



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:58 PM UTC

PDB ID : 5COX / pdb_00005cox
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

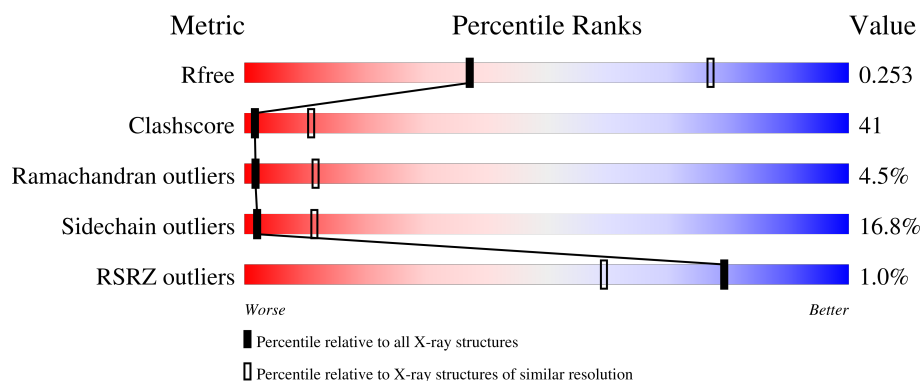
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	587	
1	B	587	
1	C	587	
1	D	587	

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.

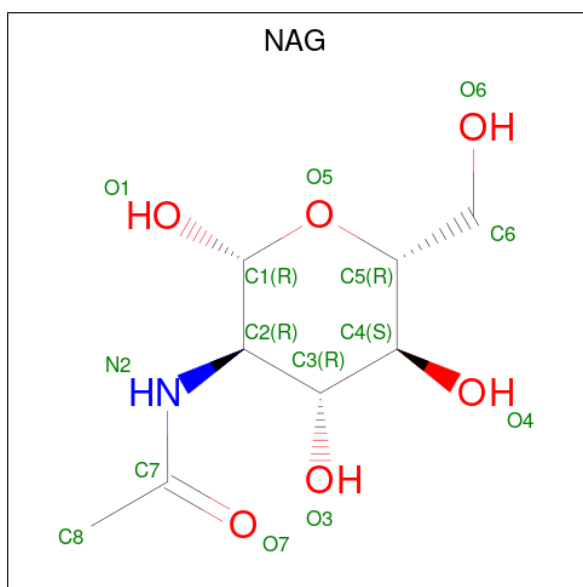
- Molecule 1 is a protein called CYCLOOXYGENASE-2.

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:

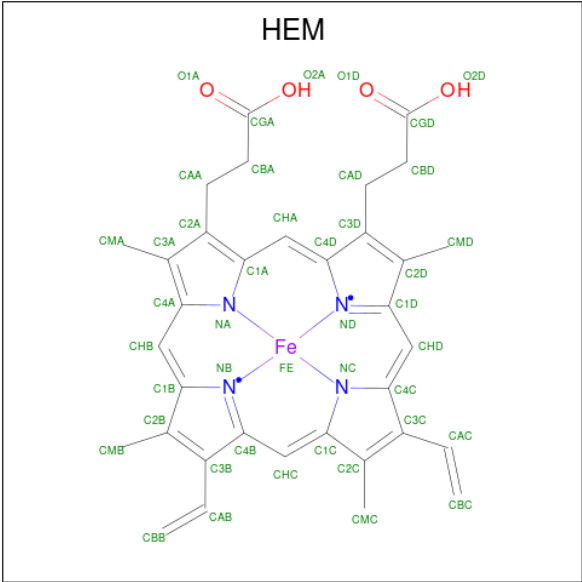
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769
C	310	GLN	ASN	conflict	UNP Q05769
C	333	LYS	ARG	conflict	UNP Q05769
D	310	GLN	ASN	conflict	UNP Q05769
D	333	LYS	ARG	conflict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

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

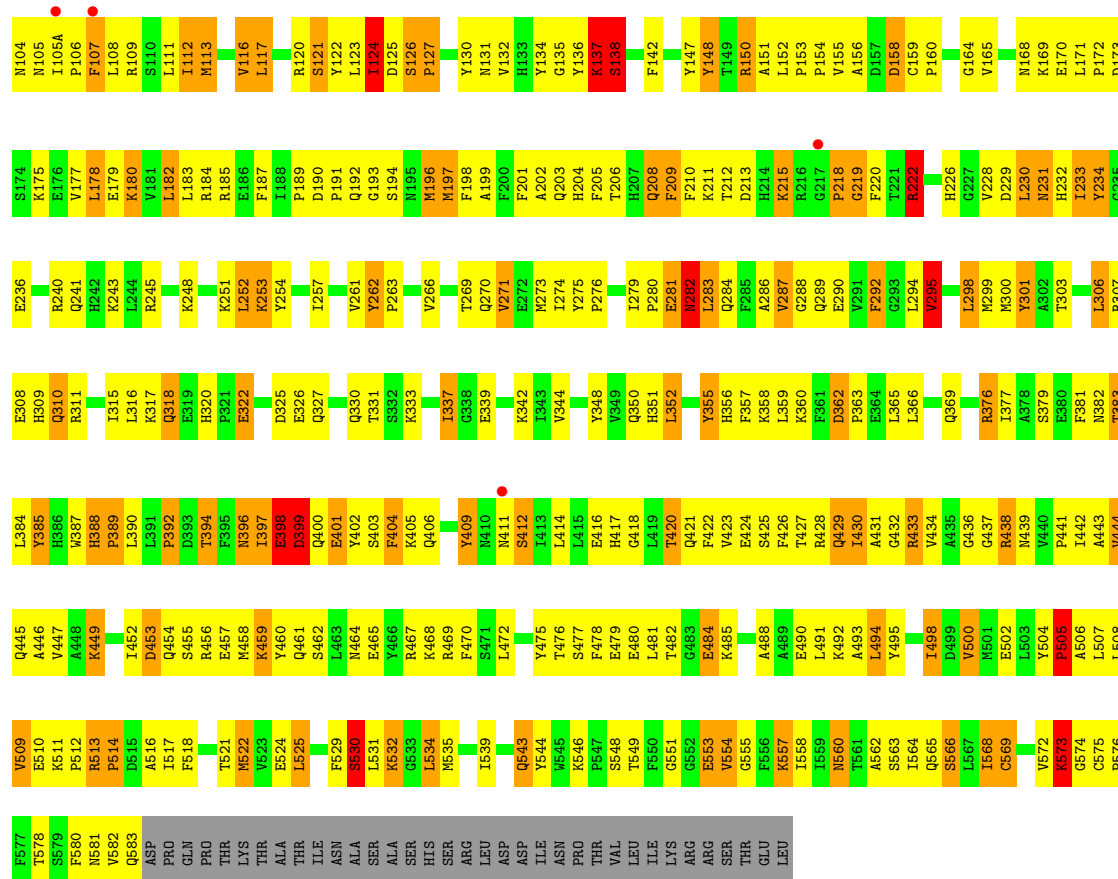


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

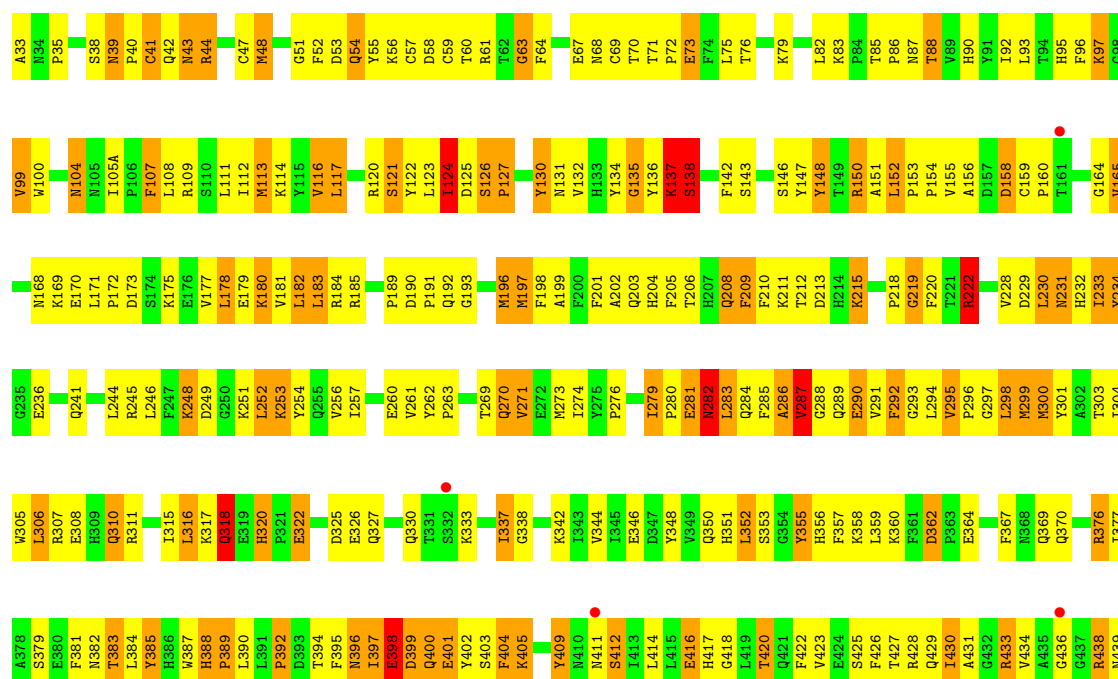
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

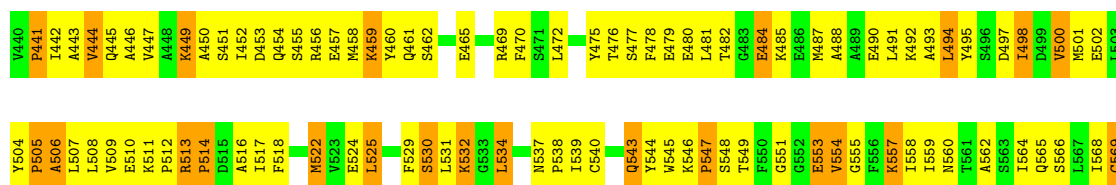


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

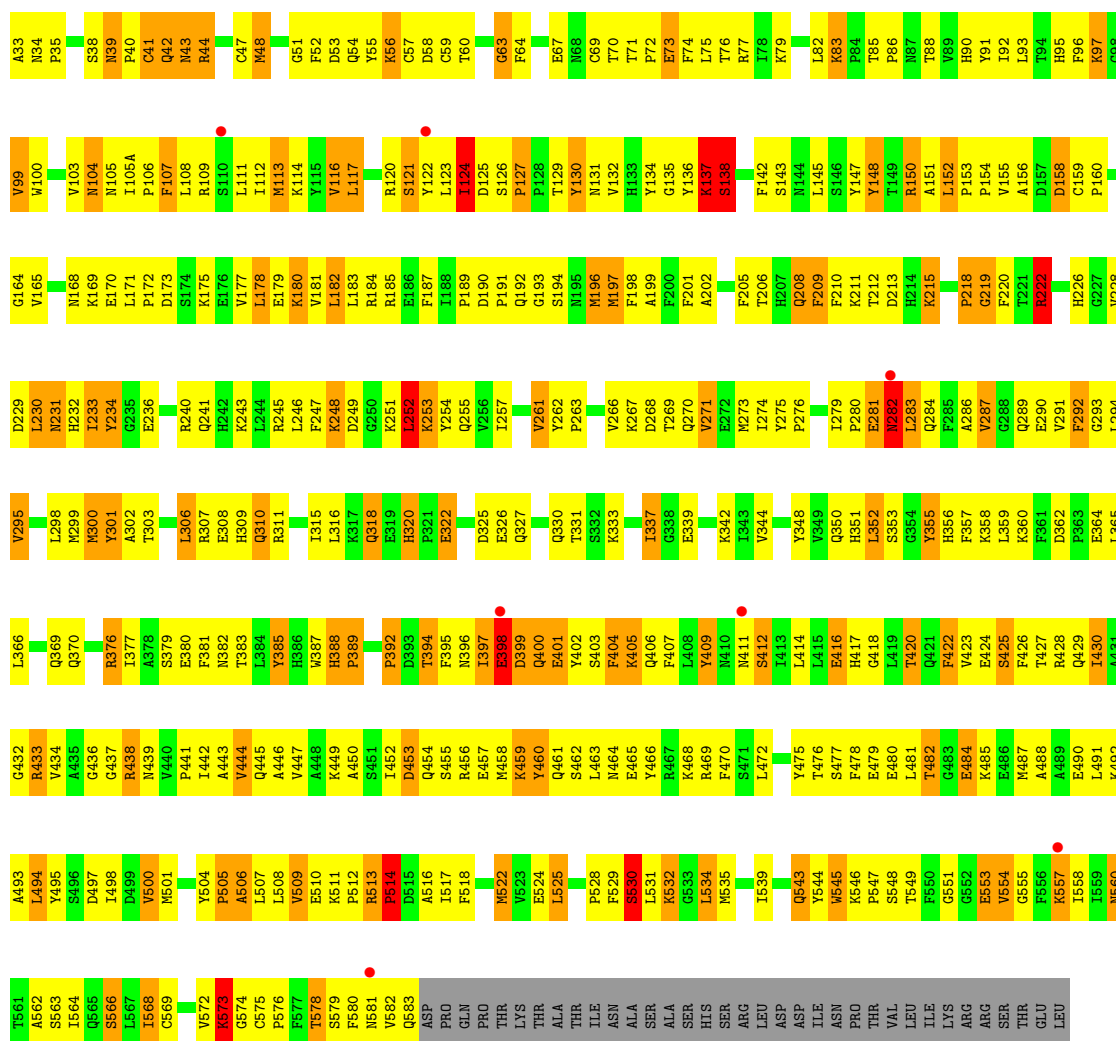


• Molecule 1: CYCLOOXYGENASE-2





● Molecule 1: CYCLOOXYGENASE-2



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	180.46Å 134.42Å 119.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 8.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	74.3 (8.00-3.00) 80.9 (8.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.98Å)	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)	0.33 , 68.9	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.88	2/4600 (0.0%)	1.30	52/6237 (0.8%)
1	B	0.88	3/4600 (0.1%)	1.31	60/6237 (1.0%)
1	C	0.85	1/4600 (0.0%)	1.30	61/6237 (1.0%)
1	D	0.85	2/4600 (0.0%)	1.30	60/6237 (1.0%)
All	All	0.87	8/18400 (0.0%)	1.30	233/24948 (0.9%)

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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	THR	CA-C	7.71	1.56	1.52
1	B	295	VAL	CA-CB	6.22	1.62	1.54
1	D	388	HIS	CG-CD2	6.14	1.42	1.35
1	A	413	ILE	CA-CB	5.45	1.60	1.54
1	B	112	ILE	CA-CB	5.43	1.60	1.54
1	B	388	HIS	CG-CD2	5.28	1.41	1.35
1	A	388	HIS	CA-C	5.16	1.59	1.52
1	C	299	MET	SD-CE	5.14	1.92	1.79

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	LYS	N-CA-C	11.79	124.13	111.28
1	B	137	LYS	N-CA-C	11.72	124.06	111.28
1	C	355	TYR	N-CA-C	11.70	127.69	113.41
1	A	137	LYS	N-CA-C	11.60	123.93	111.28
1	C	137	LYS	N-CA-C	11.02	123.29	111.28
1	B	355	TYR	N-CA-C	10.85	126.65	113.41
1	D	355	TYR	N-CA-C	10.79	126.58	113.41
1	A	355	TYR	N-CA-C	10.01	126.78	113.97
1	B	127	PRO	CA-C-N	9.93	130.02	119.89
1	B	127	PRO	C-N-CA	9.93	130.02	119.89
1	A	127	PRO	CA-C-N	9.88	129.97	119.89
1	A	127	PRO	C-N-CA	9.88	129.97	119.89
1	B	99	VAL	N-CA-C	-9.65	101.16	110.42
1	D	127	PRO	CA-C-N	9.42	129.50	119.89
1	D	127	PRO	C-N-CA	9.42	129.50	119.89
1	D	130	TYR	N-CA-C	9.21	121.62	110.19
1	D	99	VAL	N-CA-C	-9.20	101.59	110.42
1	B	130	TYR	N-CA-C	9.16	121.55	110.19
1	D	208	GLN	N-CA-C	-9.05	101.80	113.12
1	B	208	GLN	N-CA-C	-8.91	101.99	113.12
1	A	99	VAL	N-CA-C	-8.80	101.97	110.42
1	C	513	ARG	N-CA-C	-8.76	98.71	109.83
1	C	99	VAL	N-CA-C	-8.69	102.08	110.42
1	A	148	TYR	N-CA-C	-8.55	95.83	109.59
1	D	148	TYR	N-CA-C	-8.52	95.88	109.59
1	A	130	TYR	N-CA-C	8.51	120.74	110.19
1	B	148	TYR	N-CA-C	-8.35	96.15	109.59
1	B	513	ARG	N-CA-C	-8.31	98.61	110.08
1	C	318	GLN	N-CA-C	-8.30	101.81	111.03
1	C	130	TYR	N-CA-C	8.30	120.48	110.19
1	D	513	ARG	N-CA-C	-8.10	99.54	109.83
1	B	287	VAL	N-CA-C	8.05	126.08	109.34
1	B	121	SER	N-CA-C	7.96	122.25	112.23
1	C	234	TYR	N-CA-C	7.90	123.02	113.23
1	D	287	VAL	N-CA-C	7.83	125.63	109.34
1	A	287	VAL	N-CA-C	7.73	125.42	109.34
1	A	222	ARG	N-CA-C	-7.70	102.98	113.30
1	C	388	HIS	CA-CB-CG	-7.70	106.10	113.80
1	A	513	ARG	N-CA-C	-7.62	100.16	109.83
1	D	121	SER	N-CA-C	7.58	121.78	112.23
1	C	287	VAL	N-CA-C	7.51	124.97	109.34
1	A	234	TYR	N-CA-C	7.49	122.52	113.23
1	B	234	TYR	N-CA-C	7.49	122.52	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	SER	N-CA-C	7.46	121.62	112.23
1	C	148	TYR	N-CA-C	-7.44	97.55	109.76
1	C	127	PRO	CA-C-N	7.37	129.05	119.84
1	C	127	PRO	C-N-CA	7.37	129.05	119.84
1	C	121	SER	N-CA-C	7.27	121.39	112.23
1	B	553	GLU	N-CA-C	-7.26	104.57	113.50
1	B	449	LYS	N-CA-C	-7.15	103.09	111.03
1	B	560	ASN	N-CA-C	7.09	121.38	112.87
1	A	281	GLU	N-CA-C	-7.05	95.78	110.80
1	C	546	LYS	CA-C-N	7.03	128.63	119.84
1	C	546	LYS	C-N-CA	7.03	128.63	119.84
1	C	449	LYS	N-CA-C	-7.01	103.56	111.14
1	C	43	ASN	N-CA-C	6.99	121.13	111.90
1	D	234	TYR	N-CA-C	6.98	121.89	113.23
1	B	388	HIS	CA-CB-CG	-6.93	106.87	113.80
1	C	185	ARG	N-CA-C	-6.85	102.30	111.96
1	C	281	GLU	N-CA-C	-6.79	96.34	110.80
1	A	43	ASN	N-CA-C	6.78	120.84	111.90
1	A	558	ILE	N-CA-C	-6.77	103.92	110.42
1	A	388	HIS	CA-CB-CG	-6.76	107.04	113.80
1	D	388	HIS	CA-CB-CG	-6.73	107.07	113.80
1	B	63	GLY	N-CA-C	-6.71	105.85	115.64
1	B	318	GLN	N-CA-C	-6.70	103.59	111.03
1	D	553	GLU	N-CA-C	-6.68	105.28	113.50
1	A	208	GLN	N-CA-C	-6.67	103.18	112.45
1	D	63	GLY	N-CA-C	-6.66	105.66	115.72
1	B	281	GLU	N-CA-C	-6.63	96.68	110.80
1	A	125	ASP	N-CA-C	6.59	118.89	108.67
1	B	286	ALA	N-CA-C	6.58	118.34	111.03
1	A	318	GLN	N-CA-C	-6.56	103.75	111.03
1	D	573	LYS	N-CA-C	6.55	124.76	110.80
1	D	306	LEU	N-CA-C	-6.54	104.07	111.07
1	B	546	LYS	CA-C-N	6.50	127.97	119.84
1	B	546	LYS	C-N-CA	6.50	127.97	119.84
1	A	57	CYS	N-CA-C	6.49	119.31	108.73
1	A	449	LYS	N-CA-C	-6.46	104.16	111.14
1	D	449	LYS	N-CA-C	-6.46	103.86	111.03
1	C	218	PRO	N-CA-C	-6.45	101.74	111.41
1	D	222	ARG	N-CA-C	-6.44	104.67	113.30
1	B	222	ARG	N-CA-C	-6.41	104.71	113.30
1	C	222	ARG	N-CA-C	-6.39	104.74	113.30
1	A	546	LYS	CA-C-N	6.39	127.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	546	LYS	C-N-CA	6.39	127.82	119.84
1	A	573	LYS	N-CA-C	6.38	124.39	110.80
1	B	573	LYS	N-CA-C	6.37	124.37	110.80
1	D	286	ALA	N-CA-C	6.37	118.10	111.03
1	D	560	ASN	N-CA-C	6.36	120.50	112.87
1	A	73	GLU	N-CA-C	-6.34	100.18	110.20
1	C	57	CYS	N-CA-C	6.33	118.84	108.52
1	C	63	GLY	N-CA-C	-6.31	106.19	115.72
1	D	43	ASN	N-CA-C	6.30	120.30	112.24
1	A	370	GLN	N-CA-C	-6.27	99.78	109.76
1	C	125	ASP	N-CA-C	6.25	118.35	108.67
1	C	573	LYS	N-CA-C	6.21	124.03	110.80
1	A	138	SER	N-CA-C	6.19	123.98	110.80
1	C	124	ILE	N-CA-C	6.17	118.25	108.87
1	D	283	LEU	N-CA-C	-6.16	105.04	114.16
1	D	546	LYS	CA-C-N	6.10	127.47	119.84
1	D	546	LYS	C-N-CA	6.10	127.47	119.84
1	B	138	SER	N-CA-C	6.10	123.80	110.80
1	B	43	ASN	N-CA-C	6.08	119.93	111.90
1	C	208	GLN	N-CA-C	-6.07	104.02	112.45
1	D	218	PRO	N-CA-C	-6.05	102.34	111.41
1	D	138	SER	N-CA-C	5.99	123.55	110.80
1	B	219	GLY	N-CA-C	-5.97	107.59	114.69
1	C	138	SER	N-CA-C	5.97	123.51	110.80
1	D	281	GLU	N-CA-C	-5.95	98.13	110.80
1	D	266	VAL	N-CA-C	-5.92	103.65	111.05
1	C	558	ILE	N-CA-C	-5.91	104.75	110.42
1	D	558	ILE	N-CA-C	-5.91	104.75	110.42
1	C	283	LEU	N-CA-C	-5.87	105.48	114.16
1	A	423	VAL	N-CA-C	-5.86	104.61	111.00
1	B	433	ARG	N-CA-C	-5.84	102.26	110.50
1	D	528	PRO	N-CA-C	-5.83	105.13	113.47
1	B	423	VAL	N-CA-C	-5.83	104.65	111.00
1	C	182	LEU	N-CA-C	5.83	120.17	111.96
1	B	41	CYS	N-CA-C	5.79	117.90	108.63
1	B	306	LEU	N-CA-C	-5.79	104.87	111.07
1	D	404	PHE	N-CA-C	-5.79	104.87	111.07
1	B	558	ILE	N-CA-C	-5.78	104.29	110.36
1	A	182	LEU	N-CA-C	5.77	120.09	111.96
1	C	165	VAL	N-CA-C	-5.77	108.23	113.71
1	A	440	VAL	N-CA-C	5.76	112.81	107.56
1	B	498	ILE	N-CA-C	-5.76	104.90	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	GLU	N-CA-C	-5.76	101.10	110.20
1	C	180	LYS	N-CA-C	5.76	117.25	110.97
1	B	218	PRO	N-CA-C	-5.74	102.81	111.41
1	D	57	CYS	N-CA-C	5.72	118.29	109.07
1	D	401	GLU	N-CA-C	-5.72	99.10	108.76
1	B	57	CYS	N-CA-C	5.72	118.27	109.07
1	C	370	GLN	N-CA-C	-5.71	100.51	109.25
1	B	362	ASP	CA-C-N	5.68	126.94	119.84
1	B	362	ASP	C-N-CA	5.68	126.94	119.84
1	A	498	ILE	N-CA-C	-5.67	104.00	111.09
1	B	388	HIS	ND1-CE1-NE2	5.66	114.06	108.40
1	B	432	GLY	N-CA-C	5.63	119.40	112.14
1	C	41	CYS	N-CA-C	5.62	117.62	108.63
1	B	125	ASP	N-CA-C	5.62	117.38	108.67
1	D	182	LEU	N-CA-C	5.60	119.86	111.96
1	D	482	THR	N-CA-C	5.60	117.47	111.36
1	C	433	ARG	N-CA-C	-5.59	102.61	110.50
1	D	433	ARG	N-CA-C	-5.59	102.62	110.50
1	D	73	GLU	N-CA-C	-5.59	101.37	110.20
1	C	143	SER	N-CA-C	5.58	118.55	111.69
1	B	502	GLU	N-CA-C	5.58	117.27	110.41
1	C	362	ASP	CA-C-N	5.57	126.81	119.84
1	C	362	ASP	C-N-CA	5.57	126.81	119.84
1	C	359	LEU	N-CA-C	-5.57	102.78	110.35
1	B	404	PHE	N-CA-C	-5.55	105.13	111.07
1	D	135	GLY	N-CA-C	-5.54	107.03	115.66
1	A	41	CYS	N-CA-C	5.53	117.48	108.63
1	C	135	GLY	N-CA-C	-5.52	108.09	115.32
1	A	124	ILE	N-CA-C	5.51	117.83	109.12
1	C	388	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	B	266	VAL	N-CA-C	-5.50	104.17	111.05
1	D	388	HIS	CB-CG-CD2	-5.50	124.06	131.20
1	D	530	SER	N-CA-C	5.49	118.44	111.69
1	B	180	LYS	N-CA-C	5.48	116.94	110.97
1	B	212	THR	N-CA-C	5.47	117.95	110.24
1	B	453	ASP	N-CA-C	5.47	117.24	111.28
1	C	279	ILE	N-CA-C	-5.45	103.02	108.96
1	B	401	GLU	N-CA-C	-5.42	99.60	108.76
1	D	422	PHE	N-CA-C	-5.41	99.28	110.80
1	D	432	GLY	N-CA-C	5.40	119.11	112.14
1	C	212	THR	N-CA-C	5.40	117.91	110.35
1	D	125	ASP	N-CA-C	5.40	117.03	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	180	LYS	N-CA-C	5.40	116.85	110.97
1	C	233	ILE	CB-CA-C	-5.39	105.15	111.94
1	D	252	LEU	N-CA-C	-5.39	103.28	110.55
1	C	401	GLU	N-CA-C	-5.37	99.68	108.76
1	D	212	THR	N-CA-C	5.36	117.86	110.35
1	D	219	GLY	N-CA-C	-5.36	108.31	114.69
1	A	63	GLY	N-CA-C	-5.35	107.64	115.72
1	B	283	LEU	N-CA-C	-5.34	106.25	114.16
1	D	359	LEU	N-CA-C	-5.33	102.98	110.50
1	A	212	THR	N-CA-C	5.33	117.76	110.24
1	A	180	LYS	N-CA-C	5.32	116.77	110.97
1	A	306	LEU	N-CA-C	-5.31	105.39	111.07
1	D	364	GLU	N-CA-C	5.31	117.97	111.82
1	C	286	ALA	N-CA-C	5.30	116.91	111.03
1	A	207	HIS	N-CA-C	5.29	119.61	113.20
1	B	530	SER	N-CA-C	5.29	118.20	111.69
1	D	388	HIS	ND1-CE1-NE2	5.29	113.69	108.40
1	B	135	GLY	N-CA-C	-5.28	107.43	115.66
1	C	395	PHE	N-CA-C	-5.26	99.94	108.52
1	B	73	GLU	N-CA-C	-5.26	101.89	110.20
1	B	124	ILE	N-CA-C	5.25	117.42	109.12
1	C	88	THR	N-CA-C	-5.25	105.25	110.97
1	D	370	GLN	N-CA-C	-5.24	101.23	109.25
1	C	502	GLU	N-CA-C	5.22	116.83	110.41
1	D	233	ILE	CB-CA-C	-5.22	105.36	111.94
1	B	182	LEU	N-CA-C	5.21	119.31	111.96
1	C	553	GLU	N-CA-C	-5.21	106.78	113.23
1	B	359	LEU	N-CA-C	-5.20	103.17	110.50
1	C	404	PHE	N-CA-C	-5.20	105.51	111.07
1	C	306	LEU	N-CA-C	-5.19	105.51	111.07
1	A	179	GLU	N-CA-C	5.18	116.74	111.14
1	D	453	ASP	N-CA-C	5.18	116.93	111.28
1	D	41	CYS	N-CA-C	5.17	116.90	108.63
1	D	124	ILE	N-CA-C	5.17	117.29	109.12
1	A	135	GLY	N-CA-C	-5.16	108.26	114.66
1	A	218	PRO	N-CA-C	-5.16	103.67	111.41
1	D	423	VAL	N-CA-C	-5.15	105.38	111.00
1	A	422	PHE	N-CA-C	-5.14	99.85	110.80
1	C	346	GLU	N-CA-C	5.14	119.40	113.18
1	C	183	LEU	N-CA-C	5.14	116.92	110.24
1	A	401	GLU	N-CA-C	-5.14	100.08	108.76
1	A	320	HIS	CA-C-N	5.13	124.93	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	HIS	C-N-CA	5.13	124.93	119.28
1	B	85	THR	CA-C-N	5.13	125.17	119.32
1	B	85	THR	C-N-CA	5.13	125.17	119.32
1	C	320	HIS	CA-C-N	5.13	124.92	119.28
1	C	320	HIS	C-N-CA	5.13	124.92	119.28
1	A	283	LEU	N-CA-C	-5.12	106.58	114.16
1	C	498	ILE	N-CA-C	-5.12	104.69	111.09
1	B	233	ILE	CB-CA-C	-5.11	105.50	111.94
1	B	298	LEU	N-CA-C	-5.11	104.65	111.24
1	C	530	SER	N-CA-C	5.10	117.96	111.69
1	D	143	SER	N-CA-C	5.10	117.96	111.69
1	A	233	ILE	CB-CA-C	-5.09	105.25	111.92
1	C	219	GLY	N-CA-C	-5.08	108.64	114.69
1	D	320	HIS	CA-C-N	5.06	124.72	119.56
1	D	320	HIS	C-N-CA	5.06	124.72	119.56
1	A	432	GLY	N-CA-C	5.04	118.64	112.14
1	A	502	GLU	N-CA-C	5.02	116.59	110.41
1	B	388	HIS	CA-C-N	5.02	126.12	119.84
1	B	388	HIS	C-N-CA	5.02	126.12	119.84
1	A	219	GLY	N-CA-C	-5.02	108.72	114.69
1	A	346	GLU	N-CA-C	5.02	119.25	113.18
1	A	388	HIS	CB-CG-CD2	-5.01	124.69	131.20

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	369	0
1	B	4473	0	4375	362	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4473	0	4374	368	0
1	D	4473	0	4374	405	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	1466	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 41.

All (1466) 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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:83:LYS:HZ2	1:D:83:LYS:HA	1.52	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:A:211:LYS:HZ1	1:A:236:GLU:HG3	1.54	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:185:ARG:HE	1:D:438:ARG:HD3	1.55	0.71
1:D:211:LYS:NZ	1:D:236:GLU:HG3	2.05	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:458:MET:HE3	1:C:460:TYR:HE1	1.53	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: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:C:211:LYS:HZ1	1:C:236:GLU:HG3	1.56	0.70
1:D:506:ALA:O	1:D:510:GLU:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:283:LEU:HD13	1:A:411:ASN:HD21	1.56	0.69
1:A:398:GLU:O	1:A:399:ASP:HB2	1.91	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:A:458:MET:HE3	1:A:460:TYR:HE1	1.58	0.68
1:A:578:THR:O	1:D:267:LYS:NZ	2.26	0.68
1:B:510:GLU:O	1:B:512:PRO:HD3	1.93	0.68
1:C:211:LYS:HE2	1:C:222:ARG:HG2	1.75	0.68
1:B:97:LYS:HD3	1:B:356:HIS:CD2	2.28	0.68
1:B:557:LYS:HD3	1:B:560:ASN:HD22	1.58	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:342:LYS:HG2	1:C:562:ALA:HB3	1.74	0.68
1:C:405:LYS:H	1:C:405:LYS:HD2	1.57	0.68
1:C:454:GLN:HA	1:C:457:GLU:HG2	1.75	0.68
1:C:507:LEU:HD22	1:C:522:MET:HE3	1.76	0.68
1:D:428:ARG:HD2	1:D:428:ARG:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:406:GLN:HA	2:D:681:NAG:C8	2.24	0.67
1:D:470:PHE:CG	1:D:525:LEU:HD22	2.29	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: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
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:283:LEU:HD13	1:D:411:ASN:ND2	2.10	0.65
1:D:405:LYS:H	1:D:405:LYS:HD2	1.61	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:509:VAL:HG12	1:A:509:VAL:O	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:458:MET:HE3	1:D:460:TYR:HE1	1.61	0.64
1:A:507:LEU:HD22	1:A:522:MET:HE3	1.79	0.64
1:A:551:GLY:C	1:B:48:MET:HE1	2.22	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
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:67:GLU:HB3	2:C:661:NAG:H82	1.80	0.63
1:C:477:SER:HB2	1:C:479:GLU:OE1	1.98	0.63
1:C:230:LEU:HG	1:C:337:ILE:HG12	1.81	0.63
1:D:215:LYS:HD3	1:D:215:LYS:N	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:D:104:ASN:CG	1:D:358:LYS:HE2	2.24	0.63
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.10	0.63
1:C:306:LEU:HD23	1:C:306:LEU:C	2.24	0.63
1:B:113:MET:HE2	1:B:360:LYS:O	1.98	0.62
1:B:342:LYS:CG	1:B:562:ALA:HB3	2.29	0.62
1:A:283:LEU:HD22	1:A:411:ASN:CG	2.24	0.62
1:B:108:LEU:O	1:B:112:ILE:HG12	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:THR:OG1	1:B:488:ALA:HB2	2.00	0.62
1:C:283:LEU:HD22	1:C:411:ASN:CG	2.24	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:D:411:ASN:CG	1:D:412:SER:N	2.56	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:H	1:A:405:LYS:HD2	1.63	0.62
1:A:454:GLN:HA	1:A:457:GLU:HG2	1.80	0.62
1:B:39:ASN:N	1:B:40:PRO:HD3	2.15	0.62
1:B:131:ASN:ND2	1:B:147:TYR:CD2	2.68	0.62
1:C:58:ASP:HB2	1:D:548:SER:OG	2.00	0.61
1:C:131:ASN:HA	1:C:150:ARG:HB2	1.82	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:B:190:ASP:OD1	1:B:517:ILE:HB	2.00	0.61
1:B:281:GLU:HA	1:B:284:GLN:HE21	1.65	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
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:A:582:VAL:O	1:A:582:VAL:HG13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:ARG:HH11	1:B:44:ARG:CG	2.14	0.61
1:B:282:ASN:OD1	1:B:282:ASN:N	2.31	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:A:577:PHE:HE1	1:D:267:LYS:HD2	1.65	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: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:D:113:MET:HE2	1:D:360:LYS:O	2.01	0.60
1:D:180:LYS:HD3	1:D:490:GLU:CD	2.26	0.60
1:A:113:MET:HE2	1:A:360:LYS:O	2.01	0.60
1:B:398:GLU:HB2	1:B:425:SER:OG	2.00	0.60
1:C:197:MET:HA	1:C:197:MET:HE3	1.82	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:B:458:MET:HE3	1:B:460:TYR:HE1	1.66	0.60
1:C:160:PRO:HG2	1:C:165:VAL:HA	1.83	0.60
1:C:411:ASN:CG	1:C:412:SER:N	2.59	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:D:306:LEU:C	1:D:306:LEU:HD23	2.27	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:C:211:LYS:HZ1	1:C:236:GLU:CG	2.15	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:43:ASN:HB2	1:D:69:CYS:O	2.02	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:B:160:PRO:HG2	1:B:165:VAL:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:411:ASN:CG	1:A:412:SER:N	2.60	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:A:168:ASN:CG	1:A:169:LYS:N	2.60	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:H	1:A:405:LYS:CD	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:B:306:LEU:C	1:B:306:LEU:HD23	2.27	0.59
1:C:113:MET:HE2	1:C:360:LYS:O	2.02	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:N	1:A:525:LEU:HD23	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:43:ASN:ND2	1:C:64:PHE:CD2	2.72	0.58
1:C:208:GLN:HE21	1:C:228:VAL:HA	1.64	0.58
1:D:211:LYS:HE2	1:D:222:ARG:HG2	1.85	0.58
1:D:500:VAL:HG12	1:D:500:VAL:O	2.03	0.58
1:B:35:PRO:HD3	1:B:52:PHE:O	2.02	0.58
1:B:182:LEU:O	1:B:438:ARG:HA	2.03	0.58
1:B:434:VAL:H	1:B:517:ILE:HG13	1.67	0.58
1:C:206:THR:HB	1:C:210:PHE:CD2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASP:HB2	1:D:54:GLN:OE1	2.03	0.58
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:N	1:A:282:ASN:OD1	2.36	0.58
1:C:95:HIS:O	1:C:100:TRP:HD1	1.87	0.58
1:D:507:LEU:HD22	1:D:522:MET:CE	2.33	0.58
1:D:509:VAL:HG12	1:D:509:VAL:O	2.02	0.58
1:C:112:ILE:HB	1:C:357:PHE:CZ	2.39	0.58
1:D:230:LEU:N	1:D:230:LEU:HD23	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: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:CD1	1:B:107:PHE:N	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: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:43:ASN:HB2	1:B:69:CYS:O	2.03	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: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:C:509:VAL:HG12	1:C:509:VAL:O	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:LYS:HD3	1:C:356:HIS:NE2	2.19	0.57
1:C:160:PRO:HG3	1:C:165:VAL:HG23	1.87	0.57
1:D:160:PRO:HG3	1:D:165:VAL:HG23	1.86	0.57
1:D:282:ASN:N	1:D:282:ASN:OD1	2.36	0.57
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.17	0.57
1:A:107:PHE:CD1	1:A:107:PHE:N	2.73	0.57
1:A:306:LEU:HD23	1:A:306:LEU:C	2.30	0.57
1:C:44:ARG:CG	1:C:44:ARG:HH11	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: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:48:MET:HE1	1:B:551:GLY:C	2.30	0.56
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.41	0.56
1:B:64:PHE:CE2	1:B:72:PRO:HB3	2.39	0.56
1:B:418:GLY:O	1:B:422:PHE:HB2	2.05	0.56
1:C:136:TYR:CE2	1:D:327:GLN:HG3	2.40	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:D:394:THR:HA	1:D:402:TYR:O	2.05	0.56
1:D:574:GLY:C	1:D:576:PRO:HD3	2.31	0.56
1:A:172:PRO:HG2	1:A:495:TYR:CE1	2.41	0.56
1:A:178:LEU:O	1:A:182:LEU:HB2	2.05	0.56
1:B:183:LEU:HD22	1:B:442:ILE:HG13	1.87	0.56
1:C:48:MET:HE1	1:D:551:GLY:C	2.30	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:A:443:ALA:C	1:A:445:GLN:H	2.14	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
1:C:303:THR:HG22	1:C:307:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:VAL:O	1:C:582:VAL:HG13	2.05	0.56
1:D:192:GLN:HG3	1:D:516:ALA:HA	1.87	0.56
1:D:261:VAL:O	1:D:307:ARG:NH1	2.39	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:411:ASN:CG	1:B:412:SER:N	2.64	0.56
1:B:428:ARG:HD2	1:B:428:ARG:N	2.21	0.56
1:D:85:THR:HG23	1:D:88:THR:H	1.70	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:B:428:ARG:HA	1:B:582:VAL:HG23	1.88	0.56
1:C:35:PRO:HD3	1:C:52:PHE:O	2.06	0.56
1:C:178:LEU:HA	1:C:182:LEU:HD12	1.86	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:O	1:D:582:VAL:HG13	2.05	0.56
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:107:PHE:CD1	1:D:107:PHE:N	2.75	0.55
1:A:404:PHE:H	1:A:405:LYS:HZ2	1.54	0.55
1:A:418:GLY:O	1:A:422:PHE:HB2	2.06	0.55
1:B:494:LEU:H	1:B:494:LEU:HD12	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:203:GLN:HE22	3:C:682:HEM:HBB2	1.72	0.55
1:C:229:ASP:OD1	1:C:231:ASN:HB3	2.07	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:35:PRO:HD3	1:D:52:PHE:O	2.07	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
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:C:276:PRO:HG2	1:C:409:TYR:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:TYR:O	1:D:95:HIS:HD2	1.90	0.55
1:D:230:LEU:HD23	1:D:230:LEU:H	1.71	0.55
1:B:180:LYS:HD3	1:B:490:GLU:CD	2.32	0.55
1:B:500:VAL:HG12	1:B:500:VAL:O	2.05	0.55
1:B:554:VAL:HG12	1:B:555:GLY:N	2.21	0.55
1:C:197:MET:HA	1:C:197:MET:CE	2.37	0.55
1:B:35:PRO:HG3	1:B:54:GLN:O	2.06	0.55
1:B:196:MET:HE1	1:B:392:PRO:HD3	1.89	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:B:443:ALA:C	1:B:445:GLN:H	2.15	0.55
1:C:420:THR:HG22	1:C:576:PRO:HG3	1.89	0.55
1:C:443:ALA:C	1:C:445:GLN:H	2.14	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:97:LYS:HB2	1:A:356:HIS:CE1	2.42	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: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:HD12	1:D:494:LEU:H	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:427:THR:HG22	1:A:583:GLN:HE22	1.73	0.54
1:A:436:GLY:HA2	1:A:512:PRO:HD3	1.89	0.54
1:B:95:HIS:O	1:B:100:TRP:HD1	1.91	0.54
1:B:104:ASN:CG	1:B:358:LYS:HE2	2.33	0.54
1:B:381:PHE:HD1	1:B:529:PHE:HD2	1.55	0.54
1:C:525:LEU:N	1:C:525:LEU:HD23	2.22	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:190:ASP:O	1:B:430:ILE:HD11	2.08	0.54
1:B:303:THR:HG22	1:B:307:ARG:HD2	1.90	0.54
1:B:406:GLN:HG2	2:B:681:NAG:O7	2.07	0.54
1:C:180:LYS:HD3	1:C:490:GLU:CD	2.33	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:H	1:D:405:LYS:CD	2.19	0.54
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.43	0.53
1:B:197:MET:HE3	1:B:197:MET:HA	1.89	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:281:GLU:C	1:A:283:LEU:H	2.15	0.53
1:A:148:TYR:HD2	1:A:219:GLY:C	2.15	0.53
1:A:208:GLN:HE21	1:A:228:VAL:HA	1.73	0.53
1:A:292:PHE:O	1:A:299:MET:HE2	2.08	0.53
1:B:85:THR:OG1	1:B:86:PRO:HD2	2.08	0.53
1:B:479:GLU:HG3	1:B:488:ALA:HB1	1.91	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:B:582:VAL:O	1:B:582:VAL:HG13	2.07	0.53
1:C:85:THR:OG1	1:C:86:PRO:HD2	2.08	0.53
1:D:198:PHE:CD1	1:D:198:PHE:C	2.86	0.53
1:D:254:TYR:CD1	1:D:254:TYR:C	2.87	0.53
1:C:198:PHE:C	1:C:198:PHE:CD1	2.87	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:33:ALA:N	1:D:158:ASP:O	2.41	0.53
1:D:142:PHE:O	1:D:376:ARG:NH2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:N	1:A:39:ASN:HD22	2.07	0.53
1:A:192:GLN:HG3	1:A:516:ALA:HA	1.90	0.53
1:D:95:HIS:O	1:D:100:TRP:HD1	1.91	0.53
1:A:43:ASN:HB2	1:A:69:CYS:O	2.08	0.53
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.43	0.53
1:D:320:HIS:HE1	1:D:551:GLY:O	1.91	0.53
1:A:85:THR:HG23	1:A:88:THR:H	1.74	0.53
1:B:74:PHE:O	1:B:77:ARG:HB2	2.09	0.53
1:B:412:SER:O	1:B:416:GLU:N	2.42	0.53
1:A:453:ASP:O	1:A:456:ARG:HB2	2.08	0.52
1:A:494:LEU:HD12	1:A:494:LEU:H	1.74	0.52
1:B:281:GLU:HG2	1:B:282:ASN:H	1.73	0.52
1:C:39:ASN:N	1:C:39:ASN:HD22	2.07	0.52
1:C:127:PRO:HD2	1:D:543:GLN:HE22	1.75	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:197:MET:HE3	1:D:197:MET:HA	1.89	0.52
1:D:557:LYS:HA	1:D:560:ASN:HB2	1.90	0.52
1:A:198:PHE:HB2	1:A:580:PHE:HB3	1.91	0.52
1:A:457:GLU:C	1:A:459:LYS:H	2.17	0.52
1:A:510:GLU:HG2	1:A:511:LYS:N	2.23	0.52
1:B:120:ARG:HG2	1:B:531:LEU:HD12	1.90	0.52
1:B:198:PHE:CD1	1:B:198:PHE:C	2.88	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:428:ARG:HA	1:D:582:VAL:HG23	1.91	0.52
1:D:477:SER:HB2	1:D:479:GLU:OE1	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:GLN:HE22	3:A:682:HEM:HBB2	1.75	0.52
1:A:428:ARG:HA	1:A:582:VAL:HG23	1.92	0.52
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:A:172:PRO:HG2	1:A:495:TYR:CD1	2.45	0.52
1:A:198:PHE:CD1	1:A:198:PHE:C	2.88	0.52
1:A:251:LYS:CG	1:A:310:GLN:HG3	2.38	0.52
1:A:308:GLU:OE1	1:A:311:ARG:HD3	2.09	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:193:GLY:HA3	1:B:581:ASN:OD1	2.11	0.51
1:B:226:HIS:ND1	1:B:376:ARG:HD2	2.25	0.51
1:B:281:GLU:C	1:B:283:LEU:H	2.16	0.51
1:B:507:LEU:HD22	1:B:522:MET:HE3	1.93	0.51
1:B:575:CYS:N	1:B:576:PRO:HD3	2.24	0.51
1:C:281:GLU:C	1:C:283:LEU:H	2.18	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:148:TYR:HD2	1:C:219:GLY:C	2.18	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:197:MET:HE3	1:A:197:MET:HA	1.92	0.51
1:A:276:PRO:HG2	1:A:409:TYR:CD2	2.45	0.51
1:D:281:GLU:C	1:D:283:LEU:H	2.18	0.51
1:A:322:GLU:HB3	1:B:52:PHE:CD1	2.45	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: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:196:MET:HE1	1:C:392:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:507:LEU:HD22	1:D:522:MET:HE3	1.91	0.51
1:B:191:PRO:HD2	1:B:433:ARG:HG3	1.92	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:A:444:VAL:O	1:A:444:VAL:HG12	2.09	0.51
1:B:48:MET:O	1:B:48:MET:HG3	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
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: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: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: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:C:68:ASN:ND2	2:C:661:NAG:O7	2.44	0.51
1:C:105(A):ILE:HD12	1:C:108:LEU:HD12	1.93	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:C:104:ASN:CG	1:C:358:LYS:HE2	2.36	0.51
1:A:104:ASN:CG	1:A:358:LYS:HE2	2.36	0.50
1:A:462:SER:HB3	1:A:465:GLU:HG2	1.93	0.50
1:B:51:GLY:O	1:B:52:PHE:HB2	2.11	0.50
1:B:213:ASP:OD1	1:B:215:LYS:HG2	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:NH1	1:A:150:ARG:HG2	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:254:TYR:CD1	1:B:254:TYR:C	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:168:ASN:C	1:C:170:GLU:N	2.68	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:420:THR:HG22	1:D:576:PRO:HG3	1.92	0.50
1:D:464:ASN:O	1:D:468:LYS:HG3	2.11	0.50
1:C:387:TRP:HB2	3:C:682:HEM:CBC	2.41	0.50
1:A:150:ARG:CG	1:A:150:ARG:HH11	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:273:MET:HE2	1:A:287:VAL:HG22	1.92	0.50
1:A:479:GLU:HG2	1:A:485:LYS:CE	2.42	0.50
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: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:443:ALA:C	1:D:445:GLN:H	2.20	0.50
1:D:462:SER:HB3	1:D:465:GLU:HG2	1.93	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: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:B:478:PHE:HD1	1:B:478:PHE:H	1.60	0.50
1:B:498:ILE:C	1:B:500:VAL:H	2.20	0.50
1:C:286:ALA:O	1:C:287:VAL:HG22	2.12	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:153:PRO:O	1:D:461:GLN:NE2	2.45	0.50
1:D:318:GLN:C	1:D:318:GLN:CD	2.79	0.50
1:D:452:ILE:O	1:D:456:ARG:HG2	2.11	0.50
1:A:172:PRO:HG2	1:A:495:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:HA	1:A:183:LEU:HD12	1.94	0.49
1:A:190:ASP:OD1	1:A:517:ILE:HB	2.12	0.49
1:C:88:THR:O	1:C:92:ILE:HG13	2.11	0.49
1:C:444:VAL:HG12	1:C:444:VAL:O	2.12	0.49
1:D:39:ASN:N	1:D:39:ASN:HD22	2.10	0.49
1:D:196:MET:HB3	1:D:426:PHE:CG	2.47	0.49
1:D:454:GLN:HA	1:D:457:GLU:CG	2.41	0.49
1:A:327:GLN:HG3	1:B:136:TYR:CE2	2.47	0.49
1:A:428:ARG:HG3	1:A:583:GLN:OE1	2.12	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:82:LEU:HD12	1:B:82:LEU:N	2.28	0.49
1:B:197:MET:HA	1:B:197:MET:CE	2.42	0.49
1:C:90:HIS:HD2	1:C:513:ARG:NH1	2.11	0.49
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.94	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:196:MET:HB3	1:B:426:PHE:CG	2.48	0.49
1:B:230:LEU:N	1:B:230:LEU:HD23	2.28	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: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:D:151:ALA:O	1:D:469:ARG:NH1	2.46	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:457:GLU:C	1:D:459:LYS:H	2.20	0.49
1:B:234:TYR:HH	1:B:309:HIS:CE1	2.29	0.49
1:D:44:ARG:CG	1:D:44:ARG:NH1	2.75	0.49
1:A:196:MET:HE1	1:A:392:PRO:HD3	1.94	0.49
1:B:263:PRO:HD3	1:B:303:THR:HG23	1.94	0.49
1:C:457:GLU:C	1:C:459:LYS:H	2.19	0.49
1:D:350:GLN:HE22	1:D:358:LYS:HA	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:574:GLY:C	1:C:576:PRO:HD3	2.38	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:44:ARG:HH11	1:B:44:ARG:HG3	1.78	0.49
1:B:240:ARG:HH12	1:B:271:VAL:HG23	1.77	0.49
1:B:457:GLU:C	1:B:459:LYS:H	2.20	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:O	1:B:522:MET:HG3	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:273:MET:HE2	1:C:287:VAL:HG22	1.95	0.48
1:C:557:LYS:HA	1:C:560:ASN:HB2	1.95	0.48
1:D:152:LEU:HD23	1:D:469:ARG:HG2	1.94	0.48
1:D:201:PHE:HA	1:D:301:TYR:CE2	2.48	0.48
1:B:183:LEU:O	1:B:438:ARG:HB3	2.13	0.48
1:B:398:GLU:H	1:B:425:SER:HB3	1.78	0.48
1:D:103:VAL:C	1:D:105:ASN:H	2.21	0.48
1:D:113:MET:O	1:D:116:VAL:HG13	2.13	0.48
1:D:196:MET:HE1	1:D:392:PRO:HD3	1.95	0.48
1:D:202:ALA:HB2	1:D:348:TYR:CE2	2.49	0.48
1:D:281:GLU:CA	1:D:284:GLN:HE21	2.25	0.48
1:A:472:LEU:HD11	1:A:524:GLU:HB2	1.95	0.48
1:D:97:LYS:HB2	1:D:356:HIS:CE1	2.49	0.48
1:D:105:ASN:O	1:D:106:PRO:HD3	2.13	0.48
1:D:172:PRO:HG2	1:D:495:TYR:CD2	2.48	0.48
1:D:184:ARG:HB2	1:D:439:ASN:C	2.37	0.48
1:D:215:LYS:HD3	1:D:215:LYS:H	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:HA	1:A:83:LYS:NZ	2.28	0.48
1:D:231:ASN:OD1	1:D:231:ASN:C	2.57	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:498:ILE:C	1:D:500:VAL:H	2.22	0.48
1:D:564:ILE:HG12	1:D:580:PHE:CZ	2.49	0.48
1:A:498:ILE:C	1:A:500:VAL:H	2.22	0.48
1:B:151:ALA:O	1:B:469:ARG:NH1	2.47	0.48
1:B:168:ASN:C	1:B:170:GLU:N	2.71	0.48
1:B:462:SER:HB3	1:B:465:GLU:HG2	1.96	0.48
1:B:525:LEU:N	1:B:525:LEU:HD23	2.28	0.48
1:C:501:MET:HE3	1:C:506:ALA:HB2	1.96	0.48
1:C:551:GLY:C	1:D:48:MET:HE1	2.39	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
1:B:88:THR:O	1:B:92:ILE:HG13	2.14	0.48
1:B:153:PRO:O	1:B:461:GLN:NE2	2.47	0.48
1:C:172:PRO:HG2	1:C:495:TYR:CE2	2.48	0.48
1:D:168:ASN:CG	1:D:169:LYS:N	2.72	0.48
1:D:564:ILE:HG12	1:D:580:PHE:CE1	2.49	0.48
1:A:318:GLN:CD	1:A:318:GLN:C	2.82	0.48
1:B:442:ILE:O	1:B:445:GLN:HG2	2.13	0.48
1:C:569:CYS:HA	1:C:575:CYS:HA	1.96	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:PHE:O	1:C:299:MET:HE2	2.14	0.47
1:C:402:TYR:OH	1:C:417:HIS:CE1	2.67	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: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:B:404:PHE:HE2	1:B:444:VAL:HG23	1.80	0.47
1:D:185:ARG:HH21	1:D:438:ARG:NE	2.11	0.47
1:A:478:PHE:HD1	1:A:478:PHE:H	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:D:544:TYR:O	1:D:549:THR:OG1	2.30	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:97:LYS:HB2	1:C:356:HIS:CE1	2.50	0.47
1:C:172:PRO:HG2	1:C:495:TYR:CD2	2.49	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:338:GLY:C	1:C:559:ILE:HG23	2.40	0.47
1:C:479:GLU:HA	1:C:488:ALA:CB	2.44	0.47
1:D:51:GLY:O	1:D:52:PHE:HB2	2.14	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:283:LEU:HD22	1:B:411:ASN:OD1	2.14	0.47
1:B:574:GLY:C	1:B:576:PRO:HD3	2.40	0.47
1:C:104:ASN:HB3	1:C:358:LYS:HE2	1.96	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:D:206:THR:HG21	1:D:385:TYR:CD1	2.49	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:B:33:ALA:HB3	1:B:158:ASP:OD2	2.14	0.47
1:B:209:PHE:O	1:B:377:ILE:HD12	2.15	0.47
1:B:254:TYR:HD2	1:B:310:GLN:HE21	1.63	0.47
1:B:482:THR:HB	1:B:484:GLU:HG3	1.96	0.47
1:D:96:PHE:HB3	1:D:99:VAL:CG2	2.44	0.47
1:D:197:MET:HA	1:D:197:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HG2	1:A:360:LYS:HB3	1.97	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:300:MET:HE3	1:A:300:MET:HB3	1.79	0.47
1:A:482:THR:HB	1:A:484:GLU:HG3	1.96	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:C:403:SER:HB2	1:C:405:LYS:HZ3	1.80	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:51:GLY:O	1:C:52:PHE:HB2	2.15	0.46
1:C:281:GLU:HA	1:C:284:GLN:HG3	1.97	0.46
1:D:97:LYS:HD3	1:D:356:HIS:CG	2.51	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
1:D:412:SER:HB2	2:D:681:NAG:H62	1.97	0.46
1:D:532:LYS:O	1:D:534:LEU:N	2.48	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:HA	1:A:197:MET:CE	2.45	0.46
1:C:88:THR:HG22	1:C:92:ILE:CD1	2.41	0.46
1:C:287:VAL:HG23	1:C:288:GLY:N	2.31	0.46
1:A:204:HIS:ND1	1:A:292:PHE:CE2	2.83	0.46
1:A:522:MET:O	1:A:522:MET:HG3	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:137:LYS:NZ	1:B:543:GLN:O	2.44	0.46
1:A:190:ASP:O	1:A:430:ILE:HD11	2.16	0.46
1:A:396:ASN:ND2	1:A:401:GLU:HG2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	1:A:150:ARG:CG	2.78	0.46
1:B:117:LEU:HD21	1:B:535:MET:HE2	1.97	0.46
1:B:350:GLN:HE22	1:B:358:LYS:HA	1.81	0.46
1:C:92:ILE:HG13	1:C:92:ILE:H	1.58	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:D:578:THR:O	1:D:579:SER:HB2	2.15	0.46
1:A:44:ARG:HH11	1:A:44:ARG:HG3	1.81	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:421:GLN:HA	1:A:421:GLN:OE1	2.15	0.46
1:C:33:ALA:N	1:C:158:ASP:O	2.49	0.46
1:C:196:MET:CE	1:C:392:PRO:HD3	2.46	0.46
1:C:232:HIS:HD2	1:C:233:ILE:N	2.14	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:126:SER:CB	1:A:532:LYS:HZ1	2.29	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:38:SER:OG	1:B:40:PRO:HG3	2.16	0.46
1:B:232:HIS:HD2	1:B:233:ILE:N	2.14	0.46
1:B:464:ASN:O	1:B:468:LYS:HG3	2.15	0.46
1:C:35:PRO:HG3	1:C:54:GLN:O	2.15	0.46
1:C:204:HIS:ND1	1:C:292:PHE:CE2	2.83	0.46
1:C:263:PRO:HD3	1:C:303:THR:HG23	1.97	0.46
1:D:273:MET:HE2	1:D:287:VAL:HG22	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:HG2	1:B:283:LEU:HD12	1.97	0.45
1:C:184:ARG:HB2	1:C:439:ASN:C	2.42	0.45
1:A:92:ILE:HA	1:A:96:PHE:CE2	2.52	0.45
1:A:574:GLY:C	1:A:576:PRO:HD3	2.40	0.45
1:B:184:ARG:HB2	1:B:439:ASN:C	2.41	0.45
1:B:191:PRO:HG3	1:B:433:ARG:NH1	2.31	0.45
1:D:522:MET:HE3	1:D:522:MET:HB2	1.64	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:88:THR:HG22	1:B:92:ILE:CD1	2.42	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:C:283:LEU:CD1	1:C:411:ASN:HD21	2.23	0.45
1:C:295:VAL:HG12	1:C:297:GLY:H	1.81	0.45
1:C:510:GLU:HG2	1:C:511:LYS:N	2.32	0.45
1:D:40:PRO:HB2	1:D:55:TYR:CE2	2.51	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:A:149:THR:O	1:A:378:ALA:HA	2.17	0.45
1:A:299:MET:HE2	1:A:299:MET:HB2	1.89	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
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: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:A:184:ARG:HB2	1:A:439:ASN:C	2.42	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:C:63:GLY:HA2	1:C:73:GLU:CD	2.42	0.45
1:D:182:LEU:HD22	1:D:508:LEU:HD12	1.98	0.45
1:A:92:ILE:HA	1:A:96:PHE:HE2	1.80	0.45
1:A:151:ALA:O	1:A:469:ARG:NH1	2.49	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:86:PRO:HG2	1:C:87:ASN:ND2	2.32	0.45
1:C:320:HIS:HE1	1:C:551:GLY:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:LYS:O	1:C:534:LEU:N	2.50	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:HD2	1:D:573:LYS:O	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:83:LYS:HZ1	1:B:84:PRO:HD2	1.81	0.45
1:B:85:THR:HG22	1:B:88:THR:HG1	1.75	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:273:MET:HE2	1:B:287:VAL:HG22	1.98	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
1:D:454:GLN:C	1:D:456:ARG:N	2.75	0.45
1:D:501:MET:HE3	1:D:506:ALA:H	1.81	0.45
1:A:52:PHE:CD1	1:B:322:GLU:HB3	2.52	0.44
1:A:283:LEU:HD22	1:A:411:ASN:ND2	2.32	0.44
1:B:43:ASN:ND2	1:B:64:PHE:CD2	2.85	0.44
1:B:198:PHE:HB2	1:B:580:PHE:HB3	1.99	0.44
1:B:209:PHE:O	1:B:377:ILE:CD1	2.65	0.44
1:B:215:LYS:HD3	1:B:215:LYS:N	2.32	0.44
1:B:274:ILE:HG13	1:B:290:GLU:HB2	1.99	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:D:148:TYR:HD2	1:D:219:GLY:C	2.25	0.44
1:A:58:ASP:C	1:A:60:THR:H	2.26	0.44
1:B:107:PHE:O	1:B:111:LEU:HB2	2.17	0.44
1:B:150:ARG:CG	1:B:150:ARG:NH1	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HD23	1:B:369:GLN:HG3	2.00	0.44
1:C:109:ARG:HG3	1:C:357:PHE:CE1	2.52	0.44
1:C:351:HIS:O	1:C:353:SER:N	2.50	0.44
1:C:543:GLN:NE2	1:D:127:PRO:O	2.50	0.44
1:A:168:ASN:C	1:A:170:GLU:N	2.73	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:NH1	1:C:150:ARG:HG2	2.31	0.44
1:C:210:PHE:HB3	1:C:382:ASN:ND2	2.33	0.44
1:A:42:GLN:HE21	1:A:42:GLN:HA	1.81	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:A:360:LYS:HE2	1:A:362:ASP:HB2	1.99	0.44
1:A:537:ASN:O	1:A:540:CYS:HB2	2.18	0.44
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	2.00	0.44
1:B:218:PRO:HB2	1:B:458:MET:SD	2.57	0.44
1:B:352:LEU:HD21	1:B:387:TRP:CH2	2.52	0.44
1:B:522:MET:HE3	1:B:522:MET:HB2	1.69	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: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:D:117:LEU:HD21	1:D:535:MET:HE2	1.99	0.44
1:D:248:LYS:N	1:D:325:ASP:OD1	2.50	0.44
1:D:420:THR:HG22	1:D:576:PRO:CG	2.47	0.44
1:D:475:TYR:CD1	1:D:480:GLU:HG2	2.52	0.44
1:A:53:ASP:HB2	1:A:54:GLN:OE1	2.18	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: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:92:ILE:HA	1:D:96:PHE:HE2	1.83	0.44
1:D:168:ASN:C	1:D:170:GLU:N	2.75	0.44
1:D:275:TYR:CE2	1:D:284:GLN:HA	2.53	0.44
1:D:513:ARG:O	1:D:514:PRO:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:MET:O	1:D:56:LYS:N	2.51	0.44
1:D:152:LEU:CD2	1:D:469:ARG:HG2	2.47	0.44
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.80	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:C:450:ALA:O	1:C:451:SER:C	2.61	0.44
1:C:498:ILE:C	1:C:500:VAL:H	2.26	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:63:GLY:HA2	1:D:73:GLU:CD	2.42	0.44
1:D:91:TYR:CE2	1:D:95:HIS:CE1	3.05	0.44
1:D:169:LYS:HB3	1:D:170:GLU:OE2	2.17	0.44
1:D:215:LYS:N	1:D:215:LYS:CD	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:A:40:PRO:HB2	1:A:55:TYR:CE2	2.53	0.43
1:A:122:TYR:CD1	1:A:122:TYR:C	2.96	0.43
1:A:148:TYR:CD1	1:A:377:ILE:HG13	2.53	0.43
1:A:180:LYS:HD3	1:A:490:GLU:CD	2.43	0.43
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.47	0.43
1:C:96:PHE:HB3	1:C:99:VAL:CG2	2.48	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:D:263:PRO:HD3	1:D:303:THR:HG23	1.99	0.43
1:D:351:HIS:C	1:D:353:SER:N	2.75	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:C:121:SER:C	1:C:123:LEU:N	2.76	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:318:GLN:CD	1:C:318:GLN:C	2.85	0.43
1:C:428:ARG:HG3	1:C:583:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ASN:O	1:C:441:PRO:HD3	2.18	0.43
1:D:74:PHE:O	1:D:77:ARG:HB2	2.18	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: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:210:PHE:HB3	1:B:382:ASN:ND2	2.33	0.43
1:B:253:LYS:HB2	1:B:253:LYS:NZ	2.34	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:254:TYR:CD1	1:C:254:TYR:C	2.96	0.43
1:C:428:ARG:HG3	1:C:583:GLN:CD	2.43	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:218:PRO:HB2	1:D:458:MET:SD	2.59	0.43
1:D:402:TYR:OH	1:D:417:HIS:HE1	2.00	0.43
1:A:59:CYS:HB3	1:A:64:PHE:O	2.19	0.43
1:A:152:LEU:CD2	1:A:469:ARG:HG2	2.48	0.43
1:B:366:LEU:HA	1:B:369:GLN:HG2	2.00	0.43
1:D:59:CYS:HB3	1:D:64:PHE:O	2.19	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:A:48:MET:O	1:A:48:MET:HG3	2.18	0.43
1:A:281:GLU:HG2	1:A:282:ASN:H	1.82	0.43
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.53	0.43
1:B:148:TYR:HD2	1:B:219:GLY:C	2.25	0.43
1:B:187:PHE:CD1	1:B:187:PHE:C	2.95	0.43
1:B:194:SER:OG	1:B:351:HIS:HE1	2.01	0.43
1:C:230:LEU:HD23	1:C:230:LEU:H	1.84	0.43
1:C:478:PHE:H	1:C:478:PHE:HD1	1.67	0.43
1:D:247:PHE:O	1:D:248:LYS:HB2	2.17	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:34:ASN:HA	1:B:35:PRO:HD2	1.85	0.43
1:B:150:ARG:NH1	1:B:150:ARG:HG2	2.33	0.43
1:B:193:GLY:O	1:B:582:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HD11	1:B:518:PHE:CE2	2.54	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:513:ARG:O	1:A:514:PRO:C	2.60	0.43
1:C:276:PRO:HD2	1:C:279:ILE:CG1	2.48	0.43
1:D:42:GLN:O	1:D:69:CYS:HB2	2.19	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:A:427:THR:HB	1:A:428:ARG:HD2	2.01	0.43
1:A:522:MET:HE3	1:A:522:MET:HB2	1.71	0.43
1:C:544:TYR:O	1:C:549:THR:OG1	2.28	0.43
1:A:273:MET:CE	1:A:287:VAL:HG22	2.48	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:B:454:GLN:O	1:B:455:SER:C	2.62	0.43
1:C:201:PHE:N	1:C:301:TYR:HE2	2.16	0.43
1:C:397:ILE:O	1:C:398:GLU:C	2.62	0.43
1:D:88:THR:HG22	1:D:92:ILE:CD1	2.46	0.43
1:D:172:PRO:HG2	1:D:495:TYR:CG	2.54	0.43
1:D:198:PHE:CZ	1:D:352:LEU:HD13	2.54	0.43
1:D:234:TYR:CE1	1:D:252:LEU:HD21	2.54	0.43
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.34	0.42
1:A:428:ARG:HG3	1:A:583:GLN:CD	2.44	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
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:292:PHE:O	1:B:299:MET:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:479:GLU:HG2	1:C:485:LYS:HZ1	1.82	0.42
1:D:92:ILE:HA	1:D:96:PHE:CE2	2.54	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:A:63:GLY:HA2	1:A:73:GLU:CD	2.44	0.42
1:A:74:PHE:O	1:A:77:ARG:HB2	2.18	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:B:564:ILE:HG12	1:B:580:PHE:CZ	2.54	0.42
1:C:510:GLU:HG2	1:C:511:LYS:H	1.85	0.42
1:C:522:MET:O	1:C:522:MET:HG3	2.20	0.42
1:D:568:ILE:O	1:D:572:VAL:N	2.47	0.42
3:D:682:HEM:HBC2	3:D:682:HEM:HHD	2.00	0.42
1:A:232:HIS:HD2	1:A:233:ILE:N	2.17	0.42
1:A:543:GLN:NE2	1:B:127:PRO:O	2.52	0.42
1:A:579:SER:HB2	1:D:267:LYS:NZ	2.34	0.42
1:C:423:VAL:HG13	1:C:578:THR:HG23	2.00	0.42
1:D:35:PRO:HB3	1:D:53:ASP:O	2.20	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: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:B:437:GLY:O	1:B:438:ARG:C	2.62	0.42
1:C:58:ASP:C	1:C:60:THR:H	2.28	0.42
1:C:82:LEU:N	1:C:82:LEU:HD12	2.34	0.42
1:C:130:TYR:CE2	1:C:135:GLY:O	2.73	0.42
1:C:181:VAL:HG21	1:C:491:LEU:HD21	2.02	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:398:GLU:H	1:C:425:SER:CB	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:MET:O	1:C:48:MET:HG3	2.19	0.42
1:C:231:ASN:OD1	1:C:231:ASN:C	2.61	0.42
1:C:276:PRO:HG2	1:C:409:TYR:CG	2.55	0.42
1:C:322:GLU:HB3	1:D:52:PHE:CD1	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: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:D:437:GLY:O	1:D:438:ARG:C	2.62	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:59:CYS:HB3	1:C:64:PHE:O	2.20	0.42
1:C:202:ALA:HB2	1:C:348:TYR:CE2	2.55	0.42
1:C:256:VAL:HA	1:C:260:GLU:O	2.20	0.42
1:C:283:LEU:HD22	1:C:411:ASN:ND2	2.35	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:D:92:ILE:HG13	1:D:92:ILE:H	1.58	0.42
1:D:294:LEU:HD22	1:D:409:TYR:HD1	1.83	0.42
1:A:175:LYS:HA	1:A:175:LYS:HD3	1.88	0.42
1:A:320:HIS:CE1	1:A:551:GLY:O	2.72	0.42
1:A:450:ALA:O	1:A:451:SER:C	2.60	0.42
1:A:563:SER:OG	1:A:566:SER:HB2	2.20	0.42
1:B:58:ASP:C	1:B:60:THR:H	2.27	0.42
1:B:231:ASN:OD1	1:B:231:ASN:C	2.63	0.42
1:B:478:PHE:CD1	1:B:478:PHE:N	2.87	0.42
1:C:61:ARG:NH2	1:D:545:TRP:O	2.51	0.42
1:C:298:LEU:HD12	1:C:298:LEU:HA	1.81	0.42
1:C:454:GLN:C	1:C:456:ARG:N	2.78	0.42
1:D:82:LEU:N	1:D:82:LEU:HD12	2.35	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: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:63:GLY:HA2	1:B:73:GLU:CD	2.45	0.42
1:B:73:GLU:O	1:B:76:THR:N	2.52	0.42
1:B:122:TYR:CD1	1:B:122:TYR:C	2.97	0.42
1:B:126:SER:CB	1:B:532:LYS:HZ1	2.33	0.42
1:C:105(A):ILE:O	1:C:108:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:MET:O	1:C:117:LEU:HB2	2.20	0.42
1:C:122:TYR:CD1	1:C:122:TYR:C	2.98	0.42
1:C:522:MET:HE3	1:C:522:MET:HB2	1.75	0.42
1:C:537:ASN:O	1:C:540:CYS:HB2	2.19	0.42
1:D:145:LEU:HD23	1:D:376:ARG:CZ	2.50	0.42
1:D:194:SER:OG	1:D:351:HIS:HE1	2.02	0.42
1:D:201:PHE:CA	1:D:301:TYR:CE2	3.03	0.42
1:D:501:MET:HE3	1:D:506:ALA:HB2	2.00	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:HD23	1:B:230:LEU:H	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:38:SER:OG	1:D:40:PRO:HG3	2.20	0.41
1:D:105(A):ILE:HD12	1:D:108:LEU:HD12	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:A:138:SER:HB2	1:B:330:GLN:HB3	2.01	0.41
1:B:215:LYS:HD3	1:B:215:LYS:H	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:C:443:ALA:C	1:C:445:GLN:N	2.79	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:42:GLN:O	1:B:69:CYS:HB2	2.21	0.41
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.36	0.41
1:B:475:TYR:CD2	1:B:481:LEU:HB2	2.56	0.41
1:D:130:TYR:HB3	1:D:134:TYR:O	2.21	0.41
1:D:187:PHE:CD1	1:D:187:PHE:C	2.98	0.41
1:D:522:MET:O	1:D:522:MET:HG3	2.20	0.41
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HG2	1:A:87:ASN:ND2	2.36	0.41
1:A:215:LYS:H	1:A:215:LYS:CD	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:330:GLN:HB3	1:B:138:SER:HB2	2.03	0.41
1:B:96:PHE:O	1:B:98:GLY:N	2.53	0.41
1:B:402:TYR:OH	1:B:417:HIS:CE1	2.73	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:309:HIS:O	1:D:310:GLN:C	2.64	0.41
1:D:513:ARG:O	1:D:514:PRO:O	2.39	0.41
1:A:131:ASN:O	1:A:132:VAL:C	2.63	0.41
1:A:168:ASN:CG	1:A:169:LYS:H	2.27	0.41
1:A:231:ASN:OD1	1:A:231:ASN:C	2.63	0.41
1:B:232:HIS:CD2	1:B:233:ILE:N	2.89	0.41
1:B:443:ALA:C	1:B:445:GLN:N	2.78	0.41
1:B:481:LEU:HD11	1:B:506:ALA:HB1	2.03	0.41
1:B:544:TYR:O	1:B:549:THR:OG1	2.35	0.41
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.92	0.41
1:C:126:SER:HA	1:C:127:PRO:C	2.46	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:96:PHE:O	1:A:99:VAL:N	2.54	0.41
1:A:338:GLY:HA3	1:A:559:ILE:HD13	2.03	0.41
1:A:477:SER:C	1:A:479:GLU:N	2.76	0.41
1:B:39:ASN:N	1:B:40:PRO:CD	2.83	0.41
1:C:126:SER:CB	1:C:532:LYS:HZ1	2.34	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:92:ILE:HG13	1:A:92:ILE:H	1.61	0.41
1:A:443:ALA:C	1:A:445:GLN:N	2.79	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
1:D:300:MET:HE3	1:D:300:MET:HB3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:682:HEM:HHH	3:D:682:HEM:CBH	2.51	0.41
1:A:121:SER:C	1:A:123:LEU:N	2.77	0.41
1:A:424:GLU:HA	1:A:428:ARG:HH11	1.86	0.41
1:A:481:LEU:HD12	1:A:510:GLU:HG3	2.03	0.41
1:A:573:LYS:HD2	1:A:573:LYS:O	2.21	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:248:LYS:N	1:B:325:ASP:OD1	2.54	0.41
1:B:281:GLU:C	1:B:283:LEU:N	2.77	0.41
1:B:320:HIS:CE1	1:B:551:GLY:O	2.72	0.41
1:B:394:THR:HB	1:B:396:ASN:HD21	1.86	0.41
1:B:454:GLN:C	1:B:456:ARG:N	2.78	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: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:D:121:SER:C	1:D:123:LEU:N	2.79	0.41
1:D:122:TYR:CD1	1:D:122:TYR:C	2.99	0.41
1:D:150:ARG:CG	1:D:152:LEU:O	2.69	0.41
1:A:181:VAL:HB	1:A:509:VAL:HG22	2.02	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:396:ASN:CG	1:A:401:GLU:HG2	2.45	0.41
1:A:399:ASP:HB3	1:A:400:GLN:NE2	2.28	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:292:PHE:O	1:D:299:MET:HE2	2.21	0.41
1:D:381:PHE:CD1	1:D:529:PHE:CD2	3.09	0.41
1:B:153:PRO:HG2	1:B:461:GLN:HE22	1.86	0.40
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.56	0.40
1:B:202:ALA:HB2	1:B:348:TYR:HE2	1.85	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:454:GLN:O	1:C:455:SER:C	2.63	0.40
1:C:538:PRO:HG3	1:D:142:PHE:CE2	2.57	0.40
1:D:58:ASP:C	1:D:60:THR:H	2.29	0.40
1:D:201:PHE:HD2	1:D:301:TYR:CZ	2.39	0.40
1:A:253:LYS:HB2	1:A:253:LYS:NZ	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:ILE:HA	1:C:96:PHE:HE2	1.85	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:D:281:GLU:HA	1:D:284:GLN:NE2	2.30	0.40
1:D:394:THR:HB	1:D:401:GLU:HB3	2.04	0.40
1:D:454:GLN:O	1:D:455:SER:C	2.63	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:402:TYR:OH	1:A:417:HIS:CE1	2.73	0.40
1:A:532:LYS:C	1:A:534:LEU:N	2.79	0.40
1:A:577:PHE:CE1	1:D:267:LYS:HD2	2.51	0.40
1:B:295:VAL:HG21	3:B:682:HEM:CBB	2.51	0.40
1:B:563:SER:OG	1:B:566:SER:HB2	2.21	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:C:291:VAL:C	1:C:293:GLY:H	2.29	0.40
1:D:184:ARG:HB2	1:D:439:ASN:CA	2.49	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:CD1	1:D:478:PHE:N	2.90	0.40
1:A:210:PHE:CG	1:A:382:ASN:ND2	2.88	0.40
1:B:299:MET:O	1:B:299:MET:HG3	2.21	0.40
1:B:564:ILE:HG12	1:B:580:PHE:CE1	2.57	0.40
1:C:33:ALA:HB3	1:C:158:ASP:OD2	2.20	0.40
1:C:130:TYR:HB3	1:C:134:TYR:O	2.21	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:582:VAL:O	1:C:583:GLN:C	2.64	0.40
1:D:41:CYS:SG	1:D:47:CYS:HB2	2.62	0.40
1:D:113:MET:O	1:D:117:LEU:HB2	2.22	0.40
1:D:479:GLU:HG2	1:D:485:LYS:NZ	2.36	0.40
1:A:97:LYS:HD3	1:A:356:HIS:NE2	2.37	0.40
1:A:269:THR:O	1:A:270:GLN:CB	2.68	0.40
1:B:383:THR:HG22	1:B:384:LEU:N	2.36	0.40
1:B:477:SER:C	1:B:479:GLU:N	2.79	0.40
1:B:491:LEU:C	1:B:493:ALA:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ILE:O	1:B:500:VAL:N	2.52	0.40
1:C:64:PHE:CE2	1:C:72:PRO:HB3	2.57	0.40
1:C:181:VAL:HG12	1:C:487:MET:HB3	2.03	0.40
1:C:233:ILE:HD13	1:C:305:TRP:HB3	2.03	0.40
1:C:285:PHE:N	1:C:285:PHE:CD1	2.89	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/587 (94%)	446 (81%)	78 (14%)	26 (5%)	2	11
1	B	550/587 (94%)	442 (80%)	87 (16%)	21 (4%)	2	15
1	C	550/587 (94%)	443 (80%)	80 (14%)	27 (5%)	1	10
1	D	550/587 (94%)	440 (80%)	85 (16%)	25 (4%)	2	12
All	All	2200/2348 (94%)	1771 (80%)	330 (15%)	99 (4%)	2	12

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	407 (83%)	86 (17%)	2	10
1	B	493/525 (94%)	412 (84%)	81 (16%)	2	12
1	C	493/525 (94%)	413 (84%)	80 (16%)	2	12
1	D	493/525 (94%)	409 (83%)	84 (17%)	2	11
All	All	1972/2100 (94%)	1641 (83%)	331 (17%)	2	11

All (331) 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	56	LYS
1	A	60	THR
1	A	70	THR
1	A	71	THR
1	A	83	LYS
1	A	93	LEU
1	A	107	PHE

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Mol	Chain	Res	Type
1	A	113	MET
1	A	116	VAL
1	A	117	LEU
1	A	124	ILE
1	A	126	SER
1	A	138	SER
1	A	150	ARG
1	A	152	LEU
1	A	158	ASP
1	A	169	LYS
1	A	171	LEU
1	A	174	SER
1	A	178	LEU
1	A	196	MET
1	A	197	MET
1	A	209	PHE
1	A	215	LYS
1	A	222	ARG
1	A	230	LEU
1	A	231	ASN
1	A	241	GLN
1	A	252	LEU
1	A	253	LYS
1	A	266	VAL
1	A	270	GLN
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	295	VAL
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	331	THR
1	A	337	ILE
1	A	376	ARG
1	A	379	SER
1	A	383	THR
1	A	385	TYR
1	A	389	PRO

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Mol	Chain	Res	Type
1	A	396	ASN
1	A	397	ILE
1	A	398	GLU
1	A	400	GLN
1	A	405	LYS
1	A	409	TYR
1	A	412	SER
1	A	416	GLU
1	A	420	THR
1	A	423	VAL
1	A	441	PRO
1	A	459	LYS
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	532	LYS
1	A	534	LEU
1	A	539	ILE
1	A	543	GLN
1	A	547	PRO
1	A	557	LYS
1	A	566	SER
1	A	568	ILE
1	A	569	CYS
1	A	578	THR
1	A	583	GLN
1	B	34	ASN
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

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Mol	Chain	Res	Type
1	B	113	MET
1	B	116	VAL
1	B	117	LEU
1	B	124	ILE
1	B	126	SER
1	B	137	LYS
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	222	ARG
1	B	230	LEU
1	B	231	ASN
1	B	241	GLN
1	B	252	LEU
1	B	253	LYS
1	B	270	GLN
1	B	271	VAL
1	B	282	ASN
1	B	289	GLN
1	B	295	VAL
1	B	298	LEU
1	B	300	MET
1	B	310	GLN
1	B	316	LEU
1	B	318	GLN
1	B	322	GLU
1	B	331	THR
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	396	ASN

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Mol	Chain	Res	Type
1	B	397	ILE
1	B	398	GLU
1	B	399	ASP
1	B	400	GLN
1	B	409	TYR
1	B	412	SER
1	B	420	THR
1	B	441	PRO
1	B	459	LYS
1	B	476	THR
1	B	484	GLU
1	B	492	LYS
1	B	494	LEU
1	B	505	PRO
1	B	514	PRO
1	B	522	MET
1	B	525	LEU
1	B	530	SER
1	B	532	LYS
1	B	534	LEU
1	B	539	ILE
1	B	543	GLN
1	B	557	LYS
1	B	566	SER
1	B	568	ILE
1	B	569	CYS
1	B	578	THR
1	B	583	GLN
1	C	39	ASN
1	C	42	GLN
1	C	44	ARG
1	C	48	MET
1	C	54	GLN
1	C	56	LYS
1	C	70	THR
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

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Mol	Chain	Res	Type
1	C	124	ILE
1	C	126	SER
1	C	137	LYS
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	222	ARG
1	C	230	LEU
1	C	231	ASN
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	295	VAL
1	C	296	PRO
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	337	ILE
1	C	376	ARG
1	C	379	SER
1	C	383	THR
1	C	385	TYR
1	C	389	PRO
1	C	396	ASN
1	C	397	ILE
1	C	398	GLU
1	C	400	GLN
1	C	405	LYS

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Mol	Chain	Res	Type
1	C	409	TYR
1	C	412	SER
1	C	416	GLU
1	C	420	THR
1	C	441	PRO
1	C	459	LYS
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	532	LYS
1	C	534	LEU
1	C	539	ILE
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	34	ASN
1	D	39	ASN
1	D	42	GLN
1	D	44	ARG
1	D	48	MET
1	D	56	LYS
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
1	D	137	LYS
1	D	138	SER

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Mol	Chain	Res	Type
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	222	ARG
1	D	230	LEU
1	D	231	ASN
1	D	241	GLN
1	D	252	LEU
1	D	253	LYS
1	D	261	VAL
1	D	270	GLN
1	D	271	VAL
1	D	282	ASN
1	D	289	GLN
1	D	295	VAL
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	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	397	ILE
1	D	398	GLU
1	D	400	GLN
1	D	405	LYS
1	D	409	TYR
1	D	412	SER

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Mol	Chain	Res	Type
1	D	416	GLU
1	D	420	THR
1	D	425	SER
1	D	441	PRO
1	D	459	LYS
1	D	463	LEU
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	532	LYS
1	D	534	LEU
1	D	539	ILE
1	D	543	GLN
1	D	557	LYS
1	D	566	SER
1	D	568	ILE
1	D	569	CYS
1	D	578	THR
1	D	583	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	42	GLN
1	A	43	ASN
1	A	87	ASN
1	A	90	HIS
1	A	95	HIS
1	A	105	ASN
1	A	203	GLN
1	A	232	HIS
1	A	278	HIS
1	A	284	GLN
1	A	320	HIS
1	A	327	GLN
1	A	351	HIS

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Mol	Chain	Res	Type
1	A	356	HIS
1	A	396	ASN
1	A	400	GLN
1	A	411	ASN
1	A	417	HIS
1	A	454	GLN
1	A	464	ASN
1	A	560	ASN
1	A	571	ASN
1	B	39	ASN
1	B	42	GLN
1	B	43	ASN
1	B	87	ASN
1	B	105	ASN
1	B	232	HIS
1	B	278	HIS
1	B	284	GLN
1	B	320	HIS
1	B	327	GLN
1	B	350	GLN
1	B	351	HIS
1	B	382	ASN
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	43	ASN
1	C	87	ASN
1	C	90	HIS
1	C	95	HIS
1	C	105	ASN
1	C	203	GLN
1	C	232	HIS
1	C	242	HIS
1	C	320	HIS
1	C	327	GLN
1	C	351	HIS

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Mol	Chain	Res	Type
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	39	ASN
1	D	42	GLN
1	D	43	ASN
1	D	87	ASN
1	D	90	HIS
1	D	95	HIS
1	D	105	ASN
1	D	232	HIS
1	D	284	GLN
1	D	350	GLN
1	D	351	HIS
1	D	369	GLN
1	D	396	ASN
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 oligosaccharides 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
3	HEM	C	682	1	50,50,50	1.23	4 (8%)	67,82,82	1.10	3 (4%)
3	HEM	A	682	1	50,50,50	1.27	5 (10%)	67,82,82	1.07	3 (4%)
3	HEM	D	682	1	50,50,50	1.19	4 (8%)	67,82,82	1.05	4 (5%)
2	NAG	A	681	1	14,14,15	0.39	0	17,19,21	0.83	1 (5%)
2	NAG	B	661	1	14,14,15	0.71	1 (7%)	17,19,21	0.93	0
2	NAG	A	671	1	14,14,15	0.86	0	17,19,21	1.59	3 (17%)
3	HEM	B	682	1	50,50,50	1.11	4 (8%)	67,82,82	0.99	3 (4%)
2	NAG	B	671	1	14,14,15	0.85	0	17,19,21	1.51	3 (17%)
2	NAG	C	681	1	14,14,15	0.65	0	17,19,21	1.02	2 (11%)
2	NAG	D	661	1	14,14,15	0.62	0	17,19,21	0.85	1 (5%)
2	NAG	B	681	1	14,14,15	0.56	0	17,19,21	0.89	2 (11%)
2	NAG	C	661	1	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
2	NAG	D	671	1	14,14,15	0.65	0	17,19,21	1.43	1 (5%)
2	NAG	D	681	1	14,14,15	0.62	0	17,19,21	0.77	1 (5%)
2	NAG	A	661	1	14,14,15	0.66	0	17,19,21	0.74	0
2	NAG	C	671	1	14,14,15	0.85	0	17,19,21	1.63	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	682	1	-	4/14/54/54	-
3	HEM	A	682	1	-	4/14/54/54	-
3	HEM	D	682	1	-	4/14/54/54	-
2	NAG	A	681	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
3	HEM	B	682	1	-	4/14/54/54	-
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
2	NAG	C	681	1	-	2/6/23/26	0/1/1/1
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	2/6/23/26	0/1/1/1
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	671	1	-	2/6/23/26	0/1/1/1
2	NAG	D	681	1	-	2/6/23/26	0/1/1/1
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	671	1	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	682	HEM	CAC-C3C	-3.52	1.38	1.47
3	A	682	HEM	CBB-CAB	3.32	1.46	1.30
3	C	682	HEM	CBB-CAB	3.29	1.46	1.30
3	D	682	HEM	CBB-CAB	3.18	1.45	1.30
3	C	682	HEM	CAC-C3C	-3.08	1.39	1.47
3	A	682	HEM	CAB-C3B	-3.06	1.39	1.47
3	C	682	HEM	CBC-CAC	3.05	1.45	1.30
3	A	682	HEM	CAC-C3C	-3.01	1.39	1.47
3	C	682	HEM	CAB-C3B	-2.96	1.39	1.47
3	B	682	HEM	CAC-C3C	-2.90	1.39	1.47
3	B	682	HEM	CAB-C3B	-2.89	1.39	1.47
3	D	682	HEM	CAB-C3B	-2.87	1.39	1.47
3	A	682	HEM	CBC-CAC	2.83	1.44	1.30
3	B	682	HEM	CBB-CAB	2.55	1.42	1.30
3	A	682	HEM	CBA-CGA	2.45	1.56	1.50
3	D	682	HEM	CBC-CAC	2.35	1.41	1.30
2	B	661	NAG	C1-C2	2.22	1.55	1.52
3	B	682	HEM	CBC-CAC	2.19	1.40	1.30

All (31) 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	-3.39	118.36	122.90
3	C	682	HEM	C3B-C4B-NB	3.08	111.68	109.47
2	A	681	NAG	C2-N2-C7	-2.77	119.19	122.90
2	A	671	NAG	C2-N2-C7	-2.71	119.27	122.90
2	C	681	NAG	C2-N2-C7	-2.69	119.30	122.90
3	D	682	HEM	C3B-C4B-NB	2.69	111.40	109.47
3	B	682	HEM	C3B-C4B-NB	2.61	111.34	109.47
2	D	661	NAG	C2-N2-C7	-2.49	119.57	122.90
2	C	671	NAG	C1-O5-C5	2.48	115.51	112.19
2	A	671	NAG	C1-O5-C5	2.44	115.45	112.19
2	B	681	NAG	C2-N2-C7	-2.38	119.71	122.90
3	D	682	HEM	CMB-C2B-C1B	2.38	128.75	125.03
2	C	681	NAG	O5-C1-C2	-2.37	107.62	111.29
2	B	671	NAG	C2-N2-C7	-2.30	119.81	122.90
2	B	671	NAG	C1-O5-C5	2.25	115.20	112.19
2	D	681	NAG	C2-N2-C7	-2.23	119.92	122.90
3	A	682	HEM	CAC-C3C-C4C	2.22	130.12	124.82
3	A	682	HEM	CMC-C2C-C1C	2.22	128.63	124.73
3	C	682	HEM	CMB-C2B-C1B	2.10	128.32	125.03
3	D	682	HEM	O1A-CGA-CBA	-2.10	116.43	123.09
2	B	681	NAG	C1-O5-C5	-2.08	109.40	112.19
3	C	682	HEM	CAC-C3C-C4C	2.08	129.78	124.82
2	C	661	NAG	C1-O5-C5	2.06	114.94	112.19
3	A	682	HEM	C2A-C1A-NA	2.05	112.43	110.15
3	B	682	HEM	O1A-CGA-CBA	-2.03	116.64	123.09
3	B	682	HEM	CMB-C2B-C1B	2.03	128.20	125.03
3	D	682	HEM	O2A-CGA-CBA	2.01	120.36	114.00

There are no chirality outliers.

All (32) 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	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

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Mol	Chain	Res	Type	Atoms
2	A	681	NAG	O5-C5-C6-O6
2	D	671	NAG	C4-C5-C6-O6
2	D	681	NAG	O5-C5-C6-O6
2	D	681	NAG	C4-C5-C6-O6
2	B	671	NAG	C4-C5-C6-O6
2	A	681	NAG	C4-C5-C6-O6
2	A	671	NAG	C4-C5-C6-O6
2	C	671	NAG	C4-C5-C6-O6
3	A	682	HEM	CAA-CBA-CGA-O1A
3	B	682	HEM	CAA-CBA-CGA-O1A
3	C	682	HEM	CAA-CBA-CGA-O1A
3	D	682	HEM	CAA-CBA-CGA-O2A
3	D	682	HEM	CAA-CBA-CGA-O1A
3	C	682	HEM	CAD-CBD-CGD-O2D
3	C	682	HEM	CAA-CBA-CGA-O2A
3	A	682	HEM	CAA-CBA-CGA-O2A
3	B	682	HEM	CAA-CBA-CGA-O2A
3	A	682	HEM	CAD-CBD-CGD-O2D
3	D	682	HEM	CAD-CBD-CGD-O2D
3	A	682	HEM	CAD-CBD-CGD-O1D
3	D	682	HEM	CAD-CBD-CGD-O1D
3	C	682	HEM	CAD-CBD-CGD-O1D
3	B	682	HEM	CAD-CBD-CGD-O2D
3	B	682	HEM	CAD-CBD-CGD-O1D

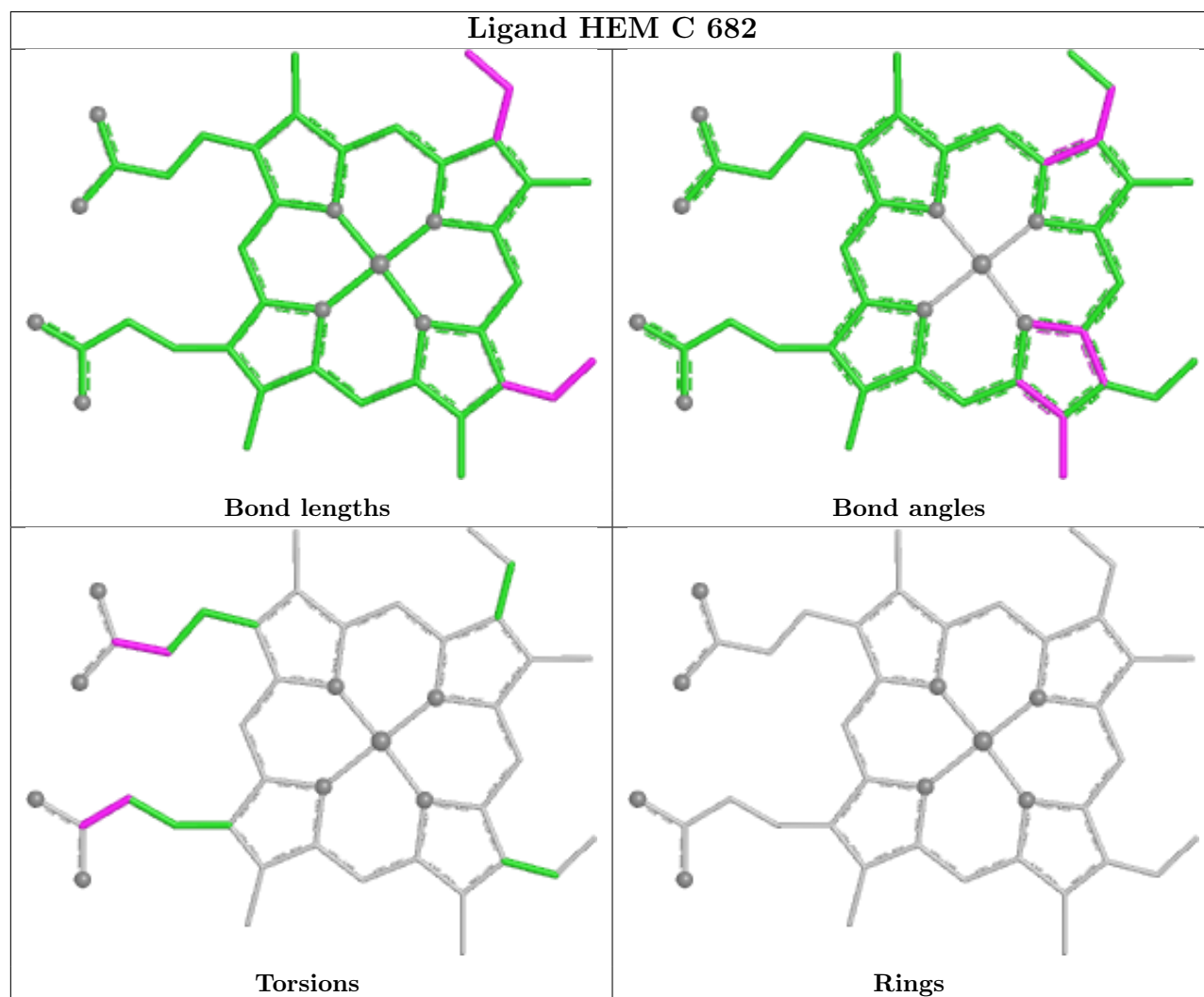
There are no ring outliers.

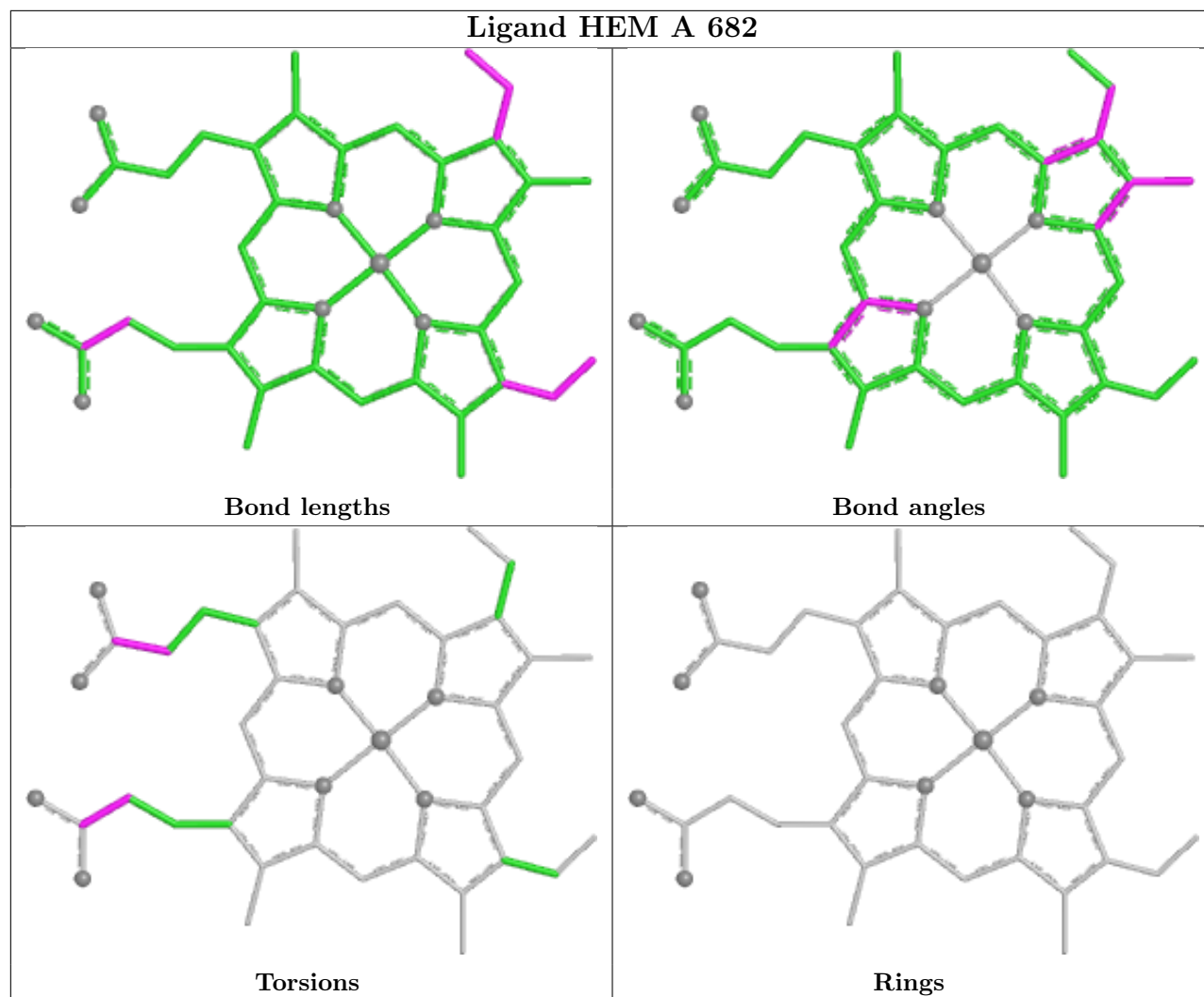
9 monomers are involved in 16 short contacts:

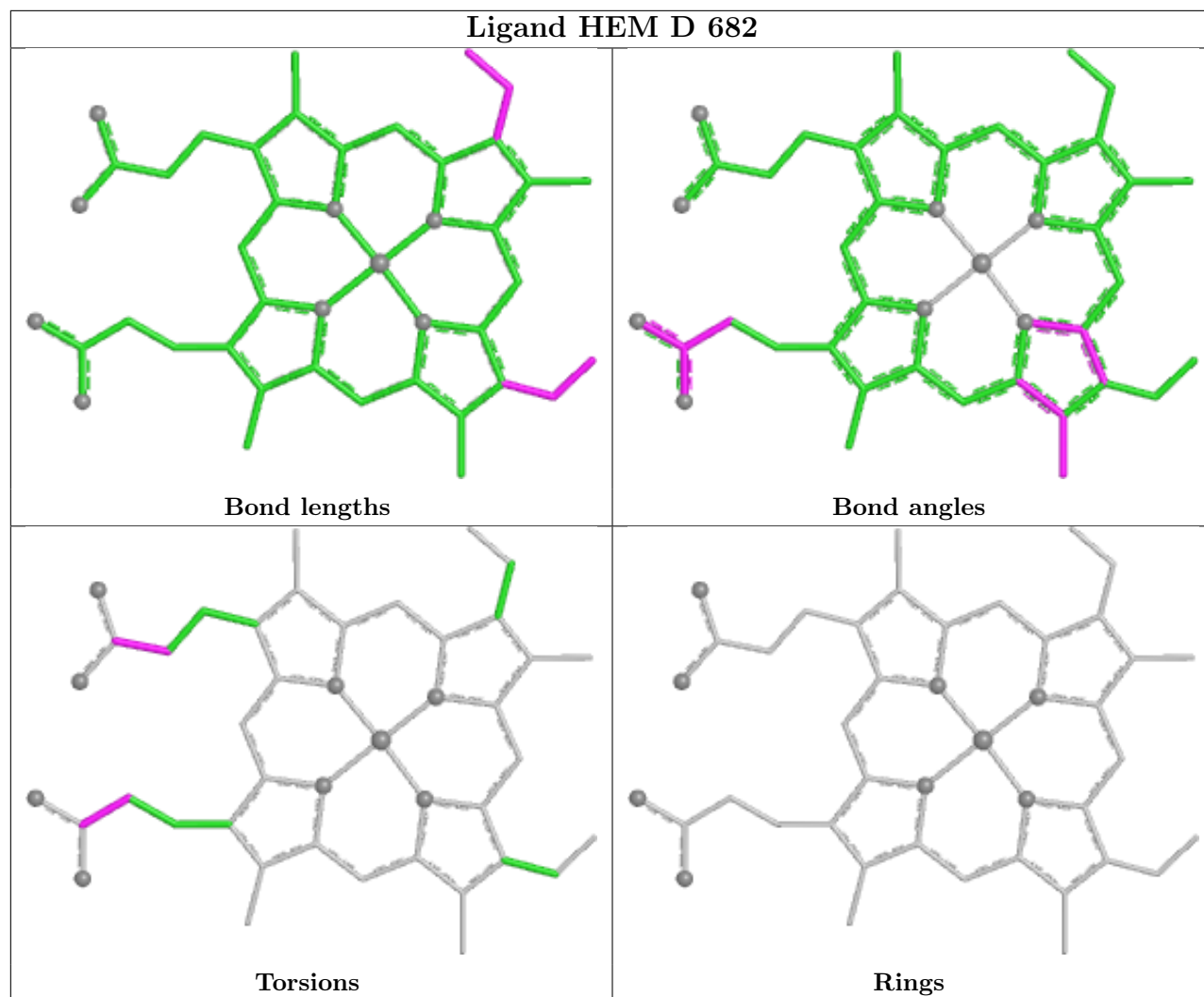
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	682	HEM	2	0
3	A	682	HEM	1	0
3	D	682	HEM	2	0
3	B	682	HEM	2	0
2	D	661	NAG	1	0
2	B	681	NAG	1	0
2	C	661	NAG	2	0
2	D	681	NAG	4	0
2	C	671	NAG	1	0

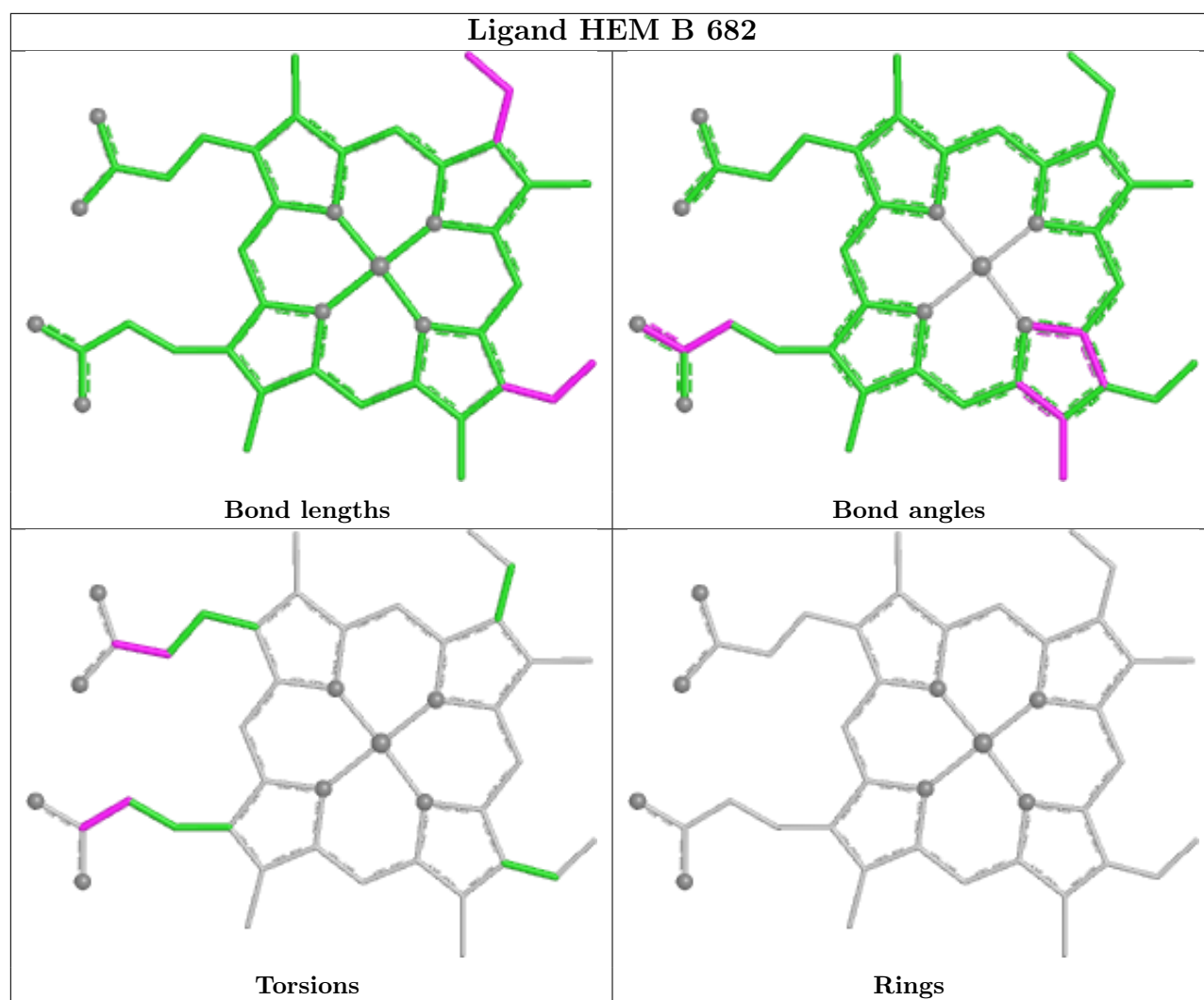
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	552/587 (94%)	-0.09	5 (0%) 81 61	2, 8, 25, 40	0
1	B	552/587 (94%)	-0.12	4 (0%) 84 66	2, 8, 26, 38	0
1	C	552/587 (94%)	-0.10	5 (0%) 81 61	2, 8, 28, 38	0
1	D	552/587 (94%)	-0.09	7 (1%) 75 53	2, 9, 27, 41	0
All	All	2208/2348 (94%)	-0.10	21 (0%) 79 59	2, 8, 27, 41	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ASN	5.1
1	B	411	ASN	4.8
1	D	411	ASN	4.2
1	C	411	ASN	3.6
1	C	581	ASN	3.5
1	D	398	GLU	3.3
1	A	581	ASN	3.0
1	C	161	THR	3.0
1	C	436	GLY	2.6
1	D	557	LYS	2.6
1	A	170	GLU	2.5
1	A	119	SER	2.4
1	D	122	TYR	2.4
1	A	107	PHE	2.3
1	B	105(A)	ILE	2.3
1	D	110	SER	2.3
1	C	332	SER	2.1
1	B	217	GLY	2.1
1	D	282	ASN	2.0
1	D	581	ASN	2.0
1	B	107	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

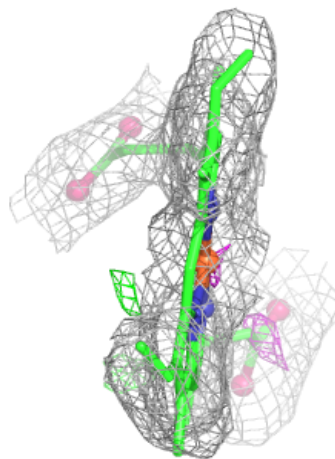
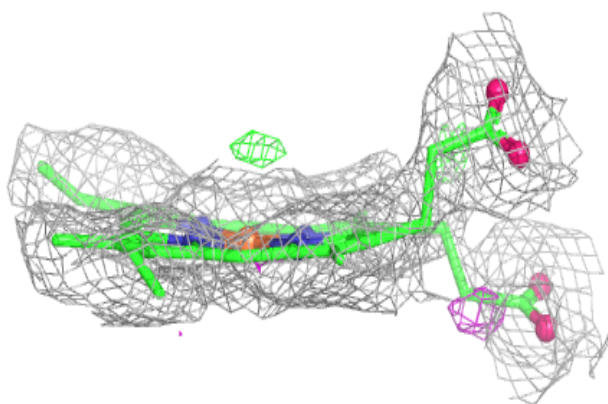
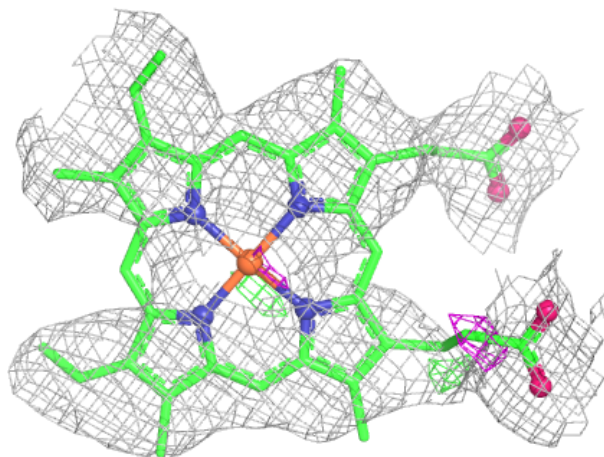
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	681	14/15	0.63	0.19	21,31,33,37	0
2	NAG	D	661	14/15	0.70	0.14	20,25,29,31	0
2	NAG	B	681	14/15	0.71	0.15	22,32,33,33	0
2	NAG	C	661	14/15	0.71	0.17	24,26,29,30	0
2	NAG	A	671	14/15	0.77	0.15	2,6,18,20	0
2	NAG	B	661	14/15	0.77	0.12	22,25,31,33	0
2	NAG	D	671	14/15	0.81	0.13	4,7,18,21	0
2	NAG	A	681	14/15	0.82	0.12	23,29,34,36	0
2	NAG	C	681	14/15	0.83	0.10	24,29,32,36	0
2	NAG	B	671	14/15	0.83	0.11	4,7,17,20	0
2	NAG	C	671	14/15	0.85	0.13	4,7,17,21	0
2	NAG	A	661	14/15	0.87	0.11	21,25,30,32	0
3	HEM	D	682	43/43	0.90	0.10	2,9,26,27	0
3	HEM	C	682	43/43	0.92	0.09	2,5,25,30	0
3	HEM	B	682	43/43	0.92	0.09	2,8,24,28	0
3	HEM	A	682	43/43	0.93	0.10	2,4,24,31	0

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.

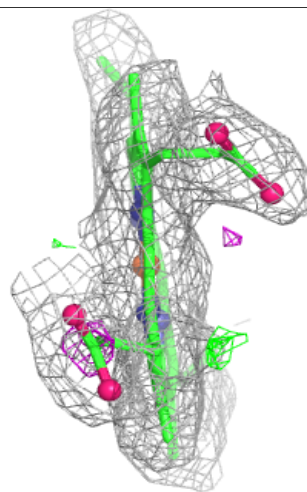
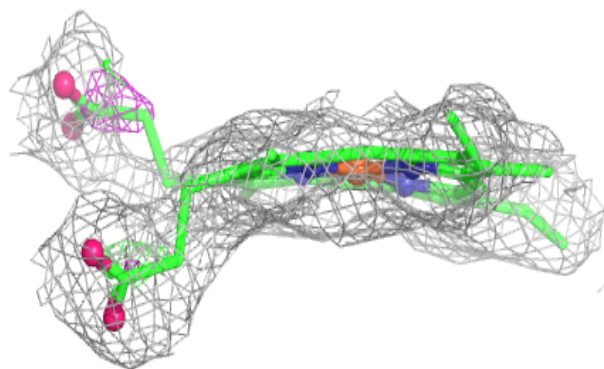
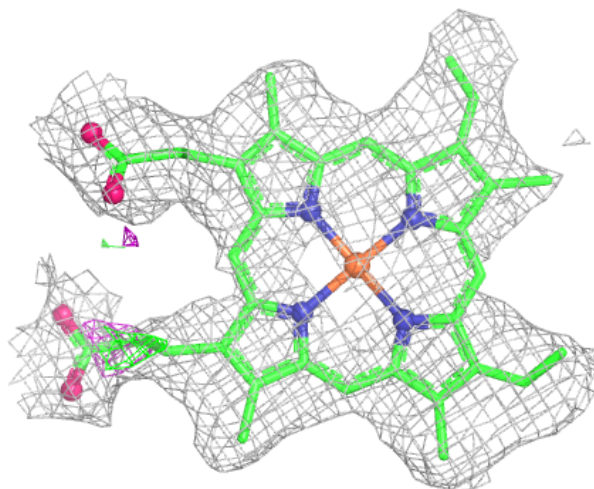
Electron density around HEM D 682:

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



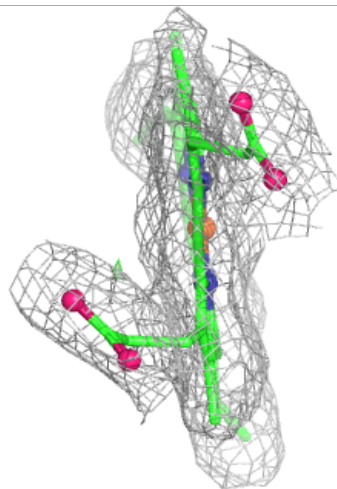
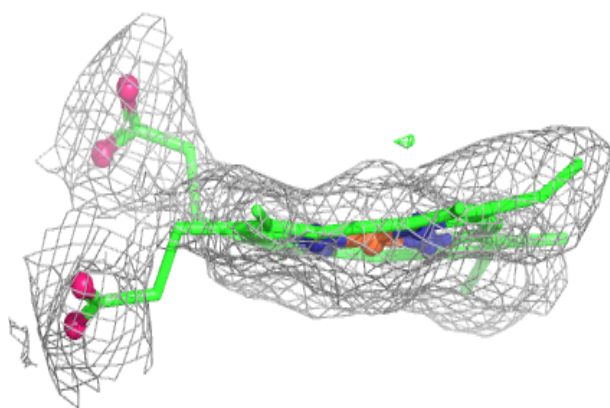
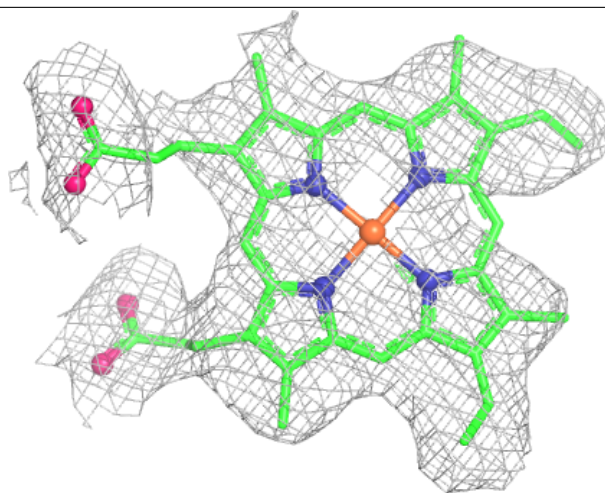
Electron density around HEM C 682:

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



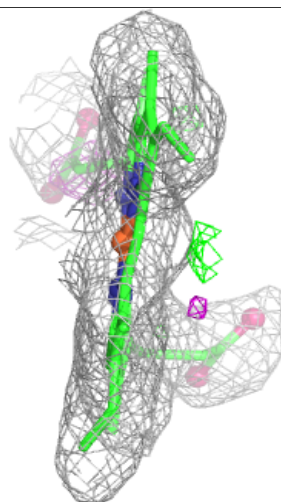
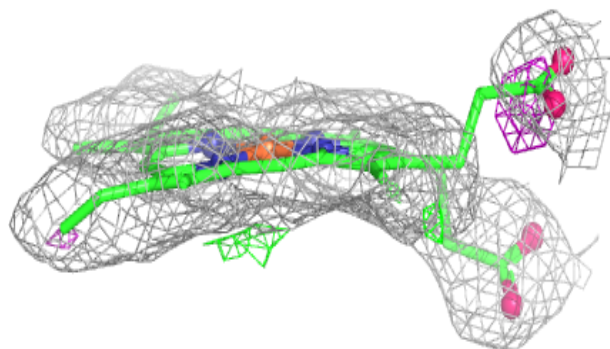
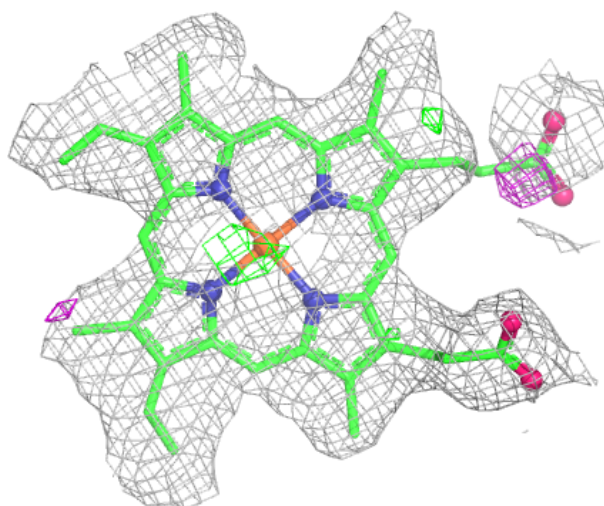
Electron density around HEM B 682:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.