



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 07:56 AM EDT

PDB ID : 1JKI  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

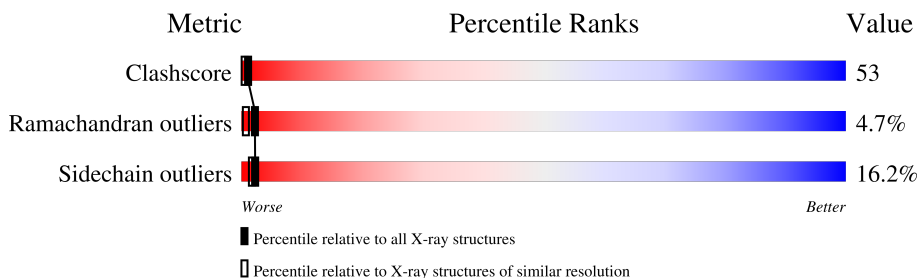
# 1 Overall quality at a glance

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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  $\geq 3$ , 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](#)

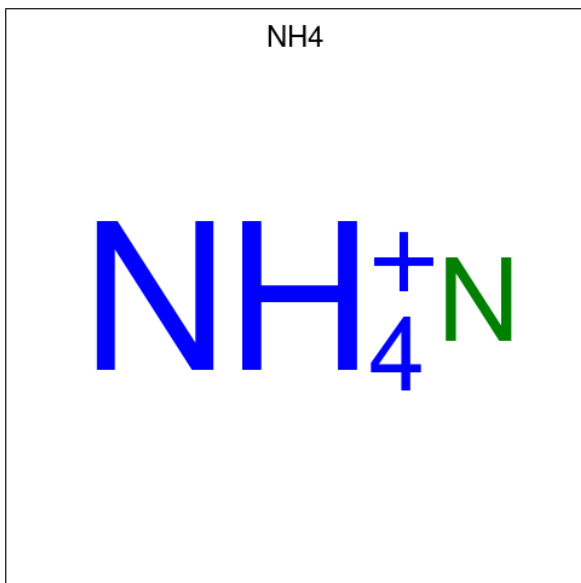
There are 5 unique types of molecules in this entry. The entry contains 9006 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

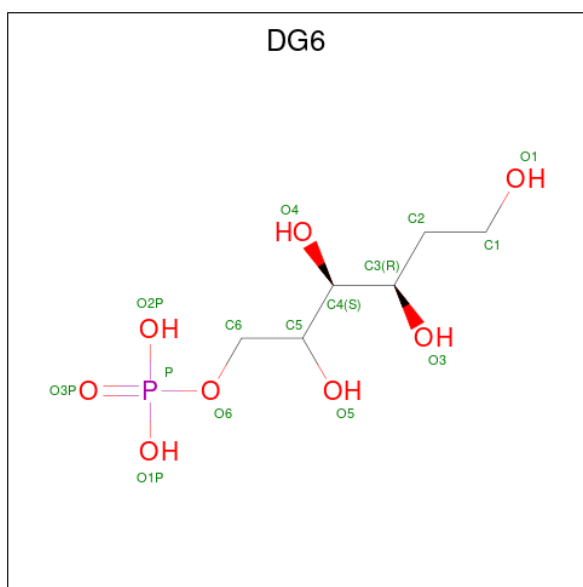
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	525	4138	2632	695	795	16	0	0	0
1	B	524	4130	2626	694	794	16	0	0	0

- Molecule 2 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



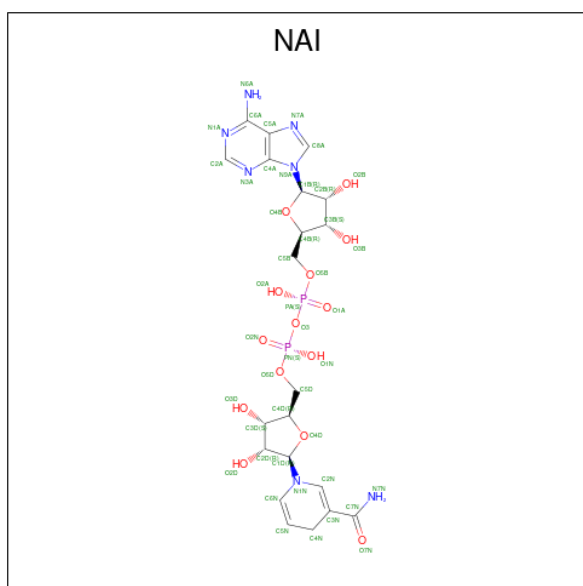
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			1	1		
2	B	1	Total	N	0	0
			1	1		

- Molecule 3 is 2-DEOXY-GLUCITOL-6-PHOSPHATE (three-letter code: DG6) (formula: C<sub>6</sub>H<sub>15</sub>O<sub>8</sub>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 (three-letter code: NAI) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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
			Total	C	N	O	P		
4	B	1	44	21	7	14	2	0	0

- Molecule 5 is water.

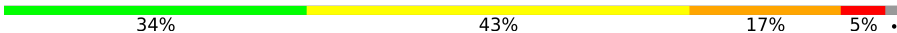
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total	O	0	0
			303	303		
5	B	315	Total	O	0	0
			315	315		

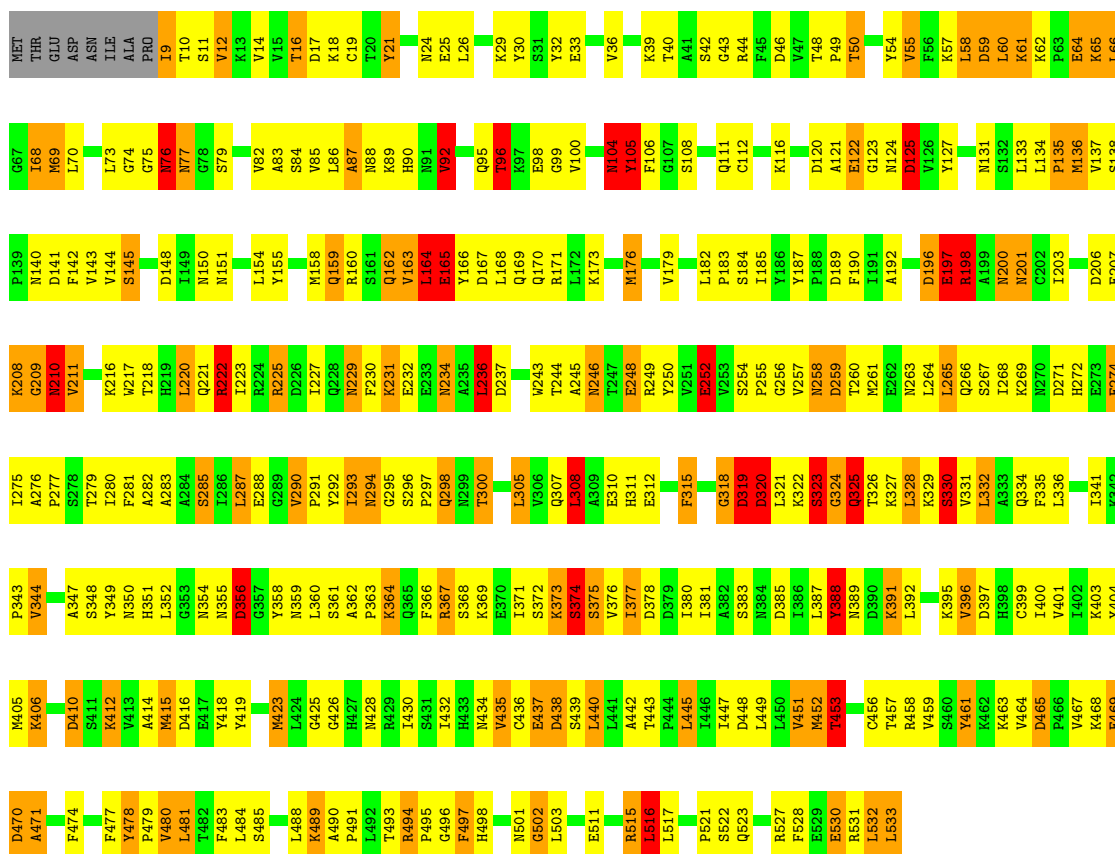
### 3 Residue-property plots

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.

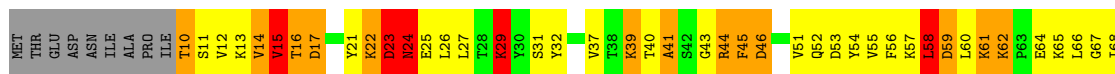
- Molecule 1: myo-inositol-1-phosphate synthase

Chain A: 



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

Chain B: 



L481	L482	F483	L484	S485	Y486	W487	L488	K489	A490	P491	L492	T493	R494	P495	G496	F497	H498	P499	V500	N501	G502	L503	N504	K505	Q506	R507	L510	E511	L514	R515	L516	L517	I518	G519	L520	P521	S522	Q523	N524	E525	L526	R527	F528	E529	E530	O531	L532	L533								
A414	M415	D416	E417	Y418	Y419	M420	G426	D427	H427	N428	H429	I430	S431	G436	E437	D438	S439	L440	L441	A442	T443	P444	L445	F446	I447	D448	L449	L450	V451	M452	T453	E454	F455	G456	T457	R458	V459	S460	Y461	K462	K463	V464	D465	P466	V467	K468	E469	D470	A471	G472	K473	F474	F477	Y478	P479	V480
A347	S348	Y349	N350	H351	L352	G353	N354	N355	D356	G357	Y358	N359	L360	S361	A362	F363	K364	Q365	F366	R367	S368	K369	E370	I371	S372	K373	S374	S375	V376	I377	D378	D379	I380	D385	I386	L387	Y388	L392	K395	V396	D397	H398	G399	V400	I401	I402	K403	Y404	M405	K406	P407	V408	S411	K412	V413	
A282	I286	L287	E288	G289	V290	P291	Y292	I293	N294	G295	S296	P297	Q298	N299	V302	P303	G304	L305	E332	E233	L236	D237	K238	V239	I240	V241	V242	F315	I316	A317	G318	D319	D320	L321	K322	S323	G324	Q325	K327	L328	K329	S330	V331	L332	A333	Q334	F335	L336	V337	D338	K342	F343	V344	S345	I346	
K208	G209	N210	V211	T212	T213	K216	W217	I149	M150	M151	A152	D153	L154	Y155	M158	Q159	R160	S161	Q162	V163	L164	E165	Y166	D167	L168	Q169	Q170	R171	L172	K173	M176	S177	A245	N246	E248	R249	Y250	V251	E252	V253	S254	P255	G256	V257	N258	D259	T260	M261	L264	L265	E273	E274	I275	A276	P277	S278
M69	L70	I71	G72	L73	G74	G75	N76	S79	T80	L81	W82	A83	S84	W85	L86	A87	V92	E93	F94	Q95	T96	K97	K101	Q102	P103	M104	Y105	E106	G107	M109	S113	T114	L115	K116	I119	E122	G123	M124	D125	V126	P129	F130	M131	S132	L133	L134	P135	M136	V137	S138	P139					
N140	D141	F142	V143	V144	W147	D148	I149	M150	M151	A152	D153	L154	Y155	M158	Q159	R160	S161	Q162	V163	L164	E165	Y166	D167	L168	Q169	Q170	R171	L172	K173	M176	S177	A184	I185	Y186	Y187	F190	I191	A192	D194	A195	M194	Q195	D196	E197	R198	A199	N200	N201	M204	L205	D206	E207				

## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	9006	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP



## 5 Model quality i

### 5.1 Standard geometry i

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	1.87	91/4219 (2.2%)	1.52	58/5719 (1.0%)
1	B	1.95	97/4211 (2.3%)	1.69	81/5708 (1.4%)
All	All	1.91	188/8430 (2.2%)	1.61	139/11427 (1.2%)

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 (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	MET	CB-CG	9.86	1.82	1.51
1	A	165	GLU	CB-CG	9.64	1.70	1.52
1	A	32	TYR	CE1-CZ	8.97	1.50	1.38
1	A	356	ASP	CB-CG	8.89	1.70	1.51
1	A	388	TYR	CE1-CZ	8.76	1.50	1.38
1	A	54	TYR	CG-CD2	-8.69	1.27	1.39
1	B	356	ASP	CB-CG	8.58	1.69	1.51
1	A	77	ASN	CB-CG	8.48	1.70	1.51
1	B	437	GLU	CB-CG	-8.37	1.36	1.52
1	A	459	VAL	CA-CB	8.27	1.72	1.54
1	A	136	MET	CG-SD	8.05	2.02	1.81
1	B	75	GLY	CA-C	-8.05	1.39	1.51
1	A	315	PHE	CB-CG	-8.04	1.37	1.51
1	B	84	SER	CB-OG	7.97	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	ILE	CA-CB	-7.91	1.36	1.54
1	A	456	CYS	CB-SG	7.76	1.95	1.82
1	B	144	VAL	CB-CG1	-7.74	1.36	1.52
1	B	166	TYR	CB-CG	7.66	1.63	1.51
1	B	155	TYR	CE1-CZ	7.53	1.48	1.38
1	A	145	SER	N-CA	-7.47	1.31	1.46
1	B	344	VAL	CB-CG1	7.26	1.68	1.52
1	B	113	SER	CB-OG	-7.25	1.32	1.42
1	B	451	VAL	CA-CB	-7.11	1.39	1.54
1	B	105	TYR	CD1-CE1	7.07	1.50	1.39
1	B	456	CYS	CB-SG	7.07	1.94	1.82
1	A	163	VAL	CB-CG2	-7.03	1.38	1.52
1	B	155	TYR	CG-CD2	7.01	1.48	1.39
1	B	158	MET	SD-CE	7.00	2.17	1.77
1	B	69	MET	CG-SD	-6.97	1.63	1.81
1	B	238	LYS	CD-CE	6.93	1.68	1.51
1	B	15	VAL	CB-CG2	-6.93	1.38	1.52
1	A	84	SER	CA-CB	6.92	1.63	1.52
1	B	231	LYS	CD-CE	6.85	1.68	1.51
1	B	81	LEU	N-CA	6.85	1.60	1.46
1	B	423	MET	SD-CE	-6.81	1.39	1.77
1	A	85	VAL	CB-CG2	6.80	1.67	1.52
1	A	79	SER	CA-CB	6.77	1.63	1.52
1	A	229	ASN	N-CA	6.72	1.59	1.46
1	B	293	ILE	CA-CB	-6.63	1.39	1.54
1	A	143	VAL	CA-CB	6.57	1.68	1.54
1	A	197	GLU	CG-CD	6.57	1.61	1.51
1	B	80	THR	CA-CB	6.55	1.70	1.53
1	B	515	ARG	CG-CD	6.55	1.68	1.51
1	A	158	MET	CG-SD	-6.54	1.64	1.81
1	A	104	ASN	CB-CG	6.53	1.66	1.51
1	B	105	TYR	CE1-CZ	-6.53	1.30	1.38
1	A	87	ALA	CA-CB	6.51	1.66	1.52
1	B	85	VAL	CB-CG2	6.50	1.66	1.52
1	A	197	GLU	CD-OE1	6.49	1.32	1.25
1	B	464	VAL	CB-CG2	-6.49	1.39	1.52
1	A	274	GLU	CG-CD	6.48	1.61	1.51
1	A	108	SER	CA-CB	6.45	1.62	1.52
1	B	138	SER	CA-CB	-6.45	1.43	1.52
1	B	239	VAL	CB-CG2	6.44	1.66	1.52
1	B	116	LYS	CE-NZ	6.43	1.65	1.49
1	A	69	MET	SD-CE	6.43	2.13	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	TYR	CD1-CE1	-6.43	1.29	1.39
1	A	292	TYR	CG-CD1	6.41	1.47	1.39
1	B	530	GLU	CG-CD	6.36	1.61	1.51
1	A	83	ALA	CA-CB	6.36	1.65	1.52
1	B	105	TYR	CE2-CZ	6.35	1.46	1.38
1	A	54	TYR	CB-CG	-6.35	1.42	1.51
1	B	228	GLN	N-CA	6.31	1.58	1.46
1	B	135	PRO	CG-CD	6.31	1.71	1.50
1	B	415	MET	CG-SD	6.31	1.97	1.81
1	A	511	GLU	CD-OE2	6.31	1.32	1.25
1	A	68	ILE	CB-CG2	6.30	1.72	1.52
1	A	437	GLU	CG-CD	6.30	1.61	1.51
1	A	105	TYR	CD2-CE2	6.28	1.48	1.39
1	A	227	ILE	CA-CB	6.26	1.69	1.54
1	A	75	GLY	CA-C	-6.25	1.41	1.51
1	B	460	SER	CA-CB	6.24	1.62	1.52
1	A	105	TYR	CB-CG	6.22	1.60	1.51
1	A	144	VAL	CB-CG1	6.22	1.66	1.52
1	B	418	TYR	CD1-CE1	-6.20	1.30	1.39
1	A	347	ALA	CA-CB	6.19	1.65	1.52
1	A	248	GLU	CG-CD	6.16	1.61	1.51
1	B	358	TYR	CE1-CZ	6.15	1.46	1.38
1	B	14	VAL	CA-CB	6.14	1.67	1.54
1	B	39	LYS	CE-NZ	6.13	1.64	1.49
1	A	64	GLU	CG-CD	6.11	1.61	1.51
1	B	245	ALA	N-CA	-6.11	1.34	1.46
1	A	293	ILE	C-O	6.09	1.34	1.23
1	B	525	GLU	CD-OE2	6.07	1.32	1.25
1	A	30	TYR	CG-CD2	-6.07	1.31	1.39
1	A	166	TYR	CD2-CE2	6.05	1.48	1.39
1	A	453	THR	CB-CG2	-6.04	1.32	1.52
1	B	358	TYR	CG-CD1	6.03	1.47	1.39
1	A	244	THR	CA-CB	-6.02	1.37	1.53
1	B	83	ALA	CA-CB	6.02	1.65	1.52
1	A	137	VAL	CB-CG1	-6.01	1.40	1.52
1	A	69	MET	CB-CG	5.99	1.70	1.51
1	A	418	TYR	CD2-CE2	5.97	1.48	1.39
1	A	232	GLU	CG-CD	5.95	1.60	1.51
1	B	106	PHE	CB-CG	-5.93	1.41	1.51
1	B	141	ASP	CA-C	-5.91	1.37	1.52
1	A	12	VAL	CA-CB	5.88	1.67	1.54
1	A	448	ASP	CB-CG	-5.86	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	ALA	C-O	-5.84	1.12	1.23
1	A	29	LYS	CD-CE	5.82	1.65	1.51
1	A	451	VAL	N-CA	-5.82	1.34	1.46
1	B	108	SER	CA-CB	5.81	1.61	1.52
1	A	344	VAL	CA-CB	5.77	1.66	1.54
1	B	217	TRP	CB-CG	5.75	1.60	1.50
1	B	527	ARG	CG-CD	5.75	1.66	1.51
1	B	79	SER	CA-CB	5.74	1.61	1.52
1	B	151	ASN	CA-C	-5.71	1.38	1.52
1	B	141	ASP	CG-OD2	5.70	1.38	1.25
1	A	414	ALA	CA-CB	5.70	1.64	1.52
1	B	136	MET	SD-CE	-5.70	1.46	1.77
1	B	315	PHE	CB-CG	-5.69	1.41	1.51
1	A	55	VAL	CB-CG1	5.68	1.64	1.52
1	B	310	GLU	CG-CD	5.67	1.60	1.51
1	B	436	CYS	CB-SG	-5.67	1.72	1.81
1	B	288	GLU	CG-CD	5.67	1.60	1.51
1	B	166	TYR	C-O	-5.66	1.12	1.23
1	A	290	VAL	CB-CG2	-5.65	1.41	1.52
1	A	288	GLU	CD-OE2	5.63	1.31	1.25
1	B	405	MET	CG-SD	5.59	1.95	1.81
1	A	252	GLU	CG-CD	5.58	1.60	1.51
1	B	230	PHE	CG-CD1	-5.58	1.30	1.38
1	A	415	MET	SD-CE	5.55	2.08	1.77
1	B	419	TYR	CD1-CE1	5.54	1.47	1.39
1	A	111	GLN	CA-C	-5.54	1.38	1.52
1	B	69	MET	SD-CE	5.52	2.08	1.77
1	B	246	ASN	CG-ND2	5.50	1.46	1.32
1	B	507	ARG	CZ-NH2	5.50	1.40	1.33
1	A	159	GLN	CG-CD	5.46	1.63	1.51
1	B	148	ASP	CB-CG	5.45	1.63	1.51
1	A	105	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	231	LYS	CD-CE	5.45	1.64	1.51
1	B	337	VAL	CA-CB	-5.44	1.43	1.54
1	A	423	MET	SD-CE	-5.44	1.47	1.77
1	B	159	GLN	CG-CD	5.43	1.63	1.51
1	A	252	GLU	CB-CG	5.43	1.62	1.52
1	B	243	TRP	CG-CD1	5.38	1.44	1.36
1	B	232	GLU	CD-OE2	5.38	1.31	1.25
1	B	93	GLU	CG-CD	-5.38	1.43	1.51
1	B	160	ARG	N-CA	-5.37	1.35	1.46
1	A	425	GLY	C-O	-5.35	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	GLU	CG-CD	5.35	1.59	1.51
1	B	288	GLU	CD-OE2	5.34	1.31	1.25
1	A	234	ASN	CG-OD1	-5.34	1.12	1.24
1	A	405	MET	CG-SD	5.33	1.95	1.81
1	A	530	GLU	CG-CD	5.32	1.59	1.51
1	B	45	PHE	CE1-CZ	5.30	1.47	1.37
1	B	511	GLU	CB-CG	-5.29	1.42	1.52
1	A	112	CYS	CB-SG	5.28	1.91	1.82
1	B	194	ASN	CB-CG	5.27	1.63	1.51
1	B	161	SER	CB-OG	5.26	1.49	1.42
1	A	330	SER	CB-OG	5.25	1.49	1.42
1	B	274	GLU	CG-CD	5.25	1.59	1.51
1	A	76	ASN	CB-CG	5.24	1.63	1.51
1	B	388	TYR	CE1-CZ	5.24	1.45	1.38
1	B	72	GLY	C-O	5.24	1.32	1.23
1	A	293	ILE	CA-CB	-5.22	1.42	1.54
1	A	366	PHE	CE1-CZ	5.22	1.47	1.37
1	A	168	LEU	CA-C	-5.21	1.39	1.52
1	B	96	THR	CA-CB	5.21	1.66	1.53
1	B	126	VAL	CB-CG2	5.20	1.63	1.52
1	A	127	TYR	CB-CG	-5.20	1.43	1.51
1	B	442	ALA	N-CA	-5.19	1.35	1.46
1	B	158	MET	CG-SD	-5.18	1.67	1.81
1	A	325	GLN	CG-CD	5.17	1.62	1.51
1	A	19	CYS	CB-SG	5.16	1.91	1.82
1	B	464	VAL	CA-CB	-5.15	1.44	1.54
1	A	435	VAL	CB-CG2	5.15	1.63	1.52
1	A	158	MET	CB-CG	-5.14	1.34	1.51
1	B	143	VAL	CA-CB	5.14	1.65	1.54
1	B	29	LYS	CE-NZ	5.12	1.61	1.49
1	A	54	TYR	CE1-CZ	-5.12	1.31	1.38
1	B	248	GLU	CD-OE2	5.12	1.31	1.25
1	A	61	LYS	CE-NZ	5.12	1.61	1.49
1	B	515	ARG	CZ-NH2	5.11	1.39	1.33
1	A	438	ASP	N-CA	-5.09	1.36	1.46
1	B	478	TYR	CA-C	5.09	1.66	1.52
1	A	95	GLN	CG-CD	-5.09	1.39	1.51
1	A	111	GLN	CG-CD	5.09	1.62	1.51
1	A	471	ALA	CA-CB	5.08	1.63	1.52
1	B	487	TRP	CG-CD1	5.08	1.43	1.36
1	A	69	MET	CG-SD	-5.07	1.68	1.81
1	B	377	ILE	CA-CB	5.06	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	190	PHE	CE2-CZ	5.06	1.47	1.37
1	A	451	VAL	CA-CB	-5.04	1.44	1.54
1	B	155	TYR	CD2-CE2	5.03	1.46	1.39
1	A	376	VAL	CA-CB	-5.03	1.44	1.54
1	A	325	GLN	CB-CG	5.02	1.66	1.52
1	B	358	TYR	CE2-CZ	5.00	1.45	1.38

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	NE-CZ-NH2	-21.35	109.62	120.30
1	B	222	ARG	NE-CZ-NH1	18.52	129.56	120.30
1	B	321	LEU	CB-CG-CD2	-13.96	87.26	111.00
1	A	423	MET	CG-SD-CE	13.56	121.90	100.20
1	B	153	ASP	CB-CG-OD2	11.97	129.07	118.30
1	B	438	ASP	CB-CG-OD2	-11.48	107.97	118.30
1	A	171	ARG	NE-CZ-NH2	11.17	125.89	120.30
1	B	507	ARG	NE-CZ-NH1	-10.83	114.88	120.30
1	B	338	ASP	CB-CG-OD1	-10.04	109.27	118.30
1	A	236	LEU	CA-CB-CG	10.01	138.32	115.30
1	B	224	ARG	NE-CZ-NH2	-9.73	115.43	120.30
1	B	321	LEU	CB-CG-CD1	9.61	127.34	111.00
1	A	494	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	198	ARG	N-CA-C	-9.18	86.22	111.00
1	B	338	ASP	CB-CG-OD2	8.78	126.20	118.30
1	B	167	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	171	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	B	526	LEU	C-N-CA	-8.62	100.15	121.70
1	B	59	ASP	CB-CG-OD1	-8.59	110.57	118.30
1	B	158	MET	CA-CB-CG	8.52	127.79	113.30
1	B	44	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	B	261	MET	CG-SD-CE	8.15	113.25	100.20
1	A	356	ASP	N-CA-CB	-8.13	95.97	110.60
1	B	59	ASP	CB-CG-OD2	8.10	125.59	118.30
1	B	158	MET	CG-SD-CE	-8.09	87.26	100.20
1	B	502	GLY	N-CA-C	-8.02	93.05	113.10
1	B	320	ASP	CB-CG-OD1	-8.00	111.10	118.30
1	B	321	LEU	CA-CB-CG	8.00	133.70	115.30
1	A	209	GLY	N-CA-C	-7.95	93.22	113.10
1	A	318	GLY	C-N-CA	7.95	141.58	121.70
1	A	125	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	B	430	ILE	CG1-CB-CG2	-7.73	94.40	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	MET	CG-SD-CE	-7.70	87.88	100.20
1	B	448	ASP	CB-CG-OD1	7.67	125.21	118.30
1	B	81	LEU	CA-CB-CG	-7.62	97.76	115.30
1	A	356	ASP	CB-CG-OD1	7.53	125.07	118.30
1	B	323	SER	N-CA-C	-7.52	90.69	111.00
1	B	73	LEU	CB-CG-CD2	7.47	123.70	111.00
1	B	136	MET	CG-SD-CE	-7.46	88.26	100.20
1	B	318	GLY	N-CA-C	7.08	130.81	113.10
1	B	167	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	B	171	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	516	LEU	CA-CB-CG	6.99	131.37	115.30
1	B	473	LYS	N-CA-C	6.99	129.87	111.00
1	B	516	LEU	CA-CB-CG	6.94	131.27	115.30
1	B	471	ALA	N-CA-C	-6.87	92.44	111.00
1	A	59	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	A	237	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	164	LEU	CA-CB-CG	6.78	130.89	115.30
1	B	470	ASP	N-CA-C	6.71	129.12	111.00
1	B	445	LEU	CB-CG-CD1	-6.69	99.62	111.00
1	B	315	PHE	CB-CA-C	-6.60	97.20	110.40
1	B	323	SER	N-CA-CB	-6.60	100.60	110.50
1	A	92	VAL	CG1-CB-CG2	6.54	121.37	110.90
1	B	459	VAL	CB-CA-C	-6.54	98.97	111.40
1	B	438	ASP	CB-CG-OD1	6.53	124.18	118.30
1	B	58	LEU	CA-CB-CG	6.49	130.23	115.30
1	B	17	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	B	325	GLN	N-CA-C	-6.45	93.59	111.00
1	A	141	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	410	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	158	MET	CA-CB-CG	6.38	124.16	113.30
1	A	320	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	356	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	96	THR	OG1-CB-CG2	6.28	124.45	110.00
1	A	448	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	167	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	210	ASN	N-CA-C	6.23	127.83	111.00
1	B	97	LYS	CD-CE-NZ	-6.21	97.41	111.70
1	B	208	LYS	N-CA-C	-6.19	94.29	111.00
1	B	158	MET	N-CA-CB	6.17	121.70	110.60
1	B	46	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	225	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	332	LEU	CA-CB-CG	-6.14	101.18	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLY	N-CA-C	-6.11	97.81	113.10
1	A	60	LEU	CA-CB-CG	6.05	129.21	115.30
1	B	163	VAL	CG1-CB-CG2	6.04	120.57	110.90
1	B	176	MET	CG-SD-CE	6.02	109.83	100.20
1	A	515	ARG	CG-CD-NE	-6.02	99.16	111.80
1	A	143	VAL	N-CA-C	-6.01	94.77	111.00
1	B	222	ARG	CG-CD-NE	-6.00	99.19	111.80
1	B	526	LEU	O-C-N	-6.00	113.09	122.70
1	B	318	GLY	C-N-CA	6.00	136.70	121.70
1	B	448	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	452	MET	CG-SD-CE	5.98	109.77	100.20
1	B	168	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	70	LEU	CA-CB-CG	5.91	128.88	115.30
1	B	153	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	B	173	LYS	CD-CE-NZ	-5.89	98.16	111.70
1	A	96	THR	N-CA-CB	-5.88	99.13	110.30
1	B	527	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	465	ASP	CB-CG-OD1	5.86	123.57	118.30
1	B	379	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	379	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	62	LYS	CD-CE-NZ	5.84	125.12	111.70
1	B	222	ARG	CD-NE-CZ	5.78	131.70	123.60
1	A	318	GLY	CA-C-N	-5.78	104.48	117.20
1	A	59	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	305	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	251	VAL	N-CA-C	-5.70	95.61	111.00
1	B	308	LEU	CA-CB-CG	5.70	128.41	115.30
1	A	46	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	196	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	308	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	323	SER	N-CA-C	5.56	126.01	111.00
1	A	419	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	A	136	MET	CG-SD-CE	-5.55	91.32	100.20
1	B	44	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	A	435	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	A	452	MET	CB-CG-SD	5.37	128.51	112.40
1	A	17	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	396	VAL	N-CA-C	-5.35	96.55	111.00
1	B	356	ASP	N-CA-CB	-5.33	101.00	110.60
1	A	410	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	B	356	ASP	OD1-CG-OD2	-5.30	113.23	123.30
1	B	133	LEU	CA-CB-CG	5.30	127.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	B	73	LEU	CB-CG-CD1	-5.26	102.06	111.00
1	B	137	VAL	CB-CA-C	-5.26	101.41	111.40
1	A	344	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	A	220	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	437	GLU	C-N-CA	-5.18	108.74	121.70
1	A	138	SER	CA-CB-OG	-5.16	97.27	111.20
1	A	182	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	430	ILE	C-N-CA	-5.16	108.81	121.70
1	A	145	SER	CB-CA-C	5.13	119.84	110.10
1	B	24	ASN	N-CA-C	-5.13	97.16	111.00
1	A	222	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	395	LYS	CD-CE-NZ	5.11	123.45	111.70
1	B	494	ARG	N-CA-C	-5.09	97.25	111.00
1	B	296	SER	CB-CA-C	-5.09	100.44	110.10
1	B	23	ASP	C-N-CA	5.08	134.41	121.70
1	B	418	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	B	187	TYR	N-CA-C	-5.06	97.33	111.00
1	A	452	MET	CG-SD-CE	-5.06	92.11	100.20
1	B	445	LEU	CB-CG-CD2	5.06	119.59	111.00
1	A	439	SER	CA-CB-OG	-5.04	97.58	111.20
1	B	172	LEU	CB-CA-C	-5.04	100.62	110.20
1	A	434	ASN	C-N-CA	-5.03	109.11	121.70

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	420	1
1	B	4130	0	4136	505	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	8	0
4	B	44	0	24	3	0
5	A	303	0	0	55	0
5	B	315	0	0	63	0
All	All	9006	0	8353	891	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 53.

All (891) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:ASP:CG	1:B:24:ASN:H	1.75	0.90
1:B:61:LYS:NZ	5:B:937:HOH:O	2.02	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:B:168:LEU:HD13	1:B:168:LEU:C	1.93	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:HA	1:B:95:GLN:NE2	1.89	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: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
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:HB2	1:B:368:SER:HB3	1.60	0.83
1:B:494:ARG:HG3	5:B:842:HOH:O	1.76	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:PRO:HD3	1:B:320:ASP:CG	2.03	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
1:A:334:GLN:HE22	1:A:380:ILE:HG12	1.48	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:365:GLN:CD	5:B:990:HOH:O	2.21	0.79
1:B:286:ILE:CG2	1:B:308:LEU:HD12	2.11	0.78
1:A:294:ASN:C	1:A:294:ASN:ND2	2.36	0.78
1:B:258:ASN:HD22	1:B:258:ASN:H	1.32	0.78
1:A:294:ASN:C	1:A:294:ASN:HD22	1.84	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:B:191:ILE:HD13	1:B:191:ILE:H	1.49	0.76
1:B:116:LYS:HE3	1:B:125:ASP:CG	2.06	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:B:261:MET:CE	1:B:308:LEU:HA	2.15	0.75
1:A:293:ILE:HD11	1:A:453:THR:HG21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:24:ASN:OD1	5:A:724:HOH:O	2.06	0.74
1:B:23:ASP:CG	1:B:24:ASN:N	2.36	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:131:ASN:HA	1:B:136:MET:HE2	1.70	0.74
1:B:480:VAL:HG21	1:B:492:LEU:HD12	1.68	0.73
1:B:373:LYS:HZ1	1:B:376:VAL:HG12	1.53	0.73
1:B:254:SER:H	1:B:258:ASN:HD21	1.36	0.73
1:B:372:SER:OG	1:B:489:LYS:HE3	1.89	0.73
1:A:207:GLU:OE1	1:A:207:GLU:HA	1.89	0.73
1:A:122:GLU:H	1:A:122:GLU:CD	1.92	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: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: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: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:109:MET:HE3	1:B:487:TRP:CZ2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:369:LYS:HZ1	3:B:640:DG6:HC62	1.54	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: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:A:122:GLU:C	1:A:124:ASN:H	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:C	1:A:516:LEU:HD23	2.15	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
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:B:131:ASN:HB2	1:B:136:MET:CE	2.26	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:B:261:MET:HE2	1:B:308:LEU:HA	1.78	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:B:58:LEU:HD13	1:B:60:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:LEU:HB3	1:A:176:MET:HE2	1.80	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: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: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:364:LYS:HE3	1:B:364:LYS:H	1.63	0.64
1:B:131:ASN:HB2	1:B:136:MET:HE1	1.78	0.64
1:A:389:ASN:OD1	1:A:391:LYS:N	2.30	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: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:451:VAL:O	1:A:451:VAL:CG1	2.47	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: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:322:LYS:HZ2	1:A:503:LEU:HD12	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:406:LYS:HD2	1:A:406:LYS:C	2.17	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: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: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:B:261:MET:HE3	1:B:308:LEU:HA	1.81	0.60
1:B:261:MET:HE1	1:B:311:HIS:HB2	1.82	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:B:109:MET:HE3	1:B:487:TRP:HZ2	1.67	0.60
1:A:68:ILE:HD13	1:A:142:PHE:CG	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLU:CD	1:A:122:GLU:N	2.55	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: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:NE2	1:B:95:GLN:CA	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
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: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:330:SER:O	1:A:331:VAL:C	2.40	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:A:399:CYS:C	1:A:400:ILE:HD12	2.23	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:131:ASN:CB	1:B:136:MET:HE1	2.32	0.59
1:B:151:ASN:C	1:B:151:ASN:HD22	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:331:VAL:C	5:A:907:HOH:O	2.41	0.58
1:B:345:SER:HA	1:B:397:ASP:O	2.04	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:261:MET:HE3	1:B:308:LEU:CA	2.34	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: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: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:494:ARG:O	1:B:497:PHE:HB2	2.04	0.57
1:A:197:GLU:C	1:A:197:GLU:OE1	2.42	0.57
1:B:365:GLN:NE2	1:B:365:GLN:N	2.52	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: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:116:LYS:HE3	1:A:125:ASP:CG	2.25	0.56
1:A:246:ASN:ND2	4:A:650:NAI:H8A	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:MET:CE	1:B:487:TRP:CZ2	2.88	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:303:PRO:CG	1:B:304:GLY:N	2.69	0.56
1:B:14:VAL:HG22	1:B:16:THR:HG22	1.88	0.56
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:168:LEU:C	1:B:168:LEU:CD1	2.71	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:LYS:NZ	5:A:970:HOH:O	2.35	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:A:261:MET:HE3	1:A:311:HIS:HB3	1.89	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
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:22:LYS:O	1:B:23:ASP:C	2.44	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:A:423:MET:CE	1:B:443:THR:HB	2.38	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:A:96:THR:HG23	1:A:98:GLU:N	2.20	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:A:104:ASN:C	1:A:104:ASN:HD22	2.11	0.53
1:A:218:THR:CG2	5:A:836:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PRO:HD2	1:A:364:LYS:CE	2.35	0.53
1:B:258:ASN:N	1:B:258:ASN:ND2	2.56	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: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
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:B:350:ASN:C	1:B:350:ASN:HD22	2.13	0.52
1:B:259:ASP:OD2	1:B:260:THR:N	2.42	0.52
1:B:130:PHE:CE2	1:B:452:MET:HE3	2.44	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:322:LYS:HZ2	1:A:503:LEU:CD1	2.23	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:A:120:ASP:O	1:A:121:ALA:C	2.47	0.52
1:A:200:ASN:C	1:A:200:ASN:HD22	2.12	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:B:327:LYS:NZ	5:B:993:HOH:O	2.42	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: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:B:261:MET:HE3	1:B:308:LEU:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:516:LEU:C	1:A:516:LEU:CD2	2.79	0.50
1:B:187:TYR:OH	1:B:219:HIS:CD2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:443:THR:CG2	1:B:423:MET:HE1	2.42	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:423:MET:HE1	1:B:443:THR:CG2	2.43	0.49
1:B:352:LEU:HA	1:B:411:SER:O	2.11	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:108:SER:OG	1:B:448:ASP:OD2	2.27	0.49
1:B:173:LYS:NZ	5:B:968:HOH:O	2.26	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:B:130:PHE:CE2	1:B:452:MET:CE	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:121:ALA:HB3	1:A:122:GLU:CD	2.34	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:B:369:LYS:HZ1	4:B:660:NAI:H2D	1.78	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: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:B:242:LEU:HD23	1:B:242:LEU:C	2.35	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:B:369:LYS:HZ2	3:B:640:DG6:HC62	1.75	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: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:B:489:LYS:C	1:B:491:PRO:HD3	2.34	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:491:PRO:CD	1:A:501:ASN:HD21	2.28	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:TRP:CZ2	1:A:245:ALA:HB3	2.50	0.46
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:354:ASN:CG	1:B:356:ASP:CG	2.74	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:353:GLY:N	1:B:408:VAL:HG23	2.31	0.46
1:B:486:TYR:CG	1:B:486:TYR:O	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:358:TYR:HD1	1:A:404:TYR:CE2	2.33	0.45
1:B:173:LYS:O	1:B:177:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:ASN:ND2	1:A:200:ASN:C	2.70	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:167:ASP:O	1:B:167:ASP:CG	2.55	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:243:TRP:CD1	1:A:243:TRP:C	2.90	0.45
1:A:250:TYR:CE1	1:A:371:ILE:HG21	2.52	0.45
1:A:412:LYS:C	5:A:956:HOH:O	2.53	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: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: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:439:SER:OG	4:B:660:NAI:O7N	2.28	0.44
1:B:481:LEU:HB3	1:B:484:LEU:HD23	1.99	0.44
1:A:21:TYR:CZ	1:A:26:LEU:HD13	2.52	0.44
1:A:389:ASN:OD1	1:A:389:ASN:C	2.55	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: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
1:A:308:LEU:CD2	1:A:312:GLU:CG	2.96	0.44
1:A:322:LYS:NZ	1:A:503:LEU:CD1	2.75	0.44
1:B:64:GLU:HG2	5:B:772:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:455:PHE:O	1:B:456:CYS:C	2.56	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: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: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:151:ASN:C	1:B:151:ASN:ND2	2.72	0.43
1:B:438:ASP:OD1	2:B:680:NH4:N	2.50	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: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:194:ASN:HD22	1:B:194:ASN:C	2.22	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:B:276:ALA:O	1:B:277:PRO:C	2.55	0.43
1:A:528:PHE:HB3	1:A:532:LEU:HD22	2.01	0.43
1:B:286:ILE:C	1:B:288:GLU:N	2.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASN:HD21	1:A:392:LEU:HG	1.82	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:A:502:GLY:O	1:A:503:LEU:C	2.58	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:372:SER:CB	5:B:801:HOH:O	2.67	0.42
1:B:303:PRO:O	1:B:306:VAL:N	2.52	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: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: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:B:455:PHE:C	1:B:457:THR:N	2.71	0.42
1:A:148:ASP:C	1:A:150:ASN:H	2.22	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: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:325:GLN:HE21	1:B:412:LYS:HE2	1.84	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:316:ILE:C	1:B:316:ILE:CD1	2.88	0.42
1:B:349:TYR:O	1:B:350:ASN:HB3	2.19	0.42
1:B:529:GLU:CD	1:B:529:GLU:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:96:THR:CG2	1:A:98:GLU:N	2.81	0.41
1:A:136:MET:HE1	1:A:452:MET:SD	2.60	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:73:LEU:HG	1:A:154:LEU:HD11	2.01	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:322:LYS:O	1:B:323:SER:C	2.56	0.41
1:B:473:LYS:HG3	1:B:474:PHE:O	2.21	0.41
1:B:306:VAL:O	1:B:310:GLU:HG3	2.21	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
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:253:VAL:HG22	1:B:302:VAL:HG12	2.02	0.41
1:A:48:THR:HA	1:A:49:PRO:HD3	1.97	0.41
1:A:197:GLU:C	1:A:197:GLU:CD	2.79	0.41
1:A:248:GLU:OE2	1:A:277:PRO:HD2	2.21	0.41
1:A:291:PRO:CG	5:A:838:HOH:O	2.57	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: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:A:281:PHE:O	1:A:285:SER:OG	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:109:MET:HE3	1:B:487:TRP:CE2	2.56	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: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:294:ASN:ND2	1:A:295:GLY:N	2.64	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
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%)	<b>2</b> <b>1</b>
1	B	522/533 (98%)	444 (85%)	52 (10%)	26 (5%)	<b>2</b> <b>0</b>
All	All	1045/1066 (98%)	907 (87%)	89 (8%)	49 (5%)	<b>2</b> <b>1</b>

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
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

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Mol	Chain	Res	Type
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 [i](#)

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%)	396 (85%)	68 (15%)	3	2
1	B	463/471 (98%)	381 (82%)	82 (18%)	2	1
All	All	927/942 (98%)	777 (84%)	150 (16%)	2	2

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	16	THR
1	A	50	THR
1	A	58	LEU
1	A	65	LYS
1	A	66	LEU
1	A	70	LEU
1	A	76	ASN
1	A	86	LEU
1	A	92	VAL
1	A	96	THR
1	A	100	VAL
1	A	104	ASN
1	A	122	GLU
1	A	135	PRO
1	A	162	GLN
1	A	164	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
1	A	252	GLU
1	A	258	ASN
1	A	259	ASP
1	A	285	SER
1	A	287	LEU
1	A	294	ASN
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	373	LYS
1	A	374	SER
1	A	377	ILE
1	A	378	ASP
1	A	387	LEU
1	A	391	LYS
1	A	397	ASP
1	A	406	LYS
1	A	412	LYS
1	A	440	LEU
1	A	445	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	453	THR
1	A	483	PHE
1	A	484	LEU
1	A	489	LYS
1	A	497	PHE
1	A	516	LEU
1	A	523	GLN
1	A	532	LEU
1	A	533	LEU
1	B	10	THR
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	58	LEU
1	B	61	LYS
1	B	62	LYS
1	B	70	LEU
1	B	73	LEU
1	B	79	SER
1	B	80	THR
1	B	95	GLN
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	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	231	LYS
1	B	233	GLU
1	B	236	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	237	ASP
1	B	257	VAL
1	B	258	ASN
1	B	265	LEU
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	323	SER
1	B	325	GLN
1	B	328	LEU
1	B	329	LYS
1	B	330	SER
1	B	332	LEU
1	B	350	ASN
1	B	356	ASP
1	B	361	SER
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	415	MET
1	B	441	LEU
1	B	457	THR
1	B	465	ASP
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	497	PHE

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Mol	Chain	Res	Type
1	B	504	ASN
1	B	510	LEU
1	B	514	LEU
1	B	515	ARG
1	B	517	LEU
1	B	522	SER
1	B	532	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
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	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	350	ASN
1	A	359	ASN
1	A	428	ASN
1	A	501	ASN
1	A	512	ASN

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Mol	Chain	Res	Type
1	A	523	GLN
1	B	24	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	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 [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	3.87	8 (57%)	18,19,19	2.22	6 (33%)
4	NAI	A	650	-	42,48,48	3.79	26 (61%)	47,73,73	2.38	15 (31%)
4	NAI	B	660	-	42,48,48	3.91	25 (59%)	47,73,73	2.42	20 (42%)
3	DG6	A	630	-	14,14,14	4.56	10 (71%)	18,19,19	2.44	5 (27%)

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	-
4	NAI	A	650	-	-	8/25/72/72	0/5/5/5
4	NAI	B	660	-	-	4/25/72/72	0/5/5/5
3	DG6	A	630	-	1/1/4/4	10/17/17/17	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	660	NAI	O4B-C1B	-11.54	1.25	1.41
4	B	660	NAI	C4A-N3A	10.81	1.50	1.35
3	A	630	DG6	C6-C5	9.39	1.65	1.51
3	B	640	DG6	C6-C5	8.92	1.64	1.51
4	A	650	NAI	O2B-C2B	-8.36	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	A	650	NAI	C2B-C1B	7.56	1.65	1.53
3	A	630	DG6	P-O6	6.79	1.82	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	630	DG6	C2-C3	6.72	1.64	1.52
4	A	650	NAI	O4B-C1B	-6.55	1.31	1.41
4	A	650	NAI	C4A-N3A	5.92	1.43	1.35
4	B	660	NAI	O2B-C2B	-5.84	1.29	1.43
4	B	660	NAI	C6N-N1N	5.80	1.51	1.37
3	B	640	DG6	P-O6	5.58	1.78	1.60
4	A	650	NAI	PA-O1A	-5.49	1.31	1.50
4	B	660	NAI	C6N-C5N	5.35	1.42	1.33
4	A	650	NAI	C3B-C4B	5.33	1.66	1.53
4	A	650	NAI	C6N-N1N	5.32	1.50	1.37
4	B	660	NAI	O4D-C4D	5.21	1.56	1.45
3	A	630	DG6	C5-C4	5.13	1.63	1.53
3	B	640	DG6	C3-C4	5.06	1.63	1.53
4	A	650	NAI	O3B-C3B	-5.01	1.31	1.43
3	B	640	DG6	C2-C3	4.95	1.61	1.52
4	A	650	NAI	C8A-N7A	4.86	1.43	1.34
4	A	650	NAI	C1D-N1N	4.78	1.59	1.46
4	B	660	NAI	O3B-C3B	-4.52	1.32	1.43
3	A	630	DG6	C3-C4	4.52	1.62	1.53
4	B	660	NAI	C3B-C4B	4.40	1.64	1.53
4	A	650	NAI	C2D-C1D	-4.37	1.39	1.53
4	B	660	NAI	PN-O2N	4.26	1.66	1.50
3	A	630	DG6	P-O1P	-4.22	1.38	1.54
3	B	640	DG6	C5-C4	4.19	1.61	1.53
4	B	660	NAI	PN-O1N	-4.00	1.36	1.55
4	B	660	NAI	C1D-N1N	3.92	1.57	1.46
4	A	650	NAI	C3D-C4D	-3.89	1.43	1.53
4	A	650	NAI	C7N-N7N	-3.88	1.22	1.33
4	A	650	NAI	PN-O1N	-3.66	1.38	1.55
4	A	650	NAI	C2D-C3D	3.66	1.63	1.53
3	A	630	DG6	C2-C1	3.63	1.64	1.51
4	B	660	NAI	C2B-C1B	3.61	1.59	1.53
4	B	660	NAI	C2A-N3A	-3.61	1.26	1.32
3	A	630	DG6	P-O3P	-3.56	1.39	1.50
4	A	650	NAI	O3D-C3D	-3.40	1.35	1.43
4	B	660	NAI	C8A-N7A	3.29	1.40	1.34
4	A	650	NAI	C4N-C3N	-3.26	1.43	1.49
4	B	660	NAI	O3D-C3D	-3.26	1.35	1.43
3	B	640	DG6	P-O1P	-3.25	1.42	1.54
4	A	650	NAI	O2D-C2D	3.21	1.50	1.43
4	A	650	NAI	PA-O2A	-3.14	1.40	1.55
3	A	630	DG6	P-O2P	-3.10	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	650	NAI	O7N-C7N	-3.10	1.17	1.24
4	B	660	NAI	O2D-C2D	2.95	1.49	1.43
4	B	660	NAI	C2B-C3B	-2.88	1.45	1.53
4	B	660	NAI	C2N-C3N	2.84	1.42	1.34
4	A	650	NAI	C5D-C4D	2.76	1.60	1.51
4	A	650	NAI	PN-O2N	2.71	1.60	1.50
4	A	650	NAI	O5D-C5D	-2.62	1.34	1.44
3	A	630	DG6	O4-C4	2.62	1.49	1.43
4	B	660	NAI	C4N-C5N	-2.42	1.42	1.48
3	B	640	DG6	O4-C4	2.41	1.48	1.43
4	B	660	NAI	C4N-C3N	2.38	1.54	1.49
4	B	660	NAI	PA-O5B	2.30	1.68	1.59
4	B	660	NAI	C6A-N6A	2.21	1.42	1.34
4	A	650	NAI	O4D-C4D	2.11	1.49	1.45
3	B	640	DG6	P-O3P	-2.08	1.43	1.50
4	B	660	NAI	O4B-C4B	2.05	1.49	1.45
4	B	660	NAI	C2D-C1D	-2.03	1.47	1.53
4	A	650	NAI	PA-O5B	2.02	1.67	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	O4D-C1D-N1N	7.65	123.00	108.06
4	A	650	NAI	O2A-PA-O1A	5.95	141.64	112.24
4	B	660	NAI	O4D-C1D-N1N	5.50	118.82	108.06
3	A	630	DG6	C6-C5-C4	5.46	122.75	112.20
4	A	650	NAI	O7N-C7N-N7N	-5.31	110.45	122.88
3	B	640	DG6	C6-C5-C4	5.30	122.45	112.20
3	A	630	DG6	O6-C6-C5	5.20	123.24	109.36
4	B	660	NAI	O2A-PA-O1A	5.04	137.15	112.24
4	B	660	NAI	C1B-N9A-C4A	-4.75	118.30	126.64
3	B	640	DG6	O5-C5-C6	4.68	120.43	109.92
4	A	650	NAI	C5A-C6A-N6A	4.65	127.42	120.35
4	B	660	NAI	O2D-C2D-C1D	-4.41	95.27	110.02
3	A	630	DG6	O5-C5-C6	4.28	119.55	109.92
4	A	650	NAI	C1B-N9A-C4A	-4.06	119.51	126.64
4	B	660	NAI	C4A-C5A-N7A	4.06	113.63	109.40
4	B	660	NAI	C2D-C1D-N1N	3.93	123.14	113.30
4	A	650	NAI	C3N-C7N-N7N	3.69	124.23	117.67
4	B	660	NAI	O7N-C7N-N7N	-3.68	114.27	122.88
4	B	660	NAI	C5A-C6A-N1A	-3.52	112.37	120.35
4	B	660	NAI	O3B-C3B-C4B	3.49	121.13	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	650	NAI	O2D-C2D-C1D	-3.48	98.39	110.02
4	A	650	NAI	C2A-N1A-C6A	3.42	124.61	118.75
3	A	630	DG6	O5-C5-C4	3.41	117.39	109.10
4	B	660	NAI	C5B-C4B-C3B	-3.38	102.53	115.18
4	B	660	NAI	C2A-N1A-C6A	3.35	124.49	118.75
4	B	660	NAI	N3A-C2A-N1A	3.31	133.86	128.68
3	B	640	DG6	O5-C5-C4	3.29	117.09	109.10
3	B	640	DG6	O6-C6-C5	3.27	118.09	109.36
4	B	660	NAI	O3D-C3D-C4D	-3.13	102.00	111.05
4	B	660	NAI	O5D-PN-O2N	2.91	120.44	109.07
4	A	650	NAI	C2D-C1D-N1N	2.83	120.39	113.30
3	B	640	DG6	O2P-P-O6	2.81	114.22	106.73
4	B	660	NAI	O7N-C7N-C3N	2.60	125.79	120.90
4	B	660	NAI	O4B-C4B-C5B	-2.58	100.89	109.37
4	A	650	NAI	O4B-C1B-C2B	-2.45	103.34	106.93
4	B	660	NAI	C3D-C2D-C1D	2.43	106.05	101.43
3	A	630	DG6	O2P-P-O6	2.41	113.15	106.73
4	B	660	NAI	N6A-C6A-N1A	2.37	123.49	118.57
4	A	650	NAI	O4B-C4B-C3B	-2.36	100.44	105.11
4	A	650	NAI	O7N-C7N-C3N	2.31	125.24	120.90
4	B	660	NAI	O2D-C2D-C3D	-2.19	104.73	111.82
4	A	650	NAI	C5A-C6A-N1A	-2.15	115.47	120.35
4	A	650	NAI	C3D-C2D-C1D	2.09	105.40	101.43
4	B	660	NAI	O2B-C2B-C3B	-2.08	105.08	111.82
3	B	640	DG6	C1-C2-C3	-2.05	109.14	113.07
4	A	650	NAI	O4B-C4B-C5B	-2.05	102.63	109.37

All (2) chirality outliers are listed below:

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

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	O3-C3-C4-O4
3	B	640	DG6	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
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	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
4	A	650	NAI	C3D-C4D-C5D-O5D
3	A	630	DG6	C3-C4-C5-O5
3	A	630	DG6	C2-C3-C4-C5
3	B	640	DG6	C2-C3-C4-C5
3	A	630	DG6	C1-C2-C3-O3
3	A	630	DG6	O3-C3-C4-C5
3	A	630	DG6	O3-C3-C4-O4
3	A	630	DG6	C3-C4-C5-C6
3	A	630	DG6	C1-C2-C3-C4
4	B	660	NAI	C5D-O5D-PN-O3
4	A	650	NAI	C5B-O5B-PA-O1A
4	A	650	NAI	C5D-O5D-PN-O1N
4	A	650	NAI	C5D-O5D-PN-O2N
4	A	650	NAI	O4B-C4B-C5B-O5B
4	B	660	NAI	O4B-C4B-C5B-O5B
3	A	630	DG6	C2-C3-C4-O4

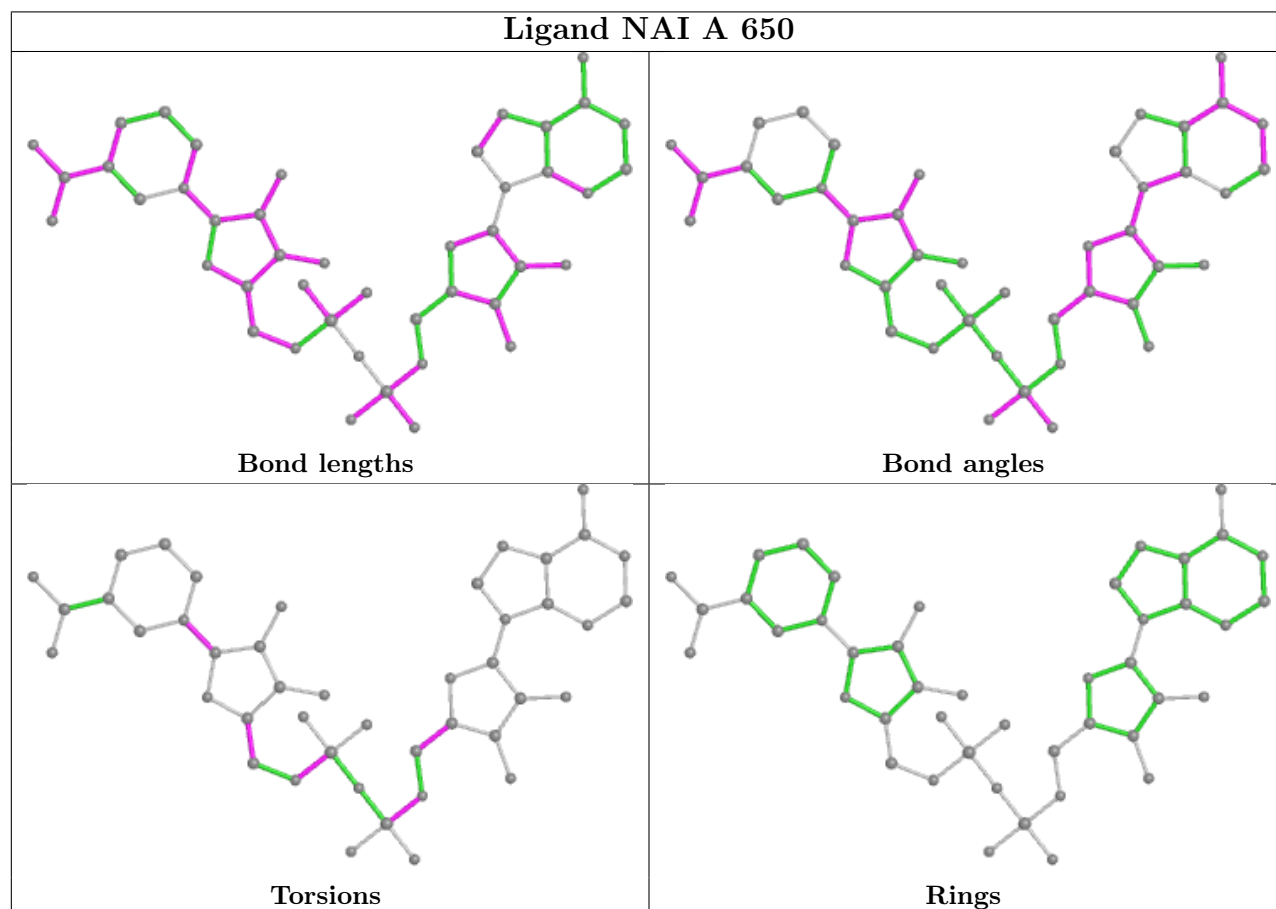
There are no ring outliers.

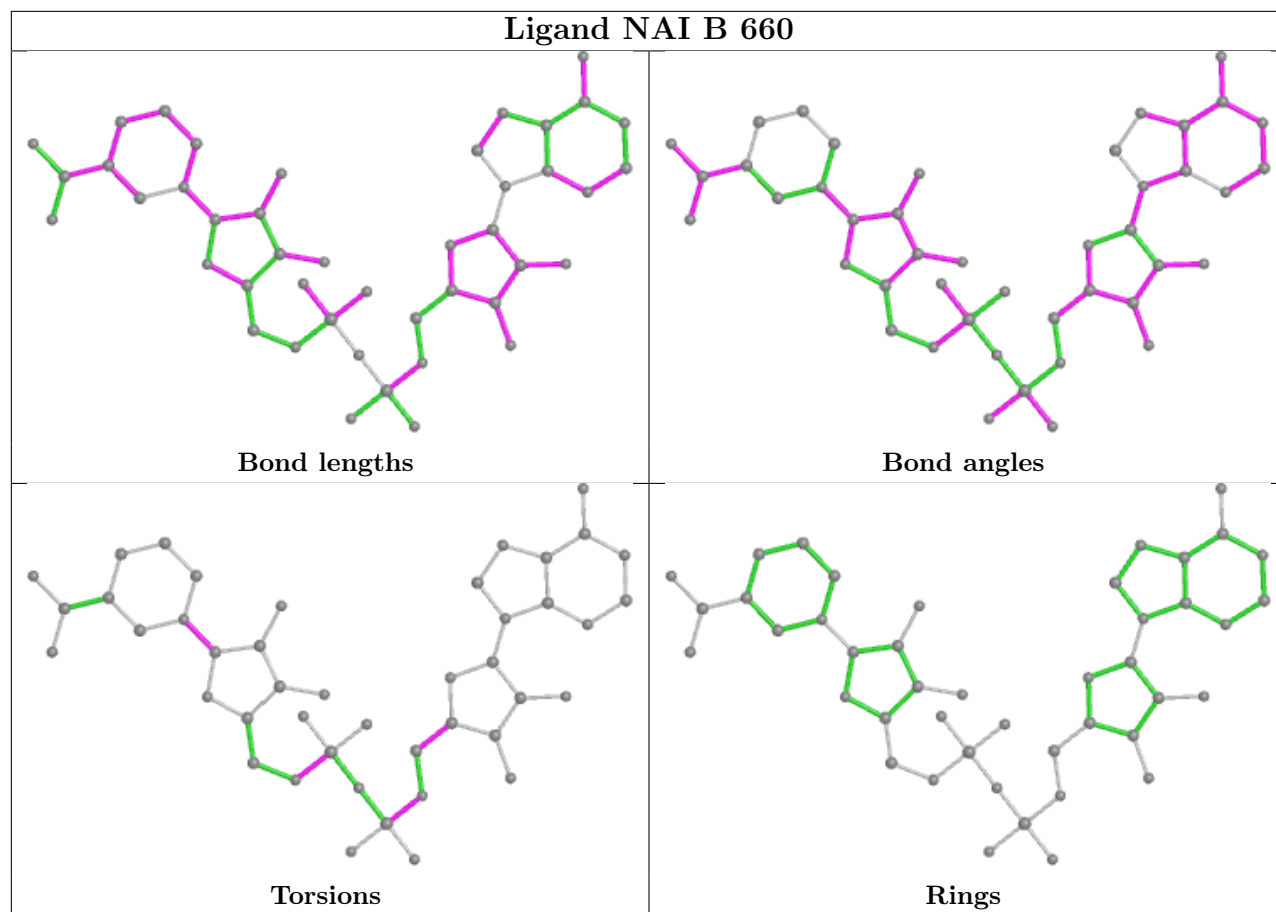
4 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	640	DG6	17	0
4	A	650	NAI	8	0
4	B	660	NAI	3	0
3	A	630	DG6	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.