



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:45 AM EDT

PDB ID : 1CT9 / pdb_00001ct9
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

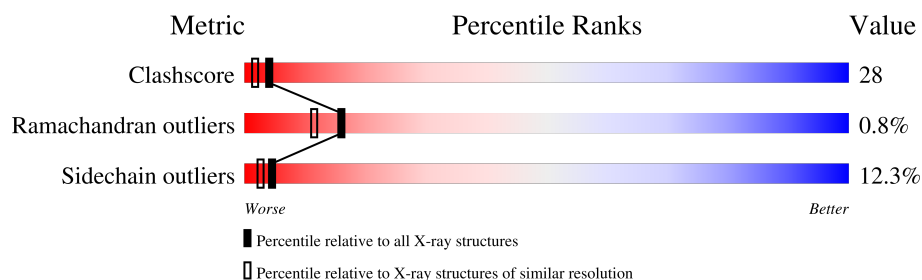
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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	
1	B	553	
1	C	553	
1	D	553	

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.

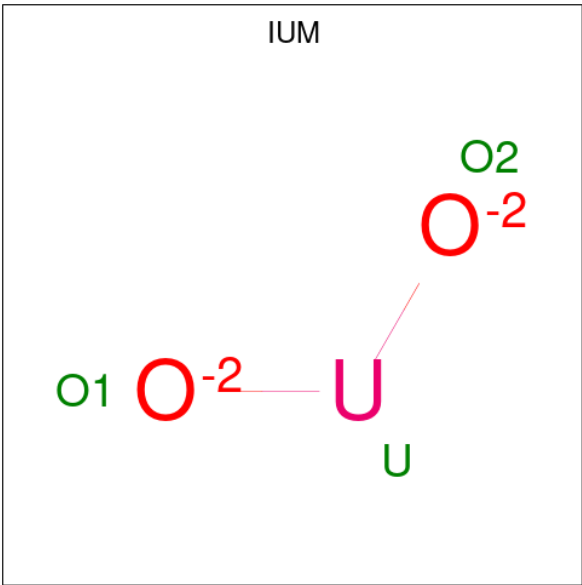
- Molecule 1 is a protein called ASPARAGINE SYNTHETASE B.

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

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 (CCD ID: 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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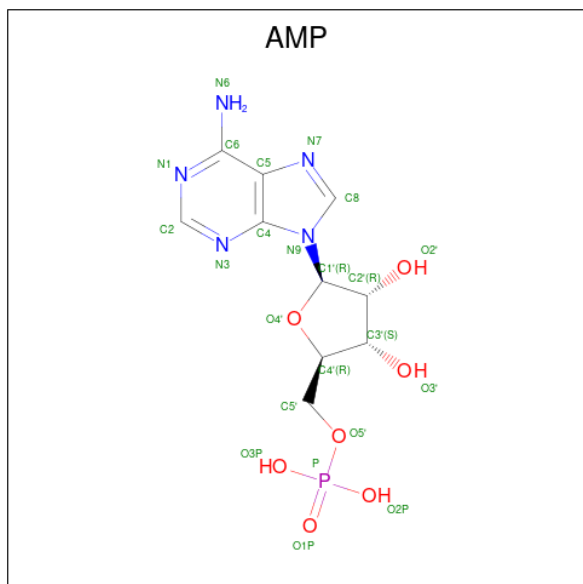
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total U 1 1	0	0
2	D	1	Total U 1 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: 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 (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



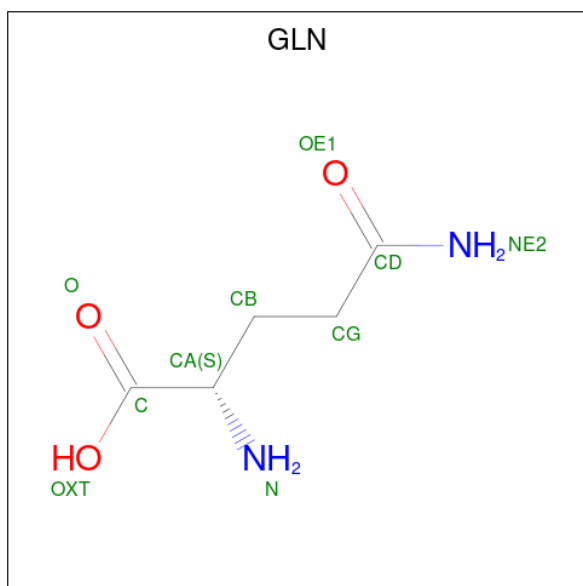
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 23 10 5 7 1	0	0
4	B	1	Total C N O P 23 10 5 7 1	0	0
4	C	1	Total C N O P 23 10 5 7 1	0	0

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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 (CCD ID: GLN) (formula: $C_5H_{10}N_2O_3$).



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.

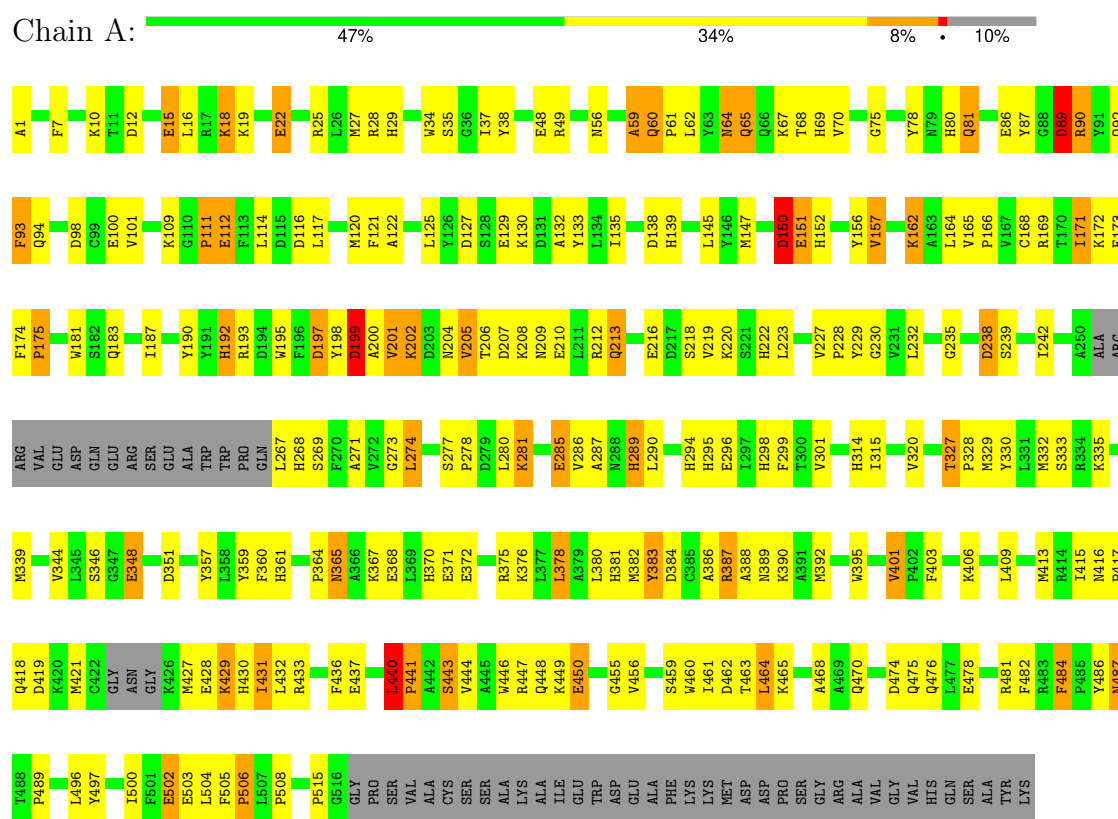
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	B	235	Total	O	0	0
			235	235		
6	C	223	Total	O	0	0
			223	223		
6	D	296	Total	O	0	0
			296	296		

3 Residue-property plots

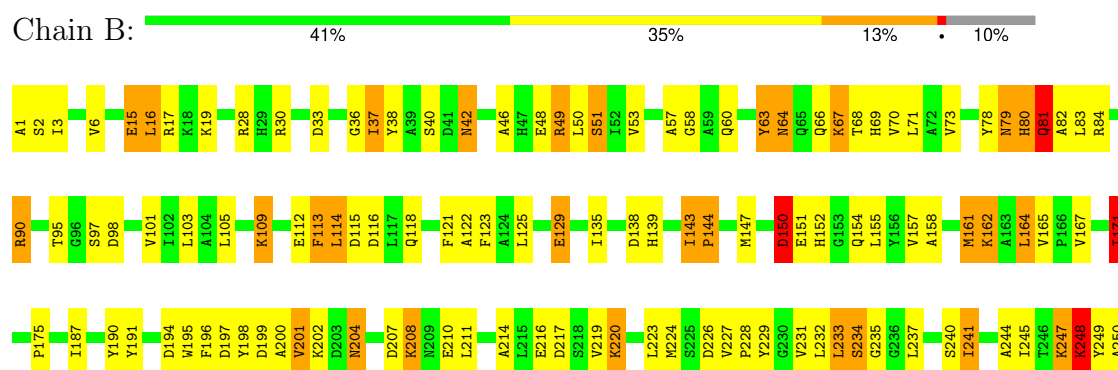
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

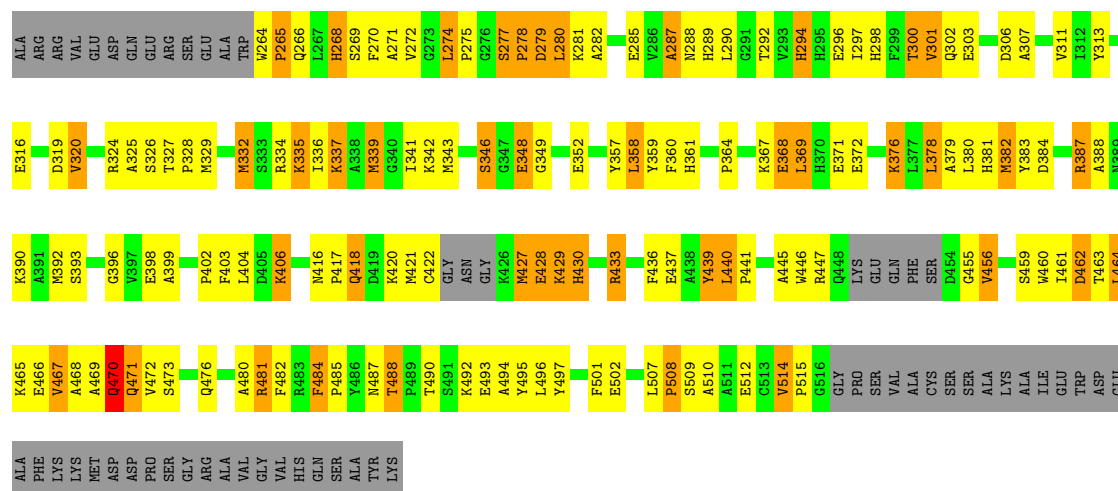
Note EDS was not executed.

• Molecule 1: ASPARAGINE SYNTHETASE B



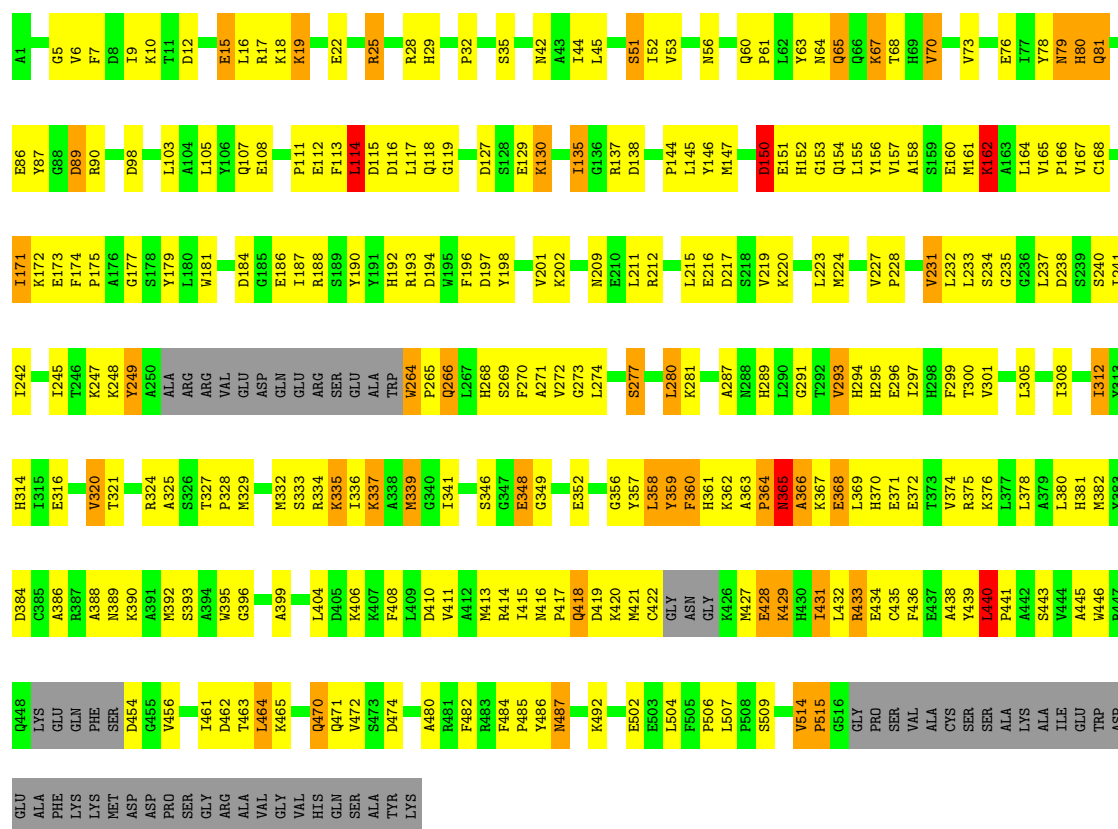
• Molecule 1: ASPARAGINE SYNTHETASE B





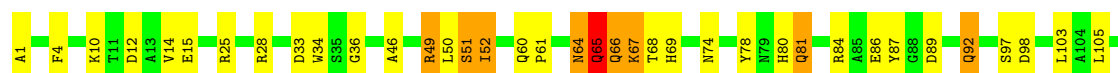
• Molecule 1: ASPARAGINE SYNTHETASE B

Chain C: 41% 40% 8% • 10%



• Molecule 1: ASPARAGINE SYNTHETASE B

Chain D: 49% 33% 7% • 10%



VAL	ALA	CYS	SER	ALA	LYS	ALA	ILE	GLU	TRP	ASP	GLU	ALA	PHE	PHE	LYS	LYS	MET	ASP	ASP	PRO	SER	GLY	ARG	ALA	VAL	ALA	GLY	VAL	HIS	GLN	SER	ALA	TYR	LYS																		
E428	K429	H430	R433	V444	Q448	LYS	GLU	GLU	TRP	ASP	GLU	ALA	PHE	D454	G455	V456	G457	Y458	S459	W460	SER	GLY	ARG	ALA	VAL	ALA	GLY	VAL	HIS	GLN	SER	ALA	TYR	LYS																		
D351	E352	V353	F354	Y357	L358	Y359	F360	H361	K362	A363	P364	K367	E368	E371	E372	R375	L380	H381	M382	Y383	D384	R387	A388	N389	W395	E398	A399	R400	V401	P402	D405	K406	K407	D410																		
K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157																		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235																
PRO	Q266	L267	H268	S269	F270	A271	V272	G273	L274	S277	P278	D279	L280	K281	V293	H294	H295	E296	I297	H298	F299	T300	D310	H314	I315	E316	T317	Y318	D319	V320	I323	T327	P328	M332	S333	R334	K335	I336	K337	A338	M339	G340	I341	K342	M343	V344	L345	S346	G347	E348	G349	S350
K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
PRO	Q266	L267	H268	S269	F270	A271	V272	G273	L274	S277	P278	D279	L280	K281	V293	H294	H295	E296	I297	H298	F299	T300	D310	H314	I315	E316	T317	Y318	D319	V320	I323	T327	P328	M332	S333	R334	K335	I336	K337	A338	M339	G340	I341	K342	M343	V344	L345	S346	G347	E348	G349	S350
K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
PRO	Q266	L267	H268	S269	F270	A271	V272	G273	L274	S277	P278	D279	L280	K281	V293	H294	H295	E296	I297	H298	F299	T300	D310	H314	I315	E316	T317	Y318	D319	V320	I323	T327	P328	M332	S333	R334	K335	I336	K337	A338	M339	G340	I341	K342	M343	V344	L345	S346	G347	E348	G349	S350
K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
PRO	Q266	L267	H268	S269	F270	A271	V272	G273	L274	S277	P278	D279	L280	K281	V293	H294	H295	E296	I297	H298	F299	T300	D310	H314	I315	E316	T317	Y318	D319	V320	I323	T327	P328	M332	S333	R334	K335	I336	K337	A338	M339	G340	I341	K342	M343	V344	L345	S346	G347	E348	G349	S350
K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
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K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
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K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
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K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
PRO	Q266	L267	H268	S269	F270	A271	V272	G273	L274	S277	P278	D279	L280	K281	V293	H294	H295	E296	I297	H298	F299	T300	D310	H314	I315	E316	T317	Y318	D319	V320	I323	T327	P328	M332	S333	R334	K335	I336	K337	A338	M339	G340	I341	K342	M343	V344	L345	S346	G347	E348	G349	S350
K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203	N204	Y205	I206	D207	E210	V219	K220	L223	M224	S225	D226	V227	P228	Y229	G230	V231	L232	L233	S234	G235	S239	K247	A251	ARG	ARG	VAL	GLU	ASP	GLN	GLU	ARG	SER	GLU	ALA	TRP	
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K109	G110	P111	E112	F113	L114	D115	D116	L117	Q118	G119	M120	L125	Y126	E129	A132	R137	D138	H139	L140	I143	P144	L145	Y146	M147	G148	Y149	D150	E151	H152	G153	Q154	L155	Y156	V157	E160	M161	K162	V165	P166	V167	C168	R169	T170	E173	F174	P175	W181	S182	Q183	D184		
G185	E186	I187	R188	S189	Y190	Y191	H192	R193	D194	D197	Y198	D199	A200	V201	K202	D203																																				

4 Data and refinement statistics

Xtriage (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.	Xtriage
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: AMP, IUM, CL

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	1.20	0/4060	1.71	50/5493 (0.9%)
1	B	1.18	1/4037 (0.0%)	1.74	64/5466 (1.2%)
1	C	1.14	1/4037 (0.0%)	1.66	51/5466 (0.9%)
1	D	1.22	6/4022 (0.1%)	1.72	58/5443 (1.1%)
All	All	1.18	8/16156 (0.0%)	1.71	223/21868 (1.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	478	GLU	CD-OE2	5.50	1.35	1.25
1	D	150	ASP	CA-CB	5.36	1.61	1.53
1	D	87	TYR	CA-C	-5.31	1.45	1.52
1	B	33	ASP	CG-OD2	5.30	1.35	1.25
1	C	231	VAL	C-O	5.24	1.29	1.24
1	D	36	GLY	CA-C	5.18	1.56	1.51
1	D	398	GLU	CD-OE2	5.09	1.35	1.25
1	D	98	ASP	CG-OD2	5.08	1.35	1.25

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CA-CB-CG	-12.34	100.26	112.60
1	A	150	ASP	CA-CB-CG	-12.23	100.37	112.60
1	D	64	ASN	CA-CB-CG	-12.21	100.39	112.60
1	A	482	PHE	CA-CB-CG	-11.83	101.97	113.80
1	B	430	HIS	CA-CB-CG	-11.27	102.53	113.80
1	B	112	GLU	N-CA-C	10.57	124.78	112.72
1	A	314	HIS	CA-CB-CG	-10.18	103.62	113.80
1	A	64	ASN	CA-CB-CG	-9.98	102.62	112.60
1	D	363	ALA	CA-C-N	9.47	129.56	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	363	ALA	C-N-CA	9.47	129.56	119.05
1	D	427	MET	N-CA-C	-9.26	99.02	110.41
1	B	268	HIS	CA-CB-CG	-9.01	104.79	113.80
1	C	150	ASP	CA-CB-CG	-8.84	103.76	112.60
1	A	440	LEU	O-C-N	8.66	127.38	121.14
1	B	64	ASN	N-CA-CB	-8.66	97.31	110.04
1	B	114	LEU	N-CA-C	8.63	121.47	111.11
1	A	487	ASN	CB-CA-C	-8.55	98.92	112.09
1	D	422	CYS	CB-CA-C	-8.53	99.33	112.12
1	C	7	PHE	CA-CB-CG	-8.44	105.36	113.80
1	B	274	LEU	N-CA-C	-8.32	99.62	109.93
1	A	162	LYS	N-CA-CB	-8.18	98.10	110.12
1	D	184	ASP	N-CA-CB	8.18	122.41	110.47
1	D	147	MET	N-CA-CB	-8.09	97.61	111.69
1	B	482	PHE	CA-CB-CG	-8.00	105.80	113.80
1	D	149	TYR	CA-C-N	7.84	134.91	120.95
1	D	149	TYR	C-N-CA	7.84	134.91	120.95
1	D	33	ASP	N-CA-C	7.77	119.53	111.14
1	A	78	TYR	N-CA-C	7.72	120.68	111.33
1	D	363	ALA	O-C-N	7.54	128.01	121.30
1	B	79	ASN	N-CA-CB	-7.50	98.17	110.40
1	B	204	ASN	CA-CB-CG	-7.50	105.10	112.60
1	C	151	GLU	N-CA-C	-7.38	104.25	113.18
1	C	144	PRO	CB-CA-C	-7.37	101.33	110.98
1	C	79	ASN	N-CA-CB	-7.35	99.19	110.44
1	C	80	HIS	N-CA-C	7.34	119.92	111.11
1	C	514	VAL	CA-C-N	7.32	127.73	119.83
1	C	514	VAL	C-N-CA	7.32	127.73	119.83
1	D	418	GLN	N-CA-C	-7.30	103.40	111.36
1	C	114	LEU	N-CA-C	7.21	119.76	111.11
1	C	162	LYS	N-CA-CB	-7.13	99.36	110.06
1	B	320	VAL	N-CA-C	7.13	117.89	110.62
1	A	89	ASP	CA-CB-CG	-7.11	105.49	112.60
1	D	416	ASN	CA-C-O	7.11	124.93	119.46
1	B	37	ILE	N-CA-C	7.07	117.11	108.06
1	B	287	ALA	N-CA-C	-7.02	103.63	111.28
1	D	194	ASP	CA-CB-CG	6.96	119.56	112.60
1	C	515	PRO	CB-CA-C	-6.96	102.88	111.64
1	A	383	TYR	N-CA-C	6.88	119.06	108.12
1	D	65	GLN	N-CA-C	-6.86	103.73	111.07
1	B	319	ASP	CA-CB-CG	-6.80	105.80	112.60
1	A	49	ARG	N-CA-C	6.80	121.11	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	514	VAL	CA-C-N	6.78	128.32	119.84
1	B	514	VAL	C-N-CA	6.78	128.32	119.84
1	A	361	HIS	CA-CB-CG	-6.73	107.07	113.80
1	B	162	LYS	N-CA-CB	-6.73	99.97	110.06
1	A	389	ASN	CA-CB-CG	-6.71	105.89	112.60
1	C	249	TYR	N-CA-C	6.70	121.29	113.18
1	B	78	TYR	CA-C-N	6.65	132.78	121.14
1	B	78	TYR	C-N-CA	6.65	132.78	121.14
1	B	49	ARG	N-CA-C	6.64	121.11	109.96
1	C	112	GLU	N-CA-C	6.61	120.04	112.57
1	D	314	HIS	CA-CB-CG	-6.61	107.19	113.80
1	B	279	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	289	HIS	CA-CB-CG	-6.53	107.27	113.80
1	D	139	HIS	N-CA-C	6.53	119.23	111.33
1	D	513	CYS	N-CA-C	-6.52	104.02	112.23
1	D	270	PHE	CA-CB-CG	-6.52	107.28	113.80
1	A	15	GLU	N-CA-CB	-6.50	99.94	109.82
1	C	365	ASN	CA-CB-CG	-6.48	106.12	112.60
1	B	139	HIS	N-CA-C	6.45	120.01	111.75
1	B	467	VAL	N-CA-C	6.45	119.11	111.05
1	C	436	PHE	CA-CB-CG	-6.44	107.36	113.80
1	A	139	HIS	N-CA-C	6.42	118.28	111.28
1	C	440	LEU	N-CA-C	6.37	117.96	110.31
1	A	235	GLY	N-CA-C	-6.37	106.93	115.21
1	A	436	PHE	CA-CB-CG	-6.34	107.46	113.80
1	D	169	ARG	N-CA-C	-6.30	105.42	113.23
1	D	363	ALA	N-CA-C	6.22	118.44	109.48
1	A	150	ASP	N-CA-CB	-6.21	101.87	110.38
1	A	151	GLU	N-CA-C	-6.20	105.70	113.20
1	B	109	LYS	N-CA-CB	-6.20	101.56	110.80
1	D	277	SER	CA-C-N	6.20	127.59	119.84
1	D	277	SER	C-N-CA	6.20	127.59	119.84
1	A	274	LEU	N-CA-C	-6.17	102.27	109.93
1	A	383	TYR	O-C-N	6.17	126.26	120.71
1	A	112	GLU	N-CA-C	6.13	119.50	112.57
1	A	93	PHE	CA-CB-CG	-6.12	107.68	113.80
1	C	29	HIS	CA-CB-CG	-6.11	107.69	113.80
1	D	336	ILE	N-CA-C	6.11	116.28	110.42
1	C	314	HIS	CA-CB-CG	-6.10	107.70	113.80
1	A	127	ASP	CA-CB-CG	6.08	118.68	112.60
1	C	370	HIS	CA-CB-CG	-6.07	107.73	113.80
1	D	116	ASP	CA-CB-CG	6.01	118.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	LEU	N-CA-C	6.00	117.50	111.07
1	C	470	GLN	CA-C-N	5.99	128.59	120.38
1	C	470	GLN	C-N-CA	5.99	128.59	120.38
1	D	314	HIS	N-CA-C	5.99	118.70	111.40
1	C	293	VAL	N-CA-C	-5.96	98.62	107.51
1	A	401	VAL	CA-C-N	5.94	126.09	119.32
1	A	401	VAL	C-N-CA	5.94	126.09	119.32
1	B	63	TYR	CA-C-N	5.93	129.70	120.75
1	B	63	TYR	C-N-CA	5.93	129.70	120.75
1	D	111	PRO	CB-CA-C	-5.92	102.63	110.27
1	C	56	ASN	N-CA-C	5.91	117.80	111.36
1	B	484	PHE	CA-C-N	5.88	125.75	119.28
1	B	484	PHE	C-N-CA	5.88	125.75	119.28
1	A	390	LYS	N-CA-C	5.87	118.46	111.71
1	D	112	GLU	N-CA-C	5.84	119.38	112.72
1	D	49	ARG	N-CA-C	5.84	119.34	109.76
1	D	336	ILE	N-CA-CB	-5.82	103.74	110.55
1	B	196	PHE	N-CA-C	-5.81	105.02	111.71
1	D	487	ASN	CB-CA-C	-5.79	103.67	111.89
1	D	247	LYS	N-CA-C	-5.78	104.89	111.14
1	C	389	ASN	CA-CB-CG	-5.78	106.82	112.60
1	B	151	GLU	N-CA-C	-5.76	106.23	113.20
1	D	334	ARG	CA-C-N	5.76	128.27	120.44
1	D	334	ARG	C-N-CA	5.76	128.27	120.44
1	C	471	GLN	N-CA-C	5.75	118.29	111.33
1	B	33	ASP	N-CA-C	5.74	117.23	110.97
1	C	32	PRO	CB-CA-C	-5.74	102.07	111.31
1	C	366	ALA	N-CA-C	5.73	117.33	111.14
1	D	157	VAL	CA-CB-CG2	5.70	120.09	110.40
1	A	450	GLU	N-CA-CB	5.69	120.64	110.80
1	A	484	PHE	O-C-N	5.67	126.38	121.34
1	B	64	ASN	CB-CA-C	-5.67	99.47	109.62
1	B	150	ASP	CB-CA-C	-5.63	98.75	110.40
1	D	501	PHE	CA-CB-CG	-5.63	108.17	113.80
1	B	144	PRO	CB-CA-C	-5.61	104.05	111.23
1	C	300	THR	N-CA-CB	5.60	119.30	110.56
1	B	204	ASN	N-CA-C	5.59	118.38	110.50
1	B	161	MET	CA-C-N	5.58	128.03	120.38
1	B	161	MET	C-N-CA	5.58	128.03	120.38
1	B	150	ASP	CB-CG-OD2	-5.57	105.59	118.40
1	C	462	ASP	CA-CB-CG	5.56	118.16	112.60
1	B	191	TYR	N-CA-C	5.54	117.68	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	ASP	CB-CA-C	-5.54	98.94	110.40
1	D	458	TYR	N-CA-C	-5.54	105.16	111.14
1	D	507	LEU	N-CA-C	5.51	116.35	109.57
1	B	470	GLN	CA-C-N	5.51	127.67	120.28
1	B	470	GLN	C-N-CA	5.51	127.67	120.28
1	B	235	GLY	N-CA-C	-5.51	107.69	113.58
1	C	235	GLY	N-CA-C	-5.51	107.34	113.79
1	D	113	PHE	CA-CB-CG	-5.50	108.30	113.80
1	A	370	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	294	HIS	N-CA-C	5.49	118.87	110.20
1	D	389	ASN	CA-CB-CG	-5.48	107.12	112.60
1	D	161	MET	CA-C-N	5.46	128.35	120.38
1	D	161	MET	C-N-CA	5.46	128.35	120.38
1	C	15	GLU	N-CA-C	-5.45	105.34	111.28
1	C	73	VAL	CB-CA-C	-5.45	102.11	110.50
1	B	113	PHE	N-CA-CB	-5.44	102.29	110.73
1	B	143	ILE	CA-C-N	5.42	125.36	119.78
1	B	143	ILE	C-N-CA	5.42	125.36	119.78
1	D	220	LYS	CB-CA-C	-5.42	102.14	110.81
1	C	360	PHE	N-CA-C	-5.41	106.68	113.28
1	B	171	ILE	CA-CB-CG2	5.41	119.70	110.50
1	D	151	GLU	N-CA-C	-5.41	106.64	113.18
1	A	60	GLN	CB-CG-CD	-5.40	103.42	112.60
1	C	51	SER	N-CA-C	5.40	117.04	108.67
1	D	157	VAL	CG1-CB-CG2	5.40	122.68	110.80
1	A	327	THR	CA-C-O	5.39	124.01	118.73
1	A	150	ASP	CB-CG-OD2	-5.37	106.05	118.40
1	B	487	ASN	CB-CA-C	-5.36	104.28	111.89
1	B	122	ALA	N-CA-CB	5.34	119.48	110.77
1	A	476	GLN	N-CA-C	-5.33	105.47	111.28
1	C	135	ILE	CA-C-N	-5.32	114.89	121.38
1	C	135	ILE	C-N-CA	-5.32	114.89	121.38
1	A	150	ASP	CB-CA-C	-5.30	98.64	110.19
1	C	174	PHE	CA-C-O	5.29	123.53	119.46
1	B	15	GLU	CA-C-O	5.28	126.10	120.24
1	A	56	ASN	N-CA-C	5.28	118.18	111.69
1	D	363	ALA	N-CA-CB	5.26	119.15	109.73
1	A	441	PRO	CB-CA-C	-5.25	105.84	111.56
1	D	205	VAL	N-CA-C	5.25	115.33	107.51
1	B	114	LEU	N-CA-CB	5.25	117.76	109.94
1	A	59	ALA	N-CA-C	5.24	117.05	110.24
1	C	378	LEU	N-CA-C	5.24	118.93	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	MET	CA-C-O	5.23	126.31	120.82
1	C	514	VAL	CB-CA-C	5.23	116.31	110.71
1	B	81	GLN	OE1-CD-NE2	-5.23	117.37	122.60
1	B	313	TYR	CA-C-O	5.22	126.09	120.55
1	A	175	PRO	N-CA-C	5.22	119.39	111.15
1	C	320	VAL	N-CA-C	5.22	115.66	110.23
1	C	487	ASN	CB-CA-C	-5.21	104.87	111.86
1	B	135	ILE	CA-C-N	-5.19	116.00	121.35
1	B	135	ILE	C-N-CA	-5.19	116.00	121.35
1	C	480	ALA	N-CA-C	5.19	118.39	111.75
1	C	440	LEU	O-C-N	5.19	125.92	120.99
1	D	52	ILE	CA-C-O	5.19	125.18	120.30
1	A	508	PRO	N-CA-CB	5.18	108.80	103.15
1	C	158	ALA	CA-C-N	5.17	127.17	120.44
1	C	158	ALA	C-N-CA	5.17	127.17	120.44
1	D	319	ASP	CA-C-N	5.17	127.55	120.77
1	D	319	ASP	C-N-CA	5.17	127.55	120.77
1	A	111	PRO	CA-C-N	-5.17	114.87	122.83
1	A	111	PRO	C-N-CA	-5.17	114.87	122.83
1	C	438	ALA	N-CA-C	5.14	119.04	112.87
1	B	471	GLN	N-CA-C	5.14	116.88	111.28
1	A	443	SER	N-CA-C	-5.13	105.69	111.28
1	B	437	GLU	CA-C-N	5.13	127.41	120.38
1	B	437	GLU	C-N-CA	5.13	127.41	120.38
1	D	186	GLU	N-CA-CB	5.13	120.31	111.13
1	A	199	ASP	N-CA-CB	5.13	119.04	110.32
1	A	489	PRO	CB-CA-C	-5.12	105.19	111.64
1	C	474	ASP	N-CA-C	-5.12	105.70	111.28
1	A	169	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	D	464	LEU	N-CA-C	-5.10	104.79	111.02
1	D	472	VAL	N-CA-C	5.10	115.19	107.75
1	C	161	MET	CA-C-N	5.09	127.36	120.38
1	C	161	MET	C-N-CA	5.09	127.36	120.38
1	D	220	LYS	CA-C-O	5.09	126.35	120.90
1	B	162	LYS	CA-CB-CG	5.08	124.25	114.10
1	D	494	ALA	CB-CA-C	-5.07	102.37	110.79
1	D	174	PHE	CA-CB-CG	-5.07	108.73	113.80
1	D	109	LYS	CB-CA-C	-5.07	101.17	109.99
1	B	42	ASN	CA-CB-CG	-5.06	107.54	112.60
1	B	64	ASN	N-CA-C	-5.04	103.50	110.35
1	A	197	ASP	CA-C-N	5.04	127.03	120.28
1	A	197	ASP	C-N-CA	5.04	127.03	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ALA	N-CA-C	-5.01	99.46	108.48
1	C	482	PHE	CA-CB-CG	-5.01	108.79	113.80
1	B	234	SER	CA-C-N	-5.00	118.00	123.30
1	B	234	SER	C-N-CA	-5.00	118.00	123.30

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	206	0
1	B	3942	0	3828	258	0
1	C	3942	0	3827	213	0
1	D	3930	0	3818	195	0
2	A	5	0	0	0	0
2	B	4	0	0	1	0
2	C	4	0	0	1	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	6	0
4	B	23	0	12	4	0
4	C	23	0	11	8	0
4	D	23	0	12	9	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	9	0
6	B	235	0	0	14	0
6	C	223	0	0	7	0
6	D	296	0	0	19	0
All	All	16980	0	15409	866	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 28.

All (866) 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: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
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:C:366:ALA:HA	1:C:421:MET:HE3	1.55	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:B:348:GLU:CD	4:B:1107:AMP:H5'1	2.03	0.83
1:D:64:ASN:HB3	1:D:67:LYS:H	1.41	0.82
1:C:238:ASP:OD1	2:C:1115:IUM:U	1.60	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:D:268:HIS:HD1	1:D:295:HIS:HE2	0.82	0.81
1:C:422:CYS:SG	1:C:428:GLU:HA	2.21	0.81
2:B:1108:IUM:U	4:B:1107:AMP:O2P	1.61	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:D:348:GLU:CD	4:D:1121:AMP:H5'1	2.08	0.80
1:A:387:ARG:HH11	1:A:387:ARG:CB	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:78:TYR:HD2	1:D:224:MET:HE2	1.49	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:B:439:TYR:C	1:B:440:LEU:HD23	2.10	0.76
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
1:C:44:ILE:C	1:C:45:LEU:HD12	2.09	0.76
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:D:78:TYR:CD2	1:D:224:MET:HE2	2.21	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:A:365:ASN:HD21	1:A:368:GLU:HG2	1.53	0.73
1:B:1:ALA:H3	5:B:1113:GLN:HE22	1.35	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:D:271:ALA:HA	4:D:1121:AMP:N1	2.04	0.73
1:C:365:ASN:O	1:C:421:MET:HE1	1.89	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:D:427:MET:HE2	1:D:448:GLN:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:348:GLU:CD	4:C:1114:AMP:H5'1	2.16	0.70
1:A:348:GLU:CD	4:A:1100:AMP:H5'1	2.17	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
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:A:365:ASN:HA	1:A:421:MET:HE1	1.74	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:117:LEU:O	1:C:406:LYS:NZ	2.26	0.66
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:454:ASP:N	6:C:1309:HOH:O	2.30	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: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:B:427:MET:HE1	1:B:446:TRP:C	2.23	0.64
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:A:213:GLN:HE21	1:A:213:GLN:C	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:SER:C	1:D:52:ILE:HD12	2.22	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:D:473:SER:HG	1:D:475:GLN:H	1.43	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
1:D:270:PHE:HE2	1:D:339:MET:HE2	1.62	0.63
1:D:84:ARG:NH2	1:D:97:SER:O	2.28	0.63
1:C:232:LEU:HD22	1:C:332:MET:HE3	1.79	0.62
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:HD12	1:D:52:ILE:N	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:229:TYR:CB	1:D:343:MET:HE3	2.31	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:507:LEU:HD12	1:D:508:PRO:HD2	1.82	0.60
1:D:197:ASP:O	1:D:200:ALA:HB3	2.02	0.59
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:C:366:ALA:CA	1:C:421:MET:HE3	2.29	0.58
1:A:381:HIS:CE1	1:A:382:MET:HG3	2.38	0.58
1:B:199:ASP:HB2	1:B:202:LYS:NZ	2.18	0.58
1:D:428:GLU:CD	1:D:428:GLU:H	2.10	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:199:ASP:HB3	1:A:202:LYS:HZ1	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:361:HIS:HE2	1:D:428:GLU:CD	2.10	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:C:361:HIS:C	1:C:363:ALA:H	2.11	0.57
1:D:125:LEU:C	1:D:125:LEU:HD23	2.29	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:A:416:ASN:OD1	1:A:417:PRO:HD2	2.05	0.57
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:384:ASP:CG	1:D:387:ARG:HH21	2.12	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:D:229:TYR:C	1:D:341:ILE:HD13	2.31	0.56
1:A:504:LEU:C	1:A:506:PRO:HD3	2.30	0.56
1:A:164:LEU:HB3	1:A:171:ILE:HD11	1.88	0.56
1:A:329:MET:HE3	1:A:388:ALA:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:MET:HE1	1:B:447:ARG:N	2.21	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:125:LEU:HD23	1:B:125:LEU:C	2.32	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:C:81:GLN:H	1:C:81:GLN:CD	2.13	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
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:D:192:HIS:C	1:D:193:ARG:HG2	2.32	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:B:496:LEU:C	1:B:496:LEU:HD23	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:427:MET:HE2	1:A:448:GLN:HG3	1.89	0.54
1:B:81:GLN:CD	1:B:82:ALA:H	2.16	0.54
1:B:216:GLU:OE1	1:B:439:TYR:OH	2.25	0.54
1:D:406:LYS:NZ	6:D:1196:HOH:O	2.33	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:A:238:ASP:CG	1:A:429:LYS:HZ1	2.15	0.53
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:C:504:LEU:C	1:C:506:PRO:HD3	2.33	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:D:1:ALA:H1	5:D:1127:GLN:HE22	1.55	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:C:5:GLY:O	1:C:156:TYR:HA	2.09	0.53
1:A:213:GLN:O	1:A:213:GLN:NE2	2.42	0.53
1:B:199:ASP:HB2	1:B:202:LYS:HZ1	1.72	0.53
1:A:60:GLN:HA	1:A:61:PRO:C	2.35	0.52
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:A:12:ASP:HB3	1:A:15:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:358:LEU:O	1:D:361:HIS:HB2	2.09	0.52
1:B:207:ASP:CG	1:B:210:GLU:HB2	2.35	0.52
1:D:4:PHE:HB3	1:D:46:ALA:HB3	1.92	0.52
1:A:329:MET:HE2	1:A:387:ARG:HD2	1.92	0.52
1:A:486:TYR:CE1	1:A:487:ASN:ND2	2.78	0.52
1:C:332:MET:HE1	4:C:1114:AMP:C2	2.44	0.52
1:A:147:MET:HE2	1:A:174:PHE:HA	1.91	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:C:264:TRP:C	1:C:266:GLN:H	2.18	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: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:229:TYR:HB3	1:D:343:MET:HE3	1.91	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:270:PHE:HE2	1:B:339:MET:HE2	1.76	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:270:PHE:CE2	1:D:339:MET:HE2	2.43	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:64:ASN:C	1:D:67:LYS:H	2.18	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:B:1:ALA:H1	5:B:1113:GLN:HE22	1.54	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:A:475:GLN:HA	1:A:478:GLU:CD	2.37	0.50
1:B:81:GLN:CD	1:B:82:ALA:N	2.70	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:337:LYS:HG2	1:C:395:TRP:O	2.12	0.50
1:C:472:VAL:O	1:C:492:LYS:NZ	2.30	0.50
1:C:127:ASP:OD1	1:C:130:LYS:HD3	2.12	0.50
1:A:428:GLU:H	1:A:428:GLU:CD	2.20	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: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:C:358:LEU:C	1:C:360:PHE:H	2.20	0.50
1:D:496:LEU:HD12	1:D:496:LEU:C	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:316:GLU:OE2	1:B:390:LYS:NZ	2.43	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:A:401:VAL:HG23	1:A:401:VAL:O	2.13	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: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:B:285:GLU:O	1:B:288:ASN:HB2	2.13	0.48
1:D:268:HIS:HD1	1:D:295:HIS:CE1	2.22	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:205:VAL:HG13	1:A:206:THR:N	2.29	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:60:GLN:HA	1:C:61:PRO:C	2.40	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:346:SER:OG	1:A:348:GLU:OE2	2.29	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: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:D:332:MET:HE1	4:D:1121:AMP:C2	2.49	0.47
1:C:274:LEU:O	1:C:277:SER:OG	2.29	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:427:MET:HE3	1:D:427:MET:HA	1.97	0.46
1:A:332:MET:HE1	4:A:1100:AMP:C2	2.50	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:364:PRO:CG	1:D:368:GLU:HG2	2.29	0.46
1:A:164:LEU:C	1:A:166:PRO:HD2	2.40	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: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
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:B:216:GLU:C	1:B:220:LYS:HD3	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:CG	1:A:212:ARG:HH12	2.24	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:A:427:MET:HE2	1:A:448:GLN:CG	2.45	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:92:GLN:CD	1:A:94:GLN:HE22	2.25	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:365:ASN:CA	1:A:421:MET:HE1	2.43	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:D:64:ASN:HB2	1:D:68:THR:N	2.32	0.45
1:B:300:THR:HG23	1:B:302:GLN:H	1.82	0.45
1:B:427:MET:HE1	1:B:446:TRP:CA	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:60:GLN:HA	1:D:61:PRO:C	2.43	0.44
1:D:514:VAL:CG1	1:D:515:PRO:HD2	2.47	0.44
1:A:416:ASN:C	1:A:418:GLN:H	2.25	0.44
1:B:49:ARG:NH2	1:B:53:VAL:O	2.51	0.44
1:B:501:PHE:CD1	1:B:501:PHE:C	2.94	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:C:358:LEU:C	1:C:360:PHE:N	2.73	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:A:416:ASN:C	1:A:418:GLN:N	2.75	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
1:B:113:PHE:C	1:B:113:PHE:CD1	2.95	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:190:TYR:CD1	1:D:190:TYR:C	2.96	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:147:MET:HE3	1:B:155:LEU:HD11	2.00	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: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:271:ALA:HA	4:A:1100:AMP:N1	2.34	0.43
1:A:496:LEU:HD23	1:A:496:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HD12	1:C:464:LEU:HA	1.69	0.43
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:C:190:TYR:CD1	1:C:190:TYR:C	2.97	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:A:213:GLN:C	1:A:213:GLN:NE2	2.76	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:A:145:LEU:HD11	1:A:157:VAL:HG13	2.01	0.42
1:A:335:LYS:NZ	6:A:1251:HOH:O	2.46	0.42
1:A:365:ASN:HA	1:A:421:MET:HE2	2.00	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: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: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:505:PHE:N	1:A:506:PRO:HD3	2.35	0.42
1:B:190:TYR:CD1	1:B:190:TYR:C	2.97	0.42
1:C:234:SER:HB3	4:C:1114:AMP:C4	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ALA:HA	1:C:421:MET:HE1	1.98	0.42
1:A:147:MET:HE3	1:A:172:LYS:HG3	2.01	0.42
1:C:114:LEU:HD22	1:C:190:TYR:CE2	2.55	0.42
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:D:198:TYR:C	1:D:200:ALA:H	2.27	0.42
1:A:192:HIS:ND1	1:A:192:HIS:C	2.78	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:81:GLN:CD	6:B:1152:HOH:O	2.63	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:302:GLN:HE21	1:B:306:ASP:CG	2.28	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: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:280:LEU:HG	1:D:296:GLU:CD	2.45	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:123:PHE:CD1	1:B:123:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:198:TYR:CD2	1:A:367:LYS:HG3	2.55	0.41
1:A:199:ASP:HA	1:A:202:LYS:HZ3	1.85	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:C:162:LYS:HB2	1:C:162:LYS:HZ2	1.85	0.41
1:D:384:ASP:CG	1:D:387:ARG:NH2	2.78	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:192:HIS:C	1:C:193:ARG:HG2	2.45	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:229:TYR:CD1	1:A:229:TYR:C	2.98	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:231:VAL:O	1:B:269:SER:HA	2.21	0.41
1:C:359:TYR:CD2	1:C:359:TYR:C	2.98	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:289:HIS:NE2	1:A:441:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:248:LYS:C	1:B:250:ALA:H	2.28	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:D:281:LYS:N	1:D:281:LYS:CD	2.78	0.41
1:A:190:TYR:CD1	1:A:190:TYR:C	2.99	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:113:PHE:CD1	1:C:113:PHE:C	2.99	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
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:125:LEU:C	1:A:125:LEU:HD23	2.46	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:194:ASP:C	1:C:196:PHE:H	2.28	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:A:195:TRP:C	1:A:197:ASP:N	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:229:TYR:CD1	1:B:229:TYR:C	2.99	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%)	30	27
1	B	487/553 (88%)	449 (92%)	31 (6%)	7 (1%)	9	4
1	C	487/553 (88%)	450 (92%)	33 (7%)	4 (1%)	16	11
1	D	487/553 (88%)	467 (96%)	18 (4%)	2 (0%)	30	27
All	All	1952/2212 (88%)	1831 (94%)	106 (5%)	15 (1%)	16	11

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	351 (85%)	63 (15%)	3	1
1	C	414/462 (90%)	361 (87%)	53 (13%)	4	2
1	D	412/462 (89%)	370 (90%)	42 (10%)	7	4
All	All	1658/1848 (90%)	1453 (88%)	205 (12%)	4	2

All (205) 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	81	GLN
1	A	89	ASP
1	A	90	ARG
1	A	112	GLU
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	150	ASP
1	A	151	GLU
1	A	157	VAL
1	A	162	LYS
1	A	171	ILE
1	A	192	HIS
1	A	199	ASP
1	A	201	VAL
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	339	MET
1	A	348	GLU
1	A	365	ASN
1	A	375	ARG
1	A	378	LEU
1	A	387	ARG
1	A	429	LYS
1	A	431	ILE
1	A	440	LEU
1	A	443	SER
1	A	447	ARG
1	A	449	LYS
1	A	450	GLU
1	A	456	VAL
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	16	LEU
1	B	19	LYS
1	B	42	ASN
1	B	51	SER
1	B	66	GLN
1	B	67	LYS

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Mol	Chain	Res	Type
1	B	80	HIS
1	B	81	GLN
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	171	ILE
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	248	LYS
1	B	277	SER
1	B	280	LEU
1	B	281	LYS
1	B	300	THR
1	B	301	VAL
1	B	329	MET
1	B	335	LYS
1	B	337	LYS
1	B	339	MET
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

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Mol	Chain	Res	Type
1	B	439	TYR
1	B	440	LEU
1	B	456	VAL
1	B	459	SER
1	B	462	ASP
1	B	464	LEU
1	B	470	GLN
1	B	471	GLN
1	B	473	SER
1	B	481	ARG
1	B	488	THR
1	B	490	THR
1	B	502	GLU
1	B	509	SER
1	C	10	LYS
1	C	19	LYS
1	C	25	ARG
1	C	42	ASN
1	C	51	SER
1	C	65	GLN
1	C	67	LYS
1	C	70	VAL
1	C	80	HIS
1	C	81	GLN
1	C	89	ASP
1	C	103	LEU
1	C	114	LEU
1	C	130	LYS
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	201	VAL
1	C	202	LYS
1	C	224	MET
1	C	242	ILE
1	C	247	LYS
1	C	264	TRP
1	C	277	SER
1	C	280	LEU

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Mol	Chain	Res	Type
1	C	312	ILE
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	365	ASN
1	C	368	GLU
1	C	369	LEU
1	C	376	LYS
1	C	393	SER
1	C	418	GLN
1	C	427	MET
1	C	428	GLU
1	C	429	LYS
1	C	431	ILE
1	C	433	ARG
1	C	440	LEU
1	C	443	SER
1	C	464	LEU
1	C	470	GLN
1	C	502	GLU
1	C	509	SER
1	D	10	LYS
1	D	25	ARG
1	D	51	SER
1	D	65	GLN
1	D	66	GLN
1	D	67	LYS
1	D	74	ASN
1	D	81	GLN
1	D	89	ASP
1	D	92	GLN
1	D	103	LEU
1	D	129	GLU
1	D	150	ASP
1	D	155	LEU
1	D	162	LYS
1	D	188	ARG
1	D	199	ASP

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Mol	Chain	Res	Type
1	D	203	ASP
1	D	205	VAL
1	D	220	LYS
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	341	ILE
1	D	357	TYR
1	D	358	LEU
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	456	VAL
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 (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
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

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Mol	Chain	Res	Type
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	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	92	GLN
1	C	94	GLN
1	C	183	GLN
1	C	192	HIS
1	C	288	ASN
1	C	302	GLN
1	C	365	ASN
1	C	430	HIS
1	C	470	GLN
1	C	471	GLN
1	D	56	ASN
1	D	74	ASN
1	D	80	HIS
1	D	81	GLN
1	D	192	HIS
1	D	213	GLN
1	D	284	GLN
1	D	288	ASN
1	D	418	GLN
1	D	430	HIS
1	D	470	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
2	IUM	A	1102	1,4	0,1,2	-	-	-		
4	AMP	C	1114	2	25,25,25	1.28	3 (12%)	37,38,38	1.69	6 (16%)
5	GLN	D	1127	-	8,9,9	1.35	1 (12%)	8,11,11	0.87	0
4	AMP	A	1100	2	25,25,25	1.28	3 (12%)	37,38,38	1.60	5 (13%)
5	GLN	B	1113	-	8,9,9	1.26	1 (12%)	8,11,11	0.92	1 (12%)
5	GLN	C	1120	-	8,9,9	1.32	2 (25%)	8,11,11	1.49	2 (25%)
4	AMP	D	1121	2	25,25,25	1.19	3 (12%)	37,38,38	1.84	7 (18%)
2	IUM	D	1122	1,2,6,4	0,1,2	-	-	-		
5	GLN	A	1106	-	8,9,9	1.33	1 (12%)	8,11,11	0.95	0
4	AMP	B	1107	2	25,25,25	1.20	3 (12%)	37,38,38	1.05	3 (8%)

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	C	1114	2	-	0/10/26/26	0/3/3/3
5	GLN	D	1127	-	-	0/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	A	1100	2	-	0/10/26/26	0/3/3/3
5	GLN	B	1113	-	-	0/9/9/9	-
5	GLN	C	1120	-	-	0/9/9/9	-
4	AMP	D	1121	2	-	6/10/26/26	0/3/3/3
5	GLN	A	1106	-	-	0/9/9/9	-
4	AMP	B	1107	2	-	0/10/26/26	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1106	GLN	CA-N	-3.08	1.33	1.48
4	C	1114	AMP	O2'-C2'	3.05	1.50	1.43
4	C	1114	AMP	O3'-C3'	3.03	1.50	1.43
4	A	1100	AMP	O2'-C2'	2.93	1.50	1.43
4	A	1100	AMP	O3'-C3'	2.91	1.50	1.43
4	B	1107	AMP	O3'-C3'	2.89	1.50	1.43
4	D	1121	AMP	O2'-C2'	2.88	1.50	1.43
4	A	1100	AMP	C2-N1	2.71	1.38	1.33
4	C	1114	AMP	C2-N1	2.54	1.38	1.33
5	B	1113	GLN	CA-N	-2.51	1.35	1.48
5	C	1120	GLN	CA-N	-2.50	1.35	1.48
4	B	1107	AMP	C2-N1	2.46	1.38	1.33
5	D	1127	GLN	CA-N	-2.41	1.36	1.48
4	B	1107	AMP	O2'-C2'	2.35	1.48	1.43
4	D	1121	AMP	O3'-C3'	2.29	1.48	1.43
5	C	1120	GLN	O-C	2.21	1.28	1.22
4	D	1121	AMP	C4-N9	2.20	1.42	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1121	AMP	O2P-P-O5'	-5.87	91.36	106.67
4	C	1114	AMP	C2'-C3'-C4'	-5.59	91.82	102.61
4	A	1100	AMP	O3'-C3'-C2'	5.17	128.39	111.82
4	D	1121	AMP	C2'-C3'-C4'	-4.51	93.90	102.61
4	C	1114	AMP	O3'-C3'-C2'	4.37	125.83	111.82
4	A	1100	AMP	O2P-P-O5'	-3.72	96.97	106.67
4	D	1121	AMP	O3'-C3'-C2'	3.58	123.28	111.82
4	C	1114	AMP	O2P-P-O5'	3.52	115.86	106.67
4	D	1121	AMP	N6-C6-N1	-3.48	110.63	118.38
4	B	1107	AMP	O3'-C3'-C2'	3.17	121.99	111.82
4	A	1100	AMP	O2'-C2'-C3'	3.06	121.64	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1120	GLN	OXT-C-O	-2.96	117.37	124.08
4	D	1121	AMP	C5-C6-N6	2.82	130.28	123.29
5	C	1120	GLN	CG-CB-CA	-2.79	107.45	113.86
4	A	1100	AMP	C2'-C3'-C4'	-2.68	97.43	102.61
4	C	1114	AMP	O4'-C4'-C3'	-2.57	100.06	105.15
4	B	1107	AMP	C2'-C3'-C4'	-2.52	97.73	102.61
4	B	1107	AMP	O2P-P-O5'	2.42	112.97	106.67
4	D	1121	AMP	O4'-C1'-N9	2.40	112.69	108.09
4	C	1114	AMP	O2'-C2'-C3'	2.32	119.24	111.82
5	B	1113	GLN	OXT-C-O	-2.19	119.10	124.08
4	D	1121	AMP	O3P-P-O2P	2.13	115.78	107.80
4	C	1114	AMP	O4'-C1'-N9	2.02	111.97	108.09
4	A	1100	AMP	O4'-C4'-C3'	-2.00	101.18	105.15

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

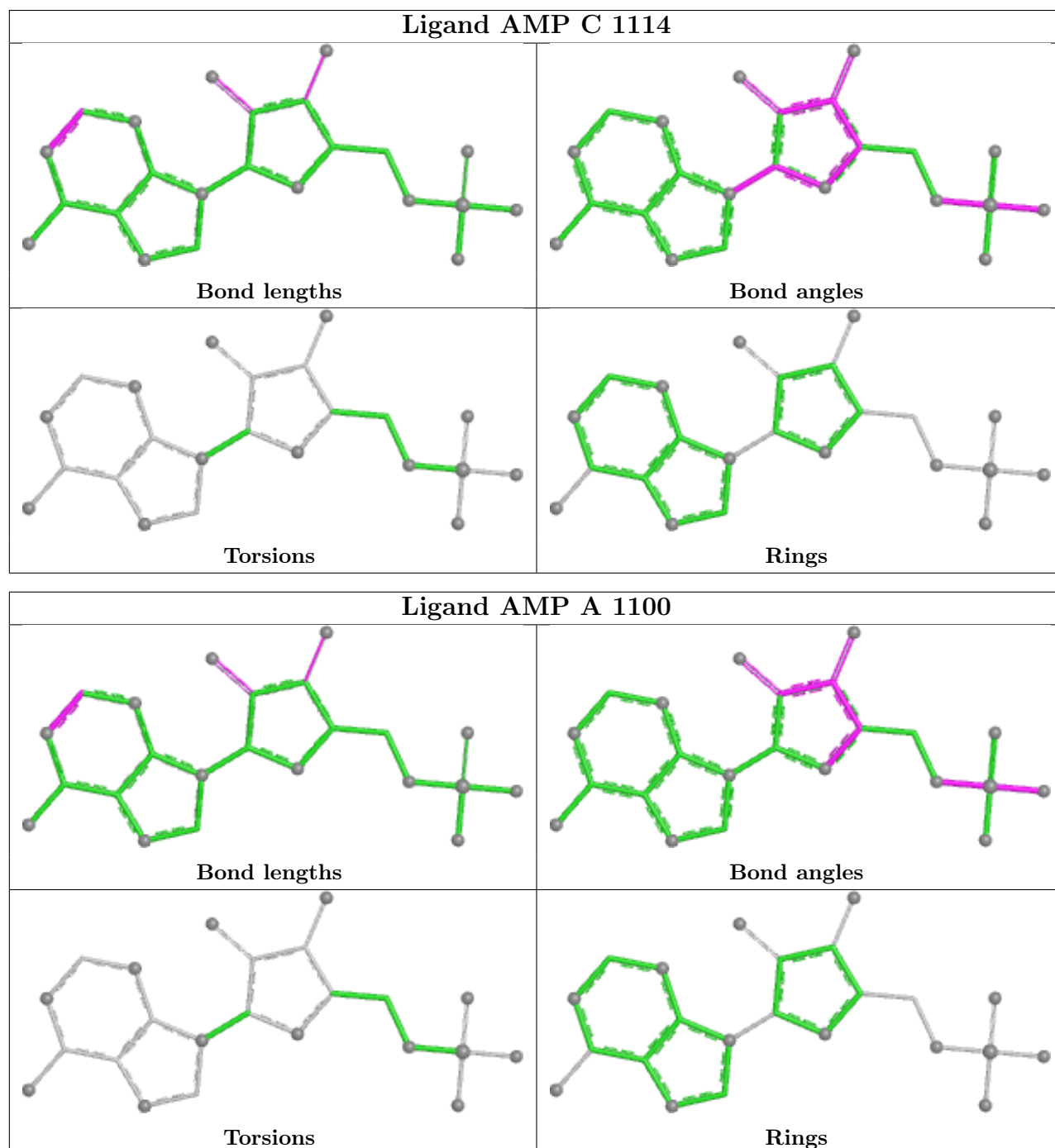
There are no ring outliers.

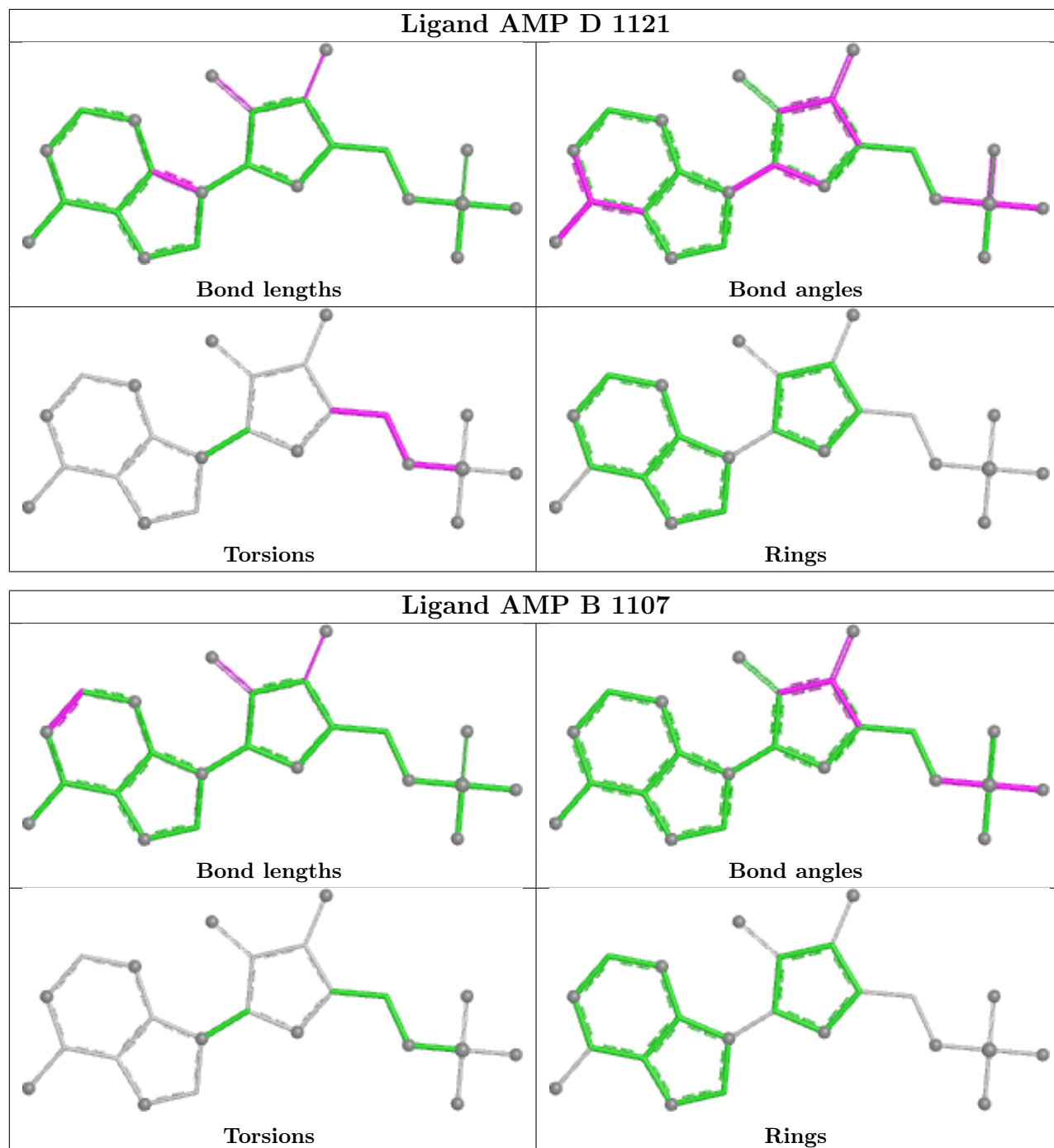
8 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1114	AMP	8	0
5	D	1127	GLN	2	0
4	A	1100	AMP	6	0
5	B	1113	GLN	4	0
5	C	1120	GLN	1	0
4	D	1121	AMP	9	0
5	A	1106	GLN	2	0
4	B	1107	AMP	4	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.