



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:13 PM UTC

PDB ID : 1JKI / pdb_00001jki
Title : myo-Inositol-1-phosphate Synthase Complexed with an Inhibitor, 2-deoxy-glucitol-6-phosphate
Authors : Stein, A.J.; Geiger, J.H.
Deposited on : 2001-07-12
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

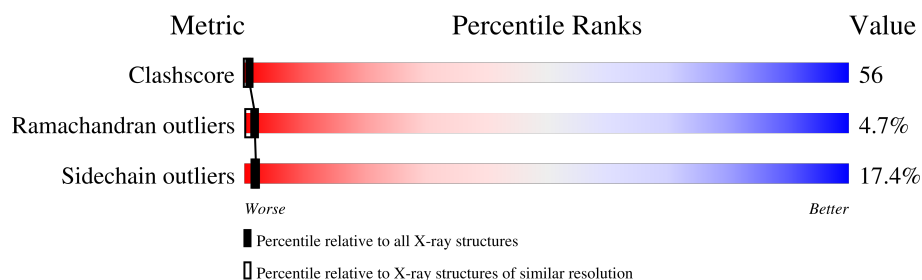
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	533	
1	B	533	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DG6	A	630	X	X	X	-
3	DG6	B	640	X	X	X	-

2 Entry composition [i](#)

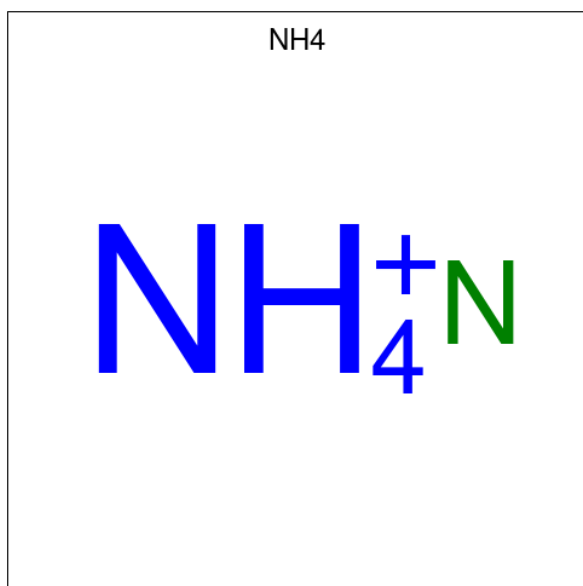
There are 5 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 myo-inositol-1-phosphate synthase.

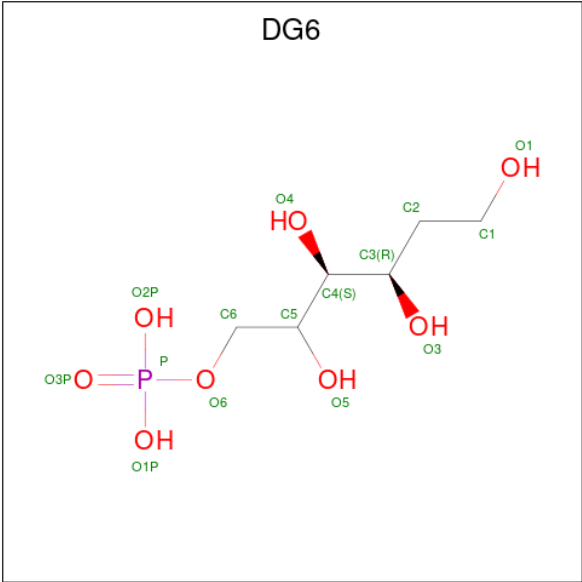
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4138	2632	695	795	16			
1	B	524	Total	C	N	O	S	0	0	0
			4130	2626	694	794	16			

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



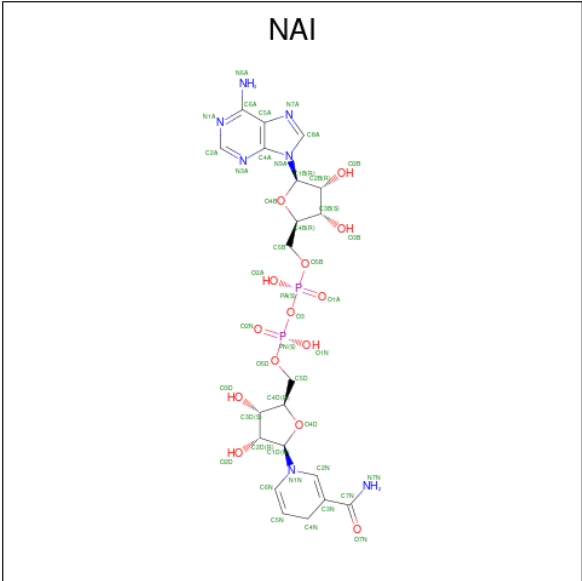
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

- Molecule 3 is 2-DEOXY-GLUCITOL-6-PHOSPHATE (CCD ID: DG6) (formula: $\text{C}_6\text{H}_{15}\text{O}_8\text{P}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			15	6	8	1		
3	B	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 4 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is water.

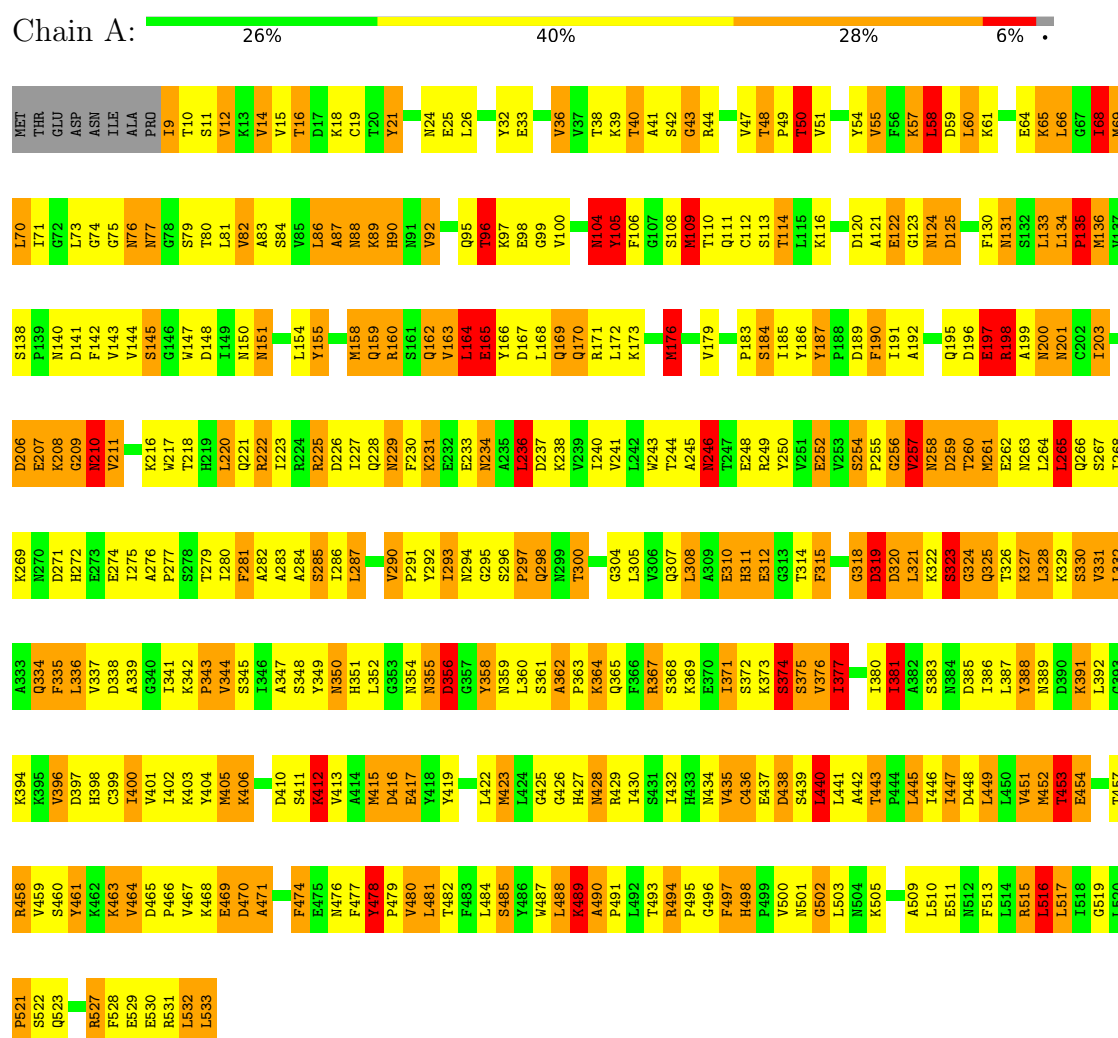
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	315	Total	O	0	0
			315	315		

3 Residue-property plots

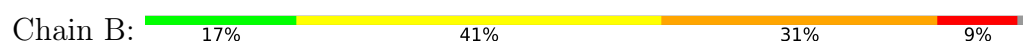
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: myo-inositol-1-phosphate synthase



• Molecule 1: myo-inositol-1-phosphate synthase



L503	L504	K505	Q506	R507		L510	E511	H512	F513	L514	R515	L516	L517	L518	G519	L520	P521	S522	Q523	N524	E525	L526	F527	F528	E529	E530	R531	E532	L533																																
A442	T443	P444	L445	I446	I447	D448	L449	L450	V451	M452	T453	E454	F455	C456	T457	R458	V459	S460	Y461	K462	V463	D464	D465	P466	V467	K468	E469	D470	A471	G472	K473	F474	F477	Y478	P479	V480	L481	T482	F483	L484	S485	Y486	W487	L488	K489	A490	P491	L492	T493	R494	P495	G496	F497	H498	P499	V500	N501	G502			
D379	I380	A381	S382	S383	S384	D385	L386	L387	Y388		K391	L392		K395	V396	D397	H398	C399	I400	V401	L402	K403	K404	Y404	M405	K406	P407	V408	G409	D410	S411	K350	L412	V413	A414	M415	D416	E417	Y418	Y419		L422	M423	L424	G425	G426	H427	N428	R429	I430	S431	I432	H433	V434	V435	C436	E437	D438	S439	L440	L441
I316	R249	Y186	Y187	F190	I191	A192	A193	N194	Q195	D196	E197	R198	A199	N200	C202	D203	N204	L205	D206	E207	K208	G209	N210	V211	T212	T213	R214	G215	K216		H219	L220	Q221	R222	I223	R224	R225	D226	I227	Q228	N229	F230	K231	E232	E233		L236	D237	K238	V239	I240	V241	L242	W243	E244	N245	A246	T247	E248		
K62	N124	Y186	P63	A128	F190	P129	F130	N131	L133	L134	P135	M136	V137	S138	N201	G202	D141	F142	V143	S145	G146	W147	D148	I149	N150	A151	A152	D153	L154	Y155	E156	A157	M158	Q159	R160	S161	Q162	V163	L164	E165	Y166	D167	L168	Q169	Q170	R171	L172	K173	A174	K175	M176	S177	L178	V179		I119	D120	A121	E122	G123	
MET	THR	GLU	ASP	ASN	ILE	ALA	PRO	PRO	ILE	T10	S11	T12	K13	V14	V15	T16	D17	K18	T19	T20	Y21	K22	D23	N24	E25	L26	N88	L27	T28	K29	T30	S31	Y32	F33		T96	K97	E98	G99	V100	K101	Q102	P103	R104	Y105	F106	G107	S108	L109	T110	Q111	T114	L115	V54	V55	F56	K57	L58	D59	L60	E61

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.73Å 98.31Å 121.86Å 90.00° 126.09° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	87.6 (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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: NH4, DG6, NAI

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	2.38	189/4219 (4.5%)	1.95	155/5719 (2.7%)
1	B	2.51	231/4211 (5.5%)	2.11	193/5708 (3.4%)
All	All	2.44	420/8430 (5.0%)	2.03	348/11427 (3.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	7
All	All	0	12

All (420) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	423	MET	SD-CE	-15.93	1.39	1.79
1	B	158	MET	SD-CE	15.00	2.17	1.79
1	B	71	ILE	CA-CB	-14.56	1.36	1.54
1	A	459	VAL	CA-CB	13.88	1.72	1.54
1	A	69	MET	SD-CE	13.73	2.13	1.79
1	B	136	MET	SD-CE	-13.44	1.46	1.79
1	A	423	MET	SD-CE	-12.86	1.47	1.79
1	A	227	ILE	CA-CB	12.69	1.69	1.54
1	B	293	ILE	CA-CB	-12.13	1.39	1.53
1	B	81	LEU	N-CA	11.85	1.60	1.46
1	A	415	MET	SD-CE	11.76	2.08	1.79
1	B	69	MET	SD-CE	11.68	2.08	1.79
1	B	478	TYR	CA-C	11.46	1.66	1.53
1	B	141	ASP	CA-C	-11.35	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	ASN	N-CA	11.19	1.59	1.46
1	B	14	VAL	CA-CB	11.17	1.67	1.54
1	A	143	VAL	CA-CB	10.96	1.68	1.54
1	B	75	GLY	CA-C	-10.88	1.39	1.51
1	A	244	THR	CA-CB	-10.59	1.37	1.53
1	A	145	SER	N-CA	-10.58	1.31	1.46
1	A	168	LEU	CA-C	-10.57	1.39	1.52
1	B	228	GLN	N-CA	10.43	1.58	1.46
1	A	344	VAL	CA-CB	10.38	1.66	1.54
1	B	151	ASN	CA-C	-10.36	1.38	1.52
1	B	377	ILE	CA-CB	10.34	1.66	1.54
1	B	419	TYR	CA-C	10.32	1.64	1.52
1	A	111	GLN	CA-C	-10.27	1.38	1.52
1	B	282	ALA	C-O	-10.23	1.12	1.24
1	B	451	VAL	CA-CB	-10.20	1.39	1.54
1	B	69	MET	CB-CG	10.15	1.82	1.52
1	B	80	THR	CA-CB	10.07	1.70	1.53
1	B	166	TYR	C-O	-9.92	1.12	1.24
1	A	293	ILE	C-O	9.84	1.34	1.24
1	B	405	MET	SD-CE	-9.57	1.55	1.79
1	B	137	VAL	CA-C	9.56	1.63	1.52
1	B	275	ILE	CA-CB	9.45	1.65	1.54
1	B	302	VAL	CA-C	9.43	1.62	1.52
1	A	286	ILE	CA-CB	9.37	1.65	1.54
1	A	451	VAL	N-CA	-9.33	1.34	1.46
1	A	293	ILE	CA-CB	-9.33	1.42	1.54
1	A	335	PHE	CA-C	9.31	1.64	1.52
1	B	104	ASN	CA-C	-9.22	1.41	1.52
1	A	347	ALA	CA-CB	9.05	1.65	1.53
1	B	227	ILE	CA-CB	9.01	1.66	1.54
1	A	136	MET	SD-CE	-9.01	1.57	1.79
1	B	231	LYS	CA-C	8.91	1.64	1.52
1	B	459	VAL	CA-C	-8.90	1.41	1.52
1	B	245	ALA	N-CA	-8.83	1.34	1.45
1	B	77	ASN	CA-C	8.76	1.63	1.52
1	A	434	ASN	CA-C	8.65	1.62	1.52
1	A	12	VAL	CA-CB	8.62	1.67	1.54
1	B	342	LYS	CA-C	8.60	1.63	1.52
1	A	136	MET	CG-SD	8.54	2.02	1.80
1	A	438	ASP	N-CA	-8.50	1.36	1.46
1	B	143	VAL	CA-CB	8.49	1.65	1.54
1	B	227	ILE	CA-C	8.47	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	VAL	CA-CB	8.44	1.64	1.54
1	A	521	PRO	CA-C	8.37	1.62	1.52
1	B	71	ILE	C-O	8.30	1.32	1.24
1	B	223	ILE	CA-CB	8.30	1.64	1.54
1	B	90	HIS	CA-C	-8.24	1.41	1.52
1	A	158	MET	SD-CE	8.24	2.00	1.79
1	A	231	LYS	CA-C	8.23	1.63	1.52
1	B	443	THR	CA-CB	8.22	1.63	1.53
1	A	88	ASN	CA-C	8.20	1.63	1.52
1	B	17	ASP	CA-C	-8.17	1.40	1.52
1	B	109	MET	SD-CE	-8.16	1.59	1.79
1	B	79	SER	CA-C	-8.15	1.42	1.52
1	A	290	VAL	C-O	-8.12	1.14	1.24
1	B	442	ALA	N-CA	-8.08	1.35	1.46
1	A	87	ALA	CA-CB	8.08	1.66	1.53
1	A	176	MET	SD-CE	-8.03	1.59	1.79
1	A	83	ALA	CA-CB	8.01	1.65	1.53
1	A	160	ARG	CA-C	8.00	1.63	1.52
1	A	113	SER	CA-C	7.97	1.62	1.52
1	A	71	ILE	CA-C	7.84	1.62	1.52
1	B	160	ARG	N-CA	-7.84	1.35	1.46
1	B	481	LEU	CA-C	7.80	1.62	1.53
1	A	147	TRP	CA-C	7.79	1.62	1.52
1	B	337	VAL	CA-CB	-7.78	1.43	1.54
1	B	464	VAL	CA-CB	-7.74	1.44	1.54
1	A	80	THR	CA-C	7.71	1.63	1.52
1	B	69	MET	N-CA	-7.70	1.36	1.46
1	A	454	GLU	CA-C	7.68	1.62	1.52
1	A	81	LEU	N-CA	7.67	1.55	1.46
1	B	331	VAL	CA-CB	-7.66	1.45	1.54
1	A	413	VAL	CA-CB	7.66	1.63	1.54
1	A	257	VAL	CA-CB	7.64	1.63	1.55
1	B	292	TYR	CA-C	7.62	1.62	1.52
1	B	109	MET	CA-C	7.59	1.62	1.52
1	B	169	GLN	CA-C	7.58	1.62	1.52
1	B	452	MET	SD-CE	-7.58	1.60	1.79
1	B	80	THR	CA-C	7.57	1.63	1.52
1	A	376	VAL	CA-CB	-7.55	1.44	1.54
1	B	211	VAL	CA-CB	-7.55	1.45	1.54
1	B	176	MET	N-CA	7.50	1.55	1.46
1	A	90	HIS	CA-C	-7.48	1.42	1.52
1	B	224	ARG	N-CA	7.46	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114	THR	CA-CB	-7.45	1.42	1.53
1	B	83	ALA	CA-CB	7.43	1.65	1.53
1	B	467	VAL	CA-CB	7.42	1.64	1.54
1	A	83	ALA	C-O	7.41	1.32	1.24
1	A	77	ASN	CB-CG	7.41	1.70	1.52
1	A	237	ASP	N-CA	7.41	1.55	1.46
1	A	141	ASP	CA-C	-7.40	1.43	1.52
1	B	422	LEU	CA-C	7.38	1.63	1.53
1	A	135	PRO	CA-C	-7.35	1.44	1.52
1	A	356	ASP	CB-CG	7.35	1.70	1.52
1	A	51	VAL	CA-CB	-7.30	1.44	1.54
1	B	500	VAL	CA-CB	7.28	1.63	1.54
1	B	344	VAL	CA-CB	7.26	1.63	1.54
1	B	435	VAL	CA-C	7.23	1.62	1.52
1	B	96	THR	CA-CB	7.22	1.66	1.53
1	B	443	THR	C-O	-7.22	1.18	1.24
1	B	84	SER	C-O	-7.22	1.15	1.24
1	A	75	GLY	CA-C	-7.21	1.41	1.52
1	A	451	VAL	CA-CB	-7.20	1.44	1.54
1	B	105	TYR	CA-C	7.19	1.62	1.52
1	B	442	ALA	CA-C	7.19	1.62	1.52
1	A	342	LYS	CA-C	7.14	1.62	1.52
1	A	167	ASP	CA-C	7.13	1.62	1.52
1	B	69	MET	CA-C	7.13	1.61	1.52
1	A	108	SER	C-O	-7.12	1.15	1.24
1	B	70	LEU	N-CA	7.11	1.54	1.46
1	B	428	ASN	C-O	-7.10	1.15	1.24
1	B	69	MET	CG-SD	-7.09	1.63	1.80
1	B	356	ASP	CB-CG	7.08	1.69	1.52
1	A	478	TYR	CA-C	7.05	1.61	1.53
1	A	89	LYS	N-CA	7.03	1.54	1.46
1	A	453	THR	N-CA	-7.03	1.37	1.46
1	A	443	THR	C-O	-7.02	1.17	1.24
1	B	347	ALA	N-CA	7.01	1.54	1.46
1	A	168	LEU	C-O	-6.93	1.16	1.24
1	B	241	VAL	CA-C	6.93	1.61	1.52
1	B	261	MET	SD-CE	-6.92	1.62	1.79
1	B	81	LEU	CA-C	6.91	1.61	1.52
1	B	141	ASP	CG-OD2	6.90	1.38	1.25
1	B	449	LEU	C-O	6.88	1.32	1.24
1	B	373	LYS	CA-C	6.87	1.61	1.53
1	B	145	SER	C-O	-6.85	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	ALA	CA-C	6.85	1.61	1.52
1	A	356	ASP	CA-C	6.84	1.61	1.52
1	B	145	SER	N-CA	-6.84	1.38	1.46
1	A	297	PRO	CA-C	-6.84	1.43	1.52
1	B	100	VAL	CA-CB	6.83	1.62	1.54
1	A	114	THR	N-CA	-6.80	1.38	1.45
1	B	160	ARG	CA-C	6.79	1.62	1.52
1	B	81	LEU	CB-CG	6.78	1.67	1.53
1	B	352	LEU	CA-C	6.78	1.61	1.52
1	B	451	VAL	CA-C	6.76	1.61	1.52
1	B	85	VAL	N-CA	6.75	1.54	1.46
1	A	68	ILE	C-O	6.73	1.31	1.24
1	B	111	GLN	CA-C	-6.73	1.43	1.52
1	B	415	MET	CG-SD	6.72	1.97	1.80
1	A	516	LEU	CA-C	6.72	1.61	1.52
1	A	429	ARG	CA-C	6.68	1.60	1.52
1	B	174	ALA	N-CA	6.68	1.54	1.46
1	A	405	MET	SD-CE	-6.66	1.62	1.79
1	A	110	THR	N-CA	6.65	1.54	1.46
1	A	158	MET	CG-SD	-6.64	1.64	1.80
1	A	48	THR	CA-CB	6.61	1.62	1.53
1	B	290	VAL	CA-C	6.59	1.58	1.53
1	A	206	ASP	CA-C	6.58	1.61	1.52
1	B	417	GLU	CA-C	6.56	1.60	1.52
1	A	419	TYR	CA-C	6.56	1.60	1.52
1	A	114	THR	CA-CB	-6.55	1.43	1.53
1	A	163	VAL	CA-C	-6.54	1.44	1.52
1	A	84	SER	CA-C	6.51	1.61	1.52
1	B	511	GLU	CA-C	6.50	1.61	1.52
1	A	337	VAL	CA-C	6.49	1.62	1.52
1	B	158	MET	C-O	6.49	1.31	1.24
1	A	436	CYS	C-O	6.49	1.30	1.23
1	B	391	LYS	CA-C	6.49	1.61	1.52
1	B	129	PRO	CA-C	-6.48	1.45	1.52
1	B	191	ILE	CA-CB	6.48	1.63	1.54
1	B	380	ILE	CA-CB	6.47	1.62	1.54
1	B	402	ILE	CA-C	6.45	1.60	1.52
1	A	108	SER	CA-CB	6.44	1.62	1.53
1	A	14	VAL	CA-C	6.38	1.60	1.52
1	A	318	GLY	C-O	6.37	1.31	1.23
1	B	323	SER	N-CA	-6.37	1.38	1.46
1	A	89	LYS	CA-C	6.36	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	ASN	CG-ND2	6.36	1.46	1.33
1	B	521	PRO	CA-C	6.35	1.60	1.52
1	A	87	ALA	CA-C	-6.35	1.44	1.52
1	A	511	GLU	CA-C	6.35	1.60	1.52
1	B	61	LYS	CA-CB	6.33	1.61	1.53
1	A	84	SER	CA-CB	6.32	1.63	1.53
1	B	430	ILE	CA-CB	6.32	1.63	1.54
1	B	106	PHE	N-CA	6.31	1.54	1.46
1	A	240	ILE	CA-CB	6.30	1.62	1.54
1	A	184	SER	CA-C	-6.30	1.44	1.52
1	A	338	ASP	C-O	6.29	1.32	1.24
1	B	69	MET	CA-CB	6.28	1.61	1.53
1	B	88	ASN	N-CA	6.27	1.53	1.46
1	B	309	ALA	CA-C	6.27	1.60	1.52
1	B	459	VAL	CA-CB	6.26	1.62	1.54
1	A	81	LEU	CA-C	6.25	1.60	1.52
1	B	12	VAL	CA-C	6.25	1.60	1.52
1	A	134	LEU	CA-C	6.22	1.58	1.52
1	A	425	GLY	C-O	-6.21	1.15	1.24
1	A	471	ALA	CA-CB	6.21	1.63	1.54
1	B	128	ALA	CA-CB	6.19	1.61	1.53
1	A	460	SER	N-CA	6.18	1.53	1.45
1	B	138	SER	C-N	6.18	1.41	1.34
1	A	79	SER	CA-CB	6.18	1.63	1.53
1	B	458	ARG	CA-C	6.17	1.62	1.52
1	B	144	VAL	CA-CB	6.15	1.62	1.54
1	B	31	SER	N-CA	-6.14	1.38	1.46
1	B	433	HIS	CA-C	6.14	1.60	1.52
1	B	442	ALA	CA-CB	-6.13	1.43	1.53
1	A	515	ARG	CA-C	6.13	1.60	1.52
1	B	228	GLN	C-O	6.13	1.31	1.24
1	A	423	MET	C-O	6.12	1.31	1.23
1	B	294	ASN	CA-C	-6.11	1.45	1.52
1	A	453	THR	CB-CG2	-6.10	1.32	1.52
1	B	135	PRO	CG-CD	6.10	1.71	1.50
1	B	451	VAL	N-CA	-6.09	1.38	1.46
1	B	270	ASN	CA-C	6.08	1.63	1.52
1	B	527	ARG	N-CA	6.07	1.55	1.46
1	A	165	GLU	C-O	6.06	1.30	1.23
1	A	170	GLN	C-O	-6.06	1.17	1.24
1	A	241	VAL	CA-C	6.05	1.59	1.52
1	A	69	MET	CB-CG	6.03	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	530	GLU	CA-C	6.02	1.59	1.52
1	A	169	GLN	CA-C	6.02	1.60	1.52
1	A	68	ILE	CB-CG2	6.01	1.72	1.52
1	A	165	GLU	CB-CG	6.00	1.70	1.52
1	B	70	LEU	CA-CB	-6.00	1.45	1.53
1	A	447	ILE	CA-CB	-6.00	1.47	1.54
1	A	57	LYS	CA-C	5.98	1.59	1.52
1	B	429	ARG	N-CA	5.98	1.53	1.46
1	B	72	GLY	C-O	5.98	1.32	1.24
1	B	223	ILE	CA-C	5.98	1.60	1.52
1	B	405	MET	CG-SD	5.97	1.95	1.80
1	A	234	ASN	CG-OD1	-5.97	1.12	1.23
1	B	280	ILE	CG1-CD1	-5.97	1.28	1.51
1	A	226	ASP	CA-C	-5.96	1.45	1.52
1	B	70	LEU	CA-C	-5.96	1.45	1.52
1	A	55	VAL	CA-C	5.94	1.60	1.52
1	A	168	LEU	N-CA	-5.93	1.39	1.46
1	B	460	SER	CA-C	5.93	1.60	1.52
1	A	109	MET	CA-C	5.92	1.60	1.52
1	A	241	VAL	CA-CB	-5.92	1.47	1.54
1	B	347	ALA	CA-CB	5.92	1.61	1.53
1	B	514	LEU	C-O	5.92	1.30	1.24
1	B	279	THR	N-CA	-5.92	1.39	1.46
1	A	155	TYR	N-CA	5.91	1.53	1.46
1	A	233	GLU	CA-C	-5.90	1.44	1.52
1	B	320	ASP	C-O	-5.89	1.16	1.24
1	B	165	GLU	N-CA	-5.87	1.38	1.46
1	A	77	ASN	CA-CB	5.87	1.62	1.53
1	A	228	GLN	N-CA	5.87	1.53	1.46
1	A	158	MET	CB-CG	-5.85	1.34	1.52
1	A	220	LEU	N-CA	5.85	1.53	1.46
1	B	136	MET	N-CA	5.84	1.53	1.45
1	B	244	THR	C-O	-5.84	1.15	1.23
1	A	452	MET	CA-C	-5.83	1.44	1.52
1	B	220	LEU	CA-C	5.82	1.60	1.52
1	B	333	ALA	N-CA	-5.82	1.39	1.46
1	B	197	GLU	CA-C	5.80	1.60	1.52
1	B	526	LEU	N-CA	5.78	1.53	1.46
1	B	169	GLN	CA-CB	-5.77	1.44	1.53
1	A	440	LEU	C-O	5.77	1.31	1.24
1	B	36	VAL	C-O	5.76	1.29	1.24
1	B	108	SER	CA-CB	5.76	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	THR	CA-C	-5.76	1.45	1.52
1	A	400	ILE	CA-CB	5.76	1.61	1.54
1	B	172	LEU	CA-C	-5.74	1.45	1.52
1	B	429	ARG	C-O	-5.74	1.17	1.24
1	A	170	GLN	CA-C	5.74	1.60	1.52
1	B	86	LEU	C-O	5.74	1.30	1.24
1	A	430	ILE	CA-C	-5.73	1.45	1.52
1	B	525	GLU	CA-C	-5.73	1.45	1.52
1	B	247	THR	C-O	-5.73	1.17	1.23
1	A	443	THR	CA-CB	5.72	1.61	1.53
1	B	77	ASN	N-CA	5.72	1.53	1.46
1	B	138	SER	CA-CB	-5.72	1.43	1.53
1	A	281	PHE	C-O	5.71	1.31	1.24
1	A	405	MET	CG-SD	5.71	1.95	1.80
1	A	513	PHE	CA-CB	-5.70	1.44	1.53
1	B	176	MET	CA-C	-5.70	1.45	1.52
1	A	76	ASN	C-O	5.69	1.30	1.24
1	A	478	TYR	N-CA	5.67	1.52	1.45
1	B	342	LYS	C-O	5.66	1.31	1.24
1	B	162	GLN	CA-CB	5.65	1.62	1.53
1	B	147	TRP	CA-C	5.65	1.59	1.52
1	A	312	GLU	CA-C	-5.64	1.44	1.52
1	A	315	PHE	CB-CG	-5.64	1.37	1.50
1	A	336	LEU	CA-C	5.63	1.60	1.52
1	A	464	VAL	CA-CB	-5.63	1.47	1.54
1	B	50	THR	CA-CB	-5.63	1.42	1.54
1	B	441	LEU	CA-C	-5.61	1.45	1.52
1	A	104	ASN	CB-CG	5.61	1.66	1.52
1	A	82	VAL	CA-CB	5.60	1.61	1.54
1	B	224	ARG	C-O	5.60	1.30	1.24
1	A	427	HIS	CA-CB	-5.59	1.44	1.53
1	A	345	SER	N-CA	5.58	1.53	1.46
1	A	105	TYR	CA-C	5.58	1.60	1.53
1	A	447	ILE	C-O	5.58	1.30	1.24
1	A	485	SER	C-O	-5.57	1.17	1.24
1	A	131	ASN	N-CA	-5.57	1.39	1.46
1	B	474	PHE	N-CA	-5.56	1.38	1.45
1	A	355	ASN	CA-C	5.56	1.60	1.52
1	A	314	THR	N-CA	5.56	1.53	1.46
1	A	509	ALA	CA-CB	-5.54	1.44	1.53
1	B	241	VAL	C-O	5.53	1.31	1.24
1	B	60	LEU	N-CA	-5.51	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	SER	CA-C	5.51	1.60	1.52
1	A	381	ILE	CA-CB	5.51	1.60	1.54
1	B	448	ASP	CG-OD1	5.50	1.35	1.25
1	A	86	LEU	N-CA	5.50	1.53	1.46
1	A	160	ARG	N-CA	-5.50	1.39	1.46
1	B	170	GLN	CA-C	5.49	1.59	1.52
1	B	257	VAL	CA-CB	5.48	1.61	1.54
1	A	422	LEU	CA-C	5.48	1.60	1.53
1	A	109	MET	C-O	-5.47	1.17	1.24
1	A	54	TYR	CG-CD2	-5.47	1.27	1.39
1	B	242	LEU	C-O	5.47	1.30	1.23
1	A	50	THR	CA-CB	-5.47	1.44	1.53
1	A	517	LEU	C-O	-5.47	1.17	1.24
1	B	238	LYS	CA-C	5.47	1.59	1.52
1	B	452	MET	C-O	5.46	1.31	1.24
1	A	509	ALA	N-CA	-5.46	1.39	1.46
1	B	15	VAL	C-O	-5.46	1.18	1.23
1	A	130	PHE	N-CA	-5.46	1.39	1.46
1	B	231	LYS	N-CA	5.46	1.52	1.46
1	B	173	LYS	CA-C	5.43	1.59	1.52
1	B	177	SER	N-CA	5.43	1.53	1.46
1	B	79	SER	C-O	5.41	1.30	1.24
1	B	376	VAL	CA-C	5.41	1.58	1.52
1	B	199	ALA	CA-CB	5.40	1.61	1.52
1	A	297	PRO	C-O	-5.40	1.17	1.24
1	A	335	PHE	N-CA	-5.40	1.40	1.46
1	B	437	GLU	CB-CG	-5.40	1.36	1.52
1	A	292	TYR	CA-CB	-5.39	1.43	1.53
1	B	145	SER	CA-C	5.39	1.58	1.53
1	B	238	LYS	CD-CE	5.38	1.68	1.52
1	A	339	ALA	CA-C	5.37	1.60	1.52
1	A	438	ASP	CA-C	5.36	1.59	1.52
1	B	458	ARG	N-CA	-5.35	1.39	1.46
1	B	66	LEU	C-N	-5.35	1.28	1.33
1	B	203	ILE	CA-C	-5.35	1.46	1.53
1	B	424	LEU	CA-C	5.34	1.59	1.53
1	B	36	VAL	CA-CB	-5.34	1.47	1.54
1	B	108	SER	N-CA	5.32	1.52	1.46
1	B	175	LYS	CA-C	-5.32	1.46	1.52
1	B	226	ASP	CA-CB	5.32	1.61	1.53
1	B	231	LYS	CD-CE	5.31	1.68	1.52
1	A	411	SER	C-O	5.31	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	ARG	C-O	-5.30	1.18	1.24
1	A	321	LEU	CA-C	-5.30	1.45	1.52
1	B	136	MET	CG-SD	5.29	1.94	1.80
1	B	515	ARG	CG-CD	5.29	1.68	1.52
1	B	78	GLY	C-O	5.28	1.29	1.23
1	A	417	GLU	C-O	-5.28	1.17	1.24
1	A	466	PRO	CA-C	5.28	1.59	1.52
1	B	446	ILE	C-O	-5.28	1.18	1.24
1	A	458	ARG	CA-C	5.27	1.61	1.52
1	B	458	ARG	C-O	5.27	1.30	1.24
1	B	146	GLY	N-CA	-5.26	1.39	1.45
1	B	116	LYS	CE-NZ	5.26	1.65	1.49
1	A	36	VAL	CA-C	5.25	1.59	1.52
1	A	438	ASP	C-O	5.25	1.30	1.24
1	B	307	GLN	C-O	5.25	1.30	1.24
1	B	447	ILE	CA-C	5.25	1.59	1.52
1	B	161	SER	C-O	-5.24	1.17	1.24
1	B	84	SER	CB-OG	5.23	1.52	1.42
1	B	158	MET	CG-SD	-5.23	1.67	1.80
1	A	490	ALA	CA-C	5.22	1.58	1.52
1	B	166	TYR	CB-CG	5.22	1.63	1.51
1	B	447	ILE	CA-CB	-5.22	1.47	1.54
1	A	428	ASN	C-O	-5.22	1.17	1.23
1	A	261	MET	SD-CE	-5.21	1.66	1.79
1	B	79	SER	CA-CB	5.21	1.61	1.53
1	B	166	TYR	CA-CB	5.20	1.61	1.53
1	B	73	LEU	C-O	-5.20	1.17	1.24
1	B	507	ARG	CZ-NH2	5.19	1.40	1.33
1	A	168	LEU	CG-CD2	5.19	1.69	1.52
1	B	301	PHE	CA-C	-5.18	1.47	1.53
1	A	394	LYS	CA-C	5.17	1.59	1.52
1	B	526	LEU	CA-C	-5.17	1.46	1.52
1	A	334	GLN	CA-CB	5.15	1.61	1.53
1	B	33	GLU	CA-CB	-5.15	1.45	1.53
1	B	436	CYS	CA-CB	5.15	1.62	1.53
1	A	133	LEU	C-O	-5.12	1.18	1.24
1	B	83	ALA	C-O	5.12	1.30	1.24
1	A	321	LEU	C-O	-5.12	1.18	1.24
1	A	510	LEU	CG-CD1	5.12	1.69	1.52
1	A	105	TYR	N-CA	5.11	1.52	1.46
1	A	435	VAL	CA-C	5.11	1.58	1.52
1	A	69	MET	CG-SD	-5.11	1.68	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	ARG	CD-NE	5.10	1.53	1.46
1	B	316	ILE	C-O	5.10	1.29	1.23
1	B	287	LEU	C-O	-5.10	1.17	1.24
1	B	86	LEU	CA-C	-5.10	1.46	1.52
1	A	327	LYS	N-CA	-5.09	1.39	1.46
1	A	377	ILE	CA-C	5.09	1.59	1.52
1	B	405	MET	CA-C	5.09	1.59	1.53
1	A	241	VAL	N-CA	-5.09	1.39	1.46
1	B	182	LEU	C-O	-5.08	1.17	1.23
1	B	518	ILE	N-CA	-5.08	1.40	1.46
1	A	95	GLN	CG-CD	-5.08	1.39	1.52
1	A	459	VAL	N-CA	-5.08	1.40	1.46
1	B	439	SER	C-O	-5.08	1.17	1.24
1	A	331	VAL	CA-C	5.07	1.59	1.52
1	B	292	TYR	CA-CB	-5.07	1.46	1.53
1	A	151	ASN	CA-C	-5.07	1.44	1.52
1	A	71	ILE	CA-CB	-5.05	1.48	1.54
1	B	82	VAL	CA-C	-5.05	1.46	1.52
1	A	32	TYR	CA-C	5.04	1.59	1.52
1	A	448	ASP	CB-CG	-5.04	1.39	1.52
1	B	400	ILE	CA-CB	5.03	1.60	1.54
1	B	84	SER	CA-C	5.02	1.59	1.52
1	B	243	TRP	N-CA	-5.02	1.40	1.46
1	B	31	SER	CA-C	5.01	1.59	1.52
1	B	39	LYS	CE-NZ	5.01	1.64	1.49
1	B	51	VAL	CA-CB	-5.01	1.46	1.55
1	A	58	LEU	C-O	5.00	1.29	1.24
1	A	284	ALA	CA-CB	5.00	1.61	1.53

All (348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	LEU	CA-C-N	-16.70	100.15	123.20
1	B	526	LEU	C-N-CA	-16.70	100.15	123.20
1	B	318	GLY	N-CA-C	15.96	130.81	110.38
1	B	325	GLN	N-CA-C	-14.71	93.59	111.69
1	B	323	SER	N-CA-C	-13.03	90.69	110.10
1	A	441	LEU	N-CA-C	-12.47	97.84	113.55
1	B	372	SER	N-CA-C	-11.74	98.21	111.71
1	A	198	ARG	N-CA-C	-11.54	86.22	110.80
1	B	222	ARG	NE-CZ-NH2	-10.64	109.62	119.20
1	B	168	LEU	N-CA-C	-10.56	100.52	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	GLY	CA-C-N	10.49	141.58	121.54
1	A	318	GLY	C-N-CA	10.49	141.58	121.54
1	A	434	ASN	CA-C-N	-9.98	109.11	122.99
1	A	434	ASN	C-N-CA	-9.98	109.11	122.99
1	A	355	ASN	CA-C-N	9.59	134.11	120.79
1	A	355	ASN	C-N-CA	9.59	134.11	120.79
1	A	423	MET	CG-SD-CE	9.54	121.90	100.90
1	A	138	SER	CA-C-N	-9.50	109.87	119.56
1	A	138	SER	C-N-CA	-9.50	109.87	119.56
1	B	441	LEU	N-CA-C	-9.21	101.83	113.43
1	A	356	ASP	N-CA-CB	-9.11	95.97	109.82
1	A	124	ASN	N-CA-C	9.10	122.78	108.67
1	B	350	ASN	N-CA-C	9.06	122.38	108.42
1	B	144	VAL	N-CA-C	9.03	120.75	108.11
1	B	473	LYS	N-CA-C	8.95	129.87	110.80
1	B	210	ASN	N-CA-C	8.90	123.45	110.28
1	A	482	THR	N-CA-C	-8.88	102.44	113.18
1	B	42	SER	N-CA-C	-8.82	99.87	113.02
1	A	143	VAL	N-CA-C	-8.78	94.77	107.77
1	B	251	VAL	N-CA-C	-8.77	95.61	109.20
1	A	318	GLY	O-C-N	8.73	130.41	122.90
1	B	492	LEU	N-CA-C	-8.73	99.00	110.43
1	A	187	TYR	CA-C-N	8.63	128.21	119.24
1	A	187	TYR	C-N-CA	8.63	128.21	119.24
1	B	471	ALA	N-CA-C	-8.62	92.44	110.80
1	B	450	LEU	N-CA-C	-8.62	101.09	111.69
1	B	470	ASP	N-CA-C	8.60	129.12	110.80
1	A	430	ILE	CA-C-N	-8.59	108.81	122.73
1	A	430	ILE	C-N-CA	-8.59	108.81	122.73
1	B	502	GLY	N-CA-C	-8.49	93.05	113.18
1	A	209	GLY	N-CA-C	-8.42	93.22	113.18
1	B	297	PRO	N-CA-C	8.42	125.02	113.65
1	B	386	ILE	N-CA-C	-8.34	102.29	110.72
1	B	14	VAL	N-CA-C	8.33	119.88	107.80
1	A	203	ILE	N-CA-C	-8.29	103.72	113.42
1	B	500	VAL	N-CA-CB	8.20	119.47	110.53
1	B	498	HIS	N-CA-C	8.15	119.91	109.65
1	A	386	ILE	N-CA-C	-8.09	102.18	111.00
1	B	222	ARG	NE-CZ-NH1	8.06	129.56	121.50
1	B	122	GLU	N-CA-C	-8.05	104.33	114.56
1	B	70	LEU	N-CA-C	8.04	121.75	108.96
1	B	526	LEU	O-C-N	-8.03	113.09	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ASN	N-CA-C	8.00	127.83	110.80
1	A	286	ILE	N-CA-C	-7.94	103.07	110.53
1	B	318	GLY	CA-C-N	7.94	136.70	121.54
1	B	318	GLY	C-N-CA	7.94	136.70	121.54
1	A	96	THR	N-CA-CB	-7.87	99.13	111.56
1	B	321	LEU	CB-CG-CD2	-7.81	87.26	110.70
1	B	158	MET	N-CA-CB	7.79	121.70	110.16
1	B	459	VAL	CB-CA-C	-7.78	98.97	110.33
1	B	208	LYS	N-CA-C	-7.75	94.29	110.80
1	A	350	ASN	N-CA-C	7.74	121.99	108.75
1	A	343	PRO	N-CA-C	-7.70	99.17	111.03
1	B	48	THR	CB-CA-C	-7.58	102.60	110.33
1	A	96	THR	OG1-CB-CG2	7.58	124.45	109.30
1	B	282	ALA	N-CA-C	-7.55	102.98	111.14
1	B	60	LEU	CA-C-N	-7.55	112.38	122.42
1	B	60	LEU	C-N-CA	-7.55	112.38	122.42
1	A	344	VAL	N-CA-C	-7.50	104.64	113.42
1	B	32	TYR	N-CA-C	7.49	121.11	108.23
1	A	171	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	A	429	ARG	CA-C-N	-7.40	112.84	123.06
1	A	429	ARG	C-N-CA	-7.40	112.84	123.06
1	A	144	VAL	N-CA-C	7.33	118.37	108.11
1	B	404	TYR	CA-C-N	7.33	133.31	123.20
1	B	404	TYR	C-N-CA	7.33	133.31	123.20
1	B	203	ILE	N-CA-C	-7.33	102.62	113.39
1	B	40	THR	N-CA-C	7.32	118.95	110.97
1	A	494	ARG	CA-C-N	7.25	128.91	119.84
1	A	494	ARG	C-N-CA	7.25	128.91	119.84
1	A	164	LEU	N-CA-C	7.24	121.23	110.52
1	B	12	VAL	N-CA-C	7.23	118.23	108.11
1	A	323	SER	N-CA-C	7.14	126.01	110.80
1	B	490	ALA	CA-C-N	7.14	128.76	119.84
1	B	490	ALA	C-N-CA	7.14	128.76	119.84
1	A	356	ASP	N-CA-C	-7.13	102.32	111.02
1	B	315	PHE	N-CA-C	7.06	119.67	110.43
1	A	138	SER	CA-CB-OG	-6.92	97.27	111.10
1	A	411	SER	CA-C-N	-6.85	112.67	122.94
1	A	411	SER	C-N-CA	-6.85	112.67	122.94
1	B	412	LYS	CA-C-N	-6.85	114.70	123.19
1	B	412	LYS	C-N-CA	-6.85	114.70	123.19
1	B	158	MET	CA-CB-CG	6.84	127.79	114.10
1	B	164	LEU	N-CA-C	6.78	121.09	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	439	SER	CA-CB-OG	-6.76	97.58	111.10
1	B	23	ASP	CA-C-N	6.74	134.41	121.54
1	B	23	ASP	C-N-CA	6.74	134.41	121.54
1	A	190	PHE	N-CA-C	6.74	121.50	113.28
1	A	130	PHE	CA-C-N	-6.73	111.89	122.73
1	A	130	PHE	C-N-CA	-6.73	111.89	122.73
1	A	474	PHE	N-CA-C	6.73	120.39	110.30
1	B	449	LEU	N-CA-C	6.72	119.61	111.82
1	B	134	LEU	CA-C-N	-6.72	112.74	119.93
1	B	134	LEU	C-N-CA	-6.72	112.74	119.93
1	B	278	SER	CA-CB-OG	-6.68	97.73	111.10
1	A	498	HIS	CA-C-N	-6.68	113.10	119.85
1	A	498	HIS	C-N-CA	-6.68	113.10	119.85
1	A	76	ASN	N-CA-C	6.67	118.63	111.36
1	B	79	SER	CA-C-N	-6.66	109.48	121.14
1	B	79	SER	C-N-CA	-6.66	109.48	121.14
1	B	137	VAL	CB-CA-C	-6.66	101.41	111.33
1	B	195	GLN	N-CA-C	-6.64	104.75	112.92
1	B	507	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	B	19	CYS	N-CA-C	6.61	119.18	108.41
1	B	437	GLU	CA-C-N	-6.58	108.74	121.58
1	B	437	GLU	C-N-CA	-6.58	108.74	121.58
1	A	394	LYS	N-CA-C	6.58	120.64	111.56
1	B	138	SER	CA-C-N	-6.58	112.92	119.56
1	B	138	SER	C-N-CA	-6.58	112.92	119.56
1	A	38	THR	N-CA-C	-6.55	98.30	109.24
1	A	416	ASP	CA-C-N	-6.53	113.79	122.99
1	A	416	ASP	C-N-CA	-6.53	113.79	122.99
1	B	199	ALA	CA-C-N	-6.53	112.30	122.67
1	B	199	ALA	C-N-CA	-6.53	112.30	122.67
1	A	386	ILE	CB-CA-C	-6.52	103.51	112.24
1	B	254	SER	CA-C-N	6.51	127.53	119.98
1	B	254	SER	C-N-CA	6.51	127.53	119.98
1	B	161	SER	N-CA-C	-6.50	105.50	113.50
1	A	402	ILE	CB-CA-C	-6.50	103.87	111.09
1	A	449	LEU	N-CA-C	6.49	119.18	111.33
1	A	324	GLY	N-CA-C	-6.48	97.81	113.18
1	B	40	THR	CB-CA-C	-6.47	101.00	110.96
1	B	381	ILE	N-CA-C	-6.44	104.06	110.30
1	A	451	VAL	CB-CA-C	-6.43	102.20	112.16
1	A	342	LYS	CA-C-N	6.42	126.77	119.83
1	A	342	LYS	C-N-CA	6.42	126.77	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	485	SER	N-CA-C	-6.42	105.60	113.50
1	B	24	ASN	N-CA-C	-6.41	97.16	110.80
1	A	304	GLY	CA-C-O	6.38	127.32	120.75
1	A	172	LEU	CA-C-O	6.37	126.41	119.15
1	A	396	VAL	N-CA-C	-6.37	96.55	107.24
1	B	158	MET	N-CA-C	-6.36	104.42	111.36
1	A	365	GLN	N-CA-C	-6.35	105.69	113.50
1	B	336	LEU	N-CA-C	-6.32	103.69	111.40
1	A	236	LEU	CA-CB-CG	6.29	138.32	116.30
1	A	54	TYR	CA-C-N	-6.26	114.94	123.14
1	A	54	TYR	C-N-CA	-6.26	114.94	123.14
1	A	342	LYS	N-CA-C	6.26	121.96	109.01
1	B	526	LEU	N-CA-C	-6.24	101.04	110.28
1	B	413	VAL	N-CA-C	-6.22	99.46	108.17
1	A	159	GLN	O-C-N	6.21	128.49	122.03
1	B	158	MET	CG-SD-CE	-6.20	87.26	100.90
1	B	232	GLU	N-CA-C	6.19	118.54	111.11
1	B	527	ARG	N-CA-C	-6.17	99.84	108.54
1	B	377	ILE	N-CA-C	-6.17	104.50	110.42
1	A	71	ILE	N-CA-C	-6.16	98.80	108.23
1	B	412	LYS	N-CA-C	-6.16	98.34	108.76
1	B	174	ALA	CA-C-N	-6.16	111.54	120.29
1	B	174	ALA	C-N-CA	-6.16	111.54	120.29
1	B	11	SER	CA-C-N	-6.15	115.08	123.14
1	B	11	SER	C-N-CA	-6.15	115.08	123.14
1	B	48	THR	CA-C-N	-6.14	113.35	119.92
1	B	48	THR	C-N-CA	-6.14	113.35	119.92
1	B	87	ALA	CA-C-N	-6.12	112.12	120.44
1	B	87	ALA	C-N-CA	-6.12	112.12	120.44
1	B	506	GLN	N-CA-C	-6.07	104.77	111.82
1	A	398	HIS	N-CA-C	6.07	118.52	108.99
1	A	246	ASN	CB-CA-C	-6.02	100.51	109.90
1	B	315	PHE	CB-CA-C	-6.02	97.20	109.65
1	A	311	HIS	N-CA-C	6.01	118.79	111.82
1	B	286	ILE	N-CA-C	-5.96	104.52	110.30
1	B	500	VAL	CB-CA-C	-5.95	103.41	111.15
1	B	323	SER	N-CA-CB	-5.94	100.60	109.69
1	A	398	HIS	CA-C-N	-5.94	112.58	122.21
1	A	398	HIS	C-N-CA	-5.94	112.58	122.21
1	A	158	MET	CG-SD-CE	-5.92	87.88	100.90
1	A	454	GLU	N-CA-C	-5.92	104.75	111.14
1	A	19	CYS	N-CA-C	5.90	118.03	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	VAL	N-CA-C	-5.90	99.24	107.80
1	A	478	TYR	N-CA-C	-5.89	102.32	109.57
1	B	197	GLU	N-CA-C	5.87	123.31	110.80
1	A	310	GLU	N-CA-C	-5.87	104.80	111.14
1	A	412	LYS	N-CA-C	-5.87	99.84	109.40
1	B	320	ASP	N-CA-C	5.87	123.29	110.80
1	B	362	ALA	CA-C-N	5.85	127.16	119.84
1	B	362	ALA	C-N-CA	5.85	127.16	119.84
1	A	151	ASN	N-CA-C	5.85	120.15	113.19
1	A	413	VAL	CA-C-N	-5.85	114.16	122.94
1	A	413	VAL	C-N-CA	-5.85	114.16	122.94
1	B	378	ASP	N-CA-C	5.85	118.44	111.71
1	B	411	SER	CA-C-O	5.84	127.62	121.19
1	A	515	ARG	CG-CD-NE	-5.83	99.16	112.00
1	B	222	ARG	CG-CD-NE	-5.82	99.19	112.00
1	B	365	GLN	N-CA-C	-5.80	104.55	111.69
1	A	244	THR	N-CA-CB	-5.80	103.53	111.65
1	B	163	VAL	N-CA-C	5.79	117.72	111.58
1	B	296	SER	CB-CA-C	-5.78	100.44	109.22
1	A	254	SER	CA-C-N	5.77	127.05	119.84
1	A	254	SER	C-N-CA	5.77	127.05	119.84
1	A	438	ASP	N-CA-C	5.77	118.03	111.11
1	B	136	MET	CG-SD-CE	-5.74	88.26	100.90
1	A	199	ALA	CA-C-N	-5.72	113.50	122.49
1	A	199	ALA	C-N-CA	-5.72	113.50	122.49
1	A	482	THR	CA-C-N	-5.72	112.05	120.28
1	A	482	THR	C-N-CA	-5.72	112.05	120.28
1	A	519	GLY	N-CA-C	5.70	123.67	114.90
1	A	356	ASP	CB-CA-C	5.67	119.94	110.92
1	B	135	PRO	N-CA-C	5.66	120.49	111.26
1	B	172	LEU	CB-CA-C	-5.65	100.62	110.17
1	B	190	PHE	N-CA-C	-5.65	107.39	114.56
1	A	70	LEU	N-CA-C	5.64	117.93	108.96
1	A	265	LEU	CA-C-N	-5.64	111.70	122.53
1	A	265	LEU	C-N-CA	-5.64	111.70	122.53
1	B	94	PHE	CA-C-O	5.64	127.09	120.89
1	A	176	MET	N-CA-C	5.63	117.42	111.28
1	A	186	TYR	CA-C-O	-5.62	114.50	120.40
1	B	261	MET	CG-SD-CE	5.61	113.25	100.90
1	B	356	ASP	N-CA-CB	-5.61	101.00	110.49
1	B	65	LYS	CA-C-N	-5.61	115.09	122.99
1	B	65	LYS	C-N-CA	-5.61	115.09	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	ASP	N-CA-C	-5.61	106.44	113.28
1	A	314	THR	N-CA-C	5.60	118.23	108.76
1	A	15	VAL	CB-CA-C	-5.60	102.10	111.29
1	A	60	LEU	N-CA-C	5.59	119.97	113.20
1	B	355	ASN	CA-C-N	5.59	132.21	121.54
1	B	355	ASN	C-N-CA	5.59	132.21	121.54
1	A	527	ARG	N-CA-C	5.59	118.90	111.30
1	B	219	HIS	N-CA-C	-5.58	105.27	111.36
1	B	437	GLU	N-CA-C	-5.58	100.72	109.25
1	B	111	GLN	CB-CG-CD	-5.57	103.13	112.60
1	B	182	LEU	CA-C-N	-5.55	114.87	120.31
1	B	182	LEU	C-N-CA	-5.55	114.87	120.31
1	A	158	MET	N-CA-C	-5.55	105.23	111.28
1	B	151	ASN	N-CA-C	5.55	119.91	113.20
1	B	321	LEU	CB-CG-CD1	5.55	127.34	110.70
1	B	289	GLY	CA-C-N	-5.54	117.26	123.02
1	B	289	GLY	C-N-CA	-5.54	117.26	123.02
1	B	413	VAL	CA-C-N	-5.53	114.64	122.94
1	B	413	VAL	C-N-CA	-5.53	114.64	122.94
1	B	158	MET	CB-CA-C	-5.53	101.45	110.85
1	A	171	ARG	NE-CZ-NH1	-5.51	115.98	121.50
1	B	354	ASN	N-CA-C	5.51	118.89	110.36
1	B	237	ASP	N-CA-C	-5.50	106.93	113.97
1	B	428	ASN	CA-C-N	-5.50	115.24	123.00
1	B	428	ASN	C-N-CA	-5.50	115.24	123.00
1	B	432	ILE	CB-CA-C	-5.50	103.54	111.19
1	B	157	ALA	N-CA-C	-5.49	105.45	111.82
1	B	245	ALA	N-CA-C	-5.49	101.32	109.94
1	B	213	THR	N-CA-CB	-5.49	103.05	110.95
1	B	419	TYR	N-CA-C	-5.49	99.47	108.41
1	A	229	ASN	CA-C-O	5.48	126.76	120.90
1	A	445	LEU	CB-CA-C	-5.45	102.32	110.88
1	B	162	GLN	CA-C-N	-5.45	112.52	121.34
1	B	162	GLN	C-N-CA	-5.45	112.52	121.34
1	B	272	HIS	N-CA-C	5.45	117.92	110.24
1	B	327	LYS	CA-C-N	5.44	128.33	120.38
1	B	327	LYS	C-N-CA	5.44	128.33	120.38
1	B	430	ILE	CG1-CB-CG2	-5.43	94.40	110.70
1	A	50	THR	N-CA-C	-5.43	101.05	109.14
1	B	504	ASN	CA-C-N	5.42	127.54	120.28
1	B	504	ASN	C-N-CA	5.42	127.54	120.28
1	B	83	ALA	CA-C-N	-5.41	112.08	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ALA	C-N-CA	-5.41	112.08	120.31
1	B	239	VAL	N-CA-C	5.41	116.27	108.48
1	A	87	ALA	CA-C-N	-5.41	112.61	120.29
1	A	87	ALA	C-N-CA	-5.41	112.61	120.29
1	B	79	SER	CA-C-O	5.40	126.14	120.42
1	B	184	SER	CA-C-N	-5.39	116.50	123.19
1	B	184	SER	C-N-CA	-5.39	116.50	123.19
1	A	312	GLU	N-CA-C	-5.38	106.56	113.23
1	B	92	VAL	N-CA-C	5.37	120.52	109.34
1	A	358	TYR	N-CA-C	-5.36	105.52	111.36
1	A	207	GLU	N-CA-C	5.35	119.07	112.54
1	A	158	MET	N-CA-CB	5.35	117.98	110.12
1	A	434	ASN	N-CA-CB	-5.35	102.05	110.77
1	A	511	GLU	CA-C-N	5.34	127.44	120.28
1	A	511	GLU	C-N-CA	5.34	127.44	120.28
1	A	32	TYR	N-CA-C	5.34	117.39	107.99
1	A	190	PHE	CA-C-N	-5.32	115.26	122.92
1	A	190	PHE	C-N-CA	-5.32	115.26	122.92
1	B	157	ALA	CA-C-O	-5.31	113.86	119.97
1	B	383	SER	N-CA-C	5.30	119.50	113.19
1	A	362	ALA	N-CA-C	-5.30	102.32	110.32
1	B	94	PHE	N-CA-C	5.30	117.13	108.76
1	B	81	LEU	CA-CB-CG	-5.30	97.76	116.30
1	B	395	LYS	N-CA-C	5.29	118.35	110.14
1	B	107	GLY	CA-C-N	-5.29	115.42	122.72
1	B	107	GLY	C-N-CA	-5.29	115.42	122.72
1	A	488	LEU	CA-C-N	5.28	127.62	120.38
1	A	488	LEU	C-N-CA	5.28	127.62	120.38
1	A	60	LEU	CD1-CG-CD2	-5.28	99.19	110.80
1	B	120	ASP	CA-C-N	-5.28	114.06	122.66
1	B	120	ASP	C-N-CA	-5.28	114.06	122.66
1	A	452	MET	CB-CG-SD	5.27	128.51	112.70
1	A	428	ASN	CA-C-N	-5.26	115.58	123.00
1	A	428	ASN	C-N-CA	-5.26	115.58	123.00
1	B	187	TYR	N-CA-C	-5.25	97.33	108.66
1	A	315	PHE	N-CA-C	5.24	117.76	109.96
1	B	432	ILE	CA-C-N	-5.21	115.80	123.00
1	B	432	ILE	C-N-CA	-5.21	115.80	123.00
1	B	222	ARG	CD-NE-CZ	5.21	131.70	124.40
1	A	97	LYS	CA-C-N	-5.20	113.61	122.56
1	A	97	LYS	C-N-CA	-5.20	113.61	122.56
1	A	47	VAL	N-CA-C	5.20	115.55	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	SER	N-CA-C	5.20	116.37	109.93
1	A	489	LYS	N-CA-C	5.19	117.61	111.33
1	B	401	VAL	CA-C-N	5.18	130.34	122.98
1	B	401	VAL	C-N-CA	5.18	130.34	122.98
1	A	163	VAL	N-CA-C	5.17	115.83	110.82
1	B	71	ILE	N-CA-C	-5.15	100.92	108.54
1	A	290	VAL	CA-C-N	5.14	125.38	119.83
1	A	290	VAL	C-N-CA	5.14	125.38	119.83
1	B	523	GLN	CA-C-N	-5.14	114.22	122.08
1	B	523	GLN	C-N-CA	-5.14	114.22	122.08
1	A	112	CYS	N-CA-C	5.13	121.25	114.12
1	A	419	TYR	N-CA-C	-5.12	100.07	108.41
1	A	155	TYR	N-CA-C	-5.11	105.79	111.36
1	B	203	ILE	CA-C-N	-5.11	114.50	122.16
1	B	203	ILE	C-N-CA	-5.11	114.50	122.16
1	A	355	ASN	CA-C-O	5.11	125.87	120.10
1	B	386	ILE	CB-CA-C	-5.10	105.18	112.22
1	B	99	GLY	CA-C-N	-5.09	113.83	120.91
1	B	99	GLY	C-N-CA	-5.09	113.83	120.91
1	A	476	ASN	N-CA-C	5.09	118.05	110.52
1	B	25	GLU	N-CA-C	-5.09	101.34	109.23
1	A	521	PRO	CA-C-N	5.09	128.30	120.82
1	A	521	PRO	C-N-CA	5.09	128.30	120.82
1	B	466	PRO	N-CA-C	5.09	122.02	114.80
1	B	86	LEU	CA-C-N	-5.08	113.08	120.29
1	B	86	LEU	C-N-CA	-5.08	113.08	120.29
1	A	43	GLY	CA-C-O	5.07	125.44	119.46
1	B	214	ARG	N-CA-C	-5.06	102.99	110.48
1	B	376	VAL	CA-C-N	5.06	126.93	120.56
1	B	376	VAL	C-N-CA	5.06	126.93	120.56
1	B	130	PHE	CA-C-N	-5.05	114.58	122.65
1	B	130	PHE	C-N-CA	-5.05	114.58	122.65
1	B	398	HIS	CA-C-N	-5.04	114.05	122.21
1	B	398	HIS	C-N-CA	-5.04	114.05	122.21
1	B	109	MET	N-CA-C	-5.03	105.70	111.14
1	A	191	ILE	CA-C-O	-5.03	116.54	121.67
1	A	158	MET	CA-CB-CG	5.03	124.16	114.10
1	A	260	THR	N-CA-C	5.03	117.02	109.23
1	A	195	GLN	N-CA-C	-5.01	107.17	113.28
1	B	74	GLY	N-CA-C	5.01	125.05	113.18
1	A	446	ILE	CA-C-N	5.01	126.87	120.56
1	A	446	ILE	C-N-CA	5.01	126.87	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	GLY	CA-C-N	-5.00	118.02	123.08
1	A	256	GLY	C-N-CA	-5.00	118.02	123.08

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	A	21	TYR	Sidechain
1	A	388	TYR	Sidechain
1	A	461	TYR	Sidechain
1	A	478	TYR	Sidechain
1	B	105	TYR	Sidechain
1	B	186	TYR	Sidechain
1	B	358	TYR	Sidechain
1	B	388	TYR	Sidechain
1	B	418	TYR	Sidechain
1	B	486	TYR	Sidechain
1	B	56	PHE	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4138	0	4147	450	1
1	B	4130	0	4136	529	0
2	A	1	0	0	1	0
2	B	1	0	0	1	0
3	A	15	0	12	10	0
3	B	15	0	12	17	0
4	A	44	0	22	9	0
4	B	44	0	24	2	0
5	A	303	0	0	57	0
5	B	315	0	0	64	0
All	All	9006	0	8353	941	1

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 56.

All (941) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:CG	1:B:69:MET:CB	1.82	1.54
1:A:136:MET:CG	1:A:136:MET:SD	2.02	1.46
1:B:69:MET:SD	1:B:69:MET:CE	2.08	1.40
1:A:415:MET:SD	1:A:415:MET:CE	2.09	1.40
1:A:69:MET:SD	1:A:69:MET:CE	2.13	1.36
1:A:449:LEU:HD22	5:A:791:HOH:O	1.16	1.32
1:B:158:MET:SD	1:B:158:MET:CE	2.17	1.31
1:B:11:SER:HB3	5:B:760:HOH:O	1.40	1.19
1:B:321:LEU:HD22	5:B:979:HOH:O	1.44	1.18
1:A:318:GLY:HA2	1:A:488:LEU:CD1	1.74	1.16
1:B:76:ASN:O	1:B:80:THR:HG23	1.47	1.14
1:B:347:ALA:HB2	5:B:989:HOH:O	1.49	1.13
1:B:417:GLU:OE2	1:B:431:SER:HB3	1.49	1.11
1:A:77:ASN:OD1	5:A:784:HOH:O	1.69	1.10
1:A:363:PRO:HG2	1:A:364:LYS:HE2	1.34	1.09
1:B:369:LYS:HD2	3:B:640:DG6:HC3	1.35	1.06
1:B:323:SER:HB2	5:B:995:HOH:O	1.53	1.06
1:B:373:LYS:HD2	1:B:374:SER:N	1.70	1.06
1:A:327:LYS:HE3	5:A:940:HOH:O	1.56	1.06
1:B:469:GLU:HG2	1:B:470:ASP:H	1.15	1.05
1:B:373:LYS:HD2	1:B:374:SER:H	1.20	1.04
4:A:650:NAI:N7N	4:A:650:NAI:O1N	1.89	1.04
1:B:76:ASN:O	1:B:80:THR:CG2	2.05	1.04
1:B:23:ASP:OD1	1:B:24:ASN:N	1.91	1.03
1:B:315:PHE:CD1	1:B:481:LEU:HD11	1.94	1.03
1:B:95:GLN:HE21	1:B:95:GLN:HA	1.26	1.00
1:A:318:GLY:HA2	1:A:488:LEU:HD13	1.37	1.00
1:A:363:PRO:CG	1:A:364:LYS:HE2	1.92	0.99
1:A:412:LYS:HE2	3:A:630:DG6:O4	1.61	0.98
1:B:469:GLU:HG2	1:B:470:ASP:N	1.76	0.98
1:B:261:MET:HE2	1:B:308:LEU:HA	1.43	0.98
4:B:660:NAI:N7N	4:B:660:NAI:O1N	1.96	0.98
1:B:437:GLU:HG3	5:B:746:HOH:O	1.63	0.97
1:B:473:LYS:HE2	1:B:474:PHE:N	1.78	0.97
1:A:318:GLY:CA	1:A:488:LEU:HD13	1.94	0.97
1:A:122:GLU:O	1:A:124:ASN:N	1.96	0.97
1:B:356:ASP:HB3	3:B:640:DG6:O1P	1.64	0.97
1:A:61:LYS:O	1:A:61:LYS:HG3	1.61	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ARG:NH1	1:B:521:PRO:O	1.98	0.96
1:B:365:GLN:HG3	5:B:990:HOH:O	1.66	0.96
1:A:151:ASN:H	1:A:200:ASN:HD21	1.14	0.95
1:B:23:ASP:CG	1:B:24:ASN:H	1.75	0.94
1:B:238:LYS:HE3	5:B:978:HOH:O	1.67	0.94
1:A:428:ASN:HD22	1:B:436:CYS:HB3	1.30	0.94
1:B:168:LEU:HD13	1:B:168:LEU:C	1.93	0.94
1:A:356:ASP:HB3	3:A:630:DG6:O3P	1.67	0.93
1:B:289:GLY:HA2	1:B:314:THR:HG21	1.51	0.93
5:A:800:HOH:O	1:B:168:LEU:HG	1.67	0.93
1:B:473:LYS:HE2	1:B:474:PHE:H	1.33	0.93
1:B:489:LYS:HZ3	3:B:640:DG6:HC12	1.34	0.92
1:A:300:THR:HG21	5:A:704:HOH:O	1.67	0.92
1:A:435:VAL:HG23	5:A:956:HOH:O	1.66	0.92
1:B:163:VAL:HG22	1:B:164:LEU:HD22	1.52	0.92
1:B:330:SER:OG	1:B:376:VAL:HG21	1.70	0.92
1:A:297:PRO:HD3	1:A:320:ASP:OD2	1.70	0.91
1:B:342:LYS:HE2	5:B:880:HOH:O	1.69	0.91
1:A:64:GLU:O	1:A:65:LYS:HD3	1.70	0.91
1:B:11:SER:CB	5:B:760:HOH:O	2.08	0.91
1:B:286:ILE:HG21	1:B:308:LEU:HD12	1.48	0.91
1:A:58:LEU:HD13	1:A:60:LEU:HD23	1.54	0.90
1:B:315:PHE:HD1	1:B:481:LEU:HD11	1.34	0.90
1:B:369:LYS:HD2	3:B:640:DG6:C3	2.01	0.90
1:A:225:ARG:HE	1:A:229:ASN:HD21	1.16	0.90
1:A:449:LEU:O	1:A:453:THR:HG23	1.71	0.90
1:B:61:LYS:NZ	5:B:937:HOH:O	2.02	0.90
1:B:369:LYS:HZ1	3:B:640:DG6:HC62	1.36	0.90
1:A:40:THR:O	1:A:43:GLY:N	2.03	0.89
1:B:286:ILE:HG21	1:B:308:LEU:CD1	2.01	0.89
1:A:449:LEU:O	1:A:453:THR:CG2	2.22	0.88
1:B:116:LYS:HE3	1:B:125:ASP:OD1	1.72	0.88
1:A:363:PRO:CD	1:A:364:LYS:HE2	2.03	0.88
1:A:260:THR:HG23	1:A:263:ASN:H	1.39	0.87
1:B:95:GLN:HE21	1:B:95:GLN:CA	1.86	0.87
1:B:115:LEU:HD22	1:B:511:GLU:HG3	1.57	0.86
1:A:423:MET:HE2	1:B:444:PRO:HD3	1.58	0.86
1:A:372:SER:HB2	1:A:489:LYS:HE3	1.56	0.85
1:A:449:LEU:CD2	5:A:791:HOH:O	1.91	0.85
1:B:237:ASP:HB2	5:B:774:HOH:O	1.76	0.85
1:A:406:LYS:HD2	1:A:406:LYS:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:LYS:NZ	3:B:640:DG6:HC62	1.91	0.85
1:B:286:ILE:CG2	1:B:308:LEU:CD1	2.54	0.85
1:B:427:HIS:HE1	5:B:906:HOH:O	1.59	0.85
1:B:297:PRO:HD3	1:B:320:ASP:CG	2.03	0.84
1:B:365:GLN:CD	5:B:990:HOH:O	2.21	0.83
1:B:297:PRO:HB2	1:B:368:SER:HB3	1.60	0.83
1:B:261:MET:HE1	1:B:311:HIS:HB2	1.60	0.83
1:B:494:ARG:HG3	5:B:842:HOH:O	1.76	0.83
1:A:294:ASN:C	1:A:294:ASN:HD22	1.84	0.83
1:B:198:ARG:HG3	5:B:966:HOH:O	1.79	0.83
1:A:327:LYS:HG2	1:A:503:LEU:HD13	1.61	0.83
5:A:800:HOH:O	1:B:168:LEU:CG	2.26	0.82
1:B:365:GLN:CG	5:B:990:HOH:O	2.23	0.82
1:A:96:THR:HG23	1:A:98:GLU:H	1.43	0.82
1:A:356:ASP:OD2	1:A:356:ASP:N	2.10	0.82
1:B:297:PRO:HD3	1:B:320:ASP:OD1	1.78	0.82
1:A:348:SER:OG	1:A:416:ASP:OD2	1.98	0.82
1:A:89:LYS:NZ	5:A:827:HOH:O	2.11	0.81
1:A:40:THR:HB	1:A:44:ARG:HB3	1.62	0.81
1:A:360:LEU:HD11	3:A:630:DG6:HC61	1.61	0.81
1:B:131:ASN:HB2	1:B:136:MET:HE3	1.60	0.81
1:B:116:LYS:HE3	1:B:125:ASP:CG	2.06	0.81
1:B:464:VAL:HG12	1:B:465:ASP:N	1.95	0.81
1:A:364:LYS:HE3	1:A:364:LYS:H	1.46	0.81
1:B:95:GLN:HA	1:B:95:GLN:NE2	1.89	0.81
1:A:234:ASN:OD1	5:A:714:HOH:O	2.00	0.80
1:B:191:ILE:N	1:B:191:ILE:HD13	1.96	0.80
1:A:136:MET:CG	1:A:136:MET:CE	2.58	0.80
1:B:315:PHE:HD1	1:B:481:LEU:CD1	1.94	0.80
1:B:61:LYS:HD2	1:B:61:LYS:O	1.81	0.80
1:A:412:LYS:CE	3:A:630:DG6:O4	2.30	0.80
1:B:23:ASP:OD1	1:B:24:ASN:HB2	1.82	0.80
1:A:257:VAL:HG22	1:A:258:ASN:ND2	1.96	0.79
1:A:533:LEU:HB2	1:B:494:ARG:HH12	1.47	0.79
1:B:251:VAL:H	1:B:299:ASN:HD21	1.29	0.79
1:A:445:LEU:HB2	5:A:754:HOH:O	1.82	0.79
1:B:303:PRO:HG2	1:B:304:GLY:H	1.45	0.79
1:A:154:LEU:HD22	1:A:179:VAL:HG11	1.64	0.79
1:A:318:GLY:CA	1:A:488:LEU:CD1	2.55	0.79
1:B:489:LYS:NZ	3:B:640:DG6:HC12	1.97	0.79
1:A:436:CYS:HB3	1:B:428:ASN:HD22	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLN:HE22	1:A:380:ILE:HG12	1.48	0.79
1:B:23:ASP:CG	1:B:24:ASN:N	2.36	0.79
1:B:115:LEU:CD2	1:B:511:GLU:HG3	2.13	0.79
1:B:464:VAL:CG1	1:B:465:ASP:N	2.45	0.79
1:B:154:LEU:HB3	1:B:176:MET:HE3	1.64	0.79
1:B:286:ILE:CG2	1:B:308:LEU:HD12	2.11	0.78
1:B:258:ASN:HD22	1:B:258:ASN:H	1.32	0.78
1:B:373:LYS:HZ1	1:B:376:VAL:HG12	1.49	0.78
1:B:206:ASP:O	1:B:208:LYS:N	2.17	0.78
1:A:258:ASN:HD22	1:A:258:ASN:H	1.29	0.77
1:B:456:CYS:HG	1:B:477:PHE:HE1	1.32	0.77
1:A:90:HIS:CE1	5:A:865:HOH:O	2.36	0.77
1:B:69:MET:CB	1:B:69:MET:SD	2.73	0.77
1:A:150:ASN:ND2	1:A:160:ARG:HH12	1.83	0.77
1:A:329:LYS:NZ	5:A:964:HOH:O	2.17	0.77
1:A:315:PHE:CD1	1:A:481:LEU:HD11	2.20	0.77
1:A:104:ASN:HD21	1:B:423:MET:HA	1.49	0.77
1:A:122:GLU:H	1:A:122:GLU:CD	1.92	0.76
1:A:294:ASN:C	1:A:294:ASN:ND2	2.36	0.76
1:B:191:ILE:HD13	1:B:191:ILE:H	1.49	0.76
1:A:231:LYS:HD3	5:A:873:HOH:O	1.86	0.76
1:B:454:GLU:O	1:B:457:THR:HG22	1.86	0.76
1:A:249:ARG:O	1:A:249:ARG:HG3	1.86	0.76
1:A:363:PRO:HD2	1:A:364:LYS:HE2	1.65	0.76
1:A:9:ILE:HD12	1:A:9:ILE:N	2.01	0.75
1:B:59:ASP:OD1	1:B:61:LYS:HE3	1.85	0.75
1:B:480:VAL:HG12	1:B:482:THR:HG22	1.66	0.75
1:A:293:ILE:HD11	1:A:453:THR:HG21	1.67	0.75
1:A:154:LEU:HD22	1:A:179:VAL:CG1	2.17	0.75
1:B:289:GLY:HA2	1:B:314:THR:CG2	2.17	0.75
1:A:318:GLY:HA2	1:A:488:LEU:CD2	2.17	0.74
1:A:437:GLU:HG3	5:A:685:HOH:O	1.88	0.74
1:B:315:PHE:CE1	1:B:481:LEU:HD11	2.21	0.74
1:B:261:MET:HE1	1:B:311:HIS:CB	2.16	0.74
1:A:24:ASN:OD1	5:A:724:HOH:O	2.06	0.74
1:B:480:VAL:CG2	1:B:492:LEU:HD12	2.18	0.74
1:B:159:GLN:O	5:B:691:HOH:O	2.06	0.74
1:B:315:PHE:CD1	1:B:481:LEU:CD1	2.70	0.74
1:B:347:ALA:HB1	1:B:349:TYR:CE2	2.23	0.74
1:B:480:VAL:HG21	1:B:492:LEU:HD12	1.68	0.73
1:B:254:SER:H	1:B:258:ASN:HD21	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:SER:OG	1:B:489:LYS:HE3	1.89	0.73
1:B:261:MET:CE	1:B:308:LEU:HA	2.15	0.73
1:B:323:SER:CB	5:B:995:HOH:O	2.20	0.73
1:B:109:MET:N	1:B:448:ASP:OD1	2.20	0.73
1:A:122:GLU:C	1:A:124:ASN:H	1.97	0.73
1:B:327:LYS:HG2	1:B:503:LEU:HD13	1.71	0.73
1:A:363:PRO:HG2	1:A:364:LYS:CE	2.15	0.72
1:B:256:GLY:N	1:B:259:ASP:OD1	2.20	0.72
1:B:264:LEU:HD21	1:B:305:LEU:HD13	1.71	0.72
1:A:516:LEU:C	1:A:516:LEU:HD23	2.15	0.72
1:A:344:VAL:HG23	5:A:728:HOH:O	1.88	0.72
1:A:493:THR:HG23	1:B:530:GLU:OE1	1.90	0.72
1:B:65:LYS:NZ	1:B:141:ASP:OD2	2.21	0.72
1:B:405:MET:O	1:B:408:VAL:HG22	1.89	0.72
1:A:261:MET:HE1	1:A:311:HIS:ND1	2.05	0.72
1:B:373:LYS:NZ	1:B:376:VAL:HG12	2.05	0.72
1:A:322:LYS:NZ	1:A:503:LEU:HD12	2.04	0.72
1:B:187:TYR:OH	1:B:219:HIS:HD2	1.73	0.72
1:B:299:ASN:HD22	1:B:299:ASN:H	1.37	0.72
1:B:158:MET:CE	1:B:158:MET:CG	2.67	0.72
1:B:62:LYS:O	5:B:772:HOH:O	2.08	0.71
1:B:297:PRO:HG3	1:B:369:LYS:HE2	1.73	0.71
1:A:192:ALA:HB3	1:A:359:ASN:HD22	1.55	0.71
1:B:302:VAL:HB	1:B:303:PRO:HD2	1.72	0.71
1:A:217:TRP:O	1:A:221:GLN:HG2	1.90	0.71
1:A:381:ILE:HD11	1:A:396:VAL:HG23	1.73	0.71
1:A:354:ASN:OD1	1:A:356:ASP:HB2	1.90	0.71
1:A:451:VAL:HG12	1:A:451:VAL:O	1.89	0.71
1:B:362:ALA:HB1	1:B:364:LYS:NZ	2.06	0.71
1:B:315:PHE:H	1:B:315:PHE:HD2	1.37	0.71
1:B:75:GLY:O	1:B:79:SER:HB3	1.91	0.71
1:B:367:ARG:O	1:B:370:GLU:HB2	1.91	0.71
1:A:503:LEU:HD22	1:B:335:PHE:HE2	1.54	0.70
1:A:207:GLU:OE1	1:A:207:GLU:HA	1.89	0.70
1:B:365:GLN:NE2	5:B:990:HOH:O	2.22	0.70
1:B:464:VAL:CG1	1:B:465:ASP:H	2.03	0.70
1:B:396:VAL:O	1:B:398:HIS:HD2	1.74	0.70
1:B:356:ASP:CB	3:B:640:DG6:O3P	2.40	0.70
1:B:12:VAL:O	5:B:911:HOH:O	2.09	0.70
1:B:303:PRO:CG	1:B:304:GLY:H	2.05	0.70
1:A:90:HIS:HE1	5:A:865:HOH:O	1.70	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:LYS:CE	5:A:940:HOH:O	2.26	0.70
1:A:255:PRO:HA	1:A:259:ASP:OD1	1.93	0.69
1:B:371:ILE:HD13	1:B:374:SER:HB3	1.75	0.69
1:B:527:ARG:H	1:B:531:ARG:HD2	1.57	0.69
1:A:203:ILE:HD12	1:A:222:ARG:HG3	1.74	0.69
1:A:341:ILE:O	1:A:343:PRO:HD2	1.92	0.69
1:B:273:GLU:HB3	5:B:876:HOH:O	1.91	0.69
1:A:372:SER:CB	1:A:489:LYS:HE3	2.23	0.69
1:B:456:CYS:SG	1:B:477:PHE:HE1	2.16	0.69
1:B:131:ASN:HA	1:B:136:MET:CE	2.22	0.69
1:B:356:ASP:HB3	3:B:640:DG6:P	2.32	0.69
1:A:294:ASN:HD22	1:A:295:GLY:N	1.90	0.69
1:A:377:ILE:O	1:A:381:ILE:HG13	1.93	0.69
1:B:168:LEU:HD13	1:B:168:LEU:O	1.91	0.69
1:B:373:LYS:O	1:B:374:SER:HB3	1.92	0.69
1:B:216:LYS:HA	1:B:219:HIS:CD2	2.28	0.69
1:B:362:ALA:HB3	1:B:365:GLN:OE1	1.91	0.69
1:A:294:ASN:ND2	1:A:296:SER:H	1.91	0.69
1:A:406:LYS:HD2	1:A:406:LYS:C	2.17	0.69
1:A:249:ARG:NH2	5:A:702:HOH:O	2.26	0.68
1:A:372:SER:CB	1:A:489:LYS:CE	2.71	0.68
1:B:325:GLN:NE2	1:B:350:ASN:OD1	2.27	0.68
1:A:331:VAL:O	5:A:907:HOH:O	2.12	0.68
1:A:297:PRO:HG3	1:A:369:LYS:HD2	1.75	0.68
1:B:469:GLU:CG	1:B:470:ASP:H	1.89	0.68
1:B:315:PHE:CE1	1:B:481:LEU:HD21	2.29	0.68
1:A:497:PHE:CE2	1:B:530:GLU:HB2	2.28	0.68
1:B:318:GLY:HA2	1:B:488:LEU:CD2	2.24	0.68
1:B:25:GLU:OE1	1:B:57:LYS:HD2	1.93	0.67
1:A:328:LEU:HD21	1:B:332:LEU:HD11	1.74	0.67
1:A:120:ASP:OD1	1:A:124:ASN:HB2	1.94	0.67
1:B:258:ASN:HD22	1:B:258:ASN:N	1.89	0.67
1:A:412:LYS:O	5:A:956:HOH:O	2.12	0.67
1:A:531:ARG:O	1:A:532:LEU:HD12	1.95	0.67
1:B:373:LYS:CD	1:B:374:SER:H	2.01	0.67
1:B:95:GLN:HB2	1:B:167:ASP:OD1	1.95	0.67
1:B:134:LEU:HD21	1:B:518:ILE:CG2	2.25	0.67
1:B:467:VAL:HG23	5:B:899:HOH:O	1.94	0.67
1:B:366:PHE:CE1	1:B:402:ILE:HG22	2.30	0.67
1:B:354:ASN:OD1	1:B:356:ASP:HB2	1.95	0.67
1:A:183:PRO:HB2	1:A:203:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:CG	1:B:69:MET:CE	2.74	0.66
1:B:249:ARG:HG3	1:B:249:ARG:O	1.95	0.66
1:B:248:GLU:OE2	1:B:278:SER:HB2	1.95	0.66
1:A:131:ASN:OD1	5:A:900:HOH:O	2.14	0.66
1:A:321:LEU:HD22	1:A:445:LEU:CD2	2.26	0.66
1:A:9:ILE:N	1:A:9:ILE:CD1	2.59	0.66
5:A:800:HOH:O	1:B:168:LEU:CD1	2.43	0.65
1:B:142:PHE:O	5:B:685:HOH:O	2.13	0.65
1:B:337:VAL:HG21	1:B:380:ILE:CG2	2.25	0.65
1:B:23:ASP:OD1	1:B:24:ASN:CB	2.44	0.65
1:B:32:TYR:O	5:B:845:HOH:O	2.14	0.65
1:B:356:ASP:HB2	3:B:640:DG6:O3P	1.96	0.65
1:B:297:PRO:HD3	1:B:320:ASP:CB	2.27	0.65
1:A:272:HIS:HD2	1:A:274:GLU:HB2	1.61	0.65
1:A:291:PRO:HG2	5:A:838:HOH:O	1.95	0.65
1:A:326:THR:HG21	1:A:489:LYS:HG3	1.79	0.65
1:A:375:SER:OG	5:A:965:HOH:O	2.14	0.65
1:A:225:ARG:NE	1:A:229:ASN:HD21	1.89	0.65
1:A:315:PHE:CZ	1:A:481:LEU:HD21	2.32	0.65
1:A:416:ASP:OD1	5:A:703:HOH:O	2.14	0.65
1:B:480:VAL:CG1	1:B:482:THR:HG22	2.26	0.65
1:A:325:GLN:NE2	3:A:630:DG6:O1	2.30	0.64
1:B:438:ASP:N	1:B:438:ASP:OD2	2.24	0.64
1:A:122:GLU:CD	1:A:122:GLU:N	2.55	0.64
1:A:166:TYR:OH	5:A:930:HOH:O	2.14	0.64
1:B:58:LEU:HD13	1:B:60:LEU:HD23	1.79	0.64
1:B:115:LEU:HD22	1:B:511:GLU:CG	2.27	0.64
1:B:480:VAL:HG12	1:B:480:VAL:O	1.97	0.64
1:A:364:LYS:HE3	1:A:364:LYS:N	2.13	0.64
1:B:361:SER:OG	5:B:921:HOH:O	2.15	0.64
1:A:120:ASP:OD1	1:A:122:GLU:O	2.15	0.64
1:A:330:SER:O	1:A:331:VAL:C	2.40	0.64
1:B:355:ASN:O	1:B:359:ASN:N	2.26	0.64
1:A:315:PHE:CE1	1:A:481:LEU:HD11	2.33	0.64
1:A:154:LEU:HB3	1:A:176:MET:HE2	1.79	0.64
1:A:372:SER:HB3	1:A:489:LYS:HE2	1.78	0.64
1:B:76:ASN:O	1:B:80:THR:HG22	1.96	0.64
1:B:131:ASN:HB2	1:B:136:MET:CE	2.26	0.64
1:B:364:LYS:HE3	1:B:364:LYS:H	1.63	0.64
1:A:261:MET:HE1	1:A:311:HIS:CG	2.33	0.64
1:A:389:ASN:OD1	1:A:391:LYS:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:CYS:C	1:A:400:ILE:HD12	2.23	0.63
1:B:153:ASP:OD2	1:B:155:TYR:HB3	1.96	0.63
1:A:87:ALA:HA	1:A:92:VAL:HG13	1.80	0.63
1:B:61:LYS:CG	5:B:958:HOH:O	2.46	0.63
1:A:503:LEU:HD22	1:B:335:PHE:CE2	2.32	0.63
1:B:295:GLY:HA2	5:B:728:HOH:O	1.98	0.63
1:A:209:GLY:O	1:A:210:ASN:HB2	1.98	0.63
1:A:364:LYS:CE	1:A:364:LYS:N	2.61	0.63
1:A:463:LYS:HB2	1:A:463:LYS:NZ	2.11	0.63
1:B:151:ASN:C	1:B:151:ASN:HD22	2.06	0.63
1:A:322:LYS:HG3	1:A:489:LYS:HA	1.80	0.63
1:B:286:ILE:CG2	1:B:308:LEU:HD13	2.28	0.63
1:B:417:GLU:OE2	1:B:431:SER:CB	2.39	0.62
1:B:261:MET:O	1:B:265:LEU:HD22	1.99	0.62
1:A:478:TYR:CE1	1:A:480:VAL:HB	2.33	0.62
1:B:297:PRO:CD	1:B:320:ASP:OD1	2.47	0.62
1:B:396:VAL:O	1:B:398:HIS:CD2	2.52	0.62
1:A:190:PHE:CE2	1:A:276:ALA:HB2	2.34	0.62
1:B:15:VAL:HG23	1:B:15:VAL:O	1.97	0.62
1:A:68:ILE:HD13	1:A:142:PHE:CD1	2.34	0.62
1:A:134:LEU:HB3	1:A:135:PRO:HD2	1.81	0.62
1:A:203:ILE:HD12	1:A:222:ARG:CG	2.30	0.62
1:A:225:ARG:CG	1:A:225:ARG:HH21	2.12	0.62
1:A:331:VAL:C	5:A:907:HOH:O	2.41	0.62
1:B:494:ARG:N	5:B:981:HOH:O	2.26	0.62
1:A:162:GLN:NE2	5:A:774:HOH:O	2.17	0.62
1:A:498:HIS:CE1	5:A:861:HOH:O	2.52	0.62
1:B:116:LYS:HD3	1:B:523:GLN:NE2	2.14	0.62
1:B:190:PHE:HE2	1:B:251:VAL:HG12	1.64	0.62
1:A:192:ALA:H	1:A:359:ASN:HD21	1.48	0.62
1:B:516:LEU:O	1:B:519:GLY:N	2.29	0.62
1:A:197:GLU:C	1:A:197:GLU:OE1	2.42	0.62
1:A:291:PRO:CD	5:A:838:HOH:O	2.48	0.62
1:A:463:LYS:NZ	1:A:463:LYS:CB	2.62	0.62
1:B:372:SER:HA	1:B:490:ALA:HB2	1.80	0.62
1:B:467:VAL:HG12	1:B:467:VAL:O	2.00	0.62
1:B:503:LEU:HA	1:B:506:GLN:NE2	2.15	0.62
3:A:630:DG6:O1P	4:A:650:NAI:H2D	1.99	0.62
1:B:489:LYS:NZ	3:B:640:DG6:C1	2.61	0.62
1:A:530:GLU:HG3	1:B:497:PHE:CD1	2.34	0.61
1:A:258:ASN:HD22	1:A:258:ASN:N	1.90	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ARG:O	1:A:532:LEU:CD1	2.48	0.61
1:A:287:LEU:HD13	1:A:308:LEU:HD11	1.80	0.61
1:B:116:LYS:CE	1:B:125:ASP:OD1	2.47	0.61
1:B:299:ASN:HD22	1:B:299:ASN:N	1.98	0.61
1:A:116:LYS:HE3	1:A:125:ASP:CG	2.25	0.61
1:A:318:GLY:HA2	1:A:488:LEU:CG	2.31	0.61
1:A:485:SER:OG	1:A:491:PRO:HB3	2.01	0.61
1:A:493:THR:HG22	1:A:494:ARG:N	2.15	0.61
1:B:40:THR:O	1:B:41:ALA:CB	2.49	0.61
1:A:283:ALA:O	1:A:287:LEU:HB2	2.00	0.61
1:A:297:PRO:CD	1:A:320:ASP:OD2	2.46	0.61
1:B:168:LEU:C	1:B:168:LEU:CD1	2.71	0.61
1:B:297:PRO:CG	1:B:369:LYS:HE2	2.31	0.61
1:A:217:TRP:HB2	1:A:269:LYS:HA	1.83	0.61
1:A:250:TYR:HD1	1:A:368:SER:HG	1.48	0.61
1:A:451:VAL:O	1:A:451:VAL:CG1	2.47	0.61
1:B:310:GLU:HG2	1:B:479:PRO:HG2	1.81	0.61
1:B:342:LYS:HB2	1:B:387:LEU:HG	1.82	0.61
1:A:399:CYS:O	1:A:400:ILE:HD12	2.01	0.60
1:B:321:LEU:HB2	5:B:979:HOH:O	1.98	0.60
1:B:364:LYS:HB2	1:B:365:GLN:HE22	1.66	0.60
1:B:377:ILE:HG21	1:B:398:HIS:CD2	2.36	0.60
1:B:385:ASP:HA	1:B:388:TYR:O	2.01	0.60
1:A:334:GLN:NE2	1:A:380:ILE:HG12	2.15	0.60
1:A:426:GLY:HA3	1:B:440:LEU:CD1	2.32	0.60
1:A:442:ALA:HB2	4:A:650:NAI:H42N	1.83	0.60
1:A:478:TYR:HE1	1:A:480:VAL:HB	1.66	0.60
1:A:308:LEU:CD2	1:A:312:GLU:HG2	2.31	0.60
1:A:68:ILE:HD13	1:A:142:PHE:CG	2.36	0.60
1:A:364:LYS:N	1:A:364:LYS:CD	2.64	0.60
1:B:252:GLU:O	1:B:274:GLU:OE2	2.19	0.60
1:B:352:LEU:CD2	1:B:402:ILE:HD11	2.32	0.60
1:B:484:LEU:N	1:B:484:LEU:CD2	2.65	0.60
1:A:61:LYS:NZ	5:A:970:HOH:O	2.35	0.60
1:A:234:ASN:HB2	1:A:236:LEU:HD22	1.83	0.60
1:B:147:TRP:HB3	1:B:184:SER:HB2	1.83	0.60
1:B:95:GLN:CA	1:B:95:GLN:NE2	2.56	0.60
1:A:183:PRO:HB2	1:A:203:ILE:CG2	2.31	0.60
1:A:285:SER:HB3	1:A:290:VAL:HG23	1.83	0.60
1:B:59:ASP:OD2	1:B:61:LYS:HG3	2.00	0.60
1:B:61:LYS:HG2	5:B:958:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASP:HA	1:B:303:PRO:HG2	1.84	0.60
1:B:291:PRO:HB3	1:B:315:PHE:HB2	1.84	0.60
1:B:315:PHE:HD2	1:B:315:PHE:N	1.99	0.60
1:B:372:SER:CA	1:B:490:ALA:HB2	2.32	0.60
1:A:323:SER:HB2	1:A:326:THR:HB	1.83	0.59
1:B:264:LEU:CD2	1:B:305:LEU:HD13	2.32	0.59
1:B:367:ARG:HA	1:B:370:GLU:HG3	1.84	0.59
1:A:423:MET:HE2	1:B:443:THR:HB	1.84	0.59
1:B:154:LEU:HD22	1:B:179:VAL:CG1	2.32	0.59
1:B:190:PHE:CE2	1:B:276:ALA:HB2	2.37	0.59
1:A:318:GLY:HA2	1:A:488:LEU:HD11	1.74	0.59
1:A:296:SER:CB	1:A:298:GLN:HE22	2.15	0.59
1:A:259:ASP:OD2	1:A:263:ASN:OD1	2.21	0.59
1:A:364:LYS:H	1:A:364:LYS:CE	2.15	0.59
1:B:129:PRO:HB2	1:B:132:SER:HB3	1.85	0.59
1:B:150:ASN:O	5:B:681:HOH:O	2.16	0.59
1:A:92:VAL:HG22	1:A:92:VAL:O	2.02	0.59
1:B:196:ASP:O	1:B:198:ARG:N	2.35	0.59
1:A:493:THR:HG21	1:A:497:PHE:HB2	1.83	0.59
1:B:15:VAL:O	1:B:15:VAL:CG2	2.51	0.59
1:B:251:VAL:HG13	5:B:940:HOH:O	2.02	0.59
1:B:473:LYS:CE	1:B:473:LYS:HA	2.33	0.59
1:A:368:SER:HA	1:A:371:ILE:CG2	2.32	0.59
1:B:22:LYS:O	1:B:23:ASP:C	2.44	0.59
1:B:347:ALA:HB1	1:B:349:TYR:HE2	1.67	0.59
1:B:352:LEU:HD21	1:B:402:ILE:HD11	1.85	0.59
1:A:438:ASP:OD1	2:A:670:NH4:N	2.36	0.59
1:B:29:LYS:HD3	1:B:54:TYR:O	2.02	0.58
1:B:204:ASN:ND2	1:B:212:THR:O	2.32	0.58
1:B:345:SER:HA	1:B:397:ASP:O	2.04	0.58
1:B:405:MET:HE2	1:B:405:MET:HA	1.84	0.58
1:B:23:ASP:OD1	1:B:24:ASN:CA	2.52	0.58
1:B:167:ASP:O	1:B:171:ARG:HG3	2.04	0.58
1:B:503:LEU:O	1:B:506:GLN:HB2	2.04	0.58
1:A:372:SER:HB3	1:A:489:LYS:CE	2.33	0.58
1:B:464:VAL:HG13	1:B:465:ASP:H	1.66	0.58
1:A:165:GLU:OE1	5:A:695:HOH:O	2.17	0.58
1:B:130:PHE:CE2	1:B:452:MET:HE3	2.38	0.58
1:B:523:GLN:HB2	5:B:902:HOH:O	2.02	0.58
1:A:50:THR:CG2	5:A:692:HOH:O	2.51	0.58
1:A:104:ASN:C	1:A:104:ASN:HD22	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HD2	1:A:327:LYS:HG3	1.86	0.58
1:A:322:LYS:HE2	5:A:906:HOH:O	2.03	0.58
1:A:480:VAL:HG12	1:A:480:VAL:O	2.02	0.58
1:B:469:GLU:CG	1:B:470:ASP:N	2.51	0.58
1:A:36:VAL:HA	1:B:119:ILE:O	2.04	0.57
1:B:40:THR:HG1	1:B:44:ARG:H	1.50	0.57
1:B:492:LEU:HD13	1:B:493:THR:H	1.69	0.57
1:A:142:PHE:O	5:A:679:HOH:O	2.17	0.57
1:A:252:GLU:O	1:A:274:GLU:OE1	2.22	0.57
1:A:321:LEU:CD2	1:A:445:LEU:HD22	2.34	0.57
1:B:307:GLN:O	1:B:310:GLU:HB2	2.03	0.57
1:A:298:GLN:H	1:A:298:GLN:NE2	2.03	0.57
1:B:109:MET:HE1	1:B:487:TRP:CZ2	2.39	0.57
1:B:494:ARG:O	1:B:497:PHE:HB2	2.04	0.57
1:B:365:GLN:NE2	1:B:365:GLN:N	2.52	0.57
1:B:350:ASN:C	1:B:350:ASN:HD22	2.13	0.57
1:A:352:LEU:N	1:A:352:LEU:HD23	2.19	0.57
1:A:355:ASN:HB3	1:A:356:ASP:OD2	2.05	0.57
1:B:297:PRO:HB2	1:B:368:SER:CB	2.34	0.57
1:B:186:TYR:HE1	1:B:191:ILE:HD11	1.69	0.57
1:A:368:SER:HA	1:A:371:ILE:HG22	1.87	0.57
1:A:469:GLU:O	1:A:470:ASP:CB	2.52	0.57
1:B:109:MET:CE	1:B:487:TRP:CZ2	2.88	0.57
1:B:503:LEU:HA	1:B:506:GLN:HE21	1.69	0.57
1:A:356:ASP:CB	3:A:630:DG6:O3P	2.48	0.56
1:A:294:ASN:HD21	1:A:296:SER:H	1.52	0.56
1:B:315:PHE:N	1:B:315:PHE:CD2	2.67	0.56
1:A:12:VAL:HG12	1:A:133:LEU:HA	1.87	0.56
1:A:120:ASP:O	1:A:121:ALA:C	2.47	0.56
1:A:200:ASN:C	1:A:200:ASN:HD22	2.12	0.56
1:A:246:ASN:ND2	4:A:650:NAI:H8A	2.19	0.56
1:A:321:LEU:HD22	1:A:445:LEU:HD22	1.88	0.56
1:B:87:ALA:HA	1:B:92:VAL:HG13	1.88	0.56
1:A:449:LEU:O	1:A:453:THR:HG22	2.03	0.56
1:A:498:HIS:HE1	5:A:861:HOH:O	1.89	0.56
1:B:198:ARG:NH2	5:B:969:HOH:O	2.38	0.56
1:B:316:ILE:O	1:B:316:ILE:HD12	2.05	0.56
1:A:291:PRO:HD2	5:A:838:HOH:O	2.05	0.56
1:A:522:SER:OG	1:B:524:ASN:HB3	2.05	0.56
1:B:130:PHE:HE2	1:B:452:MET:CE	2.19	0.56
1:B:14:VAL:HG22	1:B:16:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:N	5:B:699:HOH:O	1.96	0.56
1:A:318:GLY:HA2	1:A:488:LEU:HD22	1.87	0.56
1:A:363:PRO:HB2	1:A:367:ARG:NH2	2.20	0.56
1:B:356:ASP:OD2	1:B:356:ASP:N	2.22	0.56
1:B:255:PRO:HA	1:B:259:ASP:OD1	2.06	0.56
1:A:58:LEU:HD13	1:A:60:LEU:CD2	2.33	0.55
1:A:238:LYS:NZ	1:A:454:GLU:OE2	2.36	0.55
1:A:515:ARG:NH1	1:A:521:PRO:O	2.36	0.55
1:A:116:LYS:HE3	1:A:125:ASP:OD1	2.06	0.55
1:B:354:ASN:CG	1:B:356:ASP:CG	2.74	0.55
1:B:346:ILE:HG23	1:B:418:TYR:CE2	2.41	0.55
1:B:358:TYR:HB2	1:B:404:TYR:CE2	2.41	0.55
1:A:332:LEU:HD21	1:B:328:LEU:HD21	1.88	0.55
1:B:374:SER:O	1:B:376:VAL:N	2.40	0.55
1:A:256:GLY:HA2	1:A:263:ASN:OD1	2.07	0.55
1:A:310:GLU:OE1	1:A:478:TYR:OH	2.17	0.55
1:A:453:THR:O	1:A:457:THR:HG23	2.06	0.55
1:B:231:LYS:HG2	1:B:236:LEU:O	2.07	0.55
1:B:286:ILE:HG22	1:B:308:LEU:CD1	2.33	0.55
1:A:516:LEU:C	1:A:516:LEU:CD2	2.79	0.55
1:B:74:GLY:N	1:B:148:ASP:OD1	2.40	0.55
1:B:486:TYR:CE1	1:B:503:LEU:HG	2.40	0.55
1:A:371:ILE:O	1:A:374:SER:HB3	2.07	0.55
1:B:131:ASN:HA	1:B:136:MET:HE2	1.87	0.55
1:B:131:ASN:CB	1:B:136:MET:CE	2.84	0.55
1:B:321:LEU:HD13	1:B:445:LEU:HD22	1.88	0.55
1:B:468:LYS:HG3	1:B:468:LYS:O	2.06	0.55
1:A:92:VAL:O	1:A:92:VAL:CG2	2.55	0.55
1:A:372:SER:CB	1:A:489:LYS:HE2	2.37	0.55
1:A:151:ASN:H	1:A:200:ASN:ND2	1.95	0.55
1:A:331:VAL:HG12	5:A:907:HOH:O	2.06	0.55
1:B:106:PHE:N	1:B:106:PHE:CD1	2.74	0.55
1:B:366:PHE:HE1	1:B:402:ILE:HG22	1.70	0.55
1:A:104:ASN:ND2	1:A:106:PHE:H	2.05	0.54
1:A:134:LEU:HD11	1:A:517:LEU:HB2	1.88	0.54
1:A:88:ASN:HD21	1:A:104:ASN:CA	2.20	0.54
1:A:96:THR:HG22	1:A:99:GLY:N	2.22	0.54
1:A:14:VAL:O	1:A:16:THR:HG22	2.08	0.54
1:A:170:GLN:NE2	5:A:723:HOH:O	2.41	0.54
1:B:61:LYS:HG3	5:B:958:HOH:O	2.07	0.54
1:A:364:LYS:N	1:A:364:LYS:HD3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:THR:CG2	1:A:497:PHE:HB2	2.37	0.54
1:B:356:ASP:CB	3:B:640:DG6:P	2.96	0.54
1:B:489:LYS:HZ3	3:B:640:DG6:C1	2.12	0.54
1:B:303:PRO:HG2	1:B:304:GLY:N	2.18	0.54
1:A:12:VAL:CG1	1:A:133:LEU:HA	2.37	0.54
1:A:96:THR:CG2	1:A:98:GLU:H	2.18	0.54
1:A:246:ASN:ND2	4:A:650:NAI:H51A	2.23	0.54
1:A:246:ASN:HD22	4:A:650:NAI:H51A	1.70	0.54
1:A:222:ARG:HG2	1:A:222:ARG:HH11	1.72	0.54
1:A:327:LYS:HG2	1:A:503:LEU:CD1	2.36	0.54
1:A:325:GLN:NE2	1:A:350:ASN:OD1	2.40	0.54
1:A:344:VAL:HG21	5:A:851:HOH:O	2.07	0.54
1:A:527:ARG:HG2	1:A:527:ARG:HH11	1.73	0.54
1:B:106:PHE:N	1:B:106:PHE:HD1	2.04	0.54
1:B:134:LEU:HD11	1:B:517:LEU:HB3	1.90	0.54
1:A:350:ASN:N	1:A:401:VAL:O	2.42	0.54
1:A:527:ARG:HG2	1:A:527:ARG:NH1	2.23	0.54
1:A:44:ARG:NH2	1:B:13:LYS:HG2	2.23	0.53
1:A:218:THR:HG23	5:A:836:HOH:O	2.08	0.53
1:B:212:THR:OG1	1:B:213:THR:N	2.41	0.53
1:A:163:VAL:HG12	1:A:164:LEU:HD13	1.90	0.53
1:A:298:GLN:HG2	1:A:300:THR:HG22	1.90	0.53
1:A:246:ASN:HD22	1:A:246:ASN:N	2.07	0.53
1:B:108:SER:OG	1:B:448:ASP:OD2	2.27	0.53
1:A:96:THR:HG23	1:A:98:GLU:N	2.20	0.53
1:A:423:MET:CE	1:B:443:THR:HB	2.38	0.53
1:A:463:LYS:HB2	1:A:463:LYS:HZ2	1.71	0.53
1:B:299:ASN:H	1:B:299:ASN:ND2	2.06	0.53
1:B:369:LYS:HZ1	3:B:640:DG6:C6	2.16	0.53
1:A:218:THR:CG2	5:A:836:HOH:O	2.57	0.53
1:A:363:PRO:HD2	1:A:364:LYS:CE	2.35	0.53
1:B:259:ASP:HA	1:B:303:PRO:CG	2.39	0.53
1:A:61:LYS:O	1:A:61:LYS:CG	2.45	0.52
1:A:82:VAL:HG21	1:A:154:LEU:CD2	2.38	0.52
1:A:258:ASN:ND2	1:A:258:ASN:N	2.53	0.52
1:B:258:ASN:N	1:B:258:ASN:ND2	2.56	0.52
1:A:121:ALA:HB3	1:A:122:GLU:CD	2.34	0.52
1:A:362:ALA:CB	5:A:879:HOH:O	2.56	0.52
1:B:243:TRP:CE2	1:B:245:ALA:HB3	2.44	0.52
1:B:355:ASN:N	1:B:356:ASP:OD2	2.43	0.52
1:A:377:ILE:HD11	5:A:917:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LYS:CB	1:A:463:LYS:HZ3	2.22	0.52
1:B:105:TYR:CZ	1:B:139:PRO:HG2	2.44	0.52
1:B:315:PHE:CD1	1:B:481:LEU:CG	2.92	0.52
1:A:322:LYS:HZ2	1:A:503:LEU:HD12	1.72	0.52
1:B:259:ASP:OD2	1:B:260:THR:N	2.42	0.52
1:B:204:ASN:O	1:B:211:VAL:HA	2.09	0.52
1:B:318:GLY:HA2	1:B:488:LEU:HD21	1.91	0.52
1:A:57:LYS:NZ	5:A:823:HOH:O	2.42	0.52
1:B:473:LYS:HA	1:B:473:LYS:HE3	1.92	0.52
1:B:484:LEU:N	1:B:484:LEU:HD22	2.24	0.52
1:B:486:TYR:HA	1:B:506:GLN:NE2	2.24	0.52
1:B:439:SER:OG	4:B:660:NAI:O7N	2.28	0.52
1:B:489:LYS:C	1:B:491:PRO:HD3	2.34	0.52
1:B:14:VAL:HG11	1:B:518:ILE:O	2.10	0.52
1:B:288:GLU:OE2	5:B:977:HOH:O	2.19	0.52
1:B:327:LYS:HD2	5:B:993:HOH:O	2.09	0.52
1:B:194:ASN:HD22	1:B:195:GLN:N	2.07	0.51
1:A:328:LEU:HD13	1:A:432:ILE:HD11	1.92	0.51
1:A:104:ASN:ND2	1:B:423:MET:HA	2.22	0.51
1:A:105:TYR:OH	1:A:140:ASN:ND2	2.43	0.51
1:A:385:ASP:HA	1:A:388:TYR:O	2.11	0.51
1:A:503:LEU:CD2	1:B:335:PHE:CE2	2.94	0.51
1:B:242:LEU:HD23	1:B:242:LEU:C	2.35	0.51
1:B:318:GLY:CA	1:B:488:LEU:HD23	2.40	0.51
1:A:25:GLU:OE2	1:A:57:LYS:HD2	2.11	0.51
1:A:328:LEU:O	1:A:332:LEU:HB2	2.11	0.51
1:B:62:LYS:N	5:B:847:HOH:O	2.09	0.51
1:A:296:SER:HB3	1:A:298:GLN:HE22	1.75	0.51
5:A:793:HOH:O	1:B:533:LEU:HD13	2.10	0.51
1:A:55:VAL:HG23	1:A:464:VAL:HG21	1.93	0.51
1:A:373:LYS:O	1:A:373:LYS:HG2	2.11	0.51
1:B:455:PHE:O	1:B:457:THR:N	2.44	0.51
1:B:500:VAL:HG12	1:B:501:ASN:O	2.11	0.51
1:A:151:ASN:N	1:A:200:ASN:HD21	1.97	0.51
1:A:287:LEU:CD1	1:A:308:LEU:HD21	2.40	0.51
1:A:423:MET:HE1	1:B:443:THR:HG21	1.93	0.51
1:B:286:ILE:HG21	1:B:308:LEU:HD13	1.83	0.51
1:A:33:GLU:OE2	5:A:810:HOH:O	2.20	0.51
1:A:209:GLY:O	1:A:210:ASN:CB	2.58	0.51
1:A:59:ASP:OD1	1:A:61:LYS:HG2	2.12	0.50
1:A:296:SER:HB2	1:A:298:GLN:HE22	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:MET:HE1	1:B:443:THR:CG2	2.41	0.50
1:A:207:GLU:O	1:A:208:LYS:HB2	2.11	0.50
1:B:481:LEU:O	1:B:484:LEU:HD23	2.11	0.50
1:B:528:PHE:CG	1:B:532:LEU:HD22	2.46	0.50
1:B:21:TYR:CE2	1:B:26:LEU:HD13	2.46	0.50
1:B:52:GLN:OE1	1:B:53:ASP:N	2.43	0.50
1:B:350:ASN:HB3	1:B:414:ALA:HA	1.93	0.50
1:A:74:GLY:N	1:A:148:ASP:OD1	2.44	0.50
1:A:184:SER:OG	1:A:185:ILE:N	2.44	0.50
1:A:440:LEU:HD23	1:B:426:GLY:HA3	1.92	0.50
1:A:461:TYR:OH	1:B:533:LEU:HB2	2.11	0.50
1:B:25:GLU:HG3	1:B:57:LYS:HG3	1.94	0.50
1:B:51:VAL:HG12	1:B:52:GLN:N	2.26	0.50
1:A:216:LYS:HD2	1:A:271:ASP:HA	1.93	0.50
1:A:491:PRO:HD3	1:A:501:ASN:HD21	1.77	0.50
1:B:286:ILE:O	1:B:288:GLU:N	2.45	0.50
1:A:468:LYS:O	1:A:470:ASP:N	2.44	0.50
1:B:14:VAL:CG1	1:B:518:ILE:O	2.59	0.50
1:B:81:LEU:HA	1:B:443:THR:HG23	1.94	0.50
1:B:302:VAL:HB	1:B:303:PRO:CD	2.40	0.50
1:B:322:LYS:NZ	5:B:926:HOH:O	2.44	0.50
1:B:485:SER:OG	1:B:491:PRO:HB3	2.12	0.50
1:A:197:GLU:C	1:A:197:GLU:CD	2.79	0.50
1:B:130:PHE:HZ	1:B:510:LEU:HD12	1.77	0.50
1:B:376:VAL:CG1	1:B:377:ILE:N	2.74	0.50
1:A:327:LYS:HD3	1:B:335:PHE:CE2	2.47	0.50
1:A:497:PHE:N	1:A:497:PHE:CD1	2.80	0.50
1:B:14:VAL:O	1:B:16:THR:HG22	2.12	0.50
1:A:192:ALA:CB	1:A:359:ASN:HD22	2.22	0.50
1:A:225:ARG:CG	1:A:225:ARG:NH2	2.73	0.50
1:B:167:ASP:O	1:B:167:ASP:CG	2.55	0.50
1:B:187:TYR:OH	1:B:219:HIS:CD2	2.60	0.50
1:A:114:THR:OG1	1:B:383:SER:O	2.27	0.49
1:A:321:LEU:HD13	1:A:445:LEU:HD22	1.93	0.49
1:A:493:THR:HG22	1:A:494:ARG:H	1.77	0.49
1:B:318:GLY:CA	1:B:488:LEU:CD2	2.89	0.49
1:B:184:SER:OG	1:B:185:ILE:N	2.44	0.49
1:A:120:ASP:OD1	1:A:124:ASN:O	2.30	0.49
1:A:243:TRP:CD1	1:A:243:TRP:C	2.90	0.49
1:B:40:THR:O	1:B:41:ALA:HB3	2.12	0.49
1:B:402:ILE:O	1:B:402:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ARG:HB3	5:B:981:HOH:O	2.12	0.49
1:A:272:HIS:CD2	1:A:274:GLU:HB2	2.45	0.49
1:A:367:ARG:O	1:A:371:ILE:HG22	2.12	0.49
1:A:368:SER:CA	1:A:371:ILE:HG22	2.43	0.49
1:A:465:ASP:OD1	1:A:467:VAL:N	2.41	0.49
1:B:66:LEU:HD21	1:B:240:ILE:HD12	1.95	0.49
1:B:154:LEU:HD22	1:B:179:VAL:HG11	1.94	0.49
1:B:360:LEU:HD11	3:B:640:DG6:HC61	1.94	0.49
1:A:362:ALA:HA	5:A:879:HOH:O	2.11	0.49
1:A:412:LYS:C	5:A:956:HOH:O	2.53	0.49
1:B:352:LEU:HA	1:B:411:SER:O	2.11	0.49
1:A:389:ASN:OD1	1:A:389:ASN:C	2.55	0.49
1:A:497:PHE:CD2	1:B:530:GLU:HB2	2.48	0.49
1:A:225:ARG:HH21	1:A:225:ARG:HG2	1.78	0.49
1:A:349:TYR:HD1	1:A:401:VAL:HB	1.78	0.49
1:A:533:LEU:CB	1:B:494:ARG:HH12	2.22	0.49
1:B:499:PRO:HD2	5:B:886:HOH:O	2.13	0.49
1:B:350:ASN:O	1:B:402:ILE:HA	2.13	0.49
3:A:630:DG6:O1P	4:A:650:NAI:H3D	2.12	0.48
1:A:321:LEU:CD1	1:A:445:LEU:HD22	2.42	0.48
1:B:261:MET:H	1:B:307:GLN:NE2	2.11	0.48
1:A:43:GLY:O	1:B:10:THR:HA	2.14	0.48
1:A:68:ILE:CD1	1:A:142:PHE:CD2	2.96	0.48
1:B:130:PHE:O	1:B:130:PHE:CD2	2.66	0.48
1:A:264:LEU:HD21	1:A:305:LEU:HD13	1.95	0.48
1:A:494:ARG:HG3	1:A:497:PHE:CD1	2.48	0.48
1:A:66:LEU:HD13	1:A:68:ILE:HD11	1.95	0.48
1:B:155:TYR:OH	1:B:170:GLN:NE2	2.44	0.48
1:B:370:GLU:OE2	1:B:400:ILE:HG22	2.13	0.48
1:B:31:SER:CB	5:B:699:HOH:O	2.61	0.48
1:B:527:ARG:HD3	5:B:855:HOH:O	2.14	0.48
1:A:155:TYR:CE1	1:A:173:LYS:HG3	2.49	0.48
1:A:371:ILE:O	1:A:371:ILE:HD12	2.14	0.48
1:B:130:PHE:CE2	1:B:452:MET:CE	2.96	0.48
1:A:322:LYS:NZ	1:A:503:LEU:CD1	2.75	0.48
1:B:194:ASN:HD22	1:B:194:ASN:C	2.22	0.48
1:B:455:PHE:O	1:B:456:CYS:C	2.56	0.48
1:B:520:LEU:HD12	1:B:520:LEU:HA	1.80	0.48
1:A:383:SER:O	1:B:114:THR:OG1	2.22	0.48
1:A:471:ALA:N	5:A:963:HOH:O	2.47	0.48
1:B:243:TRP:CZ2	1:B:245:ALA:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ILE:O	1:B:450:LEU:N	2.44	0.48
1:B:460:SER:OG	5:B:914:HOH:O	2.20	0.48
1:A:136:MET:HE1	1:A:452:MET:SD	2.54	0.48
1:A:351:HIS:HA	1:A:403:LYS:O	2.14	0.48
1:B:364:LYS:HB2	1:B:365:GLN:NE2	2.29	0.48
1:A:192:ALA:CB	1:A:359:ASN:ND2	2.77	0.47
1:B:158:MET:CE	1:B:158:MET:HG3	2.45	0.47
1:B:194:ASN:ND2	1:B:195:GLN:HG2	2.30	0.47
1:B:286:ILE:C	1:B:288:GLU:N	2.70	0.47
1:A:155:TYR:CD1	1:A:173:LYS:HG3	2.48	0.47
1:B:122:GLU:HB2	1:B:124:ASN:ND2	2.28	0.47
1:B:229:ASN:ND2	1:B:233:GLU:OE2	2.42	0.47
1:A:502:GLY:O	1:A:503:LEU:C	2.58	0.47
1:B:319:ASP:N	1:B:319:ASP:OD1	2.47	0.47
1:A:298:GLN:H	1:A:298:GLN:HE21	1.61	0.47
1:A:282:ALA:HB3	1:A:305:LEU:HD21	1.97	0.47
1:A:423:MET:HA	1:B:104:ASN:OD1	2.15	0.47
1:A:443:THR:CG2	1:B:423:MET:HE1	2.45	0.47
1:B:97:LYS:HG3	5:B:722:HOH:O	2.13	0.47
1:B:258:ASN:H	1:B:258:ASN:ND2	2.07	0.47
1:A:68:ILE:CD1	1:A:142:PHE:CG	2.98	0.47
1:A:196:ASP:O	1:A:197:GLU:CB	2.63	0.47
1:A:249:ARG:O	1:A:249:ARG:CG	2.62	0.47
1:A:322:LYS:HZ3	1:A:503:LEU:HD12	1.78	0.47
1:A:491:PRO:CD	1:A:501:ASN:HD21	2.28	0.47
1:A:64:GLU:C	1:A:65:LYS:HD3	2.39	0.47
1:A:196:ASP:O	1:A:197:GLU:HB3	2.15	0.47
1:A:352:LEU:HD23	1:A:352:LEU:H	1.80	0.47
1:A:148:ASP:C	1:A:150:ASN:H	2.22	0.47
1:B:37:VAL:HA	1:B:46:ASP:O	2.15	0.47
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.73	0.47
1:B:353:GLY:CA	1:B:406:LYS:HA	2.44	0.47
1:A:360:LEU:CD1	3:A:630:DG6:HC61	2.39	0.47
1:A:10:THR:HA	1:B:43:GLY:O	2.15	0.46
1:A:40:THR:N	1:A:44:ARG:O	2.28	0.46
1:A:250:TYR:HD1	1:A:368:SER:OG	1.98	0.46
1:A:531:ARG:HD3	1:B:483:PHE:CE2	2.50	0.46
1:B:276:ALA:O	1:B:277:PRO:C	2.55	0.46
1:B:316:ILE:CD1	1:B:316:ILE:C	2.88	0.46
1:B:529:GLU:CD	1:B:529:GLU:H	2.23	0.46
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ILE:N	1:B:191:ILE:CD1	2.75	0.46
1:A:159:GLN:HA	1:A:169:GLN:HE22	1.80	0.46
1:A:185:ILE:CG2	1:A:187:TYR:CE2	2.99	0.46
1:B:131:ASN:CA	1:B:136:MET:CE	2.92	0.46
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.83	0.46
1:B:327:LYS:HG2	1:B:503:LEU:CD1	2.42	0.46
1:B:486:TYR:CD1	1:B:503:LEU:HG	2.50	0.46
1:A:327:LYS:HD3	1:B:335:PHE:CZ	2.50	0.46
1:A:374:SER:O	1:A:374:SER:OG	2.34	0.46
1:B:103:PRO:HA	5:B:933:HOH:O	2.14	0.46
1:B:149:ILE:HD12	1:B:199:ALA:HB2	1.98	0.46
1:B:206:ASP:OD1	1:B:210:ASN:HB2	2.15	0.46
1:A:82:VAL:HG21	1:A:154:LEU:HD21	1.97	0.46
1:A:136:MET:SD	1:A:136:MET:CB	2.96	0.46
1:B:408:VAL:O	1:B:411:SER:HB2	2.16	0.46
1:A:254:SER:H	1:A:258:ASN:HD21	1.63	0.46
1:B:231:LYS:HG3	1:B:239:VAL:HG21	1.98	0.46
1:B:468:LYS:O	1:B:469:GLU:O	2.33	0.46
1:B:297:PRO:HG3	1:B:369:LYS:CE	2.44	0.46
1:B:322:LYS:O	1:B:323:SER:C	2.56	0.46
1:B:353:GLY:N	1:B:408:VAL:HG23	2.31	0.46
1:B:486:TYR:O	1:B:486:TYR:CG	2.69	0.46
1:A:76:ASN:HD22	1:A:76:ASN:N	2.13	0.46
1:A:358:TYR:CD1	1:A:404:TYR:CE2	3.04	0.46
1:B:80:THR:HB	1:B:164:LEU:HD21	1.97	0.46
1:B:139:PRO:HA	1:B:142:PHE:CE2	2.51	0.46
1:B:470:ASP:O	1:B:471:ALA:HB2	2.15	0.46
1:A:96:THR:HA	1:A:165:GLU:OE2	2.16	0.46
1:B:362:ALA:HB1	1:B:364:LYS:HZ1	1.78	0.46
1:B:466:PRO:HB2	5:B:899:HOH:O	2.16	0.46
1:A:257:VAL:O	1:A:267:SER:OG	2.31	0.46
1:B:93:GLU:HB3	1:B:102:GLN:OE1	2.16	0.46
1:B:332:LEU:HD23	1:B:332:LEU:N	2.30	0.46
1:B:403:LYS:HB3	5:B:895:HOH:O	2.15	0.46
1:A:310:GLU:HA	1:A:479:PRO:HG2	1.97	0.45
1:B:166:TYR:CE2	1:B:170:GLN:HG3	2.51	0.45
1:B:369:LYS:HD2	3:B:640:DG6:O3	2.14	0.45
1:A:135:PRO:HG2	1:A:458:ARG:HH12	1.80	0.45
1:A:200:ASN:C	1:A:200:ASN:ND2	2.70	0.45
1:A:358:TYR:HD1	1:A:404:TYR:CE2	2.33	0.45
1:A:404:TYR:O	1:A:405:MET:HE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:LYS:O	1:B:177:SER:OG	2.34	0.45
1:B:332:LEU:HD22	1:B:332:LEU:HA	1.21	0.45
1:B:452:MET:HG3	1:B:487:TRP:CH2	2.51	0.45
1:A:265:LEU:O	1:A:269:LYS:HG3	2.16	0.45
1:B:353:GLY:HA3	1:B:406:LYS:HA	1.97	0.45
1:B:473:LYS:CE	1:B:473:LYS:CA	2.94	0.45
1:B:55:VAL:O	1:B:462:LYS:N	2.45	0.45
1:A:268:ILE:HG12	1:A:275:ILE:HG21	1.98	0.45
1:A:503:LEU:CD2	1:B:335:PHE:HE2	2.26	0.45
1:A:530:GLU:CG	1:B:497:PHE:CD1	3.00	0.45
1:B:198:ARG:NE	5:B:969:HOH:O	2.50	0.45
1:B:332:LEU:N	1:B:332:LEU:CD2	2.70	0.45
1:A:319:ASP:HB2	1:A:490:ALA:O	2.16	0.45
1:B:67:GLY:O	1:B:240:ILE:N	2.45	0.45
1:B:186:TYR:CE1	1:B:191:ILE:HD11	2.49	0.45
1:B:334:GLN:NE2	1:B:380:ILE:HG12	2.32	0.45
1:A:145:SER:HB3	1:A:230:PHE:CE1	2.52	0.45
1:A:250:TYR:CE1	1:A:371:ILE:HG21	2.52	0.45
1:A:443:THR:O	1:A:447:ILE:HG13	2.17	0.45
1:B:58:LEU:HA	1:B:458:ARG:O	2.17	0.45
1:B:130:PHE:CD2	1:B:130:PHE:C	2.95	0.45
1:A:264:LEU:O	1:A:266:GLN:N	2.50	0.45
1:A:428:ASN:ND2	1:B:436:CYS:HB3	2.13	0.45
1:B:447:ILE:O	1:B:448:ASP:C	2.60	0.45
1:A:318:GLY:C	1:A:488:LEU:HD13	2.43	0.44
1:A:320:ASP:O	1:A:488:LEU:HA	2.18	0.44
1:B:187:TYR:HD1	1:B:277:PRO:HD3	1.82	0.44
1:B:373:LYS:NZ	1:B:376:VAL:CG1	2.76	0.44
1:B:455:PHE:C	1:B:457:THR:N	2.71	0.44
1:B:481:LEU:HB3	1:B:484:LEU:HD23	1.99	0.44
1:B:483:PHE:C	1:B:484:LEU:HD22	2.42	0.44
1:A:21:TYR:CZ	1:A:26:LEU:HD13	2.52	0.44
1:B:109:MET:HE3	1:B:487:TRP:CZ2	2.53	0.44
1:B:22:LYS:HE3	1:B:27:LEU:HD12	1.99	0.44
1:B:443:THR:HB	1:B:444:PRO:HD3	2.00	0.44
1:B:198:ARG:CZ	5:B:969:HOH:O	2.66	0.44
1:B:303:PRO:CG	1:B:304:GLY:N	2.69	0.44
1:A:261:MET:HE1	1:A:311:HIS:HD1	1.78	0.44
1:B:372:SER:CA	5:B:801:HOH:O	2.65	0.44
1:A:18:LYS:NZ	5:A:713:HOH:O	2.50	0.44
1:A:272:HIS:CD2	1:A:274:GLU:H	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:CD2	1:A:312:GLU:CG	2.96	0.44
1:B:64:GLU:HG2	5:B:772:HOH:O	2.17	0.44
1:B:70:LEU:HD23	1:B:73:LEU:HD23	1.99	0.44
1:B:134:LEU:HD21	1:B:518:ILE:HG22	1.99	0.44
1:A:261:MET:H	1:A:307:GLN:NE2	2.15	0.44
1:A:321:LEU:CD2	1:A:445:LEU:CD2	2.93	0.44
1:B:52:GLN:OE1	1:B:52:GLN:HA	2.16	0.44
1:B:373:LYS:HZ1	1:B:376:VAL:CG1	2.24	0.44
1:A:57:LYS:HE3	1:A:474:PHE:CD1	2.53	0.44
1:A:207:GLU:OE1	1:A:207:GLU:CA	2.62	0.44
1:A:256:GLY:N	1:A:259:ASP:OD1	2.51	0.43
1:A:262:GLU:H	1:A:262:GLU:CD	2.26	0.43
1:A:285:SER:HB3	1:A:290:VAL:CG2	2.45	0.43
1:A:469:GLU:O	1:A:470:ASP:HB3	2.17	0.43
1:B:187:TYR:CD1	1:B:277:PRO:HD3	2.53	0.43
1:B:478:TYR:CE2	1:B:494:ARG:HB2	2.53	0.43
1:B:478:TYR:O	1:B:479:PRO:C	2.61	0.43
1:B:492:LEU:HD13	1:B:493:THR:N	2.33	0.43
1:A:136:MET:CE	1:A:136:MET:HG2	2.46	0.43
1:B:438:ASP:OD1	2:B:680:NH4:N	2.50	0.43
1:A:268:ILE:O	1:A:269:LYS:C	2.61	0.43
1:A:412:LYS:HZ3	1:A:412:LYS:HG3	1.13	0.43
1:B:144:VAL:O	5:B:789:HOH:O	2.21	0.43
1:B:254:SER:N	1:B:258:ASN:HD21	2.12	0.43
1:A:264:LEU:O	1:A:265:LEU:C	2.60	0.43
1:A:294:ASN:OD1	1:A:300:THR:HG23	2.18	0.43
1:A:369:LYS:NZ	3:A:630:DG6:HC62	2.33	0.43
1:B:354:ASN:OD1	1:B:356:ASP:CB	2.65	0.43
1:B:473:LYS:HE2	1:B:473:LYS:HA	2.00	0.43
1:A:165:GLU:O	1:A:169:GLN:HG3	2.18	0.43
1:B:82:VAL:HG21	1:B:154:LEU:HD23	2.01	0.43
1:B:95:GLN:HE21	1:B:96:THR:N	2.16	0.43
1:A:104:ASN:HD22	1:A:106:PHE:H	1.66	0.43
1:B:115:LEU:HD21	1:B:511:GLU:HG3	1.96	0.43
1:B:322:LYS:HB2	1:B:487:TRP:O	2.18	0.43
1:B:362:ALA:HB1	1:B:364:LYS:HZ3	1.79	0.43
1:A:528:PHE:HB3	1:A:532:LEU:HD22	2.01	0.43
1:B:354:ASN:HB2	1:B:356:ASP:OD2	2.19	0.43
1:B:368:SER:O	1:B:372:SER:HB3	2.19	0.43
1:B:454:GLU:O	1:B:457:THR:CG2	2.62	0.43
1:B:489:LYS:HZ2	3:B:640:DG6:C1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:THR:HG23	5:A:692:HOH:O	2.14	0.43
1:A:318:GLY:CA	1:A:488:LEU:HD22	2.49	0.43
1:A:389:ASN:HD21	1:A:392:LEU:HG	1.82	0.43
1:B:342:LYS:O	1:B:343:PRO:C	2.59	0.43
1:B:455:PHE:C	1:B:457:THR:H	2.26	0.43
1:A:225:ARG:NH2	1:A:225:ARG:HG3	2.34	0.42
1:A:315:PHE:CE1	1:A:481:LEU:HD21	2.54	0.42
1:A:354:ASN:HB2	1:A:356:ASP:OD1	2.19	0.42
1:B:39:LYS:HD3	1:B:45:PHE:CE2	2.54	0.42
1:B:68:ILE:HD12	1:B:450:LEU:HD13	2.01	0.42
1:B:68:ILE:HG22	1:B:70:LEU:HD13	2.00	0.42
1:B:130:PHE:CZ	1:B:452:MET:HE3	2.54	0.42
1:B:372:SER:CB	5:B:801:HOH:O	2.67	0.42
1:B:405:MET:C	1:B:407:PRO:HD2	2.44	0.42
1:B:164:LEU:O	1:B:165:GLU:C	2.61	0.42
1:B:256:GLY:H	1:B:259:ASP:CG	2.19	0.42
1:B:303:PRO:O	1:B:306:VAL:N	2.52	0.42
1:B:403:LYS:NZ	5:B:884:HOH:O	2.48	0.42
1:A:223:ILE:HD12	1:A:281:PHE:CE2	2.54	0.42
1:A:40:THR:HG22	1:A:42:SER:H	1.84	0.42
1:A:217:TRP:CE3	1:A:269:LYS:HG2	2.54	0.42
1:A:335:PHE:HE1	1:B:503:LEU:HD22	1.83	0.42
1:B:29:LYS:HE2	5:B:816:HOH:O	2.19	0.42
1:B:192:ALA:O	1:B:194:ASN:N	2.52	0.42
1:A:69:MET:CE	1:A:69:MET:CG	2.90	0.42
1:A:158:MET:HE3	1:A:158:MET:HB2	1.66	0.42
1:A:392:LEU:N	1:A:392:LEU:HD23	2.33	0.42
1:A:39:LYS:HE2	1:A:39:LYS:HB3	1.60	0.42
1:A:260:THR:O	1:A:261:MET:C	2.62	0.42
1:A:497:PHE:CD2	1:B:530:GLU:HG3	2.55	0.42
1:B:261:MET:HG3	1:B:308:LEU:HD23	2.01	0.42
1:B:352:LEU:HD22	1:B:402:ILE:HD11	2.01	0.42
1:A:332:LEU:HA	1:A:332:LEU:HD22	1.55	0.42
1:A:354:ASN:ND2	1:A:410:ASP:OD2	2.48	0.42
1:B:286:ILE:C	1:B:288:GLU:H	2.28	0.42
1:B:480:VAL:HG12	1:B:482:THR:CG2	2.42	0.42
1:A:96:THR:N	1:A:99:GLY:O	2.53	0.42
1:A:225:ARG:HE	1:A:229:ASN:ND2	1.98	0.42
1:B:40:THR:HG21	1:B:44:ARG:NH1	2.35	0.42
1:B:131:ASN:HA	1:B:136:MET:HE1	1.99	0.42
1:B:192:ALA:O	1:B:193:ALA:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLN:HE21	1:B:412:LYS:HE2	1.84	0.42
1:A:41:ALA:C	1:A:43:GLY:H	2.28	0.42
1:A:322:LYS:HG3	1:A:489:LYS:CA	2.46	0.42
1:B:250:TYR:HA	1:B:299:ASN:ND2	2.34	0.42
1:B:349:TYR:O	1:B:350:ASN:HB3	2.19	0.42
1:A:261:MET:HE1	1:A:311:HIS:CB	2.50	0.42
1:A:315:PHE:CZ	1:A:477:PHE:HB2	2.55	0.42
1:A:377:ILE:HA	1:A:377:ILE:HD13	1.72	0.42
1:B:296:SER:HA	1:B:297:PRO:HD2	1.85	0.42
1:B:297:PRO:HD3	1:B:320:ASP:HB2	2.00	0.42
1:A:11:SER:O	1:B:44:ARG:HA	2.20	0.41
1:A:323:SER:CB	1:A:326:THR:H	2.33	0.41
1:A:344:VAL:CG2	5:A:728:HOH:O	2.59	0.41
1:B:374:SER:C	1:B:376:VAL:N	2.78	0.41
1:A:77:ASN:HD21	4:A:650:NAI:C7N	2.33	0.41
1:A:163:VAL:CG1	1:A:440:LEU:HD13	2.50	0.41
1:A:246:ASN:CG	4:A:650:NAI:H8A	2.44	0.41
1:A:477:PHE:O	1:A:478:TYR:C	2.63	0.41
1:B:11:SER:CA	5:B:760:HOH:O	2.59	0.41
1:B:55:VAL:O	1:B:461:TYR:HA	2.20	0.41
1:B:165:GLU:O	1:B:169:GLN:HG3	2.20	0.41
1:B:191:ILE:HG23	1:B:191:ILE:HD12	1.70	0.41
1:B:292:TYR:O	1:B:316:ILE:HA	2.20	0.41
1:B:371:ILE:C	1:B:373:LYS:N	2.74	0.41
1:A:96:THR:CG2	1:A:98:GLU:N	2.81	0.41
1:A:264:LEU:C	1:A:266:GLN:N	2.76	0.41
1:B:61:LYS:HA	5:B:847:HOH:O	2.20	0.41
1:B:225:ARG:HH21	1:B:225:ARG:HD3	1.72	0.41
1:A:41:ALA:C	1:A:43:GLY:N	2.78	0.41
1:A:73:LEU:HG	1:A:154:LEU:HD11	2.01	0.41
1:A:104:ASN:C	1:A:104:ASN:ND2	2.75	0.41
1:A:530:GLU:HB2	1:B:497:PHE:CE1	2.56	0.41
1:B:82:VAL:HG21	1:B:154:LEU:CD2	2.51	0.41
1:B:109:MET:CE	1:B:487:TRP:HZ2	2.33	0.41
1:B:233:GLU:CD	5:B:973:HOH:O	2.62	0.41
1:B:473:LYS:HG3	1:B:474:PHE:O	2.21	0.41
1:B:261:MET:HE2	1:B:308:LEU:CA	2.32	0.41
1:B:306:VAL:O	1:B:310:GLU:HG3	2.21	0.41
1:B:310:GLU:O	1:B:311:HIS:C	2.63	0.41
1:B:322:LYS:HD3	1:B:327:LYS:HG3	2.02	0.41
1:A:150:ASN:HB2	1:A:198:ARG:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PRO:HA	1:A:201:ASN:O	2.21	0.41
1:A:352:LEU:N	1:A:352:LEU:CD2	2.83	0.41
1:B:116:LYS:CD	1:B:523:GLN:NE2	2.83	0.41
1:B:392:LEU:N	1:B:392:LEU:HD23	2.35	0.41
1:B:134:LEU:O	1:B:135:PRO:C	2.63	0.41
1:B:253:VAL:HG22	1:B:302:VAL:HG12	2.02	0.41
1:B:286:ILE:O	1:B:287:LEU:C	2.63	0.41
1:A:48:THR:HA	1:A:49:PRO:HD3	1.97	0.41
1:A:248:GLU:OE2	1:A:277:PRO:HD2	2.21	0.41
1:A:261:MET:HE1	1:A:311:HIS:HB3	2.03	0.41
1:A:291:PRO:CG	5:A:838:HOH:O	2.57	0.41
1:A:322:LYS:HZ2	1:A:503:LEU:CD1	2.34	0.41
1:A:403:LYS:HE3	1:A:403:LYS:HB3	1.74	0.41
1:A:442:ALA:O	1:A:445:LEU:HB3	2.21	0.41
1:B:105:TYR:OH	1:B:140:ASN:ND2	2.54	0.41
1:B:286:ILE:HG22	1:B:308:LEU:HD13	1.97	0.41
1:B:492:LEU:HA	1:B:492:LEU:HD22	1.51	0.41
1:B:501:ASN:N	1:B:501:ASN:HD22	2.19	0.41
1:A:21:TYR:N	1:A:21:TYR:CD1	2.88	0.41
1:A:261:MET:HE3	1:A:308:LEU:HD23	2.04	0.40
1:A:276:ALA:O	1:A:279:THR:HB	2.21	0.40
5:A:800:HOH:O	1:B:168:LEU:HD11	2.16	0.40
1:B:162:GLN:NE2	5:B:991:HOH:O	2.50	0.40
1:B:513:PHE:O	1:B:514:LEU:C	2.64	0.40
1:A:281:PHE:O	1:A:285:SER:OG	2.37	0.40
1:A:447:ILE:O	1:A:451:VAL:HG23	2.21	0.40
1:B:15:VAL:H	1:B:15:VAL:HG13	1.60	0.40
1:B:371:ILE:CG2	5:B:799:HOH:O	2.68	0.40
1:A:24:ASN:HD22	1:A:61:LYS:HB3	1.85	0.40
1:A:148:ASP:C	1:A:150:ASN:N	2.80	0.40
1:A:322:LYS:HB2	1:A:487:TRP:C	2.47	0.40
1:A:493:THR:CG2	1:A:494:ARG:N	2.84	0.40
1:B:101:LYS:HA	1:B:101:LYS:HD3	1.76	0.40
1:B:297:PRO:CG	1:B:320:ASP:OD1	2.68	0.40
1:B:307:GLN:O	1:B:310:GLU:N	2.51	0.40
1:A:109:MET:HE3	1:A:487:TRP:CZ2	2.56	0.40
1:A:294:ASN:ND2	1:A:295:GLY:N	2.64	0.40
1:B:62:LYS:O	1:B:63:PRO:C	2.63	0.40
1:B:173:LYS:NZ	5:B:968:HOH:O	2.26	0.40
1:B:443:THR:N	1:B:444:PRO:HD2	2.35	0.40
1:B:260:THR:HA	1:B:304:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:PRO:O	1:B:493:THR:HG23	2.22	0.40

All (1) 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:415:MET:CE	1:A:415:MET:CE[2_555]	2.03	0.17

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/533 (98%)	463 (88%)	37 (7%)	23 (4%)	2	1
1	B	522/533 (98%)	444 (85%)	52 (10%)	26 (5%)	1	0
All	All	1045/1066 (98%)	907 (87%)	89 (8%)	49 (5%)	2	0

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
1	A	197	GLU
1	A	198	ARG
1	A	208	LYS
1	A	210	ASN
1	A	319	ASP
1	A	323	SER
1	A	375	SER
1	B	41	ALA
1	B	196	ASP
1	B	197	GLU
1	B	207	GLU

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Mol	Chain	Res	Type
1	B	375	SER
1	B	467	VAL
1	B	469	GLU
1	B	470	ASP
1	B	471	ALA
1	A	374	SER
1	A	469	GLU
1	A	470	ASP
1	A	481	LEU
1	A	495	PRO
1	B	193	ALA
1	B	322	LYS
1	B	361	SER
1	B	496	GLY
1	A	206	ASP
1	A	265	LEU
1	A	361	SER
1	B	22	LYS
1	B	319	ASP
1	B	468	LYS
1	B	495	PRO
1	A	320	ASP
1	B	320	ASP
1	B	473	LYS
1	A	125	ASP
1	A	496	GLY
1	B	106	PHE
1	B	356	ASP
1	B	491	PRO
1	A	502	GLY
1	B	209	GLY
1	B	479	PRO
1	B	480	VAL
1	A	211	VAL
1	A	480	VAL
1	B	447	ILE
1	A	324	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	464/471 (98%)	389 (84%)	75 (16%)	2	2
1	B	463/471 (98%)	377 (81%)	86 (19%)	1	1
All	All	927/942 (98%)	766 (83%)	161 (17%)	2	2

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	16	THR
1	A	40	THR
1	A	50	THR
1	A	58	LEU
1	A	65	LYS
1	A	66	LEU
1	A	68	ILE
1	A	70	LEU
1	A	86	LEU
1	A	92	VAL
1	A	96	THR
1	A	100	VAL
1	A	104	ASN
1	A	109	MET
1	A	122	GLU
1	A	135	PRO
1	A	162	GLN
1	A	164	LEU
1	A	165	GLU
1	A	176	MET
1	A	189	ASP
1	A	197	GLU
1	A	200	ASN
1	A	201	ASN
1	A	211	VAL
1	A	220	LEU
1	A	222	ARG
1	A	225	ARG
1	A	236	LEU
1	A	246	ASN

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	257	VAL
1	A	258	ASN
1	A	259	ASP
1	A	280	ILE
1	A	285	SER
1	A	287	LEU
1	A	298	GLN
1	A	300	THR
1	A	308	LEU
1	A	319	ASP
1	A	323	SER
1	A	325	GLN
1	A	328	LEU
1	A	330	SER
1	A	332	LEU
1	A	336	LEU
1	A	356	ASP
1	A	364	LYS
1	A	367	ARG
1	A	371	ILE
1	A	374	SER
1	A	376	VAL
1	A	377	ILE
1	A	381	ILE
1	A	387	LEU
1	A	391	LYS
1	A	397	ASP
1	A	406	LYS
1	A	412	LYS
1	A	417	GLU
1	A	440	LEU
1	A	453	THR
1	A	463	LYS
1	A	484	LEU
1	A	489	LYS
1	A	497	PHE
1	A	500	VAL
1	A	505	LYS
1	A	516	LEU
1	A	523	GLN
1	A	529	GLU

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Mol	Chain	Res	Type
1	A	532	LEU
1	A	533	LEU
1	B	10	THR
1	B	14	VAL
1	B	15	VAL
1	B	16	THR
1	B	17	ASP
1	B	23	ASP
1	B	24	ASN
1	B	29	LYS
1	B	40	THR
1	B	58	LEU
1	B	62	LYS
1	B	70	LEU
1	B	73	LEU
1	B	79	SER
1	B	80	THR
1	B	92	VAL
1	B	95	GLN
1	B	97	LYS
1	B	129	PRO
1	B	135	PRO
1	B	144	VAL
1	B	151	ASN
1	B	154	LEU
1	B	162	GLN
1	B	163	VAL
1	B	168	LEU
1	B	177	SER
1	B	191	ILE
1	B	194	ASN
1	B	197	GLU
1	B	201	ASN
1	B	207	GLU
1	B	213	THR
1	B	222	ARG
1	B	233	GLU
1	B	236	LEU
1	B	237	ASP
1	B	257	VAL
1	B	258	ASN
1	B	265	LEU

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Mol	Chain	Res	Type
1	B	273	GLU
1	B	277	PRO
1	B	278	SER
1	B	299	ASN
1	B	315	PHE
1	B	316	ILE
1	B	321	LEU
1	B	322	LYS
1	B	323	SER
1	B	325	GLN
1	B	328	LEU
1	B	330	SER
1	B	332	LEU
1	B	350	ASN
1	B	356	ASP
1	B	364	LYS
1	B	365	GLN
1	B	367	ARG
1	B	371	ILE
1	B	373	LYS
1	B	376	VAL
1	B	387	LEU
1	B	395	LYS
1	B	400	ILE
1	B	402	ILE
1	B	415	MET
1	B	441	LEU
1	B	446	ILE
1	B	457	THR
1	B	468	LYS
1	B	473	LYS
1	B	479	PRO
1	B	482	THR
1	B	484	LEU
1	B	488	LEU
1	B	492	LEU
1	B	494	ARG
1	B	495	PRO
1	B	504	ASN
1	B	510	LEU
1	B	514	LEU
1	B	517	LEU

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Mol	Chain	Res	Type
1	B	520	LEU
1	B	522	SER
1	B	529	GLU
1	B	532	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	76	ASN
1	A	77	ASN
1	A	88	ASN
1	A	90	HIS
1	A	104	ASN
1	A	124	ASN
1	A	140	ASN
1	A	150	ASN
1	A	151	ASN
1	A	169	GLN
1	A	170	GLN
1	A	200	ASN
1	A	201	ASN
1	A	229	ASN
1	A	234	ASN
1	A	246	ASN
1	A	258	ASN
1	A	263	ASN
1	A	266	GLN
1	A	270	ASN
1	A	272	HIS
1	A	294	ASN
1	A	298	GLN
1	A	307	GLN
1	A	325	GLN
1	A	334	GLN
1	A	359	ASN
1	A	428	ASN
1	A	434	ASN
1	A	501	ASN
1	A	512	ASN
1	A	523	GLN
1	B	24	ASN

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Mol	Chain	Res	Type
1	B	77	ASN
1	B	91	ASN
1	B	95	GLN
1	B	124	ASN
1	B	140	ASN
1	B	151	ASN
1	B	170	GLN
1	B	194	ASN
1	B	195	GLN
1	B	201	ASN
1	B	219	HIS
1	B	228	GLN
1	B	234	ASN
1	B	258	ASN
1	B	263	ASN
1	B	299	ASN
1	B	325	GLN
1	B	334	GLN
1	B	350	ASN
1	B	355	ASN
1	B	398	HIS
1	B	428	ASN
1	B	498	HIS
1	B	501	ASN
1	B	506	GLN
1	B	523	GLN

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, 2 are modelled with single atom - leaving 4 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	DG6	B	640	-	14,14,14	4.05	9 (64%)	18,19,19	2.25	5 (27%)
3	DG6	A	630	-	14,14,14	4.76	10 (71%)	18,19,19	2.53	7 (38%)
4	NAI	A	650	-	47,48,48	3.86	32 (68%)	64,73,73	2.27	18 (28%)
4	NAI	B	660	-	47,48,48	3.76	30 (63%)	64,73,73	2.31	26 (40%)

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	DG6	B	640	-	1/1/4/4	8/17/17/17	-
3	DG6	A	630	-	1/1/4/4	10/17/17/17	-
4	NAI	A	650	-	-	7/29/72/72	0/5/5/5
4	NAI	B	660	-	-	2/29/72/72	0/5/5/5

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	630	DG6	C6-C5	9.76	1.65	1.51
3	B	640	DG6	C6-C5	9.27	1.64	1.51
4	B	660	NAI	PA-O3	8.93	1.69	1.59
4	B	660	NAI	C4A-N3A	8.64	1.50	1.34
4	A	650	NAI	PA-O3	7.95	1.68	1.59
4	A	650	NAI	O2B-C2B	-7.94	1.23	1.43
4	B	660	NAI	C7N-C3N	7.79	1.65	1.48
4	A	650	NAI	C7N-C3N	7.75	1.65	1.48
4	B	660	NAI	O4B-C1B	-7.37	1.25	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	630	DG6	C2-C3	7.12	1.64	1.52
3	A	630	DG6	P-O6	6.89	1.82	1.60
4	A	650	NAI	C8A-N7A	6.08	1.43	1.31
4	B	660	NAI	C6N-N1N	5.98	1.51	1.37
4	A	650	NAI	C8A-N9A	-5.96	1.27	1.37
3	B	640	DG6	P-O6	5.66	1.78	1.60
4	A	650	NAI	PA-O1A	-5.59	1.31	1.50
3	A	630	DG6	C5-C4	5.56	1.63	1.53
4	B	660	NAI	O2B-C2B	-5.55	1.29	1.43
4	A	650	NAI	C6N-N1N	5.49	1.50	1.37
3	B	640	DG6	C3-C4	5.48	1.63	1.53
4	A	650	NAI	C3B-C4B	5.37	1.66	1.53
3	B	640	DG6	C2-C3	5.25	1.61	1.52
4	B	660	NAI	O4D-C4D	5.24	1.56	1.45
4	A	650	NAI	C1B-N9A	-5.20	1.32	1.46
4	B	660	NAI	C1B-N9A	-5.16	1.32	1.46
4	A	650	NAI	C4A-N3A	5.03	1.43	1.34
4	A	650	NAI	C1D-N1N	4.92	1.59	1.46
4	A	650	NAI	PN-O3	-4.90	1.54	1.59
3	A	630	DG6	C3-C4	4.90	1.62	1.53
4	B	660	NAI	PN-O3	-4.85	1.54	1.59
4	A	650	NAI	O3B-C3B	-4.76	1.31	1.43
4	B	660	NAI	C8A-N7A	4.62	1.40	1.31
3	B	640	DG6	C5-C4	4.54	1.61	1.53
4	A	650	NAI	C2D-C1D	-4.45	1.39	1.53
4	B	660	NAI	C3B-C4B	4.43	1.64	1.53
4	B	660	NAI	PN-O2N	4.39	1.66	1.50
3	A	630	DG6	P-O1P	-4.37	1.38	1.54
4	A	650	NAI	O4B-C1B	-4.35	1.31	1.42
4	B	660	NAI	C2A-N3A	-4.33	1.26	1.33
4	B	660	NAI	O3B-C3B	-4.29	1.32	1.43
4	B	660	NAI	PN-O1N	-4.06	1.36	1.55
4	B	660	NAI	C1D-N1N	4.04	1.57	1.46
4	A	650	NAI	C3D-C4D	-3.92	1.43	1.53
3	A	630	DG6	C2-C1	3.91	1.64	1.51
4	B	660	NAI	C8A-N9A	-3.88	1.30	1.37
4	A	650	NAI	C2B-C1B	3.74	1.65	1.53
4	A	650	NAI	PN-O1N	-3.72	1.38	1.55
4	A	650	NAI	C2D-C3D	3.69	1.63	1.53
3	A	630	DG6	P-O3P	-3.67	1.39	1.50
4	A	650	NAI	C7N-N7N	-3.61	1.22	1.33
4	A	650	NAI	C4N-C3N	-3.43	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	640	DG6	P-O1P	-3.36	1.42	1.54
4	A	650	NAI	O3D-C3D	-3.23	1.35	1.43
3	A	630	DG6	P-O2P	-3.21	1.42	1.54
4	B	660	NAI	C6N-C5N	3.20	1.42	1.33
4	A	650	NAI	PA-O2A	-3.18	1.40	1.55
4	A	650	NAI	O7N-C7N	-3.13	1.17	1.24
4	A	650	NAI	C4A-N9A	-3.11	1.31	1.37
4	B	660	NAI	O3D-C3D	-3.09	1.35	1.43
4	B	660	NAI	C6A-N6A	3.08	1.42	1.34
4	A	650	NAI	O2D-C2D	3.07	1.50	1.43
4	B	660	NAI	C2B-C3B	-2.92	1.45	1.53
4	A	650	NAI	C5D-C4D	2.88	1.60	1.51
4	B	660	NAI	O2D-C2D	2.81	1.49	1.43
4	B	660	NAI	C2N-C3N	2.80	1.42	1.35
4	A	650	NAI	PN-O2N	2.80	1.60	1.50
4	A	650	NAI	O5D-C5D	-2.62	1.34	1.44
4	A	650	NAI	C5A-C6A	2.53	1.48	1.41
3	A	630	DG6	O4-C4	2.50	1.49	1.43
4	B	660	NAI	C4N-C5N	-2.48	1.42	1.49
4	B	660	NAI	C4N-C3N	2.43	1.54	1.50
4	B	660	NAI	PA-O5B	2.36	1.68	1.59
3	B	640	DG6	O4-C4	2.30	1.48	1.43
4	B	660	NAI	C5A-C6A	2.28	1.47	1.41
4	B	660	NAI	C4A-N9A	2.20	1.42	1.37
3	B	640	DG6	P-O3P	-2.14	1.43	1.50
4	A	650	NAI	O4D-C4D	2.12	1.49	1.45
4	B	660	NAI	C2D-C1D	-2.07	1.47	1.53
4	A	650	NAI	PA-O5B	2.06	1.67	1.59
4	B	660	NAI	O4B-C4B	2.06	1.49	1.45
3	B	640	DG6	P-O2P	-2.05	1.47	1.54

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	O4D-C1D-N1N	7.82	123.00	108.08
4	A	650	NAI	O2A-PA-O1A	6.28	141.64	112.44
4	B	660	NAI	O4D-C1D-N1N	5.63	118.82	108.08
3	A	630	DG6	C6-C5-C4	5.58	122.75	112.22
4	A	650	NAI	O7N-C7N-N7N	-5.55	110.45	122.89
3	B	640	DG6	C6-C5-C4	5.42	122.45	112.22
4	B	660	NAI	O2A-PA-O1A	5.31	137.15	112.44
3	A	630	DG6	O6-C6-C5	5.20	123.24	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	O3-PN-O2N	4.95	125.60	110.70
3	B	640	DG6	O5-C5-C6	4.74	120.43	109.99
3	A	630	DG6	O5-C5-C6	4.34	119.55	109.99
4	B	660	NAI	O2D-C2D-C1D	-4.31	95.27	110.10
4	B	660	NAI	C2D-C1D-N1N	4.00	123.14	113.31
4	B	660	NAI	O7N-C7N-N7N	-3.85	114.27	122.89
4	B	660	NAI	O3-PA-O1A	-3.80	99.27	110.70
4	B	660	NAI	C2A-N3A-C4A	-3.77	102.62	111.83
4	A	650	NAI	C3N-C7N-N7N	3.69	124.23	117.67
4	B	660	NAI	C1B-N9A-C8A	3.66	135.22	127.09
4	A	650	NAI	C2A-N1A-C6A	3.58	124.61	118.73
4	B	660	NAI	C4A-N9A-C1B	-3.56	118.30	126.63
4	B	660	NAI	C5B-C4B-C3B	-3.52	102.53	115.21
4	B	660	NAI	C2A-N1A-C6A	3.51	124.49	118.73
4	B	660	NAI	O3B-C3B-C4B	3.50	121.13	111.08
4	B	660	NAI	N3A-C2A-N1A	3.49	133.86	128.58
3	A	630	DG6	O5-C5-C4	3.48	117.39	109.25
4	A	650	NAI	O2D-C2D-C1D	-3.40	98.39	110.10
4	A	650	NAI	O3-PA-O1A	-3.37	100.55	110.70
3	B	640	DG6	O5-C5-C4	3.35	117.09	109.25
3	B	640	DG6	O6-C6-C5	3.27	118.09	109.36
4	A	650	NAI	O2A-PA-O3	-3.24	98.53	107.27
4	B	660	NAI	O2A-PA-O3	-3.18	98.69	107.27
4	B	660	NAI	O3D-C3D-C4D	-3.16	102.00	111.08
4	A	650	NAI	C5A-N7A-C8A	-3.05	98.65	103.45
4	A	650	NAI	C4A-N9A-C1B	-3.05	119.51	126.63
4	B	660	NAI	C5A-N7A-C8A	-3.01	98.72	103.45
4	B	660	NAI	O3-PN-O2N	2.97	119.63	110.70
4	B	660	NAI	O5D-PN-O2N	2.90	120.44	108.94
3	B	640	DG6	O2P-P-O6	2.89	114.22	106.67
4	A	650	NAI	C2D-C1D-N1N	2.88	120.39	113.31
4	B	660	NAI	C4A-C5A-N7A	2.66	113.63	110.58
4	B	660	NAI	O4B-C4B-C5B	-2.64	100.89	109.33
4	A	650	NAI	C1B-N9A-C8A	2.63	132.94	127.09
4	B	660	NAI	O7N-C7N-C3N	2.60	125.79	120.90
4	A	650	NAI	C5A-C4A-N9A	2.56	108.60	105.81
3	A	630	DG6	O2P-P-O6	2.48	113.15	106.67
4	B	660	NAI	C3D-C2D-C1D	2.43	106.05	101.46
4	A	650	NAI	O4B-C4B-C3B	-2.37	100.44	105.15
4	A	650	NAI	O7N-C7N-C3N	2.31	125.24	120.90
4	B	660	NAI	N6A-C6A-N1A	2.29	123.49	118.38
3	A	630	DG6	C5-C4-C3	-2.29	109.76	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	630	DG6	C2-C3-C4	-2.27	110.37	113.97
4	B	660	NAI	O2D-C2D-C3D	-2.21	104.73	111.82
4	B	660	NAI	O2B-C2B-C3B	-2.10	105.08	111.82
4	A	650	NAI	O4B-C4B-C5B	-2.09	102.63	109.33
4	A	650	NAI	C3D-C2D-C1D	2.08	105.40	101.46
4	B	660	NAI	C5A-C6A-N1A	-2.03	112.37	117.51

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	630	DG6	C5
3	B	640	DG6	C5

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	630	DG6	C2-C3-C4-C5
3	A	630	DG6	O4-C4-C5-O5
3	A	630	DG6	O5-C5-C6-O6
3	B	640	DG6	O1-C1-C2-C3
3	B	640	DG6	C2-C3-C4-O4
3	B	640	DG6	C2-C3-C4-C5
3	B	640	DG6	O3-C3-C4-O4
3	B	640	DG6	O3-C3-C4-C5
3	B	640	DG6	C3-C4-C5-O5
3	B	640	DG6	O4-C4-C5-O5
3	B	640	DG6	C4-C5-C6-O6
4	A	650	NAI	C5B-O5B-PA-O1A
4	A	650	NAI	C5D-O5D-PN-O3
4	A	650	NAI	O4D-C1D-N1N-C6N
4	B	660	NAI	C5B-O5B-PA-O1A
4	B	660	NAI	O4D-C1D-N1N-C6N
4	A	650	NAI	O4D-C4D-C5D-O5D
3	A	630	DG6	C3-C4-C5-O5
3	A	630	DG6	C1-C2-C3-O3
4	A	650	NAI	C3D-C4D-C5D-O5D
3	A	630	DG6	O3-C3-C4-O4
3	A	630	DG6	O3-C3-C4-C5
3	A	630	DG6	C1-C2-C3-C4
3	A	630	DG6	C3-C4-C5-C6
4	A	650	NAI	C5D-O5D-PN-O1N
4	A	650	NAI	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	A	630	DG6	C2-C3-C4-O4

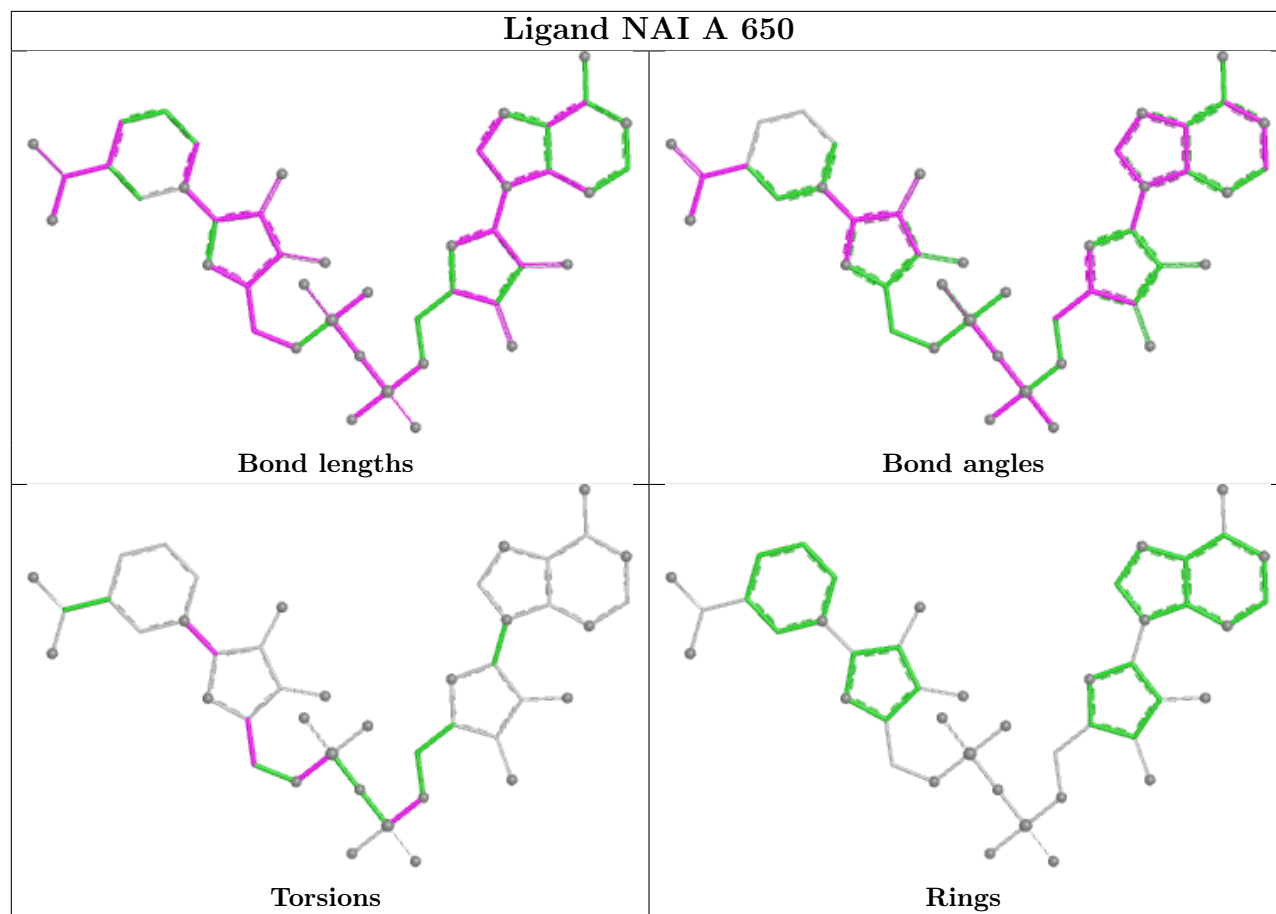
There are no ring outliers.

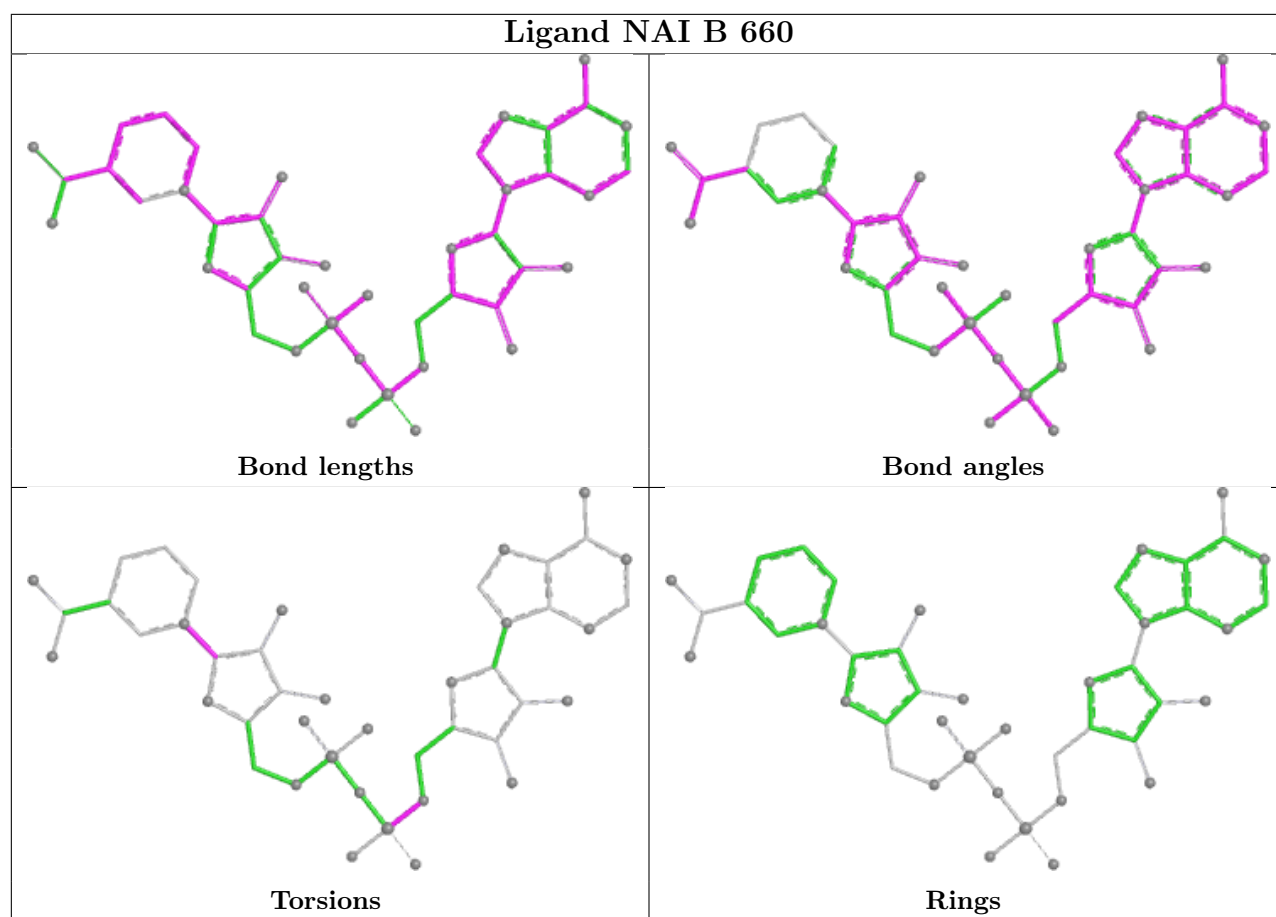
4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	640	DG6	17	0
3	A	630	DG6	10	0
4	A	650	NAI	9	0
4	B	660	NAI	2	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.

Ligand NAI A 650





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.