



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 01:49 PM EDT

PDB ID : 1CT9
Title : CRYSTAL STRUCTURE OF ASPARAGINE SYNTHETASE B FROM ES-
CHERICHIA COLI
Authors : Larsen, T.M.; Boehlein, S.K.; Schuster, S.M.; Richards, N.G.J.; Thoden, J.B.;
Holden, H.M.; Rayment, I.
Deposited on : 1999-08-20
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (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) : 2.23.2

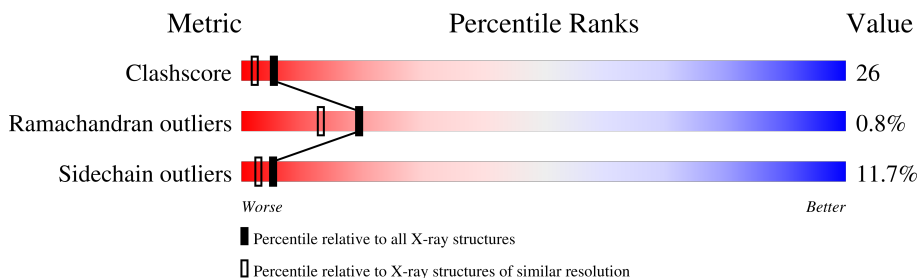
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	553	45% 35% 8% • 10%
1	B	553	39% 36% 13% • 10%
1	C	553	41% 37% 10% • 10%
1	D	553	48% 31% 9% • 10%

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
4	AMP	C	1114	-	-	X	-
4	AMP	D	1121	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16980 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.

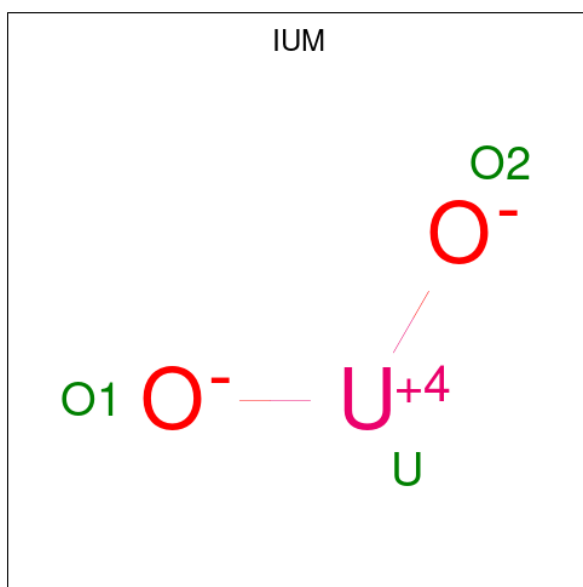
- Molecule 1 is a protein called ASPARAGINE SYNTHETASE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	497	3966	2530	671	745	20	0	0	0
1	B	495	3942	2518	665	739	20	0	0	0
1	C	495	3942	2518	665	739	20	0	0	0
1	D	495	3930	2507	664	739	20	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	CYS	engineered mutation	UNP P22106
B	1	ALA	CYS	engineered mutation	UNP P22106
C	1	ALA	CYS	engineered mutation	UNP P22106
D	1	ALA	CYS	engineered mutation	UNP P22106

- Molecule 2 is URANYL (VI) ION (three-letter code: IUM) (formula: O₂U).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total U 1 1	0	0
2	A	1	Total O U 2 1 1	0	0
2	A	1	Total U 1 1	0	0
2	A	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	B	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	C	1	Total U 1 1	0	0
2	D	1	Total O U 2 1 1	0	0
2	D	1	Total U 1 1	0	0

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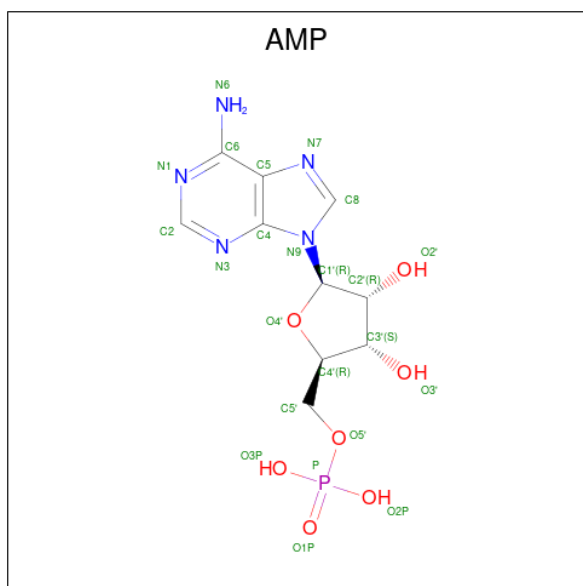
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total U 1 1	0	0
2	D	1	Total U 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



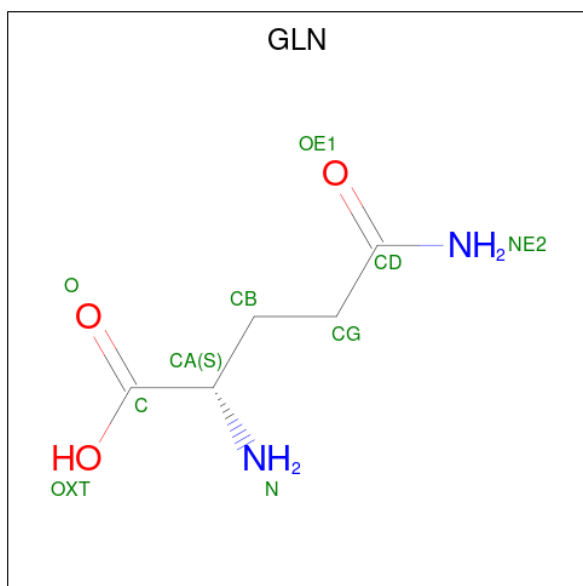
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 23 10 5 7 1	0	0
4	B	1	Total C N O P 23 10 5 7 1	0	0
4	C	1	Total C N O P 23 10 5 7 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	5	2	3		
5	B	1	Total	C	N	O	0	0
			10	5	2	3		
5	C	1	Total	C	N	O	0	0
			10	5	2	3		
5	D	1	Total	C	N	O	0	0
			10	5	2	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	B	235	Total	O	0	0
			235	235		
6	C	223	Total	O	0	0
			223	223		
6	D	296	Total	O	0	0
			296	296		

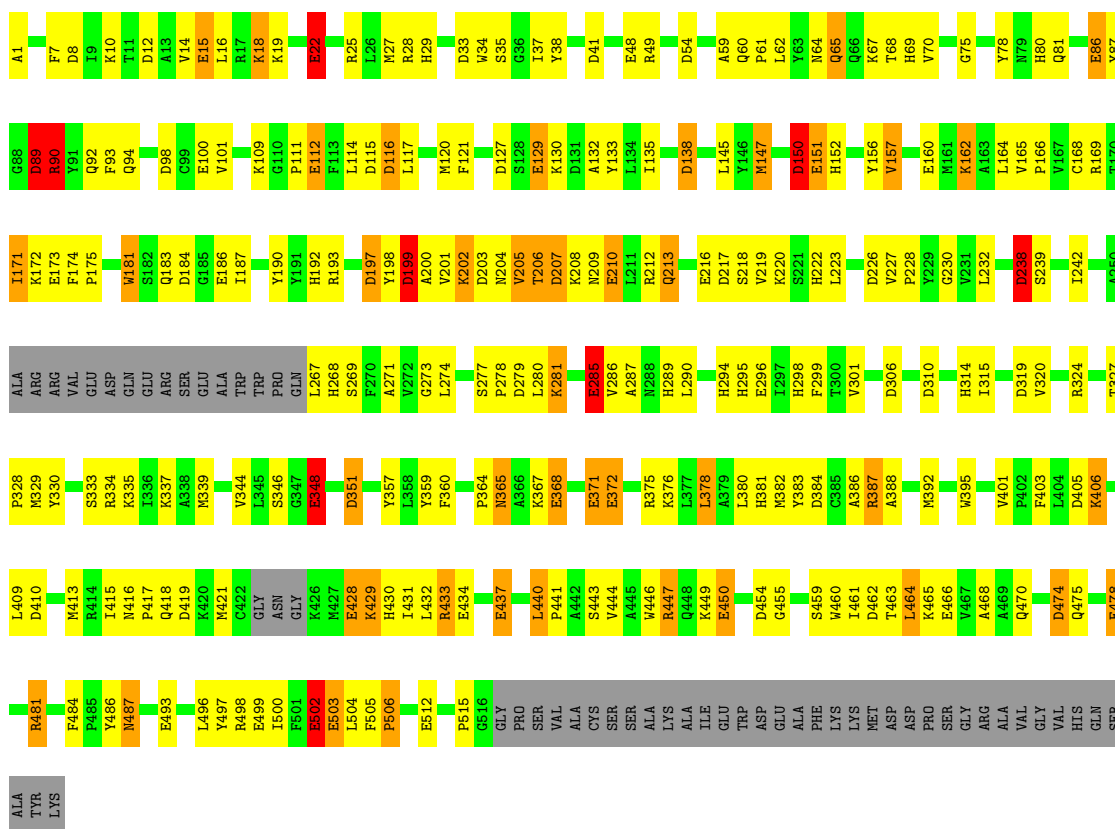
3 Residue-property plots

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 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.

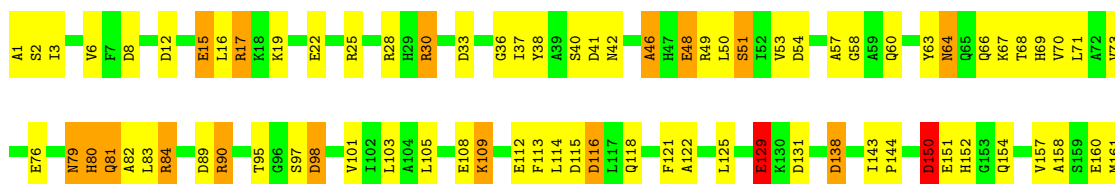
- Molecule 1: ASPARAGINE SYNTHETASE B

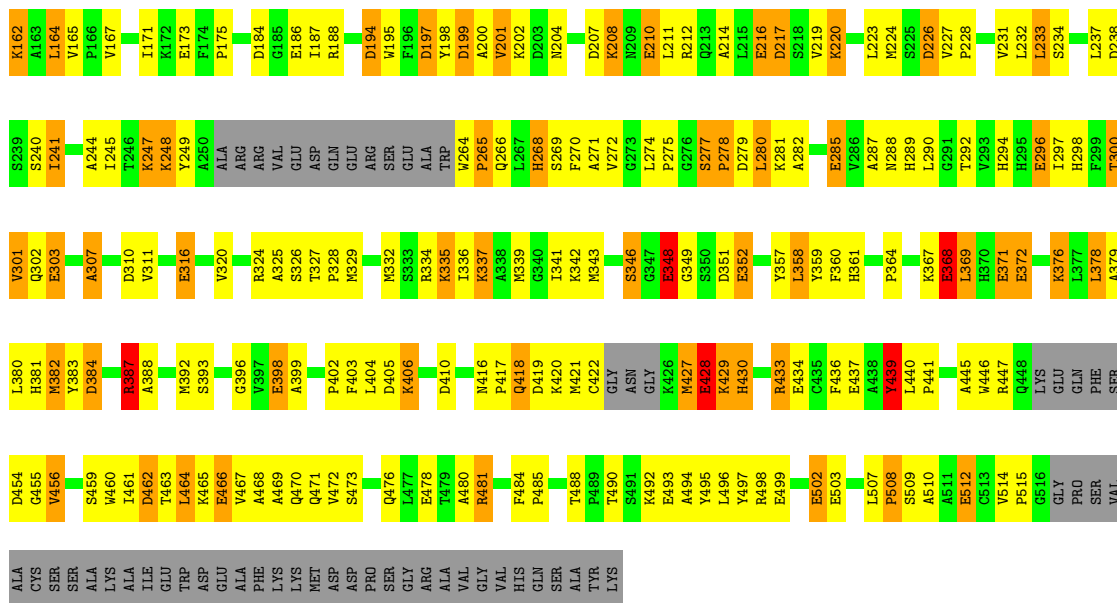
Chain A: 



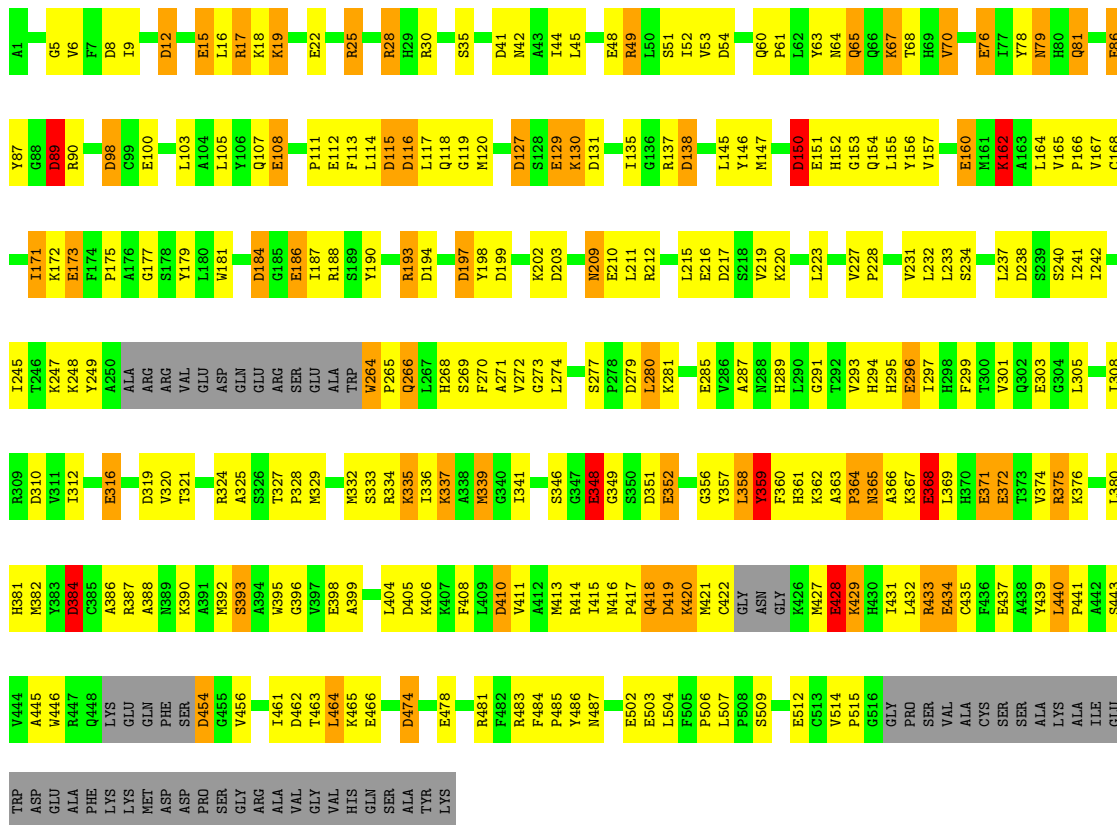
- Molecule 1: ASPARAGINE SYNTHETASE B

Chain B: 





• Molecule 1: ASPARAGINE SYNTHETASE B



• Molecule 1: ASPARAGINE SYNTHETASE B



GLY	E512	GLY	C347	Q266	S189	A1
PRO	K426	E348	E349	L267	Y190	F4
SER	K427	G349	S350	H268	Y191	D8
VAL	E428	G350	D351	S269	H192	Q118
ALA	K429	D351	E352	F270	R193	I9
CYS	P515	H430	V353	A271	D194	K10
SER	G516	R433	F354	V272	D197	K11
ALA	GLY	E434	Y357	G273	Y198	D12
LYS	PRO	E434	L358	L274	A200	M12
VAL	SER	E437	Y359	S277	V201	V14
ALA	ALA	V444	F360	P278	K202	E15
CYS	SER	Q448	H361	D279	D203	E22
LYS	ALA	LYS	K362	L280	M204	R25
ALA	ALA	GLN	A363	K281	V205	R28
ILE	GLN	GLN	P364	E285	T206	D33
GLU	PHE	PHE	N365	V293	D207	W34
TRP	SER	SER	A366	H294	E210	D41
ASP	ASP	ASP	K367	H295	E216	D46
GLU	GLU	GLU	E368	E296	D217	A46
ALA	ALA	ALA	E371	I297	P143	H47
PHE	PHE	PHE	E372	H298	L145	E48
LYS	LYS	LYS	R375	F299	L146	R49
MET	LYS	LYS	T300	T300	M147	L50
ASP	MET	ASP	H380	E303	G148	I52
ASP	ASP	ASP	H381	R309	G149	M64
PRO	PRO	PRO	M382	D310	H222	Q65
SER	SER	SER	Y383	E316	Y149	Q66
GLY	GLY	GLY	D384	T317	L155	K67
ARG	ARG	ARG	R387	Y318	L156	T68
ALA	ALA	ALA	A388	D319	V157	H69
VAL	VAL	VAL	W395	V320	E160	Y78
HIS	HIS	HIS	E398	I323	M161	N79
GLN	GLN	GLN	A399	T327	K162	H80
SER	SER	SER	R400	P328	V165	Q81
ALA	ALA	ALA	V401	M329	C168	R84
TYR	TYR	TYR	P402	Y330	R169	E86
LYS	LYS	LYS	D405	L331	T170	D89
ARG	ARG	ARG	K406	M332	ARG	R90
ALA	ALA	ALA	K407	S333	ARG	Y91
LYS	LYS	LYS	D410	R334	VAL	Q92
ARG	ARG	ARG	R414	K335	GLU	S97
ALA	ALA	ALA	P417	I336	ASP	S97
GLY	GLY	GLY	Q418	A338	GLN	E100
GLN	GLN	GLN	G340	M339	GLU	L103
TYR	TYR	TYR	D419	G340	GLU	L105
LYS	LYS	LYS	K420	I341	ASP	
			M421	K342	TRP	
			G422	M343	ALA	
			S509	V344	TRP	
				L345	TRP	
				G423	PRD	
				ASN		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.93Å 127.10Å 204.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.0 (30.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.197 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16980	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: IUM, CL, AMP

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	1.02	24/4060 (0.6%)	1.48	66/5493 (1.2%)
1	B	1.04	32/4037 (0.8%)	1.50	67/5466 (1.2%)
1	C	1.01	33/4037 (0.8%)	1.44	63/5466 (1.2%)
1	D	1.06	30/4022 (0.7%)	1.49	67/5443 (1.2%)
All	All	1.03	119/16156 (0.7%)	1.48	263/21868 (1.2%)

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	GLU	CD-OE2	9.23	1.35	1.25
1	D	398	GLU	CD-OE2	8.52	1.35	1.25
1	B	466	GLU	CD-OE2	7.96	1.34	1.25
1	D	48	GLU	CD-OE2	7.61	1.34	1.25
1	B	296	GLU	CD-OE2	7.58	1.33	1.25
1	A	15	GLU	CD-OE2	7.56	1.33	1.25
1	B	352	GLU	CD-OE2	7.49	1.33	1.25
1	C	86	GLU	CD-OE2	7.38	1.33	1.25
1	D	296	GLU	CD-OE2	7.34	1.33	1.25
1	B	316	GLU	CD-OE2	7.29	1.33	1.25
1	D	15	GLU	CD-OE2	7.21	1.33	1.25
1	D	352	GLU	CD-OE2	7.21	1.33	1.25
1	B	348	GLU	CD-OE2	7.17	1.33	1.25
1	B	285	GLU	CD-OE2	7.15	1.33	1.25
1	A	512	GLU	CD-OE2	7.14	1.33	1.25
1	B	437	GLU	CD-OE2	7.09	1.33	1.25
1	A	210	GLU	CD-OE2	7.04	1.33	1.25
1	D	503	GLU	CD-OE2	6.89	1.33	1.25
1	B	478	GLU	CD-OE2	6.89	1.33	1.25
1	B	372	GLU	CD-OE2	6.84	1.33	1.25
1	B	503	GLU	CD-OE2	6.75	1.33	1.25
1	D	512	GLU	CD-OE2	6.72	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	372	GLU	CD-OE2	6.71	1.33	1.25
1	C	393	SER	CB-OG	6.70	1.50	1.42
1	D	285	GLU	CD-OE2	6.70	1.33	1.25
1	C	112	GLU	CD-OE2	6.66	1.32	1.25
1	B	398	GLU	CD-OE2	6.66	1.32	1.25
1	C	503	GLU	CD-OE2	6.65	1.32	1.25
1	C	466	GLU	CD-OE2	6.63	1.32	1.25
1	A	186	GLU	CD-OE2	6.61	1.32	1.25
1	C	129	GLU	CD-OE2	6.57	1.32	1.25
1	D	437	GLU	CD-OE2	6.56	1.32	1.25
1	A	129	GLU	CD-OE2	6.51	1.32	1.25
1	D	502	GLU	CD-OE2	6.51	1.32	1.25
1	A	151	GLU	CD-OE2	6.50	1.32	1.25
1	D	466	GLU	CD-OE2	6.47	1.32	1.25
1	C	173	GLU	CD-OE2	6.44	1.32	1.25
1	B	434	GLU	CD-OE2	6.43	1.32	1.25
1	B	108	GLU	CD-OE2	6.43	1.32	1.25
1	C	303	GLU	CD-OE2	6.43	1.32	1.25
1	C	368	GLU	CD-OE2	6.40	1.32	1.25
1	C	151	GLU	CD-OE2	6.38	1.32	1.25
1	B	22	GLU	CD-OE2	6.36	1.32	1.25
1	C	428	GLU	CD-OE2	6.36	1.32	1.25
1	B	112	GLU	CD-OE2	6.36	1.32	1.25
1	A	466	GLU	CD-OE2	6.33	1.32	1.25
1	C	15	GLU	CD-OE2	6.32	1.32	1.25
1	B	151	GLU	CD-OE2	6.31	1.32	1.25
1	C	502	GLU	CD-OE2	6.30	1.32	1.25
1	C	434	GLU	CD-OE2	6.25	1.32	1.25
1	B	499	GLU	CD-OE2	6.25	1.32	1.25
1	A	368	GLU	CD-OE2	6.22	1.32	1.25
1	A	112	GLU	CD-OE2	6.22	1.32	1.25
1	D	372	GLU	CD-OE2	6.15	1.32	1.25
1	C	478	GLU	CD-OE2	6.15	1.32	1.25
1	B	368	GLU	CD-OE2	6.13	1.32	1.25
1	D	22	GLU	CD-OE2	6.11	1.32	1.25
1	B	15	GLU	CD-OE2	6.07	1.32	1.25
1	A	371	GLU	CD-OE2	6.07	1.32	1.25
1	B	186	GLU	CD-OE2	6.03	1.32	1.25
1	A	478	GLU	CD-OE2	6.01	1.32	1.25
1	D	428	GLU	CD-OE2	6.01	1.32	1.25
1	B	129	GLU	CD-OE2	6.01	1.32	1.25
1	D	434	GLU	CD-OE2	6.00	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	398	GLU	CD-OE2	5.96	1.32	1.25
1	C	437	GLU	CD-OE2	5.95	1.32	1.25
1	D	186	GLU	CD-OE2	5.89	1.32	1.25
1	B	371	GLU	CD-OE2	5.88	1.32	1.25
1	D	129	GLU	CD-OE2	5.88	1.32	1.25
1	C	285	GLU	CD-OE2	5.88	1.32	1.25
1	A	348	GLU	CD-OE2	5.87	1.32	1.25
1	D	210	GLU	CD-OE2	5.84	1.32	1.25
1	B	48	GLU	CD-OE2	5.83	1.32	1.25
1	A	22	GLU	CD-OE2	5.82	1.32	1.25
1	B	428	GLU	CD-OE2	5.82	1.32	1.25
1	C	398	GLU	CD-OE1	-5.80	1.19	1.25
1	C	371	GLU	CD-OE2	5.79	1.32	1.25
1	B	502	GLU	CD-OE2	5.77	1.31	1.25
1	D	151	GLU	CD-OE2	5.74	1.31	1.25
1	A	493	GLU	CD-OE2	5.73	1.31	1.25
1	C	512	GLU	CD-OE2	5.71	1.31	1.25
1	D	368	GLU	CD-OE2	5.71	1.31	1.25
1	D	112	GLU	CD-OE2	5.70	1.31	1.25
1	A	285	GLU	CD-OE2	5.69	1.31	1.25
1	D	348	GLU	CD-OE2	5.68	1.31	1.25
1	C	210	GLU	CD-OE2	5.68	1.31	1.25
1	B	210	GLU	CD-OE2	5.67	1.31	1.25
1	C	186	GLU	CD-OE2	5.67	1.31	1.25
1	B	76	GLU	CD-OE2	5.66	1.31	1.25
1	A	503	GLU	CD-OE2	5.62	1.31	1.25
1	B	512	GLU	CD-OE2	5.61	1.31	1.25
1	B	173	GLU	CD-OE2	5.60	1.31	1.25
1	C	100	GLU	CD-OE2	5.58	1.31	1.25
1	A	502	GLU	CD-OE2	5.53	1.31	1.25
1	A	434	GLU	CD-OE2	5.52	1.31	1.25
1	A	428	GLU	CD-OE2	5.51	1.31	1.25
1	B	216	GLU	CD-OE2	5.50	1.31	1.25
1	A	160	GLU	CD-OE2	5.48	1.31	1.25
1	C	76	GLU	CD-OE2	5.47	1.31	1.25
1	D	160	GLU	CD-OE2	5.41	1.31	1.25
1	D	303	GLU	CD-OE2	5.39	1.31	1.25
1	A	86	GLU	CD-OE2	5.37	1.31	1.25
1	D	100	GLU	CD-OE1	-5.34	1.19	1.25
1	C	296	GLU	CD-OE2	5.32	1.31	1.25
1	D	493	GLU	CD-OE2	5.25	1.31	1.25
1	C	316	GLU	CD-OE2	5.24	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	GLU	CD-OE2	5.24	1.31	1.25
1	C	372	GLU	CD-OE2	5.23	1.31	1.25
1	C	352	GLU	CD-OE2	5.22	1.31	1.25
1	D	499	GLU	CD-OE2	5.21	1.31	1.25
1	A	437	GLU	CD-OE2	5.18	1.31	1.25
1	C	160	GLU	CD-OE2	5.12	1.31	1.25
1	A	499	GLU	CD-OE2	5.10	1.31	1.25
1	B	303	GLU	CD-OE2	5.08	1.31	1.25
1	D	216	GLU	CD-OE2	5.08	1.31	1.25
1	C	48	GLU	CD-OE2	5.07	1.31	1.25
1	B	160	GLU	CD-OE2	5.05	1.31	1.25
1	D	173	GLU	CD-OE2	5.02	1.31	1.25
1	C	348	GLU	CD-OE2	5.00	1.31	1.25

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CB-CG-OD2	-14.12	105.59	118.30
1	A	150	ASP	CB-CG-OD2	-13.62	106.05	118.30
1	C	150	ASP	CB-CG-OD2	-10.79	108.59	118.30
1	D	194	ASP	CB-CG-OD1	10.22	127.50	118.30
1	B	238	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	A	238	ASP	CB-CG-OD1	9.77	127.09	118.30
1	C	238	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	D	410	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	B	351	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	A	238	ASP	CB-CG-OD2	-9.67	109.59	118.30
1	A	481	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	B	387	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	A	474	ASP	CB-CG-OD2	-9.47	109.78	118.30
1	D	150	ASP	CB-CG-OD1	9.15	126.54	118.30
1	D	150	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	B	351	ASP	CB-CG-OD1	8.94	126.35	118.30
1	A	190	TYR	CB-CG-CD2	-8.76	115.75	121.00
1	D	309	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	C	49	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	150	ASP	CB-CG-OD1	8.39	125.85	118.30
1	D	387	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	310	ASP	CB-CG-OD2	-8.36	110.77	118.30
1	C	193	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	194	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	B	439	TYR	CB-CG-CD1	-8.31	116.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	306	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	C	138	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	C	410	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	184	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	C	28	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	C	116	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	D	384	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	B	8	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	319	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	B	197	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	351	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	C	310	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	B	199	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	197	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	116	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	D	194	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	8	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	D	238	ASP	CB-CG-OD1	7.64	125.18	118.30
1	D	8	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	217	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	C	483	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	D	90	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	184	ASP	CB-CG-OD1	7.57	125.12	118.30
1	C	319	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	199	ASP	CB-CG-OD1	7.51	125.06	118.30
1	C	115	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	410	ASP	CB-CG-OD1	7.49	125.04	118.30
1	B	405	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	B	8	ASP	CB-CG-OD1	7.43	124.99	118.30
1	D	199	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	64	ASN	N-CA-CB	-7.38	97.31	110.60
1	D	8	ASP	CB-CG-OD1	7.37	124.94	118.30
1	A	8	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	116	ASP	CB-CG-OD1	7.36	124.93	118.30
1	D	157	VAL	CG1-CB-CG2	7.36	122.68	110.90
1	D	184	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	B	498	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	D	147	MET	N-CA-CB	-7.22	97.61	110.60
1	C	387	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	194	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	54	ASP	CB-CG-OD2	-7.18	111.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	B	17	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	D	351	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	199	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	B	138	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	8	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	C	150	ASP	CB-CG-OD1	7.05	124.65	118.30
1	C	454	ASP	CB-CG-OD1	7.04	124.64	118.30
1	B	98	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	169	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	197	ASP	CB-CG-OD1	6.99	124.59	118.30
1	D	375	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	162	LYS	N-CA-CB	-6.95	98.10	110.60
1	A	351	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	79	ASN	N-CA-CB	-6.91	98.17	110.60
1	B	188	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	279	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	324	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	405	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	498	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	188	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	41	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	C	131	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	122	ALA	N-CA-CB	6.70	119.48	110.10
1	D	279	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	474	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	184	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	410	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	C	98	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	197	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	D	184	ASP	N-CA-CB	6.56	122.41	110.60
1	C	41	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	B	17	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	C	199	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	199	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	430	HIS	CA-CB-CG	-6.51	102.53	113.60
1	B	33	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	310	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	46	ALA	N-CA-CB	6.47	119.16	110.10
1	C	138	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	419	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	D	363	ALA	N-CA-CB	6.46	119.15	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	279	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	410	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	116	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	54	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	98	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	30	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	49	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	C	79	ASN	N-CA-CB	-6.34	99.19	110.60
1	C	41	ASP	CB-CG-OD1	6.34	124.00	118.30
1	C	116	ASP	CB-CG-OD1	6.33	123.99	118.30
1	C	184	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	212	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	115	ASP	CB-CG-OD1	6.28	123.95	118.30
1	C	351	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	D	462	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	C	162	LYS	N-CA-CB	-6.25	99.36	110.60
1	D	319	ASP	CB-CG-OD1	6.22	123.90	118.30
1	D	89	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	197	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	54	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	207	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	41	ASP	CB-CG-OD1	6.13	123.82	118.30
1	D	474	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	310	ASP	CB-CG-OD1	6.13	123.81	118.30
1	D	157	VAL	CA-CB-CG2	6.13	120.09	110.90
1	A	279	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	89	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	498	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	330	TYR	CB-CG-CD2	6.08	124.65	121.00
1	A	33	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	131	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	D	433	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	334	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	84	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	351	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	410	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	25	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	90	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	150	ASP	CA-CB-CG	-5.97	100.26	113.40
1	D	89	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	D	454	ASP	CB-CG-OD2	-5.96	112.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	B	89	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	150	ASP	CA-CB-CG	-5.92	100.37	113.40
1	A	15	GLU	N-CA-CB	-5.92	99.94	110.60
1	D	64	ASN	CA-CB-CG	-5.91	100.39	113.40
1	B	162	LYS	N-CA-CB	-5.91	99.97	110.60
1	A	150	ASP	CB-CA-C	-5.88	98.64	110.40
1	A	314	HIS	CA-CB-CG	-5.87	103.62	113.60
1	B	184	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	197	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	41	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	33	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	17	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	89	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	B	150	ASP	CB-CA-C	-5.83	98.75	110.40
1	A	319	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	49	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	190	TYR	CB-CG-CD1	5.80	124.48	121.00
1	D	131	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	D	41	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	C	405	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	439	TYR	CB-CG-CD2	5.78	124.47	121.00
1	D	12	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	115	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	405	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	487	ASN	CB-CA-C	-5.74	98.92	110.40
1	C	150	ASP	CB-CA-C	-5.73	98.94	110.40
1	D	184	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	226	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	C	184	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	89	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	279	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	462	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	116	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	498	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	217	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	131	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	207	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	454	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	226	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	28	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	217	ASP	CB-CG-OD1	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	481	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	D	207	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	199	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	131	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	450	GLU	N-CA-CB	5.58	120.64	110.60
1	C	474	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	203	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	419	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	41	ASP	CB-CG-OD1	5.55	123.29	118.30
1	D	147	MET	CA-CB-CG	5.54	122.72	113.30
1	D	422	CYS	CB-CA-C	-5.54	99.33	110.40
1	C	194	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	474	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	138	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	131	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	120	MET	CG-SD-CE	5.50	109.00	100.20
1	A	410	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	98	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	197	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	64	ASN	CB-CA-C	-5.46	99.47	110.40
1	C	193	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	375	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	C	351	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	33	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	419	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	186	GLU	N-CA-CB	5.40	120.31	110.60
1	C	12	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	138	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	D	238	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	127	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	33	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	C	203	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	30	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	78	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	310	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	405	ASP	CB-CG-OD2	-5.28	113.54	118.30
1	C	8	ASP	CB-CG-OD1	5.28	123.06	118.30
1	D	149	TYR	C-N-CA	5.28	134.91	121.70
1	B	454	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	206	THR	CA-CB-CG2	-5.27	105.02	112.40
1	A	226	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	238	ASP	CB-CG-OD1	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	190	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	C	127	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	339	MET	CB-CA-C	-5.23	99.93	110.40
1	B	217	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	419	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	89	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	25	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	199	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	146	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	B	268	HIS	CA-CB-CG	-5.18	104.79	113.60
1	C	319	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	419	ASP	CB-CG-OD1	5.17	122.95	118.30
1	D	217	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	D	494	ALA	CB-CA-C	-5.15	102.37	110.10
1	B	387	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	447	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	375	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	433	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	112	GLU	N-CA-C	5.10	124.78	111.00
1	D	419	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	384	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	B	307	ALA	CB-CA-C	-5.07	102.49	110.10
1	B	12	ASP	CB-CG-OD1	5.06	122.85	118.30
1	B	138	ASP	CB-CG-OD1	5.04	122.84	118.30
1	D	427	MET	CA-CB-CG	5.03	121.84	113.30
1	B	109	LYS	N-CA-CB	-5.02	101.56	110.60
1	D	319	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3966	0	3862	192	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3942	0	3828	247	0
1	C	3942	0	3827	204	0
1	D	3930	0	3818	186	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	11	5	0
4	B	23	0	12	3	0
4	C	23	0	11	7	0
4	D	23	0	12	8	0
5	A	10	0	7	2	0
5	B	10	0	7	4	0
5	C	10	0	7	1	0
5	D	10	0	7	2	0
6	A	292	0	0	8	0
6	B	235	0	0	13	0
6	C	223	0	0	7	0
6	D	296	0	0	19	0
All	All	16980	0	15409	822	0

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 26.

All (822) 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:C:364:PRO:HG2	1:C:368:GLU:HG2	1.26	1.17
1:D:472:VAL:HB	1:D:492:LYS:HG2	1.22	1.12
1:D:364:PRO:HG2	1:D:368:GLU:HG2	1.40	1.01
1:B:300:THR:HG22	1:B:303:GLU:H	1.29	0.96
1:D:64:ASN:HB3	1:D:67:LYS:N	1.80	0.95
1:D:427:MET:H	1:D:430:HIS:HD2	1.14	0.95
1:C:366:ALA:HA	1:C:421:MET:HE3	1.46	0.95
1:B:198:TYR:CE2	1:B:367:LYS:HB2	2.04	0.92
1:A:387:ARG:HB3	1:A:387:ARG:HH11	1.35	0.90
1:C:81:GLN:H	1:C:81:GLN:NE2	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LEU:HD12	1:C:411:VAL:HG12	1.54	0.90
1:A:207:ASP:HB3	1:A:210:GLU:HB3	1.56	0.88
1:C:193:ARG:HH22	1:C:406:LYS:HE3	1.38	0.87
1:C:366:ALA:HA	1:C:421:MET:CE	2.04	0.87
1:D:472:VAL:CB	1:D:492:LYS:HG2	2.03	0.87
1:B:83:LEU:HD13	1:B:101:VAL:HG11	1.57	0.86
1:C:168:CYS:HB2	1:C:171:ILE:HD11	1.59	0.85
1:D:64:ASN:HB2	1:D:69:HIS:H	1.41	0.84
1:B:1:ALA:N	5:B:1113:GLN:HE22	1.75	0.84
1:D:272:VAL:H	4:D:1121:AMP:HN62	1.22	0.84
1:D:64:ASN:HB3	1:D:67:LYS:H	1.41	0.82
1:D:279:ASP:OD2	1:D:455:GLY:HA3	1.80	0.82
1:A:175:PRO:HG2	1:A:187:ILE:HG21	1.59	0.82
1:B:300:THR:HG21	6:B:1187:HOH:O	1.80	0.82
1:B:198:TYR:CD2	1:B:367:LYS:HB2	2.15	0.81
1:C:234:SER:HB3	4:C:1114:AMP:C5	2.14	0.81
1:C:422:CYS:SG	1:C:428:GLU:HA	2.21	0.81
1:B:81:GLN:NE2	1:B:82:ALA:H	1.79	0.80
1:C:320:VAL:HG12	1:C:324:ARG:HD2	1.61	0.80
1:B:83:LEU:CD1	1:B:101:VAL:HG11	2.12	0.80
1:C:364:PRO:HG2	1:C:368:GLU:CG	2.10	0.80
1:A:387:ARG:HH11	1:A:387:ARG:CB	1.94	0.79
1:A:199:ASP:HB3	1:A:202:LYS:NZ	1.96	0.79
1:B:150:ASP:HB3	1:B:152:HIS:H	1.45	0.79
1:B:348:GLU:CD	4:B:1107:AMP:H5'1	2.03	0.79
1:B:278:PRO:HG2	1:B:455:GLY:HA2	1.64	0.79
1:D:50:LEU:HG	1:D:52:ILE:HD11	1.64	0.79
1:D:277:SER:O	1:D:281:LYS:HE2	1.83	0.79
1:C:433:ARG:HD2	1:C:446:TRP:CE3	2.19	0.78
1:C:248:LYS:HG2	1:C:249:TYR:CD1	2.18	0.78
1:B:216:GLU:HG2	1:B:249:TYR:HE1	1.48	0.78
1:C:380:LEU:CD2	1:C:384:ASP:HB2	2.14	0.77
1:C:440:LEU:HB3	1:C:441:PRO:HD2	1.66	0.77
1:A:150:ASP:HB3	1:A:152:HIS:H	1.48	0.77
1:B:49:ARG:CZ	1:B:51:SER:HB3	2.14	0.77
1:A:440:LEU:HB3	1:A:441:PRO:HD2	1.65	0.77
1:D:349:GLY:O	1:D:353:VAL:HG23	1.85	0.77
1:C:232:LEU:HD12	1:C:346:SER:HB3	1.65	0.77
1:C:211:LEU:CD1	1:C:411:VAL:HG12	2.15	0.76
1:A:227:VAL:HB	1:A:228:PRO:HD2	1.66	0.76
1:C:150:ASP:HB3	1:C:152:HIS:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:HIS:NE2	1:D:428:GLU:HG3	2.00	0.76
1:B:300:THR:CG2	1:B:303:GLU:H	1.98	0.76
1:B:380:LEU:CD2	1:B:384:ASP:HB2	2.16	0.76
1:B:508:PRO:O	1:B:512:GLU:HG3	1.85	0.76
1:C:380:LEU:HD22	1:C:384:ASP:HB2	1.68	0.76
1:A:199:ASP:HB3	1:A:202:LYS:HZ1	1.50	0.75
1:D:348:GLU:CD	4:D:1121:AMP:H5'1	2.08	0.75
1:D:381:HIS:CE1	1:D:382:MET:HG3	2.22	0.74
1:D:372:GLU:OE2	1:D:375:ARG:HD2	1.87	0.74
1:D:268:HIS:ND1	1:D:295:HIS:NE2	2.34	0.74
1:A:365:ASN:HD21	1:A:368:GLU:HG2	1.53	0.73
1:A:418:GLN:HB2	6:A:1392:HOH:O	1.88	0.73
1:C:193:ARG:NH2	1:C:406:LYS:HE3	2.04	0.73
1:B:336:ILE:HG22	1:B:341:ILE:HB	1.71	0.73
1:C:44:ILE:C	1:C:45:LEU:HD12	2.09	0.73
1:D:271:ALA:HA	4:D:1121:AMP:N1	2.04	0.73
1:D:342:LYS:NZ	6:D:1276:HOH:O	2.22	0.73
1:B:171:ILE:HD12	1:B:507:LEU:CD2	2.19	0.72
1:B:64:ASN:HB3	1:B:67:LYS:H	1.55	0.72
1:A:64:ASN:HB3	1:A:67:LYS:N	2.05	0.72
1:C:366:ALA:CA	1:C:421:MET:HE3	2.19	0.72
1:A:207:ASP:HB3	1:A:210:GLU:CB	2.19	0.72
1:B:64:ASN:HB3	1:B:67:LYS:N	2.05	0.72
1:A:64:ASN:HB2	1:A:69:HIS:H	1.54	0.72
1:B:439:TYR:C	1:B:440:LEU:HD23	2.10	0.72
1:B:358:LEU:HA	1:B:361:HIS:HD2	1.54	0.71
1:A:132:ALA:HB2	1:A:183:GLN:NE2	2.06	0.71
1:A:387:ARG:HG3	1:A:388:ALA:N	2.06	0.71
1:A:268:HIS:ND1	1:A:295:HIS:NE2	2.39	0.71
1:B:80:HIS:CD2	1:B:98:ASP:HA	2.26	0.71
1:A:64:ASN:HB3	1:A:67:LYS:H	1.55	0.71
1:C:248:LYS:HE2	1:C:249:TYR:CZ	2.25	0.71
1:A:267:LEU:N	6:A:1379:HOH:O	2.24	0.71
1:C:81:GLN:HE21	1:C:81:GLN:N	1.88	0.70
1:C:248:LYS:HG2	1:C:249:TYR:CE1	2.26	0.70
1:C:417:PRO:HA	1:C:420:LYS:HG3	1.73	0.70
1:C:89:ASP:OD1	1:C:90:ARG:HG3	1.92	0.70
1:C:364:PRO:HB2	1:C:365:ASN:ND2	2.07	0.70
1:A:109:LYS:HE3	1:A:116:ASP:OD1	1.91	0.69
1:B:113:PHE:O	1:B:116:ASP:HB2	1.92	0.69
1:C:211:LEU:HD12	1:C:411:VAL:CG1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:PHE:HE2	1:D:339:MET:CE	2.05	0.69
1:C:308:ILE:O	1:C:312:ILE:HG13	1.92	0.69
1:A:81:GLN:HB2	6:A:1292:HOH:O	1.92	0.69
1:B:194:ASP:OD1	1:B:195:TRP:N	2.25	0.69
1:B:297:ILE:HG23	1:B:335:LYS:HD3	1.74	0.69
1:B:427:MET:O	1:B:430:HIS:HB2	1.92	0.69
1:C:81:GLN:H	1:C:81:GLN:HE21	1.40	0.68
1:C:367:LYS:O	1:C:371:GLU:HG3	1.94	0.68
1:D:199:ASP:HA	1:D:202:LYS:HE2	1.74	0.68
1:D:281:LYS:HD3	1:D:281:LYS:N	2.07	0.68
1:A:168:CYS:HB2	1:A:171:ILE:HD12	1.74	0.68
1:D:201:VAL:HA	1:D:204:ASN:ND2	2.09	0.68
1:D:496:LEU:HD12	1:D:496:LEU:O	1.93	0.68
1:A:173:GLU:OE1	1:A:381:HIS:ND1	2.23	0.68
1:D:318:TYR:OH	1:D:487:ASN:ND2	2.26	0.68
1:D:193:ARG:HH11	1:D:193:ARG:HG2	1.59	0.68
1:A:86:GLU:HG2	1:A:87:TYR:CD1	2.29	0.68
1:B:233:LEU:O	1:B:271:ALA:HB2	1.94	0.68
1:D:364:PRO:HG2	1:D:368:GLU:CG	2.22	0.68
1:D:493:GLU:HG2	1:D:497:TYR:CE2	2.29	0.67
1:A:289:HIS:CD2	1:A:441:PRO:HD3	2.29	0.67
1:B:211:LEU:O	1:B:214:ALA:HB3	1.94	0.67
1:D:272:VAL:H	4:D:1121:AMP:N6	1.93	0.67
1:C:63:TYR:CE2	1:C:70:VAL:HG13	2.30	0.67
1:A:365:ASN:HA	1:A:421:MET:CE	2.25	0.67
1:B:336:ILE:CG2	1:B:341:ILE:HB	2.24	0.67
1:D:81:GLN:HB2	6:D:1256:HOH:O	1.95	0.67
1:C:232:LEU:HD22	1:C:332:MET:HE1	1.75	0.67
1:C:410:ASP:O	1:C:414:ARG:HD2	1.94	0.67
1:D:232:LEU:HB3	4:D:1121:AMP:N3	2.10	0.67
1:C:171:ILE:HD12	1:C:507:LEU:CD2	2.26	0.66
1:C:173:GLU:O	1:C:175:PRO:HD3	1.95	0.66
1:B:472:VAL:HG21	1:B:492:LYS:O	1.96	0.66
1:D:332:MET:O	1:D:336:ILE:HG13	1.95	0.66
1:C:209:ASN:OD1	1:C:212:ARG:NH1	2.28	0.66
1:D:78:TYR:HA	1:D:224:MET:HE1	1.77	0.66
1:B:63:TYR:CD2	1:B:70:VAL:HG22	2.31	0.66
1:B:227:VAL:HB	1:B:228:PRO:HD2	1.77	0.66
1:A:360:PHE:CZ	1:A:372:GLU:HG3	2.30	0.66
1:C:115:ASP:OD2	1:C:193:ARG:NH2	2.28	0.66
1:B:1:ALA:H1	5:B:1113:GLN:HE22	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ALA:O	1:B:392:MET:HG2	1.95	0.65
1:C:392:MET:HG3	1:C:399:ALA:HB2	1.79	0.65
1:D:320:VAL:HG22	1:D:497:TYR:CD2	2.30	0.65
1:D:361:HIS:HE2	1:D:428:GLU:HG3	1.59	0.65
1:C:232:LEU:HD22	1:C:332:MET:CE	2.26	0.65
1:C:348:GLU:CD	4:C:1114:AMP:H5'1	2.16	0.65
1:C:454:ASP:N	6:C:1309:HOH:O	2.30	0.65
1:A:348:GLU:CD	4:A:1100:AMP:H5'1	2.17	0.65
1:D:473:SER:OG	1:D:475:GLN:N	2.30	0.65
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.61	0.65
1:C:117:LEU:O	1:C:406:LYS:NZ	2.26	0.65
1:C:198:TYR:CD2	1:C:367:LYS:HG3	2.31	0.65
1:C:81:GLN:NE2	1:C:81:GLN:N	2.43	0.65
1:D:361:HIS:NE2	1:D:428:GLU:OE2	2.30	0.64
1:A:199:ASP:HB3	1:A:202:LYS:CE	2.27	0.64
1:B:427:MET:HE1	1:B:447:ARG:N	2.12	0.64
1:B:81:GLN:NE2	6:B:1255:HOH:O	2.27	0.64
1:B:264:TRP:O	1:B:266:GLN:N	2.28	0.64
1:B:300:THR:HG22	1:B:303:GLU:N	2.08	0.64
1:B:440:LEU:HD23	1:B:440:LEU:N	2.13	0.64
1:C:281:LYS:HE3	6:C:1288:HOH:O	1.98	0.64
1:C:364:PRO:CG	1:C:368:GLU:HG2	2.17	0.64
1:B:80:HIS:HD2	1:B:84:ARG:HE	1.46	0.64
1:B:418:GLN:O	1:B:421:MET:HB2	1.97	0.64
1:C:289:HIS:NE2	1:C:439:TYR:O	2.31	0.64
1:D:64:ASN:HB3	1:D:67:LYS:CA	2.28	0.64
1:B:1:ALA:H3	5:B:1113:GLN:HE22	1.46	0.64
1:D:49:ARG:HD3	6:D:1173:HOH:O	1.97	0.63
1:C:415:ILE:HD11	1:C:420:LYS:HE3	1.81	0.63
1:B:307:ALA:O	1:B:311:VAL:HG23	1.98	0.63
1:D:277:SER:O	1:D:280:LEU:HB2	1.97	0.63
1:A:12:ASP:HB3	1:A:15:GLU:CB	2.28	0.63
1:B:83:LEU:HD13	1:B:101:VAL:CG1	2.28	0.63
1:B:199:ASP:HA	1:B:202:LYS:HD3	1.81	0.63
1:C:44:ILE:O	1:C:45:LEU:HD12	1.99	0.63
1:C:64:ASN:OD1	1:C:67:LYS:N	2.31	0.63
1:C:271:ALA:HA	4:C:1114:AMP:N1	2.13	0.63
1:C:416:ASN:HB3	1:C:419:ASP:OD2	1.98	0.63
1:A:277:SER:HB2	1:A:278:PRO:HD2	1.80	0.63
1:B:358:LEU:HA	1:B:361:HIS:CD2	2.33	0.63
1:B:81:GLN:HE21	1:B:81:GLN:N	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:ARG:NH2	1:D:97:SER:O	2.28	0.63
1:A:382:MET:SD	1:A:515:PRO:HG3	2.38	0.62
1:D:12:ASP:OD1	1:D:14:VAL:HB	2.00	0.62
1:C:234:SER:HB3	4:C:1114:AMP:N7	2.15	0.62
1:D:52:ILE:N	1:D:52:ILE:HD12	2.14	0.62
1:A:359:TYR:OH	1:A:376:LYS:HE3	1.99	0.62
1:C:168:CYS:HB2	1:C:171:ILE:CD1	2.29	0.62
1:C:219:VAL:O	1:C:223:LEU:HG	2.00	0.62
1:C:415:ILE:HD11	1:C:420:LYS:CE	2.29	0.62
1:D:12:ASP:OD1	1:D:15:GLU:N	2.27	0.62
1:A:500:ILE:O	1:A:503:GLU:HB3	1.99	0.62
1:B:232:LEU:HD12	1:B:346:SER:HB2	1.82	0.62
1:C:287:ALA:O	1:C:291:GLY:N	2.32	0.62
1:B:461:ILE:O	1:B:464:LEU:N	2.33	0.61
1:A:86:GLU:HG2	1:A:87:TYR:CE1	2.35	0.61
1:B:216:GLU:HG2	1:B:249:TYR:CE1	2.32	0.61
1:D:473:SER:HG	1:D:475:GLN:H	1.45	0.61
1:A:365:ASN:HA	1:A:421:MET:HE1	1.81	0.61
1:B:461:ILE:HG22	1:B:465:LYS:HE2	1.83	0.61
1:D:1:ALA:N	5:D:1127:GLN:HE22	1.99	0.61
1:D:64:ASN:CB	1:D:68:THR:H	2.14	0.61
1:A:365:ASN:HD21	1:A:368:GLU:CG	2.13	0.61
1:A:461:ILE:HG22	1:A:465:LYS:HE2	1.82	0.61
1:B:287:ALA:HB1	1:B:294:HIS:HB2	1.83	0.61
1:B:514:VAL:CG1	1:B:515:PRO:HD2	2.31	0.61
1:A:351:ASP:HB2	1:A:357:TYR:CZ	2.36	0.60
1:C:63:TYR:CD2	1:C:70:VAL:HG13	2.36	0.60
1:D:353:VAL:O	1:D:420:LYS:HE2	2.01	0.60
1:C:211:LEU:HA	1:C:411:VAL:HG11	1.83	0.60
1:D:65:GLN:HG2	1:D:92:GLN:O	2.01	0.60
1:C:6:VAL:HA	1:C:155:LEU:O	2.01	0.60
1:A:168:CYS:HB2	1:A:171:ILE:CD1	2.32	0.60
1:A:460:TRP:CZ2	1:A:464:LEU:HD21	2.37	0.60
1:D:427:MET:H	1:D:430:HIS:CD2	2.05	0.60
1:B:463:THR:O	1:B:467:VAL:HG23	2.00	0.60
1:C:241:ILE:O	1:C:245:ILE:HG13	2.02	0.60
1:D:466:GLU:O	1:D:470:GLN:HG3	2.02	0.60
1:D:51:SER:C	1:D:52:ILE:HD12	2.22	0.60
1:D:507:LEU:HD12	1:D:508:PRO:HD2	1.82	0.60
1:A:213:GLN:HE21	1:A:213:GLN:C	2.06	0.59
1:D:197:ASP:O	1:D:200:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:GLU:O	1:D:466:GLU:HG2	2.00	0.59
1:B:165:VAL:HB	6:B:1164:HOH:O	2.01	0.59
1:B:216:GLU:O	1:B:220:LYS:HD3	2.02	0.59
1:B:282:ALA:O	1:B:285:GLU:HB2	2.01	0.59
1:A:111:PRO:HG3	1:A:181:TRP:CD1	2.37	0.59
1:C:336:ILE:O	1:C:339:MET:HB2	2.03	0.59
1:B:428:GLU:HB2	1:B:433:ARG:HH21	1.67	0.59
1:C:431:ILE:O	1:C:434:GLU:HB3	2.02	0.59
1:B:248:LYS:HE2	1:B:249:TYR:CZ	2.38	0.58
1:C:150:ASP:HB3	1:C:152:HIS:N	2.17	0.58
1:A:381:HIS:CE1	1:A:382:MET:HG3	2.38	0.58
1:A:329:MET:HE3	1:A:388:ALA:HA	1.85	0.58
1:B:199:ASP:HB2	1:B:202:LYS:NZ	2.18	0.58
1:B:105:LEU:O	1:B:109:LYS:HB2	2.03	0.58
1:B:237:LEU:O	1:B:241:ILE:HG13	2.04	0.58
1:B:278:PRO:HD2	1:B:455:GLY:O	2.04	0.58
1:B:279:ASP:HB2	1:B:455:GLY:O	2.04	0.58
1:B:64:ASN:HD22	1:B:68:THR:H	1.50	0.58
1:B:81:GLN:HE21	1:B:81:GLN:H	1.50	0.58
1:B:358:LEU:CA	1:B:361:HIS:HD2	2.15	0.58
1:D:387:ARG:HG2	1:D:388:ALA:N	2.18	0.58
1:A:281:LYS:HD3	1:A:285:GLU:OE1	2.04	0.58
1:B:79:ASN:HD22	1:B:118:GLN:CB	2.16	0.58
1:B:81:GLN:NE2	6:B:1152:HOH:O	2.29	0.58
1:B:358:LEU:O	1:B:361:HIS:HB2	2.03	0.58
1:C:19:LYS:HE3	1:C:167:VAL:CG1	2.33	0.58
1:C:357:TYR:O	1:C:360:PHE:HB2	2.04	0.58
1:C:365:ASN:ND2	1:C:365:ASN:N	2.52	0.58
1:B:277:SER:HB2	1:B:278:PRO:HD2	1.86	0.57
1:C:440:LEU:HB3	1:C:441:PRO:CD	2.32	0.57
1:A:367:LYS:HE3	1:A:371:GLU:OE1	2.04	0.57
1:A:395:TRP:HH2	1:D:28:ARG:HD3	1.68	0.57
1:D:183:GLN:NE2	6:D:1260:HOH:O	2.35	0.57
1:D:358:LEU:HA	1:D:361:HIS:HD2	1.70	0.57
1:D:279:ASP:HB3	6:D:1413:HOH:O	2.04	0.57
1:D:50:LEU:CG	1:D:52:ILE:HD11	2.34	0.57
1:C:264:TRP:CD1	1:C:265:PRO:HD2	2.39	0.57
1:D:66:GLN:HB2	6:D:1255:HOH:O	2.05	0.57
1:A:89:ASP:OD1	1:A:90:ARG:HG3	2.04	0.57
1:D:270:PHE:HE2	1:D:339:MET:HE2	1.68	0.57
1:A:416:ASN:OD1	1:A:417:PRO:HD2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:HIS:CG	1:B:441:PRO:HG3	2.39	0.57
1:D:361:HIS:HE2	1:D:428:GLU:CG	2.18	0.57
1:D:81:GLN:HA	1:D:81:GLN:NE2	2.19	0.57
1:D:50:LEU:HG	1:D:52:ILE:CD1	2.33	0.56
1:A:192:HIS:O	1:A:193:ARG:HD3	2.04	0.56
1:A:199:ASP:HA	1:A:202:LYS:HE2	1.86	0.56
1:A:201:VAL:HA	1:A:204:ASN:OD1	2.06	0.56
1:A:280:LEU:HD22	1:A:296:GLU:HG3	1.88	0.56
1:D:120:MET:HB2	1:D:143:ILE:HG12	1.86	0.56
1:A:315:ILE:HD13	1:A:315:ILE:N	2.19	0.56
1:B:30:ARG:HG2	1:B:393:SER:HB3	1.86	0.56
1:C:212:ARG:HB2	1:C:435:CYS:HB3	1.87	0.56
1:A:164:LEU:HB3	1:A:171:ILE:HD11	1.88	0.56
1:B:121:PHE:H	1:B:138:ASP:HB3	1.71	0.56
1:B:300:THR:HG22	1:B:303:GLU:HB2	1.88	0.56
1:A:199:ASP:CA	1:A:202:LYS:HE2	2.36	0.56
1:B:364:PRO:HG2	1:B:368:GLU:CG	2.36	0.56
1:D:50:LEU:CD2	1:D:52:ILE:HD11	2.35	0.56
1:B:420:LYS:HE3	6:B:1221:HOH:O	2.06	0.55
1:C:90:ARG:HD2	1:C:108:GLU:HG3	1.88	0.55
1:D:65:GLN:OE1	1:D:92:GLN:HB2	2.07	0.55
1:D:233:LEU:O	1:D:271:ALA:HB2	2.05	0.55
1:A:98:ASP:O	1:A:101:VAL:HG22	2.06	0.55
1:C:150:ASP:HB2	1:C:154:GLN:H	1.72	0.55
1:A:301:VAL:HG11	1:A:463:THR:HG21	1.88	0.55
1:B:427:MET:HE1	1:B:446:TRP:C	2.27	0.55
1:A:277:SER:HB2	1:A:455:GLY:O	2.06	0.55
1:A:416:ASN:HB3	1:A:419:ASP:OD2	2.06	0.55
1:B:57:ALA:O	1:B:95:THR:HB	2.07	0.55
1:B:234:SER:HB3	4:B:1107:AMP:C5	2.41	0.55
1:A:269:SER:O	1:A:295:HIS:HD2	1.90	0.55
1:B:325:ALA:O	1:B:328:PRO:HD2	2.07	0.55
1:C:155:LEU:HD12	1:C:156:TYR:N	2.21	0.55
1:C:233:LEU:O	1:C:271:ALA:HB2	2.06	0.55
1:C:337:LYS:HE3	1:C:396:GLY:O	2.06	0.55
1:A:286:VAL:O	1:A:290:LEU:HD13	2.07	0.55
1:A:7:PHE:HB3	1:A:133:TYR:CE2	2.42	0.55
1:A:60:GLN:HB3	1:A:61:PRO:HA	1.89	0.55
1:A:320:VAL:HG22	1:A:497:TYR:CE2	2.42	0.55
1:B:467:VAL:O	1:B:470:GLN:HB2	2.06	0.55
1:D:348:GLU:HG2	1:D:384:ASP:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:THR:HB	1:C:129:GLU:HG2	1.89	0.55
1:C:105:LEU:HD22	1:C:113:PHE:HB2	1.88	0.55
1:B:352:GLU:OE1	1:B:357:TYR:OH	2.25	0.55
1:B:224:MET:HG3	1:B:224:MET:O	2.08	0.54
1:A:289:HIS:CG	1:A:441:PRO:HD3	2.43	0.54
1:A:274:LEU:HD23	1:A:299:PHE:O	2.07	0.54
1:C:107:GLN:O	1:C:107:GLN:HG2	2.06	0.54
1:D:277:SER:HB2	1:D:455:GLY:O	2.07	0.54
1:B:367:LYS:O	1:B:371:GLU:HG3	2.08	0.54
1:C:301:VAL:HG11	1:C:463:THR:HG21	1.88	0.54
1:A:333:SER:HB2	1:A:392:MET:CE	2.37	0.54
1:B:197:ASP:O	1:B:200:ALA:HB3	2.07	0.54
1:C:388:ALA:O	1:C:392:MET:HG2	2.07	0.54
1:C:433:ARG:HD3	1:C:445:ALA:O	2.08	0.54
1:D:192:HIS:O	1:D:193:ARG:HG2	2.08	0.54
1:B:216:GLU:OE1	1:B:439:TYR:OH	2.25	0.54
1:A:117:LEU:O	1:A:406:LYS:NZ	2.36	0.54
1:A:468:ALA:HA	1:A:496:LEU:HD12	1.90	0.54
1:D:494:ALA:HB1	6:D:1238:HOH:O	2.08	0.54
1:B:90:ARG:HG3	6:B:1312:HOH:O	2.07	0.54
1:D:337:LYS:NZ	6:D:1168:HOH:O	2.31	0.54
1:D:428:GLU:CD	1:D:428:GLU:H	2.10	0.54
1:C:150:ASP:HB2	1:C:154:GLN:N	2.24	0.53
1:B:332:MET:O	1:B:336:ILE:HG13	2.08	0.53
1:A:365:ASN:ND2	1:A:368:GLU:HG2	2.22	0.53
1:A:365:ASN:HD22	1:A:368:GLU:H	1.57	0.53
1:B:380:LEU:HD22	1:B:384:ASP:HB2	1.87	0.53
1:B:81:GLN:NE2	1:B:81:GLN:N	2.55	0.53
1:B:201:VAL:CG1	1:B:417:PRO:HD3	2.39	0.53
1:C:334:ARG:HD2	1:C:395:TRP:CZ2	2.44	0.53
1:D:227:VAL:HB	1:D:228:PRO:CD	2.37	0.53
1:A:12:ASP:HB3	1:A:15:GLU:HB3	1.90	0.53
1:A:242:ILE:HD11	1:A:403:PHE:CE2	2.44	0.53
1:B:468:ALA:HA	1:B:496:LEU:HD12	1.90	0.53
1:A:268:HIS:HD1	1:A:295:HIS:CE1	2.27	0.53
1:B:199:ASP:HB2	1:B:202:LYS:HE2	1.90	0.53
1:D:367:LYS:O	1:D:371:GLU:HG3	2.09	0.53
1:D:361:HIS:HE2	1:D:428:GLU:CD	2.10	0.53
1:C:5:GLY:O	1:C:156:TYR:HA	2.09	0.53
1:D:125:LEU:C	1:D:125:LEU:HD23	2.29	0.53
1:A:213:GLN:O	1:A:213:GLN:NE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ASP:HB2	1:B:202:LYS:HZ1	1.72	0.53
1:A:415:ILE:HG22	6:A:1398:HOH:O	2.08	0.52
1:B:80:HIS:CG	1:B:98:ASP:HA	2.44	0.52
1:B:403:PHE:HB2	6:B:1287:HOH:O	2.08	0.52
1:D:422:CYS:SG	1:D:428:GLU:HA	2.49	0.52
1:B:247:LYS:HD3	1:B:290:LEU:O	2.10	0.52
1:C:361:HIS:C	1:C:363:ALA:H	2.11	0.52
1:A:12:ASP:HB3	1:A:15:GLU:HB2	1.91	0.52
1:B:300:THR:HG23	1:B:302:GLN:N	2.24	0.52
1:B:429:LYS:O	1:B:433:ARG:HG2	2.08	0.52
1:C:79:ASN:HB2	1:C:118:GLN:HB3	1.89	0.52
1:D:297:ILE:HG12	1:D:335:LYS:HG2	1.91	0.52
1:A:239:SER:HB3	4:A:1100:AMP:H2'	1.92	0.52
1:C:356:GLY:HA2	1:C:429:LYS:HG3	1.90	0.52
1:B:240:SER:HB3	1:B:440:LEU:HD13	1.92	0.52
1:B:2:SER:OG	1:B:48:GLU:HB2	2.10	0.52
1:B:199:ASP:HB2	1:B:202:LYS:CE	2.39	0.52
1:D:384:ASP:CG	1:D:387:ARG:HH21	2.12	0.52
1:D:358:LEU:O	1:D:361:HIS:HB2	2.09	0.52
1:D:4:PHE:HB3	1:D:46:ALA:HB3	1.92	0.52
1:A:486:TYR:CE1	1:A:487:ASN:ND2	2.78	0.52
1:C:216:GLU:OE1	1:C:439:TYR:OH	2.27	0.52
1:C:264:TRP:CD1	1:C:265:PRO:CD	2.93	0.52
1:D:444:VAL:HG13	6:D:1362:HOH:O	2.09	0.52
1:A:327:THR:HB	1:A:328:PRO:HD3	1.90	0.51
1:A:504:LEU:C	1:A:506:PRO:HD3	2.30	0.51
1:D:354:PHE:HA	1:D:420:LYS:HE2	1.92	0.51
1:A:268:HIS:ND1	1:A:295:HIS:CE1	2.79	0.51
1:D:300:THR:HB	6:D:1226:HOH:O	2.10	0.51
1:B:171:ILE:HD12	1:B:507:LEU:HD21	1.91	0.51
1:B:364:PRO:HG2	1:B:368:GLU:HG2	1.92	0.51
1:C:264:TRP:HD1	1:C:265:PRO:HD3	1.75	0.51
1:C:171:ILE:HD12	1:C:507:LEU:HD22	1.91	0.51
1:D:327:THR:HB	1:D:328:PRO:HD3	1.93	0.51
1:D:229:TYR:C	1:D:341:ILE:HD13	2.31	0.51
1:C:358:LEU:O	1:C:361:HIS:N	2.32	0.51
1:D:80:HIS:HD2	1:D:84:ARG:HE	1.59	0.51
1:B:161:MET:HG2	1:B:316:GLU:OE2	2.11	0.51
1:B:289:HIS:CB	1:B:441:PRO:HG3	2.41	0.51
1:B:289:HIS:ND1	1:B:441:PRO:HG3	2.26	0.51
1:B:379:ALA:O	1:B:383:TYR:HD1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:GLU:HG2	1:C:87:TYR:CD1	2.46	0.51
1:C:215:LEU:HB2	1:C:408:PHE:CE1	2.45	0.51
1:D:181:TRP:NE1	1:D:183:GLN:HB2	2.25	0.51
1:B:357:TYR:HE2	1:B:376:LYS:HD2	1.75	0.51
1:C:19:LYS:O	1:C:22:GLU:HB2	2.11	0.51
1:B:175:PRO:HG2	1:B:187:ILE:HG21	1.93	0.51
1:C:25:ARG:O	1:C:25:ARG:HG3	2.09	0.51
1:C:78:TYR:CD1	1:C:119:GLY:HA2	2.46	0.51
1:C:416:ASN:OD1	1:C:418:GLN:HB2	2.11	0.51
1:B:125:LEU:HD23	1:B:125:LEU:C	2.32	0.51
1:B:433:ARG:HB3	1:B:445:ALA:O	2.10	0.51
1:C:359:TYR:CZ	1:C:360:PHE:CE1	2.99	0.51
1:D:472:VAL:CG1	1:D:492:LYS:HG2	2.40	0.51
1:A:19:LYS:HE3	1:A:22:GLU:OE1	2.11	0.50
1:A:93:PHE:CD2	1:A:100:GLU:HG2	2.46	0.50
1:B:36:GLY:HA3	1:B:60:GLN:O	2.11	0.50
1:B:360:PHE:HD2	1:B:369:LEU:HD12	1.76	0.50
1:D:346:SER:OG	1:D:348:GLU:OE2	2.29	0.50
1:C:358:LEU:O	1:C:360:PHE:N	2.45	0.50
1:D:269:SER:O	1:D:295:HIS:HD2	1.94	0.50
1:D:387:ARG:NH1	6:D:1342:HOH:O	2.37	0.50
1:B:289:HIS:HB2	1:B:441:PRO:HG3	1.93	0.50
1:B:337:LYS:HE3	1:B:396:GLY:O	2.12	0.50
1:C:81:GLN:H	1:C:81:GLN:CD	2.13	0.50
1:C:337:LYS:HG2	1:C:395:TRP:O	2.12	0.50
1:C:127:ASP:OD1	1:C:130:LYS:HD3	2.12	0.50
1:B:204:ASN:O	1:B:416:ASN:ND2	2.44	0.50
1:C:486:TYR:CD1	1:C:487:ASN:HB2	2.47	0.50
1:D:1:ALA:H3	5:D:1127:GLN:HE22	1.59	0.50
1:D:320:VAL:HG22	1:D:497:TYR:CE2	2.46	0.50
1:A:80:HIS:ND1	1:A:98:ASP:HA	2.25	0.50
1:D:205:VAL:O	1:D:205:VAL:HG12	2.11	0.50
1:A:68:THR:HB	1:A:129:GLU:HG2	1.94	0.50
1:B:84:ARG:NH2	1:B:97:SER:O	2.37	0.50
1:B:496:LEU:C	1:B:496:LEU:HD23	2.32	0.50
1:A:147:MET:HE2	1:A:174:PHE:HA	1.93	0.50
1:A:209:ASN:HA	1:A:212:ARG:NH1	2.27	0.50
1:B:342:LYS:N	6:B:1274:HOH:O	2.42	0.50
1:D:192:HIS:C	1:D:193:ARG:HG2	2.32	0.50
1:A:329:MET:HE2	1:A:387:ARG:HD2	1.94	0.49
1:A:365:ASN:HA	1:A:421:MET:HE2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ASN:CB	1:D:68:THR:N	2.75	0.49
1:A:227:VAL:HB	1:A:228:PRO:CD	2.40	0.49
1:A:365:ASN:ND2	1:A:368:GLU:CG	2.75	0.49
1:B:38:TYR:OH	1:B:40:SER:HB3	2.12	0.49
1:B:115:ASP:OD2	1:B:406:LYS:HE2	2.11	0.49
1:C:175:PRO:HG2	1:C:187:ILE:HG21	1.94	0.49
1:C:352:GLU:OE1	1:C:357:TYR:OH	2.31	0.49
1:D:371:GLU:O	1:D:375:ARG:HB2	2.13	0.49
1:C:217:ASP:HA	1:C:220:LYS:HD3	1.94	0.49
1:A:218:SER:O	1:A:222:HIS:ND1	2.46	0.49
1:B:81:GLN:CD	1:B:82:ALA:H	2.16	0.49
1:A:401:VAL:HG23	1:A:401:VAL:O	2.13	0.49
1:B:270:PHE:HE2	1:B:339:MET:HE2	1.78	0.49
1:B:349:GLY:HA3	1:B:404:LEU:HD21	1.95	0.49
1:D:147:MET:HA	1:D:156:TYR:O	2.13	0.49
1:A:1:ALA:HB1	1:A:48:GLU:O	2.12	0.49
1:A:289:HIS:CD2	1:A:290:LEU:HD12	2.47	0.49
1:C:186:GLU:HB2	1:C:188:ARG:NH2	2.27	0.49
1:A:199:ASP:HA	1:A:202:LYS:CE	2.42	0.49
1:A:474:ASP:O	1:A:478:GLU:HG3	2.13	0.49
1:A:238:ASP:CG	1:A:429:LYS:HZ1	2.15	0.49
1:B:79:ASN:HD22	1:B:118:GLN:HB2	1.78	0.49
1:B:201:VAL:HA	1:B:204:ASN:OD1	2.13	0.49
1:C:234:SER:HB3	4:C:1114:AMP:C8	2.48	0.49
1:C:504:LEU:C	1:C:506:PRO:HD3	2.33	0.48
1:B:285:GLU:O	1:B:288:ASN:HB2	2.13	0.48
1:C:365:ASN:O	1:C:421:MET:HE1	2.13	0.48
1:D:348:GLU:CG	4:D:1121:AMP:H5'1	2.43	0.48
1:A:64:ASN:ND2	1:A:68:THR:OG1	2.45	0.48
1:A:320:VAL:HG22	1:A:497:TYR:CD2	2.49	0.48
1:A:440:LEU:HB3	1:A:441:PRO:CD	2.41	0.48
1:C:111:PRO:HG3	1:C:181:TRP:CE2	2.48	0.48
1:B:167:VAL:HG22	1:B:167:VAL:O	2.14	0.48
1:C:418:GLN:O	1:C:421:MET:HB2	2.14	0.48
1:D:464:LEU:HD12	1:D:464:LEU:HA	1.62	0.48
1:B:430:HIS:CD2	1:B:446:TRP:HZ3	2.31	0.48
1:D:81:GLN:NE2	1:D:81:GLN:CA	2.76	0.48
1:D:165:VAL:N	1:D:166:PRO:CD	2.77	0.48
1:D:274:LEU:HD23	1:D:299:PHE:O	2.14	0.48
1:A:60:GLN:HA	1:A:61:PRO:C	2.35	0.48
1:A:205:VAL:HG13	1:A:206:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:HG23	1:A:432:LEU:N	2.29	0.48
1:A:242:ILE:HD11	1:A:403:PHE:CD2	2.49	0.48
1:B:357:TYR:O	1:B:360:PHE:HB2	2.14	0.48
1:B:68:THR:O	1:B:69:HIS:HD2	1.97	0.47
1:C:264:TRP:HD1	1:C:265:PRO:CD	2.26	0.47
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.79	0.47
1:D:80:HIS:O	1:D:84:ARG:HG3	2.14	0.47
1:A:199:ASP:HB3	1:A:202:LYS:HE2	1.95	0.47
1:B:17:ARG:HD3	6:B:1121:HOH:O	2.14	0.47
1:B:49:ARG:NH2	1:B:51:SER:HB3	2.29	0.47
1:B:158:ALA:HB3	1:B:164:LEU:HD13	1.96	0.47
1:D:387:ARG:CG	1:D:388:ALA:N	2.77	0.47
1:A:383:TYR:O	1:A:386:ALA:HB3	2.14	0.47
1:B:484:PHE:O	1:B:488:THR:HG23	2.14	0.47
1:A:209:ASN:O	1:A:213:GLN:HB2	2.14	0.47
1:A:387:ARG:CG	1:A:388:ALA:N	2.77	0.47
1:B:334:ARG:NH1	1:C:35:SER:OG	2.48	0.47
1:B:83:LEU:CB	1:B:101:VAL:HG11	2.43	0.47
1:B:301:VAL:HG12	1:B:302:GLN:N	2.30	0.47
1:B:467:VAL:O	1:B:467:VAL:HG12	2.14	0.47
1:C:147:MET:SD	1:C:172:LYS:HE3	2.55	0.47
1:A:28:ARG:HD3	1:D:395:TRP:HH2	1.80	0.47
1:A:378:LEU:CD1	1:A:378:LEU:N	2.77	0.47
1:A:381:HIS:CE1	1:A:382:MET:CG	2.98	0.47
1:B:207:ASP:CG	1:B:210:GLU:HB2	2.35	0.47
1:C:264:TRP:C	1:C:266:GLN:H	2.18	0.47
1:C:272:VAL:HA	1:C:297:ILE:O	2.14	0.47
1:C:321:THR:HB	6:C:1343:HOH:O	2.14	0.47
1:D:210:GLU:HA	6:D:1273:HOH:O	2.14	0.47
1:D:273:GLY:O	1:D:298:HIS:HA	2.14	0.47
1:C:358:LEU:H	1:C:358:LEU:HG	1.44	0.47
1:B:81:GLN:NE2	1:B:82:ALA:N	2.58	0.47
1:B:219:VAL:O	1:B:223:LEU:HG	2.15	0.47
1:B:514:VAL:HG12	1:B:515:PRO:HD2	1.95	0.47
1:C:386:ALA:O	1:C:390:LYS:HB2	2.15	0.47
1:C:410:ASP:O	1:C:414:ARG:HB2	2.14	0.47
1:A:333:SER:HB2	1:A:392:MET:HE3	1.95	0.47
1:B:79:ASN:HB2	1:B:118:GLN:HB3	1.96	0.47
1:B:289:HIS:CG	1:B:441:PRO:HD3	2.50	0.47
1:B:372:GLU:OE2	1:B:372:GLU:HA	2.15	0.47
1:C:162:LYS:HB2	1:C:316:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:HIS:HA	1:C:293:VAL:O	2.15	0.47
1:C:374:VAL:HG23	1:C:413:MET:CE	2.45	0.47
1:D:233:LEU:HD22	1:D:235:GLY:H	1.80	0.47
1:D:193:ARG:HH11	1:D:193:ARG:CG	2.28	0.46
1:D:280:LEU:HD12	1:D:280:LEU:HA	1.78	0.46
1:D:334:ARG:HB2	1:D:395:TRP:CE2	2.50	0.46
1:A:287:ALA:HB1	1:A:294:HIS:HB2	1.97	0.46
1:A:289:HIS:HD2	1:A:290:LEU:HD12	1.79	0.46
1:A:335:LYS:HE3	1:D:34:TRP:CZ3	2.50	0.46
1:B:1:ALA:HB1	1:B:48:GLU:O	2.16	0.46
1:B:324:ARG:NH2	1:B:461:ILE:CG2	2.78	0.46
1:B:507:LEU:O	1:B:510:ALA:N	2.37	0.46
1:C:184:ASP:OD1	1:C:188:ARG:NH2	2.39	0.46
1:D:118:GLN:NE2	1:D:405:ASP:OD1	2.48	0.46
1:D:268:HIS:CE1	1:D:293:VAL:HG11	2.51	0.46
1:B:240:SER:HB3	1:B:440:LEU:CD1	2.46	0.46
1:C:433:ARG:HD2	1:C:446:TRP:CZ3	2.49	0.46
1:D:12:ASP:OD1	1:D:15:GLU:HG3	2.15	0.46
1:A:409:LEU:O	1:A:413:MET:HB2	2.14	0.46
1:B:241:ILE:HD13	1:B:436:PHE:HB2	1.97	0.46
1:B:245:ILE:HG23	1:B:249:TYR:CE1	2.50	0.46
1:B:494:ALA:HB2	6:B:1298:HOH:O	2.15	0.46
1:A:280:LEU:CD1	1:A:298:HIS:CD2	2.98	0.46
1:A:464:LEU:HD12	6:A:1342:HOH:O	2.15	0.46
1:B:277:SER:HB2	1:B:455:GLY:O	2.16	0.46
1:B:427:MET:SD	1:B:433:ARG:NE	2.89	0.46
1:D:64:ASN:C	1:D:67:LYS:H	2.18	0.46
1:B:199:ASP:CB	1:B:202:LYS:NZ	2.78	0.46
1:C:227:VAL:HB	1:C:228:PRO:HD2	1.98	0.46
1:D:78:TYR:CD2	1:D:224:MET:HE2	2.50	0.46
1:D:364:PRO:CG	1:D:368:GLU:HG2	2.29	0.46
1:D:406:LYS:NZ	6:D:1196:HOH:O	2.33	0.46
1:B:79:ASN:HD22	1:B:118:GLN:N	2.14	0.46
1:B:248:LYS:HG2	1:B:249:TYR:N	2.31	0.46
1:D:351:ASP:OD2	1:D:429:LYS:HE3	2.16	0.46
1:D:472:VAL:HB	1:D:492:LYS:CG	2.16	0.46
1:A:213:GLN:NE2	1:A:213:GLN:CA	2.79	0.46
1:A:277:SER:HB2	1:A:278:PRO:CD	2.46	0.46
1:B:81:GLN:CD	1:B:82:ALA:N	2.70	0.46
1:C:335:LYS:HG3	6:C:1328:HOH:O	2.16	0.46
1:D:129:GLU:OE2	1:D:129:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:O	1:D:175:PRO:HD3	2.15	0.46
1:B:49:ARG:NH1	1:B:58:GLY:HA3	2.31	0.46
1:A:430:HIS:O	1:A:433:ARG:HB2	2.16	0.45
1:A:437:GLU:OE1	1:A:446:TRP:NE1	2.49	0.45
1:A:475:GLN:HA	1:A:478:GLU:CD	2.37	0.45
1:B:64:ASN:HB2	1:B:69:HIS:H	1.81	0.45
1:D:224:MET:O	1:D:400:ARG:NH1	2.43	0.45
1:B:300:THR:HG22	1:B:303:GLU:CB	2.46	0.45
1:D:357:TYR:O	1:D:360:PHE:HB2	2.16	0.45
1:A:165:VAL:N	1:A:166:PRO:CD	2.79	0.45
1:A:351:ASP:OD2	1:A:429:LYS:NZ	2.43	0.45
1:C:280:LEU:HG	1:C:296:GLU:HG3	1.99	0.45
1:D:514:VAL:HG13	1:D:515:PRO:HD2	1.97	0.45
1:A:1:ALA:N	5:A:1106:GLN:HE22	2.14	0.45
1:A:165:VAL:N	1:A:166:PRO:HD2	2.32	0.45
1:B:28:ARG:HG3	1:B:48:GLU:OE2	2.15	0.45
1:B:269:SER:OG	1:B:294:HIS:ND1	2.43	0.45
1:C:19:LYS:HE3	1:C:167:VAL:HG11	1.98	0.45
1:C:171:ILE:CD1	1:C:507:LEU:HD22	2.46	0.45
1:C:198:TYR:CD2	1:C:367:LYS:CG	2.99	0.45
1:A:428:GLU:H	1:A:428:GLU:CD	2.20	0.45
1:A:464:LEU:HD13	1:A:464:LEU:HA	1.80	0.45
1:B:150:ASP:HB2	1:B:154:GLN:H	1.82	0.45
1:B:248:LYS:CG	1:B:249:TYR:N	2.78	0.45
1:B:296:GLU:HG2	1:B:298:HIS:NE2	2.32	0.45
1:C:358:LEU:C	1:C:360:PHE:H	2.20	0.45
1:D:64:ASN:HB2	1:D:68:THR:N	2.32	0.45
1:D:78:TYR:HD2	1:D:224:MET:HE2	1.82	0.45
1:D:496:LEU:HD12	1:D:496:LEU:C	2.37	0.45
1:B:300:THR:HG23	1:B:302:GLN:H	1.82	0.45
1:B:79:ASN:ND2	1:B:118:GLN:CB	2.79	0.45
1:B:105:LEU:O	1:B:109:LYS:N	2.45	0.45
1:C:76:GLU:O	1:C:119:GLY:HA3	2.16	0.45
1:C:135:ILE:O	1:C:179:TYR:HA	2.17	0.45
1:D:509:SER:HB2	6:D:1211:HOH:O	2.17	0.45
1:A:25:ARG:HG2	1:A:25:ARG:NH1	2.30	0.45
1:A:34:TRP:CE3	1:D:335:LYS:HD2	2.51	0.45
1:B:6:VAL:HG11	1:B:16:LEU:HD13	1.99	0.45
1:B:201:VAL:O	1:B:204:ASN:OD1	2.34	0.45
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.57	0.45
1:B:481:ARG:N	1:B:488:THR:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:PHE:CD2	1:C:295:HIS:HB2	2.51	0.45
1:D:234:SER:HB3	4:D:1121:AMP:C5	2.51	0.45
1:B:427:MET:SD	1:B:433:ARG:HD2	2.56	0.45
1:D:232:LEU:O	1:D:239:SER:HB2	2.17	0.45
1:A:59:ALA:O	1:A:62:LEU:HD23	2.17	0.45
1:D:380:LEU:CD2	1:D:384:ASP:HB2	2.47	0.45
1:A:475:GLN:HA	1:A:478:GLU:OE2	2.17	0.44
1:C:150:ASP:OD1	1:C:154:GLN:NE2	2.39	0.44
1:C:358:LEU:O	1:C:361:HIS:HB2	2.17	0.44
1:C:514:VAL:CG1	1:C:515:PRO:HD2	2.46	0.44
1:D:64:ASN:HB3	1:D:68:THR:H	1.82	0.44
1:D:125:LEU:HD23	1:D:126:TYR:N	2.33	0.44
1:D:319:ASP:O	1:D:323:ILE:HD12	2.17	0.44
1:D:361:HIS:CD2	1:D:428:GLU:HG3	2.52	0.44
1:A:372:GLU:HA	1:A:372:GLU:OE2	2.17	0.44
1:C:198:TYR:CD2	1:C:367:LYS:HA	2.53	0.44
1:D:514:VAL:CG1	1:D:515:PRO:HD2	2.47	0.44
1:B:49:ARG:NH2	1:B:53:VAL:O	2.51	0.44
1:D:227:VAL:HB	1:D:228:PRO:HD2	1.99	0.44
1:A:65:GLN:OE1	1:A:92:GLN:N	2.36	0.44
1:B:28:ARG:HB3	6:B:1344:HOH:O	2.16	0.44
1:B:327:THR:N	1:B:328:PRO:CD	2.81	0.44
1:B:367:LYS:HG2	1:B:368:GLU:OE2	2.17	0.44
1:C:146:TYR:OH	1:C:390:LYS:NZ	2.51	0.44
1:C:165:VAL:N	1:C:166:PRO:CD	2.79	0.44
1:C:333:SER:OG	1:C:395:TRP:HB2	2.18	0.44
1:A:290:LEU:HD12	1:A:290:LEU:N	2.33	0.44
1:A:395:TRP:CH2	1:D:28:ARG:HD3	2.50	0.44
1:B:241:ILE:HD13	1:B:436:PHE:CB	2.48	0.44
1:B:244:ALA:HA	1:B:290:LEU:HD21	1.99	0.44
1:B:357:TYR:CD2	1:B:359:TYR:CE1	3.05	0.44
1:B:461:ILE:O	1:B:464:LEU:HB2	2.18	0.44
1:B:472:VAL:HB	1:B:492:LYS:HB3	1.98	0.44
1:D:207:ASP:O	1:D:210:GLU:HB3	2.18	0.44
1:D:427:MET:HB3	1:D:433:ARG:NE	2.32	0.44
1:A:120:MET:O	1:A:121:PHE:HB3	2.17	0.44
1:A:130:LYS:HG3	6:A:1273:HOH:O	2.17	0.44
1:B:49:ARG:HG2	1:B:50:LEU:N	2.32	0.44
1:C:165:VAL:N	1:C:166:PRO:HD2	2.33	0.44
1:C:356:GLY:HA3	1:C:429:LYS:HE3	1.98	0.44
1:B:79:ASN:ND2	1:B:118:GLN:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ASP:HB3	1:D:152:HIS:H	1.83	0.44
1:D:160:GLU:HB3	1:D:316:GLU:OE1	2.18	0.44
1:D:204:ASN:ND2	6:D:1324:HOH:O	2.30	0.44
1:D:320:VAL:HG22	1:D:497:TYR:HD2	1.78	0.44
1:A:351:ASP:CB	1:A:357:TYR:CE1	3.00	0.44
1:B:217:ASP:HA	1:B:220:LYS:HD3	1.99	0.44
1:B:343:MET:HA	1:B:398:GLU:O	2.18	0.44
1:D:233:LEU:CD2	1:D:235:GLY:H	2.31	0.44
1:D:234:SER:HB3	4:D:1121:AMP:C4	2.53	0.44
1:A:37:ILE:HG12	1:A:38:TYR:N	2.33	0.44
1:B:248:LYS:HE2	1:B:249:TYR:CE1	2.52	0.44
1:B:469:ALA:HA	1:B:492:LYS:HD2	2.00	0.44
1:B:481:ARG:NH2	6:B:1198:HOH:O	2.49	0.44
1:C:301:VAL:O	1:C:305:LEU:HG	2.18	0.44
1:A:216:GLU:O	1:A:220:LYS:HD3	2.18	0.43
1:B:143:ILE:HG23	1:B:144:PRO:HD2	2.00	0.43
1:B:484:PHE:N	1:B:485:PRO:CD	2.79	0.43
1:C:28:ARG:NH2	6:C:1292:HOH:O	2.50	0.43
1:C:325:ALA:O	1:C:328:PRO:HD2	2.18	0.43
1:C:433:ARG:HD3	1:C:433:ARG:HH11	1.69	0.43
1:D:78:TYR:CD2	1:D:224:MET:CE	3.01	0.43
1:A:165:VAL:HG11	6:A:1156:HOH:O	2.18	0.43
1:A:232:LEU:HB3	4:A:1100:AMP:N3	2.32	0.43
1:A:289:HIS:CE1	1:A:441:PRO:HD3	2.53	0.43
1:A:301:VAL:CG1	1:A:463:THR:HG21	2.48	0.43
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.79	0.43
1:B:270:PHE:CD1	1:B:270:PHE:N	2.84	0.43
1:B:357:TYR:HD2	1:B:359:TYR:CE1	2.35	0.43
1:C:145:LEU:HG	1:C:146:TYR:N	2.32	0.43
1:D:118:GLN:OE1	1:D:407:LYS:HD2	2.18	0.43
1:A:387:ARG:HH11	1:A:387:ARG:CG	2.31	0.43
1:C:138:ASP:O	1:C:177:GLY:N	2.49	0.43
1:A:14:VAL:HG12	1:A:15:GLU:N	2.32	0.43
1:A:271:ALA:HA	4:A:1100:AMP:N1	2.34	0.43
1:B:493:GLU:HG2	1:B:497:TYR:CE2	2.53	0.43
1:B:245:ILE:HG22	1:B:249:TYR:HD1	1.84	0.43
1:B:268:HIS:CD2	1:B:268:HIS:N	2.86	0.43
1:B:320:VAL:O	1:B:324:ARG:HG3	2.18	0.43
1:C:65:GLN:H	1:C:65:GLN:HG3	1.14	0.43
1:C:105:LEU:HB3	1:C:113:PHE:CG	2.53	0.43
1:C:464:LEU:HD12	1:C:464:LEU:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:ALA:HA	1:D:364:PRO:HD3	1.73	0.43
1:A:199:ASP:CB	1:A:202:LYS:HE2	2.47	0.43
1:A:348:GLU:CG	4:A:1100:AMP:H5'1	2.48	0.43
1:B:49:ARG:NH1	1:B:58:GLY:CA	2.82	0.43
1:B:277:SER:CB	1:B:278:PRO:HD2	2.48	0.43
1:D:64:ASN:ND2	1:D:68:THR:OG1	2.51	0.43
1:A:273:GLY:O	1:A:298:HIS:HA	2.18	0.43
1:B:3:ILE:HD13	1:B:3:ILE:HG21	1.68	0.43
1:B:381:HIS:CE1	1:B:382:MET:HG2	2.54	0.43
1:C:17:ARG:HD3	6:C:1144:HOH:O	2.19	0.43
1:C:327:THR:N	1:C:328:PRO:CD	2.82	0.43
1:D:68:THR:O	1:D:69:HIS:HD2	2.01	0.43
1:D:168:CYS:HB3	1:D:170:THR:O	2.18	0.43
1:A:238:ASP:OD2	1:A:429:LYS:HE2	2.18	0.43
1:A:280:LEU:HD11	1:A:298:HIS:CD2	2.54	0.43
1:A:365:ASN:ND2	1:A:368:GLU:H	2.16	0.43
1:A:268:HIS:CG	1:A:295:HIS:HE2	2.35	0.43
1:D:78:TYR:HD2	1:D:224:MET:CE	2.32	0.43
1:A:145:LEU:HD11	1:A:157:VAL:HG13	2.01	0.42
1:B:38:TYR:CZ	1:B:40:SER:HB3	2.54	0.42
1:B:49:ARG:NE	1:B:51:SER:HB3	2.34	0.42
1:B:357:TYR:O	1:B:360:PHE:N	2.46	0.42
1:C:232:LEU:HB3	4:C:1114:AMP:N3	2.34	0.42
1:C:504:LEU:O	1:C:506:PRO:HD3	2.19	0.42
1:D:105:LEU:HD22	1:D:113:PHE:HB2	2.01	0.42
1:D:152:HIS:HB2	1:D:154:GLN:HG3	2.00	0.42
1:D:476:GLN:HB3	1:D:495:TYR:CZ	2.54	0.42
1:B:361:HIS:HA	1:B:422:CYS:SG	2.59	0.42
1:C:60:GLN:HA	1:C:61:PRO:C	2.40	0.42
1:C:248:LYS:HE2	1:C:249:TYR:OH	2.20	0.42
1:A:135:ILE:HD13	1:A:157:VAL:HG21	2.00	0.42
1:B:68:THR:HG21	1:B:129:GLU:OE2	2.19	0.42
1:B:480:ALA:HB1	1:B:488:THR:HG22	2.02	0.42
1:C:162:LYS:HB2	1:C:162:LYS:HZ2	1.85	0.42
1:D:52:ILE:N	1:D:52:ILE:CD1	2.82	0.42
1:D:230:GLY:O	1:D:344:VAL:HA	2.18	0.42
1:A:147:MET:HE3	1:A:172:LYS:HG3	2.01	0.42
1:A:505:PHE:N	1:A:506:PRO:HD3	2.35	0.42
1:C:234:SER:HB3	4:C:1114:AMP:C4	2.54	0.42
1:A:164:LEU:C	1:A:166:PRO:HD2	2.40	0.42
1:C:114:LEU:HD22	1:C:190:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:TYR:HD2	1:C:367:LYS:HG3	1.81	0.42
1:C:415:ILE:CD1	1:C:420:LYS:HE3	2.48	0.42
1:A:197:ASP:O	1:A:200:ALA:HB3	2.18	0.42
1:A:280:LEU:HD22	1:A:296:GLU:CG	2.48	0.42
1:C:461:ILE:O	1:C:465:LYS:HG3	2.20	0.42
1:D:410:ASP:O	1:D:414:ARG:HB2	2.20	0.42
1:A:329:MET:CE	1:A:388:ALA:HA	2.48	0.42
1:A:364:PRO:HG2	1:A:368:GLU:HG3	2.01	0.42
1:A:380:LEU:HD22	1:A:384:ASP:HB2	2.01	0.42
1:B:264:TRP:HD1	1:B:265:PRO:HD2	1.85	0.42
1:B:277:SER:HB2	1:B:278:PRO:CD	2.49	0.42
1:B:464:LEU:HD12	1:B:464:LEU:HA	1.43	0.42
1:B:287:ALA:HA	1:B:292:THR:HG22	2.01	0.42
1:B:324:ARG:NH2	1:B:461:ILE:HG21	2.35	0.42
1:C:111:PRO:HG3	1:C:181:TRP:CD1	2.55	0.42
1:C:198:TYR:CE2	1:C:367:LYS:HB2	2.54	0.42
1:C:231:VAL:O	1:C:269:SER:HA	2.19	0.42
1:A:18:LYS:HD2	6:A:1113:HOH:O	2.19	0.42
1:A:461:ILE:CG2	1:A:465:LYS:HE2	2.48	0.42
1:C:422:CYS:HG	1:C:428:GLU:HA	1.85	0.42
1:C:433:ARG:HB3	1:C:445:ALA:O	2.19	0.42
1:D:132:ALA:HB1	1:D:182:SER:OG	2.20	0.42
1:D:198:TYR:HE1	1:D:417:PRO:HG2	1.85	0.42
1:D:358:LEU:H	1:D:358:LEU:HG	1.61	0.42
1:A:27:MET:HA	1:A:29:HIS:CE1	2.55	0.42
1:A:330:TYR:HE1	6:D:1134:HOH:O	2.03	0.42
1:B:324:ARG:CZ	1:B:461:ILE:HG21	2.49	0.42
1:C:137:ARG:NH2	6:C:1283:HOH:O	2.52	0.42
1:C:160:GLU:HB3	1:C:316:GLU:OE1	2.19	0.42
1:C:349:GLY:HA3	1:C:404:LEU:HD21	2.02	0.42
1:C:381:HIS:CE1	1:C:382:MET:HG3	2.55	0.42
1:D:475:GLN:HB2	6:D:1400:HOH:O	2.20	0.42
1:A:75:GLY:N	5:A:1106:GLN:OE1	2.53	0.41
1:B:277:SER:CB	1:B:278:PRO:CD	2.98	0.41
1:C:237:LEU:O	1:C:240:SER:HB2	2.20	0.41
1:C:372:GLU:HA	1:C:375:ARG:NH1	2.35	0.41
1:D:201:VAL:HG12	6:D:1324:HOH:O	2.20	0.41
1:D:86:GLU:O	1:D:86:GLU:HG2	2.20	0.41
1:D:277:SER:OG	1:D:280:LEU:HD22	2.20	0.41
1:A:129:GLU:OE2	1:A:129:GLU:HA	2.21	0.41
1:C:305:LEU:HD23	1:C:305:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:TYR:CD2	1:A:367:LYS:HG3	2.55	0.41
1:B:49:ARG:NH2	5:B:1113:GLN:O	2.53	0.41
1:B:245:ILE:CG2	1:B:249:TYR:CD1	3.04	0.41
1:B:464:LEU:HG	1:B:497:TYR:OH	2.20	0.41
1:C:52:ILE:HG22	1:C:53:VAL:HG23	2.02	0.41
1:A:431:ILE:CG2	1:A:432:LEU:N	2.83	0.41
1:B:240:SER:CB	1:B:440:LEU:CD1	2.98	0.41
1:B:379:ALA:HB1	1:B:383:TYR:CE1	2.55	0.41
1:C:15:GLU:O	1:C:18:LYS:HB3	2.20	0.41
1:C:289:HIS:CD2	1:C:441:PRO:HD3	2.56	0.41
1:D:137:ARG:HD2	1:D:145:LEU:HB3	2.02	0.41
1:A:460:TRP:CE2	1:A:464:LEU:HD21	2.55	0.41
1:B:64:ASN:ND2	1:B:68:THR:OG1	2.53	0.41
1:B:81:GLN:HG3	6:B:1255:HOH:O	2.20	0.41
1:B:216:GLU:C	1:B:220:LYS:HD3	2.41	0.41
1:B:231:VAL:O	1:B:269:SER:HA	2.21	0.41
1:B:121:PHE:N	1:B:138:ASP:HB3	2.34	0.41
1:B:274:LEU:HG	1:B:456:VAL:O	2.20	0.41
1:B:337:LYS:HD3	1:B:337:LYS:HA	1.75	0.41
1:D:345:LEU:HD23	1:D:402:PRO:HG3	2.02	0.41
1:D:507:LEU:HA	1:D:508:PRO:HD2	1.79	0.41
1:A:219:VAL:O	1:A:223:LEU:HG	2.21	0.41
1:B:71:LEU:HG	1:B:73:VAL:HG23	2.02	0.41
1:B:326:SER:OG	1:B:387:ARG:HB2	2.20	0.41
1:D:318:TYR:CZ	1:D:514:VAL:HB	2.56	0.41
1:A:147:MET:HA	1:A:156:TYR:O	2.21	0.41
1:A:199:ASP:CB	1:A:202:LYS:NZ	2.76	0.41
1:A:209:ASN:CG	1:A:212:ARG:HH12	2.24	0.41
1:A:289:HIS:NE2	1:A:441:PRO:HD3	2.35	0.41
1:B:49:ARG:NE	1:B:51:SER:CB	2.84	0.41
1:B:208:LYS:H	1:B:208:LYS:HG2	1.56	0.41
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.90	0.41
1:C:86:GLU:HG2	1:C:87:TYR:CE1	2.55	0.41
1:C:358:LEU:C	1:C:360:PHE:N	2.73	0.41
1:D:281:LYS:N	1:D:281:LYS:CD	2.78	0.41
1:A:484:PHE:HD1	1:A:502:GLU:OE1	2.04	0.41
1:B:234:SER:HB3	4:B:1107:AMP:C4	2.56	0.41
1:B:392:MET:HG3	1:B:399:ALA:HB2	2.02	0.41
1:C:45:LEU:HD12	1:C:45:LEU:N	2.36	0.41
1:C:115:ASP:O	1:C:406:LYS:NZ	2.38	0.41
1:C:150:ASP:HB3	1:C:153:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLY:HA2	1:C:456:VAL:HG22	2.02	0.41
1:C:484:PHE:HA	1:C:485:PRO:HD2	1.77	0.41
1:A:92:GLN:CD	1:A:94:GLN:HE22	2.25	0.40
1:A:230:GLY:O	1:A:344:VAL:HA	2.21	0.40
1:A:441:PRO:O	1:A:444:VAL:N	2.52	0.40
1:B:28:ARG:HD3	1:C:395:TRP:HH2	1.86	0.40
1:B:476:GLN:NE2	1:B:495:TYR:CE1	2.89	0.40
1:C:186:GLU:HB2	1:C:188:ARG:CZ	2.51	0.40
1:C:287:ALA:HB1	1:C:294:HIS:HB2	2.02	0.40
1:C:320:VAL:HG12	1:C:324:ARG:CD	2.43	0.40
1:C:337:LYS:HA	1:C:337:LYS:HD3	1.64	0.40
1:C:364:PRO:HG2	1:C:368:GLU:OE2	2.22	0.40
1:C:432:LEU:HD12	1:C:432:LEU:HA	1.83	0.40
1:D:219:VAL:O	1:D:223:LEU:HG	2.21	0.40
1:A:65:GLN:H	1:A:65:GLN:HG3	1.32	0.40
1:B:199:ASP:CB	1:B:202:LYS:CE	2.99	0.40
1:B:245:ILE:CG2	1:B:249:TYR:HD1	2.34	0.40
1:B:346:SER:O	1:B:402:PRO:HD2	2.22	0.40
1:B:462:ASP:O	1:B:466:GLU:HB2	2.22	0.40
1:C:9:ILE:HG23	1:C:16:LEU:HD12	2.03	0.40
1:C:98:ASP:OD1	5:C:1120:GLN:N	2.55	0.40
1:C:274:LEU:HD23	1:C:299:PHE:O	2.20	0.40
1:D:139:HIS:HB2	1:D:191:TYR:CG	2.55	0.40
1:C:113:PHE:O	1:C:116:ASP:HB2	2.22	0.40
1:D:140:LEU:HD23	1:D:140:LEU:HA	1.94	0.40
1:D:165:VAL:HG11	1:D:506:PRO:HD2	2.04	0.40
1:A:187:ILE:HG21	1:A:187:ILE:HD13	1.83	0.40
1:B:37:ILE:HD12	1:B:46:ALA:HB2	2.04	0.40
1:B:272:VAL:HG23	1:B:297:ILE:HG22	2.04	0.40
1:C:12:ASP:OD1	1:C:15:GLU:HB2	2.21	0.40
1:C:114:LEU:HB3	1:C:190:TYR:CE2	2.57	0.40
1:D:137:ARG:NH1	1:D:174:PHE:O	2.44	0.40
1:D:418:GLN:NE2	6:D:1286:HOH:O	2.54	0.40

There are no symmetry-related clashes.

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	491/553 (89%)	465 (95%)	24 (5%)	2 (0%)	34	30
1	B	487/553 (88%)	449 (92%)	31 (6%)	7 (1%)	11	5
1	C	487/553 (88%)	450 (92%)	33 (7%)	4 (1%)	19	13
1	D	487/553 (88%)	467 (96%)	18 (4%)	2 (0%)	34	30
All	All	1952/2212 (88%)	1831 (94%)	106 (5%)	15 (1%)	19	13

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	428	GLU
1	C	266	GLN
1	A	138	ASP
1	B	265	PRO
1	B	460	TRP
1	C	364	PRO
1	A	506	PRO
1	C	359	TYR
1	D	202	LYS
1	B	248	LYS
1	B	275	PRO
1	C	362	LYS
1	D	460	TRP
1	B	508	PRO
1	B	278	PRO

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	418/462 (90%)	371 (89%)	47 (11%)	6	3
1	B	414/462 (90%)	358 (86%)	56 (14%)	4	2
1	C	414/462 (90%)	364 (88%)	50 (12%)	5	2
1	D	412/462 (89%)	371 (90%)	41 (10%)	7	4
All	All	1658/1848 (90%)	1464 (88%)	194 (12%)	5	3

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	16	LEU
1	A	18	LYS
1	A	22	GLU
1	A	35	SER
1	A	65	GLN
1	A	70	VAL
1	A	89	ASP
1	A	90	ARG
1	A	112	GLU
1	A	114	LEU
1	A	147	MET
1	A	150	ASP
1	A	151	GLU
1	A	157	VAL
1	A	162	LYS
1	A	171	ILE
1	A	181	TRP
1	A	199	ASP
1	A	202	LYS
1	A	205	VAL
1	A	208	LYS
1	A	213	GLN
1	A	238	ASP
1	A	281	LYS
1	A	285	GLU
1	A	337	LYS
1	A	339	MET
1	A	346	SER
1	A	348	GLU
1	A	365	ASN

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Mol	Chain	Res	Type
1	A	375	ARG
1	A	378	LEU
1	A	387	ARG
1	A	406	LYS
1	A	429	LYS
1	A	440	LEU
1	A	443	SER
1	A	447	ARG
1	A	449	LYS
1	A	450	GLU
1	A	459	SER
1	A	462	ASP
1	A	464	LEU
1	A	470	GLN
1	A	481	ARG
1	A	502	GLU
1	B	15	GLU
1	B	19	LYS
1	B	42	ASN
1	B	51	SER
1	B	66	GLN
1	B	80	HIS
1	B	81	GLN
1	B	84	ARG
1	B	90	ARG
1	B	103	LEU
1	B	114	LEU
1	B	129	GLU
1	B	150	ASP
1	B	157	VAL
1	B	162	LYS
1	B	164	LEU
1	B	201	VAL
1	B	208	LYS
1	B	220	LYS
1	B	226	ASP
1	B	233	LEU
1	B	241	ILE
1	B	247	LYS
1	B	277	SER
1	B	280	LEU
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	300	THR
1	B	301	VAL
1	B	329	MET
1	B	335	LYS
1	B	337	LYS
1	B	346	SER
1	B	348	GLU
1	B	358	LEU
1	B	368	GLU
1	B	369	LEU
1	B	376	LYS
1	B	378	LEU
1	B	382	MET
1	B	387	ARG
1	B	406	LYS
1	B	418	GLN
1	B	427	MET
1	B	429	LYS
1	B	433	ARG
1	B	439	TYR
1	B	456	VAL
1	B	459	SER
1	B	462	ASP
1	B	464	LEU
1	B	471	GLN
1	B	473	SER
1	B	481	ARG
1	B	490	THR
1	B	502	GLU
1	B	509	SER
1	C	19	LYS
1	C	25	ARG
1	C	42	ASN
1	C	49	ARG
1	C	51	SER
1	C	65	GLN
1	C	67	LYS
1	C	70	VAL
1	C	81	GLN
1	C	89	ASP
1	C	103	LEU
1	C	130	LYS

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Mol	Chain	Res	Type
1	C	150	ASP
1	C	157	VAL
1	C	162	LYS
1	C	164	LEU
1	C	171	ILE
1	C	197	ASP
1	C	202	LYS
1	C	209	ASN
1	C	242	ILE
1	C	247	LYS
1	C	264	TRP
1	C	277	SER
1	C	280	LEU
1	C	329	MET
1	C	335	LYS
1	C	337	LYS
1	C	339	MET
1	C	341	ILE
1	C	348	GLU
1	C	358	LEU
1	C	359	TYR
1	C	365	ASN
1	C	368	GLU
1	C	369	LEU
1	C	376	LYS
1	C	384	ASP
1	C	393	SER
1	C	418	GLN
1	C	420	LYS
1	C	427	MET
1	C	428	GLU
1	C	429	LYS
1	C	433	ARG
1	C	440	LEU
1	C	443	SER
1	C	464	LEU
1	C	474	ASP
1	C	509	SER
1	D	10	LYS
1	D	25	ARG
1	D	51	SER
1	D	65	GLN

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Mol	Chain	Res	Type
1	D	67	LYS
1	D	81	GLN
1	D	89	ASP
1	D	103	LEU
1	D	129	GLU
1	D	150	ASP
1	D	162	LYS
1	D	166	PRO
1	D	184	ASP
1	D	188	ARG
1	D	199	ASP
1	D	203	ASP
1	D	220	LYS
1	D	222	HIS
1	D	225	SER
1	D	233	LEU
1	D	266	GLN
1	D	280	LEU
1	D	281	LYS
1	D	310	ASP
1	D	335	LYS
1	D	337	LYS
1	D	341	ILE
1	D	357	TYR
1	D	358	LEU
1	D	365	ASN
1	D	387	ARG
1	D	418	GLN
1	D	427	MET
1	D	428	GLU
1	D	429	LYS
1	D	454	ASP
1	D	459	SER
1	D	464	LEU
1	D	473	SER
1	D	496	LEU
1	D	502	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN

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Mol	Chain	Res	Type
1	A	81	GLN
1	A	94	GLN
1	A	183	GLN
1	A	213	GLN
1	A	284	GLN
1	A	288	ASN
1	A	365	ASN
1	A	448	GLN
1	A	451	GLN
1	A	471	GLN
1	B	64	ASN
1	B	69	HIS
1	B	74	ASN
1	B	79	ASN
1	B	80	HIS
1	B	81	GLN
1	B	183	GLN
1	B	192	HIS
1	B	288	ASN
1	B	302	GLN
1	B	361	HIS
1	B	470	GLN
1	B	476	GLN
1	C	42	ASN
1	C	56	ASN
1	C	65	GLN
1	C	81	GLN
1	C	183	GLN
1	C	288	ASN
1	C	365	ASN
1	C	470	GLN
1	C	471	GLN
1	D	56	ASN
1	D	80	HIS
1	D	81	GLN
1	D	152	HIS
1	D	192	HIS
1	D	284	GLN
1	D	288	ASN
1	D	430	HIS
1	D	470	GLN
1	D	471	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 [i](#)

Of 28 ligands modelled in this entry, 14 are modelled with single atom and 4 are monoatomic - leaving 10 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
4	AMP	B	1107	2	22,25,25	1.19	3 (13%)	25,38,38	1.49	4 (16%)
2	IUM	A	1102	-	0,1,2	-	-	-		
5	GLN	C	1120	-	5,9,9	2.28	1 (20%)	5,11,11	1.29	1 (20%)
2	IUM	D	1122	4	0,1,2	-	-	-		
5	GLN	A	1106	-	5,9,9	2.86	1 (20%)	5,11,11	0.86	0
4	AMP	D	1121	2	22,25,25	1.00	2 (9%)	25,38,38	2.44	6 (24%)
5	GLN	B	1113	-	5,9,9	2.25	1 (20%)	5,11,11	0.46	0
4	AMP	A	1100	-	22,25,25	1.20	3 (13%)	25,38,38	1.87	4 (16%)
4	AMP	C	1114	-	22,25,25	1.19	3 (13%)	25,38,38	2.12	7 (28%)
5	GLN	D	1127	-	5,9,9	2.21	1 (20%)	5,11,11	0.45	0

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
4	AMP	B	1107	2	-	0/6/26/26	0/3/3/3
5	GLN	C	1120	-	-	0/5/9/9	-
5	GLN	A	1106	-	-	0/5/9/9	-
4	AMP	D	1121	2	-	6/6/26/26	0/3/3/3
5	GLN	B	1113	-	-	0/5/9/9	-
4	AMP	A	1100	-	-	0/6/26/26	0/3/3/3
4	AMP	C	1114	-	-	0/6/26/26	0/3/3/3
5	GLN	D	1127	-	-	0/5/9/9	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	GLN	CA-N	-6.31	1.33	1.47
5	B	1113	GLN	CA-N	-5.00	1.35	1.47
5	C	1120	GLN	CA-N	-4.99	1.35	1.47
5	D	1127	GLN	CA-N	-4.77	1.36	1.47
4	C	1114	AMP	O2'-C2'	3.19	1.50	1.43
4	C	1114	AMP	O3'-C3'	3.18	1.50	1.43
4	A	1100	AMP	O2'-C2'	3.07	1.50	1.43
4	A	1100	AMP	O3'-C3'	3.05	1.50	1.43
4	B	1107	AMP	O3'-C3'	3.03	1.50	1.43
4	D	1121	AMP	O2'-C2'	3.02	1.50	1.43
4	A	1100	AMP	C2-N1	2.60	1.38	1.33
4	B	1107	AMP	O2'-C2'	2.46	1.48	1.43
4	C	1114	AMP	C2-N1	2.44	1.38	1.33
4	D	1121	AMP	O3'-C3'	2.39	1.48	1.43
4	B	1107	AMP	C2-N1	2.36	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1121	AMP	C5-C6-N6	6.53	130.28	120.35
4	D	1121	AMP	O2P-P-O5'	-5.78	91.36	106.73
4	C	1114	AMP	C2'-C3'-C4'	-5.57	91.82	102.64
4	A	1100	AMP	O3'-C3'-C2'	5.12	128.39	111.82
4	D	1121	AMP	C2'-C3'-C4'	-4.50	93.90	102.64
4	C	1114	AMP	O3'-C3'-C2'	4.33	125.83	111.82
4	C	1114	AMP	C5-C6-N6	3.91	126.30	120.35
4	D	1121	AMP	N6-C6-N1	-3.83	110.63	118.57
4	A	1100	AMP	O2P-P-O5'	-3.67	96.97	106.73
4	D	1121	AMP	O3'-C3'-C2'	3.54	123.28	111.82
4	B	1107	AMP	C5-C6-N6	3.49	125.65	120.35
4	C	1114	AMP	O2P-P-O5'	3.43	115.86	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1107	AMP	O3'-C3'-C2'	3.14	121.99	111.82
4	C	1114	AMP	O4'-C1'-C2'	-3.06	102.45	106.93
4	A	1100	AMP	O2'-C2'-C3'	3.03	121.64	111.82
5	C	1120	GLN	CG-CB-CA	-2.74	107.45	113.84
4	A	1100	AMP	C2'-C3'-C4'	-2.68	97.43	102.64
4	C	1114	AMP	O4'-C4'-C3'	-2.55	100.06	105.11
4	B	1107	AMP	C2'-C3'-C4'	-2.53	97.73	102.64
4	B	1107	AMP	O2P-P-O5'	2.34	112.97	106.73
4	C	1114	AMP	O2'-C2'-C3'	2.29	119.24	111.82
4	D	1121	AMP	O3P-P-O2P	2.13	115.78	107.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1121	AMP	C5'-O5'-P-O1P
4	D	1121	AMP	C5'-O5'-P-O2P
4	D	1121	AMP	C5'-O5'-P-O3P
4	D	1121	AMP	O4'-C4'-C5'-O5'
4	D	1121	AMP	C3'-C4'-C5'-O5'
4	D	1121	AMP	C4'-C5'-O5'-P

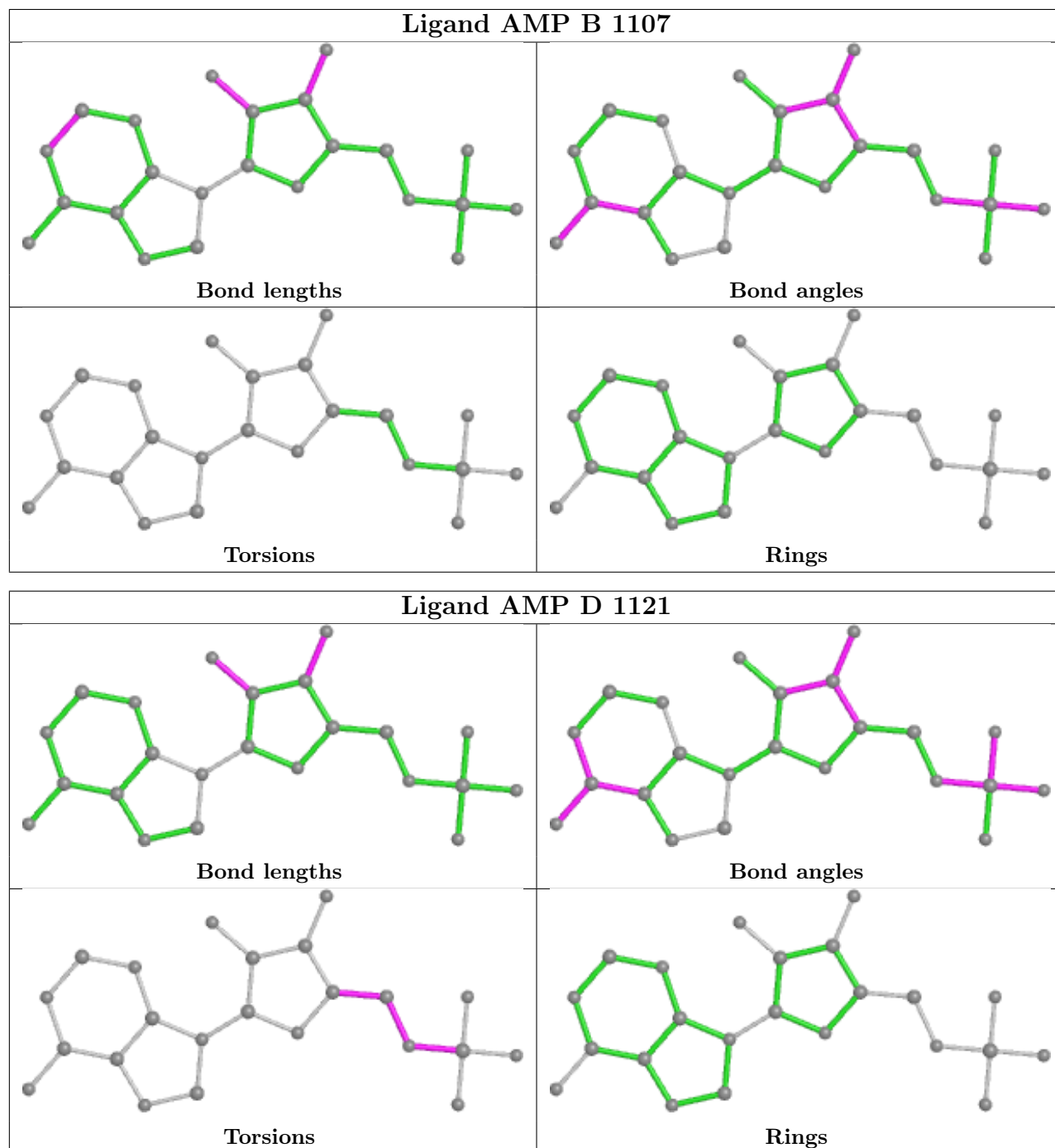
There are no ring outliers.

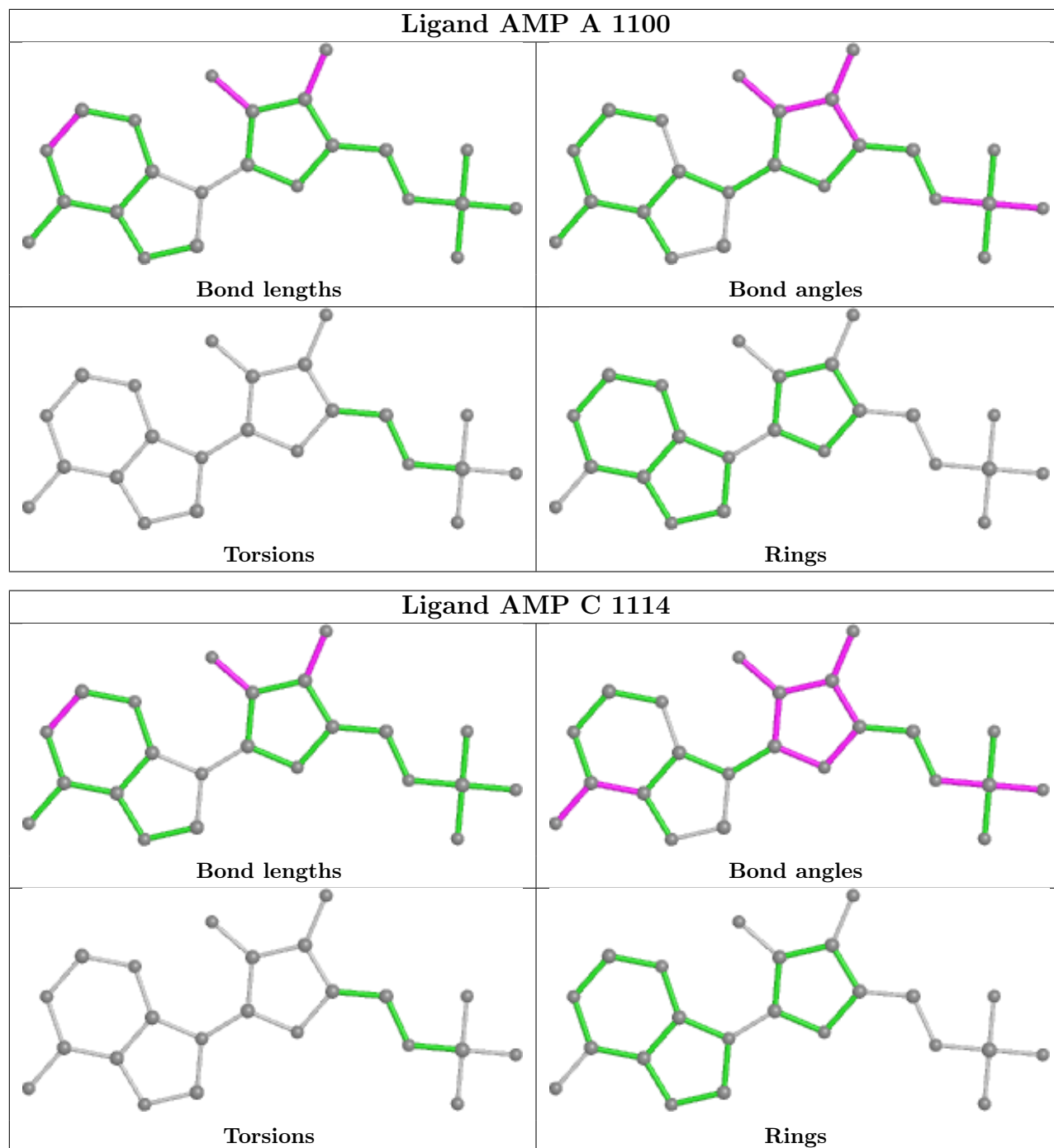
8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1107	AMP	3	0
5	C	1120	GLN	1	0
5	A	1106	GLN	2	0
4	D	1121	AMP	8	0
5	B	1113	GLN	4	0
4	A	1100	AMP	5	0
4	C	1114	AMP	7	0
5	D	1127	GLN	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.





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.