



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:12 AM BST

PDB ID : 5COX
Title : UNINHIBITED MOUSE CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2)
Authors : Kurumbail, R.; Stallings, W.
Deposited on : 1996-12-18
Resolution : 3.00 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)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

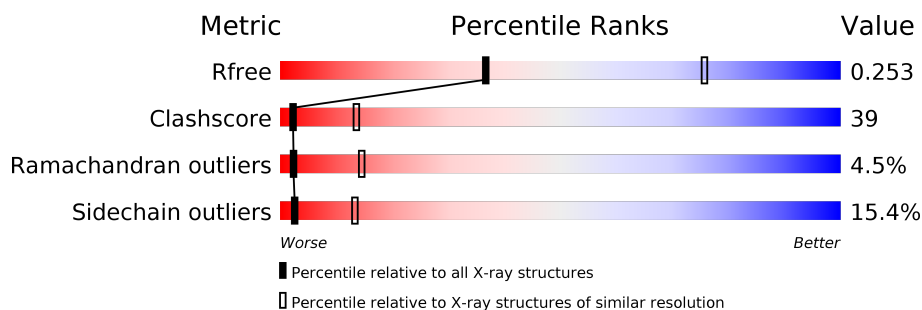
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	587	<div> <div>35%</div> <div>45%</div> <div>13%</div> <div>6%</div> </div>
1	B	587	<div> <div>35%</div> <div>47%</div> <div>11%</div> <div>6%</div> </div>
1	C	587	<div> <div>33%</div> <div>47%</div> <div>13%</div> <div>6%</div> </div>
1	D	587	<div> <div>33%</div> <div>49%</div> <div>12%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18232 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769
C	310	GLN	ASN	conflict	UNP Q05769
C	333	LYS	ARG	conflict	UNP Q05769
D	310	GLN	ASN	conflict	UNP Q05769
D	333	LYS	ARG	conflict	UNP Q05769

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

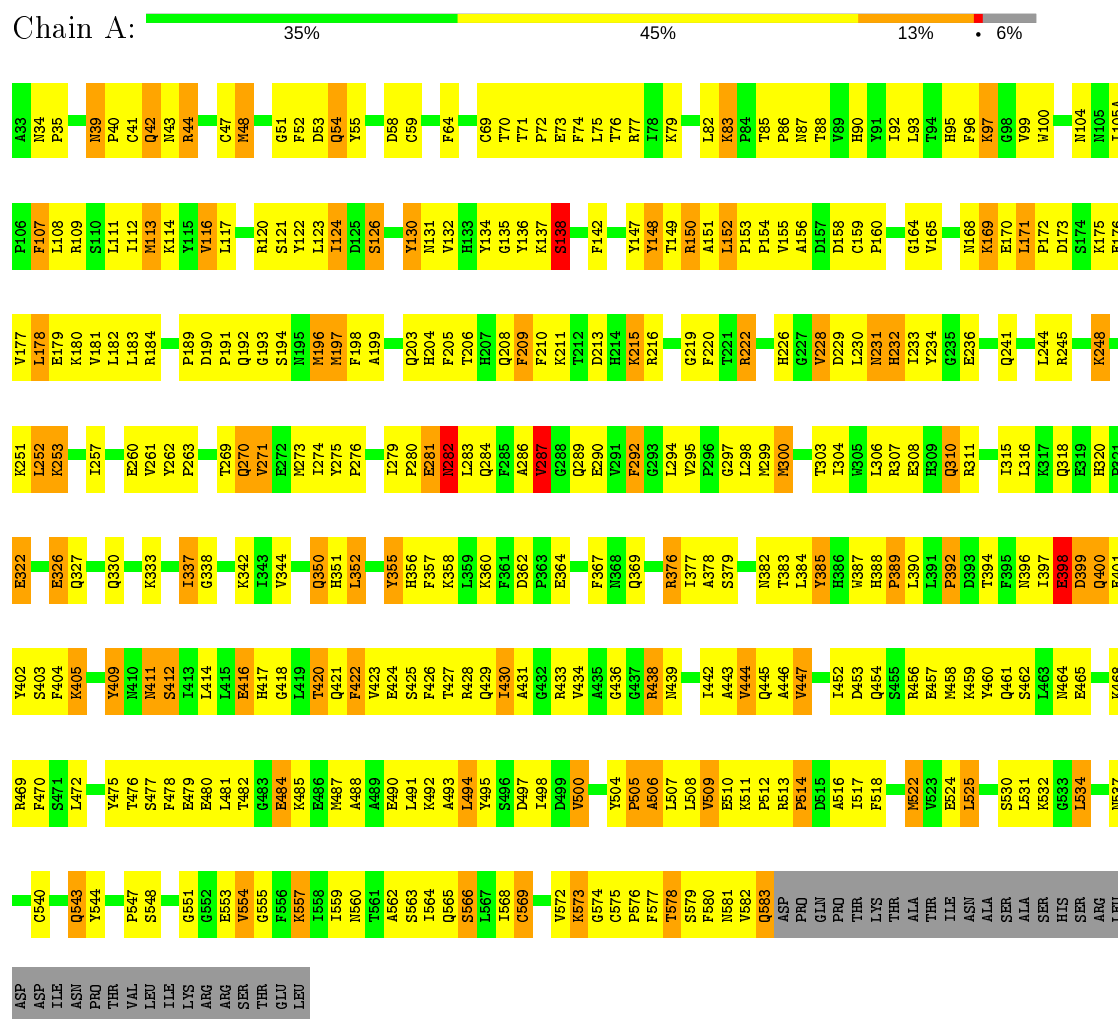


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

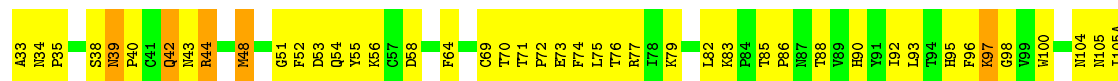
3 Residue-property plots

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.

• Molecule 1: CYCLOOXYGENASE-2



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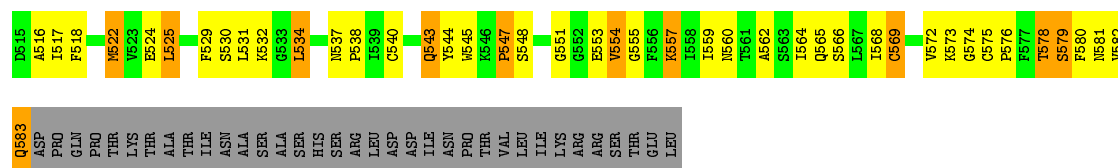


SER	ALA	HIS	SER	ARG	LEU	ASP	ASP	ILE	ASN	PRO	THR	VAL	LEU	ILE	LYS	ARG	ARG	SER	THR	GLU	LEU																																				
M522	V523	E524	L525	F529	S530	L531	K532	G533	L534	M535	Q543	S548	G551	G552	S553	V554	F555	F556	K557	M560	T561	A562	S563	F564	S565	C566	C567	V572	K573	G574	C575	P576	F577	T578	S579	F580	N581	V582	Q583	ASP	PRO	GLN	THR	ILE	ASN	ALA											
R456	E457	M458	K459	Y460	Q461	S462	L463	N464	E465	Y466	K467	K468	R469	F470	S471	L472	Y475	T476	F478	E479	E480	L481	T482	G483	E484	K485	A488	A489	E490	L491	K492	Q493	L494	Y495	T498	D499	V500	Y504	P505	A506	L507	L508	V509	E510	K511	P512	THR	P514	D515	A516	I517	F518	T521				
T394	F395	N396	I397	E398	D399	Q400	E401	Y402	S403	F404	K405	Q406	F407	L408	Y409	N410	N411	S412	L413	L414	L415	E416	H417	G418	L419	T420	Q421	F422	V423	E424	S425	F426	T427	K428	Q429	L430	A431	G432	R433	V434	A435	G436	G437	R438	N439	I442	F443	N444	Q445	A446	V447	A448	K449	I452	D453	Q454	S455
P106	F107	L108	R109	S110	L111	I112	M113	V116	V117	R120	S121	Y122	L123	I124	S126	P127	N131	V132	H133	Y134	G135	Y136	K137	S138	F142	Y147	Y148	R150	K215	R216	G217	L152	P153	P154	V155	A156	D157	C158	P160	G164	V165	M168	K169	E170	L171	P172	D173	S174	K175	E176	V177						
L178	E179	K180	V181	L182	L183	R184	R185	P189	D190	Q191	Q192	G193	S194	N195	M196	M197	F198	A199	F200	F201	A202	Q203	H204	F205	T206	G207	Q208	F209	K211	T212	D213	H214	T149	K215	R216	G217	P218	G219	F220	T221	R222	H226	G227	V228	D229	L230	J031	H232	I233	G235	E236	R240	Q241	K243			
L244	E245	K248	K251	L252	K253	Y254	I257	V261	Y262	P263	T269	Q270	V271	E272	M273	I274	Y275	P276	I279	P280	E281	R282	L283	F285	Q286	K287	L288	E289	E290	V291	F292	G293	V295	L298	M299	K300	Y301	T303	L306	K307	E308	H309	Q310	R311	I315	L316	K317	Q318									
E319	H320	P321	E322	D325	E326	Q327	Q330	K333	I337	G338	E339	K342	I343	V344	Y348	Q350	E480	H351	L352	Y355	H356	F357	L263	K358	L359	K360	F361	K362	P363	E364	L365	L366	Q369	R376	I377	A378	S379	F381	N382	T383	L384	Y385	H386	W387	H388	L389	L390	L391	P392	D393							

• Molecule 1: CYCLOOXYGENASE-2

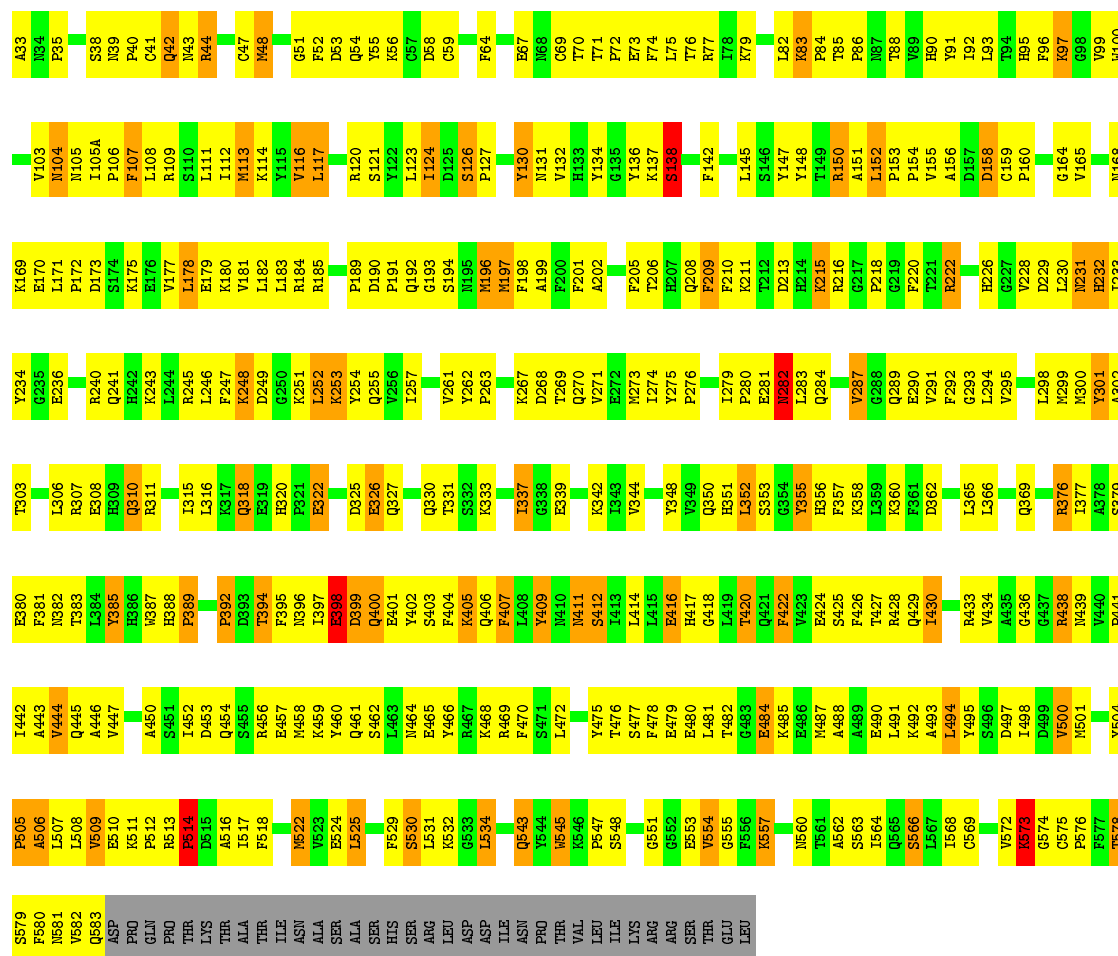
Chain C:  33% 47% 13% 6%

V447	Y385	E308	Q241	K169	V99	A33
A448	H386	H309		E170	W100	A33
K449	R387	Q310	L244	L171		P35
	H388	R311	R245	P172		
I452	P389	T315	L246	D173	M104	S38
D453	L390	T315	F247	S174	I105A	N39
Q454	D453	L316	K248	K175	P106	P40
Q455	P392	K317	D249	E176	P107	C41
A456	D393	Q318	Q250	V177	L108	Q42
E457	T394	E319	K251	L178	R109	N43
M458	P395	H320	L252	E179	S110	R44
K459	N396	P321	K253	K180	L111	
V460	L397	E322	Y254	V181	L112	C47
Q461	E398		Q255	L182	M113	M48
S462	Q400	D325	V256	L183	K114	
E465	E401	Q327	I257	R184	Y115	G51
	Y402				L117	F52
R469	S403	Q330	E260	P189		F53
F470	F404	K333	V261	D190	R120	Q54
	K405		P263	Q192	S121	K56
L472				G193	Y122	G57
	Y409	I337	T269		L123	D58
Y475	N410	G338	Q270	M196	I124	C59
T476	M411		V271	M197	D125	
S477	S412	K342	E272	F198	T60	T60
F478	I413	L343	M273	A199	S126	R61
E479	L414	V344	L274	F201	P127	T62
E480	L415		Y275	F200		G63
	E416	Y348	P276	F201	Y130	F64
L481	H417	Y349		A202	N131	
T482	G418	Q350	L279	Q203	V132	E67
A483	L419	H351	P280	H204	H133	N68
K484	T420	L352	E281	F205	C69	
Q485	Q421	S353	N282	T206	G135	T70
E486	F422	G354	L283	Q207	V136	T71
M487	V423	Y355	Q284	Q208	K137	P72
A488	E424	H356	F285	F209	S138	E73
E489	S425	F357	A286	F210		F74
E490	F426	K358	L286	K211	F142	T76
L491	T427	L359	V287	T212		
K492	R428	K360	Q289	H214	S146	K79
A493	Q429	F361	E290	R215	Y147	
L494	L430	D362	V291	K216	T149	L82
E495	A431	P363	F292	R216	R150	K83
S496	G432	E364	G293	G219	A151	P84
D497	R433	V434	L294	F220	L152	T85
	A435	F367	V295	T221	P153	P86
V500	G436	N368	P296	R222	P154	N87
	G437	Q369	L298		V155	T88
Y504	P505		G297	V228	A156	V89
A506	R438	R376	M299	D229	D157	H90
L507	N439	L377	K300	L230	D158	Y91
L508	V440	A378	Y301	N231	C159	I92
V509	P441	S379	A302	H232	P160	L93
E510	L442	E380	T303	L233		T94
K511	A443	F381	I304	G234	G164	H95
P512	N444	N382	V305	E235	V165	F96
R513	Q445	T383	L306	E236		K97
E514	A446	L284	P307		V168	C98



• Molecule 1: CYCLOOXYGENASE-2

Chain D: 33% 49% 12% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	180.46 Å 134.42 Å 119.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	74.3 (8.00-3.00) 86.0 (20.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.98 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.321 , 0.308 0.254 , 0.253	Depositor DCC
R_{free} test set	5077 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18232	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1137e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.73	0/4600	0.87	4/6237 (0.1%)
1	B	0.73	0/4600	0.88	4/6237 (0.1%)
1	C	0.71	0/4600	0.87	3/6237 (0.0%)
1	D	0.72	0/4600	0.88	4/6237 (0.1%)
All	All	0.72	0/18400	0.87	15/24948 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	TYR	N-CA-C	6.18	127.69	111.00
1	A	355	TYR	N-CA-C	5.84	126.78	111.00
1	B	355	TYR	N-CA-C	5.79	126.65	111.00
1	D	355	TYR	N-CA-C	5.77	126.58	111.00
1	A	281	GLU	N-CA-C	-5.64	95.78	111.00
1	A	148	TYR	N-CA-C	-5.62	95.83	111.00
1	D	148	TYR	N-CA-C	-5.60	95.88	111.00
1	B	287	VAL	N-CA-C	5.58	126.08	111.00
1	B	148	TYR	N-CA-C	-5.50	96.15	111.00
1	C	281	GLU	N-CA-C	-5.43	96.34	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	VAL	N-CA-C	5.42	125.63	111.00
1	A	287	VAL	N-CA-C	5.34	125.42	111.00
1	B	281	GLU	N-CA-C	-5.30	96.68	111.00
1	C	287	VAL	N-CA-C	5.17	124.97	111.00
1	D	573	LYS	N-CA-C	5.09	124.76	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	262	TYR	Sidechain
1	B	301	TYR	Sidechain
1	D	301	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4473	0	4374	353	0
1	B	4473	0	4375	341	0
1	C	4473	0	4374	343	0
1	D	4473	0	4374	386	0
2	A	42	0	39	0	0
2	B	42	0	39	1	0
2	C	42	0	39	3	0
2	D	42	0	39	5	0
3	A	43	0	30	1	0
3	B	43	0	30	2	0
3	C	43	0	30	2	0
3	D	43	0	30	2	0
All	All	18232	0	17773	1388	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 39.

All (1388) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:HG2	1:B:52:PHE:H	1.23	1.00
1:C:322:GLU:HG2	1:D:52:PHE:H	1.29	0.94
1:C:52:PHE:H	1:D:322:GLU:HG2	1.32	0.91
1:A:52:PHE:H	1:B:322:GLU:HG2	1.35	0.90
1:D:189:PRO:HB2	1:D:430:ILE:HD13	1.54	0.90
1:B:189:PRO:HB2	1:B:430:ILE:HD13	1.55	0.88
1:B:273:MET:SD	1:B:290:GLU:HA	2.14	0.88
1:B:85:THR:HG22	1:B:88:THR:OG1	1.75	0.87
1:A:322:GLU:HG2	1:B:52:PHE:N	1.88	0.87
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.56	0.86
1:C:189:PRO:HB2	1:C:430:ILE:HD13	1.58	0.86
1:C:478:PHE:HE2	1:C:495:TYR:HB2	1.39	0.85
1:B:478:PHE:HE2	1:B:495:TYR:HB2	1.38	0.85
1:C:283:LEU:HD13	1:C:411:ASN:ND2	1.90	0.85
1:A:478:PHE:HE2	1:A:495:TYR:HB2	1.40	0.85
1:B:283:LEU:HD13	1:B:411:ASN:HD21	1.42	0.84
1:A:85:THR:HG22	1:A:88:THR:OG1	1.78	0.84
1:D:85:THR:HG22	1:D:88:THR:OG1	1.78	0.83
1:A:189:PRO:HB2	1:A:430:ILE:HD13	1.59	0.83
1:D:251:LYS:HG2	1:D:310:GLN:HG3	1.60	0.83
1:B:251:LYS:HG2	1:B:310:GLN:HG3	1.59	0.83
1:D:478:PHE:HE2	1:D:495:TYR:HB2	1.43	0.82
1:C:146:SER:OG	2:C:671:NAG:H82	1.79	0.82
1:D:342:LYS:HG2	1:D:562:ALA:HB3	1.61	0.82
1:B:398:GLU:O	1:B:399:ASP:HB2	1.81	0.81
1:D:479:GLU:HG2	1:D:485:LYS:HE3	1.63	0.81
1:D:156:ALA:HB3	1:D:159:CYS:SG	2.20	0.81
1:C:283:LEU:HD13	1:C:411:ASN:HD21	1.45	0.81
1:B:269:THR:OG1	1:B:271:VAL:HG13	1.80	0.80
1:A:52:PHE:N	1:B:322:GLU:HG2	1.96	0.80
1:C:388:HIS:CE1	1:C:447:VAL:HG11	2.15	0.80
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.17	0.80
1:C:85:THR:HG22	1:C:88:THR:OG1	1.81	0.80
1:C:322:GLU:HG2	1:D:52:PHE:N	1.97	0.80
1:C:88:THR:HG22	1:C:92:ILE:HD11	1.64	0.80
1:C:53:ASP:HB2	1:C:54:GLN:OE1	1.82	0.79
1:B:211:LYS:HZ1	1:B:236:GLU:HG3	1.48	0.79
1:C:273:MET:SD	1:C:290:GLU:HA	2.23	0.79
1:B:281:GLU:HA	1:B:284:GLN:HG3	1.65	0.78
1:C:191:PRO:HD2	1:C:433:ARG:HG3	1.63	0.78
1:B:478:PHE:CE2	1:B:495:TYR:HB2	2.18	0.78
1:D:75:LEU:HG	1:D:79:LYS:HE2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:ASP:HB3	1:C:400:GLN:HE21	1.48	0.78
1:A:283:LEU:HD13	1:A:411:ASN:ND2	1.99	0.78
1:A:75:LEU:HG	1:A:79:LYS:HE2	1.65	0.77
1:B:342:LYS:HG2	1:B:562:ALA:HB3	1.65	0.77
1:A:478:PHE:CE2	1:A:495:TYR:HB2	2.20	0.77
1:C:434:VAL:HG23	1:C:517:ILE:HD11	1.66	0.77
1:C:478:PHE:CE2	1:C:495:TYR:HB2	2.18	0.77
1:D:434:VAL:HG23	1:D:517:ILE:HD11	1.65	0.77
1:C:398:GLU:O	1:C:399:ASP:HB2	1.84	0.76
1:A:434:VAL:HG23	1:A:517:ILE:HD11	1.65	0.76
1:B:283:LEU:HD13	1:B:411:ASN:ND2	1.99	0.76
1:A:97:LYS:HD3	1:A:356:HIS:CD2	2.21	0.76
1:C:205:PHE:CE1	1:C:344:VAL:HG21	2.20	0.76
1:A:281:GLU:HA	1:A:284:GLN:HG3	1.67	0.76
1:A:251:LYS:HG2	1:A:310:GLN:HG3	1.66	0.76
1:D:388:HIS:CE1	1:D:447:VAL:HG11	2.20	0.76
1:A:88:THR:HG22	1:A:92:ILE:HD11	1.67	0.75
1:A:205:PHE:CE1	1:A:344:VAL:HG21	2.21	0.75
1:D:273:MET:SD	1:D:290:GLU:HA	2.26	0.75
1:B:434:VAL:HG23	1:B:517:ILE:HD11	1.69	0.75
1:C:52:PHE:N	1:D:322:GLU:HG2	2.00	0.75
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.27	0.74
1:D:398:GLU:O	1:D:399:ASP:HB2	1.86	0.74
1:D:424:GLU:HA	1:D:428:ARG:NH1	2.02	0.74
1:C:479:GLU:HG2	1:C:485:LYS:HE3	1.69	0.74
1:C:75:LEU:HG	1:C:79:LYS:HE2	1.69	0.74
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.02	0.74
1:C:283:LEU:HD22	1:C:411:ASN:OD1	1.88	0.74
1:B:211:LYS:NZ	1:B:236:GLU:HG3	2.03	0.74
1:D:88:THR:HG22	1:D:92:ILE:HD11	1.70	0.74
1:A:557:LYS:HD3	1:A:560:ASN:HD22	1.53	0.73
1:C:251:LYS:HG2	1:C:310:GLN:HG3	1.69	0.73
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.24	0.73
1:A:399:ASP:HB3	1:A:400:GLN:HE21	1.52	0.73
1:D:191:PRO:HG3	1:D:433:ARG:CZ	2.19	0.72
1:B:88:THR:HG22	1:B:92:ILE:HD11	1.70	0.72
1:C:208:GLN:NE2	1:C:228:VAL:HA	2.05	0.72
1:D:245:ARG:HH12	1:D:326:GLU:HG2	1.55	0.72
1:C:108:LEU:O	1:C:112:ILE:HG12	1.89	0.72
1:A:280:PRO:O	1:A:281:GLU:HB3	1.89	0.71
1:D:211:LYS:NZ	1:D:236:GLU:HG3	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ARG:HE	1:D:438:ARG:HD3	1.55	0.71
1:B:405:LYS:H	1:B:405:LYS:HD2	1.54	0.71
1:D:478:PHE:CE2	1:D:495:TYR:HB2	2.23	0.71
1:C:479:GLU:HG2	1:C:485:LYS:CE	2.20	0.71
1:D:269:THR:OG1	1:D:271:VAL:HG13	1.91	0.71
1:B:134:TYR:HD1	1:B:136:TYR:CE1	2.09	0.71
1:A:283:LEU:HD22	1:A:411:ASN:OD1	1.90	0.71
1:A:184:ARG:HA	1:A:438:ARG:O	1.89	0.71
1:C:182:LEU:O	1:C:438:ARG:HA	1.89	0.71
1:A:211:LYS:HZ1	1:A:236:GLU:HG3	1.56	0.70
1:A:211:LYS:HE2	1:A:222:ARG:HG2	1.73	0.70
1:A:273:MET:SD	1:A:290:GLU:HA	2.31	0.70
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.26	0.70
1:B:73:GLU:O	1:B:76:THR:HB	1.91	0.70
1:A:191:PRO:HG3	1:A:433:ARG:CZ	2.22	0.70
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.73	0.70
1:D:510:GLU:O	1:D:512:PRO:HD3	1.90	0.70
1:A:548:SER:OG	1:B:58:ASP:HB2	1.91	0.70
1:D:506:ALA:O	1:D:510:GLU:HB2	1.92	0.70
1:D:281:GLU:HA	1:D:284:GLN:HE21	1.56	0.70
1:A:276:PRO:O	1:A:279:ILE:HG12	1.92	0.70
1:B:253:LYS:HE2	1:B:269:THR:HG22	1.74	0.70
1:D:97:LYS:HD3	1:D:356:HIS:CD2	2.27	0.70
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.21	0.69
1:C:211:LYS:HZ1	1:C:236:GLU:HG3	1.56	0.69
1:A:173:ASP:O	1:A:177:VAL:HG23	1.91	0.69
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.74	0.69
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.74	0.69
1:D:414:LEU:HA	1:D:422:PHE:CE2	2.26	0.69
1:C:504:TYR:HB3	1:C:505:PRO:HD3	1.72	0.69
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.22	0.69
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.33	0.69
1:A:398:GLU:O	1:A:399:ASP:HB2	1.91	0.69
1:A:283:LEU:HD13	1:A:411:ASN:HD21	1.56	0.69
1:B:75:LEU:HG	1:B:79:LYS:HE2	1.72	0.69
1:B:229:ASP:OD1	1:B:231:ASN:HB3	1.92	0.69
1:B:453:ASP:O	1:B:456:ARG:HB2	1.92	0.69
1:C:173:ASP:O	1:C:177:VAL:HG23	1.93	0.69
1:B:475:TYR:HA	1:B:480:GLU:OE2	1.93	0.69
1:C:97:LYS:HD3	1:C:356:HIS:CD2	2.28	0.69
1:B:510:GLU:O	1:B:512:PRO:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:LYS:HE2	1:C:222:ARG:HG2	1.75	0.68
1:A:578:THR:O	1:D:267:LYS:NZ	2.26	0.68
1:B:557:LYS:HD3	1:B:560:ASN:HD22	1.58	0.68
1:B:97:LYS:HD3	1:B:356:HIS:CD2	2.28	0.68
1:D:73:GLU:O	1:D:76:THR:HB	1.93	0.68
1:D:453:ASP:O	1:D:456:ARG:HB2	1.94	0.68
1:D:479:GLU:HG2	1:D:485:LYS:CE	2.23	0.68
1:B:156:ALA:HB3	1:B:159:CYS:SG	2.34	0.68
1:A:35:PRO:HB2	1:A:55:TYR:HB3	1.74	0.68
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.28	0.68
1:D:205:PHE:CE1	1:D:344:VAL:HG21	2.29	0.68
1:D:150:ARG:NH2	1:D:154:PRO:HB3	2.08	0.68
1:D:281:GLU:HA	1:D:284:GLN:HG3	1.76	0.68
1:B:509:VAL:HG12	1:B:509:VAL:O	1.93	0.68
1:C:405:LYS:HD2	1:C:405:LYS:H	1.57	0.68
1:C:454:GLN:HA	1:C:457:GLU:HG2	1.75	0.68
1:C:342:LYS:HG2	1:C:562:ALA:HB3	1.74	0.68
1:D:428:ARG:N	1:D:428:ARG:HD2	2.09	0.68
1:A:182:LEU:O	1:A:438:ARG:HA	1.94	0.67
1:A:506:ALA:O	1:A:510:GLU:HB2	1.93	0.67
1:C:184:ARG:HA	1:C:438:ARG:O	1.93	0.67
1:D:229:ASP:OD1	1:D:231:ASN:HB3	1.95	0.67
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.76	0.67
1:A:507:LEU:HD22	1:A:522:MET:CE	2.25	0.67
1:D:470:PHE:CG	1:D:525:LEU:HD22	2.29	0.67
1:D:406:GLN:HA	2:D:681:NAG:C8	2.24	0.67
1:C:211:LYS:NZ	1:C:236:GLU:HG3	2.09	0.67
1:A:73:GLU:O	1:A:76:THR:HB	1.95	0.67
1:D:208:GLN:NE2	1:D:228:VAL:HA	2.10	0.67
1:A:123:LEU:O	1:A:469:ARG:NH2	2.27	0.67
1:B:184:ARG:HA	1:B:438:ARG:O	1.93	0.67
1:A:510:GLU:O	1:A:512:PRO:HD3	1.95	0.67
1:C:507:LEU:HD22	1:C:522:MET:CE	2.25	0.67
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.29	0.66
1:D:280:PRO:CG	1:D:283:LEU:HD12	2.25	0.66
1:A:281:GLU:O	1:A:283:LEU:N	2.28	0.66
1:C:470:PHE:CG	1:C:525:LEU:HD22	2.31	0.66
1:A:509:VAL:O	1:A:509:VAL:HG12	1.96	0.66
1:C:360:LYS:HE2	1:C:362:ASP:HB2	1.78	0.66
1:D:185:ARG:HH21	1:D:438:ARG:HE	1.44	0.66
1:D:427:THR:HB	1:D:428:ARG:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:GLU:O	1:C:512:PRO:HD3	1.96	0.66
1:D:108:LEU:O	1:D:112:ILE:HG12	1.96	0.66
1:D:405:LYS:HD2	1:D:405:LYS:H	1.61	0.65
1:D:283:LEU:HD13	1:D:411:ASN:ND2	2.10	0.65
1:C:398:GLU:HB2	1:C:425:SER:OG	1.95	0.65
1:D:35:PRO:HB2	1:D:55:TYR:HB3	1.79	0.65
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.32	0.65
1:D:206:THR:HG21	1:D:385:TYR:CE1	2.31	0.65
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.11	0.65
1:D:454:GLN:HA	1:D:457:GLU:HG2	1.77	0.65
1:D:434:VAL:H	1:D:517:ILE:HG13	1.62	0.65
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.32	0.65
1:A:475:TYR:HA	1:A:480:GLU:OE2	1.96	0.65
1:B:506:ALA:O	1:B:510:GLU:HB2	1.95	0.65
1:D:504:TYR:HB3	1:D:505:PRO:HD3	1.78	0.65
1:C:191:PRO:HG3	1:C:433:ARG:CZ	2.27	0.64
1:C:280:PRO:O	1:C:281:GLU:HB3	1.97	0.64
1:D:283:LEU:HD13	1:D:411:ASN:HD21	1.62	0.64
1:B:211:LYS:HZ1	1:B:236:GLU:CG	2.08	0.64
1:C:123:LEU:O	1:C:469:ARG:NH2	2.31	0.64
1:D:253:LYS:HE2	1:D:269:THR:HG22	1.79	0.64
1:C:35:PRO:HB2	1:C:55:TYR:HB3	1.77	0.64
1:D:281:GLU:O	1:D:283:LEU:N	2.31	0.64
1:A:134:TYR:HD1	1:A:136:TYR:CE1	2.15	0.64
1:C:206:THR:HG21	1:C:385:TYR:CE1	2.32	0.64
1:B:414:LEU:HA	1:B:422:PHE:CE2	2.33	0.64
1:C:73:GLU:O	1:C:76:THR:HB	1.96	0.64
1:C:183:LEU:O	1:C:438:ARG:HB3	1.98	0.64
1:D:134:TYR:HD1	1:D:136:TYR:CE1	2.15	0.64
1:C:355:TYR:O	1:C:356:HIS:HB2	1.96	0.64
1:A:229:ASP:OD1	1:A:231:ASN:HB3	1.97	0.64
1:B:281:GLU:O	1:B:283:LEU:N	2.30	0.64
1:D:211:LYS:HZ1	1:D:236:GLU:HG3	1.63	0.64
1:D:280:PRO:O	1:D:281:GLU:HB3	1.97	0.64
1:B:479:GLU:HG2	1:B:485:LYS:HE3	1.79	0.64
1:D:173:ASP:O	1:D:177:VAL:HG23	1.97	0.64
1:B:205:PHE:CE1	1:B:344:VAL:HG21	2.33	0.63
1:D:355:TYR:O	1:D:356:HIS:HB2	1.97	0.63
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.33	0.63
1:B:454:GLN:HA	1:B:457:GLU:HG2	1.79	0.63
1:C:405:LYS:H	1:C:405:LYS:CD	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HE2	1:A:269:THR:HG22	1.80	0.63
1:B:557:LYS:HA	1:B:560:ASN:HB2	1.80	0.63
1:C:477:SER:HB2	1:C:479:GLU:OE1	1.98	0.63
1:C:67:GLU:HB3	2:C:661:NAG:H82	1.80	0.63
1:C:230:LEU:HG	1:C:337:ILE:HG12	1.81	0.63
1:D:215:LYS:N	1:D:215:LYS:HD3	2.14	0.63
1:D:294:LEU:HD22	1:D:409:TYR:CD1	2.33	0.63
1:A:213:ASP:OD1	1:A:215:LYS:HG2	1.97	0.63
1:C:197:MET:HE3	1:C:197:MET:HA	1.79	0.63
1:B:342:LYS:CG	1:B:562:ALA:HB3	2.29	0.62
1:B:108:LEU:O	1:B:112:ILE:HG12	1.97	0.62
1:B:482:THR:OG1	1:B:488:ALA:HB2	2.00	0.62
1:D:67:GLU:HB3	2:D:661:NAG:H82	1.82	0.62
1:A:35:PRO:HD3	1:A:52:PHE:O	1.98	0.62
1:B:184:ARG:HB2	1:B:439:ASN:HA	1.82	0.62
1:A:178:LEU:HA	1:A:182:LEU:HD12	1.81	0.62
1:A:398:GLU:HB2	1:A:425:SER:OG	1.99	0.62
1:A:479:GLU:HG2	1:A:485:LYS:HE3	1.80	0.62
1:C:134:TYR:HD1	1:C:136:TYR:CE1	2.16	0.62
1:D:123:LEU:O	1:D:469:ARG:NH2	2.31	0.62
1:A:108:LEU:O	1:A:112:ILE:HG12	1.99	0.62
1:A:150:ARG:NH2	1:A:458:MET:O	2.33	0.62
1:D:44:ARG:HH11	1:D:44:ARG:CG	2.12	0.62
1:D:85:THR:OG1	1:D:86:PRO:HD2	2.00	0.62
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.81	0.62
1:A:355:TYR:O	1:A:356:HIS:HB2	2.00	0.62
1:A:405:LYS:HD2	1:A:405:LYS:H	1.63	0.62
1:A:454:GLN:HA	1:A:457:GLU:HG2	1.80	0.62
1:B:131:ASN:ND2	1:B:147:TYR:CD2	2.68	0.62
1:B:39:ASN:N	1:B:40:PRO:HD3	2.15	0.62
1:C:131:ASN:HA	1:C:150:ARG:HB2	1.82	0.61
1:C:58:ASP:HB2	1:D:548:SER:OG	2.00	0.61
1:B:208:GLN:NE2	1:B:228:VAL:HA	2.16	0.61
1:A:142:PHE:O	1:A:376:ARG:NH2	2.29	0.61
1:D:183:LEU:HD22	1:D:442:ILE:HG13	1.80	0.61
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.82	0.61
1:A:582:VAL:O	1:A:582:VAL:HG13	1.99	0.61
1:B:281:GLU:HA	1:B:284:GLN:HE21	1.65	0.61
1:B:190:ASP:OD1	1:B:517:ILE:HB	2.00	0.61
1:C:198:PHE:HB2	1:C:580:PHE:HB3	1.83	0.61
1:A:58:ASP:HB2	1:B:548:SER:OG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLU:HA	1:B:428:ARG:NH1	2.14	0.61
1:C:269:THR:OG1	1:C:271:VAL:HG13	2.01	0.61
1:C:453:ASP:O	1:C:456:ARG:HB2	1.99	0.61
1:D:160:PRO:HG2	1:D:165:VAL:HA	1.83	0.61
1:B:191:PRO:HG3	1:B:433:ARG:CZ	2.31	0.61
1:C:39:ASN:N	1:C:40:PRO:HD3	2.16	0.61
1:C:506:ALA:O	1:C:510:GLU:HB2	2.01	0.61
1:D:182:LEU:O	1:D:438:ARG:HA	2.00	0.61
1:A:108:LEU:O	1:A:111:LEU:HB3	2.01	0.61
1:A:477:SER:HB2	1:A:479:GLU:OE1	2.01	0.61
1:B:112:ILE:HB	1:B:357:PHE:CZ	2.36	0.61
1:A:424:GLU:HA	1:A:428:ARG:NH1	2.16	0.61
1:B:282:ASN:OD1	1:B:282:ASN:N	2.31	0.61
1:B:44:ARG:CG	1:B:44:ARG:HH11	2.14	0.61
1:C:434:VAL:H	1:C:517:ILE:HG13	1.65	0.61
1:A:434:VAL:H	1:A:517:ILE:HG13	1.66	0.60
1:C:475:TYR:HA	1:C:480:GLU:OE2	2.00	0.60
1:D:108:LEU:O	1:D:111:LEU:HB3	2.01	0.60
1:A:577:PHE:HE1	1:D:267:LYS:HD2	1.65	0.60
1:A:183:LEU:O	1:A:438:ARG:HB3	2.01	0.60
1:B:173:ASP:O	1:B:177:VAL:HG23	2.01	0.60
1:B:257:ILE:HB	1:B:262:TYR:CD2	2.36	0.60
1:C:311:ARG:O	1:C:315:ILE:HG13	2.01	0.60
1:B:398:GLU:HB2	1:B:425:SER:OG	2.00	0.60
1:B:261:VAL:O	1:B:307:ARG:NH1	2.34	0.60
1:B:355:TYR:O	1:B:356:HIS:HB2	2.02	0.60
1:C:160:PRO:HG2	1:C:165:VAL:HA	1.83	0.60
1:D:206:THR:HB	1:D:210:PHE:CD2	2.37	0.60
1:D:226:HIS:CE1	1:D:376:ARG:HD2	2.36	0.60
1:A:131:ASN:HA	1:A:150:ARG:HB2	1.82	0.60
1:A:294:LEU:O	1:A:295:VAL:HG23	2.01	0.60
1:C:190:ASP:OD1	1:C:517:ILE:HB	2.00	0.60
1:B:155:VAL:HB	1:B:459:LYS:NZ	2.15	0.60
1:C:281:GLU:O	1:C:283:LEU:N	2.35	0.60
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.82	0.60
1:B:108:LEU:O	1:B:111:LEU:HB3	2.02	0.60
1:B:123:LEU:O	1:B:469:ARG:NH2	2.34	0.60
1:C:280:PRO:CG	1:C:283:LEU:HD12	2.32	0.60
1:D:245:ARG:HD2	1:D:247:PHE:CD1	2.37	0.60
1:D:399:ASP:HB3	1:D:400:GLN:HE21	1.67	0.60
1:D:43:ASN:HB2	1:D:69:CYS:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:PRO:HG2	1:B:165:VAL:HA	1.82	0.59
1:D:232:HIS:CD2	1:D:233:ILE:HG13	2.37	0.59
1:D:475:TYR:HA	1:D:480:GLU:OE2	2.02	0.59
1:A:112:ILE:HB	1:A:357:PHE:CZ	2.37	0.59
1:C:211:LYS:HZ1	1:C:236:GLU:CG	2.15	0.59
1:C:294:LEU:HD22	1:C:409:TYR:CD1	2.36	0.59
1:D:254:TYR:HD2	1:D:310:GLN:HE21	1.50	0.59
1:C:509:VAL:HG12	1:C:509:VAL:O	2.03	0.59
1:B:35:PRO:HB2	1:B:55:TYR:HB3	1.83	0.59
1:C:150:ARG:NH2	1:C:458:MET:O	2.35	0.59
1:C:482:THR:OG1	1:C:488:ALA:HB2	2.02	0.59
1:D:39:ASN:N	1:D:40:PRO:HD3	2.17	0.59
1:A:245:ARG:HH12	1:A:326:GLU:HG2	1.67	0.59
1:A:405:LYS:CD	1:A:405:LYS:H	2.14	0.59
1:B:206:THR:HB	1:B:210:PHE:CD2	2.36	0.59
1:C:553:GLU:O	1:C:557:LYS:HE3	2.03	0.59
1:D:184:ARG:HB2	1:D:439:ASN:HA	1.83	0.59
1:D:190:ASP:OD1	1:D:517:ILE:HB	2.02	0.59
1:C:245:ARG:HH12	1:C:326:GLU:HG2	1.67	0.59
1:D:240:ARG:HH12	1:D:271:VAL:HG23	1.68	0.59
1:C:500:VAL:HG12	1:C:500:VAL:O	2.03	0.59
1:D:226:HIS:ND1	1:D:376:ARG:HD2	2.18	0.59
1:B:294:LEU:HD22	1:B:409:TYR:CD1	2.37	0.59
1:C:414:LEU:HA	1:C:422:PHE:CE1	2.38	0.59
1:C:294:LEU:O	1:C:295:VAL:HG23	2.02	0.59
1:A:191:PRO:CD	1:A:433:ARG:HG3	2.31	0.59
1:A:525:LEU:HD23	1:A:525:LEU:N	2.17	0.59
1:B:491:LEU:HD11	1:B:509:VAL:HG11	1.85	0.59
1:D:211:LYS:HZ1	1:D:236:GLU:CG	2.16	0.59
1:D:554:VAL:HG12	1:D:555:GLY:N	2.18	0.59
1:A:445:GLN:HG3	1:A:446:ALA:N	2.18	0.58
1:B:339:GLU:O	1:B:342:LYS:HB3	2.03	0.58
1:C:208:GLN:HE21	1:C:228:VAL:HA	1.64	0.58
1:C:43:ASN:ND2	1:C:64:PHE:CD2	2.72	0.58
1:D:211:LYS:HE2	1:D:222:ARG:HG2	1.85	0.58
1:D:500:VAL:O	1:D:500:VAL:HG12	2.03	0.58
1:B:434:VAL:H	1:B:517:ILE:HG13	1.67	0.58
1:B:182:LEU:O	1:B:438:ARG:HA	2.03	0.58
1:B:35:PRO:HD3	1:B:52:PHE:O	2.02	0.58
1:C:206:THR:HB	1:C:210:PHE:CD2	2.37	0.58
1:D:53:ASP:HB2	1:D:54:GLN:OE1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLU:OE1	1:C:311:ARG:HD3	2.03	0.58
1:D:178:LEU:HA	1:D:182:LEU:HD12	1.84	0.58
1:A:280:PRO:HG3	1:A:283:LEU:HD12	1.84	0.58
1:A:482:THR:OG1	1:A:488:ALA:HB2	2.03	0.58
1:B:150:ARG:NH2	1:B:154:PRO:HB3	2.19	0.58
1:C:142:PHE:O	1:C:376:ARG:NH2	2.33	0.58
1:A:282:ASN:OD1	1:A:282:ASN:N	2.36	0.58
1:C:95:HIS:O	1:C:100:TRP:HD1	1.87	0.58
1:D:104:ASN:CG	1:D:358:LYS:HE2	2.24	0.58
1:D:509:VAL:HG12	1:D:509:VAL:O	2.02	0.58
1:D:507:LEU:HD22	1:D:522:MET:CE	2.33	0.58
1:C:306:LEU:C	1:C:306:LEU:HD23	2.24	0.58
1:C:112:ILE:HB	1:C:357:PHE:CZ	2.39	0.58
1:C:507:LEU:HD22	1:C:522:MET:HE2	1.84	0.58
1:D:230:LEU:HD23	1:D:230:LEU:N	2.19	0.58
1:D:418:GLY:O	1:D:422:PHE:HB2	2.04	0.58
1:A:193:GLY:HA3	1:A:581:ASN:OD1	2.04	0.58
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.16	0.58
1:B:53:ASP:HB2	1:B:54:GLN:OE1	2.04	0.58
1:D:193:GLY:HA3	1:D:581:ASN:OD1	2.04	0.58
1:A:160:PRO:HD2	1:A:164:GLY:O	2.04	0.58
1:A:403:SER:HB2	1:A:405:LYS:HD2	1.85	0.58
1:C:43:ASN:HB2	1:C:69:CYS:O	2.04	0.58
1:B:452:ILE:O	1:B:456:ARG:HG2	2.04	0.58
1:B:107:PHE:N	1:B:107:PHE:CD1	2.72	0.58
1:B:131:ASN:HA	1:B:150:ARG:HB2	1.86	0.58
1:A:414:LEU:HA	1:A:422:PHE:CE2	2.38	0.57
1:C:283:LEU:HD22	1:C:411:ASN:CG	2.24	0.57
1:C:554:VAL:HG12	1:C:555:GLY:N	2.18	0.57
1:D:112:ILE:HB	1:D:357:PHE:CZ	2.39	0.57
1:D:445:GLN:HG3	1:D:446:ALA:N	2.19	0.57
1:B:280:PRO:O	1:B:281:GLU:HB3	2.04	0.57
1:B:280:PRO:CG	1:B:283:LEU:HD12	2.34	0.57
1:B:43:ASN:HB2	1:B:69:CYS:O	2.03	0.57
1:C:281:GLU:HG2	1:C:282:ASN:H	1.68	0.57
1:C:491:LEU:HD11	1:C:509:VAL:HG11	1.85	0.57
1:A:121:SER:O	1:A:124:ILE:HD12	2.05	0.57
1:B:192:GLN:HG3	1:B:516:ALA:HA	1.86	0.57
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.87	0.57
1:C:403:SER:HB2	1:C:405:LYS:HD2	1.87	0.57
1:D:411:ASN:CG	1:D:412:SER:N	2.56	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:THR:OG1	1:D:488:ALA:HB2	2.04	0.57
1:A:206:THR:HB	1:A:210:PHE:CD2	2.39	0.57
1:B:160:PRO:HG3	1:B:165:VAL:HG23	1.86	0.57
1:B:472:LEU:HD11	1:B:524:GLU:HB2	1.86	0.57
1:C:192:GLN:HG3	1:C:516:ALA:HA	1.86	0.57
1:D:183:LEU:O	1:D:438:ARG:HB3	2.05	0.57
1:A:95:HIS:O	1:A:100:TRP:HD1	1.87	0.57
1:C:160:PRO:HG3	1:C:165:VAL:HG23	1.87	0.57
1:C:97:LYS:HD3	1:C:356:HIS:NE2	2.19	0.57
1:D:160:PRO:HG3	1:D:165:VAL:HG23	1.86	0.57
1:D:282:ASN:OD1	1:D:282:ASN:N	2.36	0.57
1:A:107:PHE:N	1:A:107:PHE:CD1	2.73	0.57
1:A:44:ARG:CG	1:A:44:ARG:HH11	2.17	0.57
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.17	0.57
1:C:183:LEU:HD22	1:C:442:ILE:HG13	1.85	0.57
1:D:150:ARG:NH2	1:D:458:MET:O	2.37	0.57
1:B:150:ARG:NH2	1:B:458:MET:O	2.37	0.57
1:C:113:MET:O	1:C:116:VAL:HG13	2.05	0.57
1:C:445:GLN:HG3	1:C:446:ALA:N	2.18	0.57
1:A:283:LEU:HD22	1:A:411:ASN:CG	2.24	0.56
1:A:554:VAL:HG12	1:A:555:GLY:N	2.20	0.56
1:A:311:ARG:O	1:A:315:ILE:HG13	2.04	0.56
1:B:311:ARG:O	1:B:315:ILE:HG13	2.05	0.56
1:C:108:LEU:O	1:C:111:LEU:HB3	2.03	0.56
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.41	0.56
1:B:418:GLY:O	1:B:422:PHE:HB2	2.05	0.56
1:B:64:PHE:CE2	1:B:72:PRO:HB3	2.39	0.56
1:C:136:TYR:CE2	1:D:327:GLN:HG3	2.40	0.56
1:D:394:THR:HA	1:D:402:TYR:O	2.05	0.56
1:C:244:LEU:CD2	1:C:271:VAL:HG11	2.34	0.56
1:D:257:ILE:HB	1:D:262:TYR:CD2	2.40	0.56
1:D:283:LEU:HD22	1:D:411:ASN:OD1	2.06	0.56
1:A:178:LEU:O	1:A:182:LEU:HB2	2.05	0.56
1:A:172:PRO:HG2	1:A:495:TYR:CE1	2.41	0.56
1:B:183:LEU:HD22	1:B:442:ILE:HG13	1.87	0.56
1:B:500:VAL:HG12	1:B:500:VAL:O	2.05	0.56
1:C:548:SER:OG	1:D:58:ASP:HB2	2.06	0.56
1:D:198:PHE:HD1	1:D:199:ALA:N	2.03	0.56
1:D:308:GLU:OE1	1:D:311:ARG:HD3	2.05	0.56
1:B:245:ARG:HH12	1:B:326:GLU:HG2	1.69	0.56
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:THR:HG22	1:C:307:ARG:HD2	1.88	0.56
1:C:582:VAL:O	1:C:582:VAL:HG13	2.05	0.56
1:D:261:VAL:O	1:D:307:ARG:NH1	2.39	0.56
1:D:192:GLN:HG3	1:D:516:ALA:HA	1.87	0.56
1:A:39:ASN:N	1:A:40:PRO:HD3	2.20	0.56
1:C:184:ARG:HB2	1:C:439:ASN:HA	1.87	0.56
1:C:452:ILE:O	1:C:456:ARG:HG2	2.06	0.56
1:D:184:ARG:HA	1:D:438:ARG:O	2.04	0.56
1:D:279:ILE:HG22	1:D:280:PRO:HD2	1.87	0.56
1:D:436:GLY:HA2	1:D:512:PRO:HD3	1.88	0.56
1:B:428:ARG:HD2	1:B:428:ARG:N	2.21	0.56
1:D:191:PRO:HG3	1:D:433:ARG:NH2	2.21	0.56
1:D:208:GLN:HE21	1:D:228:VAL:HA	1.71	0.56
1:D:397:ILE:HG22	1:D:417:HIS:CD2	2.41	0.56
1:D:85:THR:HG23	1:D:88:THR:H	1.70	0.56
1:A:507:LEU:HD22	1:A:522:MET:HE2	1.87	0.56
1:B:428:ARG:HA	1:B:582:VAL:HG23	1.88	0.56
1:C:178:LEU:HA	1:C:182:LEU:HD12	1.86	0.56
1:C:411:ASN:CG	1:C:412:SER:N	2.59	0.56
1:C:35:PRO:HD3	1:C:52:PHE:O	2.06	0.56
1:D:131:ASN:HA	1:D:150:ARG:HB2	1.88	0.56
1:D:557:LYS:HD3	1:D:560:ASN:HD22	1.71	0.56
1:D:582:VAL:HG13	1:D:582:VAL:O	2.05	0.56
1:A:404:PHE:H	1:A:405:LYS:HZ2	1.54	0.55
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.88	0.55
1:A:352:LEU:HD11	1:A:518:PHE:CE2	2.42	0.55
1:B:39:ASN:N	1:B:39:ASN:HD22	2.04	0.55
1:D:180:LYS:HD3	1:D:490:GLU:CD	2.26	0.55
1:D:306:LEU:HD23	1:D:306:LEU:C	2.27	0.55
1:D:107:PHE:CD1	1:D:107:PHE:N	2.75	0.55
1:A:418:GLY:O	1:A:422:PHE:HB2	2.06	0.55
1:B:494:LEU:HD12	1:B:494:LEU:H	1.71	0.55
1:C:232:HIS:CD2	1:C:233:ILE:HG13	2.41	0.55
1:D:210:PHE:CE1	1:D:382:ASN:HA	2.41	0.55
1:B:85:THR:HG23	1:B:88:THR:H	1.71	0.55
1:C:229:ASP:OD1	1:C:231:ASN:HB3	2.07	0.55
1:C:203:GLN:HE22	3:C:682:HEM:HBB2	1.72	0.55
1:B:33:ALA:N	1:B:158:ASP:O	2.40	0.55
1:B:178:LEU:HA	1:B:182:LEU:HD12	1.89	0.55
1:D:279:ILE:CG2	1:D:280:PRO:HD2	2.36	0.55
1:D:406:GLN:HA	2:D:681:NAG:H82	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:PRO:HD3	1:D:52:PHE:O	2.07	0.55
1:A:500:VAL:HG12	1:A:500:VAL:O	2.05	0.55
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.71	0.55
1:B:554:VAL:HG12	1:B:555:GLY:N	2.21	0.55
1:C:276:PRO:HG2	1:C:409:TYR:CD2	2.42	0.55
1:D:230:LEU:HD23	1:D:230:LEU:H	1.71	0.55
1:D:91:TYR:O	1:D:95:HIS:HD2	1.90	0.55
1:C:197:MET:HA	1:C:197:MET:CE	2.37	0.55
1:A:168:ASN:CG	1:A:169:LYS:N	2.60	0.55
1:A:411:ASN:CG	1:A:412:SER:N	2.60	0.55
1:B:35:PRO:HG3	1:B:54:GLN:O	2.06	0.55
1:B:397:ILE:HG22	1:B:417:HIS:CD2	2.41	0.55
1:B:198:PHE:HD1	1:B:199:ALA:N	2.05	0.55
1:C:420:THR:HG22	1:C:576:PRO:HG3	1.89	0.55
1:A:137:LYS:O	1:A:138:SER:O	2.25	0.54
1:B:211:LYS:HE2	1:B:222:ARG:HG2	1.87	0.54
1:D:303:THR:HG22	1:D:307:ARG:HD2	1.88	0.54
1:D:472:LEU:HD11	1:D:524:GLU:HB2	1.89	0.54
1:A:160:PRO:HG3	1:A:165:VAL:HG23	1.88	0.54
1:A:261:VAL:O	1:A:307:ARG:NH1	2.40	0.54
1:A:97:LYS:HB2	1:A:356:HIS:CE1	2.42	0.54
1:B:306:LEU:C	1:B:306:LEU:HD23	2.27	0.54
1:B:582:VAL:HG13	1:B:582:VAL:O	2.07	0.54
1:C:244:LEU:HD21	1:C:271:VAL:HG11	1.89	0.54
1:D:424:GLU:HA	1:D:428:ARG:HH11	1.72	0.54
1:A:252:LEU:O	1:A:310:GLN:NE2	2.40	0.54
1:C:479:GLU:HG2	1:C:485:LYS:NZ	2.22	0.54
1:D:444:VAL:HG12	1:D:444:VAL:O	2.08	0.54
1:D:494:LEU:H	1:D:494:LEU:HD12	1.72	0.54
1:B:427:THR:HB	1:B:428:ARG:HD2	1.90	0.54
1:C:85:THR:HG23	1:C:88:THR:H	1.71	0.54
1:D:398:GLU:H	1:D:425:SER:HB3	1.72	0.54
1:C:121:SER:O	1:C:124:ILE:HD12	2.08	0.54
1:D:294:LEU:O	1:D:295:VAL:HG23	2.08	0.54
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.08	0.54
1:A:303:THR:HG22	1:A:307:ARG:HD2	1.90	0.54
1:A:436:GLY:HA2	1:A:512:PRO:HD3	1.89	0.54
1:A:427:THR:HG22	1:A:583:GLN:HE22	1.73	0.54
1:B:381:PHE:HD1	1:B:529:PHE:HD2	1.55	0.54
1:B:95:HIS:O	1:B:100:TRP:HD1	1.91	0.54
1:C:525:LEU:N	1:C:525:LEU:HD23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:CYS:N	1:C:576:PRO:HD3	2.22	0.54
1:B:320:HIS:HE1	1:B:551:GLY:O	1.90	0.54
1:C:436:GLY:HA2	1:C:512:PRO:HD3	1.90	0.54
1:D:131:ASN:ND2	1:D:147:TYR:CD2	2.75	0.54
1:D:507:LEU:HD22	1:D:522:MET:HE2	1.89	0.54
1:B:303:THR:HG22	1:B:307:ARG:HD2	1.90	0.54
1:B:190:ASP:O	1:B:430:ILE:HD11	2.08	0.54
1:B:406:GLN:HG2	2:B:681:NAG:O7	2.07	0.54
1:C:479:GLU:HA	1:C:488:ALA:HB1	1.90	0.54
1:D:575:CYS:N	1:D:576:PRO:HD3	2.22	0.54
1:D:90:HIS:HD2	1:D:513:ARG:NH1	2.05	0.54
1:A:394:THR:HA	1:A:402:TYR:O	2.07	0.54
1:A:575:CYS:N	1:A:576:PRO:HD3	2.23	0.54
1:C:276:PRO:O	1:C:279:ILE:HG12	2.07	0.54
1:D:155:VAL:HB	1:D:459:LYS:NZ	2.23	0.54
1:D:405:LYS:CD	1:D:405:LYS:H	2.19	0.54
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.43	0.53
1:B:232:HIS:CD2	1:B:233:ILE:HG13	2.43	0.53
1:B:308:GLU:OE1	1:B:311:ARG:HD3	2.08	0.53
1:B:436:GLY:HA2	1:B:512:PRO:HD3	1.89	0.53
1:C:402:TYR:OH	1:C:417:HIS:HE1	1.91	0.53
1:A:208:GLN:HE21	1:A:228:VAL:HA	1.73	0.53
1:B:479:GLU:HG3	1:B:488:ALA:HB1	1.91	0.53
1:B:85:THR:OG1	1:B:86:PRO:HD2	2.08	0.53
1:D:281:GLU:HG2	1:D:282:ASN:H	1.73	0.53
1:D:491:LEU:HD11	1:D:509:VAL:HG11	1.90	0.53
1:B:403:SER:HB2	1:B:405:LYS:HD2	1.90	0.53
1:B:479:GLU:HA	1:B:488:ALA:HB1	1.91	0.53
1:C:85:THR:OG1	1:C:86:PRO:HD2	2.08	0.53
1:A:90:HIS:HD2	1:A:513:ARG:NH1	2.07	0.53
1:C:364:GLU:HG2	1:C:367:PHE:CE2	2.44	0.53
1:B:507:LEU:HD22	1:B:522:MET:CE	2.38	0.53
1:C:107:PHE:CD1	1:C:107:PHE:N	2.77	0.53
1:D:142:PHE:O	1:D:376:ARG:NH2	2.37	0.53
1:D:33:ALA:N	1:D:158:ASP:O	2.41	0.53
1:A:192:GLN:HG3	1:A:516:ALA:HA	1.90	0.53
1:A:39:ASN:HD22	1:A:39:ASN:N	2.07	0.53
1:D:95:HIS:O	1:D:100:TRP:HD1	1.91	0.53
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.43	0.53
1:A:43:ASN:HB2	1:A:69:CYS:O	2.08	0.53
1:D:320:HIS:HE1	1:D:551:GLY:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:THR:HG23	1:A:88:THR:H	1.74	0.53
1:B:412:SER:O	1:B:416:GLU:N	2.42	0.53
1:B:74:PHE:O	1:B:77:ARG:HB2	2.09	0.53
1:A:453:ASP:O	1:A:456:ARG:HB2	2.08	0.52
1:A:494:LEU:H	1:A:494:LEU:HD12	1.74	0.52
1:B:281:GLU:HG2	1:B:282:ASN:H	1.73	0.52
1:C:127:PRO:HD2	1:D:543:GLN:HE22	1.75	0.52
1:C:39:ASN:N	1:C:39:ASN:HD22	2.07	0.52
1:A:444:VAL:HG12	1:A:444:VAL:O	2.09	0.52
1:A:88:THR:O	1:A:92:ILE:HG13	2.09	0.52
1:B:121:SER:O	1:B:124:ILE:HD12	2.09	0.52
1:B:172:PRO:HG2	1:B:495:TYR:CE1	2.44	0.52
1:C:418:GLY:O	1:C:422:PHE:HB2	2.09	0.52
1:D:109:ARG:HG3	1:D:357:PHE:CE1	2.45	0.52
1:D:557:LYS:HA	1:D:560:ASN:HB2	1.90	0.52
1:A:306:LEU:HD23	1:A:306:LEU:C	2.30	0.52
1:A:510:GLU:HG2	1:A:511:LYS:N	2.23	0.52
1:A:198:PHE:HB2	1:A:580:PHE:HB3	1.91	0.52
1:B:120:ARG:HG2	1:B:531:LEU:HD12	1.90	0.52
1:C:150:ARG:NH2	1:C:154:PRO:HB3	2.24	0.52
1:C:404:PHE:HE2	1:C:444:VAL:HG23	1.74	0.52
1:D:190:ASP:O	1:D:430:ILE:HD11	2.09	0.52
1:D:404:PHE:HE2	1:D:444:VAL:HG23	1.75	0.52
1:D:477:SER:HB2	1:D:479:GLU:OE1	2.08	0.52
1:D:428:ARG:HA	1:D:582:VAL:HG23	1.91	0.52
1:C:190:ASP:O	1:C:430:ILE:HD11	2.09	0.52
1:D:403:SER:HB2	1:D:405:LYS:HD2	1.90	0.52
1:A:35:PRO:HG3	1:A:54:GLN:O	2.09	0.52
1:B:507:LEU:HD22	1:B:522:MET:HE2	1.92	0.52
1:A:136:TYR:CE2	1:B:327:GLN:HG3	2.44	0.52
1:A:191:PRO:HG3	1:A:433:ARG:NH1	2.24	0.52
1:C:38:SER:OG	1:C:40:PRO:HG3	2.10	0.52
1:A:114:LYS:HD3	1:A:369:GLN:NE2	2.24	0.52
1:A:320:HIS:HE1	1:A:551:GLY:O	1.93	0.52
1:C:472:LEU:HD21	1:C:524:GLU:HG3	1.91	0.52
1:C:544:TYR:OH	1:D:142:PHE:HB2	2.10	0.52
1:D:150:ARG:HG2	1:D:152:LEU:O	2.10	0.52
1:D:198:PHE:HB2	1:D:580:PHE:HB3	1.91	0.52
1:A:51:GLY:O	1:A:52:PHE:HB2	2.10	0.52
1:A:428:ARG:HA	1:A:582:VAL:HG23	1.92	0.52
1:A:203:GLN:HE22	3:A:682:HEM:HBB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:THR:HG22	1:B:576:PRO:HG3	1.92	0.52
1:C:210:PHE:CE1	1:C:382:ASN:HA	2.45	0.52
1:D:251:LYS:CG	1:D:310:GLN:HG3	2.37	0.52
1:D:574:GLY:C	1:D:576:PRO:HD3	2.31	0.52
1:A:308:GLU:OE1	1:A:311:ARG:HD3	2.09	0.52
1:A:251:LYS:CG	1:A:310:GLN:HG3	2.38	0.52
1:A:172:PRO:HG2	1:A:495:TYR:CD1	2.45	0.52
1:B:147:TYR:HE1	1:B:220:PHE:CZ	2.28	0.52
1:C:178:LEU:O	1:C:182:LEU:HB2	2.10	0.52
1:C:494:LEU:HD12	1:C:494:LEU:H	1.75	0.52
1:D:342:LYS:CG	1:D:562:ALA:HB3	2.38	0.52
1:B:226:HIS:ND1	1:B:376:ARG:HD2	2.25	0.51
1:B:575:CYS:N	1:B:576:PRO:HD3	2.24	0.51
1:B:193:GLY:HA3	1:B:581:ASN:OD1	2.11	0.51
1:A:150:ARG:NH2	1:A:154:PRO:HB3	2.26	0.51
1:A:420:THR:HG22	1:A:576:PRO:HG3	1.91	0.51
1:B:294:LEU:O	1:B:295:VAL:HG23	2.11	0.51
1:C:251:LYS:CG	1:C:310:GLN:HG3	2.37	0.51
1:C:252:LEU:O	1:C:310:GLN:NE2	2.43	0.51
1:C:557:LYS:HD3	1:C:560:ASN:HD22	1.75	0.51
1:D:113:MET:HG2	1:D:360:LYS:HB3	1.92	0.51
1:D:525:LEU:HD23	1:D:525:LEU:N	2.25	0.51
1:A:276:PRO:HG2	1:A:409:TYR:CD2	2.45	0.51
1:A:443:ALA:C	1:A:445:GLN:H	2.14	0.51
1:A:464:ASN:O	1:A:468:LYS:HG3	2.10	0.51
1:B:196:MET:CE	1:B:392:PRO:HD3	2.41	0.51
1:A:322:GLU:HB3	1:B:52:PHE:CD1	2.45	0.51
1:C:155:VAL:HB	1:C:459:LYS:NZ	2.25	0.51
1:C:412:SER:O	1:C:416:GLU:N	2.41	0.51
1:C:232:HIS:HD2	1:C:233:ILE:H	1.57	0.51
1:D:147:TYR:HE1	1:D:220:PHE:CZ	2.28	0.51
1:D:191:PRO:HG3	1:D:433:ARG:NH1	2.24	0.51
1:B:191:PRO:HD2	1:B:433:ARG:HG3	1.92	0.51
1:B:411:ASN:CG	1:B:412:SER:N	2.64	0.51
1:B:445:GLN:HG3	1:B:446:ALA:N	2.24	0.51
1:C:192:GLN:OE1	1:C:517:ILE:HG22	2.11	0.51
1:C:389:PRO:HB2	1:C:434:VAL:HA	1.93	0.51
1:A:198:PHE:HD1	1:A:199:ALA:N	2.09	0.51
1:B:48:MET:HG3	1:B:48:MET:O	2.10	0.51
1:D:178:LEU:O	1:D:182:LEU:HB2	2.11	0.51
1:D:215:LYS:CD	1:D:215:LYS:H	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:LEU:HD12	1:D:510:GLU:HG3	1.91	0.51
1:C:568:ILE:HG13	1:C:572:VAL:HG21	1.93	0.51
1:D:411:ASN:ND2	1:D:412:SER:N	2.59	0.51
1:D:482:THR:HB	1:D:484:GLU:HG3	1.91	0.51
1:D:64:PHE:CE2	1:D:72:PRO:HB3	2.46	0.51
1:D:88:THR:O	1:D:92:ILE:HG13	2.11	0.51
1:A:152:LEU:HD23	1:A:469:ARG:HG2	1.93	0.51
1:A:404:PHE:HE2	1:A:444:VAL:HG23	1.76	0.51
1:A:507:LEU:HD22	1:A:522:MET:HE3	1.92	0.51
1:C:105(A):ILE:HD12	1:C:108:LEU:HD12	1.93	0.51
1:C:68:ASN:ND2	2:C:661:NAG:O7	2.44	0.51
1:D:121:SER:O	1:D:124:ILE:HD12	2.09	0.51
1:D:213:ASP:OD1	1:D:215:LYS:HG2	2.11	0.51
1:D:424:GLU:O	1:D:428:ARG:HD3	2.10	0.51
1:A:155:VAL:HB	1:A:459:LYS:NZ	2.26	0.51
1:A:364:GLU:HG2	1:A:367:PHE:CD2	2.46	0.51
1:A:411:ASN:ND2	1:A:412:SER:N	2.59	0.51
1:A:462:SER:HB3	1:A:465:GLU:HG2	1.93	0.50
1:B:213:ASP:OD1	1:B:215:LYS:HG2	2.11	0.50
1:B:51:GLY:O	1:B:52:PHE:HB2	2.11	0.50
1:C:213:ASP:OD1	1:C:215:LYS:HG2	2.11	0.50
1:D:248:LYS:HG2	1:D:249:ASP:OD2	2.12	0.50
1:D:381:PHE:HD1	1:D:529:PHE:HD2	1.59	0.50
1:A:150:ARG:HG2	1:A:150:ARG:NH1	2.26	0.50
1:B:105:ASN:O	1:B:106:PRO:HD3	2.12	0.50
1:B:179:GLU:HA	1:B:183:LEU:HD12	1.92	0.50
1:B:510:GLU:HG2	1:B:511:LYS:N	2.26	0.50
1:C:114:LYS:HD3	1:C:369:GLN:NE2	2.27	0.50
1:C:175:LYS:O	1:C:178:LEU:HB3	2.12	0.50
1:C:193:GLY:HA3	1:C:581:ASN:OD1	2.11	0.50
1:D:388:HIS:N	1:D:389:PRO:HD2	2.26	0.50
1:C:398:GLU:H	1:C:425:SER:HB3	1.77	0.50
1:D:120:ARG:HG2	1:D:531:LEU:HD12	1.93	0.50
1:D:464:ASN:O	1:D:468:LYS:HG3	2.11	0.50
1:D:420:THR:HG22	1:D:576:PRO:HG3	1.92	0.50
1:C:387:TRP:HB2	3:C:682:HEM:CBC	2.41	0.50
1:A:150:ARG:HH11	1:A:150:ARG:CG	2.24	0.50
1:B:97:LYS:HB2	1:B:356:HIS:CE1	2.47	0.50
1:D:44:ARG:HH11	1:D:44:ARG:HG3	1.77	0.50
1:A:479:GLU:HG2	1:A:485:LYS:CE	2.42	0.50
1:B:180:LYS:HD3	1:B:490:GLU:CD	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.46	0.50
1:B:251:LYS:CG	1:B:310:GLN:HG3	2.35	0.50
1:C:261:VAL:O	1:C:307:ARG:NH1	2.45	0.50
1:B:405:LYS:H	1:B:405:LYS:CD	2.17	0.50
1:B:443:ALA:C	1:B:445:GLN:H	2.15	0.50
1:C:352:LEU:HD21	1:C:387:TRP:CH2	2.46	0.50
1:D:274:ILE:HG13	1:D:290:GLU:HB2	1.94	0.50
1:A:113:MET:O	1:A:117:LEU:HB2	2.12	0.50
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.94	0.50
1:B:281:GLU:CA	1:B:284:GLN:HG3	2.41	0.50
1:D:462:SER:HB3	1:D:465:GLU:HG2	1.93	0.50
1:A:105(A):ILE:HD12	1:A:108:LEU:HD12	1.94	0.50
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.95	0.50
1:A:564:ILE:HG12	1:A:580:PHE:CZ	2.47	0.50
1:A:82:LEU:N	1:A:82:LEU:HD12	2.26	0.50
1:A:85:THR:OG1	1:A:86:PRO:HD2	2.11	0.50
1:B:478:PHE:HD1	1:B:478:PHE:H	1.60	0.50
1:C:286:ALA:O	1:C:287:VAL:HG22	2.12	0.50
1:C:443:ALA:C	1:C:445:GLN:H	2.14	0.50
1:C:472:LEU:HD11	1:C:524:GLU:HB2	1.94	0.50
1:D:150:ARG:HH11	1:D:150:ARG:CG	2.25	0.50
1:D:452:ILE:O	1:D:456:ARG:HG2	2.11	0.50
1:D:153:PRO:O	1:D:461:GLN:NE2	2.45	0.50
1:A:179:GLU:HA	1:A:183:LEU:HD12	1.94	0.49
1:A:172:PRO:HG2	1:A:495:TYR:CZ	2.47	0.49
1:A:190:ASP:OD1	1:A:517:ILE:HB	2.12	0.49
1:C:444:VAL:HG12	1:C:444:VAL:O	2.12	0.49
1:C:88:THR:O	1:C:92:ILE:HG13	2.11	0.49
1:D:196:MET:HB3	1:D:426:PHE:CG	2.47	0.49
1:D:39:ASN:N	1:D:39:ASN:HD22	2.10	0.49
1:D:454:GLN:HA	1:D:457:GLU:CG	2.41	0.49
1:A:428:ARG:HG3	1:A:583:GLN:OE1	2.12	0.49
1:A:327:GLN:HG3	1:B:136:TYR:CE2	2.47	0.49
1:B:160:PRO:HD2	1:B:164:GLY:O	2.12	0.49
1:B:381:PHE:CD1	1:B:529:PHE:CB	2.96	0.49
1:C:282:ASN:OD1	1:C:282:ASN:N	2.44	0.49
1:C:428:ARG:HD2	1:C:428:ARG:N	2.26	0.49
1:D:208:GLN:OE1	1:D:232:HIS:CE1	2.64	0.49
1:B:197:MET:CE	1:B:197:MET:HA	2.42	0.49
1:B:82:LEU:HD12	1:B:82:LEU:N	2.28	0.49
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:HIS:HD2	1:C:513:ARG:NH1	2.11	0.49
1:D:210:PHE:HB3	1:D:382:ASN:ND2	2.27	0.49
1:A:553:GLU:O	1:A:557:LYS:HE3	2.12	0.49
1:B:230:LEU:N	1:B:230:LEU:HD23	2.28	0.49
1:B:104:ASN:CG	1:B:358:LYS:HE2	2.33	0.49
1:B:196:MET:HB3	1:B:426:PHE:CG	2.48	0.49
1:C:120:ARG:HG2	1:C:531:LEU:HD12	1.94	0.49
1:D:43:ASN:ND2	1:D:64:PHE:CD2	2.80	0.49
1:A:281:GLU:C	1:A:283:LEU:H	2.15	0.49
1:B:172:PRO:HG2	1:B:495:TYR:CD1	2.47	0.49
1:C:481:LEU:HD12	1:C:510:GLU:HG3	1.93	0.49
1:D:395:PHE:CD2	1:D:407:PHE:CD2	3.01	0.49
1:D:411:ASN:ND2	1:D:412:SER:H	2.10	0.49
1:B:388:HIS:N	1:B:389:PRO:HD2	2.26	0.49
1:C:180:LYS:HD3	1:C:490:GLU:CD	2.33	0.49
1:D:276:PRO:O	1:D:279:ILE:HG12	2.12	0.49
1:D:276:PRO:HG2	1:D:409:TYR:CD2	2.48	0.49
1:D:151:ALA:O	1:D:469:ARG:NH1	2.46	0.49
1:B:234:TYR:HH	1:B:309:HIS:CE1	2.29	0.49
1:D:44:ARG:NH1	1:D:44:ARG:CG	2.75	0.49
1:B:263:PRO:HD3	1:B:303:THR:HG23	1.94	0.49
1:D:350:GLN:HE22	1:D:358:LYS:HA	1.77	0.49
1:A:148:TYR:HD2	1:A:219:GLY:C	2.15	0.49
1:B:287:VAL:HG23	1:B:288:GLY:N	2.28	0.49
1:C:150:ARG:CG	1:C:150:ARG:HH11	2.26	0.49
1:C:151:ALA:O	1:C:469:ARG:NH1	2.45	0.49
1:C:254:TYR:HD2	1:C:310:GLN:HE21	1.61	0.49
1:D:352:LEU:HD21	1:D:387:TRP:CH2	2.47	0.49
1:A:109:ARG:HG3	1:A:357:PHE:CE1	2.47	0.49
1:B:240:ARG:HH12	1:B:271:VAL:HG23	1.77	0.49
1:B:44:ARG:HG3	1:B:44:ARG:HH11	1.78	0.49
1:C:198:PHE:HD1	1:C:199:ALA:N	2.11	0.49
1:D:198:PHE:CD1	1:D:199:ALA:N	2.81	0.49
1:A:423:VAL:HG13	1:A:578:THR:HG23	1.95	0.48
1:B:396:ASN:HD22	1:B:401:GLU:HA	1.77	0.48
1:B:444:VAL:HG12	1:B:444:VAL:O	2.12	0.48
1:B:522:MET:HG3	1:B:522:MET:O	2.13	0.48
1:A:183:LEU:HD22	1:A:442:ILE:HG13	1.95	0.48
1:B:208:GLN:OE1	1:B:232:HIS:CE1	2.67	0.48
1:B:479:GLU:HA	1:B:488:ALA:CB	2.43	0.48
1:C:557:LYS:HA	1:C:560:ASN:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:LEU:HD23	1:D:469:ARG:HG2	1.94	0.48
1:D:198:PHE:C	1:D:198:PHE:CD1	2.86	0.48
1:D:201:PHE:HA	1:D:301:TYR:CE2	2.48	0.48
1:D:254:TYR:CD1	1:D:254:TYR:C	2.87	0.48
1:B:398:GLU:H	1:B:425:SER:HB3	1.78	0.48
1:B:183:LEU:O	1:B:438:ARG:HB3	2.13	0.48
1:C:198:PHE:CD1	1:C:198:PHE:C	2.87	0.48
1:D:113:MET:O	1:D:116:VAL:HG13	2.13	0.48
1:D:197:MET:HA	1:D:197:MET:HE3	1.94	0.48
1:D:281:GLU:CA	1:D:284:GLN:HE21	2.25	0.48
1:D:202:ALA:HB2	1:D:348:TYR:CE2	2.49	0.48
1:D:196:MET:HE1	1:D:392:PRO:HD3	1.95	0.48
1:A:472:LEU:HD11	1:A:524:GLU:HB2	1.95	0.48
1:D:105:ASN:O	1:D:106:PRO:HD3	2.13	0.48
1:D:215:LYS:HD3	1:D:215:LYS:H	1.75	0.48
1:D:172:PRO:HG2	1:D:495:TYR:CD2	2.48	0.48
1:D:97:LYS:HB2	1:D:356:HIS:CE1	2.49	0.48
1:B:113:MET:O	1:B:116:VAL:HG13	2.12	0.48
1:B:479:GLU:HG2	1:B:485:LYS:NZ	2.28	0.48
1:C:152:LEU:HD23	1:C:469:ARG:HG2	1.93	0.48
1:C:182:LEU:HD22	1:C:508:LEU:HD12	1.95	0.48
1:C:383:THR:HG22	1:C:384:LEU:N	2.28	0.48
1:D:568:ILE:HG13	1:D:572:VAL:HG21	1.95	0.48
1:A:64:PHE:CE2	1:A:72:PRO:HB3	2.49	0.48
1:A:83:LYS:NZ	1:A:83:LYS:HA	2.28	0.48
1:D:351:HIS:O	1:D:353:SER:N	2.47	0.48
1:A:263:PRO:HD3	1:A:303:THR:HG23	1.94	0.48
1:B:201:PHE:HA	1:B:301:TYR:CE2	2.48	0.48
1:B:317:LYS:O	1:B:317:LYS:HG2	2.12	0.48
1:C:179:GLU:HA	1:C:183:LEU:HD12	1.95	0.48
1:C:330:GLN:HB3	1:D:138:SER:HB2	1.96	0.48
1:C:564:ILE:HG12	1:C:580:PHE:CZ	2.49	0.48
1:D:564:ILE:HG12	1:D:580:PHE:CZ	2.49	0.48
1:B:462:SER:HB3	1:B:465:GLU:HG2	1.96	0.48
1:B:151:ALA:O	1:B:469:ARG:NH1	2.47	0.48
1:B:525:LEU:N	1:B:525:LEU:HD23	2.28	0.48
1:D:35:PRO:HG3	1:D:54:GLN:O	2.13	0.48
1:D:398:GLU:HB2	1:D:425:SER:OG	2.13	0.48
1:A:134:TYR:CD1	1:A:136:TYR:CE1	3.00	0.48
1:A:479:GLU:HA	1:A:488:ALA:HB1	1.96	0.48
1:A:568:ILE:HG13	1:A:572:VAL:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PRO:O	1:B:461:GLN:NE2	2.47	0.48
1:B:88:THR:O	1:B:92:ILE:HG13	2.14	0.48
1:C:172:PRO:HG2	1:C:495:TYR:CE2	2.48	0.48
1:D:564:ILE:HG12	1:D:580:PHE:CE1	2.49	0.48
1:A:457:GLU:C	1:A:459:LYS:H	2.17	0.48
1:B:442:ILE:O	1:B:445:GLN:HG2	2.13	0.48
1:C:507:LEU:HD22	1:C:522:MET:HE3	1.95	0.48
1:C:569:CYS:HA	1:C:575:CYS:HA	1.96	0.48
1:B:198:PHE:C	1:B:198:PHE:CD1	2.88	0.47
1:B:381:PHE:CD1	1:B:529:PHE:HB3	2.49	0.47
1:C:428:ARG:HA	1:C:582:VAL:HG23	1.96	0.47
1:A:194:SER:OG	1:A:351:HIS:HE1	1.96	0.47
1:A:257:ILE:HB	1:A:262:TYR:CD2	2.48	0.47
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.96	0.47
1:C:394:THR:HA	1:C:402:TYR:O	2.14	0.47
1:C:578:THR:O	1:C:579:SER:HB2	2.14	0.47
1:D:147:TYR:CE1	1:D:220:PHE:CE1	3.02	0.47
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.81	0.47
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.96	0.47
1:C:402:TYR:OH	1:C:417:HIS:CE1	2.67	0.47
1:D:197:MET:HA	1:D:197:MET:CE	2.45	0.47
1:D:339:GLU:O	1:D:342:LYS:HB3	2.14	0.47
1:D:479:GLU:HA	1:D:488:ALA:HB1	1.96	0.47
1:A:113:MET:O	1:A:116:VAL:HG13	2.14	0.47
1:A:209:PHE:O	1:A:377:ILE:HD12	2.14	0.47
1:B:404:PHE:HE2	1:B:444:VAL:HG23	1.80	0.47
1:B:44:ARG:CG	1:B:44:ARG:NH1	2.77	0.47
1:B:90:HIS:HD2	1:B:513:ARG:NH1	2.11	0.47
1:B:124:ILE:HD13	1:B:532:LYS:HG3	1.97	0.47
1:D:185:ARG:HH21	1:D:438:ARG:NE	2.11	0.47
1:A:478:PHE:H	1:A:478:PHE:HD1	1.62	0.47
1:B:202:ALA:HB2	1:B:348:TYR:CE2	2.50	0.47
1:C:352:LEU:HD11	1:C:518:PHE:CE2	2.48	0.47
1:D:381:PHE:CD1	1:D:529:PHE:HB3	2.49	0.47
1:B:198:PHE:CD1	1:B:199:ALA:N	2.81	0.47
1:B:243:LYS:O	1:B:269:THR:HB	2.14	0.47
1:C:234:TYR:CE1	1:C:252:LEU:HD21	2.49	0.47
1:C:253:LYS:HE2	1:C:269:THR:HG22	1.96	0.47
1:C:479:GLU:HA	1:C:488:ALA:CB	2.44	0.47
1:C:172:PRO:HG2	1:C:495:TYR:CD2	2.49	0.47
1:C:97:LYS:HB2	1:C:356:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:GLY:O	1:D:52:PHE:HB2	2.14	0.47
1:C:104:ASN:HB3	1:C:358:LYS:HE2	1.96	0.47
1:D:232:HIS:HD2	1:D:233:ILE:N	2.12	0.47
1:D:280:PRO:HG3	1:D:283:LEU:HD12	1.95	0.47
1:D:206:THR:HG21	1:D:385:TYR:CD1	2.49	0.47
1:D:501:MET:HE3	1:D:506:ALA:H	1.79	0.47
1:A:198:PHE:CD1	1:A:198:PHE:C	2.88	0.47
1:A:442:ILE:O	1:A:445:GLN:HG2	2.14	0.47
1:B:134:TYR:CD1	1:B:136:TYR:CE1	2.96	0.47
1:B:196:MET:HE1	1:B:392:PRO:HD3	1.96	0.47
1:B:283:LEU:HD22	1:B:411:ASN:OD1	2.14	0.47
1:C:209:PHE:O	1:C:377:ILE:HD12	2.15	0.47
1:C:230:LEU:N	1:C:230:LEU:HD23	2.29	0.47
1:B:33:ALA:HB3	1:B:158:ASP:OD2	2.14	0.47
1:B:254:TYR:HD2	1:B:310:GLN:HE21	1.63	0.47
1:B:209:PHE:O	1:B:377:ILE:HD12	2.15	0.47
1:B:482:THR:HB	1:B:484:GLU:HG3	1.96	0.47
1:C:148:TYR:HD2	1:C:219:GLY:C	2.18	0.47
1:C:281:GLU:C	1:C:283:LEU:H	2.18	0.47
1:D:96:PHE:HB3	1:D:99:VAL:CG2	2.44	0.47
1:A:175:LYS:O	1:A:178:LEU:HB3	2.15	0.47
1:A:215:LYS:HD3	1:A:215:LYS:N	2.30	0.47
1:A:280:PRO:O	1:A:281:GLU:CB	2.59	0.47
1:A:113:MET:HG2	1:A:360:LYS:HB3	1.97	0.47
1:A:482:THR:HB	1:A:484:GLU:HG3	1.96	0.47
1:B:281:GLU:C	1:B:283:LEU:H	2.16	0.47
1:B:394:THR:HA	1:B:402:TYR:O	2.14	0.47
1:B:573:LYS:HD2	1:B:573:LYS:O	2.15	0.47
1:C:249:ASP:OD1	1:C:317:LYS:HD2	2.15	0.47
1:D:124:ILE:HD13	1:D:532:LYS:HG3	1.96	0.47
1:A:88:THR:HG22	1:A:92:ILE:CD1	2.41	0.47
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.50	0.47
1:B:530:SER:O	1:B:534:LEU:HB2	2.15	0.47
1:C:390:LEU:O	1:C:431:ALA:HB1	2.15	0.47
1:D:281:GLU:C	1:D:283:LEU:H	2.18	0.47
1:A:153:PRO:O	1:A:461:GLN:NE2	2.49	0.46
1:B:201:PHE:N	1:B:301:TYR:HE2	2.13	0.46
1:C:281:GLU:HA	1:C:284:GLN:HG3	1.97	0.46
1:C:51:GLY:O	1:C:52:PHE:HB2	2.15	0.46
1:D:403:SER:OG	1:D:406:GLN:HG3	2.15	0.46
1:D:412:SER:O	1:D:416:GLU:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LYS:O	1:D:534:LEU:N	2.48	0.46
1:D:412:SER:HB2	2:D:681:NAG:H62	1.97	0.46
1:D:97:LYS:HD3	1:D:356:HIS:CG	2.51	0.46
1:C:244:LEU:O	1:C:252:LEU:HD12	2.15	0.46
1:C:257:ILE:HB	1:C:262:TYR:CD2	2.50	0.46
1:C:350:GLN:HE22	1:C:358:LYS:HA	1.81	0.46
1:A:197:MET:CE	1:A:197:MET:HA	2.45	0.46
1:C:287:VAL:HG23	1:C:288:GLY:N	2.31	0.46
1:C:88:THR:HG22	1:C:92:ILE:CD1	2.41	0.46
1:A:204:HIS:ND1	1:A:292:PHE:CE2	2.83	0.46
1:A:522:MET:HG3	1:A:522:MET:O	2.14	0.46
1:B:97:LYS:HD3	1:B:356:HIS:NE2	2.30	0.46
1:C:134:TYR:CD1	1:C:136:TYR:CE1	3.02	0.46
1:D:134:TYR:CD1	1:D:136:TYR:CE1	3.02	0.46
1:D:191:PRO:HD2	1:D:433:ARG:HG3	1.98	0.46
1:A:396:ASN:ND2	1:A:401:GLU:HG2	2.31	0.46
1:A:190:ASP:O	1:A:430:ILE:HD11	2.16	0.46
1:B:203:GLN:HE22	3:B:682:HEM:HBB2	1.80	0.46
1:D:388:HIS:N	1:D:389:PRO:CD	2.78	0.46
1:D:578:THR:O	1:D:579:SER:HB2	2.15	0.46
1:A:397:ILE:HG22	1:A:417:HIS:CD2	2.50	0.46
1:B:360:LYS:HE2	1:B:362:ASP:HB2	1.98	0.46
1:B:388:HIS:N	1:B:389:PRO:CD	2.78	0.46
1:C:150:ARG:CG	1:C:150:ARG:NH1	2.78	0.46
1:C:153:PRO:O	1:C:461:GLN:NE2	2.48	0.46
1:C:181:VAL:HB	1:C:509:VAL:HG22	1.98	0.46
1:D:333:LYS:O	1:D:337:ILE:HG13	2.16	0.46
1:D:381:PHE:CD1	1:D:529:PHE:CB	2.98	0.46
1:A:150:ARG:CG	1:A:150:ARG:NH1	2.78	0.46
1:B:350:GLN:HE22	1:B:358:LYS:HA	1.81	0.46
1:C:137:LYS:O	1:C:138:SER:O	2.33	0.46
1:C:147:TYR:HE1	1:C:220:PHE:CZ	2.33	0.46
1:C:295:VAL:HG12	1:C:295:VAL:O	2.15	0.46
1:C:104:ASN:CG	1:C:358:LYS:HE2	2.36	0.46
1:C:92:ILE:H	1:C:92:ILE:HG13	1.58	0.46
1:A:107:PHE:O	1:A:111:LEU:HB2	2.16	0.46
1:A:274:ILE:HG13	1:A:290:GLU:HB2	1.98	0.46
1:A:104:ASN:CG	1:A:358:LYS:HE2	2.36	0.46
1:A:421:GLN:HA	1:A:421:GLN:OE1	2.15	0.46
1:A:44:ARG:HH11	1:A:44:ARG:HG3	1.81	0.46
1:C:196:MET:CE	1:C:392:PRO:HD3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:HIS:HD2	1:C:233:ILE:N	2.14	0.46
1:C:33:ALA:N	1:C:158:ASP:O	2.49	0.46
1:C:475:TYR:CD1	1:C:480:GLU:HG2	2.51	0.46
1:D:276:PRO:HG2	1:D:409:TYR:CG	2.51	0.46
1:D:352:LEU:HD11	1:D:518:PHE:CE2	2.51	0.46
1:D:553:GLU:O	1:D:557:LYS:HE3	2.16	0.46
1:A:248:LYS:HB2	1:A:248:LYS:HE3	1.54	0.46
1:A:352:LEU:HD21	1:A:387:TRP:HH2	1.80	0.46
1:A:394:THR:HB	1:A:401:GLU:HB3	1.97	0.46
1:B:232:HIS:HD2	1:B:233:ILE:N	2.14	0.46
1:B:254:TYR:CD1	1:B:254:TYR:C	2.89	0.46
1:B:38:SER:OG	1:B:40:PRO:HG3	2.16	0.46
1:B:464:ASN:O	1:B:468:LYS:HG3	2.15	0.46
1:C:168:ASN:C	1:C:170:GLU:N	2.68	0.46
1:C:263:PRO:HD3	1:C:303:THR:HG23	1.97	0.46
1:C:204:HIS:ND1	1:C:292:PHE:CE2	2.83	0.46
1:C:35:PRO:HG3	1:C:54:GLN:O	2.15	0.46
1:A:83:LYS:HA	1:A:83:LYS:HZ1	1.80	0.46
1:B:232:HIS:HD2	1:B:233:ILE:H	1.64	0.46
1:D:497:ASP:HB3	1:D:500:VAL:HG23	1.98	0.46
1:A:211:LYS:HE2	1:A:222:ARG:CG	2.45	0.45
1:A:126:SER:CB	1:A:532:LYS:HZ1	2.29	0.45
1:B:280:PRO:HG2	1:B:283:LEU:HD12	1.97	0.45
1:A:92:ILE:HA	1:A:96:PHE:CE2	2.52	0.45
1:B:191:PRO:HG3	1:B:433:ARG:NH1	2.31	0.45
1:A:120:ARG:HG2	1:A:531:LEU:HD12	1.98	0.45
1:A:398:GLU:H	1:A:425:SER:HB3	1.81	0.45
1:A:452:ILE:O	1:A:456:ARG:HG2	2.15	0.45
1:B:150:ARG:HH11	1:B:150:ARG:CG	2.30	0.45
1:B:475:TYR:CD1	1:B:480:GLU:HG2	2.51	0.45
1:B:88:THR:HG22	1:B:92:ILE:CD1	2.42	0.45
1:C:295:VAL:HG12	1:C:297:GLY:H	1.81	0.45
1:C:283:LEU:CD1	1:C:411:ASN:HD21	2.23	0.45
1:C:510:GLU:HG2	1:C:511:LYS:N	2.32	0.45
1:D:114:LYS:HD3	1:D:369:GLN:NE2	2.31	0.45
1:D:232:HIS:HD2	1:D:233:ILE:H	1.62	0.45
1:D:40:PRO:HB2	1:D:55:TYR:CE2	2.51	0.45
1:A:149:THR:O	1:A:378:ALA:HA	2.17	0.45
1:A:197:MET:HA	1:A:197:MET:HE3	1.98	0.45
1:A:350:GLN:HE22	1:A:358:LYS:HA	1.81	0.45
1:B:276:PRO:HG2	1:B:409:TYR:CD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LEU:CD2	1:C:469:ARG:HG2	2.47	0.45
1:C:232:HIS:CD2	1:C:233:ILE:N	2.85	0.45
1:C:457:GLU:C	1:C:459:LYS:H	2.19	0.45
1:C:482:THR:HB	1:C:484:GLU:HG3	1.97	0.45
1:D:196:MET:CE	1:D:392:PRO:HD3	2.45	0.45
1:B:137:LYS:O	1:B:138:SER:O	2.34	0.45
1:B:178:LEU:O	1:B:182:LEU:HB2	2.17	0.45
1:D:182:LEU:HD22	1:D:508:LEU:HD12	1.98	0.45
1:D:443:ALA:C	1:D:445:GLN:H	2.20	0.45
1:A:151:ALA:O	1:A:469:ARG:NH1	2.49	0.45
1:A:92:ILE:HA	1:A:96:PHE:HE2	1.80	0.45
1:B:498:ILE:C	1:B:500:VAL:H	2.20	0.45
1:D:406:GLN:HG2	2:D:681:NAG:O7	2.16	0.45
1:A:215:LYS:HD3	1:A:215:LYS:H	1.82	0.45
1:B:113:MET:HB3	1:B:365:LEU:HD13	1.99	0.45
1:B:234:TYR:CE1	1:B:252:LEU:HD21	2.52	0.45
1:B:470:PHE:CD1	1:B:525:LEU:HD22	2.52	0.45
1:C:320:HIS:HE1	1:C:551:GLY:O	1.99	0.45
1:C:532:LYS:O	1:C:534:LEU:N	2.50	0.45
1:C:86:PRO:HG2	1:C:87:ASN:ND2	2.32	0.45
1:D:150:ARG:HG2	1:D:150:ARG:NH1	2.32	0.45
1:D:202:ALA:HB2	1:D:348:TYR:HE2	1.80	0.45
1:A:232:HIS:HD2	1:A:233:ILE:H	1.64	0.45
1:A:333:LYS:O	1:A:337:ILE:HG13	2.16	0.45
1:B:201:PHE:CA	1:B:301:TYR:CE2	3.00	0.45
1:B:565:GLN:O	1:B:569:CYS:HB2	2.16	0.45
1:D:104:ASN:HB3	1:D:358:LYS:HE2	1.99	0.45
1:D:563:SER:OG	1:D:566:SER:HB2	2.17	0.45
1:D:573:LYS:O	1:D:573:LYS:HD2	2.17	0.45
1:A:300:MET:O	1:A:304:ILE:HG13	2.17	0.45
1:A:510:GLU:HG2	1:A:511:LYS:H	1.82	0.45
1:B:366:LEU:HA	1:B:369:GLN:CG	2.47	0.45
1:D:380:GLU:HG2	1:D:466:TYR:CE2	2.52	0.45
1:A:569:CYS:HA	1:A:575:CYS:HA	1.99	0.45
1:B:172:PRO:HG2	1:B:495:TYR:CZ	2.52	0.45
1:B:208:GLN:HE21	1:B:228:VAL:HA	1.79	0.45
1:B:467:ARG:NH1	1:B:521:THR:OG1	2.48	0.45
1:C:107:PHE:O	1:C:111:LEU:HB2	2.17	0.45
1:C:196:MET:HB3	1:C:426:PHE:CG	2.52	0.45
1:D:240:ARG:NH1	1:D:271:VAL:HG23	2.31	0.45
1:D:366:LEU:HA	1:D:369:GLN:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HB2	1:D:439:ASN:C	2.37	0.45
1:A:283:LEU:HD22	1:A:411:ASN:ND2	2.32	0.44
1:A:52:PHE:CD1	1:B:322:GLU:HB3	2.52	0.44
1:B:198:PHE:HB2	1:B:580:PHE:HB3	1.99	0.44
1:B:215:LYS:N	1:B:215:LYS:HD3	2.32	0.44
1:B:274:ILE:HG13	1:B:290:GLU:HB2	1.99	0.44
1:B:209:PHE:O	1:B:377:ILE:CD1	2.65	0.44
1:B:43:ASN:ND2	1:B:64:PHE:CD2	2.85	0.44
1:C:147:TYR:CE1	1:C:220:PHE:CE1	3.05	0.44
1:C:411:ASN:ND2	1:C:412:SER:N	2.65	0.44
1:D:91:TYR:O	1:D:95:HIS:CD2	2.69	0.44
1:B:107:PHE:O	1:B:111:LEU:HB2	2.17	0.44
1:B:150:ARG:NH1	1:B:150:ARG:CG	2.80	0.44
1:B:366:LEU:HD23	1:B:369:GLN:HG3	2.00	0.44
1:C:351:HIS:O	1:C:353:SER:N	2.50	0.44
1:C:109:ARG:HG3	1:C:357:PHE:CE1	2.52	0.44
1:C:543:GLN:NE2	1:D:127:PRO:O	2.50	0.44
1:D:457:GLU:C	1:D:459:LYS:H	2.20	0.44
1:A:182:LEU:HD22	1:A:508:LEU:HD12	1.99	0.44
1:A:196:MET:HB3	1:A:426:PHE:CG	2.53	0.44
1:A:230:LEU:HD23	1:A:230:LEU:N	2.31	0.44
1:A:403:SER:CB	1:A:405:LYS:HD2	2.47	0.44
1:B:257:ILE:HB	1:B:262:TYR:HD2	1.81	0.44
1:B:490:GLU:O	1:B:493:ALA:HB3	2.18	0.44
1:C:150:ARG:HG2	1:C:150:ARG:NH1	2.31	0.44
1:C:210:PHE:HB3	1:C:382:ASN:ND2	2.33	0.44
1:A:360:LYS:HE2	1:A:362:ASP:HB2	1.99	0.44
1:A:42:GLN:HA	1:A:42:GLN:HE21	1.81	0.44
1:A:537:ASN:O	1:A:540:CYS:HB2	2.18	0.44
1:A:95:HIS:O	1:A:100:TRP:CD1	2.69	0.44
1:A:97:LYS:HD3	1:A:356:HIS:CG	2.50	0.44
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	2.00	0.44
1:B:352:LEU:HD21	1:B:387:TRP:CH2	2.52	0.44
1:B:218:PRO:HB2	1:B:458:MET:SD	2.57	0.44
1:C:333:LYS:O	1:C:337:ILE:HG13	2.18	0.44
1:B:276:PRO:O	1:B:279:ILE:HG12	2.18	0.44
1:B:457:GLU:C	1:B:459:LYS:H	2.20	0.44
1:C:160:PRO:HD2	1:C:164:GLY:O	2.18	0.44
1:C:388:HIS:N	1:C:389:PRO:HD2	2.33	0.44
1:C:574:GLY:C	1:C:576:PRO:HD3	2.38	0.44
1:D:248:LYS:N	1:D:325:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:TYR:CD1	1:D:480:GLU:HG2	2.52	0.44
1:D:420:THR:HG22	1:D:576:PRO:CG	2.47	0.44
1:A:176:GLU:HG2	1:A:180:LYS:HE3	1.98	0.44
1:A:383:THR:HG22	1:A:384:LEU:N	2.32	0.44
1:A:532:LYS:O	1:A:534:LEU:N	2.51	0.44
1:A:53:ASP:HB2	1:A:54:GLN:OE1	2.18	0.44
1:B:142:PHE:O	1:B:376:ARG:NH2	2.44	0.44
1:B:147:TYR:CE1	1:B:220:PHE:CE1	3.05	0.44
1:B:481:LEU:HD12	1:B:510:GLU:HG3	2.00	0.44
1:D:247:PHE:O	1:D:248:LYS:HB2	2.17	0.44
1:D:275:TYR:CE2	1:D:284:GLN:HA	2.53	0.44
1:D:92:ILE:HA	1:D:96:PHE:HE2	1.83	0.44
1:A:279:ILE:CG2	1:A:280:PRO:HD2	2.48	0.44
1:A:281:GLU:CA	1:A:284:GLN:HG3	2.40	0.44
1:D:152:LEU:CD2	1:D:469:ARG:HG2	2.47	0.44
1:D:48:MET:O	1:D:56:LYS:N	2.51	0.44
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.77	0.44
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.80	0.44
1:B:241:GLN:HG3	1:B:242:HIS:N	2.31	0.44
1:B:35:PRO:HB3	1:B:53:ASP:O	2.18	0.44
1:C:95:HIS:O	1:C:100:TRP:CD1	2.70	0.44
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.18	0.44
1:A:275:TYR:HA	1:A:276:PRO:HD3	1.91	0.44
1:A:286:ALA:O	1:A:287:VAL:HG22	2.18	0.44
1:B:104:ASN:HB3	1:B:358:LYS:HE2	1.98	0.44
1:B:381:PHE:CD1	1:B:529:PHE:CD2	3.06	0.44
1:B:553:GLU:O	1:B:557:LYS:HE3	2.18	0.44
1:C:201:PHE:HA	1:C:301:TYR:CE2	2.53	0.44
1:D:103:VAL:C	1:D:105:ASN:H	2.21	0.44
1:D:169:LYS:HB3	1:D:170:GLU:OE2	2.17	0.44
1:D:215:LYS:CD	1:D:215:LYS:N	2.78	0.44
1:D:478:PHE:HD1	1:D:478:PHE:H	1.64	0.44
1:D:479:GLU:HA	1:D:488:ALA:CB	2.48	0.44
1:D:91:TYR:CE2	1:D:95:HIS:CE1	3.05	0.44
1:A:148:TYR:CD1	1:A:377:ILE:HG13	2.53	0.43
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.47	0.43
1:A:273:MET:CE	1:A:287:VAL:HG22	2.48	0.43
1:A:40:PRO:HB2	1:A:55:TYR:CE2	2.53	0.43
1:C:172:PRO:HG2	1:C:495:TYR:CZ	2.52	0.43
1:C:397:ILE:HG22	1:C:417:HIS:CD2	2.53	0.43
1:C:96:PHE:HB3	1:C:99:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:PRO:HD3	1:D:303:THR:HG23	1.99	0.43
1:D:530:SER:O	1:D:534:LEU:HB2	2.17	0.43
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.53	0.43
1:B:532:LYS:O	1:B:534:LEU:N	2.51	0.43
1:D:150:ARG:CG	1:D:150:ARG:NH1	2.81	0.43
1:A:198:PHE:CD1	1:A:199:ALA:N	2.85	0.43
1:A:295:VAL:HG12	1:A:297:GLY:H	1.83	0.43
1:C:439:ASN:O	1:C:441:PRO:HD3	2.18	0.43
1:C:428:ARG:HG3	1:C:583:GLN:OE1	2.19	0.43
1:D:113:MET:HB3	1:D:365:LEU:HD13	2.00	0.43
1:D:252:LEU:HD13	1:D:252:LEU:HA	1.87	0.43
1:D:74:PHE:O	1:D:77:ARG:HB2	2.18	0.43
1:A:234:TYR:CE1	1:A:252:LEU:HD21	2.53	0.43
1:B:109:ARG:HG3	1:B:357:PHE:CE1	2.54	0.43
1:B:168:ASN:C	1:B:170:GLU:N	2.71	0.43
1:B:253:LYS:HB2	1:B:253:LYS:NZ	2.34	0.43
1:B:210:PHE:HB3	1:B:382:ASN:ND2	2.33	0.43
1:B:390:LEU:O	1:B:431:ALA:HB1	2.19	0.43
1:B:402:TYR:OH	1:B:417:HIS:HE1	2.01	0.43
1:B:427:THR:HB	1:B:428:ARG:NH1	2.34	0.43
1:C:487:MET:HA	1:C:490:GLU:HB3	2.01	0.43
1:D:105(A):ILE:HG22	1:D:108:LEU:H	1.83	0.43
1:D:172:PRO:HG2	1:D:495:TYR:CE2	2.54	0.43
1:D:231:ASN:C	1:D:231:ASN:OD1	2.57	0.43
1:D:402:TYR:OH	1:D:417:HIS:HE1	2.00	0.43
1:D:218:PRO:HB2	1:D:458:MET:SD	2.59	0.43
1:A:152:LEU:CD2	1:A:469:ARG:HG2	2.48	0.43
1:A:498:ILE:C	1:A:500:VAL:H	2.22	0.43
1:A:59:CYS:HB3	1:A:64:PHE:O	2.19	0.43
1:B:126:SER:CB	1:B:532:LYS:HZ1	2.31	0.43
1:B:366:LEU:HA	1:B:369:GLN:HG2	2.00	0.43
1:D:352:LEU:HD21	1:D:387:TRP:HH2	1.84	0.43
1:D:389:PRO:HB2	1:D:434:VAL:HA	1.98	0.43
1:D:510:GLU:HG2	1:D:511:LYS:N	2.33	0.43
1:D:59:CYS:HB3	1:D:64:PHE:O	2.19	0.43
1:A:281:GLU:HG2	1:A:282:ASN:H	1.82	0.43
1:A:196:MET:HE1	1:A:392:PRO:HD3	2.00	0.43
1:A:48:MET:HG3	1:A:48:MET:O	2.18	0.43
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.53	0.43
1:B:194:SER:OG	1:B:351:HIS:HE1	2.01	0.43
1:C:230:LEU:H	1:C:230:LEU:HD23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:PHE:HD1	1:C:478:PHE:H	1.67	0.43
1:D:168:ASN:CG	1:D:169:LYS:N	2.72	0.43
1:A:130:TYR:CE2	1:A:135:GLY:O	2.71	0.43
1:A:181:VAL:HG12	1:A:487:MET:HB3	2.01	0.43
1:A:184:ARG:HB2	1:A:439:ASN:CA	2.47	0.43
1:A:578:THR:O	1:A:579:SER:HB2	2.18	0.43
1:B:150:ARG:NH1	1:B:150:ARG:HG2	2.33	0.43
1:B:352:LEU:HD11	1:B:518:PHE:CE2	2.54	0.43
1:B:34:ASN:HA	1:B:35:PRO:HD2	1.85	0.43
1:B:193:GLY:O	1:B:582:VAL:HG12	2.18	0.43
1:C:44:ARG:CG	1:C:44:ARG:NH1	2.80	0.43
1:C:92:ILE:HA	1:C:96:PHE:CE2	2.54	0.43
1:D:179:GLU:HA	1:D:183:LEU:HD12	2.01	0.43
1:D:232:HIS:CD2	1:D:233:ILE:N	2.87	0.43
1:D:487:MET:O	1:D:491:LEU:N	2.48	0.43
1:A:130:TYR:HB3	1:A:134:TYR:O	2.18	0.43
1:A:292:PHE:O	1:A:299:MET:HE2	2.18	0.43
1:C:276:PRO:HD2	1:C:279:ILE:CG1	2.48	0.43
1:D:181:VAL:HB	1:D:509:VAL:HG22	2.01	0.43
1:D:209:PHE:O	1:D:377:ILE:CD1	2.67	0.43
1:D:280:PRO:HG2	1:D:283:LEU:HD12	1.99	0.43
1:D:360:LYS:HE2	1:D:362:ASP:HB2	2.01	0.43
1:D:490:GLU:O	1:D:493:ALA:HB3	2.19	0.43
1:D:42:GLN:O	1:D:69:CYS:HB2	2.19	0.43
1:A:427:THR:HB	1:A:428:ARG:HD2	2.01	0.43
1:A:579:SER:HB2	1:D:267:LYS:HZ1	1.84	0.43
1:D:498:ILE:C	1:D:500:VAL:H	2.22	0.43
1:A:477:SER:O	1:A:480:GLU:N	2.52	0.43
1:A:582:VAL:O	1:A:582:VAL:CG1	2.66	0.43
1:C:201:PHE:N	1:C:301:TYR:HE2	2.16	0.43
1:D:234:TYR:CE1	1:D:252:LEU:HD21	2.54	0.43
1:D:198:PHE:CZ	1:D:352:LEU:HD13	2.54	0.43
1:D:172:PRO:HG2	1:D:495:TYR:CG	2.54	0.43
1:D:88:THR:HG22	1:D:92:ILE:CD1	2.46	0.43
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.34	0.42
1:B:175:LYS:HE2	1:B:449:LYS:HE3	2.01	0.42
1:C:180:LYS:HD3	1:C:490:GLU:OE1	2.19	0.42
1:C:381:PHE:CD1	1:C:529:PHE:HB3	2.54	0.42
1:D:137:LYS:O	1:D:138:SER:O	2.36	0.42
1:A:210:PHE:HB3	1:A:382:ASN:ND2	2.34	0.42
1:B:333:LYS:O	1:B:337:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ARG:O	1:B:429:GLN:HB2	2.19	0.42
1:C:168:ASN:O	1:C:170:GLU:N	2.52	0.42
1:A:196:MET:CE	1:A:392:PRO:HD3	2.49	0.42
1:A:475:TYR:CD1	1:A:480:GLU:HG2	2.54	0.42
1:B:424:GLU:O	1:B:428:ARG:HD3	2.19	0.42
1:C:260:GLU:HB2	1:C:262:TYR:CE2	2.54	0.42
1:C:449:LYS:HD3	1:C:453:ASP:OD2	2.19	0.42
1:D:295:VAL:O	1:D:295:VAL:HG12	2.19	0.42
1:D:450:ALA:O	1:D:453:ASP:N	2.52	0.42
1:D:92:ILE:HA	1:D:96:PHE:CE2	2.54	0.42
1:A:147:TYR:HE1	1:A:220:PHE:CZ	2.37	0.42
1:A:276:PRO:HG2	1:A:409:TYR:CG	2.54	0.42
1:A:565:GLN:HG2	1:D:268:ASP:HB2	2.02	0.42
1:A:74:PHE:O	1:A:77:ARG:HB2	2.18	0.42
1:A:137:LYS:NZ	1:B:543:GLN:O	2.44	0.42
1:B:564:ILE:HG12	1:B:580:PHE:CZ	2.54	0.42
1:C:338:GLY:C	1:C:559:ILE:HG23	2.40	0.42
1:C:510:GLU:HG2	1:C:511:LYS:H	1.85	0.42
1:C:522:MET:HG3	1:C:522:MET:O	2.20	0.42
1:D:568:ILE:O	1:D:572:VAL:N	2.47	0.42
3:D:682:HEM:HHD	3:D:682:HEM:HBC2	2.00	0.42
1:A:232:HIS:HD2	1:A:233:ILE:N	2.17	0.42
1:A:579:SER:HB2	1:D:267:LYS:NZ	2.34	0.42
1:A:543:GLN:NE2	1:B:127:PRO:O	2.52	0.42
1:C:423:VAL:HG13	1:C:578:THR:HG23	2.00	0.42
1:D:175:LYS:O	1:D:178:LEU:HB3	2.19	0.42
1:D:211:LYS:HE2	1:D:222:ARG:CG	2.49	0.42
1:D:35:PRO:HB3	1:D:53:ASP:O	2.20	0.42
1:A:168:ASN:O	1:A:170:GLU:N	2.53	0.42
1:A:171:LEU:HD12	1:A:171:LEU:HA	1.86	0.42
1:A:244:LEU:O	1:A:252:LEU:HD12	2.19	0.42
1:A:352:LEU:HD11	1:A:518:PHE:CZ	2.54	0.42
1:A:411:ASN:ND2	1:A:412:SER:H	2.16	0.42
1:B:421:GLN:OE1	1:B:421:GLN:HA	2.19	0.42
1:C:130:TYR:CE2	1:C:135:GLY:O	2.73	0.42
1:C:198:PHE:CD1	1:C:199:ALA:N	2.88	0.42
1:C:352:LEU:HD21	1:C:387:TRP:HH2	1.84	0.42
1:C:283:LEU:HD22	1:C:411:ASN:ND2	2.35	0.42
1:C:398:GLU:H	1:C:425:SER:CB	2.32	0.42
1:C:181:VAL:HG21	1:C:491:LEU:HD21	2.02	0.42
1:C:82:LEU:N	1:C:82:LEU:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:SER:CB	1:D:532:LYS:HZ1	2.32	0.42
1:D:83:LYS:HA	1:D:83:LYS:NZ	2.34	0.42
1:A:544:TYR:OH	1:B:142:PHE:HB2	2.19	0.42
1:B:182:LEU:HD22	1:B:508:LEU:HD12	2.01	0.42
1:B:510:GLU:HG2	1:B:511:LYS:H	1.83	0.42
1:B:574:GLY:C	1:B:576:PRO:HD3	2.40	0.42
1:C:276:PRO:HG2	1:C:409:TYR:CG	2.55	0.42
1:C:403:SER:HB2	1:C:405:LYS:CD	2.50	0.42
1:C:427:THR:HB	1:C:428:ARG:HD2	2.02	0.42
1:C:442:ILE:O	1:C:445:GLN:HG2	2.20	0.42
1:C:48:MET:HG3	1:C:48:MET:O	2.19	0.42
1:C:505:PRO:O	1:C:507:LEU:N	2.52	0.42
1:D:107:PHE:O	1:D:111:LEU:HB2	2.19	0.42
1:C:322:GLU:HB3	1:D:52:PHE:CD1	2.55	0.42
1:A:412:SER:O	1:A:416:GLU:N	2.47	0.42
1:B:204:HIS:ND1	1:B:292:PHE:CE2	2.88	0.42
1:C:256:VAL:HA	1:C:260:GLU:O	2.20	0.42
1:C:202:ALA:HB2	1:C:348:TYR:CE2	2.55	0.42
1:C:388:HIS:N	1:C:389:PRO:CD	2.82	0.42
1:C:396:ASN:HD22	1:C:401:GLU:HA	1.85	0.42
1:C:59:CYS:HB3	1:C:64:PHE:O	2.20	0.42
1:D:294:LEU:HD22	1:D:409:TYR:HD1	1.83	0.42
1:D:92:ILE:H	1:D:92:ILE:HG13	1.58	0.42
1:A:175:LYS:HD3	1:A:175:LYS:HA	1.88	0.42
1:A:320:HIS:CE1	1:A:551:GLY:O	2.72	0.42
1:A:563:SER:OG	1:A:566:SER:HB2	2.20	0.42
1:B:197:MET:HE3	1:B:197:MET:HA	2.01	0.42
1:B:478:PHE:N	1:B:478:PHE:CD1	2.87	0.42
1:C:298:LEU:HD12	1:C:298:LEU:HA	1.81	0.42
1:D:243:LYS:O	1:D:269:THR:HB	2.20	0.42
1:D:487:MET:HA	1:D:490:GLU:HB3	2.01	0.42
1:C:61:ARG:NH2	1:D:545:TRP:O	2.51	0.42
1:D:82:LEU:N	1:D:82:LEU:HD12	2.35	0.42
1:A:300:MET:HB3	1:A:300:MET:HE3	1.85	0.42
1:A:388:HIS:N	1:A:389:PRO:HD2	2.34	0.42
1:A:388:HIS:CG	1:A:444:VAL:HG11	2.54	0.42
1:B:40:PRO:HB2	1:B:55:TYR:CE2	2.55	0.42
1:B:73:GLU:O	1:B:76:THR:N	2.52	0.42
1:C:105(A):ILE:O	1:C:108:LEU:HB2	2.20	0.42
1:C:113:MET:O	1:C:117:LEU:HB2	2.20	0.42
1:C:537:ASN:O	1:C:540:CYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:PHE:CA	1:D:301:TYR:CE2	3.03	0.42
1:D:194:SER:OG	1:D:351:HIS:HE1	2.02	0.42
1:D:145:LEU:HD23	1:D:376:ARG:CZ	2.50	0.42
1:A:478:PHE:CD1	1:A:478:PHE:N	2.88	0.41
1:B:206:THR:HG21	1:B:385:TYR:CD1	2.55	0.41
1:B:230:LEU:H	1:B:230:LEU:HD23	1.84	0.41
1:B:275:TYR:HA	1:B:276:PRO:HD3	1.93	0.41
1:C:248:LYS:N	1:C:325:ASP:OD1	2.53	0.41
1:C:462:SER:HB3	1:C:465:GLU:HG2	2.02	0.41
1:D:201:PHE:N	1:D:301:TYR:HE2	2.18	0.41
1:A:168:ASN:ND2	1:A:169:LYS:H	2.18	0.41
1:A:390:LEU:O	1:A:431:ALA:HB1	2.20	0.41
1:A:565:GLN:O	1:A:569:CYS:HB2	2.20	0.41
1:C:138:SER:HB2	1:D:330:GLN:HB3	2.01	0.41
1:C:206:THR:HG21	1:C:385:TYR:CD1	2.56	0.41
1:C:300:MET:O	1:C:304:ILE:HG13	2.21	0.41
1:D:105(A):ILE:HD12	1:D:108:LEU:HD12	2.01	0.41
1:D:38:SER:OG	1:D:40:PRO:HG3	2.20	0.41
1:A:138:SER:HB2	1:B:330:GLN:HB3	2.01	0.41
1:A:43:ASN:ND2	1:A:64:PHE:CD2	2.88	0.41
1:A:96:PHE:HB3	1:A:99:VAL:CG2	2.50	0.41
1:B:215:LYS:H	1:B:215:LYS:HD3	1.85	0.41
1:B:381:PHE:HD1	1:B:529:PHE:CD2	2.35	0.41
1:B:433:ARG:HH21	1:B:512:PRO:CB	2.33	0.41
1:B:568:ILE:HG13	1:B:572:VAL:HG21	2.01	0.41
1:C:211:LYS:HE2	1:C:222:ARG:CG	2.45	0.41
1:D:210:PHE:HZ	1:D:381:PHE:CD2	2.38	0.41
1:A:490:GLU:O	1:A:493:ALA:HB3	2.21	0.41
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.36	0.41
1:B:42:GLN:O	1:B:69:CYS:HB2	2.21	0.41
1:B:475:TYR:CD2	1:B:481:LEU:HB2	2.56	0.41
1:D:104:ASN:CB	1:D:358:LYS:HE2	2.51	0.41
1:D:130:TYR:HB3	1:D:134:TYR:O	2.21	0.41
1:D:522:MET:O	1:D:522:MET:HG3	2.20	0.41
1:D:83:LYS:HZ1	1:D:84:PRO:HD2	1.85	0.41
1:A:113:MET:HE2	1:A:360:LYS:O	2.20	0.41
1:A:215:LYS:CD	1:A:215:LYS:H	2.32	0.41
1:A:260:GLU:HB2	1:A:262:TYR:CE2	2.55	0.41
1:A:294:LEU:HD22	1:A:409:TYR:HD1	1.83	0.41
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.61	0.41
1:A:86:PRO:HG2	1:A:87:ASN:ND2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLN:HB3	1:B:138:SER:HB2	2.03	0.41
1:B:402:TYR:OH	1:B:417:HIS:CE1	2.73	0.41
1:B:96:PHE:O	1:B:98:GLY:N	2.53	0.41
1:C:403:SER:HB2	1:C:405:LYS:HZ3	1.85	0.41
1:C:41:CYS:SG	1:C:47:CYS:HB2	2.61	0.41
1:C:565:GLN:O	1:C:569:CYS:HB2	2.21	0.41
1:D:209:PHE:O	1:D:377:ILE:HD12	2.19	0.41
1:D:513:ARG:O	1:D:514:PRO:O	2.39	0.41
1:A:168:ASN:C	1:A:170:GLU:N	2.73	0.41
1:B:232:HIS:CD2	1:B:233:ILE:N	2.89	0.41
1:B:481:LEU:HD11	1:B:506:ALA:HB1	2.03	0.41
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.92	0.41
1:C:209:PHE:O	1:C:377:ILE:CD1	2.69	0.41
1:C:352:LEU:HD11	1:C:518:PHE:CZ	2.55	0.41
1:C:491:LEU:HD11	1:C:509:VAL:CG1	2.49	0.41
1:D:160:PRO:HD2	1:D:164:GLY:O	2.21	0.41
1:D:291:VAL:O	1:D:293:GLY:N	2.54	0.41
1:D:352:LEU:HD11	1:D:518:PHE:CZ	2.56	0.41
1:A:338:GLY:HA3	1:A:559:ILE:HD13	2.03	0.41
1:A:96:PHE:O	1:A:99:VAL:N	2.54	0.41
1:B:39:ASN:N	1:B:40:PRO:CD	2.83	0.41
1:C:246:LEU:HD23	1:C:251:LYS:HB2	2.02	0.41
1:C:394:THR:HB	1:C:401:GLU:HB3	2.02	0.41
1:D:299:MET:HA	1:D:302:ALA:HB3	2.03	0.41
1:D:311:ARG:O	1:D:315:ILE:HG13	2.20	0.41
1:A:396:ASN:N	1:A:396:ASN:ND2	2.69	0.41
1:A:92:ILE:HG13	1:A:92:ILE:H	1.61	0.41
1:C:280:PRO:HG2	1:C:283:LEU:HD12	2.02	0.41
1:D:130:TYR:CD1	1:D:130:TYR:N	2.88	0.41
3:D:682:HEM:HHH	3:D:682:HEM:CBC	2.51	0.41
1:A:481:LEU:HD12	1:A:510:GLU:HG3	2.03	0.41
1:B:113:MET:O	1:B:117:LEU:HB2	2.21	0.41
1:B:168:ASN:O	1:B:170:GLU:N	2.54	0.41
1:B:184:ARG:HB2	1:B:439:ASN:C	2.41	0.41
1:B:320:HIS:CE1	1:B:551:GLY:O	2.72	0.41
1:C:184:ARG:HB2	1:C:439:ASN:C	2.42	0.41
1:C:208:GLN:OE1	1:C:232:HIS:CE1	2.74	0.41
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.86	0.41
1:C:490:GLU:O	1:C:493:ALA:HB3	2.21	0.41
1:A:424:GLU:HA	1:A:428:ARG:HH11	1.86	0.41
1:A:573:LYS:O	1:A:573:LYS:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LYS:N	1:B:325:ASP:OD1	2.54	0.41
1:B:394:THR:HB	1:B:396:ASN:HD21	1.86	0.41
1:B:479:GLU:HG3	1:B:488:ALA:CB	2.50	0.41
1:B:482:THR:HG22	1:B:509:VAL:HG12	2.03	0.41
1:D:150:ARG:CG	1:D:152:LEU:O	2.69	0.41
1:A:232:HIS:CD2	1:A:233:ILE:N	2.89	0.41
1:A:295:VAL:HG12	1:A:295:VAL:O	2.20	0.41
1:A:399:ASP:HB3	1:A:400:GLN:NE2	2.28	0.41
1:A:181:VAL:HB	1:A:509:VAL:HG22	2.02	0.41
1:A:574:GLY:C	1:A:576:PRO:HD3	2.40	0.41
1:B:113:MET:HE2	1:B:360:LYS:O	2.21	0.41
1:D:109:ARG:HG3	1:D:357:PHE:HE1	1.86	0.41
1:D:254:TYR:HD1	1:D:255:GLN:N	2.19	0.41
1:D:273:MET:CE	1:D:287:VAL:HG22	2.51	0.41
1:D:381:PHE:CD1	1:D:529:PHE:CD2	3.09	0.41
1:B:202:ALA:HB2	1:B:348:TYR:HE2	1.85	0.40
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.56	0.40
1:B:153:PRO:HG2	1:B:461:GLN:HE22	1.86	0.40
1:C:172:PRO:HG2	1:C:495:TYR:CG	2.56	0.40
1:C:269:THR:O	1:C:270:GLN:CB	2.69	0.40
1:C:433:ARG:NH2	1:C:516:ALA:O	2.54	0.40
1:C:126:SER:CB	1:C:532:LYS:HZ1	2.34	0.40
1:C:538:PRO:HG3	1:D:142:PHE:CE2	2.57	0.40
1:D:201:PHE:HD2	1:D:301:TYR:CZ	2.39	0.40
1:D:48:MET:HG3	1:D:48:MET:O	2.20	0.40
1:A:184:ARG:HB2	1:A:439:ASN:C	2.42	0.40
1:A:253:LYS:NZ	1:A:253:LYS:HB2	2.37	0.40
1:A:281:GLU:HA	1:A:284:GLN:HE21	1.86	0.40
1:B:412:SER:O	1:B:416:GLU:HB2	2.20	0.40
1:B:420:THR:HG22	1:B:576:PRO:CG	2.51	0.40
1:B:472:LEU:HD21	1:B:524:GLU:HG3	2.02	0.40
1:B:531:LEU:O	1:B:535:MET:HB2	2.21	0.40
1:C:274:ILE:HG13	1:C:290:GLU:HB2	2.01	0.40
1:C:389:PRO:CB	1:C:434:VAL:HA	2.51	0.40
1:C:92:ILE:HA	1:C:96:PHE:HE2	1.85	0.40
1:D:281:GLU:HA	1:D:284:GLN:NE2	2.30	0.40
1:D:318:GLN:CD	1:D:318:GLN:C	2.79	0.40
1:D:394:THR:HB	1:D:401:GLU:HB3	2.04	0.40
1:D:487:MET:O	1:D:490:GLU:HB3	2.21	0.40
1:D:505:PRO:O	1:D:507:LEU:N	2.55	0.40
1:A:273:MET:HE2	1:A:287:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TYR:OH	1:A:417:HIS:CE1	2.73	0.40
1:B:292:PHE:O	1:B:299:MET:HE2	2.22	0.40
1:B:563:SER:OG	1:B:566:SER:HB2	2.21	0.40
1:B:295:VAL:HG21	3:B:682:HEM:CBB	2.51	0.40
1:C:204:HIS:ND1	1:C:292:PHE:HE2	2.18	0.40
1:C:210:PHE:CG	1:C:382:ASN:ND2	2.85	0.40
1:D:184:ARG:HB2	1:D:439:ASN:CA	2.49	0.40
1:A:577:PHE:CE1	1:D:267:LYS:HD2	2.51	0.40
1:D:366:LEU:HD23	1:D:369:GLN:HG3	2.03	0.40
1:D:472:LEU:HD21	1:D:524:GLU:HG3	2.03	0.40
1:D:478:PHE:N	1:D:478:PHE:CD1	2.90	0.40
1:A:210:PHE:CG	1:A:382:ASN:ND2	2.88	0.40
1:B:299:MET:HG3	1:B:299:MET:O	2.21	0.40
1:B:564:ILE:HG12	1:B:580:PHE:CE1	2.57	0.40
1:C:130:TYR:HB3	1:C:134:TYR:O	2.21	0.40
1:C:33:ALA:HB3	1:C:158:ASP:OD2	2.20	0.40
1:C:291:VAL:O	1:C:293:GLY:N	2.54	0.40
1:C:327:GLN:HG3	1:D:136:TYR:CE2	2.57	0.40
1:C:479:GLU:HG2	1:C:485:LYS:HZ1	1.85	0.40
1:C:63:GLY:HA2	1:C:73:GLU:CD	2.42	0.40
1:D:113:MET:O	1:D:117:LEU:HB2	2.22	0.40
1:D:41:CYS:SG	1:D:47:CYS:HB2	2.62	0.40
1:D:479:GLU:HG2	1:D:485:LYS:NZ	2.36	0.40
1:A:269:THR:O	1:A:270:GLN:CB	2.68	0.40
1:A:97:LYS:HD3	1:A:356:HIS:NE2	2.37	0.40
1:B:383:THR:HG22	1:B:384:LEU:N	2.36	0.40
1:B:498:ILE:O	1:B:500:VAL:N	2.52	0.40
1:C:233:ILE:HD13	1:C:305:TRP:HB3	2.03	0.40
1:C:285:PHE:CD1	1:C:285:PHE:N	2.89	0.40
1:C:181:VAL:HG12	1:C:487:MET:HB3	2.03	0.40
1:C:64:PHE:CE2	1:C:72:PRO:HB3	2.57	0.40
1:D:103:VAL:O	1:D:105:ASN:N	2.54	0.40
1:D:246:LEU:HD23	1:D:251:LYS:HB2	2.03	0.40
1:D:320:HIS:CE1	1:D:551:GLY:O	2.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/587 (94%)	446 (81%)	78 (14%)	26 (5%)	2	14
1	B	550/587 (94%)	442 (80%)	87 (16%)	21 (4%)	3	18
1	C	550/587 (94%)	443 (80%)	80 (14%)	27 (5%)	2	13
1	D	550/587 (94%)	440 (80%)	85 (16%)	25 (4%)	2	14
All	All	2200/2348 (94%)	1771 (80%)	330 (15%)	99 (4%)	2	14

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	429	GLN
1	A	438	ARG
1	A	514	PRO
1	A	573	LYS
1	B	138	SER
1	B	429	GLN
1	B	438	ARG
1	B	514	PRO
1	B	573	LYS
1	C	138	SER
1	C	429	GLN
1	C	514	PRO
1	C	573	LYS
1	D	138	SER
1	D	429	GLN
1	D	514	PRO
1	D	573	LYS
1	A	97	LYS
1	A	282	ASN
1	A	398	GLU
1	A	399	ASP

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Mol	Chain	Res	Type
1	B	97	LYS
1	B	282	ASN
1	B	398	GLU
1	B	399	ASP
1	B	444	VAL
1	C	97	LYS
1	C	292	PHE
1	C	398	GLU
1	C	399	ASP
1	C	438	ARG
1	D	97	LYS
1	D	282	ASN
1	D	292	PHE
1	D	352	LEU
1	D	398	GLU
1	D	399	ASP
1	D	438	ARG
1	A	292	PHE
1	A	352	LEU
1	A	444	VAL
1	A	506	ALA
1	B	169	LYS
1	B	292	PHE
1	B	500	VAL
1	B	554	VAL
1	C	132	VAL
1	C	282	ASN
1	C	500	VAL
1	D	104	ASN
1	D	392	PRO
1	D	460	TYR
1	A	169	LYS
1	A	392	PRO
1	A	460	TYR
1	B	392	PRO
1	C	352	LEU
1	C	392	PRO
1	C	444	VAL
1	C	506	ALA
1	C	554	VAL
1	D	132	VAL
1	D	248	LYS

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Mol	Chain	Res	Type
1	D	444	VAL
1	D	500	VAL
1	D	506	ALA
1	A	132	VAL
1	A	248	LYS
1	A	500	VAL
1	C	169	LYS
1	C	290	GLU
1	C	545	TRP
1	C	579	SER
1	D	545	TRP
1	D	554	VAL
1	A	554	VAL
1	B	352	LEU
1	C	104	ASN
1	C	248	LYS
1	D	505	PRO
1	A	430	ILE
1	A	509	VAL
1	B	132	VAL
1	C	547	PRO
1	D	509	VAL
1	D	547	PRO
1	A	505	PRO
1	B	505	PRO
1	C	505	PRO
1	A	228	VAL
1	B	509	VAL
1	D	430	ILE
1	A	447	VAL
1	B	363	PRO
1	B	430	ILE
1	C	287	VAL
1	C	430	ILE
1	A	287	VAL

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	493/525 (94%)	417 (85%)	76 (15%)	2	13
1	B	493/525 (94%)	418 (85%)	75 (15%)	3	14
1	C	493/525 (94%)	416 (84%)	77 (16%)	2	13
1	D	493/525 (94%)	417 (85%)	76 (15%)	2	13
All	All	1972/2100 (94%)	1668 (85%)	304 (15%)	2	13

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	39	ASN
1	A	42	GLN
1	A	44	ARG
1	A	48	MET
1	A	54	GLN
1	A	70	THR
1	A	71	THR
1	A	83	LYS
1	A	93	LEU
1	A	107	PHE
1	A	113	MET
1	A	116	VAL
1	A	122	TYR
1	A	124	ILE
1	A	126	SER
1	A	130	TYR
1	A	138	SER
1	A	150	ARG
1	A	152	LEU
1	A	158	ASP
1	A	171	LEU
1	A	178	LEU
1	A	196	MET
1	A	197	MET
1	A	209	PHE
1	A	215	LYS
1	A	216	ARG
1	A	222	ARG
1	A	231	ASN
1	A	232	HIS

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	252	LEU
1	A	253	LYS
1	A	270	GLN
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	298	LEU
1	A	300	MET
1	A	310	GLN
1	A	316	LEU
1	A	318	GLN
1	A	322	GLU
1	A	326	GLU
1	A	337	ILE
1	A	350	GLN
1	A	376	ARG
1	A	379	SER
1	A	385	TYR
1	A	389	PRO
1	A	398	GLU
1	A	400	GLN
1	A	405	LYS
1	A	409	TYR
1	A	411	ASN
1	A	412	SER
1	A	416	GLU
1	A	420	THR
1	A	422	PHE
1	A	476	THR
1	A	484	GLU
1	A	492	LYS
1	A	494	LEU
1	A	514	PRO
1	A	522	MET
1	A	525	LEU
1	A	530	SER
1	A	534	LEU
1	A	543	GLN
1	A	547	PRO
1	A	557	LYS
1	A	566	SER

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Mol	Chain	Res	Type
1	A	569	CYS
1	A	578	THR
1	A	583	GLN
1	B	39	ASN
1	B	42	GLN
1	B	44	ARG
1	B	48	MET
1	B	56	LYS
1	B	70	THR
1	B	71	THR
1	B	83	LYS
1	B	93	LEU
1	B	107	PHE
1	B	113	MET
1	B	116	VAL
1	B	117	LEU
1	B	122	TYR
1	B	124	ILE
1	B	126	SER
1	B	136	TYR
1	B	138	SER
1	B	150	ARG
1	B	152	LEU
1	B	158	ASP
1	B	171	LEU
1	B	178	LEU
1	B	196	MET
1	B	197	MET
1	B	209	PHE
1	B	215	LYS
1	B	216	ARG
1	B	222	ARG
1	B	231	ASN
1	B	232	HIS
1	B	241	GLN
1	B	252	LEU
1	B	253	LYS
1	B	270	GLN
1	B	282	ASN
1	B	289	GLN
1	B	298	LEU
1	B	300	MET

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Mol	Chain	Res	Type
1	B	310	GLN
1	B	316	LEU
1	B	318	GLN
1	B	322	GLU
1	B	326	GLU
1	B	337	ILE
1	B	376	ARG
1	B	379	SER
1	B	383	THR
1	B	385	TYR
1	B	389	PRO
1	B	394	THR
1	B	398	GLU
1	B	399	ASP
1	B	400	GLN
1	B	405	LYS
1	B	407	PHE
1	B	409	TYR
1	B	412	SER
1	B	420	THR
1	B	422	PHE
1	B	476	THR
1	B	484	GLU
1	B	492	LYS
1	B	494	LEU
1	B	514	PRO
1	B	522	MET
1	B	525	LEU
1	B	530	SER
1	B	534	LEU
1	B	543	GLN
1	B	557	LYS
1	B	566	SER
1	B	569	CYS
1	B	578	THR
1	B	583	GLN
1	C	42	GLN
1	C	44	ARG
1	C	48	MET
1	C	54	GLN
1	C	56	LYS
1	C	70	THR

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Mol	Chain	Res	Type
1	C	71	THR
1	C	83	LYS
1	C	93	LEU
1	C	107	PHE
1	C	113	MET
1	C	116	VAL
1	C	117	LEU
1	C	122	TYR
1	C	124	ILE
1	C	126	SER
1	C	130	TYR
1	C	138	SER
1	C	150	ARG
1	C	152	LEU
1	C	158	ASP
1	C	171	LEU
1	C	178	LEU
1	C	196	MET
1	C	197	MET
1	C	209	PHE
1	C	215	LYS
1	C	216	ARG
1	C	222	ARG
1	C	231	ASN
1	C	232	HIS
1	C	241	GLN
1	C	252	LEU
1	C	253	LYS
1	C	270	GLN
1	C	271	VAL
1	C	282	ASN
1	C	289	GLN
1	C	298	LEU
1	C	300	MET
1	C	310	GLN
1	C	316	LEU
1	C	318	GLN
1	C	322	GLU
1	C	326	GLU
1	C	337	ILE
1	C	350	GLN
1	C	376	ARG

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Mol	Chain	Res	Type
1	C	379	SER
1	C	385	TYR
1	C	389	PRO
1	C	398	GLU
1	C	400	GLN
1	C	405	LYS
1	C	409	TYR
1	C	411	ASN
1	C	412	SER
1	C	416	GLU
1	C	420	THR
1	C	422	PHE
1	C	441	PRO
1	C	476	THR
1	C	484	GLU
1	C	492	LYS
1	C	494	LEU
1	C	514	PRO
1	C	522	MET
1	C	525	LEU
1	C	530	SER
1	C	534	LEU
1	C	543	GLN
1	C	547	PRO
1	C	557	LYS
1	C	566	SER
1	C	569	CYS
1	C	578	THR
1	C	583	GLN
1	D	42	GLN
1	D	44	ARG
1	D	48	MET
1	D	70	THR
1	D	71	THR
1	D	83	LYS
1	D	93	LEU
1	D	107	PHE
1	D	113	MET
1	D	116	VAL
1	D	117	LEU
1	D	124	ILE
1	D	126	SER

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Mol	Chain	Res	Type
1	D	130	TYR
1	D	138	SER
1	D	150	ARG
1	D	152	LEU
1	D	158	ASP
1	D	171	LEU
1	D	178	LEU
1	D	196	MET
1	D	197	MET
1	D	209	PHE
1	D	215	LYS
1	D	216	ARG
1	D	222	ARG
1	D	231	ASN
1	D	232	HIS
1	D	241	GLN
1	D	252	LEU
1	D	253	LYS
1	D	270	GLN
1	D	282	ASN
1	D	289	GLN
1	D	298	LEU
1	D	300	MET
1	D	310	GLN
1	D	316	LEU
1	D	318	GLN
1	D	322	GLU
1	D	326	GLU
1	D	331	THR
1	D	337	ILE
1	D	376	ARG
1	D	379	SER
1	D	383	THR
1	D	385	TYR
1	D	389	PRO
1	D	394	THR
1	D	396	ASN
1	D	398	GLU
1	D	400	GLN
1	D	405	LYS
1	D	407	PHE
1	D	409	TYR

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Mol	Chain	Res	Type
1	D	411	ASN
1	D	412	SER
1	D	416	GLU
1	D	420	THR
1	D	422	PHE
1	D	441	PRO
1	D	476	THR
1	D	484	GLU
1	D	492	LYS
1	D	494	LEU
1	D	514	PRO
1	D	522	MET
1	D	525	LEU
1	D	530	SER
1	D	534	LEU
1	D	543	GLN
1	D	557	LYS
1	D	566	SER
1	D	569	CYS
1	D	578	THR
1	D	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	87	ASN
1	A	95	HIS
1	A	203	GLN
1	A	232	HIS
1	A	278	HIS
1	A	284	GLN
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	369	GLN
1	A	396	ASN
1	A	400	GLN
1	A	417	HIS
1	A	454	GLN
1	A	560	ASN
1	B	42	GLN

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Mol	Chain	Res	Type
1	B	87	ASN
1	B	95	HIS
1	B	203	GLN
1	B	232	HIS
1	B	278	HIS
1	B	284	GLN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	396	ASN
1	B	400	GLN
1	B	411	ASN
1	B	417	HIS
1	B	454	GLN
1	B	543	GLN
1	B	560	ASN
1	C	39	ASN
1	C	42	GLN
1	C	95	HIS
1	C	203	GLN
1	C	232	HIS
1	C	242	HIS
1	C	320	HIS
1	C	350	GLN
1	C	369	GLN
1	C	396	ASN
1	C	400	GLN
1	C	411	ASN
1	C	417	HIS
1	C	454	GLN
1	C	543	GLN
1	C	560	ASN
1	D	42	GLN
1	D	90	HIS
1	D	95	HIS
1	D	203	GLN
1	D	232	HIS
1	D	284	GLN
1	D	350	GLN
1	D	351	HIS
1	D	369	GLN
1	D	396	ASN

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Mol	Chain	Res	Type
1	D	400	GLN
1	D	411	ASN
1	D	417	HIS
1	D	454	GLN
1	D	543	GLN
1	D	560	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

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	NAG	C	661	1	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
2	NAG	D	661	1	14,14,15	0.62	0	17,19,21	0.84	1 (5%)
3	HEM	D	682	1	27,50,50	1.91	5 (18%)	17,82,82	1.02	1 (5%)
2	NAG	B	661	1	14,14,15	0.67	1 (7%)	17,19,21	0.91	0
3	HEM	B	682	1	27,50,50	1.75	5 (18%)	17,82,82	0.95	0
2	NAG	D	681	1	14,14,15	0.62	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	682	1	27,50,50	1.99	6 (22%)	17,82,82	0.83	0
2	NAG	B	671	1	14,14,15	0.83	0	17,19,21	1.49	3 (17%)
2	NAG	A	671	1	14,14,15	0.86	0	17,19,21	1.57	3 (17%)
2	NAG	D	671	1	14,14,15	0.65	0	17,19,21	1.40	1 (5%)
2	NAG	B	681	1	14,14,15	0.57	0	17,19,21	0.87	2 (11%)
2	NAG	A	681	1	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
2	NAG	C	681	1	14,14,15	0.61	0	17,19,21	0.99	2 (11%)
2	NAG	C	671	1	14,14,15	0.83	0	17,19,21	1.60	3 (17%)
2	NAG	A	661	1	14,14,15	0.64	0	17,19,21	0.74	0
3	HEM	C	682	1	27,50,50	1.99	6 (22%)	17,82,82	0.78	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
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
3	HEM	D	682	1	-	0/6/54/54	-
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/6/54/54	-
2	NAG	D	681	1	-	2/6/23/26	0/1/1/1
3	HEM	A	682	1	-	0/6/54/54	-
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
2	NAG	D	671	1	-	2/6/23/26	0/1/1/1
2	NAG	B	681	1	-	2/6/23/26	0/1/1/1
2	NAG	A	681	1	-	2/6/23/26	0/1/1/1
2	NAG	C	681	1	-	2/6/23/26	0/1/1/1
2	NAG	C	671	1	-	2/6/23/26	0/1/1/1
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
3	HEM	C	682	1	-	0/6/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3C-C2C	-5.12	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	682	HEM	C3C-CAC	-4.79	1.38	1.47
3	A	682	HEM	C3B-C2B	-4.69	1.33	1.40
3	C	682	HEM	C3C-C2C	-4.44	1.34	1.40
3	C	682	HEM	C3B-C2B	-4.43	1.34	1.40
3	A	682	HEM	C3B-CAB	-4.27	1.39	1.47
3	C	682	HEM	C3C-CAC	-4.21	1.39	1.47
3	C	682	HEM	C3B-CAB	-4.14	1.39	1.47
3	A	682	HEM	C3C-CAC	-4.13	1.39	1.47
3	B	682	HEM	C3B-CAB	-4.06	1.39	1.47
3	D	682	HEM	C3B-CAB	-4.03	1.39	1.47
3	B	682	HEM	C3C-CAC	-3.97	1.39	1.47
3	D	682	HEM	C3B-C2B	-3.91	1.34	1.40
3	B	682	HEM	C3B-C2B	-3.45	1.35	1.40
3	B	682	HEM	C3C-C2C	-3.28	1.35	1.40
3	D	682	HEM	C3C-C2C	-2.70	1.36	1.40
3	A	682	HEM	CBB-CAB	2.58	1.46	1.29
3	C	682	HEM	CBB-CAB	2.56	1.46	1.29
3	D	682	HEM	CBB-CAB	2.47	1.45	1.29
3	C	682	HEM	CBC-CAC	2.38	1.45	1.29
3	A	682	HEM	CBC-CAC	2.22	1.44	1.29
2	B	661	NAG	C1-C2	2.03	1.55	1.52
3	B	682	HEM	CBB-CAB	2.02	1.42	1.29

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	671	NAG	C4-C3-C2	-5.09	103.55	111.02
2	C	671	NAG	C4-C3-C2	-4.72	104.10	111.02
2	D	671	NAG	C4-C3-C2	-4.60	104.28	111.02
2	B	671	NAG	C4-C3-C2	-4.53	104.38	111.02
2	C	671	NAG	C2-N2-C7	-3.19	118.36	122.90
2	A	681	NAG	C2-N2-C7	-2.61	119.19	122.90
2	A	671	NAG	C2-N2-C7	-2.55	119.27	122.90
2	C	681	NAG	C2-N2-C7	-2.53	119.30	122.90
2	C	671	NAG	C1-O5-C5	2.45	115.51	112.19
2	A	671	NAG	C1-O5-C5	2.41	115.45	112.19
2	D	661	NAG	C2-N2-C7	-2.34	119.57	122.90
2	C	681	NAG	O5-C1-C2	-2.32	107.62	111.29
2	B	681	NAG	C2-N2-C7	-2.24	119.71	122.90
2	B	671	NAG	C1-O5-C5	2.22	115.20	112.19
2	B	671	NAG	C2-N2-C7	-2.17	119.81	122.90
2	D	681	NAG	C2-N2-C7	-2.10	119.92	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	681	NAG	C1-O5-C5	-2.06	109.40	112.19
3	D	682	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
2	C	661	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	671	NAG	O5-C5-C6-O6
2	D	671	NAG	O5-C5-C6-O6
2	A	671	NAG	O5-C5-C6-O6
2	D	671	NAG	C4-C5-C6-O6
2	B	681	NAG	C4-C5-C6-O6
2	C	681	NAG	C4-C5-C6-O6
2	B	681	NAG	O5-C5-C6-O6
2	C	681	NAG	O5-C5-C6-O6
2	C	671	NAG	O5-C5-C6-O6
2	B	671	NAG	C4-C5-C6-O6
2	A	681	NAG	O5-C5-C6-O6
2	D	681	NAG	O5-C5-C6-O6
2	A	671	NAG	C4-C5-C6-O6
2	D	681	NAG	C4-C5-C6-O6
2	A	681	NAG	C4-C5-C6-O6
2	C	671	NAG	C4-C5-C6-O6

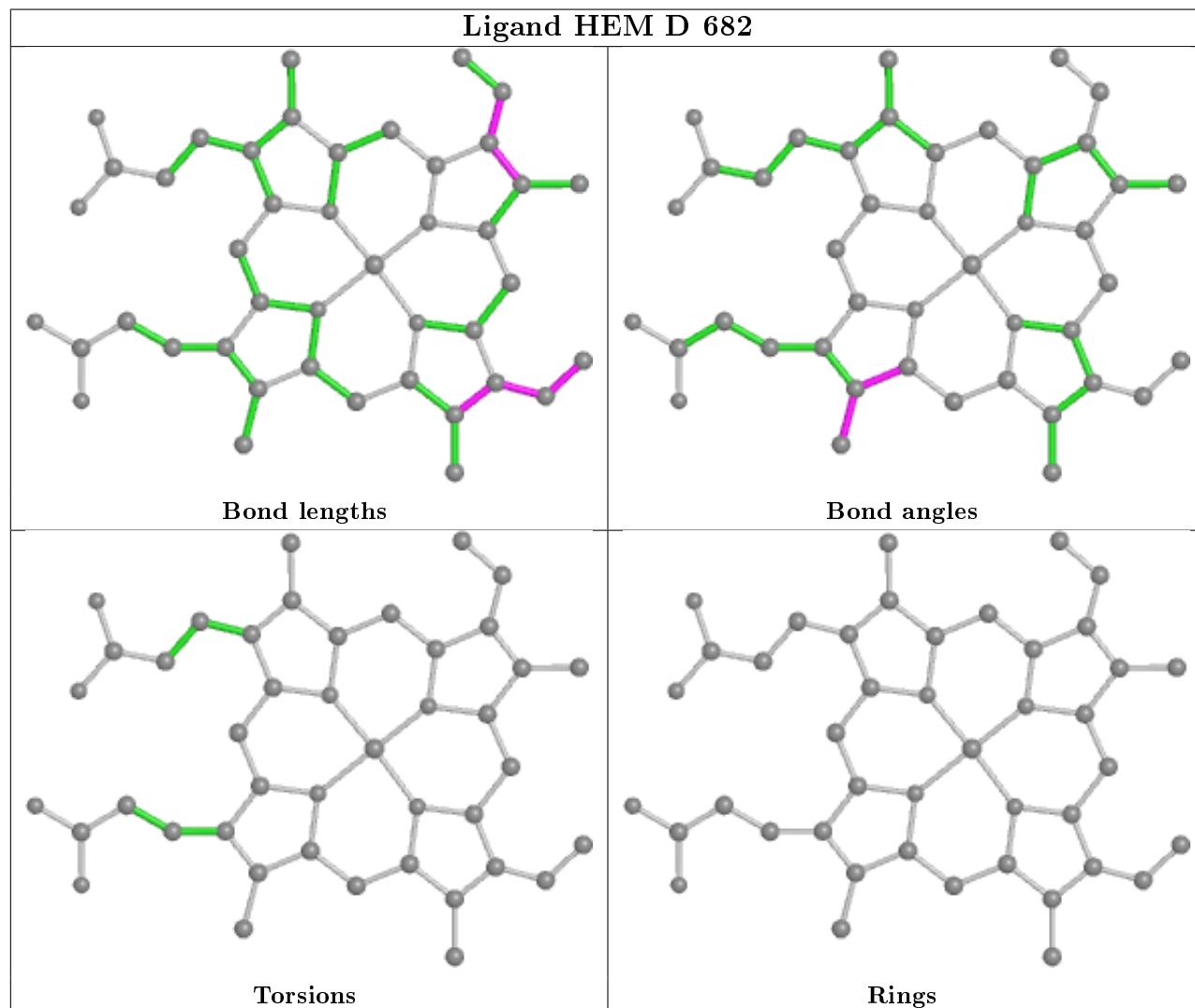
There are no ring outliers.

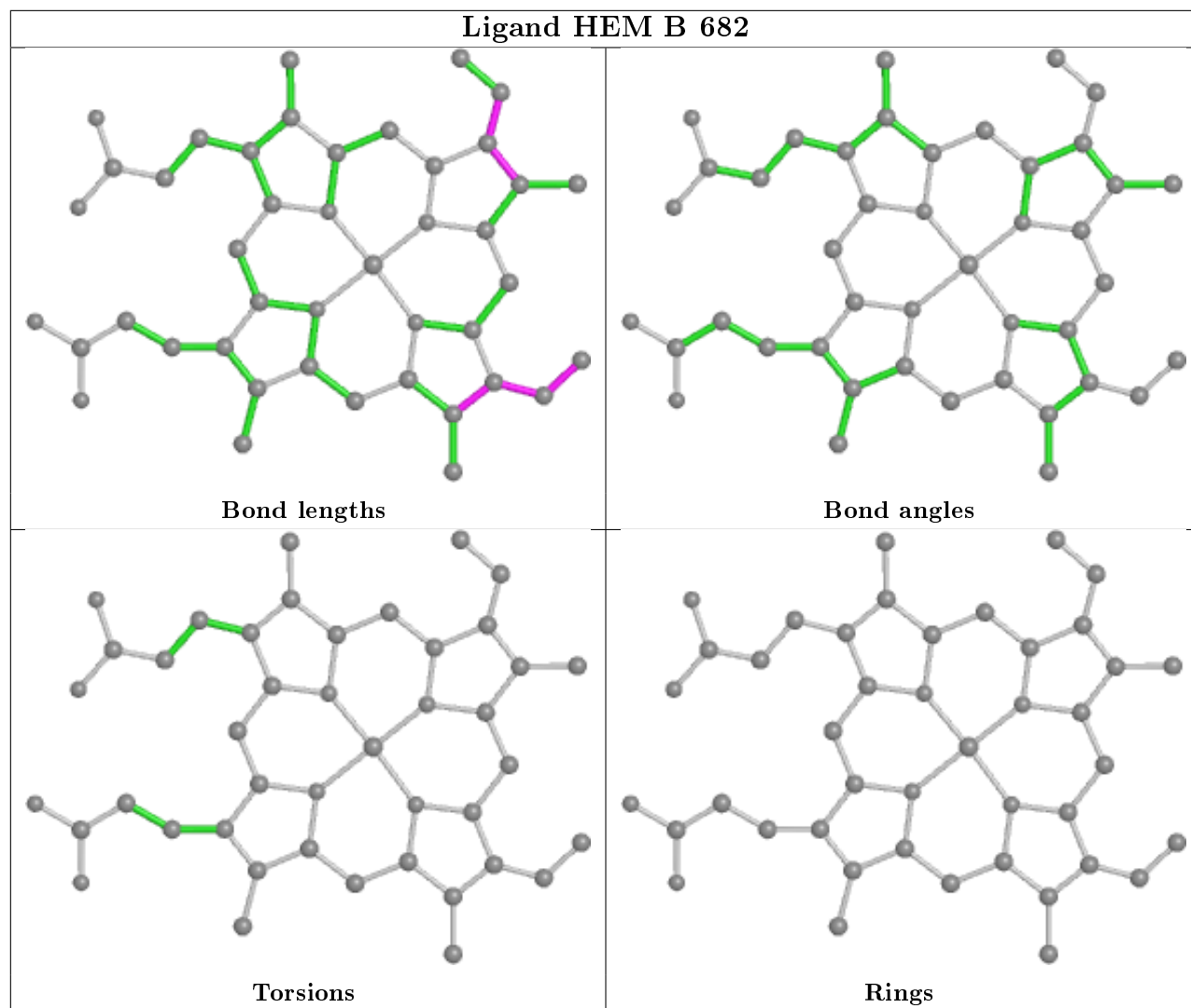
9 monomers are involved in 16 short contacts:

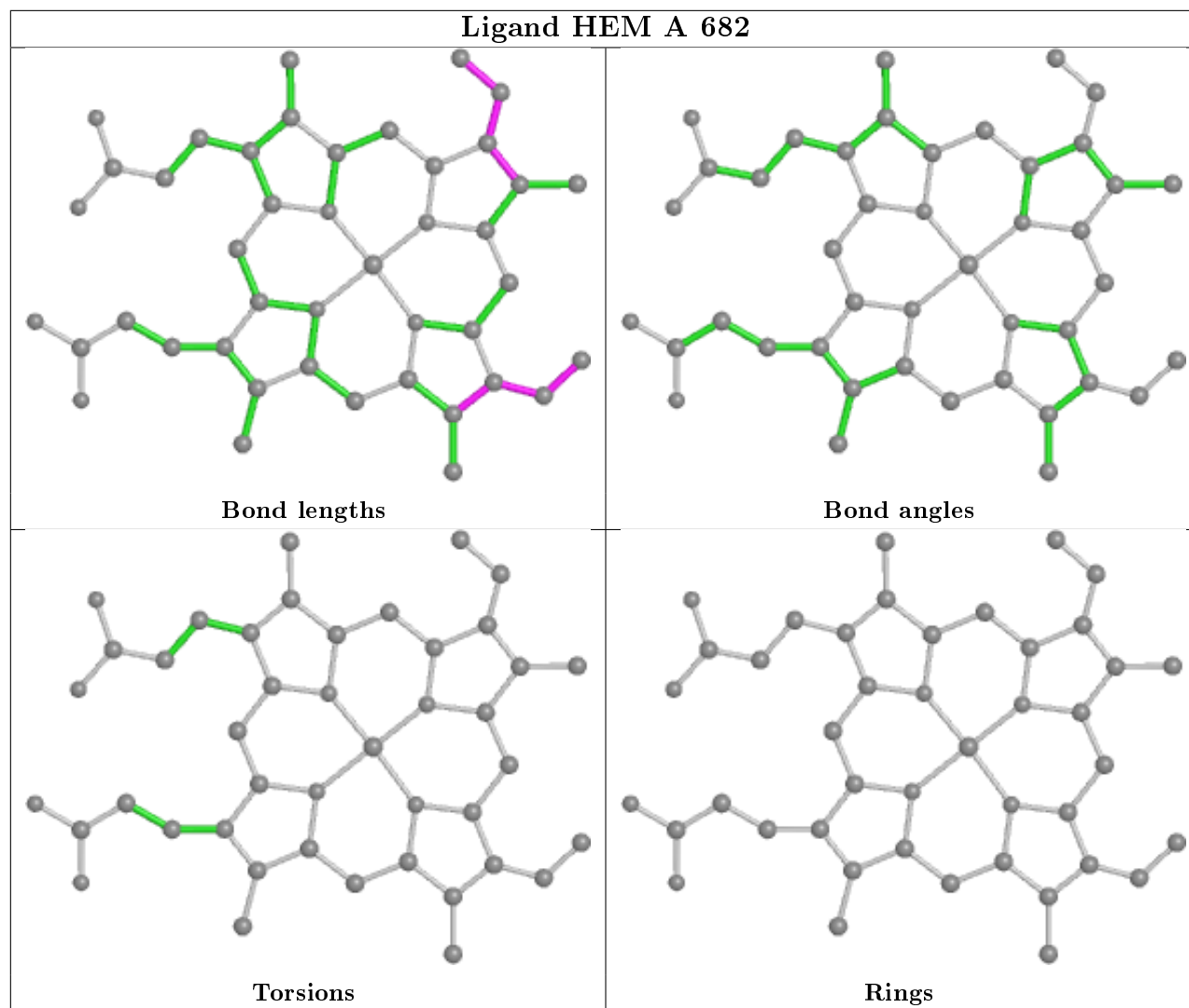
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	661	NAG	2	0
2	D	661	NAG	1	0
3	D	682	HEM	2	0
3	B	682	HEM	2	0
2	D	681	NAG	4	0
3	A	682	HEM	1	0
2	B	681	NAG	1	0
2	C	671	NAG	1	0
3	C	682	HEM	2	0

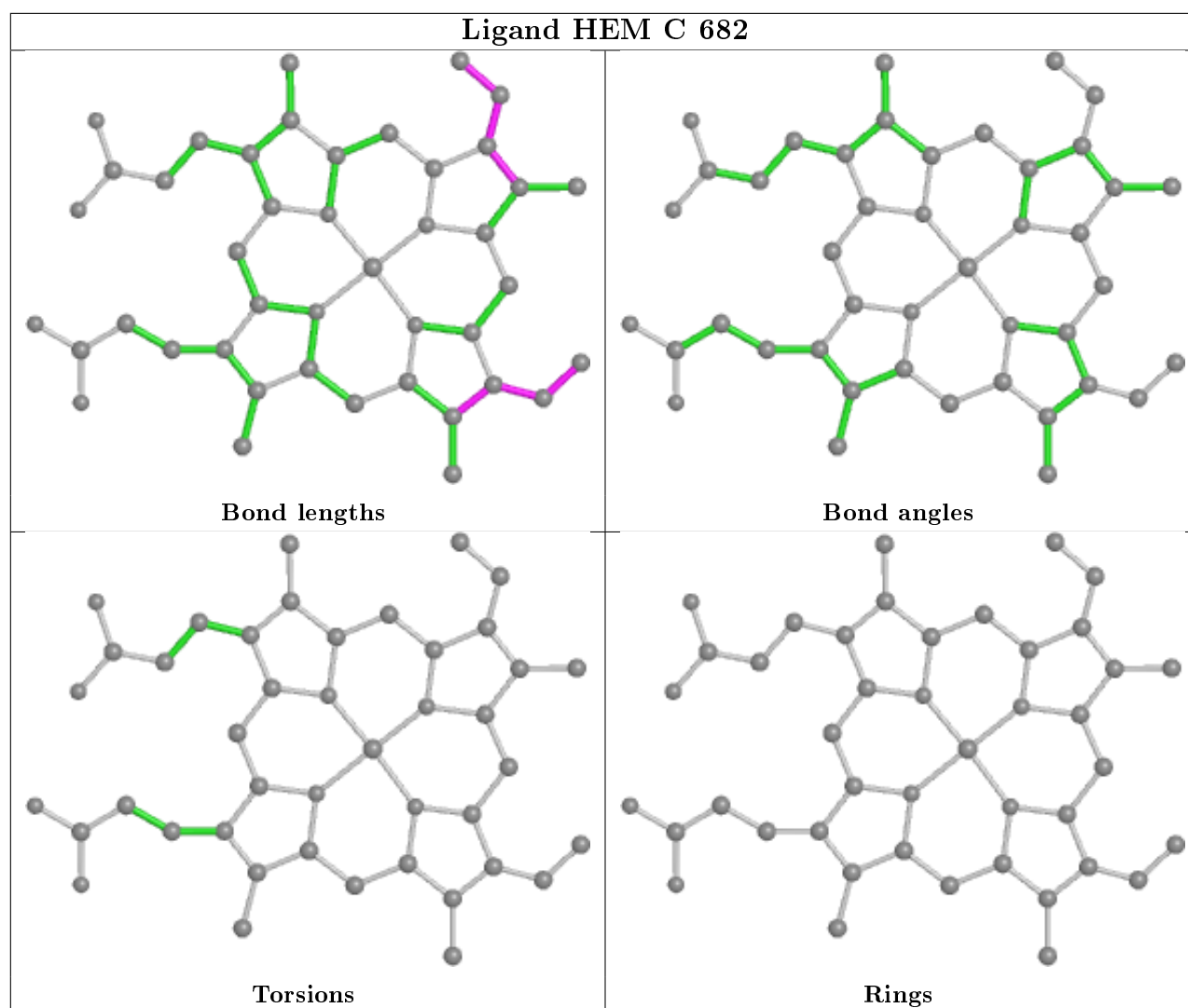
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

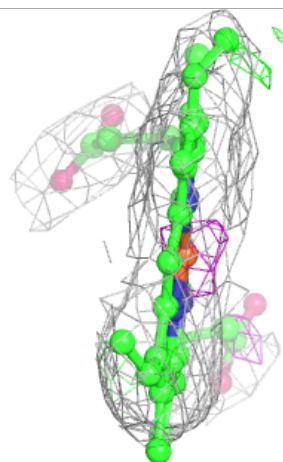
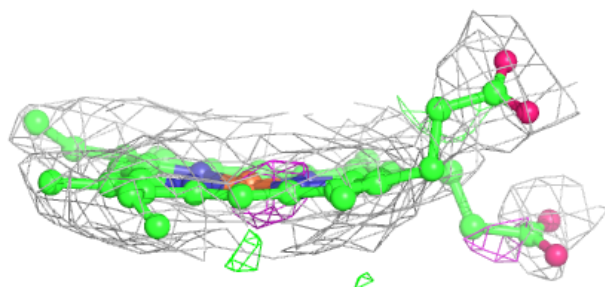
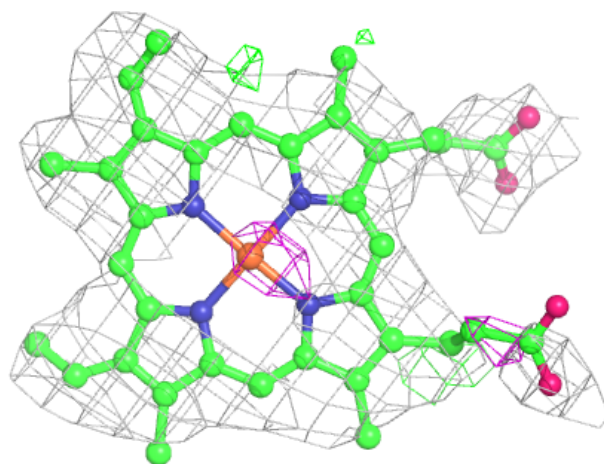
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

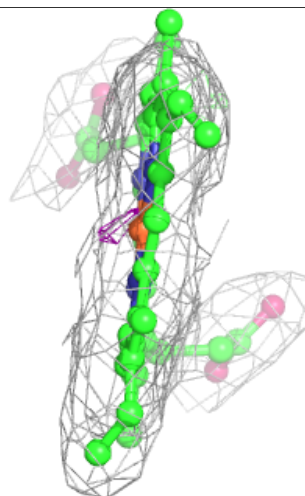
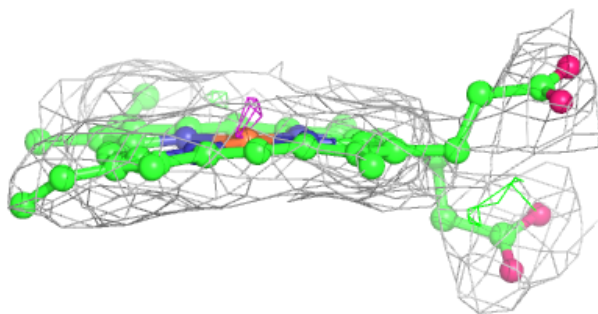
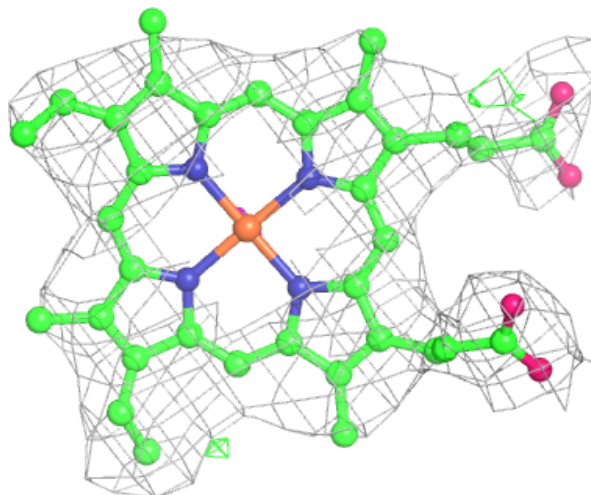
Electron density around HEM D 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



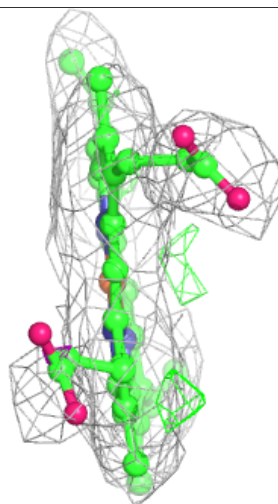
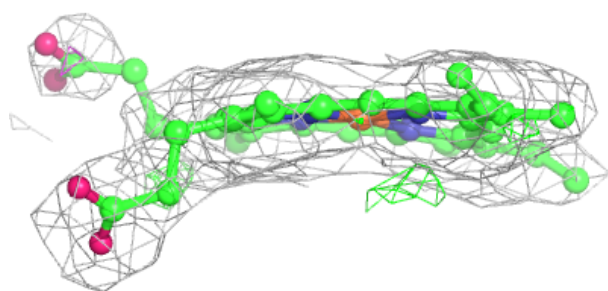
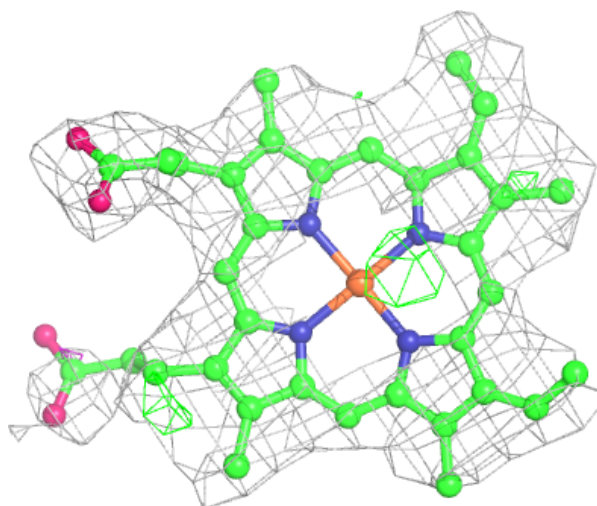
Electron density around HEM B 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



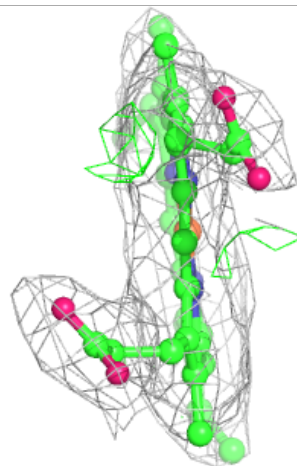
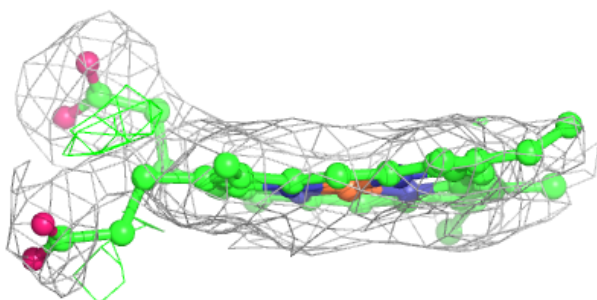
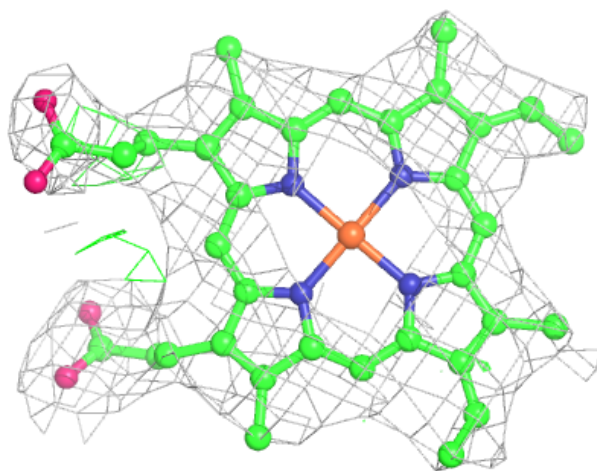
Electron density around HEM A 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 682:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.