
1:B:348:PHE:O	1:B:361:ALA:HA	2.14	0.47
1:B:357:LYS:HD2	1:B:357:LYS:HA	1.64	0.46
1:B:317:PHE:O	1:B:318:SER:C	2.58	0.46
1:A:229:ASP:OD1	1:A:230:ARG:O	2.32	0.46
1:B:118:ASP:CA	1:B:134:LYS:HD2	2.40	0.46
1:B:286:ASP:OD2	1:B:380:ARG:NH2	2.49	0.46
1:A:78:SER:HB3	1:A:124:THR:HG22	1.97	0.46
1:B:538:GLN:HB3	1:B:543:TYR:CE1	2.51	0.46
1:B:57:GLN:O	1:B:58:ARG:HB2	2.15	0.45
1:B:164:GLY:H	1:B:258:ASN:HD21	1.64	0.45
1:A:419:TYR:HB2	1:A:426:PHE:CE1	2.51	0.45
1:B:220:ASP:HB3	1:B:224:PRO:HD2	1.97	0.45
1:A:61:GLU:OE2	3:A:701:PQQ:O2A	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:TYR:HB2	1:B:160:ILE:HG13	1.98	0.45
1:B:146:ALA:HB1	1:B:152:TYR:CD2	2.52	0.45
1:A:117:GLY:O	1:A:134:LYS:NZ	2.49	0.45
1:B:56:LYS:NZ	1:B:56:LYS:HB2	2.31	0.44
1:B:564:LEU:O	1:B:567:PRO:HD2	2.16	0.44
1:A:200:ARG:HA	1:A:201:PRO:HD3	1.86	0.44
1:A:34:LYS:HD2	1:A:497:GLY:HA2	2.00	0.44
1:B:144:LYS:HZ2	1:B:148:HIS:HD2	1.64	0.44
1:A:43:LYS:HD2	1:B:582:TRP:CE3	2.52	0.44
1:A:11:ASP:O	1:A:12:ASP:C	2.59	0.44
1:B:44:LEU:HD23	1:B:521:TRP:CH2	2.53	0.44
1:A:120:VAL:HG23	1:A:132:LEU:HB2	1.98	0.44
1:B:202:PHE:O	1:B:289:TYR:HB2	2.18	0.44
1:A:21:TYR:HA	1:A:63:GLN:NE2	2.32	0.44
1:A:227:PRO:O	1:A:237:VAL:HB	2.18	0.44
1:B:420:SER:HB2	1:B:427:TYR:HE2	1.83	0.44
1:A:572:GLY:O	1:A:573:SER:HB3	2.15	0.44
1:A:55:GLU:H	1:B:57:GLN:HE21	1.66	0.43
1:A:202:PHE:O	1:A:289:TYR:HB2	2.17	0.43
1:A:43:LYS:HB3	1:B:582:TRP:CZ2	2.53	0.43
1:B:383:GLU:OE2	1:B:388:ARG:NH2	2.32	0.43
1:A:397:LYS:O	1:A:398:HIS:HB3	2.18	0.43
1:B:6:GLU:HA	1:B:9:ALA:HB3	2.00	0.43
1:B:560:ASP:O	1:B:563:ASP:HB2	2.17	0.43
1:B:177:GLY:O	1:B:178:ASP:C	2.61	0.43
1:B:157:ALA:HA	1:B:158:PRO:HD3	1.81	0.43
1:B:163:ASP:OD2	1:B:299:SER:HB3	2.18	0.43
1:B:210:LEU:HD12	1:B:211:ASN:N	2.34	0.43
1:B:405:SER:HB2	1:B:434:LYS:CB	2.47	0.43
1:A:136:THR:CG2	1:A:138:LYS:HG3	2.48	0.43
1:B:41:VAL:HG11	1:B:520:LEU:HB3	2.00	0.43
1:B:292:GLY:HA2	1:B:309:HIS:ND1	2.34	0.43
1:B:393:GLU:HB3	1:B:394:PRO:CD	2.48	0.43
1:A:420:SER:HB3	1:A:423:THR:OG1	2.18	0.42
1:B:80:LEU:C	1:B:80:LEU:HD23	2.44	0.42
1:B:561:MET:O	1:B:565:THR:HB	2.18	0.42
1:A:318:SER:O	1:A:344:ARG:HG3	2.19	0.42
1:B:48:TRP:CZ2	1:B:576:VAL:HG21	2.54	0.42
1:B:544:LEU:O	1:B:576:VAL:HA	2.20	0.42
1:A:249:GLN:HE22	1:A:321:ASN:HA	1.84	0.42
1:B:18:VAL:O	1:B:65:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ALA:O	1:B:224:PRO:C	2.62	0.42
1:A:398:HIS:HD2	1:A:399:GLY:O	2.00	0.42
1:B:246:ALA:HA	1:B:247:PRO:HD3	1.90	0.42
1:B:63:GLN:HB2	1:B:532:PRO:HG2	2.01	0.42
1:B:370:TRP:CE3	1:B:371:ALA:HB2	2.55	0.42
1:B:389:PRO:HA	1:B:390:PRO:HD3	1.83	0.42
1:B:406:PRO:HB2	1:B:407:PRO:HD2	2.01	0.42
1:A:84:ASP:O	1:A:87:THR:O	2.38	0.42
1:A:349:TYR:CD1	1:A:349:TYR:N	2.88	0.42
1:B:509:PHE:O	1:B:522:LYS:HA	2.20	0.42
1:A:50:TYR:OH	1:A:90:ARG:HD3	2.20	0.42
1:A:55:GLU:H	1:B:57:GLN:NE2	2.17	0.42
1:A:306:PHE:CZ	1:A:308:GLN:HG3	2.54	0.42
1:A:266:ASN:HB2	1:A:267:PRO:CD	2.47	0.41
1:B:442:VAL:CG2	1:B:452:GLY:HA3	2.41	0.41
1:A:507:GLY:HA3	1:A:524:GLN:HE22	1.85	0.41
1:A:246:ALA:HA	1:A:247:PRO:HD3	1.83	0.41
1:B:222:LYS:HE2	1:B:222:LYS:HB3	1.93	0.41
1:A:453:MET:HE3	1:A:453:MET:HB3	1.88	0.41
1:B:163:ASP:HB3	1:B:166:THR:HG22	2.02	0.41
1:A:352:ASP:OD1	1:A:354:SER:OG	2.28	0.41
1:B:288:LEU:HD23	1:B:288:LEU:HA	1.85	0.41
1:A:339:THR:CG2	4:A:775:HOH:O	2.62	0.41
1:B:190:ASP:HA	1:B:191:PRO:HD3	1.90	0.41
1:A:63:GLN:HB2	1:A:532:PRO:HG2	2.03	0.41
1:B:277:ALA:O	1:B:278:LYS:C	2.62	0.41
1:B:306:PHE:CE2	1:B:308:GLN:HB2	2.56	0.41
1:B:543:TYR:CZ	1:B:578:LYS:NZ	2.87	0.41
1:B:62:SER:HB2	1:B:74:THR:OG1	2.20	0.41
1:B:144:LYS:NZ	1:B:148:HIS:CD2	2.87	0.41
1:B:203:VAL:HG22	1:B:206:HIS:ND1	2.36	0.41
1:B:152:TYR:CZ	1:B:182:VAL:HG22	2.56	0.40
1:B:5:TRP:CZ3	1:B:161:VAL:HA	2.56	0.40
1:B:71:ILE:HG22	1:B:73:VAL:HG22	2.04	0.40
1:A:457:ILE:N	1:A:457:ILE:CD1	2.84	0.40
1:B:128:SER:HA	1:B:144:LYS:HA	2.04	0.40
1:A:200:ARG:HD3	1:A:201:PRO:CD	2.50	0.40
1:A:334:LYS:HE3	1:A:334:LYS:CA	2.47	0.40
1:B:59:GLY:HA3	1:B:551:GLY:HA3	2.03	0.40

All (6) 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:A:373:HIS:CD2	1:A:456:ARG:NH2[2_665]	1.57	0.63
1:A:372:SER:OG	1:A:456:ARG:NH2[2_665]	1.92	0.28
1:A:372:SER:OG	1:A:456:ARG:NH1[2_665]	2.04	0.16
1:A:373:HIS:CG	1:A:456:ARG:NH2[2_665]	2.08	0.12
1:A:373:HIS:CD2	1:A:456:ARG:CZ[2_665]	2.13	0.07
1:A:372:SER:OG	1:A:456:ARG:CZ[2_665]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/582 (100%)	530 (91%)	45 (8%)	5 (1%)	14	30
1	B	580/582 (100%)	514 (89%)	47 (8%)	19 (3%)	3	5
All	All	1160/1164 (100%)	1044 (90%)	92 (8%)	24 (2%)	5	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	ALA
1	A	385	GLU
1	B	217	VAL
1	B	289	TYR
1	B	330	ALA
1	B	332	ASP
1	B	366	ASP
1	B	385	GLU
1	B	107	ASP
1	B	280	GLY
1	B	331	LYS
1	A	107	ASP
1	B	313	ASP
1	B	3	VAL
1	B	15	THR

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Mol	Chain	Res	Type
1	B	211	ASN
1	B	269	PRO
1	B	496	ALA
1	A	108	VAL
1	B	375	ASP
1	B	459	ARG
1	A	3	VAL
1	B	108	VAL
1	B	572	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	469/469 (100%)	404 (86%)	65 (14%)	3	7
1	B	469/469 (100%)	393 (84%)	76 (16%)	2	4
All	All	938/938 (100%)	797 (85%)	141 (15%)	3	5

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	34	LYS
1	A	43	LYS
1	A	58	ARG
1	A	73	VAL
1	A	83	LEU
1	A	87	THR
1	A	89	LYS
1	A	97	ARG
1	A	102	ILE
1	A	103	ARG
1	A	125	LEU
1	A	134	LYS
1	A	138	LYS

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Mol	Chain	Res	Type
1	A	153	THR
1	A	154	MET
1	A	159	THR
1	A	161	VAL
1	A	162	LYS
1	A	166	THR
1	A	168	LYS
1	A	182	VAL
1	A	203	VAL
1	A	217	VAL
1	A	221	VAL
1	A	237	VAL
1	A	258	ASN
1	A	261	ILE
1	A	262	VAL
1	A	269	PRO
1	A	296	VAL
1	A	299	SER
1	A	308	GLN
1	A	312	ASN
1	A	320	ASN
1	A	324	VAL
1	A	332	ASP
1	A	334	LYS
1	A	335	ILE
1	A	337	LYS
1	A	339	THR
1	A	357	LYS
1	A	376	LEU
1	A	377	LYS
1	A	378	THR
1	A	400	LYS
1	A	407	PRO
1	A	433	TRP
1	A	439	THR
1	A	446	LYS
1	A	456	ARG
1	A	457	ILE
1	A	477	LYS
1	A	478	VAL
1	A	483	LYS
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	502	THR
1	A	541	GLU
1	A	544	LEU
1	A	556	LEU
1	A	561	MET
1	A	564	LEU
1	A	565	THR
1	A	578	LYS
1	A	581	SER
1	B	1	LYS
1	B	34	LYS
1	B	41	VAL
1	B	43	LYS
1	B	45	THR
1	B	51	SER
1	B	56	LYS
1	B	63	GLN
1	B	65	ILE
1	B	68	ASP
1	B	73	VAL
1	B	83	LEU
1	B	86	LYS
1	B	89	LYS
1	B	90	ARG
1	B	93	THR
1	B	103	ARG
1	B	120	VAL
1	B	136	THR
1	B	142	LYS
1	B	153	THR
1	B	154	MET
1	B	161	VAL
1	B	166	THR
1	B	182	VAL
1	B	195	GLU
1	B	203	VAL
1	B	213	LYS
1	B	218	THR
1	B	221	VAL
1	B	222	LYS
1	B	230	ARG
1	B	237	VAL

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Mol	Chain	Res	Type
1	B	256	GLU
1	B	259	THR
1	B	262	VAL
1	B	269	PRO
1	B	294	VAL
1	B	299	SER
1	B	312	ASN
1	B	320	ASN
1	B	323	LEU
1	B	324	VAL
1	B	326	PHE
1	B	329	LYS
1	B	331	LYS
1	B	334	LYS
1	B	337	LYS
1	B	339	THR
1	B	377	LYS
1	B	378	THR
1	B	397	LYS
1	B	398	HIS
1	B	402	VAL
1	B	433	TRP
1	B	445	THR
1	B	446	LYS
1	B	456	ARG
1	B	458	LYS
1	B	460	MET
1	B	472	ASP
1	B	477	LYS
1	B	483	LYS
1	B	493	LEU
1	B	495	THR
1	B	500	VAL
1	B	502	THR
1	B	513	ASP
1	B	538	GLN
1	B	544	LEU
1	B	556	LEU
1	B	563	ASP
1	B	564	LEU
1	B	565	THR
1	B	566	ARG

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Mol	Chain	Res	Type
1	B	578	LYS

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	57	GLN
1	A	63	GLN
1	A	95	ASN
1	A	96	HIS
1	A	173	HIS
1	A	206	HIS
1	A	231	ASN
1	A	242	HIS
1	A	249	GLN
1	A	258	ASN
1	A	293	GLN
1	A	312	ASN
1	A	320	ASN
1	A	367	ASN
1	A	373	HIS
1	A	398	HIS
1	A	432	HIS
1	A	464	HIS
1	A	524	GLN
1	B	20	GLN
1	B	28	GLN
1	B	57	GLN
1	B	63	GLN
1	B	95	ASN
1	B	96	HIS
1	B	148	HIS
1	B	173	HIS
1	B	249	GLN
1	B	258	ASN
1	B	266	ASN
1	B	312	ASN
1	B	320	ASN
1	B	367	ASN
1	B	373	HIS
1	B	421	GLN
1	B	432	HIS

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Mol	Chain	Res	Type
1	B	464	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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PQQ	A	701	2	26,26,26	3.88	10 (38%)	34,40,40	4.73	20 (58%)
3	PQQ	B	702	2	26,26,26	3.59	12 (46%)	34,40,40	4.54	22 (64%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PQQ	A	701	2	-	4/12/28/28	0/3/3/3
3	PQQ	B	702	2	-	1/12/28/28	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	PQQ	C5-C4	-9.84	1.40	1.54
3	A	701	PQQ	C5-C4	-9.15	1.41	1.54
3	A	701	PQQ	C6A-C5	-9.12	1.39	1.50
3	B	702	PQQ	O5-C5	8.46	1.40	1.23
3	A	701	PQQ	O4-C4	8.35	1.42	1.23
3	A	701	PQQ	O5-C5	7.77	1.39	1.23
3	B	702	PQQ	O4-C4	6.99	1.39	1.23
3	B	702	PQQ	C6A-C5	-6.60	1.42	1.50
3	A	701	PQQ	C9-C9X	-4.68	1.39	1.49
3	A	701	PQQ	C7-C7X	-4.17	1.43	1.50
3	B	702	PQQ	C7-C7X	-4.05	1.43	1.50
3	A	701	PQQ	C3-C3A	-3.13	1.35	1.42
3	A	701	PQQ	C9A-C6A	3.10	1.45	1.41
3	B	702	PQQ	C9-C9X	-2.92	1.43	1.49
3	A	701	PQQ	O9B-C9X	-2.84	1.22	1.30
3	B	702	PQQ	C2-N1	-2.82	1.33	1.37
3	B	702	PQQ	C2-C2X	-2.73	1.42	1.48
3	B	702	PQQ	C3-C3A	-2.52	1.36	1.42
3	B	702	PQQ	O7A-C7X	2.27	1.29	1.22
3	A	701	PQQ	C2-C2X	-2.23	1.43	1.48
3	B	702	PQQ	C9A-C1A	-2.09	1.43	1.46
3	B	702	PQQ	O9B-C9X	-2.00	1.24	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	PQQ	C9-C8-C7	13.40	130.93	119.93
3	A	701	PQQ	C8-C7-N6	-10.00	106.05	123.41
3	B	702	PQQ	O7B-C7X-O7A	-9.88	102.12	123.35
3	B	702	PQQ	O5-C5-C4	-9.66	105.53	118.14
3	A	701	PQQ	O4-C4-C5	-8.44	107.97	118.37
3	A	701	PQQ	C9A-C6A-C5	-8.42	113.75	121.59
3	B	702	PQQ	C8-C7-N6	-8.42	108.79	123.41
3	A	701	PQQ	O7B-C7X-C7	8.25	134.30	114.71
3	A	701	PQQ	O7B-C7X-O7A	-8.25	105.61	123.35
3	A	701	PQQ	O5-C5-C4	-7.68	108.12	118.14
3	B	702	PQQ	C6A-N6-C7	7.67	128.09	118.01
3	B	702	PQQ	O5-C5-C6A	7.14	129.91	121.76
3	B	702	PQQ	C8-C7-C7X	6.26	133.46	119.61
3	B	702	PQQ	O7B-C7X-C7	5.93	128.78	114.71
3	B	702	PQQ	O2A-C2X-C2	-5.81	109.21	121.01
3	B	702	PQQ	O9B-C9X-C9	5.80	131.77	115.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	PQQ	C9-C8-C7	5.15	124.16	119.93
3	A	701	PQQ	C1A-C3A-C4	-4.91	118.20	122.33
3	B	702	PQQ	O9A-C9X-C9	-4.32	111.65	121.97
3	A	701	PQQ	C8-C7-C7X	4.30	129.13	119.61
3	B	702	PQQ	C9A-C6A-C5	-4.03	117.83	121.59
3	B	702	PQQ	C5-C6A-N6	3.76	121.33	115.06
3	B	702	PQQ	C3A-C3-C2	-3.66	104.17	107.94
3	A	701	PQQ	O2B-C2X-O2A	-3.66	115.18	123.90
3	B	702	PQQ	C3-C2-N1	3.64	113.81	107.74
3	B	702	PQQ	C1A-N1-C2	-3.61	104.37	110.20
3	A	701	PQQ	C3A-C4-C5	-3.58	112.98	117.03
3	B	702	PQQ	C3A-C4-C5	-3.55	113.01	117.03
3	B	702	PQQ	C3-C2-C2X	-3.47	124.53	132.53
3	B	702	PQQ	O9B-C9X-O9A	-3.36	116.13	123.35
3	B	702	PQQ	O2B-C2X-C2	3.25	121.28	114.27
3	A	701	PQQ	C3A-C3-C2	-3.20	104.65	107.94
3	A	701	PQQ	C6A-N6-C7	3.10	122.08	118.01
3	B	702	PQQ	O7A-C7X-C7	2.79	126.91	121.30
3	A	701	PQQ	O9B-C9X-C9	2.55	122.54	115.28
3	A	701	PQQ	C9A-C9-C9X	2.47	126.92	121.49
3	A	701	PQQ	O9A-C9X-C9	-2.39	116.27	121.97
3	B	702	PQQ	O4-C4-C3A	2.11	127.08	121.92
3	A	701	PQQ	C5-C6A-N6	2.10	118.56	115.06
3	A	701	PQQ	C1A-N1-C2	-2.09	106.83	110.20
3	A	701	PQQ	C3A-C1A-N1	-2.07	104.51	107.23
3	A	701	PQQ	C9A-C6A-N6	2.05	126.54	123.58

There are no chirality outliers.

All (5) torsion outliers are listed below:

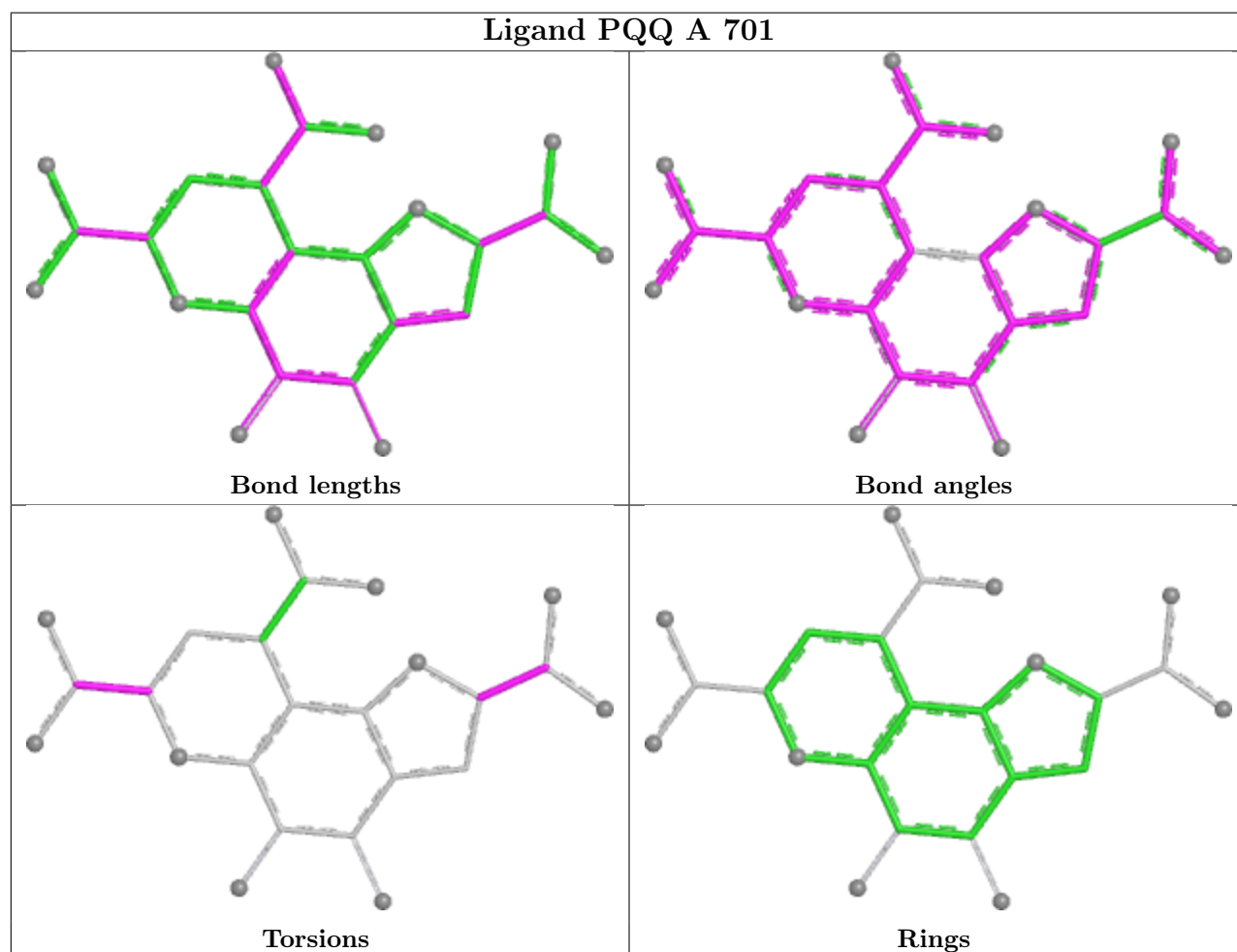
Mol	Chain	Res	Type	Atoms
3	A	701	PQQ	N1-C2-C2X-O2B
3	A	701	PQQ	C3-C2-C2X-O2B
3	B	702	PQQ	C8-C7-C7X-O7A
3	A	701	PQQ	C8-C7-C7X-O7A
3	A	701	PQQ	C8-C7-C7X-O7B

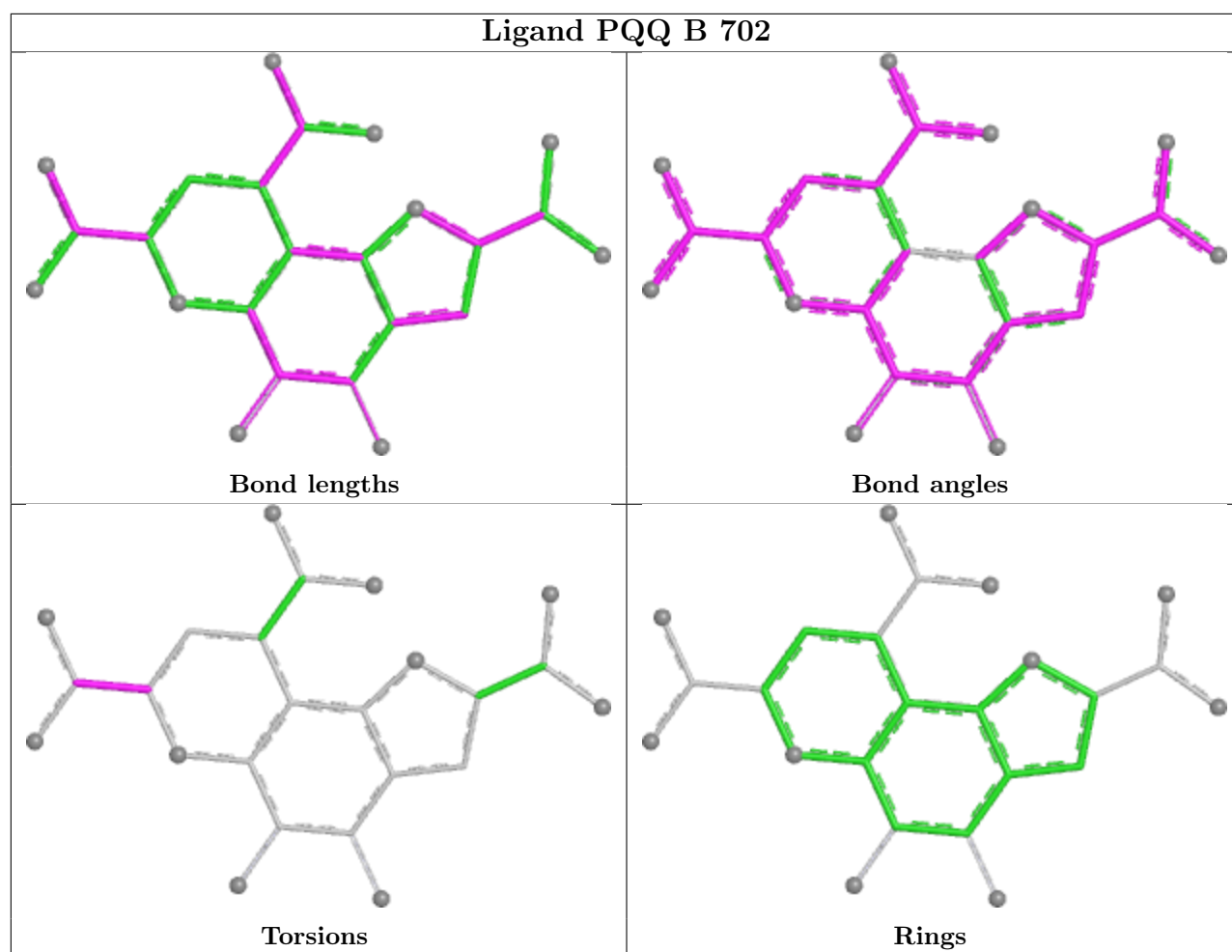
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	PQQ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.