



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:47 PM UTC

PDB ID : 4BLC / pdb_00004blc
Title : THE STRUCTURE OF ORTHORHOMBIC CRYSTALS OF BEEF LIVER CATALASE
Authors : Ko, T.P.; Day, J.; Malkin, A.; McPherson, A.
Deposited on : 1998-09-27
Resolution : 2.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

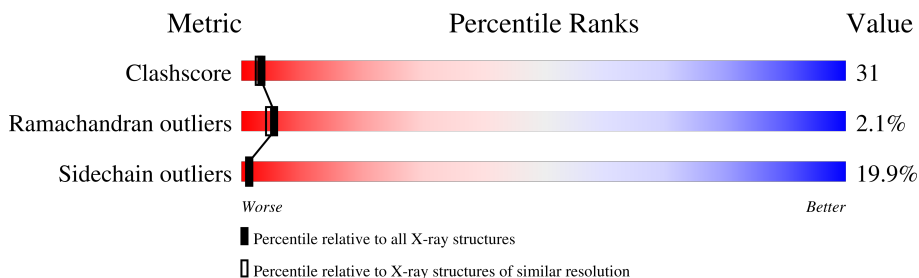
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	53% (green), 38% (yellow), 8% (orange), 0% (red), 0% (grey)
1	B	506	36% (green), 45% (yellow), 17% (orange), 0% (red), 0% (grey)
1	C	506	40% (green), 43% (yellow), 15% (orange), 0% (red), 0% (grey)
1	D	506	43% (green), 45% (yellow), 10% (orange), 0% (red), 0% (grey)

2 Entry composition [i](#)

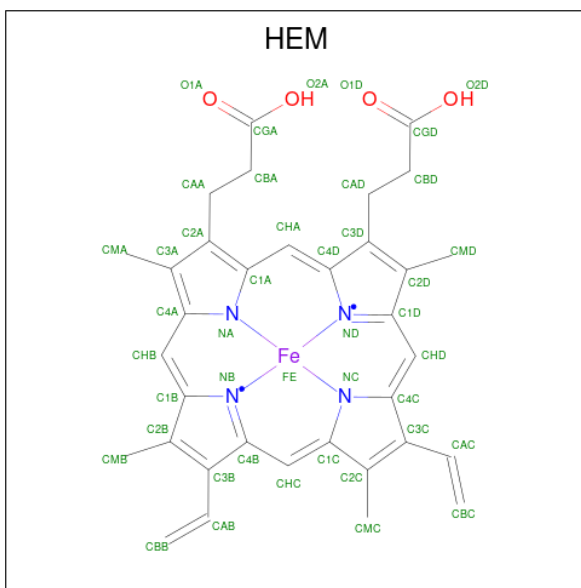
There are 4 unique types of molecules in this entry. The entry contains 16816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	B	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	C	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0
1	D	499	Total 4017	C 2548	N 715	O 740	S 14	0	0	0

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



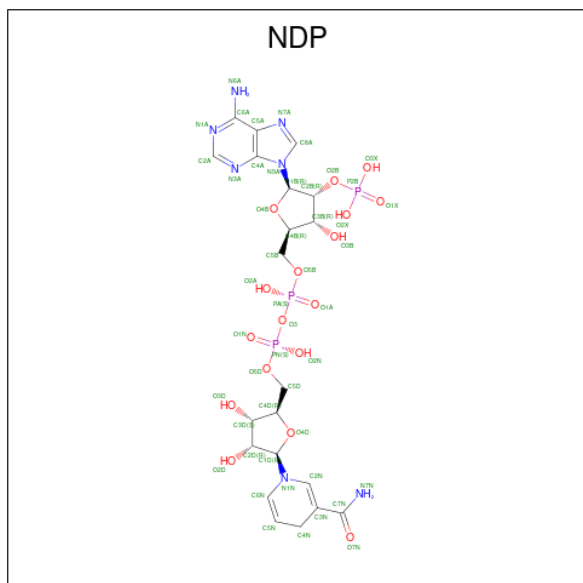
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	89	Total	O	0	0
			89	89		
4	C	83	Total	O	0	0
			83	83		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	93	Total	O	0	0
			93	93		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.80Å 140.60Å 232.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (20.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	16816	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 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	0.49	0/4137	0.96	11/5619 (0.2%)
1	B	0.45	0/4137	0.94	12/5619 (0.2%)
1	C	0.46	0/4137	0.98	26/5619 (0.5%)
1	D	0.47	0/4137	0.94	12/5619 (0.2%)
All	All	0.47	0/16548	0.96	61/22476 (0.3%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	ILE	N-CA-C	-8.30	103.14	111.77
1	D	356	ALA	N-CA-C	8.22	121.28	111.33
1	C	55	VAL	N-CA-C	-8.13	102.89	110.53
1	A	356	ALA	N-CA-C	7.56	121.43	111.75
1	B	55	VAL	N-CA-C	-7.35	103.62	110.53
1	C	123	ASP	N-CA-C	7.20	118.92	111.14
1	C	281	GLN	N-CA-C	-7.00	100.15	110.52
1	C	145	VAL	N-CA-C	6.82	113.50	106.21
1	D	55	VAL	N-CA-C	-6.62	103.79	111.00
1	C	372	ILE	N-CA-C	-6.51	101.86	108.96
1	A	372	ILE	N-CA-C	-6.50	101.87	108.96
1	A	291	PHE	CA-C-N	6.41	126.10	119.82
1	A	291	PHE	C-N-CA	6.41	126.10	119.82
1	D	452	GLU	N-CA-C	6.33	119.85	111.75
1	C	484	VAL	N-CA-C	-6.32	104.99	110.74
1	B	215	GLY	N-CA-C	-6.31	105.91	113.99
1	C	388	ASP	N-CA-C	6.22	117.20	108.00
1	C	394	MET	CB-CA-C	-6.21	108.78	117.23
1	B	169	ARG	N-CA-C	6.21	118.57	110.43
1	D	484	VAL	N-CA-C	-6.20	103.61	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	N-CA-C	6.18	120.34	109.96
1	D	90	ILE	N-CA-C	-6.16	106.76	112.43
1	A	114	THR	N-CA-C	-6.15	100.29	109.94
1	D	18	ARG	N-CA-C	-6.08	104.57	111.07
1	D	169	ARG	N-CA-C	6.07	119.47	110.48
1	A	484	VAL	N-CA-C	-6.07	105.22	110.74
1	C	485	HIS	CA-C-N	5.79	127.08	119.84
1	C	485	HIS	C-N-CA	5.79	127.08	119.84
1	B	116	ALA	N-CA-C	5.76	117.56	111.28
1	B	313	GLY	N-CA-C	5.75	118.98	110.42
1	C	341	GLY	N-CA-C	-5.69	107.17	114.85
1	A	51	VAL	N-CA-C	-5.69	105.54	112.76
1	C	378	TYR	N-CA-C	5.67	119.46	112.54
1	A	273	TYR	N-CA-C	5.65	116.52	109.57
1	A	113	SER	N-CA-C	5.64	116.71	108.14
1	C	188	ARG	CA-C-N	5.63	125.72	119.87
1	C	188	ARG	C-N-CA	5.63	125.72	119.87
1	B	92	ARG	N-CA-C	-5.62	106.41	113.20
1	A	238	ASP	N-CA-C	-5.58	106.48	113.28
1	B	432	ASN	N-CA-C	5.49	117.66	109.59
1	B	307	TYR	CA-C-N	5.48	125.43	119.78
1	B	307	TYR	C-N-CA	5.48	125.43	119.78
1	C	124	THR	N-CA-C	5.42	119.11	110.70
1	C	67	ARG	N-CA-C	5.42	118.94	110.32
1	B	51	VAL	N-CA-C	-5.35	104.52	110.62
1	D	67	ARG	N-CA-C	5.31	118.88	109.96
1	C	68	ILE	N-CA-C	-5.28	103.04	109.01
1	C	44	GLY	CA-C-N	5.28	125.59	119.47
1	C	44	GLY	C-N-CA	5.28	125.59	119.47
1	D	289	GLU	N-CA-C	-5.28	106.54	112.87
1	B	273	TYR	N-CA-C	5.26	117.23	109.50
1	C	307	TYR	CA-C-N	5.22	125.20	120.03
1	C	307	TYR	C-N-CA	5.22	125.20	120.03
1	B	356	ALA	N-CA-C	5.16	117.58	111.33
1	C	409	SER	N-CA-C	5.14	118.49	111.39
1	C	324	TYR	N-CA-C	5.12	116.87	111.28
1	D	29	GLY	N-CA-C	-5.12	107.43	113.99
1	D	139	ASP	N-CA-C	-5.11	106.36	112.59
1	C	327	GLU	N-CA-C	5.07	119.59	113.41
1	C	483	ASP	N-CA-C	-5.04	106.23	112.38
1	D	434	ALA	N-CA-C	5.03	117.49	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4017	0	3839	185	0
1	B	4017	0	3839	319	0
1	C	4017	0	3839	292	0
1	D	4017	0	3839	276	0
2	A	43	0	30	5	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	48	0	26	3	0
3	B	48	0	26	3	0
3	C	48	0	26	2	0
3	D	48	0	26	1	0
4	A	119	0	0	8	0
4	B	89	0	0	16	0
4	C	83	0	0	8	0
4	D	93	0	0	11	0
All	All	16816	0	15580	979	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 31.

All (979) 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:D:223:ASN:HD21	1:D:227:GLU:HB3	0.98	1.12
1:A:451:ASN:H	1:A:454:GLN:HE21	1.06	1.01
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.79	0.98
1:B:169:ARG:HG2	1:B:169:ARG:HH11	1.30	0.95
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.28	0.95
1:C:251:ARG:HD2	1:C:255:GLU:HG3	1.50	0.93
1:A:92:ARG:HH11	1:A:92:ARG:HB3	1.33	0.93
1:B:457:ARG:HB2	1:B:457:ARG:NH1	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:PHE:HD1	1:D:293:PHE:H	1.17	0.92
1:D:85:GLU:HG2	1:D:105:ARG:HG3	1.52	0.92
1:C:402:ASN:H	1:C:402:ASN:HD22	1.09	0.90
1:B:4:ARG:HH22	1:C:470:GLN:HE21	1.21	0.89
1:C:466:LEU:O	1:C:466:LEU:HD12	1.74	0.88
1:C:485:HIS:CE1	1:C:487:GLU:HB3	2.08	0.87
1:B:100:GLU:HB3	1:B:104:LYS:HG3	1.56	0.86
1:B:129:ARG:HB2	1:B:148:ASN:ND2	1.90	0.85
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.40	0.85
1:C:438:ASN:N	1:C:438:ASN:HD22	1.71	0.85
1:B:148:ASN:HD22	1:B:211:MET:CE	1.90	0.84
1:C:487:GLU:O	1:C:491:ARG:HG3	1.77	0.84
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.42	0.82
1:A:353:ARG:HG3	2:A:507:HEM:HBB2	1.62	0.82
1:C:208:HIS:HA	1:C:211:MET:HE2	1.61	0.82
1:B:454:GLN:HA	1:B:457:ARG:NH1	1.95	0.81
1:A:43:VAL:O	1:A:47:GLY:HA3	1.78	0.81
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.63	0.81
1:D:170:ASN:ND2	1:D:172:GLN:H	1.77	0.81
1:A:451:ASN:N	1:A:454:GLN:HE21	1.78	0.81
1:B:495:LEU:HD23	1:B:495:LEU:H	1.46	0.81
1:C:151:ILE:HD12	1:C:194:GLN:HG2	1.62	0.81
1:A:487:GLU:O	1:A:491:ARG:HG3	1.81	0.79
1:A:451:ASN:H	1:A:454:GLN:NE2	1.80	0.79
1:D:221:LEU:HD11	1:D:231:CYS:HB3	1.64	0.79
1:B:223:ASN:ND2	1:B:227:GLU:HB2	1.99	0.78
1:B:178:PRO:HD3	4:B:762:HOH:O	1.83	0.78
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.47	0.78
1:C:476:LYS:NZ	1:C:476:LYS:HB3	1.98	0.78
1:D:284:THR:OG1	1:D:287:GLU:HG2	1.83	0.78
1:B:241:ILE:HG22	1:B:242:LYS:H	1.47	0.77
1:A:485:HIS:HD2	1:A:487:GLU:H	1.28	0.77
1:B:37:LYS:HE3	1:B:59:GLU:OE2	1.84	0.77
1:D:202:ARG:NH1	1:D:241:ILE:HG21	1.99	0.77
1:B:191:SER:O	1:B:195:VAL:HG23	1.85	0.77
1:D:244:LEU:HD21	1:D:248:ASP:HB2	1.67	0.76
1:C:488:TYR:O	1:C:492:ILE:HG12	1.86	0.76
1:A:35:GLY:HA2	1:C:414:GLN:O	1.86	0.75
1:B:304:HIS:HD2	1:B:309:LEU:HD21	1.51	0.75
1:A:36:ASP:HA	1:C:413:HIS:ND1	2.01	0.75
1:C:110:VAL:HG22	1:C:133:VAL:HG22	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:HIS:HB3	1:C:242:LYS:H	1.52	0.75
1:C:222:VAL:HG22	1:C:228:ALA:HB2	1.68	0.75
1:C:244:LEU:HD13	1:C:248:ASP:HB3	1.69	0.74
1:D:145:VAL:O	2:D:507:HEM:HBC2	1.88	0.74
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.68	0.74
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.03	0.73
1:C:191:SER:O	1:C:195:VAL:HG23	1.87	0.73
1:B:182:TRP:O	1:B:186:SER:HB3	1.88	0.72
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.54	0.72
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.71	0.72
1:B:89:ASP:HB2	1:B:102:ILE:HD11	1.72	0.72
1:B:414:GLN:HE21	1:B:416:SER:CB	2.03	0.72
1:B:78:ALA:HB2	1:B:261:LEU:HG	1.71	0.72
1:B:6:PRO:HG2	1:B:266:ASN:OD1	1.89	0.71
1:D:78:ALA:HB2	1:D:261:LEU:HG	1.72	0.71
1:D:170:ASN:HD22	1:D:173:THR:H	1.39	0.71
1:B:241:ILE:HG22	1:B:242:LYS:N	2.06	0.71
1:C:72:VAL:HG13	1:C:73:VAL:HG22	1.73	0.71
1:C:491:ARG:O	1:C:495:LEU:HD12	1.90	0.71
1:A:129:ARG:H	1:A:148:ASN:ND2	1.88	0.71
1:B:241:ILE:O	1:B:242:LYS:HB2	1.91	0.70
1:B:281:GLN:OE1	1:B:302:TRP:HB2	1.89	0.70
1:C:183:ASP:O	1:C:187:LEU:HG	1.90	0.70
1:D:137:THR:HA	1:D:379:ARG:HH21	1.56	0.70
1:B:190:GLU:HA	1:B:438:ASN:HB3	1.74	0.70
1:C:301:VAL:HG22	1:C:441:GLN:OE1	1.90	0.70
1:C:189:PRO:O	1:C:192:LEU:HG	1.92	0.70
1:D:286:SER:O	1:D:290:ILE:HD12	1.91	0.70
1:C:289:GLU:HG2	4:C:898:HOH:O	1.92	0.70
1:B:220:LYS:C	1:B:221:LEU:HD23	2.16	0.70
1:B:112:PHE:HA	1:B:130:GLY:O	1.91	0.69
1:A:82:GLY:HA3	1:A:316:VAL:O	1.92	0.69
1:B:126:ARG:HE	1:B:199:PHE:HA	1.58	0.69
1:C:402:ASN:HD22	1:C:402:ASN:N	1.84	0.69
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.72	0.69
1:C:74:HIS:O	1:C:111:ARG:NH2	2.24	0.69
1:D:84:PHE:O	1:D:105:ARG:HA	1.92	0.69
1:A:92:ARG:HH11	1:A:92:ARG:CB	2.04	0.69
1:B:391:MET:HE3	1:D:366:GLY:HA3	1.75	0.69
1:B:100:GLU:HB2	1:B:104:LYS:HZ3	1.57	0.69
1:C:273:TYR:HB3	1:C:317:LEU:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:ARG:HG2	1:D:387:ARG:HH11	1.56	0.68
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.74	0.68
1:A:425:SER:HA	1:B:424:PHE:O	1.93	0.68
1:D:367:PRO:HG2	1:D:390:PRO:CG	2.23	0.68
1:C:232:LYS:HB2	1:C:281:GLN:HB2	1.76	0.68
1:D:221:LEU:HD11	1:D:231:CYS:SG	2.33	0.68
1:A:51:VAL:HG13	1:B:49:LEU:O	1.93	0.68
4:A:718:HOH:O	1:D:363:HIS:HD2	1.77	0.68
1:B:37:LYS:O	1:C:158:LEU:HD13	1.93	0.68
1:D:364:ARG:HD2	4:D:1022:HOH:O	1.93	0.67
1:C:92:ARG:HG3	1:C:92:ARG:HH11	1.59	0.67
1:B:264:LEU:HD12	1:B:264:LEU:O	1.95	0.67
1:D:60:MET:HE1	1:D:63:PHE:CD2	2.29	0.67
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.77	0.67
1:B:301:VAL:H	1:B:441:GLN:NE2	1.92	0.67
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.59	0.67
1:B:301:VAL:H	1:B:441:GLN:HE22	1.41	0.67
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.58	0.66
1:C:471:LEU:HA	1:C:474:GLN:HG3	1.75	0.66
1:B:47:GLY:HA2	1:C:424:PHE:CE1	2.30	0.66
4:B:787:HOH:O	1:C:44:GLY:HA2	1.94	0.66
1:B:414:GLN:HE21	1:B:416:SER:HB2	1.61	0.66
1:B:148:ASN:HD22	1:B:211:MET:HE2	1.59	0.66
1:D:383:ALA:HB1	1:D:411:PRO:HG3	1.78	0.66
1:D:220:LYS:HE3	1:D:343:GLU:HB2	1.78	0.66
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.06	0.66
1:B:360:THR:HG23	1:C:64:ASP:O	1.95	0.66
1:C:6:PRO:HD2	1:C:266:ASN:OD1	1.95	0.65
1:B:273:TYR:HB3	1:B:317:LEU:O	1.96	0.65
1:D:221:LEU:HD11	1:D:231:CYS:CB	2.26	0.65
1:C:470:GLN:O	1:C:473:ILE:HB	1.96	0.65
1:D:18:ARG:HB3	4:D:841:HOH:O	1.97	0.65
1:A:280:ILE:HG23	1:A:312:VAL:HG21	1.77	0.65
1:D:94:SER:HB2	1:D:221:LEU:HB3	1.79	0.65
1:A:419:GLU:OE2	1:B:430:ARG:NH1	2.30	0.65
1:D:287:GLU:HA	1:D:290:ILE:HB	1.78	0.65
1:A:170:ASN:HB3	1:A:173:THR:OG1	1.96	0.65
1:D:83:TYR:CE1	1:D:85:GLU:HG3	2.32	0.65
1:B:318:ASN:HD22	1:B:318:ASN:N	1.95	0.64
1:D:223:ASN:HD21	1:D:227:GLU:CB	1.93	0.64
1:A:471:LEU:HA	1:A:474:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:HB3	1:B:138:GLU:OE1	1.97	0.64
1:D:284:THR:HG23	1:D:287:GLU:OE2	1.98	0.64
1:D:487:GLU:HA	1:D:490:SER:OG	1.97	0.64
1:A:485:HIS:CD2	1:A:487:GLU:H	2.12	0.64
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.79	0.64
1:A:15:LYS:HD2	4:A:936:HOH:O	1.98	0.64
1:A:95:LYS:HG2	1:A:222:VAL:O	1.98	0.64
1:A:333:PHE:O	1:A:361:HIS:HE1	1.81	0.64
1:C:331:LEU:HD13	1:C:333:PHE:CZ	2.33	0.64
1:C:437:ASP:C	1:C:438:ASN:HD22	2.06	0.63
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.81	0.63
1:C:221:LEU:O	1:C:228:ALA:HA	1.98	0.63
1:C:208:HIS:CA	1:C:211:MET:HE2	2.28	0.63
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.80	0.63
1:D:76:LYS:O	1:D:113:SER:HB2	1.99	0.63
1:D:285:PHE:HD1	1:D:285:PHE:H	1.46	0.63
1:D:347:ASP:HB3	1:D:350:LEU:CB	2.27	0.63
1:A:18:ARG:HG2	4:A:935:HOH:O	1.98	0.63
1:A:498:LYS:HD2	4:A:725:HOH:O	1.97	0.63
1:C:451:ASN:OD1	1:C:454:GLN:HG2	1.99	0.63
1:B:41:LEU:HB3	1:B:53:ASP:HB2	1.80	0.63
1:B:15:LYS:HD3	1:D:408:PHE:HA	1.80	0.63
1:B:402:ASN:C	1:B:402:ASN:HD22	2.06	0.63
1:D:338:MET:CE	1:D:342:ILE:HG22	2.29	0.63
1:D:432:ASN:C	1:D:432:ASN:ND2	2.57	0.63
1:C:154:ILE:HG13	1:C:349:MET:CE	2.29	0.62
1:C:445:PHE:O	1:C:450:LEU:HB2	1.99	0.62
1:D:338:MET:HE1	1:D:343:GLU:C	2.24	0.62
1:A:25:VAL:HG13	1:C:414:GLN:HG2	1.80	0.62
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.80	0.62
1:B:321:PRO:HG2	4:C:996:HOH:O	2.00	0.62
1:B:447:LEU:O	1:B:448:LYS:HB2	1.98	0.62
1:C:4:ARG:HD3	1:C:9:ASP:OD1	2.00	0.62
1:D:63:PHE:O	1:D:66:GLU:HG3	2.00	0.62
1:D:404:TYR:CD1	1:D:405:PRO:HA	2.34	0.62
1:B:466:LEU:CD2	1:B:474:GLN:HG2	2.30	0.62
1:B:229:VAL:HG23	1:B:284:THR:HA	1.81	0.62
1:B:304:HIS:CD2	1:B:309:LEU:HD21	2.32	0.62
1:D:445:PHE:HA	1:D:449:VAL:CG2	2.30	0.62
1:B:223:ASN:C	1:B:225:ASP:H	2.08	0.62
1:A:451:ASN:N	1:A:454:GLN:NE2	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:O	1:B:47:GLY:HA3	2.00	0.61
1:B:38:LEU:HG	1:D:413:HIS:CE1	2.35	0.61
1:C:165:HIS:HB3	1:D:402:ASN:ND2	2.15	0.61
1:D:154:ILE:HG13	1:D:349:MET:HE2	1.82	0.61
1:A:414:GLN:O	1:C:35:GLY:HA2	1.99	0.61
1:D:154:ILE:HG13	1:D:349:MET:CE	2.31	0.61
1:C:358:PRO:O	1:C:362:ARG:HG3	2.00	0.61
1:C:451:ASN:H	1:C:454:GLN:HE21	1.48	0.61
1:D:156:ASP:OD1	1:D:158:LEU:HB2	2.01	0.61
1:B:142:TRP:CZ2	1:B:144:LEU:HD23	2.36	0.61
1:B:318:ASN:N	1:B:318:ASN:ND2	2.49	0.61
1:C:437:ASP:OD2	1:C:440:THR:HB	2.00	0.61
1:D:244:LEU:CD2	1:D:248:ASP:HB2	2.31	0.61
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.83	0.61
1:C:485:HIS:NE2	1:C:487:GLU:HB3	2.16	0.61
1:B:397:GLN:HG2	4:B:835:HOH:O	2.00	0.61
1:C:138:GLU:HA	1:C:379:ARG:O	2.01	0.61
1:C:251:ARG:HG3	1:C:252:LEU:N	2.16	0.61
1:B:160:PHE:O	1:B:164:ILE:HG12	2.01	0.61
1:A:148:ASN:HD22	1:A:148:ASN:H	1.49	0.60
1:B:430:ARG:HH22	1:C:53:ASP:CG	2.08	0.60
1:C:26:LEU:HD21	1:C:37:LYS:HD3	1.83	0.60
1:C:425:SER:HB2	1:D:425:SER:OG	2.01	0.60
1:C:391:MET:HE3	1:C:393:MET:HE1	1.83	0.60
1:D:170:ASN:ND2	1:D:173:THR:H	1.98	0.60
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.36	0.60
1:C:329:GLU:OE1	1:C:329:GLU:HA	2.01	0.60
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.32	0.60
1:C:235:TYR:HA	1:C:277:THR:O	2.00	0.60
1:A:197:PHE:HD2	4:A:1043:HOH:O	1.83	0.60
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.82	0.60
1:C:252:LEU:HA	1:C:255:GLU:HB2	1.83	0.60
1:B:323:ASN:O	1:B:327:GLU:HG3	2.01	0.60
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.84	0.60
1:A:206:ASP:O	1:A:210:HIS:HD2	1.85	0.60
1:C:89:ASP:OD1	1:C:91:THR:HB	2.02	0.59
1:C:351:GLN:O	1:C:354:LEU:HB2	2.01	0.59
1:D:150:PRO:HB3	1:D:214:TYR:CD2	2.37	0.59
1:A:97:LYS:O	1:A:100:GLU:HB2	2.02	0.59
1:A:150:PRO:HG3	3:A:1102:NDP:H41N	1.83	0.59
1:B:317:LEU:C	1:B:318:ASN:HD22	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ARG:C	1:C:445:PHE:H	2.10	0.59
1:D:170:ASN:HD22	1:D:172:GLN:H	1.51	0.59
1:D:222:VAL:HG11	1:D:420:HIS:HB2	1.84	0.59
1:C:153:PHE:HZ	1:C:198:LEU:HD22	1.67	0.59
1:C:402:ASN:H	1:C:402:ASN:ND2	1.90	0.59
1:D:60:MET:HE3	1:D:60:MET:HA	1.85	0.59
1:D:455:ARG:HD2	1:D:491:ARG:HH12	1.67	0.59
1:C:476:LYS:HB3	1:C:476:LYS:HZ3	1.67	0.59
1:B:351:GLN:HE22	1:D:52:GLN:HG3	1.68	0.59
1:C:197:PHE:HB2	4:C:1074:HOH:O	2.03	0.59
1:B:4:ARG:NH2	1:C:470:GLN:HE21	1.94	0.59
1:D:83:TYR:HE1	1:D:85:GLU:HG3	1.67	0.59
1:B:206:ASP:OD2	1:B:244:LEU:HD21	2.03	0.58
1:C:72:VAL:HG11	2:C:507:HEM:HMA3	1.84	0.58
1:C:374:VAL:HG13	4:C:752:HOH:O	2.03	0.58
1:B:34:VAL:HG13	1:B:55:VAL:HG11	1.84	0.58
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.38	0.58
1:B:138:GLU:H	1:B:138:GLU:CD	2.12	0.58
1:C:438:ASN:N	1:C:438:ASN:ND2	2.41	0.58
1:B:495:LEU:H	1:B:495:LEU:CD2	2.17	0.58
1:B:322:VAL:O	1:C:172:GLN:HG3	2.03	0.58
1:A:42:THR:HG22	1:A:49:LEU:HA	1.85	0.58
1:B:232:LYS:O	1:B:280:ILE:HA	2.04	0.58
1:C:188:ARG:HD3	1:C:190:GLU:OE2	2.04	0.58
1:C:284:THR:OG1	1:C:287:GLU:HG3	2.02	0.58
1:C:327:GLU:HA	1:C:374:VAL:HG11	1.86	0.58
1:D:108:ILE:HA	1:D:134:LYS:O	2.04	0.58
1:D:329:GLU:HA	1:D:329:GLU:OE1	2.02	0.58
1:D:488:TYR:O	1:D:492:ILE:HD12	2.04	0.58
1:C:446:TYR:CE1	1:C:455:ARG:HG2	2.39	0.57
1:D:415:PRO:O	1:D:418:LEU:HD12	2.04	0.57
1:A:147:ASN:ND2	2:A:507:HEM:HAC	2.20	0.57
1:B:148:ASN:HD22	1:B:211:MET:HE1	1.69	0.57
1:B:159:LEU:HD21	1:C:38:LEU:HD22	1.85	0.57
1:C:291:PHE:CD1	1:C:292:PRO:HD2	2.40	0.57
1:A:437:ASP:OD2	1:A:440:THR:HB	2.05	0.57
1:B:322:VAL:C	1:C:172:GLN:HG3	2.29	0.57
1:B:82:GLY:HA3	1:B:316:VAL:O	2.04	0.57
1:B:491:ARG:O	1:B:495:LEU:HD23	2.05	0.57
1:C:162:SER:HG	1:D:404:TYR:H	1.48	0.57
1:A:15:LYS:HD3	1:C:408:PHE:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:LYS:NZ	1:D:343:GLU:OE1	2.37	0.57
1:D:213:GLY:HA3	1:D:235:TYR:CD2	2.39	0.57
1:C:462:ILE:HD13	1:C:481:PHE:HE2	1.70	0.57
1:D:95:LYS:HG2	1:D:222:VAL:O	2.05	0.57
1:D:212:ASP:HB2	1:D:214:TYR:CE1	2.40	0.57
1:A:52:GLN:HB2	4:C:907:HOH:O	2.03	0.57
1:C:287:GLU:HA	1:C:290:ILE:CD1	2.35	0.57
1:D:97:LYS:O	1:D:100:GLU:HB2	2.05	0.57
1:D:108:ILE:HD13	1:D:315:LEU:HD22	1.86	0.57
1:D:217:HIS:CE1	1:D:298:LEU:HD22	2.40	0.57
1:D:237:THR:HA	1:D:276:TRP:CD1	2.39	0.57
1:C:462:ILE:HD13	1:C:481:PHE:CE2	2.40	0.57
1:D:177:ASP:O	1:D:181:VAL:HG23	2.05	0.57
1:D:391:MET:HE3	1:D:393:MET:HE3	1.86	0.57
1:A:402:ASN:C	1:A:402:ASN:HD22	2.12	0.56
1:D:432:ASN:C	1:D:432:ASN:HD22	2.12	0.56
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.87	0.56
1:B:18:ARG:HD2	1:D:409:SER:O	2.05	0.56
1:B:372:ILE:HB	1:B:375:ASN:HD22	1.70	0.56
1:C:251:ARG:HG2	1:C:251:ARG:NH1	2.20	0.56
1:C:287:GLU:HA	1:C:290:ILE:HD11	1.88	0.56
1:C:462:ILE:HG21	1:C:481:PHE:HE2	1.69	0.56
1:D:60:MET:HE1	1:D:63:PHE:HD2	1.70	0.56
1:C:178:PRO:HA	1:C:181:VAL:HB	1.87	0.56
1:B:279:TYR:HB3	1:B:309:LEU:HB3	1.87	0.56
1:B:294:ASN:HA	1:C:46:ARG:HH12	1.70	0.56
1:A:446:TYR:OH	1:A:487:GLU:HG2	2.06	0.56
1:C:394:MET:HE3	1:C:394:MET:HA	1.88	0.56
1:B:455:ARG:HG3	1:B:455:ARG:HH11	1.71	0.56
1:B:466:LEU:HD23	1:B:466:LEU:O	2.06	0.56
1:C:110:VAL:HG13	1:C:132:ALA:O	2.06	0.56
1:D:391:MET:HE3	1:D:393:MET:CE	2.34	0.56
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.05	0.56
1:C:207:GLY:HA3	4:C:919:HOH:O	2.05	0.56
1:B:37:LYS:C	1:C:158:LEU:HD13	2.31	0.55
1:A:335:PRO:HD2	4:A:712:HOH:O	2.05	0.55
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.89	0.55
1:B:391:MET:HE3	1:D:366:GLY:CA	2.36	0.55
1:C:223:ASN:HD21	1:C:227:GLU:HB3	1.72	0.55
1:D:18:ARG:HD3	4:D:887:HOH:O	2.06	0.55
1:D:93:TYR:CE1	1:D:282:VAL:HG11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:HIS:HD2	1:A:487:GLU:N	2.01	0.55
1:B:126:ARG:HH11	1:B:126:ARG:HB2	1.71	0.55
1:A:232:LYS:HB2	1:A:281:GLN:HB2	1.88	0.55
1:B:382:VAL:HG13	1:B:382:VAL:O	2.05	0.55
1:C:169:ARG:HD3	1:C:174:HIS:CE1	2.41	0.55
1:A:384:ASN:HA	1:C:26:LEU:HD13	1.89	0.55
1:B:160:PHE:CE1	1:B:164:ILE:HD11	2.42	0.55
1:C:97:LYS:O	1:C:104:LYS:NZ	2.39	0.55
1:A:60:MET:HE1	1:D:161:PRO:HD3	1.89	0.55
1:B:388:ASP:H	1:B:396:ASN:HD21	1.53	0.55
1:B:491:ARG:O	1:B:494:ALA:HB3	2.06	0.55
1:B:334:ASP:O	1:B:337:ASN:HB2	2.07	0.55
1:B:495:LEU:HD23	1:B:495:LEU:N	2.20	0.55
1:A:254:HIS:ND1	1:A:255:GLU:N	2.55	0.55
1:B:38:LEU:HD21	1:D:404:TYR:CD2	2.42	0.55
1:B:283:MET:HB2	1:B:302:TRP:CH2	2.42	0.55
1:B:386:GLN:C	1:B:387:ARG:HG2	2.32	0.55
1:D:26:LEU:O	1:D:34:VAL:HG13	2.06	0.54
1:C:206:ASP:HB2	1:C:244:LEU:HD23	1.89	0.54
1:D:211:MET:O	1:D:237:THR:HB	2.08	0.54
1:D:284:THR:HG23	1:D:287:GLU:CD	2.32	0.54
1:D:447:LEU:HD11	1:D:485:HIS:CD2	2.42	0.54
1:D:498:LYS:HB3	4:D:1084:HOH:O	2.05	0.54
1:B:208:HIS:O	1:B:211:MET:HG2	2.07	0.54
1:C:169:ARG:HH11	1:C:169:ARG:HG2	1.73	0.54
1:C:283:MET:HE2	1:C:307:TYR:CZ	2.43	0.54
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.43	0.54
1:B:241:ILE:CG2	1:B:242:LYS:H	2.20	0.54
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.89	0.54
1:B:439:VAL:O	1:B:442:VAL:N	2.38	0.54
1:C:195:VAL:O	1:C:199:PHE:HD1	1.91	0.54
1:D:279:TYR:C	1:D:280:ILE:HG22	2.32	0.54
1:A:72:VAL:HG13	1:A:73:VAL:HG22	1.90	0.54
1:B:4:ARG:HH22	1:C:470:GLN:NE2	1.99	0.54
1:C:91:THR:HG22	1:C:92:ARG:N	2.21	0.54
1:C:112:PHE:HA	1:C:130:GLY:O	2.08	0.54
1:B:95:LYS:HB3	1:B:224:ALA:HB2	1.89	0.54
1:C:94:SER:HA	1:C:222:VAL:O	2.07	0.54
1:D:285:PHE:N	1:D:285:PHE:CD1	2.75	0.54
1:A:148:ASN:HD22	1:A:148:ASN:N	2.05	0.54
1:B:160:PHE:N	1:B:161:PRO:HD2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:GLY:O	1:B:467:LYS:HE3	2.07	0.54
1:B:76:LYS:HD3	1:B:121:SER:O	2.07	0.54
1:B:101:HIS:O	1:B:104:LYS:HB2	2.07	0.54
1:B:221:LEU:HD23	1:B:221:LEU:N	2.23	0.54
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.90	0.54
1:C:444:THR:HG21	4:C:801:HOH:O	2.07	0.54
1:C:206:ASP:HB3	1:C:242:LYS:HG2	1.89	0.53
1:C:453:GLU:O	1:C:456:LYS:HB3	2.08	0.53
1:C:281:GLN:OE1	1:C:302:TRP:HB2	2.09	0.53
1:D:73:VAL:O	1:D:74:HIS:HB2	2.08	0.53
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.91	0.53
1:C:310:ILE:N	1:C:310:ILE:HD12	2.24	0.53
1:C:406:ASN:ND2	1:C:410:ALA:HB3	2.19	0.53
1:D:437:ASP:HA	4:D:827:HOH:O	2.07	0.53
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.69	0.53
1:C:446:TYR:O	1:C:455:ARG:HD3	2.08	0.53
1:C:466:LEU:HD12	1:C:469:ALA:HB3	1.91	0.53
1:C:493:GLN:HA	1:C:496:LEU:HD23	1.90	0.53
1:D:338:MET:HE3	1:D:342:ILE:HG22	1.90	0.53
1:A:141:ASN:O	1:A:337:ASN:HB3	2.09	0.53
1:B:153:PHE:CE2	1:B:194:GLN:HG3	2.43	0.53
4:B:998:HOH:O	1:D:386:GLN:HA	2.08	0.53
1:C:88:HIS:ND1	1:C:311:PRO:HB2	2.24	0.53
1:D:439:VAL:HG23	1:D:440:THR:N	2.24	0.53
1:D:445:PHE:HA	1:D:449:VAL:HG23	1.89	0.53
1:D:471:LEU:O	1:D:475:LYS:HG3	2.09	0.53
1:A:280:ILE:HG23	1:A:312:VAL:CG2	2.37	0.53
1:B:456:LYS:HB2	1:B:491:ARG:NH2	2.23	0.53
1:D:34:VAL:HG21	1:D:37:LYS:HB2	1.89	0.53
1:A:424:PHE:CE2	1:D:48:PRO:HD3	2.43	0.53
1:B:4:ARG:HD2	1:B:8:SER:HB2	1.90	0.53
1:A:419:GLU:CD	1:A:419:GLU:H	2.17	0.53
1:B:338:MET:HE1	1:B:343:GLU:C	2.33	0.53
1:B:235:TYR:N	1:B:235:TYR:CD1	2.77	0.52
1:C:245:SER:OG	1:C:248:ASP:HB2	2.09	0.52
1:D:6:PRO:HD2	1:D:266:ASN:OD1	2.09	0.52
1:D:391:MET:O	1:D:393:MET:HE2	2.09	0.52
1:C:108:ILE:HD13	1:C:315:LEU:HD22	1.91	0.52
1:C:145:VAL:CG1	1:C:353:ARG:HH22	2.22	0.52
1:B:485:HIS:CE1	1:B:487:GLU:HB3	2.44	0.52
1:B:201:ASP:O	1:B:243:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:THR:HG22	1:C:441:GLN:N	2.25	0.52
1:D:327:GLU:O	1:D:331:LEU:HG	2.09	0.52
1:A:215:GLY:O	1:A:216:SER:HB2	2.08	0.52
1:B:264:LEU:HD12	1:B:264:LEU:C	2.34	0.52
1:D:164:ILE:HG22	1:D:168:LYS:HD2	1.91	0.52
1:B:327:GLU:O	1:B:374:VAL:HG11	2.10	0.52
1:D:401:PRO:HA	4:D:995:HOH:O	2.09	0.52
1:B:64:ASP:HB3	1:C:360:THR:HB	1.91	0.52
1:B:368:ASN:O	1:B:371:GLN:HB2	2.09	0.52
1:B:100:GLU:HB2	1:B:104:LYS:NZ	2.24	0.52
1:B:110:VAL:HG11	1:B:131:PHE:HE1	1.74	0.52
1:C:49:LEU:HG	1:D:51:VAL:HG21	1.92	0.52
1:B:36:ASP:HB3	1:C:430:ARG:HD2	1.92	0.52
1:B:164:ILE:O	1:B:168:LYS:HG3	2.09	0.52
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.34	0.52
1:B:280:ILE:CD1	1:B:282:VAL:HG22	2.40	0.52
1:C:462:ILE:HG21	1:C:481:PHE:CE2	2.45	0.52
1:A:36:ASP:OD2	1:A:39:ASN:HB2	2.09	0.51
1:B:402:ASN:C	1:B:402:ASN:ND2	2.66	0.51
1:C:479:LYS:HG3	1:C:480:ASN:N	2.23	0.51
1:D:232:LYS:HB2	1:D:281:GLN:HG3	1.90	0.51
1:D:478:VAL:HG21	1:D:493:GLN:OE1	2.10	0.51
1:C:449:VAL:HG21	3:C:1302:NDP:O4D	2.10	0.51
1:D:12:LYS:O	1:D:16:GLU:HG3	2.10	0.51
1:C:19:ALA:O	1:C:20:ALA:HB3	2.09	0.51
1:C:239:GLN:HE22	1:C:275:SER:H	1.56	0.51
1:C:291:PHE:CG	1:C:292:PRO:HD2	2.45	0.51
1:C:463:ALA:O	1:C:467:LYS:HB3	2.10	0.51
1:D:500:ASN:C	1:D:501:GLU:HG3	2.34	0.51
1:A:37:LYS:NZ	1:D:158:LEU:HD22	2.24	0.51
1:A:424:PHE:CD2	1:D:48:PRO:HD3	2.46	0.51
1:B:205:PRO:HA	1:B:243:ASN:HA	1.92	0.51
1:C:73:VAL:O	1:C:74:HIS:HB2	2.09	0.51
1:A:446:TYR:OH	1:A:491:ARG:HD2	2.11	0.51
1:D:447:LEU:HD11	1:D:485:HIS:HD2	1.75	0.51
1:A:73:VAL:O	1:A:74:HIS:HB2	2.09	0.51
1:A:92:ARG:H	1:A:92:ARG:NH1	2.08	0.51
1:A:385:TYR:HE1	1:C:26:LEU:HD22	1.75	0.51
1:C:303:PRO:HA	3:C:1302:NDP:O2N	2.11	0.51
1:D:277:THR:HB	1:D:279:TYR:CE1	2.46	0.51
1:D:376:CYS:SG	1:D:394:MET:HE1	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLU:HG2	1:C:387:ARG:O	2.10	0.51
1:D:267:ALA:O	1:D:272:ASN:HB3	2.10	0.51
1:D:280:ILE:HG12	1:D:281:GLN:N	2.19	0.51
1:A:472:PHE:HA	1:A:475:LYS:HD3	1.93	0.51
1:B:444:THR:O	1:B:448:LYS:HB3	2.10	0.51
1:A:276:TRP:HB2	1:A:315:LEU:HD12	1.92	0.51
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.46	0.51
1:B:419:GLU:CD	1:B:419:GLU:H	2.19	0.51
1:B:495:LEU:CD2	1:B:495:LEU:N	2.74	0.51
1:C:34:VAL:HG21	1:C:37:LYS:HB2	1.92	0.51
1:D:394:MET:HE3	4:D:1069:HOH:O	2.11	0.51
1:A:88:HIS:CD2	1:A:311:PRO:HG2	2.46	0.50
1:A:139:ASP:O	1:C:32:ASN:HA	2.11	0.50
1:A:213:GLY:HA3	1:A:235:TYR:CE2	2.46	0.50
1:A:411:PRO:HA	1:C:24:ASP:O	2.10	0.50
1:B:198:LEU:O	1:B:203:GLY:HA3	2.10	0.50
1:D:188:ARG:HB3	1:D:190:GLU:OE1	2.11	0.50
1:D:202:ARG:HB3	4:D:1019:HOH:O	2.11	0.50
1:B:221:LEU:HD21	1:B:231:CYS:SG	2.51	0.50
1:B:345:SER:C	1:B:347:ASP:H	2.19	0.50
1:C:239:GLN:CD	1:C:239:GLN:H	2.19	0.50
1:C:449:VAL:O	1:C:449:VAL:HG12	2.11	0.50
1:D:74:HIS:O	1:D:111:ARG:NH2	2.44	0.50
1:D:189:PRO:C	1:D:191:SER:H	2.19	0.50
1:D:443:ARG:NE	1:D:484:VAL:O	2.44	0.50
1:B:11:MET:HB3	1:D:408:PHE:CE2	2.47	0.50
1:D:213:GLY:HA3	1:D:235:TYR:CE2	2.46	0.50
1:B:11:MET:HE1	1:C:180:MET:HG2	1.93	0.50
1:B:248:ASP:O	1:B:251:ARG:HB3	2.11	0.50
1:B:450:LEU:HD22	1:B:454:GLN:HG3	1.92	0.50
4:B:787:HOH:O	1:C:45:PRO:HD3	2.12	0.50
1:C:225:ASP:HB2	4:C:895:HOH:O	2.10	0.50
1:D:391:MET:C	1:D:393:MET:HE2	2.36	0.50
1:B:16:GLU:C	1:B:18:ARG:H	2.19	0.50
1:B:223:ASN:HD21	1:B:227:GLU:CD	2.20	0.50
1:C:61:ALA:O	1:C:65:ARG:HG3	2.11	0.50
1:C:88:HIS:HD1	1:C:311:PRO:HB2	1.77	0.50
1:C:124:THR:O	1:C:249:ALA:HB1	2.12	0.50
1:D:296:PHE:CE1	1:D:346:PRO:HD2	2.45	0.50
1:B:155:ARG:HD2	4:B:1005:HOH:O	2.12	0.50
1:C:487:GLU:HA	1:C:490:SER:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:MET:CE	1:D:63:PHE:HD2	2.24	0.50
1:D:282:VAL:HG12	1:D:283:MET:N	2.26	0.50
1:A:445:PHE:HA	1:A:449:VAL:CG2	2.42	0.50
1:C:349:MET:HE3	2:C:507:HEM:HBB1	1.94	0.50
1:B:430:ARG:NH2	1:C:53:ASP:OD2	2.44	0.50
1:D:153:PHE:HE2	1:D:185:TRP:CZ2	2.30	0.50
1:B:301:VAL:CG2	1:B:441:GLN:HE22	2.25	0.50
1:B:466:LEU:HD21	1:B:474:GLN:HA	1.94	0.50
1:C:208:HIS:HA	1:C:211:MET:CE	2.35	0.50
1:D:367:PRO:CG	1:D:390:PRO:HG2	2.42	0.50
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.12	0.49
1:A:182:TRP:O	1:A:186:SER:HB3	2.12	0.49
1:C:451:ASN:H	1:C:454:GLN:NE2	2.09	0.49
1:D:441:GLN:HA	1:D:444:THR:CG2	2.42	0.49
1:A:402:ASN:C	1:A:402:ASN:ND2	2.68	0.49
1:B:207:GLY:HA3	4:B:763:HOH:O	2.11	0.49
1:B:301:VAL:HG22	1:B:441:GLN:HE22	1.77	0.49
1:C:287:GLU:O	1:C:290:ILE:HG12	2.12	0.49
1:C:466:LEU:CD1	1:C:469:ALA:HB3	2.42	0.49
1:D:205:PRO:HA	1:D:243:ASN:HA	1.94	0.49
1:D:338:MET:HE2	1:D:342:ILE:C	2.37	0.49
1:D:440:THR:O	1:D:444:THR:HG22	2.11	0.49
1:B:442:VAL:O	1:B:445:PHE:HB3	2.13	0.49
1:C:26:LEU:HD12	1:C:27:THR:N	2.28	0.49
1:C:334:ASP:OD1	1:C:361:HIS:ND1	2.45	0.49
1:A:87:THR:HG23	1:A:313:GLY:HA2	1.95	0.49
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.95	0.49
1:A:499:TYR:C	1:A:501:GLU:H	2.21	0.49
1:D:106:THR:O	1:D:108:ILE:HG23	2.12	0.49
1:A:108:ILE:HA	1:A:134:LYS:O	2.12	0.49
1:A:120:GLY:H	1:D:120:GLY:H	1.60	0.49
1:B:283:MET:HE1	1:B:295:PRO:HB3	1.95	0.49
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.09	0.49
1:D:112:PHE:HA	1:D:130:GLY:O	2.13	0.49
1:B:40:SER:O	1:C:430:ARG:HA	2.12	0.49
1:B:41:LEU:CB	1:B:53:ASP:HB2	2.43	0.49
1:B:51:VAL:HG23	1:B:52:GLN:N	2.27	0.49
1:B:492:ILE:HG22	1:B:493:GLN:N	2.28	0.49
1:B:97:LYS:HD2	1:B:138:GLU:HB2	1.95	0.49
1:B:128:PRO:O	1:B:129:ARG:HD2	2.12	0.49
1:C:88:HIS:CE1	1:C:311:PRO:HB2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ARG:HD2	1:C:433:SER:HB2	1.94	0.49
1:B:275:SER:HA	1:B:315:LEU:O	2.13	0.49
1:B:406:ASN:ND2	1:B:410:ALA:HB3	2.20	0.49
1:C:223:ASN:HD21	1:C:227:GLU:CB	2.26	0.49
1:C:293:PHE:CD1	1:C:293:PHE:N	2.72	0.49
1:C:423:HIS:HA	1:D:427:ASP:HA	1.94	0.49
1:D:357:TYR:O	1:D:360:THR:HG22	2.13	0.49
1:D:439:VAL:HG23	1:D:440:THR:H	1.78	0.49
1:D:442:VAL:O	1:D:445:PHE:HB3	2.13	0.49
1:D:442:VAL:CG1	1:D:484:VAL:HG11	2.43	0.49
1:B:36:ASP:OD1	1:B:36:ASP:C	2.56	0.48
1:B:180:MET:HG3	1:C:11:MET:HE2	1.95	0.48
1:D:86:VAL:HG23	1:D:104:LYS:O	2.12	0.48
1:D:148:ASN:C	1:D:148:ASN:ND2	2.68	0.48
1:A:54:VAL:HG11	1:C:336:SER:HB2	1.95	0.48
1:B:148:ASN:CB	1:B:211:MET:HE2	2.42	0.48
1:B:241:ILE:CG2	1:B:242:LYS:N	2.76	0.48
1:B:328:VAL:O	1:B:331:LEU:HB2	2.12	0.48
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.43	0.48
1:B:456:LYS:HB2	1:B:491:ARG:HH22	1.78	0.48
1:C:126:ARG:CZ	1:C:126:ARG:HB2	2.42	0.48
1:D:471:LEU:O	1:D:474:GLN:HB2	2.13	0.48
1:B:245:SER:O	1:B:246:VAL:C	2.55	0.48
1:C:197:PHE:HD1	1:C:197:PHE:O	1.95	0.48
1:C:419:GLU:CD	1:C:419:GLU:H	2.22	0.48
1:B:127:ASP:O	1:B:129:ARG:NH1	2.45	0.48
1:D:85:GLU:O	1:D:313:GLY:HA3	2.13	0.48
1:B:440:THR:O	1:B:444:THR:HG23	2.14	0.48
1:D:244:LEU:HD23	1:D:245:SER:N	2.29	0.48
1:B:439:VAL:O	1:B:442:VAL:HG23	2.14	0.48
1:A:37:LYS:O	1:D:158:LEU:HD22	2.13	0.48
1:B:17:GLN:HG2	4:B:1026:HOH:O	2.14	0.48
1:B:201:ASP:HB3	1:B:243:ASN:HD22	1.79	0.48
1:B:205:PRO:HB3	4:B:1001:HOH:O	2.13	0.48
1:B:452:GLU:HB2	1:B:455:ARG:NH2	2.28	0.48
1:B:463:ALA:O	1:B:467:LYS:HG2	2.14	0.48
1:C:476:LYS:HB3	1:C:476:LYS:HZ2	1.78	0.48
1:D:397:GLN:HE21	1:D:397:GLN:HB2	1.54	0.48
1:D:491:ARG:O	1:D:495:LEU:HD12	2.14	0.48
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.77	0.48
1:A:97:LYS:HG2	1:A:100:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:TYR:CE1	1:A:328:VAL:HG11	2.49	0.48
1:A:496:LEU:O	1:A:497:ASP:C	2.57	0.48
1:B:100:GLU:CB	1:B:104:LYS:HG3	2.38	0.48
1:B:326:ALA:O	1:B:374:VAL:HG21	2.12	0.48
1:C:154:ILE:HG13	1:C:349:MET:HE1	1.95	0.48
1:D:86:VAL:HB	1:D:102:ILE:HA	1.95	0.48
1:B:206:ASP:HB2	1:B:244:LEU:HG	1.95	0.48
1:D:81:PHE:HZ	1:D:327:GLU:HB3	1.79	0.48
1:D:387:ARG:HG2	1:D:387:ARG:NH1	2.27	0.48
1:B:319:ARG:HD2	1:B:319:ARG:O	2.14	0.48
1:C:310:ILE:HD12	1:C:310:ILE:H	1.79	0.48
1:A:50:LEU:C	1:A:52:GLN:N	2.71	0.47
1:A:248:ASP:O	1:A:251:ARG:N	2.46	0.47
1:B:396:ASN:HB3	1:D:323:ASN:ND2	2.28	0.47
1:B:472:PHE:CE2	1:B:473:ILE:HG13	2.49	0.47
1:C:94:SER:OG	1:C:221:LEU:HD22	2.14	0.47
1:C:345:SER:O	1:C:347:ASP:N	2.47	0.47
1:D:235:TYR:N	1:D:235:TYR:CD1	2.81	0.47
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.49	0.47
1:C:202:ARG:HA	1:C:243:ASN:ND2	2.28	0.47
1:C:466:LEU:HD12	1:C:466:LEU:C	2.38	0.47
1:D:189:PRO:C	1:D:191:SER:N	2.71	0.47
1:A:464:GLY:O	1:A:467:LYS:HD3	2.14	0.47
1:B:125:VAL:HG22	1:B:126:ARG:N	2.28	0.47
1:B:297:ASP:HB3	1:B:300:LYS:HG3	1.95	0.47
1:C:126:ARG:O	1:C:126:ARG:HG3	2.13	0.47
1:C:439:VAL:HG12	1:C:484:VAL:HA	1.95	0.47
1:C:480:ASN:O	1:C:484:VAL:HG23	2.15	0.47
1:D:298:LEU:HD23	1:D:349:MET:HG3	1.96	0.47
1:A:42:THR:O	1:D:431:PHE:HE1	1.97	0.47
1:B:176:LYS:HG2	4:B:800:HOH:O	2.13	0.47
1:D:212:ASP:OD1	1:D:237:THR:HG22	2.14	0.47
1:D:265:PHE:CD1	1:D:320:ASN:ND2	2.83	0.47
1:B:229:VAL:CG2	1:B:284:THR:HA	2.43	0.47
1:B:351:GLN:O	1:B:354:LEU:HB2	2.14	0.47
1:A:60:MET:HB3	1:D:355:PHE:HE2	1.79	0.47
1:A:357:TYR:O	1:A:360:THR:HG22	2.14	0.47
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.95	0.47
1:C:433:SER:C	1:C:435:ASN:H	2.22	0.47
1:C:444:THR:HG22	1:C:444:THR:O	2.14	0.47
1:D:19:ALA:N	4:D:841:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ARG:HH11	1:D:65:ARG:HG3	1.79	0.47
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.49	0.47
1:D:279:TYR:O	1:D:280:ILE:HG22	2.14	0.47
1:B:270:THR:O	1:B:272:ASN:N	2.48	0.47
1:C:151:ILE:CD1	1:C:194:GLN:HG2	2.41	0.47
1:C:191:SER:C	1:C:195:VAL:HG23	2.39	0.47
1:C:239:GLN:CD	1:C:239:GLN:N	2.73	0.47
1:A:271:GLY:HA2	1:A:273:TYR:CE1	2.50	0.47
1:A:277:THR:OG1	1:A:314:LYS:NZ	2.48	0.47
1:B:46:ARG:HD2	4:B:1056:HOH:O	2.15	0.47
1:B:235:TYR:HA	1:B:277:THR:O	2.15	0.47
1:D:419:GLU:H	1:D:419:GLU:CD	2.23	0.47
1:A:177:ASP:HB3	1:A:180:MET:HB2	1.97	0.47
1:A:451:ASN:OD1	1:A:451:ASN:C	2.57	0.47
1:C:391:MET:HE3	1:C:393:MET:CE	2.43	0.47
1:D:443:ARG:HG3	1:D:484:VAL:O	2.15	0.47
1:A:265:PHE:CE2	1:D:173:THR:HG22	2.50	0.47
1:A:467:LYS:HG2	1:A:468:ASP:N	2.30	0.47
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.80	0.47
1:B:95:LYS:HG3	1:B:222:VAL:O	2.15	0.47
1:B:391:MET:HE1	1:D:369:TYR:HA	1.96	0.47
1:D:214:TYR:N	1:D:214:TYR:CD1	2.83	0.47
1:D:245:SER:HB3	1:D:248:ASP:OD2	2.15	0.47
1:D:279:TYR:C	1:D:280:ILE:CG2	2.87	0.47
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.80	0.46
1:B:430:ARG:NH2	1:C:53:ASP:CG	2.73	0.46
1:C:290:ILE:O	1:C:291:PHE:C	2.57	0.46
1:D:20:ALA:O	1:D:21:GLN:C	2.58	0.46
1:D:95:LYS:O	1:D:96:ALA:C	2.58	0.46
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.96	0.46
1:B:485:HIS:CE1	1:B:487:GLU:HG2	2.50	0.46
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.98	0.46
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.97	0.46
1:D:210:HIS:HB3	1:D:242:LYS:H	1.81	0.46
1:A:39:ASN:C	1:D:158:LEU:HD12	2.40	0.46
1:A:155:ARG:NH2	1:A:438:ASN:OD1	2.49	0.46
1:B:19:ALA:HB3	1:B:21:GLN:HG3	1.97	0.46
1:B:268:ILE:HB	1:B:320:ASN:HD21	1.80	0.46
1:C:219:PHE:O	1:C:230:TYR:HA	2.15	0.46
1:C:367:PRO:HG2	1:C:390:PRO:CG	2.46	0.46
1:C:446:TYR:OH	1:C:488:TYR:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:TRP:HA	1:D:337:ASN:O	2.14	0.46
1:D:476:LYS:O	1:D:480:ASN:OD1	2.34	0.46
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.46	0.46
1:A:51:VAL:HG11	1:B:49:LEU:HD13	1.98	0.46
1:B:254:HIS:ND1	1:C:254:HIS:ND1	2.64	0.46
1:B:359:ASP:O	1:B:362:ARG:HB2	2.16	0.46
1:C:156:ASP:OD1	1:C:158:LEU:HB2	2.15	0.46
1:A:20:ALA:O	1:A:21:GLN:C	2.59	0.46
1:B:280:ILE:O	1:B:280:ILE:HG13	2.15	0.46
1:C:83:TYR:CD1	1:C:83:TYR:C	2.94	0.46
1:C:244:LEU:HD11	1:C:252:LEU:HD12	1.98	0.46
1:C:250:ALA:O	1:C:253:ALA:HB3	2.16	0.46
1:C:428:VAL:O	1:C:429:GLN:HB3	2.15	0.46
1:C:459:CYS:SG	1:C:492:ILE:HD13	2.54	0.46
1:D:71:ARG:HG3	4:D:1078:HOH:O	2.15	0.46
1:D:118:GLU:OE1	1:D:118:GLU:N	2.44	0.46
1:D:209:ARG:HB2	4:D:1020:HOH:O	2.15	0.46
1:A:223:ASN:OD1	1:A:223:ASN:C	2.59	0.46
1:B:33:PRO:HD2	1:D:340:PRO:HD3	1.98	0.46
1:C:446:TYR:O	1:C:447:LEU:HD23	2.16	0.46
1:D:148:ASN:C	1:D:148:ASN:HD22	2.23	0.46
1:D:369:TYR:O	1:D:372:ILE:HG13	2.16	0.46
1:D:455:ARG:HD2	1:D:491:ARG:NH1	2.29	0.46
1:A:42:THR:HG22	1:A:48:PRO:O	2.16	0.46
1:B:35:GLY:O	1:D:413:HIS:HB3	2.16	0.46
1:B:209:ARG:HG2	1:B:274:PRO:CG	2.46	0.46
1:D:284:THR:O	1:D:288:ALA:N	2.48	0.46
1:D:492:ILE:HA	1:D:495:LEU:HD12	1.98	0.46
1:B:393:MET:HB3	1:B:394:MET:H	1.55	0.46
1:C:63:PHE:CD1	1:C:63:PHE:C	2.94	0.46
1:D:96:ALA:HB3	1:D:99:PHE:CD2	2.51	0.46
1:D:217:HIS:HE1	1:D:298:LEU:HD22	1.81	0.46
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.80	0.45
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.27	0.45
1:C:212:ASP:OD1	1:C:237:THR:HG22	2.16	0.45
1:C:459:CYS:SG	1:C:492:ILE:CD1	3.04	0.45
1:D:153:PHE:CE2	1:D:185:TRP:CZ2	3.05	0.45
1:B:16:GLU:C	1:B:18:ARG:N	2.73	0.45
1:B:73:VAL:HG11	1:B:164:ILE:HD12	1.98	0.45
1:B:281:GLN:HB2	1:B:302:TRP:CE3	2.51	0.45
1:C:82:GLY:HA3	1:C:316:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:HH11	1:D:241:ILE:HG21	1.78	0.45
1:D:297:ASP:OD1	1:D:297:ASP:C	2.59	0.45
1:B:381:ARG:CG	1:B:381:ARG:HH11	2.29	0.45
1:C:90:ILE:O	1:C:93:TYR:HB2	2.16	0.45
1:D:334:ASP:OD1	1:D:361:HIS:ND1	2.49	0.45
1:D:410:ALA:HB1	1:D:411:PRO:HD2	1.98	0.45
1:A:304:HIS:HB2	3:A:1102:NDP:O2A	2.17	0.45
1:B:273:TYR:HA	1:B:274:PRO:HD3	1.78	0.45
1:B:290:ILE:O	1:B:291:PHE:C	2.59	0.45
1:B:316:VAL:HG12	1:B:318:ASN:ND2	2.31	0.45
1:D:3:ASN:HB2	1:D:4:ARG:H	1.62	0.45
1:A:4:ARG:HD3	1:A:9:ASP:OD1	2.16	0.45
1:B:67:ARG:HB2	4:B:753:HOH:O	2.15	0.45
1:B:452:GLU:OE2	1:B:491:ARG:NH2	2.50	0.45
1:C:89:ASP:CG	1:C:91:THR:HB	2.41	0.45
1:C:220:LYS:HA	1:C:229:VAL:O	2.17	0.45
1:C:446:TYR:HE2	1:C:485:HIS:ND1	2.15	0.45
1:D:378:TYR:C	1:D:380:ALA:H	2.24	0.45
1:D:475:LYS:HG3	1:D:475:LYS:H	1.53	0.45
1:B:16:GLU:O	1:B:18:ARG:N	2.49	0.45
1:C:251:ARG:HG3	1:C:252:LEU:H	1.80	0.45
1:A:280:ILE:O	1:A:280:ILE:HG13	2.14	0.45
1:B:287:GLU:O	1:B:290:ILE:N	2.44	0.45
1:B:451:ASN:OD1	1:B:451:ASN:O	2.35	0.45
1:C:90:ILE:O	1:C:91:THR:C	2.59	0.45
1:C:480:ASN:O	1:C:483:ASP:HB2	2.16	0.45
1:D:98:VAL:HG13	1:D:99:PHE:CD1	2.52	0.45
1:D:343:GLU:HB3	1:D:344:PRO:HD2	1.99	0.45
1:A:39:ASN:OD1	1:D:432:ASN:HA	2.17	0.45
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.16	0.45
1:B:110:VAL:HG11	1:B:131:PHE:CE1	2.52	0.45
1:C:179:ASP:O	1:C:183:ASP:HB2	2.17	0.45
1:C:280:ILE:O	1:C:280:ILE:HG13	2.17	0.45
1:D:63:PHE:HA	1:D:66:GLU:HG3	1.98	0.45
1:D:71:ARG:HG3	1:D:71:ARG:HH11	1.82	0.45
1:D:228:ALA:HB2	1:D:420:HIS:CE1	2.52	0.45
1:D:271:GLY:HA2	1:D:273:TYR:CE1	2.52	0.45
1:D:345:SER:C	1:D:347:ASP:H	2.25	0.45
1:A:156:ASP:OD1	1:A:158:LEU:HB2	2.17	0.45
1:A:15:LYS:O	1:A:16:GLU:C	2.60	0.45
1:A:24:ASP:OD1	1:A:24:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLN:HG3	1:D:4:ARG:NH2	2.32	0.45
1:B:38:LEU:HG	1:D:413:HIS:HE1	1.81	0.45
1:B:90:ILE:O	1:B:93:TYR:HB2	2.17	0.45
1:B:92:ARG:H	1:B:92:ARG:HG3	1.43	0.45
1:B:155:ARG:NH1	1:B:299:THR:OG1	2.50	0.45
1:B:280:ILE:HD12	1:B:282:VAL:HG22	1.99	0.45
1:C:126:ARG:HA	1:C:204:ILE:HG12	1.98	0.45
1:C:148:ASN:HA	1:C:212:ASP:O	2.16	0.45
1:D:331:LEU:HD23	1:D:331:LEU:HA	1.81	0.45
1:A:498:LYS:O	1:A:501:GLU:N	2.49	0.44
1:B:364:ARG:HD3	4:B:961:HOH:O	2.17	0.44
1:C:73:VAL:HB	1:C:74:HIS:HD2	1.81	0.44
1:D:291:PHE:CD1	1:D:292:PRO:HD2	2.52	0.44
1:B:403:TYR:OH	1:D:11:MET:HE1	2.17	0.44
1:C:14:TRP:O	1:C:18:ARG:HB2	2.17	0.44
1:C:52:GLN:HE21	1:C:52:GLN:HB3	1.52	0.44
1:A:422:THR:O	1:B:428:VAL:HG22	2.16	0.44
1:B:218:THR:O	1:B:345:SER:HB3	2.18	0.44
1:B:278:LEU:O	1:B:312:VAL:HG13	2.17	0.44
1:B:283:MET:SD	1:B:288:ALA:HA	2.58	0.44
1:D:206:ASP:HB3	1:D:242:LYS:HG2	1.99	0.44
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.86	0.44
1:A:273:TYR:HB3	1:A:317:LEU:O	2.17	0.44
1:A:428:VAL:HG23	1:B:424:PHE:HD1	1.82	0.44
1:A:445:PHE:HB2	3:A:1102:NDP:O2D	2.17	0.44
1:B:189:PRO:C	1:B:191:SER:N	2.75	0.44
1:B:477:ALA:O	1:B:481:PHE:CD2	2.70	0.44
1:C:73:VAL:HG11	1:C:164:ILE:HD12	2.00	0.44
1:C:154:ILE:H	1:C:154:ILE:HG12	1.68	0.44
1:C:155:ARG:NH2	1:C:190:GLU:HB3	2.32	0.44
1:C:446:TYR:CE2	1:C:485:HIS:ND1	2.86	0.44
1:C:481:PHE:N	1:C:481:PHE:HD1	2.16	0.44
1:A:76:LYS:HD3	1:A:121:SER:O	2.17	0.44
1:A:278:LEU:HD23	1:A:312:VAL:HB	1.99	0.44
1:A:291:PHE:HD2	1:A:293:PHE:O	2.00	0.44
1:B:202:ARG:HD3	3:B:1202:NDP:C6A	2.48	0.44
1:C:481:PHE:N	1:C:481:PHE:CD1	2.85	0.44
1:D:5:ASP:N	1:D:5:ASP:OD1	2.50	0.44
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.52	0.44
1:A:235:TYR:CD1	1:A:235:TYR:N	2.85	0.44
1:A:322:VAL:O	1:D:172:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:THR:OG1	1:B:239:GLN:NE2	2.51	0.44
1:B:252:LEU:HD23	1:B:259:TYR:CD2	2.53	0.44
1:C:17:GLN:HE21	1:C:17:GLN:HB3	1.61	0.44
1:D:150:PRO:HB3	1:D:214:TYR:HD2	1.80	0.44
1:D:284:THR:O	1:D:288:ALA:HB2	2.18	0.44
1:B:16:GLU:O	1:B:19:ALA:N	2.46	0.44
1:B:162:SER:O	1:B:165:HIS:HB2	2.18	0.44
1:B:245:SER:O	1:B:248:ASP:N	2.51	0.44
1:B:283:MET:CE	1:B:295:PRO:HB3	2.48	0.44
1:C:143:ASP:HB2	1:C:334:ASP:O	2.18	0.44
1:D:281:GLN:HG2	1:D:309:LEU:HD12	2.00	0.44
1:A:216:SER:HB3	1:A:298:LEU:HD11	1.99	0.44
1:B:69:PRO:HD3	1:C:69:PRO:HG3	2.00	0.44
1:B:251:ARG:NH1	1:B:251:ARG:HG2	2.33	0.44
1:D:220:LYS:HB3	1:D:343:GLU:HB2	2.00	0.44
1:A:221:LEU:O	1:A:228:ALA:HA	2.17	0.44
1:A:436:ASP:O	1:A:437:ASP:C	2.61	0.44
1:B:319:ARG:HD2	1:B:319:ARG:C	2.43	0.44
1:C:110:VAL:HG11	1:C:131:PHE:CE1	2.53	0.44
1:C:110:VAL:HG11	1:C:131:PHE:HE1	1.83	0.44
1:C:168:LYS:HB3	1:C:169:ARG:H	1.71	0.44
1:D:228:ALA:HB1	1:D:285:PHE:HZ	1.82	0.44
1:B:18:ARG:HH11	1:B:18:ARG:CG	2.30	0.43
1:B:55:VAL:CG2	1:C:430:ARG:NH2	2.81	0.43
1:C:470:GLN:CB	1:C:473:ILE:HD12	2.48	0.43
1:A:155:ARG:NH1	1:A:297:ASP:OD2	2.51	0.43
1:B:158:LEU:HD13	1:C:37:LYS:C	2.42	0.43
1:B:382:VAL:O	1:B:382:VAL:CG1	2.66	0.43
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.54	0.43
1:D:151:ILE:HD13	1:D:193:HIS:CD2	2.53	0.43
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.83	0.43
1:A:74:HIS:HA	1:A:114:THR:O	2.18	0.43
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.48	0.43
1:B:26:LEU:HD22	1:D:385:TYR:HE1	1.83	0.43
1:B:37:LYS:O	1:C:158:LEU:HB3	2.19	0.43
1:C:91:THR:C	1:C:93:TYR:H	2.26	0.43
1:C:154:ILE:CD1	1:C:160:PHE:HA	2.48	0.43
1:D:301:VAL:O	1:D:303:PRO:HD3	2.18	0.43
1:D:439:VAL:O	1:D:440:THR:C	2.61	0.43
1:D:442:VAL:HB	1:D:484:VAL:HG13	2.00	0.43
1:A:436:ASP:O	1:A:437:ASP:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TRP:HA	1:B:337:ASN:O	2.19	0.43
1:B:161:PRO:HD3	1:C:60:MET:HE1	2.00	0.43
1:C:197:PHE:CD1	1:C:197:PHE:C	2.96	0.43
1:A:343:GLU:HB3	1:A:344:PRO:HD2	2.00	0.43
1:A:498:LYS:O	1:A:499:TYR:C	2.60	0.43
1:B:14:TRP:HA	1:B:17:GLN:CD	2.44	0.43
1:C:89:ASP:OD1	1:C:89:ASP:C	2.61	0.43
1:C:337:ASN:HD22	1:C:337:ASN:HA	1.70	0.43
1:B:218:THR:OG1	1:B:232:LYS:HE3	2.19	0.43
1:B:358:PRO:HD3	4:B:965:HOH:O	2.19	0.43
1:C:15:LYS:O	1:C:15:LYS:HG2	2.19	0.43
1:C:232:LYS:O	1:C:280:ILE:HA	2.18	0.43
1:D:85:GLU:OE2	1:D:105:ARG:NH1	2.52	0.43
1:B:214:TYR:C	1:B:216:SER:N	2.77	0.43
1:B:220:LYS:HB3	1:B:343:GLU:HB2	2.01	0.43
1:C:43:VAL:O	1:C:47:GLY:HA3	2.18	0.43
1:C:291:PHE:HD2	1:C:293:PHE:O	2.01	0.43
1:D:210:HIS:CG	1:D:242:LYS:HB3	2.54	0.43
1:D:381:ARG:HH11	1:D:381:ARG:HG2	1.84	0.43
1:B:414:GLN:O	1:D:35:GLY:HA2	2.18	0.43
1:C:169:ARG:HG2	1:C:169:ARG:NH1	2.33	0.43
1:C:275:SER:C	1:C:276:TRP:CE3	2.97	0.43
1:C:426:GLY:O	1:C:427:ASP:O	2.37	0.43
1:C:445:PHE:HD1	1:C:449:VAL:HB	1.83	0.43
1:A:100:GLU:HB3	1:A:104:LYS:HE3	2.01	0.43
1:A:445:PHE:HA	1:A:449:VAL:HG23	2.01	0.43
1:B:51:VAL:CG2	1:B:52:GLN:N	2.82	0.43
1:B:193:HIS:HB2	4:B:941:HOH:O	2.19	0.43
1:B:236:LYS:H	1:B:236:LYS:HG2	1.45	0.43
1:C:496:LEU:O	1:C:500:ASN:OD1	2.37	0.43
1:B:439:VAL:O	1:B:440:THR:C	2.62	0.43
1:C:282:VAL:HG12	1:C:283:MET:N	2.33	0.43
1:D:241:ILE:O	1:D:241:ILE:HG22	2.19	0.43
1:B:26:LEU:O	1:B:34:VAL:HG23	2.19	0.42
1:B:212:ASP:OD1	1:B:236:LYS:HA	2.19	0.42
1:A:50:LEU:C	1:A:52:GLN:H	2.27	0.42
1:B:437:ASP:HA	4:B:1007:HOH:O	2.18	0.42
1:C:197:PHE:HD1	1:C:197:PHE:C	2.27	0.42
1:D:170:ASN:HD22	1:D:172:GLN:N	2.16	0.42
1:D:478:VAL:O	1:D:479:LYS:C	2.62	0.42
1:A:279:TYR:HA	1:A:310:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLN:O	1:B:387:ARG:HG2	2.19	0.42
1:B:466:LEU:HD23	1:B:474:GLN:HG2	2.01	0.42
1:C:202:ARG:O	1:C:204:ILE:N	2.53	0.42
1:A:235:TYR:HA	1:A:277:THR:O	2.20	0.42
1:A:281:GLN:HG3	1:A:309:LEU:HD13	2.02	0.42
1:A:501:GLU:OE1	1:A:501:GLU:HA	2.19	0.42
1:A:160:PHE:CD1	2:A:507:HEM:HAB	2.55	0.42
1:C:22:LYS:CD	1:C:23:PRO:HD2	2.50	0.42
1:C:443:ARG:C	1:C:445:PHE:N	2.77	0.42
1:A:18:ARG:H	1:A:18:ARG:HG3	1.58	0.42
1:A:169:ARG:HD2	1:A:174:HIS:CE1	2.55	0.42
1:B:262:ARG:HB3	1:C:175:LEU:HD11	2.00	0.42
1:C:108:ILE:HA	1:C:134:LYS:O	2.20	0.42
1:C:286:SER:O	1:C:289:GLU:N	2.53	0.42
1:D:220:LYS:HB2	1:D:344:PRO:O	2.20	0.42
1:A:37:LYS:HZ2	1:D:158:LEU:HD22	1.84	0.42
1:A:139:ASP:HB3	1:A:340:PRO:HD2	2.02	0.42
1:A:209:ARG:CG	1:A:274:PRO:HB3	2.46	0.42
1:A:430:ARG:HA	1:D:40:SER:O	2.19	0.42
1:B:74:HIS:O	1:B:111:ARG:NH2	2.53	0.42
1:B:95:LYS:HG3	1:B:95:LYS:H	1.50	0.42
1:D:442:VAL:HB	1:D:484:VAL:CG1	2.49	0.42
1:B:166:SER:HA	1:B:180:MET:HE3	2.02	0.42
1:D:415:PRO:HA	1:D:418:LEU:CD1	2.50	0.42
1:A:393:MET:O	1:A:394:MET:HB2	2.19	0.42
1:B:169:ARG:HD3	1:B:174:HIS:CE1	2.55	0.42
1:B:347:ASP:HB3	1:B:350:LEU:HB3	2.01	0.42
1:B:355:PHE:CD2	1:B:356:ALA:N	2.88	0.42
1:B:451:ASN:C	1:B:453:GLU:N	2.78	0.42
1:C:348:LYS:O	1:C:349:MET:C	2.62	0.42
1:D:76:LYS:O	1:D:113:SER:CB	2.67	0.42
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.50	0.42
1:C:472:PHE:HA	1:C:475:LYS:HG3	2.02	0.42
1:D:252:LEU:O	1:D:253:ALA:C	2.62	0.42
1:D:283:MET:HE2	1:D:291:PHE:HD2	1.85	0.42
1:B:122:ALA:CB	1:B:257:PRO:HB3	2.44	0.41
1:B:279:TYR:HA	1:B:310:ILE:O	2.20	0.41
1:B:414:GLN:HG2	1:B:416:SER:OG	2.20	0.41
1:C:440:THR:O	1:C:441:GLN:C	2.61	0.41
1:D:99:PHE:O	1:D:100:GLU:C	2.63	0.41
1:D:451:ASN:OD1	1:D:451:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:O	1:A:56:PHE:C	2.62	0.41
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.85	0.41
1:B:126:ARG:HA	1:B:204:ILE:HG12	2.02	0.41
1:B:231:CYS:HA	1:B:281:GLN:O	2.20	0.41
1:B:239:GLN:H	1:B:239:GLN:CD	2.27	0.41
1:B:268:ILE:HB	1:B:320:ASN:ND2	2.35	0.41
1:C:180:MET:HB3	1:D:403:TYR:CE1	2.55	0.41
1:D:197:PHE:CD1	1:D:197:PHE:C	2.98	0.41
1:A:72:VAL:CG1	2:A:507:HEM:HMA1	2.50	0.41
1:A:296:PHE:CD1	1:A:346:PRO:HD2	2.55	0.41
1:B:26:LEU:HD13	1:D:384:ASN:HA	2.00	0.41
1:C:499:TYR:C	1:C:501:GLU:H	2.28	0.41
1:D:221:LEU:HD21	1:D:231:CYS:SG	2.60	0.41
1:A:350:LEU:O	1:A:353:ARG:HB2	2.21	0.41
1:A:374:VAL:HB	4:A:929:HOH:O	2.20	0.41
1:C:345:SER:C	1:C:347:ASP:H	2.28	0.41
1:D:104:LYS:NZ	1:D:138:GLU:OE1	2.54	0.41
1:A:391:MET:HE3	1:A:393:MET:CE	2.50	0.41
1:B:94:SER:HB3	1:B:221:LEU:HD13	2.02	0.41
1:B:158:LEU:O	1:C:37:LYS:NZ	2.54	0.41
1:B:304:HIS:HB2	3:B:1202:NDP:O2A	2.21	0.41
1:C:71:ARG:HG3	1:C:71:ARG:HH11	1.86	0.41
1:C:87:THR:OG1	1:C:313:GLY:HA2	2.19	0.41
1:C:284:THR:HG23	1:C:287:GLU:OE2	2.20	0.41
1:D:170:ASN:ND2	1:D:172:GLN:N	2.58	0.41
1:D:296:PHE:CD1	1:D:346:PRO:HD2	2.55	0.41
1:A:173:THR:O	1:A:174:HIS:HB3	2.20	0.41
1:D:189:PRO:O	1:D:192:LEU:HG	2.21	0.41
1:A:26:LEU:CD1	1:C:384:ASN:HA	2.50	0.41
1:B:393:MET:HG3	1:D:373:PRO:HD3	2.03	0.41
1:C:72:VAL:HG12	2:C:507:HEM:HAA2	2.03	0.41
1:C:126:ARG:HD3	1:C:198:LEU:HG	2.02	0.41
1:C:496:LEU:O	1:C:498:LYS:N	2.53	0.41
1:A:15:LYS:HD3	1:C:408:PHE:C	2.46	0.41
1:A:423:HIS:HA	1:B:427:ASP:HA	2.03	0.41
1:A:444:THR:HG21	4:A:972:HOH:O	2.21	0.41
1:B:11:MET:HE3	1:B:11:MET:HB2	1.95	0.41
1:B:221:LEU:O	1:B:228:ALA:HA	2.21	0.41
1:B:338:MET:HE2	1:B:342:ILE:HG22	2.02	0.41
1:B:439:VAL:HG12	1:B:484:VAL:HG22	2.02	0.41
1:C:191:SER:O	1:C:192:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:GLU:HG2	1:C:495:LEU:HD21	2.03	0.41
1:A:14:TRP:O	1:A:17:GLN:HB3	2.21	0.41
1:A:237:THR:HA	1:A:276:TRP:CD1	2.56	0.41
1:A:385:TYR:OH	1:A:411:PRO:O	2.36	0.41
1:A:404:TYR:CD1	1:A:405:PRO:HA	2.56	0.41
1:B:107:PRO:HD2	1:B:379:ARG:HE	1.85	0.41
1:B:188:ARG:HA	1:B:189:PRO:HD2	1.91	0.41
1:B:301:VAL:HB	3:B:1202:NDP:N7N	2.36	0.41
1:B:410:ALA:HB1	1:B:411:PRO:HD2	2.02	0.41
1:C:152:PHE:HA	1:C:194:GLN:HG3	2.02	0.41
1:C:232:LYS:HG3	1:C:302:TRP:CE3	2.56	0.41
1:D:93:TYR:CZ	1:D:282:VAL:HG21	2.56	0.41
1:D:347:ASP:O	1:D:348:LYS:C	2.63	0.41
1:D:440:THR:HG22	1:D:441:GLN:N	2.35	0.41
1:B:83:TYR:CD1	1:B:83:TYR:C	2.99	0.41
1:B:209:ARG:HG2	1:B:274:PRO:HB3	2.03	0.41
1:B:327:GLU:O	1:B:331:LEU:HG	2.21	0.41
1:B:343:GLU:HB3	1:B:344:PRO:HD2	2.02	0.41
1:C:347:ASP:O	1:C:350:LEU:HB3	2.21	0.41
1:D:93:TYR:CE1	1:D:282:VAL:HG21	2.56	0.41
1:D:372:ILE:O	1:D:373:PRO:C	2.64	0.41
1:D:450:LEU:HD21	3:D:1402:NDP:N6A	2.36	0.41
1:D:496:LEU:HD23	1:D:496:LEU:HA	1.94	0.41
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.86	0.40
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.19	0.40
1:B:118:GLU:O	1:B:121:SER:HB3	2.21	0.40
1:B:381:ARG:HH11	1:B:381:ARG:HB2	1.86	0.40
1:C:72:VAL:CG1	2:C:507:HEM:HMA3	2.50	0.40
1:C:172:GLN:HE21	1:C:172:GLN:HB3	1.69	0.40
1:C:234:HIS:O	1:C:279:TYR:N	2.43	0.40
1:C:485:HIS:CD2	1:C:485:HIS:C	2.97	0.40
1:D:206:ASP:OD1	1:D:206:ASP:C	2.65	0.40
1:D:442:VAL:HG12	1:D:484:VAL:HG11	2.03	0.40
1:A:355:PHE:O	1:A:358:PRO:HD2	2.21	0.40
1:B:129:ARG:CB	1:B:211:MET:HE1	2.51	0.40
1:B:469:ALA:HB1	1:B:473:ILE:HG21	2.04	0.40
1:C:310:ILE:HA	1:C:311:PRO:HD3	1.96	0.40
1:D:160:PHE:CD1	2:D:507:HEM:HAB	2.56	0.40
1:D:220:LYS:HE3	1:D:343:GLU:CB	2.48	0.40
1:D:331:LEU:HD13	1:D:333:PHE:CZ	2.56	0.40
1:A:127:ASP:C	1:A:128:PRO:O	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:PHE:HA	1:A:292:PRO:HD3	1.88	0.40
1:A:338:MET:HE1	1:A:344:PRO:HB3	2.02	0.40
1:A:370:LEU:HA	1:A:370:LEU:HD23	1.89	0.40
1:A:431:PHE:CE2	1:D:44:GLY:C	2.99	0.40
1:B:188:ARG:HB3	1:B:190:GLU:OE2	2.21	0.40
1:B:439:VAL:HG23	1:B:440:THR:H	1.86	0.40
1:B:446:TYR:CZ	1:B:455:ARG:HD2	2.56	0.40
1:C:264:LEU:O	1:C:264:LEU:HD12	2.21	0.40
1:C:474:GLN:O	1:C:475:LYS:C	2.64	0.40
1:D:145:VAL:CG1	1:D:353:ARG:NH2	2.85	0.40
1:A:4:ARG:HH22	1:D:179:ASP:CG	2.29	0.40
1:A:155:ARG:HD3	1:A:297:ASP:OD1	2.21	0.40
1:B:55:VAL:HG21	1:C:430:ARG:NH2	2.36	0.40
1:B:384:ASN:HB2	1:B:385:TYR:H	1.66	0.40
1:C:384:ASN:OD1	1:C:397:GLN:NE2	2.55	0.40
1:D:288:ALA:C	1:D:290:ILE:N	2.80	0.40
1:D:414:GLN:O	1:D:415:PRO:C	2.64	0.40
1:D:488:TYR:CE1	1:D:492:ILE:HD11	2.56	0.40
1:A:265:PHE:CD1	1:A:265:PHE:C	3.00	0.40
1:A:283:MET:HE2	1:A:307:TYR:CZ	2.57	0.40
1:A:428:VAL:HG23	1:B:424:PHE:CD1	2.56	0.40
1:B:205:PRO:O	1:B:244:LEU:HD12	2.22	0.40
1:B:447:LEU:O	1:B:448:LYS:HE2	2.21	0.40
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.50	0.40
1:D:189:PRO:HG3	1:D:480:ASN:ND2	2.37	0.40
1:D:228:ALA:HB1	1:D:285:PHE:CZ	2.56	0.40
1:D:414:GLN:O	1:D:416:SER:N	2.53	0.40
1:D:499:TYR:O	1:D:501:GLU:HG3	2.22	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	497/506 (98%)	442 (89%)	50 (10%)	5 (1%)	12	15
1	B	497/506 (98%)	423 (85%)	58 (12%)	16 (3%)	3	2
1	C	497/506 (98%)	417 (84%)	65 (13%)	15 (3%)	3	2
1	D	497/506 (98%)	442 (89%)	49 (10%)	6 (1%)	10	12
All	All	1988/2024 (98%)	1724 (87%)	222 (11%)	42 (2%)	5	4

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	437	ASP
1	B	124	THR
1	B	242	LYS
1	B	394	MET
1	B	448	LYS
1	C	292	PRO
1	C	427	ASP
1	B	100	GLU
1	B	271	GLY
1	B	348	LYS
1	B	437	ASP
1	C	440	THR
1	C	444	THR
1	C	496	LEU
1	C	497	ASP
1	D	411	PRO
1	D	413	HIS
1	A	21	GLN
1	A	121	SER
1	B	17	GLN
1	B	224	ALA
1	B	241	ILE
1	B	393	MET
1	B	470	GLN
1	C	92	ARG
1	C	226	GLY
1	C	346	PRO
1	C	437	ASP
1	D	437	ASP
1	B	452	GLU
1	C	19	ALA
1	C	203	GLY

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Mol	Chain	Res	Type
1	D	394	MET
1	C	192	LEU
1	D	216	SER
1	A	100	GLU
1	B	19	ALA
1	D	100	GLU
1	C	486	PRO
1	B	373	PRO
1	C	373	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/437 (99%)	359 (83%)	72 (17%)	2	2
1	B	431/437 (99%)	320 (74%)	111 (26%)	0	0
1	C	431/437 (99%)	347 (80%)	84 (20%)	1	1
1	D	431/437 (99%)	355 (82%)	76 (18%)	2	2
All	All	1724/1748 (99%)	1381 (80%)	343 (20%)	1	1

All (343) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	12	LYS
1	A	15	LYS
1	A	18	ARG
1	A	21	GLN
1	A	22	LYS
1	A	24	ASP
1	A	26	LEU
1	A	34	VAL
1	A	37	LYS
1	A	40	SER
1	A	41	LEU

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Mol	Chain	Res	Type
1	A	43	VAL
1	A	49	LEU
1	A	51	VAL
1	A	60	MET
1	A	65	ARG
1	A	70	GLU
1	A	73	VAL
1	A	92	ARG
1	A	95	LYS
1	A	97	LYS
1	A	102	ILE
1	A	104	LYS
1	A	105	ARG
1	A	137	THR
1	A	148	ASN
1	A	149	THR
1	A	162	SER
1	A	169	ARG
1	A	194	GLN
1	A	196	SER
1	A	209	ARG
1	A	227	GLU
1	A	229	VAL
1	A	235	TYR
1	A	236	LYS
1	A	237	THR
1	A	242	LYS
1	A	247	GLU
1	A	254	HIS
1	A	255	GLU
1	A	261	LEU
1	A	263	ASP
1	A	286	SER
1	A	289	GLU
1	A	290	ILE
1	A	309	LEU
1	A	327	GLU
1	A	374	VAL
1	A	394	MET
1	A	402	ASN
1	A	407	SER
1	A	413	HIS

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Mol	Chain	Res	Type
1	A	421	ARG
1	A	435	ASN
1	A	438	ASN
1	A	442	VAL
1	A	448	LYS
1	A	453	GLU
1	A	460	GLU
1	A	467	LYS
1	A	471	LEU
1	A	474	GLN
1	A	475	LYS
1	A	476	LYS
1	A	479	LYS
1	A	490	SER
1	A	492	ILE
1	A	495	LEU
1	A	498	LYS
1	A	501	GLU
1	B	4	ARG
1	B	11	MET
1	B	12	LYS
1	B	16	GLU
1	B	17	GLN
1	B	18	ARG
1	B	21	GLN
1	B	25	VAL
1	B	26	LEU
1	B	36	ASP
1	B	37	LYS
1	B	41	LEU
1	B	43	VAL
1	B	46	ARG
1	B	49	LEU
1	B	50	LEU
1	B	55	VAL
1	B	59	GLU
1	B	67	ARG
1	B	72	VAL
1	B	73	VAL
1	B	76	LYS
1	B	85	GLU
1	B	86	VAL

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Mol	Chain	Res	Type
1	B	90	ILE
1	B	92	ARG
1	B	94	SER
1	B	95	LYS
1	B	97	LYS
1	B	102	ILE
1	B	104	LYS
1	B	121	SER
1	B	124	THR
1	B	126	ARG
1	B	137	THR
1	B	144	LEU
1	B	151	ILE
1	B	162	SER
1	B	169	ARG
1	B	173	THR
1	B	186	SER
1	B	193	HIS
1	B	200	SER
1	B	201	ASP
1	B	202	ARG
1	B	220	LYS
1	B	221	LEU
1	B	225	ASP
1	B	229	VAL
1	B	232	LYS
1	B	235	TYR
1	B	236	LYS
1	B	241	ILE
1	B	242	LYS
1	B	245	SER
1	B	247	GLU
1	B	248	ASP
1	B	252	LEU
1	B	255	GLU
1	B	263	ASP
1	B	264	LEU
1	B	280	ILE
1	B	282	VAL
1	B	283	MET
1	B	286	SER
1	B	290	ILE

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Mol	Chain	Res	Type
1	B	309	LEU
1	B	312	VAL
1	B	314	LYS
1	B	315	LEU
1	B	318	ASN
1	B	319	ARG
1	B	337	ASN
1	B	342	ILE
1	B	374	VAL
1	B	381	ARG
1	B	393	MET
1	B	396	ASN
1	B	397	GLN
1	B	402	ASN
1	B	413	HIS
1	B	416	SER
1	B	422	THR
1	B	433	SER
1	B	438	ASN
1	B	439	VAL
1	B	441	GLN
1	B	442	VAL
1	B	443	ARG
1	B	444	THR
1	B	447	LEU
1	B	448	LYS
1	B	450	LEU
1	B	453	GLU
1	B	454	GLN
1	B	455	ARG
1	B	457	ARG
1	B	458	LEU
1	B	459	CYS
1	B	467	LYS
1	B	471	LEU
1	B	473	ILE
1	B	476	LYS
1	B	478	VAL
1	B	479	LYS
1	B	482	SER
1	B	487	GLU
1	B	492	ILE

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Mol	Chain	Res	Type
1	B	495	LEU
1	B	498	LYS
1	B	500	ASN
1	C	4	ARG
1	C	12	LYS
1	C	16	GLU
1	C	17	GLN
1	C	18	ARG
1	C	22	LYS
1	C	26	LEU
1	C	34	VAL
1	C	43	VAL
1	C	46	ARG
1	C	52	GLN
1	C	65	ARG
1	C	68	ILE
1	C	73	VAL
1	C	76	LYS
1	C	91	THR
1	C	92	ARG
1	C	95	LYS
1	C	97	LYS
1	C	102	ILE
1	C	104	LYS
1	C	126	ARG
1	C	138	GLU
1	C	149	THR
1	C	151	ILE
1	C	154	ILE
1	C	155	ARG
1	C	179	ASP
1	C	180	MET
1	C	188	ARG
1	C	194	GLN
1	C	195	VAL
1	C	202	ARG
1	C	227	GLU
1	C	232	LYS
1	C	235	TYR
1	C	237	THR
1	C	239	GLN
1	C	244	LEU

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Mol	Chain	Res	Type
1	C	246	VAL
1	C	247	GLU
1	C	251	ARG
1	C	261	LEU
1	C	286	SER
1	C	289	GLU
1	C	293	PHE
1	C	309	LEU
1	C	314	LYS
1	C	331	LEU
1	C	345	SER
1	C	355	PHE
1	C	374	VAL
1	C	381	ARG
1	C	394	MET
1	C	402	ASN
1	C	413	HIS
1	C	418	LEU
1	C	421	ARG
1	C	425	SER
1	C	429	GLN
1	C	433	SER
1	C	436	ASP
1	C	437	ASP
1	C	438	ASN
1	C	439	VAL
1	C	442	VAL
1	C	451	ASN
1	C	453	GLU
1	C	454	GLN
1	C	456	LYS
1	C	457	ARG
1	C	458	LEU
1	C	466	LEU
1	C	467	LYS
1	C	470	GLN
1	C	471	LEU
1	C	473	ILE
1	C	474	GLN
1	C	475	LYS
1	C	476	LYS
1	C	478	VAL

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Mol	Chain	Res	Type
1	C	485	HIS
1	C	496	LEU
1	C	497	ASP
1	D	3	ASN
1	D	4	ARG
1	D	15	LYS
1	D	18	ARG
1	D	26	LEU
1	D	27	THR
1	D	34	VAL
1	D	37	LYS
1	D	43	VAL
1	D	52	GLN
1	D	85	GLU
1	D	86	VAL
1	D	89	ASP
1	D	90	ILE
1	D	92	ARG
1	D	94	SER
1	D	100	GLU
1	D	105	ARG
1	D	144	LEU
1	D	148	ASN
1	D	155	ARG
1	D	158	LEU
1	D	193	HIS
1	D	202	ARG
1	D	214	TYR
1	D	216	SER
1	D	220	LYS
1	D	221	LEU
1	D	222	VAL
1	D	225	ASP
1	D	229	VAL
1	D	235	TYR
1	D	236	LYS
1	D	245	SER
1	D	246	VAL
1	D	247	GLU
1	D	261	LEU
1	D	263	ASP
1	D	275	SER

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Mol	Chain	Res	Type
1	D	280	ILE
1	D	281	GLN
1	D	283	MET
1	D	285	PHE
1	D	289	GLU
1	D	290	ILE
1	D	300	LYS
1	D	301	VAL
1	D	309	LEU
1	D	314	LYS
1	D	334	ASP
1	D	336	SER
1	D	368	ASN
1	D	374	VAL
1	D	379	ARG
1	D	381	ARG
1	D	387	ARG
1	D	394	MET
1	D	397	GLN
1	D	412	GLU
1	D	416	SER
1	D	421	ARG
1	D	429	GLN
1	D	432	ASN
1	D	435	ASN
1	D	440	THR
1	D	444	THR
1	D	456	LYS
1	D	460	GLU
1	D	467	LYS
1	D	475	LYS
1	D	476	LYS
1	D	479	LYS
1	D	490	SER
1	D	495	LEU
1	D	498	LYS
1	D	501	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS

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Mol	Chain	Res	Type
1	A	32	ASN
1	A	148	ASN
1	A	167	GLN
1	A	210	HIS
1	A	320	ASN
1	A	337	ASN
1	A	386	GLN
1	A	402	ASN
1	A	420	HIS
1	A	429	GLN
1	A	454	GLN
1	A	470	GLN
1	A	485	HIS
1	B	3	ASN
1	B	13	HIS
1	B	17	GLN
1	B	21	GLN
1	B	32	ASN
1	B	101	HIS
1	B	148	ASN
1	B	167	GLN
1	B	208	HIS
1	B	243	ASN
1	B	272	ASN
1	B	318	ASN
1	B	320	ASN
1	B	337	ASN
1	B	396	ASN
1	B	402	ASN
1	B	414	GLN
1	B	435	ASN
1	B	441	GLN
1	B	461	ASN
1	C	3	ASN
1	C	17	GLN
1	C	52	GLN
1	C	88	HIS
1	C	172	GLN
1	C	239	GLN
1	C	243	ASN
1	C	337	ASN
1	C	402	ASN

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Mol	Chain	Res	Type
1	C	420	HIS
1	C	429	GLN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	470	GLN
1	C	480	ASN
1	D	17	GLN
1	D	21	GLN
1	D	32	ASN
1	D	148	ASN
1	D	167	GLN
1	D	170	ASN
1	D	193	HIS
1	D	243	ASN
1	D	254	HIS
1	D	363	HIS
1	D	368	ASN
1	D	413	HIS
1	D	420	HIS
1	D	432	ASN
1	D	500	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	507	1	50,50,50	1.25	5 (10%)	67,82,82	1.00	1 (1%)
3	NDP	B	1202	-	51,52,52	1.66	10 (19%)	71,80,80	2.06	18 (25%)
2	HEM	D	507	1	50,50,50	1.25	5 (10%)	67,82,82	1.25	6 (8%)
3	NDP	A	1102	-	51,52,52	1.51	7 (13%)	71,80,80	1.91	14 (19%)
2	HEM	B	507	1	50,50,50	1.13	4 (8%)	67,82,82	1.07	5 (7%)
3	NDP	D	1402	-	51,52,52	1.59	10 (19%)	71,80,80	1.85	12 (16%)
3	NDP	C	1302	-	51,52,52	1.53	10 (19%)	71,80,80	2.08	16 (22%)
2	HEM	A	507	1	50,50,50	1.15	5 (10%)	67,82,82	0.94	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	507	1	-	5/14/54/54	-
3	NDP	B	1202	-	-	10/34/77/77	0/5/5/5
2	HEM	D	507	1	-	4/14/54/54	-
3	NDP	A	1102	-	-	7/34/77/77	0/5/5/5
2	HEM	B	507	1	-	8/14/54/54	-
3	NDP	D	1402	-	-	9/34/77/77	0/5/5/5
3	NDP	C	1302	-	-	7/34/77/77	0/5/5/5
2	HEM	A	507	1	-	5/14/54/54	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	NDP	PN-O3	4.31	1.64	1.59
3	D	1402	NDP	P2B-O1X	4.20	1.63	1.50
3	C	1302	NDP	P2B-O1X	3.94	1.62	1.50
3	A	1102	NDP	P2B-O1X	3.91	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1202	NDP	C4N-C3N	-3.84	1.42	1.50
3	C	1302	NDP	C4N-C3N	-3.78	1.42	1.50
3	B	1202	NDP	PA-O3	3.69	1.63	1.59
3	B	1202	NDP	P2B-O1X	3.66	1.61	1.50
2	C	507	HEM	CBB-CAB	3.65	1.47	1.30
2	B	507	HEM	CBC-CAC	3.51	1.47	1.30
2	D	507	HEM	CBC-CAC	3.51	1.47	1.30
3	A	1102	NDP	C7N-C3N	3.45	1.56	1.48
2	C	507	HEM	CBC-CAC	3.42	1.46	1.30
3	D	1402	NDP	C5A-N7A	-3.39	1.32	1.39
3	D	1402	NDP	PA-O3	3.39	1.63	1.59
3	D	1402	NDP	PN-O3	3.35	1.63	1.59
3	A	1102	NDP	C4N-C3N	-3.27	1.43	1.50
3	D	1402	NDP	C4N-C3N	-3.26	1.43	1.50
3	B	1202	NDP	C5A-N7A	-3.24	1.33	1.39
2	D	507	HEM	CBB-CAB	3.22	1.45	1.30
2	A	507	HEM	CAB-C3B	-3.21	1.38	1.47
3	A	1102	NDP	PA-O3	3.18	1.62	1.59
2	A	507	HEM	CBC-CAC	3.13	1.45	1.30
2	B	507	HEM	CBB-CAB	3.12	1.45	1.30
3	D	1402	NDP	C7N-C3N	3.11	1.55	1.48
3	A	1102	NDP	C5A-N7A	-3.08	1.33	1.39
3	B	1202	NDP	C7N-C3N	3.04	1.55	1.48
2	A	507	HEM	CAC-C3C	-3.03	1.39	1.47
3	C	1302	NDP	C5A-N7A	-3.00	1.33	1.39
3	C	1302	NDP	C6N-C5N	2.95	1.42	1.33
3	C	1302	NDP	C7N-C3N	2.85	1.54	1.48
3	D	1402	NDP	C6N-N1N	2.84	1.44	1.37
3	D	1402	NDP	C6N-C5N	2.83	1.41	1.33
3	A	1102	NDP	C6N-C5N	2.82	1.41	1.33
3	B	1202	NDP	C6N-C5N	2.77	1.41	1.33
3	C	1302	NDP	C6N-N1N	2.76	1.44	1.37
3	A	1102	NDP	C6N-N1N	2.70	1.43	1.37
3	B	1202	NDP	C4N-C5N	-2.67	1.42	1.49
3	C	1302	NDP	C4N-C5N	-2.62	1.42	1.49
2	C	507	HEM	FE-NC	2.58	2.03	1.95
2	A	507	HEM	CBB-CAB	2.54	1.42	1.30
3	C	1302	NDP	PA-O3	2.51	1.62	1.59
3	C	1302	NDP	C2N-C3N	2.34	1.41	1.35
3	B	1202	NDP	C2N-C3N	2.33	1.41	1.35
2	D	507	HEM	FE-NA	2.30	2.02	1.95
3	D	1402	NDP	C4N-C5N	-2.30	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	507	HEM	CAB-C3B	-2.29	1.41	1.47
2	D	507	HEM	CAB-C3B	-2.26	1.41	1.47
3	B	1202	NDP	C6N-N1N	2.24	1.42	1.37
2	D	507	HEM	CAC-C3C	-2.19	1.41	1.47
3	D	1402	NDP	C2N-C3N	2.16	1.41	1.35
3	C	1302	NDP	PN-O3	2.16	1.61	1.59
2	A	507	HEM	FE-NB	2.16	2.01	1.94
2	C	507	HEM	CAC-C3C	-2.12	1.41	1.47
2	B	507	HEM	CAB-C3B	-2.07	1.41	1.47
2	B	507	HEM	CAC-C3C	-2.06	1.41	1.47

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	NDP	C5A-C4A-N3A	-6.37	117.95	126.72
3	C	1302	NDP	O4D-C1D-N1N	6.20	119.91	108.08
3	A	1102	NDP	C5A-C4A-N3A	-5.95	118.52	126.72
3	C	1302	NDP	C5A-C4A-N3A	-5.94	118.54	126.72
3	B	1202	NDP	C2B-C1B-N9A	5.78	123.26	113.75
3	B	1202	NDP	N3A-C2A-N1A	-5.75	119.88	128.58
3	D	1402	NDP	C2B-C1B-N9A	5.53	122.86	113.75
3	C	1302	NDP	N3A-C4A-N9A	5.52	136.55	127.17
3	B	1202	NDP	O4D-C1D-N1N	5.51	118.60	108.08
3	A	1102	NDP	N3A-C4A-N9A	5.46	136.45	127.17
3	A	1102	NDP	O4B-C1B-N9A	5.37	118.40	108.09
3	B	1202	NDP	C5A-C4A-N3A	-5.36	119.34	126.72
3	C	1302	NDP	C2B-C1B-N9A	5.28	122.44	113.75
3	D	1402	NDP	N3A-C4A-N9A	5.16	135.94	127.17
3	C	1302	NDP	N3A-C2A-N1A	-5.05	120.94	128.58
3	D	1402	NDP	N3A-C2A-N1A	-4.44	121.86	128.58
3	A	1102	NDP	N3A-C2A-N1A	-4.39	121.93	128.58
3	B	1202	NDP	N3A-C4A-N9A	4.38	134.62	127.17
3	A	1102	NDP	O4D-C1D-N1N	4.10	115.91	108.08
3	D	1402	NDP	O4D-C1D-N1N	3.98	115.68	108.08
2	D	507	HEM	C3B-C4B-NB	3.96	112.31	109.47
3	D	1402	NDP	C6A-C5A-N7A	-3.91	124.56	132.09
2	B	507	HEM	C3B-C4B-NB	3.90	112.27	109.47
3	B	1202	NDP	C3D-C2D-C1D	3.85	108.75	101.46
3	B	1202	NDP	C2A-N3A-C4A	3.79	121.08	111.83
3	A	1102	NDP	C3B-C2B-C1B	3.77	110.03	102.81
3	C	1302	NDP	C2A-N3A-C4A	3.77	121.03	111.83
3	C	1302	NDP	C3D-C2D-C1D	3.62	108.31	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	NDP	C2A-N3A-C4A	3.58	120.58	111.83
3	A	1102	NDP	C3D-C2D-C1D	3.47	108.03	101.46
3	A	1102	NDP	C2A-N3A-C4A	3.45	120.26	111.83
3	B	1202	NDP	C6A-C5A-N7A	-3.36	125.61	132.09
3	C	1302	NDP	C3B-C2B-C1B	3.25	109.03	102.81
3	C	1302	NDP	P2B-O2B-C2B	-3.21	114.86	123.43
3	C	1302	NDP	O3X-P2B-O2X	3.14	119.58	107.80
3	A	1102	NDP	O3X-P2B-O2X	3.08	119.35	107.80
3	D	1402	NDP	O3X-P2B-O2X	3.06	119.26	107.80
3	A	1102	NDP	C6A-C5A-N7A	-3.00	126.30	132.09
3	D	1402	NDP	C6A-C5A-C4A	2.94	121.19	117.18
3	B	1202	NDP	C4A-N9A-C8A	2.87	108.76	105.74
3	B	1202	NDP	C4A-N9A-C1B	-2.87	119.93	126.63
3	A	1102	NDP	C2B-C1B-N9A	2.84	118.42	113.75
3	B	1202	NDP	O4B-C1B-N9A	2.76	113.38	108.09
3	B	1202	NDP	O3X-P2B-O2X	2.75	118.10	107.80
2	D	507	HEM	C4B-C3B-C2B	-2.60	104.89	107.28
3	C	1302	NDP	O4B-C1B-N9A	2.53	112.94	108.09
3	C	1302	NDP	O4B-C4B-C3B	2.52	110.16	105.15
3	A	1102	NDP	C6A-C5A-C4A	2.52	120.62	117.18
2	C	507	HEM	C3B-C4B-NB	2.51	111.27	109.47
3	C	1302	NDP	C6A-C5A-N7A	-2.50	127.27	132.09
3	B	1202	NDP	C2A-N1A-C6A	2.47	122.78	118.73
2	A	507	HEM	CMB-C2B-C1B	2.46	128.88	125.03
3	A	1102	NDP	P2B-O2B-C2B	-2.46	116.85	123.43
3	D	1402	NDP	C3D-C2D-C1D	2.45	106.10	101.46
3	B	1202	NDP	O5D-C5D-C4D	2.44	117.31	108.99
3	D	1402	NDP	C3B-C2B-C1B	2.43	107.47	102.81
3	C	1302	NDP	C6A-C5A-C4A	2.39	120.45	117.18
3	B	1202	NDP	C5D-C4D-C3D	-2.33	106.81	115.21
3	B	1202	NDP	N9A-C8A-N7A	-2.30	110.67	113.94
2	B	507	HEM	C3D-C4D-ND	2.30	112.69	110.17
3	A	1102	NDP	O2B-C2B-C1B	-2.26	102.10	110.05
2	D	507	HEM	C3B-C2B-C1B	2.20	108.07	106.41
2	D	507	HEM	CAC-C3C-C4C	2.18	130.02	124.82
2	D	507	HEM	CHC-C1C-C2C	-2.17	120.98	125.49
2	B	507	HEM	CHA-C4D-C3D	-2.16	121.25	125.23
2	D	507	HEM	C3D-C4D-ND	2.14	112.52	110.17
3	C	1302	NDP	C2A-N1A-C6A	2.10	122.19	118.73
3	B	1202	NDP	C4B-O4B-C1B	-2.10	104.83	109.47
2	B	507	HEM	CHC-C1C-C2C	-2.09	121.13	125.49
2	B	507	HEM	C4B-C3B-C2B	-2.07	105.37	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1302	NDP	O4B-C4B-C5B	-2.06	102.75	109.33
2	A	507	HEM	CHC-C1C-C2C	-2.05	121.22	125.49
3	D	1402	NDP	C4A-N9A-C1B	-2.05	121.84	126.63
3	B	1202	NDP	O5B-C5B-C4B	-2.00	102.18	108.99

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	507	HEM	C2B-C3B-CAB-CBB
2	A	507	HEM	C4B-C3B-CAB-CBB
2	A	507	HEM	C2C-C3C-CAC-CBC
2	B	507	HEM	C2B-C3B-CAB-CBB
2	D	507	HEM	C2B-C3B-CAB-CBB
2	D	507	HEM	C4B-C3B-CAB-CBB
3	A	1102	NDP	C5D-O5D-PN-O3
3	A	1102	NDP	C5D-O5D-PN-O1N
3	A	1102	NDP	C5D-O5D-PN-O2N
3	B	1202	NDP	C5D-O5D-PN-O3
3	B	1202	NDP	C5D-O5D-PN-O1N
3	B	1202	NDP	C5D-O5D-PN-O2N
3	B	1202	NDP	O4D-C1D-N1N-C6N
3	C	1302	NDP	C5D-O5D-PN-O3
3	C	1302	NDP	C5D-O5D-PN-O2N
3	C	1302	NDP	O4D-C1D-N1N-C6N
3	D	1402	NDP	C5D-O5D-PN-O2N
3	D	1402	NDP	O4D-C1D-N1N-C6N
3	A	1102	NDP	O4D-C1D-N1N-C6N
2	C	507	HEM	C2B-C3B-CAB-CBB
2	A	507	HEM	C4C-C3C-CAC-CBC
2	B	507	HEM	C4B-C3B-CAB-CBB
3	D	1402	NDP	O4B-C4B-C5B-O5B
3	D	1402	NDP	C4D-C5D-O5D-PN
3	C	1302	NDP	C5D-O5D-PN-O1N
3	D	1402	NDP	C5D-O5D-PN-O3
3	B	1202	NDP	C4D-C5D-O5D-PN
3	B	1202	NDP	C2B-O2B-P2B-O3X
3	D	1402	NDP	C2B-O2B-P2B-O3X
2	C	507	HEM	C4C-C3C-CAC-CBC
2	B	507	HEM	C4D-C3D-CAD-CBD
3	A	1102	NDP	C2B-C1B-N9A-C8A
2	B	507	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
2	B	507	HEM	CAD-CBD-CGD-O1D
2	D	507	HEM	CAD-CBD-CGD-O1D
3	A	1102	NDP	C4D-C5D-O5D-PN
2	D	507	HEM	CAD-CBD-CGD-O2D
3	D	1402	NDP	C2N-C3N-C7N-N7N
2	B	507	HEM	CAD-CBD-CGD-O2D
2	C	507	HEM	CAD-CBD-CGD-O2D
3	B	1202	NDP	PN-O3-PA-O1A
3	C	1302	NDP	PN-O3-PA-O2A
3	A	1102	NDP	O4B-C1B-N9A-C8A
2	C	507	HEM	CAD-CBD-CGD-O1D
2	B	507	HEM	C4C-C3C-CAC-CBC
2	C	507	HEM	C4B-C3B-CAB-CBB
3	B	1202	NDP	O4B-C4B-C5B-O5B
3	B	1202	NDP	PN-O3-PA-O2A
3	D	1402	NDP	PA-O3-PN-O2N
3	B	1202	NDP	O4B-C1B-N9A-C8A
3	D	1402	NDP	C2B-C1B-N9A-C4A
3	C	1302	NDP	O4B-C1B-N9A-C8A
3	C	1302	NDP	C4D-C5D-O5D-PN
2	A	507	HEM	CAA-CBA-CGA-O2A
2	B	507	HEM	C2C-C3C-CAC-CBC

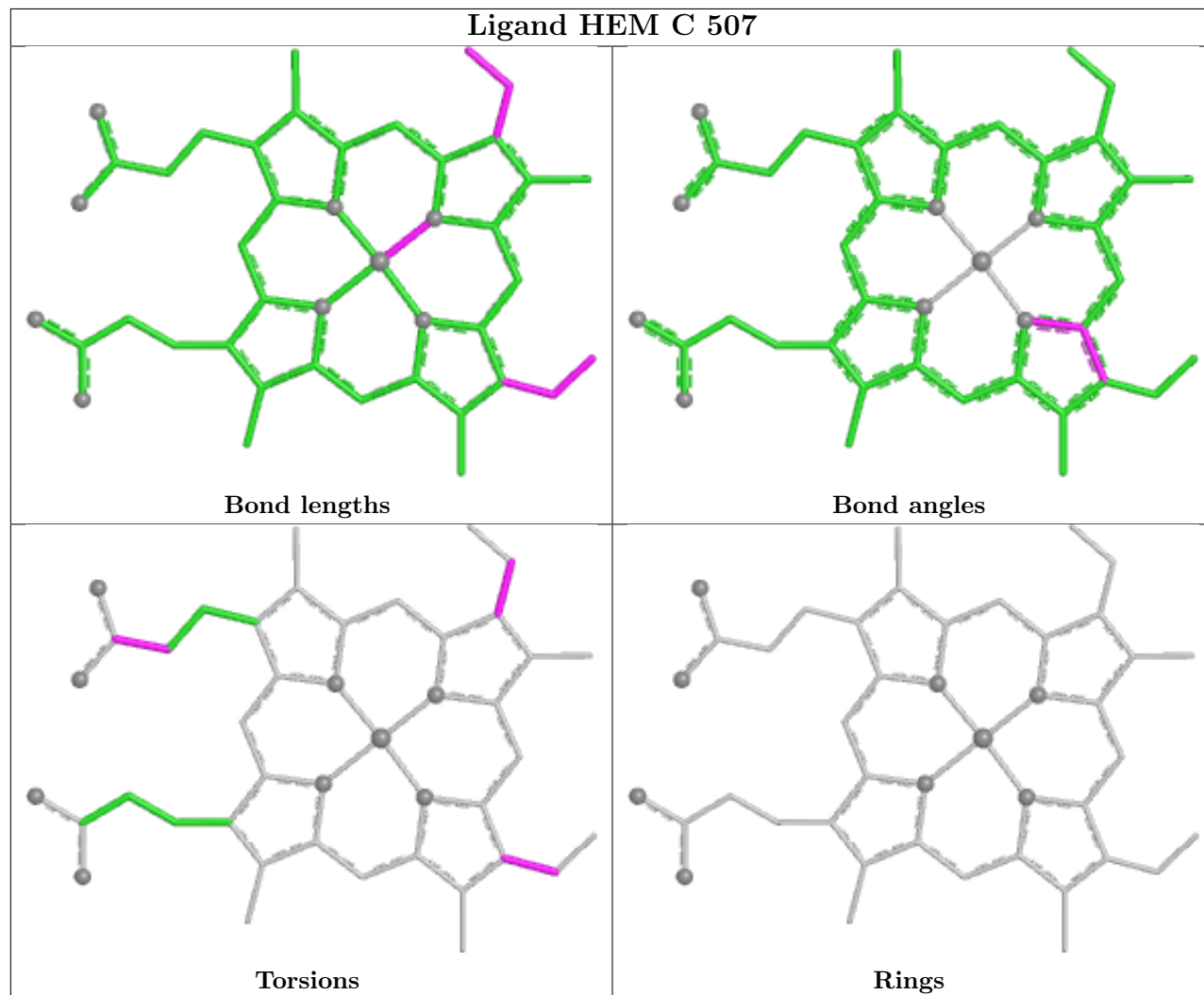
There are no ring outliers.

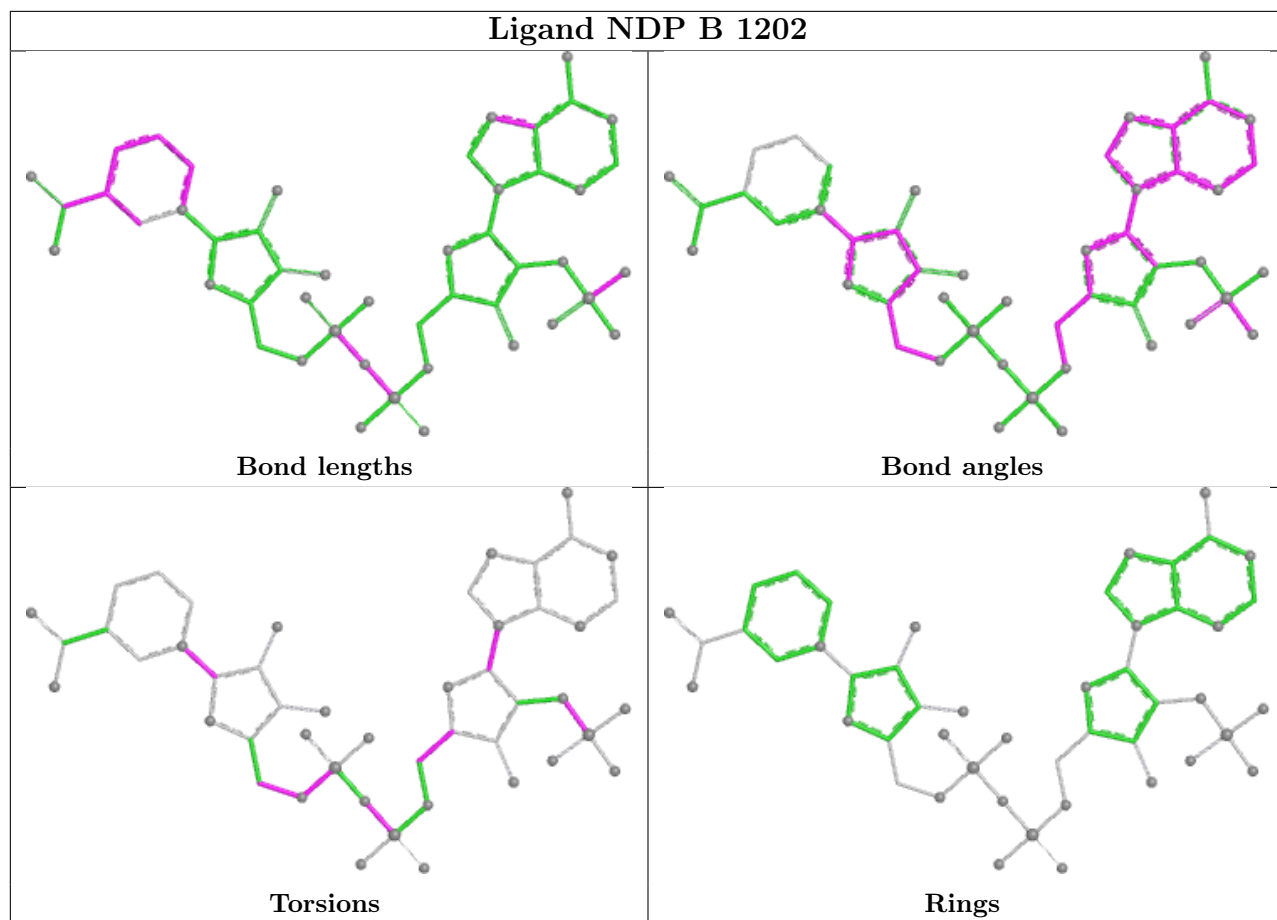
7 monomers are involved in 20 short contacts:

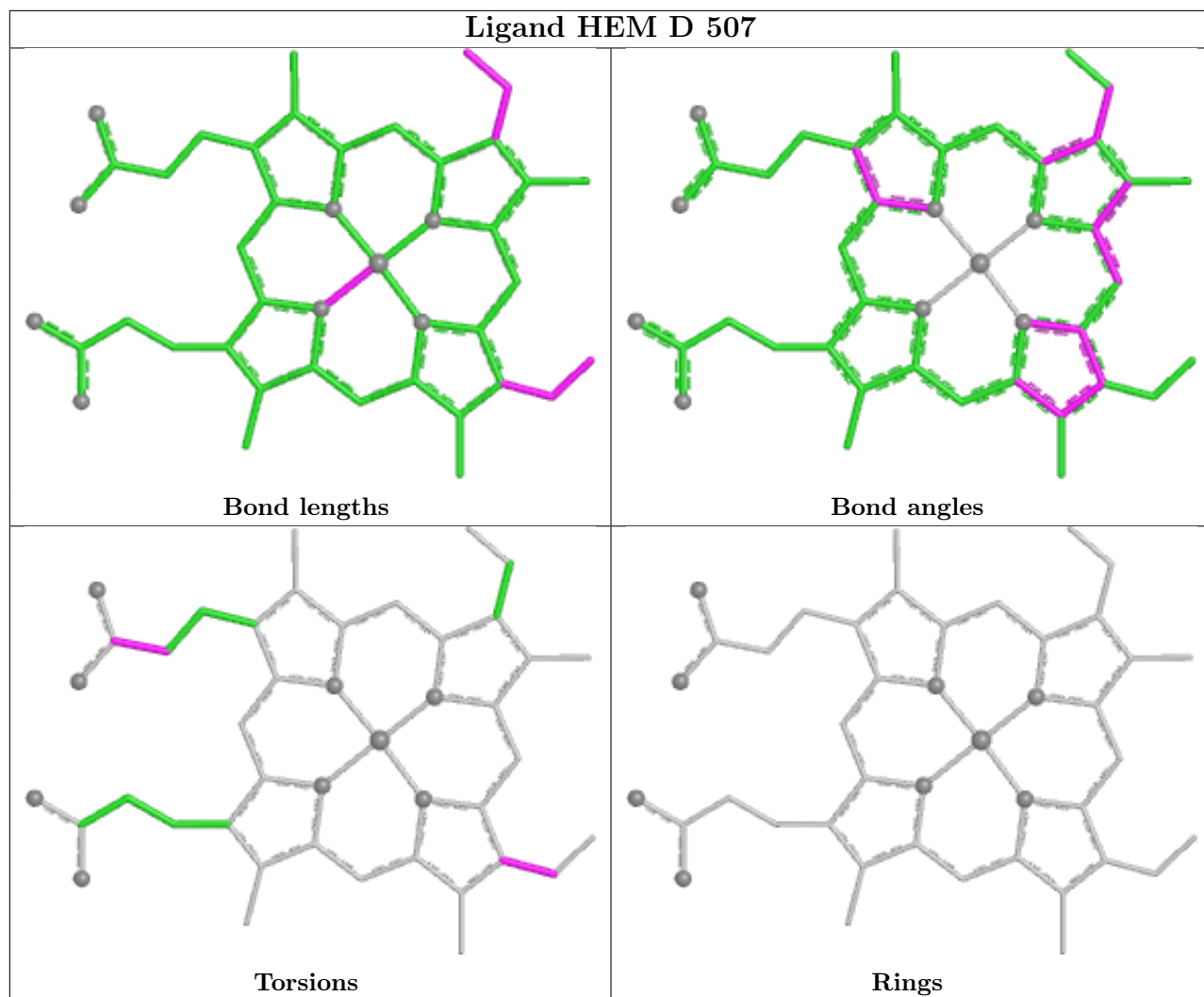
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	507	HEM	4	0
3	B	1202	NDP	3	0
2	D	507	HEM	2	0
3	A	1102	NDP	3	0
3	D	1402	NDP	1	0
3	C	1302	NDP	2	0
2	A	507	HEM	5	0

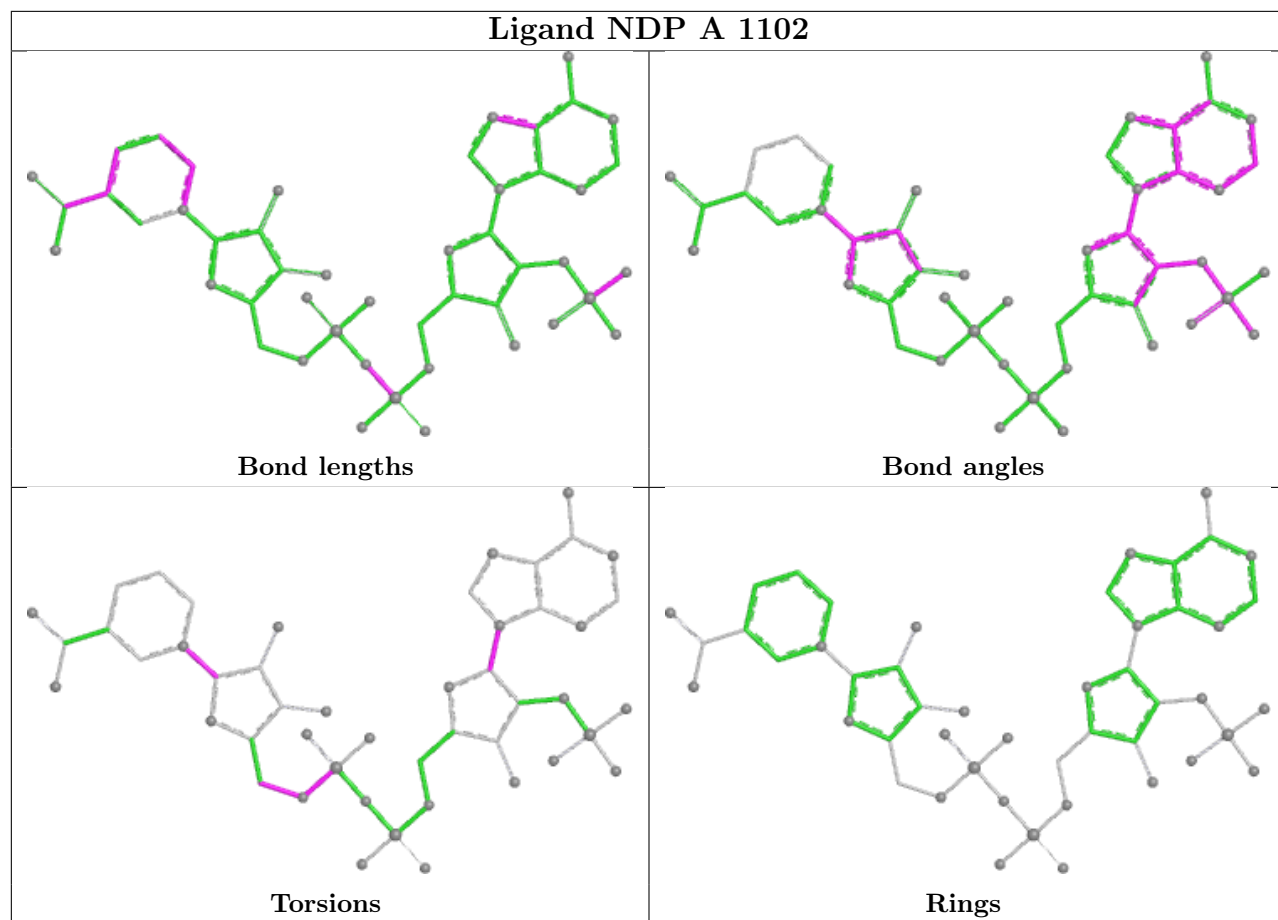
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

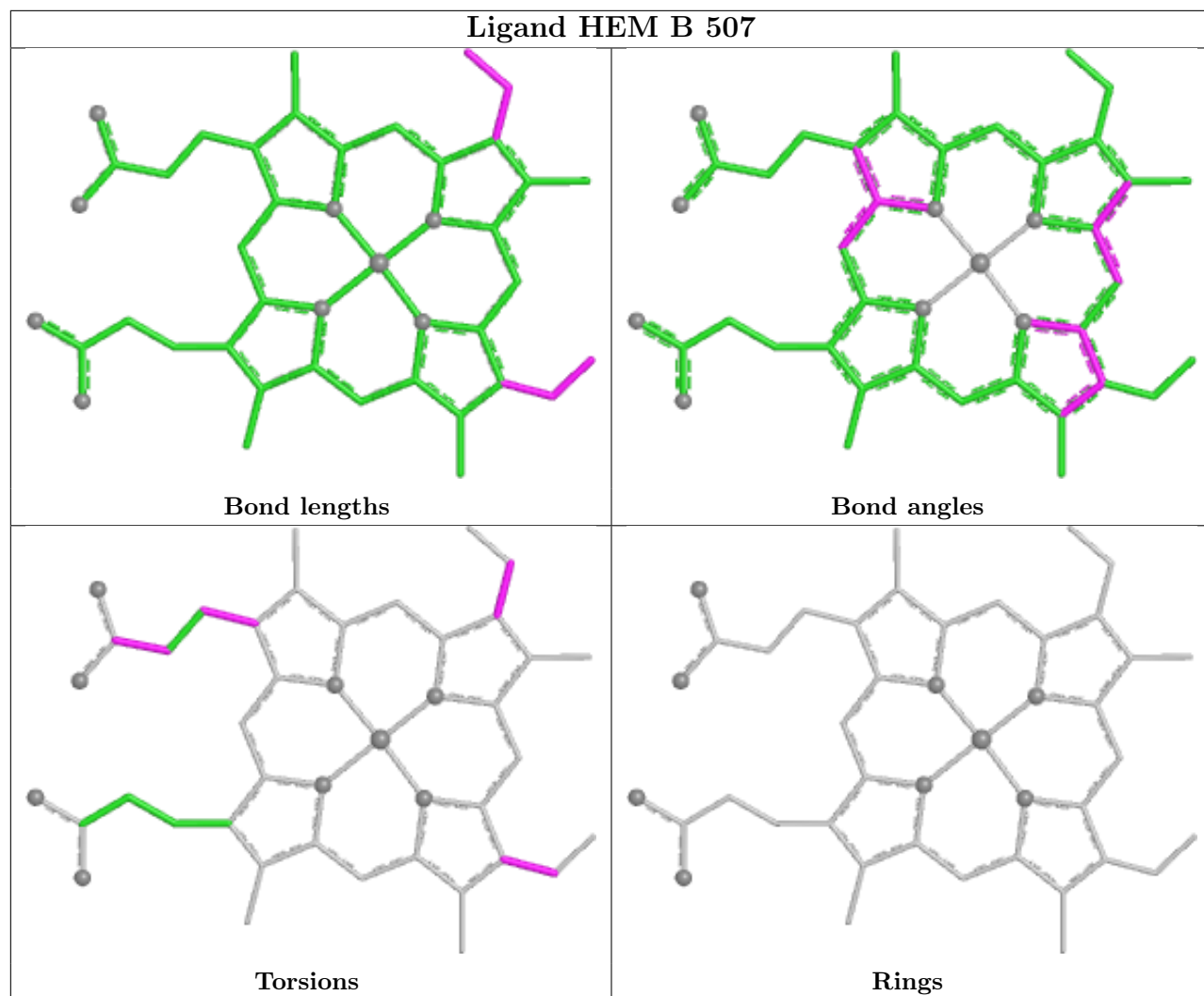
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

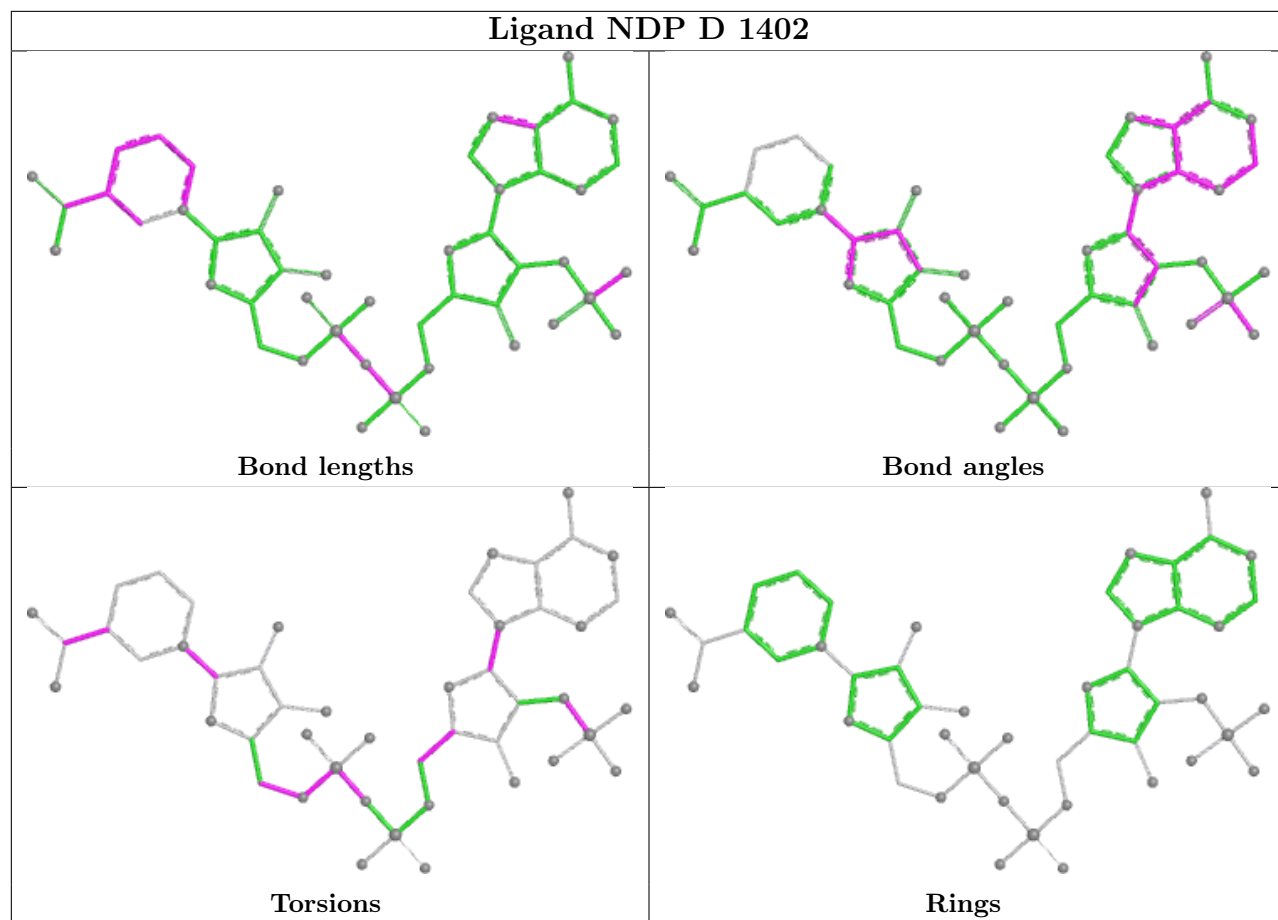


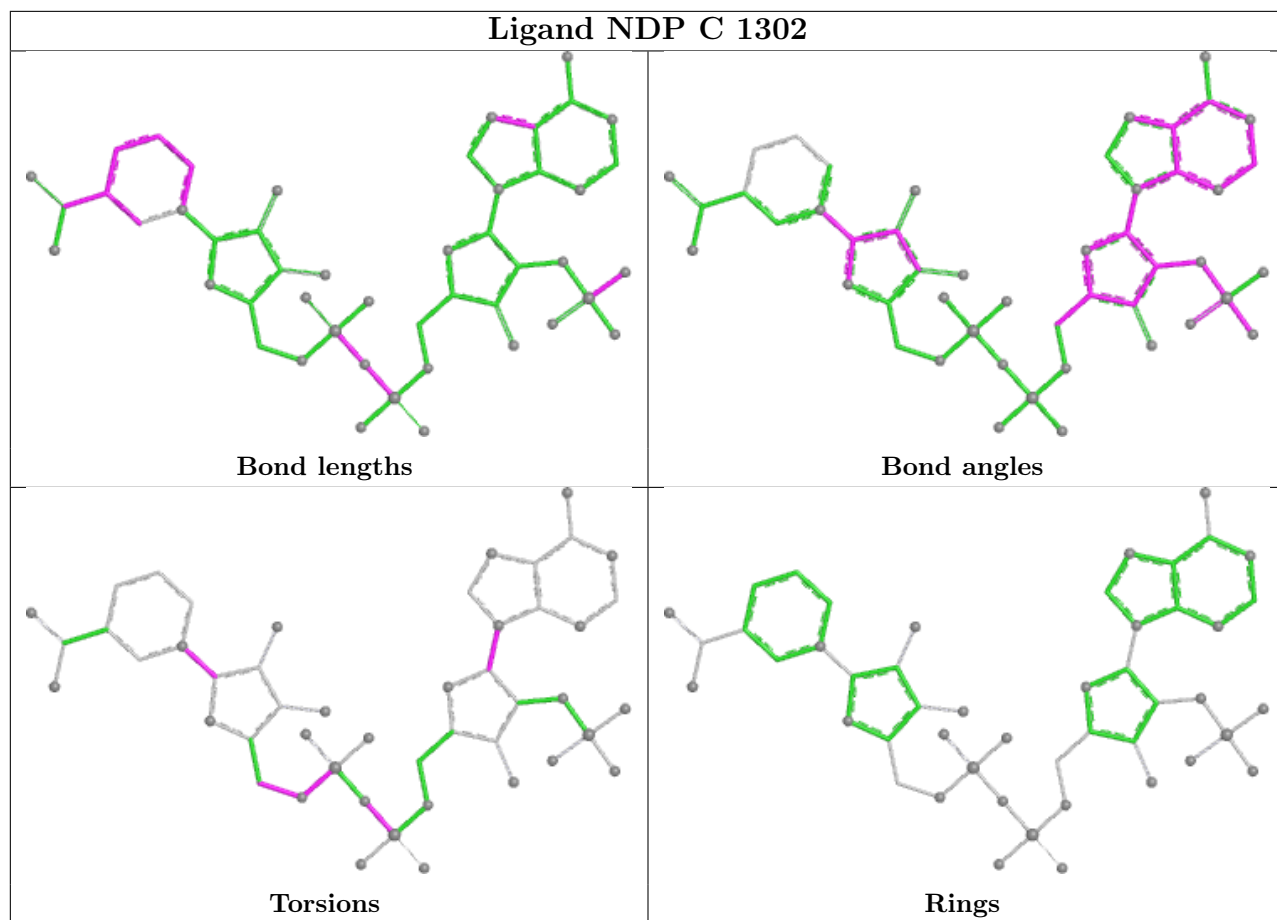


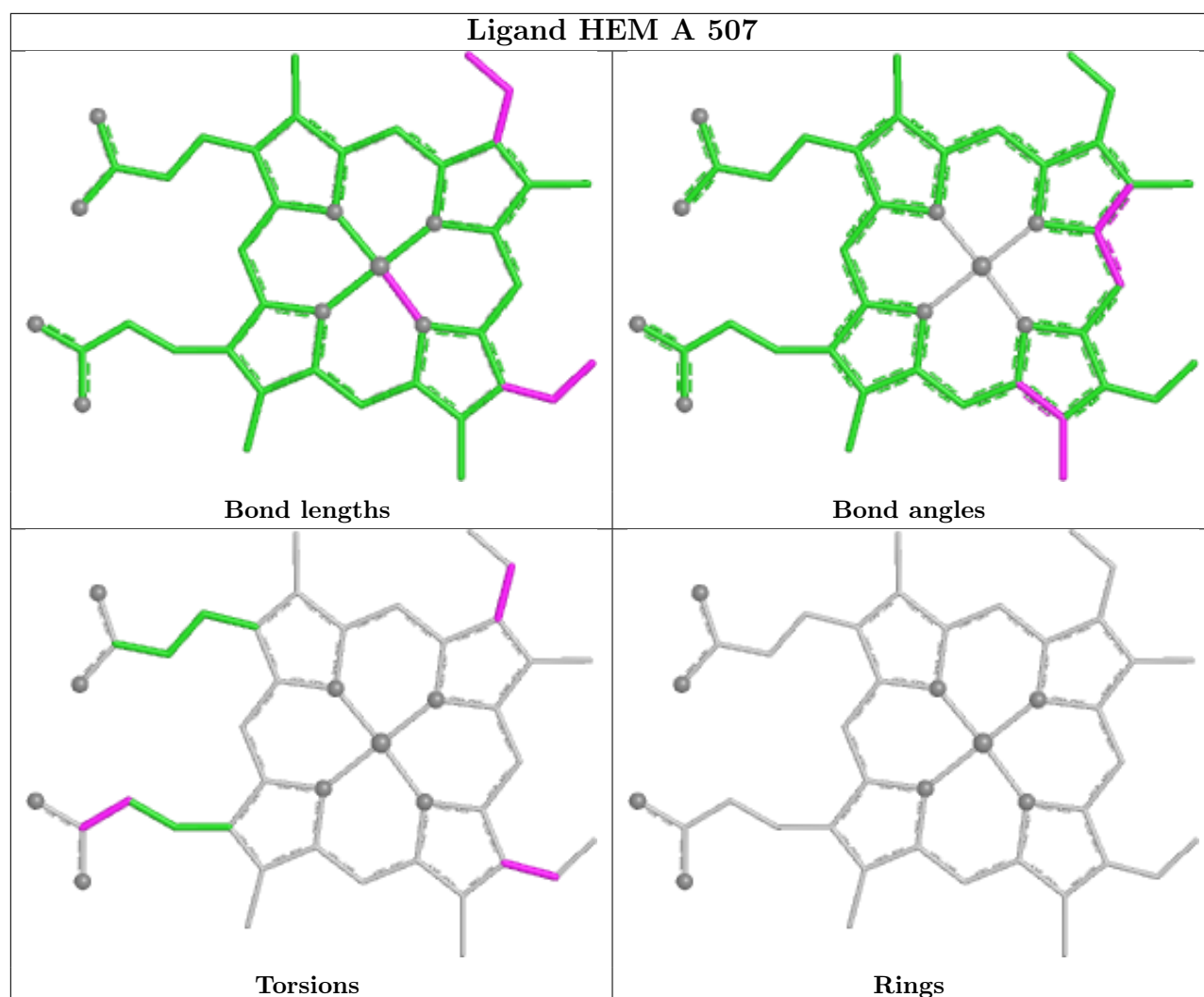












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.