



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:47 PM UTC

PDB ID : 2BHJ / pdb_00002bhj
Title : murine iNO synthase with coumarin inhibitor
Authors : Mathieu, M.; Guilloteau, J.P.
Deposited on : 2005-01-12
Resolution : 3.20 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)	:	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

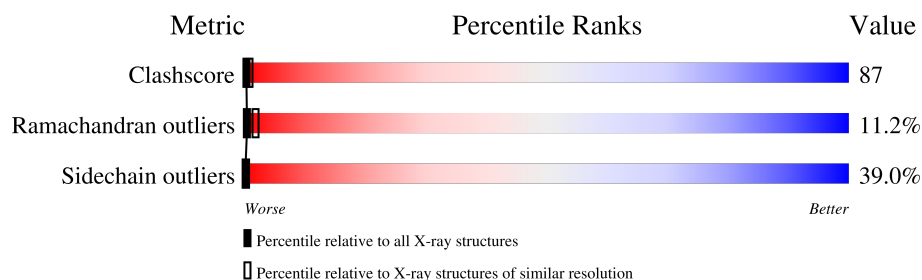
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

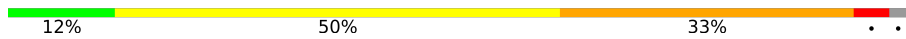
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	422	

2 Entry composition [i](#)

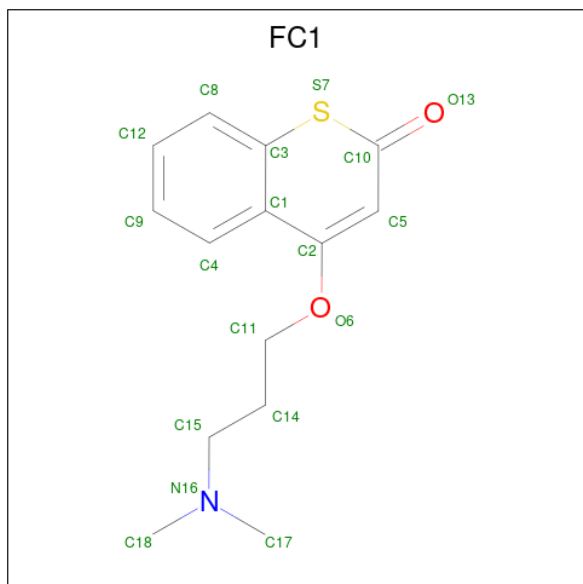
There are 5 unique types of molecules in this entry. The entry contains 3474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NITRIC OXIDE SYNTHASE.

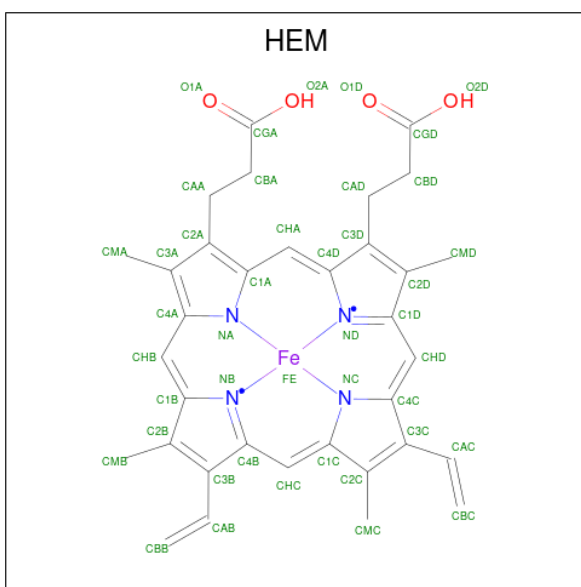
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3381	2165	583	613	20	0	0	0

- Molecule 2 is THIOCOUMARIN (CCD ID: FC1) (formula: C₁₄H₁₇NO₂S).



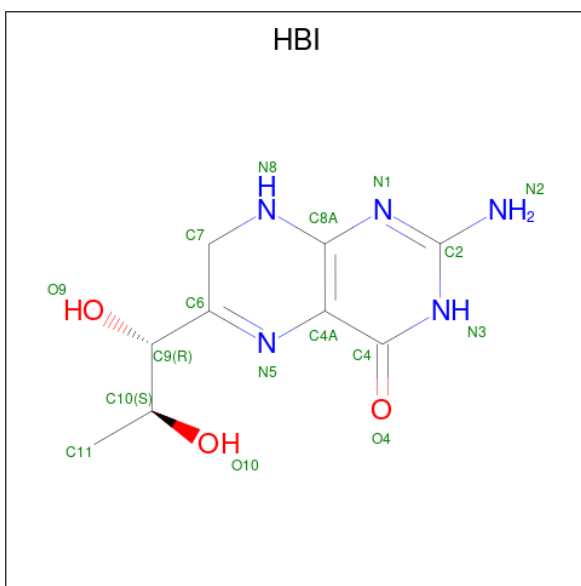
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	18	14	1	2	1	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 4 is 7,8-DIHYDROBIOPTERIN (CCD ID: HBI) (formula: $C_9H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O		
			17	9	5	3		
							0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	15	Total 15	O 15	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	213.54Å 213.54Å 115.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.40 – 3.20	Depositor
% Data completeness (in resolution range)	92.7 (29.40-3.20)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.276 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3474	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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: FC1, HEM, HBI

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	0.45	0/3479	1.07	26/4727 (0.6%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	MET	N-CA-C	-8.32	103.14	113.38
1	A	424	ASN	N-CA-C	7.90	122.33	111.90
1	A	368	MET	N-CA-C	-7.16	96.75	108.41
1	A	149	LYS	N-CA-C	-7.00	104.71	113.18
1	A	358	PHE	CA-C-N	6.82	128.36	119.84
1	A	358	PHE	C-N-CA	6.82	128.36	119.84
1	A	290	LYS	CA-C-N	6.80	128.34	119.84
1	A	290	LYS	C-N-CA	6.80	128.34	119.84
1	A	370	THR	N-CA-C	6.68	120.30	111.75
1	A	191	ALA	N-CA-C	-6.59	101.49	109.72
1	A	78	TYR	N-CA-C	6.31	119.09	107.73
1	A	214	ALA	N-CA-C	-6.01	104.41	110.97
1	A	367	TYR	N-CA-C	5.94	118.22	110.43
1	A	365	GLY	N-CA-C	-5.85	99.62	110.73
1	A	305	ALA	N-CA-C	5.76	120.33	112.04
1	A	378	CYS	N-CA-C	5.65	118.29	111.40
1	A	252	ARG	N-CA-C	5.60	118.33	108.75
1	A	176	THR	N-CA-C	-5.36	102.11	110.10
1	A	191	ALA	CA-C-N	-5.33	113.18	119.84
1	A	191	ALA	C-N-CA	-5.33	113.18	119.84
1	A	256	SER	N-CA-C	-5.30	105.40	111.07
1	A	151	ALA	N-CA-C	5.28	118.53	110.20
1	A	248	LYS	N-CA-C	-5.23	105.77	113.61
1	A	188	TRP	N-CA-C	-5.18	104.56	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	HIS	N-CA-C	-5.11	106.89	112.72
1	A	290	LYS	N-CA-C	5.07	116.04	109.65

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	3381	0	3272	594	1
2	A	18	0	17	2	0
3	A	43	0	30	3	0
4	A	17	0	13	1	0
5	A	15	0	0	0	0
All	All	3474	0	3332	594	1

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 87.

All (594) 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:393:MET:HE1	1:A:411:GLU:HG2	1.31	1.05
1:A:84:TRP:HE1	1:A:114:MET:HG3	1.20	1.05
1:A:120:THR:HG22	1:A:121:ARG:H	1.23	1.01
1:A:308:GLN:CD	1:A:308:GLN:H	1.70	0.99
1:A:393:MET:HG2	1:A:395:LEU:HD22	1.39	0.99
1:A:260:ARG:HH21	1:A:277:THR:HG22	1.26	0.98
1:A:330:TYR:HB3	1:A:332:TRP:NE1	1.79	0.98
1:A:375:ARG:O	1:A:379:ASP:HB2	1.63	0.97
1:A:203:LEU:HD12	1:A:204:GLN:H	1.31	0.94
1:A:332:TRP:HE3	1:A:392:ARG:HH11	1.10	0.93
1:A:488:GLU:HB2	1:A:491:LYS:HG3	1.50	0.93
1:A:327:HIS:HB2	1:A:333:PHE:CD2	2.04	0.93
1:A:381:GLN:H	1:A:381:GLN:NE2	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:HD1	1:A:148:PHE:H	1.14	0.91
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.05	0.91
1:A:236:SER:HA	1:A:364:ASN:ND2	1.86	0.91
1:A:381:GLN:H	1:A:381:GLN:HE21	0.92	0.91
1:A:327:HIS:HB2	1:A:333:PHE:HD2	1.33	0.90
1:A:385:ILE:HG13	1:A:386:LEU:H	1.36	0.90
1:A:181:ILE:HG12	1:A:205:VAL:HG21	1.51	0.90
1:A:381:GLN:HE21	1:A:381:GLN:N	1.69	0.89
1:A:159:ARG:O	1:A:163:VAL:HG23	1.72	0.89
1:A:163:VAL:HG12	1:A:167:ILE:HD11	1.54	0.89
1:A:393:MET:HE1	1:A:411:GLU:CG	2.02	0.89
1:A:333:PHE:HD1	1:A:336:LEU:HD23	1.37	0.87
1:A:255:ASN:HD21	1:A:301:LEU:HA	1.40	0.87
1:A:144:TYR:HE2	1:A:179:GLU:HG2	1.38	0.87
1:A:437:PHE:HE2	1:A:441:MET:HE3	1.37	0.87
1:A:333:PHE:HE2	1:A:415:ALA:CB	1.88	0.86
1:A:255:ASN:O	1:A:347:ALA:HB3	1.76	0.85
1:A:257:GLN:HB2	1:A:345:ALA:O	1.76	0.85
1:A:263:GLY:H	1:A:281:THR:HG21	1.42	0.85
1:A:327:HIS:ND1	1:A:328:PRO:HD2	1.92	0.85
1:A:134:LEU:O	1:A:138:ILE:HG12	1.76	0.85
1:A:441:MET:HE1	1:A:474:MET:HE2	1.59	0.85
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.12	0.84
1:A:236:SER:HA	1:A:364:ASN:HD21	1.41	0.84
1:A:342:ALA:HB1	1:A:425:VAL:HG11	1.61	0.83
1:A:265:GLN:HG3	1:A:265:GLN:O	1.78	0.83
1:A:389:VAL:O	1:A:393:MET:HB2	1.79	0.83
1:A:84:TRP:HE1	1:A:114:MET:CG	1.93	0.82
1:A:175:LEU:HD12	1:A:175:LEU:H	1.44	0.81
1:A:242:PRO:HG2	1:A:251:PHE:CD1	2.16	0.81
1:A:295:ARG:HD3	1:A:295:ARG:N	1.95	0.81
1:A:78:TYR:CD1	1:A:78:TYR:O	2.35	0.80
1:A:181:ILE:CG1	1:A:205:VAL:HG21	2.12	0.79
1:A:477:TYR:HD2	1:A:479:LEU:HD21	1.47	0.79
1:A:196:GLY:O	1:A:198:ILE:N	2.15	0.79
1:A:144:TYR:CE2	1:A:179:GLU:HG2	2.18	0.79
1:A:203:LEU:HD12	1:A:204:GLN:N	1.97	0.79
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.65	0.79
1:A:393:MET:HG2	1:A:395:LEU:CD2	2.13	0.79
1:A:399:THR:O	1:A:399:THR:HG22	1.81	0.79
1:A:332:TRP:HE3	1:A:392:ARG:NH1	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:HD3	1:A:357:GLU:OE2	1.84	0.78
1:A:249:HIS:HA	1:A:306:ASP:O	1.84	0.77
1:A:308:GLN:HA	1:A:496:GLN:HG2	1.66	0.77
1:A:255:ASN:ND2	1:A:301:LEU:HA	1.98	0.77
1:A:260:ARG:NH2	1:A:277:THR:HG22	2.01	0.75
1:A:323:VAL:CG2	1:A:425:VAL:HG21	2.15	0.75
1:A:332:TRP:CZ3	1:A:392:ARG:HB2	2.20	0.75
1:A:186:MET:HE1	1:A:189:ARG:HH11	1.51	0.75
1:A:203:LEU:HD12	1:A:237:ALA:HA	1.69	0.74
1:A:333:PHE:HE2	1:A:415:ALA:HB2	1.51	0.74
1:A:350:LEU:N	1:A:486:GLN:HE21	1.85	0.74
1:A:167:ILE:HG23	1:A:171:GLY:O	1.87	0.74
1:A:470:PHE:HD1	1:A:471:HIS:CD2	2.06	0.73
1:A:422:LYS:C	1:A:424:ASN:H	1.95	0.73
1:A:440:HIS:O	1:A:443:ASN:HB2	1.89	0.73
1:A:407:ARG:HG3	1:A:407:ARG:HH11	1.53	0.73
1:A:134:LEU:HD13	1:A:138:ILE:HD11	1.68	0.73
1:A:163:VAL:HG12	1:A:167:ILE:CD1	2.18	0.72
1:A:308:GLN:H	1:A:308:GLN:NE2	1.87	0.72
1:A:480:SER:HA	1:A:481:PRO:C	2.14	0.72
1:A:410:THR:O	1:A:414:VAL:HG23	1.89	0.72
1:A:438:MET:CE	1:A:469:VAL:HG12	2.19	0.72
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.89	0.72
1:A:167:ILE:O	1:A:171:GLY:N	2.22	0.72
1:A:266:MET:SD	1:A:272:ARG:HG3	2.30	0.72
1:A:270:THR:HG22	1:A:271:ILE:H	1.55	0.71
1:A:123:PRO:HA	1:A:244:ARG:HH22	1.54	0.71
1:A:140:PHE:HE2	1:A:175:LEU:HD23	1.56	0.71
1:A:260:ARG:HE	1:A:277:THR:CG2	2.03	0.70
1:A:438:MET:SD	1:A:469:VAL:HG12	2.32	0.70
1:A:120:THR:HG22	1:A:121:ARG:N	2.04	0.70
1:A:316:PRO:HB2	1:A:319:LEU:HD12	1.73	0.70
1:A:478:VAL:C	1:A:479:LEU:HD23	2.17	0.70
1:A:488:GLU:HB2	1:A:491:LYS:CG	2.21	0.70
1:A:266:MET:CG	1:A:267:PRO:HD2	2.22	0.69
1:A:333:PHE:CD1	1:A:336:LEU:HD23	2.26	0.69
1:A:114:MET:HE2	1:A:457:TRP:HZ2	1.57	0.69
1:A:373:GLY:O	1:A:377:PHE:HB2	1.92	0.69
1:A:326:GLU:HB2	1:A:334:GLN:CD	2.18	0.69
1:A:348:ASN:O	1:A:348:ASN:ND2	2.26	0.69
1:A:263:GLY:N	1:A:281:THR:HG21	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:TYR:CD2	1:A:479:LEU:HD21	2.29	0.68
1:A:253:LEU:HD11	1:A:362:PRO:HG3	1.76	0.68
1:A:134:LEU:HD23	1:A:167:ILE:HG21	1.76	0.68
1:A:296:PHE:CD1	1:A:339:LYS:HE2	2.29	0.68
1:A:350:LEU:HD21	1:A:357:GLU:HB2	1.76	0.68
1:A:236:SER:HB3	1:A:365:GLY:HA2	1.75	0.68
1:A:438:MET:HE1	1:A:469:VAL:HG12	1.75	0.68
1:A:195:ILE:HG22	1:A:437:PHE:HB2	1.76	0.67
1:A:272:ARG:NH1	1:A:295:ARG:HD2	2.09	0.67
1:A:291:PRO:C	1:A:293:TYR:H	2.00	0.67
1:A:148:PHE:CD1	1:A:148:PHE:N	2.58	0.67
1:A:422:LYS:O	1:A:424:ASN:N	2.26	0.67
1:A:418:HIS:HA	1:A:421:GLN:OE1	1.94	0.67
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.76	0.66
1:A:325:MET:SD	1:A:416:VAL:HA	2.34	0.66
1:A:437:PHE:CE2	1:A:441:MET:HE3	2.27	0.66
1:A:342:ALA:CB	1:A:425:VAL:HG11	2.24	0.66
1:A:203:LEU:CD1	1:A:237:ALA:HA	2.25	0.66
1:A:261:TYR:HD1	1:A:296:PHE:C	2.04	0.66
1:A:257:GLN:HE22	2:A:1499:FC1:H141	1.60	0.65
1:A:186:MET:HE3	1:A:186:MET:HA	1.78	0.65
1:A:306:ASP:CB	1:A:308:GLN:HE22	2.09	0.65
1:A:177:LEU:HD12	1:A:207:ASP:OD2	1.96	0.65
1:A:218:PHE:CE1	1:A:222:CYS:SG	2.90	0.65
1:A:180:LEU:HD21	1:A:240:VAL:HG21	1.79	0.65
1:A:341:TYR:CE2	1:A:367:TYR:OH	2.49	0.64
1:A:253:LEU:HD11	1:A:362:PRO:CG	2.28	0.64
1:A:194:CYS:O	1:A:197:ARG:HG3	1.96	0.64
1:A:254:TRP:CZ2	1:A:310:PRO:HG3	2.33	0.64
1:A:218:PHE:CD2	1:A:313:PHE:CD1	2.86	0.64
1:A:372:ILE:HA	1:A:376:ASP:OD2	1.97	0.64
1:A:371:GLU:O	1:A:375:ARG:HB2	1.98	0.64
1:A:252:ARG:HH12	1:A:486:GLN:HB3	1.62	0.63
1:A:350:LEU:HB2	1:A:486:GLN:NE2	2.13	0.63
1:A:282:GLN:OE1	1:A:282:GLN:HA	1.97	0.63
1:A:191:ALA:O	1:A:197:ARG:HD3	1.98	0.63
1:A:204:GLN:HB2	1:A:237:ALA:HB2	1.81	0.63
1:A:180:LEU:HD23	1:A:180:LEU:O	1.99	0.63
1:A:402:SER:O	1:A:403:LEU:HB2	1.99	0.63
1:A:206:PHE:HB2	1:A:239:THR:HA	1.81	0.62
1:A:233:ASN:C	1:A:233:ASN:HD22	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:O	1:A:197:ARG:NH1	2.32	0.62
1:A:469:VAL:HG23	1:A:469:VAL:O	1.99	0.62
1:A:322:GLU:OE2	1:A:339:LYS:HE3	1.99	0.62
1:A:77:GLN:HE21	1:A:78:TYR:HB3	1.65	0.62
1:A:327:HIS:ND1	1:A:328:PRO:CD	2.62	0.62
1:A:496:GLN:HE21	1:A:497:ASN:N	1.97	0.62
1:A:399:THR:O	1:A:402:SER:OG	2.17	0.62
1:A:459:VAL:HG23	1:A:469:VAL:O	1.99	0.62
1:A:96:HIS:C	1:A:98:ALA:H	2.08	0.62
1:A:385:ILE:CG1	1:A:386:LEU:H	2.12	0.62
1:A:285:ILE:CG1	1:A:291:PRO:HG3	2.31	0.61
1:A:417:LEU:HD21	1:A:429:ASP:HB3	1.80	0.61
1:A:221:ILE:HG22	1:A:222:CYS:N	2.14	0.61
1:A:78:TYR:O	1:A:78:TYR:HD1	1.79	0.61
1:A:228:ALA:HB1	1:A:343:LEU:HD11	1.83	0.61
1:A:306:ASP:HB3	1:A:308:GLN:HE22	1.65	0.61
1:A:110:LEU:HD12	1:A:110:LEU:H	1.64	0.61
1:A:242:PRO:HG2	1:A:251:PHE:CE1	2.34	0.60
1:A:308:GLN:CD	1:A:308:GLN:N	2.48	0.60
1:A:309:ASP:OD2	1:A:497:ASN:HB2	2.00	0.60
1:A:326:GLU:HB2	1:A:334:GLN:NE2	2.16	0.60
1:A:438:MET:O	1:A:442:GLN:HG2	2.01	0.60
1:A:416:VAL:HG12	1:A:417:LEU:N	2.17	0.60
1:A:253:LEU:HG	1:A:347:ALA:HB1	1.82	0.60
1:A:81:ILE:HD11	1:A:90:LEU:HD12	1.82	0.60
1:A:304:GLN:O	1:A:304:GLN:HG3	2.00	0.60
1:A:382:ARG:HG3	1:A:382:ARG:HH11	1.66	0.60
1:A:126:LYS:O	1:A:127:PRO:O	2.20	0.60
1:A:186:MET:HE1	1:A:189:ARG:NH1	2.15	0.60
1:A:148:PHE:HD1	1:A:148:PHE:N	1.93	0.60
1:A:215:GLN:O	1:A:219:GLN:HG2	2.02	0.60
1:A:251:PHE:O	1:A:252:ARG:HG2	2.01	0.60
1:A:333:PHE:CE2	1:A:415:ALA:CB	2.77	0.60
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.04	0.59
1:A:188:TRP:CH2	1:A:200:TRP:HA	2.37	0.59
1:A:230:ASN:HB3	1:A:233:ASN:O	2.02	0.59
1:A:306:ASP:CA	1:A:308:GLN:HE22	2.14	0.59
1:A:323:VAL:HG22	1:A:425:VAL:HG21	1.83	0.59
1:A:180:LEU:HD11	1:A:240:VAL:HG11	1.83	0.59
1:A:192:PRO:HA	1:A:452:PRO:O	2.03	0.59
1:A:215:GLN:HG3	1:A:219:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:TYR:HA	1:A:148:PHE:CE1	2.37	0.59
1:A:265:GLN:O	1:A:265:GLN:CG	2.50	0.59
1:A:84:TRP:NE1	1:A:114:MET:SD	2.76	0.59
1:A:254:TRP:CH2	1:A:310:PRO:HG3	2.37	0.58
1:A:214:ALA:O	1:A:217:MET:HB2	2.03	0.58
1:A:116:PRO:HB2	1:A:118:SER:OG	2.03	0.58
1:A:124:ARG:NH1	1:A:357:GLU:OE1	2.36	0.58
1:A:266:MET:HG3	1:A:267:PRO:HD2	1.84	0.58
1:A:272:ARG:CZ	1:A:295:ARG:HD2	2.33	0.58
1:A:175:LEU:HD12	1:A:175:LEU:N	2.17	0.58
1:A:260:ARG:HE	1:A:277:THR:HG21	1.67	0.58
1:A:344:PRO:HD2	1:A:365:GLY:O	2.03	0.58
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.38	0.58
1:A:186:MET:CE	1:A:189:ARG:HH11	2.17	0.58
1:A:233:ASN:C	1:A:233:ASN:ND2	2.61	0.57
1:A:246:ASP:OD1	1:A:248:LYS:HB3	2.04	0.57
1:A:496:GLN:HE21	1:A:496:GLN:C	2.12	0.57
1:A:390:GLY:O	1:A:393:MET:HB3	2.03	0.57
1:A:297:ASP:N	1:A:297:ASP:OD1	2.37	0.57
1:A:438:MET:HE3	1:A:438:MET:HA	1.86	0.57
1:A:204:GLN:HG3	1:A:227:TYR:CZ	2.40	0.57
1:A:420:PHE:CD2	1:A:427:ILE:HB	2.40	0.57
1:A:79:VAL:HG23	1:A:95:HIS:NE2	2.20	0.57
1:A:268:ASP:C	1:A:270:THR:H	2.12	0.57
1:A:328:PRO:O	1:A:329:LYS:HD2	2.04	0.57
1:A:221:ILE:HG21	1:A:301:LEU:CD2	2.35	0.57
1:A:123:PRO:HA	1:A:244:ARG:NH2	2.18	0.57
1:A:148:PHE:HB3	1:A:150:GLU:O	2.06	0.56
1:A:208:ALA:O	1:A:211:CYS:HB2	2.03	0.56
1:A:376:ASP:O	1:A:383:TYR:HB2	2.05	0.56
1:A:437:PHE:O	1:A:440:HIS:HB3	2.04	0.56
1:A:271:ILE:HD13	1:A:278:LEU:HD11	1.87	0.56
1:A:292:ARG:O	1:A:294:GLY:N	2.38	0.56
1:A:326:GLU:OE2	1:A:422:LYS:HE2	2.05	0.56
1:A:243:GLN:NE2	1:A:356:LEU:HD22	2.20	0.56
1:A:257:GLN:HG2	1:A:260:ARG:HG3	1.87	0.56
1:A:261:TYR:CE2	1:A:341:TYR:HD1	2.23	0.56
1:A:430:HIS:CD2	1:A:431:HIS:CD2	2.93	0.56
1:A:478:VAL:O	1:A:479:LEU:HD23	2.05	0.56
1:A:173:TYR:C	1:A:174:GLN:HE21	2.14	0.56
1:A:198:ILE:O	1:A:198:ILE:HG13	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLY:C	1:A:295:ARG:HD3	2.30	0.56
1:A:431:HIS:O	1:A:435:GLU:HG2	2.04	0.56
1:A:453:ALA:O	1:A:476:ASN:HB3	2.04	0.56
1:A:180:LEU:CD2	1:A:240:VAL:HG21	2.35	0.56
1:A:80:ARG:HG3	1:A:91:HIS:HD2	1.71	0.56
1:A:144:TYR:HE2	1:A:179:GLU:CG	2.16	0.56
1:A:330:TYR:HD2	1:A:332:TRP:CZ2	2.24	0.56
1:A:132:GLU:O	1:A:135:PRO:HD2	2.06	0.56
1:A:251:PHE:CD1	1:A:305:ALA:O	2.58	0.56
1:A:176:THR:O	1:A:179:GLU:HG3	2.06	0.56
1:A:177:LEU:HA	1:A:209:ARG:NH2	2.21	0.56
1:A:204:GLN:NE2	1:A:206:PHE:HE1	2.04	0.56
1:A:419:SER:O	1:A:422:LYS:HB3	2.06	0.56
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.41	0.56
1:A:189:ARG:HE	1:A:444:GLU:CD	2.14	0.55
1:A:224:HIS:HB2	1:A:239:THR:HG21	1.86	0.55
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.36	0.55
1:A:342:ALA:HB1	1:A:425:VAL:CG1	2.34	0.55
1:A:349:MET:HE2	1:A:483:TYR:HB3	1.88	0.55
1:A:93:THR:O	1:A:95:HIS:N	2.39	0.55
1:A:382:ARG:HG3	1:A:382:ARG:NH1	2.22	0.55
1:A:84:TRP:O	1:A:85:GLY:C	2.50	0.55
1:A:370:THR:O	1:A:374:VAL:HG13	2.07	0.55
1:A:176:THR:O	1:A:179:GLU:N	2.37	0.55
1:A:261:TYR:CE2	1:A:341:TYR:CD1	2.95	0.55
1:A:189:ARG:HD3	1:A:444:GLU:OE2	2.07	0.55
1:A:203:LEU:HD11	1:A:238:ILE:HG22	1.89	0.55
1:A:386:LEU:CD1	1:A:409:VAL:HG23	2.37	0.55
1:A:285:ILE:HG13	1:A:291:PRO:HG3	1.89	0.54
1:A:217:MET:SD	1:A:241:PHE:HE2	2.29	0.54
1:A:229:THR:HG22	1:A:231:ASN:H	1.72	0.54
1:A:306:ASP:H	1:A:308:GLN:CD	2.14	0.54
1:A:379:ASP:HB3	1:A:381:GLN:NE2	2.22	0.54
1:A:84:TRP:O	1:A:87:GLY:N	2.37	0.54
1:A:204:GLN:HB2	1:A:237:ALA:CB	2.37	0.54
1:A:385:ILE:O	1:A:387:GLU:N	2.40	0.54
1:A:153:ILE:HD12	1:A:153:ILE:H	1.73	0.54
1:A:322:GLU:CD	1:A:339:LYS:HE3	2.33	0.54
1:A:120:THR:CG2	1:A:121:ARG:H	2.05	0.54
1:A:200:TRP:CD1	1:A:200:TRP:H	2.25	0.54
1:A:82:LYS:CB	1:A:89:ILE:HG23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:O	1:A:121:ARG:HD3	2.07	0.54
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.21	0.54
1:A:161:GLU:HG3	1:A:162:ALA:N	2.22	0.54
1:A:134:LEU:HD23	1:A:167:ILE:CG2	2.38	0.53
1:A:144:TYR:C	1:A:146:GLY:H	2.16	0.53
1:A:268:ASP:OD2	1:A:268:ASP:N	2.40	0.53
1:A:110:LEU:HD12	1:A:110:LEU:N	2.22	0.53
1:A:153:ILE:O	1:A:156:HIS:HB3	2.09	0.53
1:A:298:VAL:CG1	1:A:315:ILE:HD12	2.38	0.53
1:A:395:LEU:HD13	1:A:395:LEU:H	1.72	0.53
1:A:306:ASP:N	1:A:308:GLN:OE1	2.36	0.53
1:A:292:ARG:HB2	1:A:297:ASP:OD2	2.09	0.53
1:A:374:VAL:HA	1:A:378:CYS:SG	2.48	0.53
1:A:460:PRO:HG2	1:A:467:THR:HG21	1.90	0.53
1:A:77:GLN:HE21	1:A:78:TYR:CB	2.22	0.53
1:A:165:LYS:O	1:A:169:THR:HG23	2.09	0.53
1:A:330:TYR:HB3	1:A:332:TRP:HE1	1.69	0.53
1:A:86:SER:OG	1:A:88:GLU:HB2	2.09	0.53
1:A:252:ARG:NH1	1:A:486:GLN:HB3	2.24	0.53
1:A:253:LEU:CD2	1:A:253:LEU:H	2.21	0.53
1:A:399:THR:O	1:A:400:LEU:C	2.51	0.53
1:A:204:GLN:NE2	1:A:206:PHE:CE1	2.77	0.53
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.90	0.53
1:A:114:MET:CE	1:A:457:TRP:HZ2	2.21	0.52
1:A:437:PHE:CZ	1:A:458:LEU:HD13	2.43	0.52
1:A:289:TRP:CD1	1:A:300:PRO:HB3	2.45	0.52
1:A:418:HIS:O	1:A:419:SER:C	2.52	0.52
1:A:215:GLN:OE1	1:A:219:GLN:NE2	2.42	0.52
1:A:332:TRP:HA	1:A:335:GLU:OE2	2.09	0.52
1:A:330:TYR:O	1:A:332:TRP:N	2.43	0.52
1:A:218:PHE:HD2	1:A:313:PHE:CD1	2.27	0.52
1:A:301:LEU:HD12	1:A:313:PHE:O	2.08	0.52
1:A:152:LYS:HB3	1:A:155:GLU:HG3	1.92	0.52
1:A:480:SER:HA	1:A:481:PRO:O	2.09	0.52
1:A:221:ILE:O	1:A:224:HIS:HB3	2.10	0.52
1:A:95:HIS:O	1:A:98:ALA:HB2	2.09	0.51
1:A:133:LEU:C	1:A:135:PRO:HD2	2.34	0.51
1:A:217:MET:SD	1:A:241:PHE:CE2	3.03	0.51
1:A:391:ARG:C	1:A:393:MET:H	2.17	0.51
1:A:252:ARG:NH1	1:A:486:GLN:OE1	2.44	0.51
1:A:453:ALA:O	1:A:474:MET:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ALA:HB2	1:A:481:PRO:HB2	1.91	0.51
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.92	0.51
1:A:404:TRP:CD2	1:A:405:LYS:HG2	2.45	0.51
1:A:386:LEU:HD11	1:A:409:VAL:HG23	1.91	0.51
1:A:144:TYR:C	1:A:144:TYR:CD1	2.89	0.51
1:A:249:HIS:CA	1:A:306:ASP:O	2.57	0.51
1:A:306:ASP:C	1:A:308:GLN:HE22	2.19	0.51
1:A:324:THR:H	1:A:423:GLN:HE22	1.58	0.51
1:A:415:ALA:O	1:A:418:HIS:HB3	2.11	0.51
1:A:470:PHE:HD1	1:A:471:HIS:HD2	1.54	0.51
1:A:176:THR:HG23	1:A:179:GLU:CD	2.36	0.51
1:A:134:LEU:O	1:A:138:ILE:CG1	2.56	0.51
1:A:140:PHE:O	1:A:143:GLN:N	2.43	0.51
1:A:291:PRO:C	1:A:293:TYR:N	2.69	0.51
1:A:350:LEU:HB2	1:A:486:GLN:CD	2.36	0.51
1:A:176:THR:O	1:A:177:LEU:C	2.53	0.51
1:A:243:GLN:HB3	1:A:358:PHE:CD2	2.46	0.51
1:A:195:ILE:HA	1:A:437:PHE:CD1	2.46	0.51
1:A:351:LEU:HD12	1:A:352:GLU:N	2.26	0.51
1:A:351:LEU:HD12	1:A:352:GLU:H	1.76	0.51
1:A:175:LEU:HA	1:A:179:GLU:OE1	2.10	0.50
1:A:296:PHE:CE1	1:A:339:LYS:N	2.79	0.50
1:A:370:THR:HG22	1:A:374:VAL:CG1	2.42	0.50
1:A:82:LYS:HB2	1:A:89:ILE:HG23	1.94	0.50
1:A:353:VAL:O	1:A:356:LEU:N	2.38	0.50
1:A:218:PHE:HE1	1:A:222:CYS:SG	2.32	0.50
1:A:377:PHE:O	1:A:384:ASN:N	2.44	0.50
1:A:309:ASP:OD1	1:A:496:GLN:HG3	2.12	0.50
1:A:371:GLU:OE1	1:A:375:ARG:HG3	2.10	0.50
1:A:82:LYS:HD3	1:A:84:TRP:CZ3	2.46	0.50
1:A:288:GLY:O	1:A:289:TRP:C	2.54	0.50
1:A:430:HIS:HD2	1:A:431:HIS:CD2	2.29	0.50
1:A:89:ILE:N	1:A:89:ILE:HD12	2.27	0.50
1:A:316:PRO:CB	1:A:319:LEU:HD12	2.41	0.50
1:A:372:ILE:HG22	1:A:416:VAL:HG21	1.94	0.50
1:A:325:MET:HB2	1:A:338:LEU:HB3	1.94	0.50
1:A:144:TYR:C	1:A:146:GLY:N	2.70	0.50
1:A:266:MET:HE1	1:A:272:ARG:NE	2.27	0.50
1:A:253:LEU:HD23	1:A:253:LEU:O	2.12	0.49
1:A:165:LYS:O	1:A:169:THR:CG2	2.60	0.49
1:A:217:MET:O	1:A:220:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:TYR:N	1:A:330:TYR:CD1	2.80	0.49
1:A:346:VAL:HG21	1:A:363:PHE:CZ	2.48	0.49
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.93	0.49
1:A:188:TRP:CD2	1:A:200:TRP:HA	2.47	0.49
1:A:307:GLY:N	1:A:308:GLN:NE2	2.60	0.49
1:A:144:TYR:C	1:A:144:TYR:HD1	2.20	0.49
1:A:144:TYR:HE1	1:A:148:PHE:HZ	1.61	0.49
1:A:166:GLU:HG2	1:A:173:TYR:HB2	1.94	0.49
1:A:306:ASP:HB3	1:A:308:GLN:NE2	2.27	0.49
1:A:138:ILE:O	1:A:142:ASN:ND2	2.41	0.49
1:A:404:TRP:CZ2	1:A:405:LYS:HD3	2.47	0.49
1:A:221:ILE:HD13	1:A:301:LEU:HD22	1.93	0.48
1:A:327:HIS:C	1:A:329:LYS:H	2.21	0.48
1:A:352:GLU:O	1:A:481:PRO:HB3	2.12	0.48
1:A:81:ILE:HG13	1:A:90:LEU:O	2.12	0.48
1:A:173:TYR:C	1:A:174:GLN:NE2	2.70	0.48
1:A:188:TRP:C	1:A:190:ASN:N	2.68	0.48
1:A:276:ALA:HB2	1:A:382:ARG:CD	2.43	0.48
1:A:295:ARG:O	1:A:296:PHE:CD2	2.65	0.48
1:A:307:GLY:N	1:A:308:GLN:HE22	2.11	0.48
1:A:163:VAL:C	1:A:167:ILE:HD12	2.39	0.48
1:A:264:TYR:CD1	1:A:264:TYR:N	2.80	0.48
1:A:422:LYS:HG2	1:A:423:GLN:N	2.28	0.48
1:A:200:TRP:CD1	1:A:200:TRP:N	2.81	0.48
1:A:454:ASP:C	1:A:454:ASP:OD1	2.56	0.48
1:A:218:PHE:CD1	1:A:218:PHE:C	2.90	0.48
1:A:229:THR:HG22	1:A:231:ASN:N	2.29	0.48
1:A:268:ASP:O	1:A:270:THR:N	2.47	0.48
1:A:333:PHE:CE2	1:A:415:ALA:HB1	2.49	0.48
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.24	0.48
1:A:92:ASP:OD2	1:A:95:HIS:HB3	2.13	0.48
1:A:308:GLN:NE2	1:A:308:GLN:N	2.57	0.48
1:A:371:GLU:HA	1:A:375:ARG:CG	2.43	0.48
1:A:206:PHE:HE2	1:A:224:HIS:HA	1.78	0.48
1:A:134:LEU:N	1:A:135:PRO:HD2	2.29	0.47
1:A:78:TYR:O	1:A:79:VAL:C	2.57	0.47
1:A:296:PHE:HE1	1:A:339:LYS:N	2.12	0.47
1:A:221:ILE:O	1:A:224:HIS:N	2.48	0.47
1:A:251:PHE:CE1	1:A:305:ALA:O	2.67	0.47
1:A:254:TRP:N	1:A:254:TRP:CD1	2.81	0.47
1:A:129:PRO:O	1:A:132:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TRP:CH2	3:A:1500:HEM:HMC1	2.50	0.47
1:A:430:HIS:O	1:A:431:HIS:C	2.56	0.47
1:A:439:LYS:HA	1:A:442:GLN:HG3	1.97	0.47
1:A:330:TYR:HD2	1:A:332:TRP:HZ2	1.62	0.47
1:A:388:GLU:C	1:A:390:GLY:N	2.69	0.47
1:A:289:TRP:HB2	1:A:312:VAL:HG11	1.95	0.47
1:A:338:LEU:HG	1:A:377:PHE:CE1	2.49	0.47
1:A:437:PHE:C	1:A:437:PHE:CD2	2.91	0.47
1:A:193:ARG:NH1	1:A:485:TYR:OH	2.47	0.47
1:A:420:PHE:O	1:A:421:GLN:C	2.58	0.47
1:A:494:ILE:HD12	1:A:494:ILE:O	2.15	0.47
1:A:265:GLN:HB3	1:A:278:LEU:HD21	1.96	0.47
1:A:393:MET:O	1:A:395:LEU:HD13	2.15	0.47
1:A:419:SER:O	1:A:420:PHE:C	2.57	0.46
1:A:189:ARG:HG3	1:A:200:TRP:CE3	2.50	0.46
1:A:395:LEU:H	1:A:395:LEU:CD1	2.29	0.46
1:A:462:VAL:O	1:A:463:SER:CB	2.63	0.46
1:A:188:TRP:CZ3	1:A:200:TRP:CA	2.89	0.46
1:A:206:PHE:HB2	1:A:239:THR:CB	2.45	0.46
1:A:206:PHE:CD2	1:A:239:THR:HG22	2.50	0.46
1:A:258:LEU:HD22	1:A:345:ALA:HB1	1.97	0.46
1:A:140:PHE:O	1:A:141:ILE:C	2.58	0.46
1:A:181:ILE:HG13	1:A:205:VAL:HG21	1.96	0.46
1:A:252:ARG:HH12	1:A:486:GLN:CB	2.28	0.46
1:A:275:ALA:O	1:A:278:LEU:HB2	2.16	0.46
1:A:134:LEU:CD1	1:A:138:ILE:HD11	2.42	0.46
1:A:268:ASP:C	1:A:270:THR:N	2.73	0.46
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.97	0.46
1:A:296:PHE:HE2	1:A:383:TYR:CE2	2.34	0.46
1:A:388:GLU:C	1:A:390:GLY:H	2.23	0.46
1:A:399:THR:O	1:A:399:THR:CG2	2.51	0.46
1:A:430:HIS:O	1:A:433:ALA:HB3	2.16	0.46
1:A:188:TRP:CE3	3:A:1500:HEM:HMC2	2.52	0.45
1:A:415:ALA:O	1:A:416:VAL:C	2.58	0.45
1:A:441:MET:O	1:A:442:GLN:C	2.59	0.45
1:A:403:LEU:N	1:A:403:LEU:HD23	2.30	0.45
1:A:457:TRP:HA	4:A:1501:HBI:N1	2.31	0.45
1:A:81:ILE:CD1	1:A:90:LEU:HD12	2.45	0.45
1:A:163:VAL:O	1:A:164:THR:C	2.58	0.45
1:A:218:PHE:O	1:A:221:ILE:HB	2.15	0.45
1:A:251:PHE:CG	1:A:305:ALA:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:NH2	1:A:489:PRO:HG3	2.32	0.45
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.50	0.45
1:A:408:ALA:O	1:A:409:VAL:C	2.59	0.45
1:A:188:TRP:CZ2	3:A:1500:HEM:HMC1	2.51	0.45
1:A:272:ARG:HD2	1:A:295:ARG:HB3	1.98	0.45
1:A:330:TYR:HD1	1:A:330:TYR:H	1.65	0.45
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.82	0.45
1:A:401:ALA:O	1:A:403:LEU:HD23	2.17	0.45
1:A:186:MET:O	1:A:189:ARG:N	2.50	0.45
1:A:217:MET:CE	1:A:303:LEU:HB3	2.47	0.45
1:A:332:TRP:CD1	1:A:332:TRP:H	2.35	0.45
1:A:157:LEU:O	1:A:160:LEU:HB2	2.16	0.45
1:A:255:ASN:OD1	1:A:280:PHE:CZ	2.69	0.45
1:A:294:GLY:HA3	1:A:297:ASP:OD1	2.16	0.45
1:A:330:TYR:O	1:A:333:PHE:N	2.49	0.45
1:A:330:TYR:CB	1:A:332:TRP:NE1	2.65	0.45
1:A:195:ILE:HA	1:A:437:PHE:HD1	1.80	0.45
1:A:275:ALA:HB1	1:A:278:LEU:HD12	1.98	0.45
1:A:295:ARG:HH11	1:A:295:ARG:H	1.65	0.45
1:A:217:MET:HE3	1:A:303:LEU:CB	2.47	0.44
1:A:252:ARG:O	1:A:304:GLN:HG2	2.16	0.44
1:A:281:THR:HG22	1:A:299:LEU:HD21	2.00	0.44
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	0.44
1:A:260:ARG:HE	1:A:277:THR:HG22	1.80	0.44
1:A:344:PRO:HG2	1:A:365:GLY:O	2.17	0.44
1:A:92:ASP:O	1:A:95:HIS:CD2	2.70	0.44
1:A:217:MET:O	1:A:218:PHE:C	2.60	0.44
1:A:217:MET:HE3	1:A:303:LEU:HB2	1.99	0.44
1:A:218:PHE:CD2	1:A:313:PHE:HD1	2.36	0.44
1:A:402:SER:O	1:A:403:LEU:CB	2.65	0.44
1:A:257:GLN:NE2	2:A:1499:FC1:H141	2.31	0.44
1:A:315:ILE:O	1:A:317:PRO:HD3	2.17	0.44
1:A:464:GLY:O	1:A:467:THR:HG23	2.17	0.44
1:A:204:GLN:HG3	1:A:227:TYR:CE2	2.53	0.44
1:A:298:VAL:HG11	1:A:315:ILE:HD12	1.99	0.44
1:A:437:PHE:CZ	1:A:458:LEU:CD1	3.01	0.44
1:A:495:TRP:C	1:A:497:ASN:N	2.75	0.44
1:A:85:GLY:HA2	1:A:381:GLN:HB3	2.00	0.44
1:A:89:ILE:HD12	1:A:89:ILE:H	1.83	0.44
1:A:96:HIS:C	1:A:98:ALA:N	2.74	0.44
1:A:266:MET:SD	1:A:272:ARG:CG	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ARG:C	1:A:393:MET:N	2.76	0.44
1:A:206:PHE:HB2	1:A:239:THR:CA	2.47	0.44
1:A:283:LEU:O	1:A:286:ASP:N	2.51	0.44
1:A:395:LEU:CD1	1:A:395:LEU:N	2.81	0.44
1:A:417:LEU:HB3	1:A:421:GLN:HE22	1.83	0.44
1:A:144:TYR:HE1	1:A:148:PHE:CZ	2.36	0.43
1:A:363:PHE:N	1:A:363:PHE:CD2	2.85	0.43
1:A:213:THR:HB	1:A:216:GLU:H	1.82	0.43
1:A:251:PHE:O	1:A:360:ALA:HB2	2.17	0.43
1:A:459:VAL:HG12	1:A:459:VAL:O	2.16	0.43
1:A:494:ILE:H	1:A:494:ILE:HG13	1.43	0.43
1:A:144:TYR:O	1:A:146:GLY:N	2.51	0.43
1:A:186:MET:O	1:A:187:ALA:C	2.61	0.43
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.18	0.43
1:A:121:ARG:CG	1:A:121:ARG:NH1	2.79	0.43
1:A:340:TRP:HZ3	1:A:383:TYR:CZ	2.36	0.43
1:A:353:VAL:HG23	1:A:481:PRO:HG3	2.00	0.43
1:A:161:GLU:OE1	1:A:165:LYS:HG2	2.18	0.43
1:A:167:ILE:O	1:A:171:GLY:CA	2.66	0.43
1:A:213:THR:OG1	1:A:216:GLU:HB2	2.18	0.43
1:A:217:MET:CG	1:A:241:PHE:CE2	3.01	0.43
1:A:340:TRP:CZ3	1:A:383:TYR:CE1	3.06	0.43
1:A:495:TRP:C	1:A:497:ASN:H	2.25	0.43
1:A:285:ILE:HD11	1:A:291:PRO:HG3	2.00	0.43
1:A:458:LEU:O	1:A:469:VAL:HG21	2.19	0.43
1:A:159:ARG:O	1:A:162:ALA:HB3	2.19	0.43
1:A:197:ARG:NH2	1:A:451:CYS:SG	2.91	0.43
1:A:217:MET:O	1:A:220:HIS:N	2.51	0.43
1:A:429:ASP:OD2	1:A:432:THR:OG1	2.37	0.43
1:A:385:ILE:HG13	1:A:386:LEU:N	2.18	0.43
1:A:416:VAL:O	1:A:417:LEU:C	2.62	0.43
1:A:451:CYS:O	1:A:453:ALA:N	2.51	0.43
1:A:476:ASN:ND2	1:A:476:ASN:C	2.75	0.43
1:A:131:GLU:O	1:A:135:PRO:HG3	2.19	0.43
1:A:207:ASP:C	1:A:209:ARG:H	2.26	0.43
1:A:327:HIS:CB	1:A:333:PHE:HD2	2.16	0.43
1:A:358:PHE:HA	1:A:359:PRO:HD3	1.73	0.43
1:A:496:GLN:C	1:A:496:GLN:NE2	2.77	0.43
1:A:186:MET:C	1:A:188:TRP:N	2.76	0.42
1:A:245:SER:OG	1:A:246:ASP:N	2.43	0.42
1:A:175:LEU:HD11	1:A:356:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:CB	1:A:308:GLN:NE2	2.79	0.42
1:A:397:THR:O	1:A:397:THR:CG2	2.67	0.42
1:A:437:PHE:HD2	1:A:438:MET:HE3	1.84	0.42
1:A:128:THR:O	1:A:129:PRO:C	2.61	0.42
1:A:218:PHE:O	1:A:219:GLN:C	2.62	0.42
1:A:453:ALA:HB3	1:A:474:MET:HB2	2.00	0.42
1:A:152:LYS:HD2	1:A:155:GLU:OE2	2.19	0.42
1:A:185:LYS:HE2	1:A:203:LEU:H	1.85	0.42
1:A:186:MET:O	1:A:190:ASN:N	2.51	0.42
1:A:227:TYR:CD2	1:A:227:TYR:C	2.97	0.42
1:A:407:ARG:NH1	1:A:407:ARG:CG	2.82	0.42
1:A:180:LEU:O	1:A:183:ALA:HB3	2.20	0.42
1:A:217:MET:HE1	1:A:304:GLN:N	2.34	0.42
1:A:338:LEU:HD21	1:A:385:ILE:HG21	2.02	0.42
1:A:378:CYS:O	1:A:379:ASP:C	2.63	0.42
1:A:441:MET:HE1	1:A:474:MET:CE	2.41	0.42
1:A:261:TYR:CD1	1:A:296:PHE:HA	2.55	0.42
1:A:261:TYR:CD1	1:A:296:PHE:C	2.91	0.42
1:A:348:ASN:O	1:A:349:MET:HG3	2.19	0.42
1:A:374:VAL:O	1:A:378:CYS:HB2	2.20	0.42
1:A:140:PHE:CE2	1:A:353:VAL:CG2	3.02	0.42
1:A:164:THR:O	1:A:165:LYS:C	2.63	0.42
1:A:175:LEU:H	1:A:175:LEU:CD1	2.24	0.42
1:A:200:TRP:CG	1:A:201:SER:N	2.88	0.42
1:A:348:ASN:HD22	1:A:348:ASN:C	2.19	0.42
1:A:193:ARG:HB3	1:A:457:TRP:CB	2.50	0.42
1:A:330:TYR:N	1:A:330:TYR:HD1	2.17	0.42
1:A:370:THR:HG22	1:A:374:VAL:HG12	2.02	0.42
1:A:112:SER:HA	1:A:456:ILE:HD12	2.02	0.42
1:A:144:TYR:CE2	1:A:179:GLU:HA	2.55	0.42
1:A:244:ARG:NH1	1:A:357:GLU:OE2	2.51	0.42
1:A:301:LEU:HD12	1:A:301:LEU:H	1.85	0.42
1:A:213:THR:HG1	1:A:216:GLU:HB2	1.85	0.41
1:A:299:LEU:HD22	1:A:300:PRO:HD2	2.02	0.41
1:A:324:THR:H	1:A:423:GLN:NE2	2.17	0.41
1:A:257:GLN:OE1	1:A:260:ARG:NH1	2.44	0.41
1:A:333:PHE:O	1:A:334:GLN:C	2.62	0.41
1:A:383:TYR:O	1:A:384:ASN:HB3	2.21	0.41
1:A:441:MET:C	1:A:443:ASN:N	2.77	0.41
1:A:136:HIS:O	1:A:139:GLU:HB2	2.20	0.41
1:A:446:ARG:HG3	1:A:446:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:O	1:A:135:PRO:CD	2.68	0.41
1:A:189:ARG:HG3	1:A:200:TRP:CD2	2.55	0.41
1:A:215:GLN:O	1:A:219:GLN:CG	2.66	0.41
1:A:340:TRP:HZ3	1:A:383:TYR:CE1	2.38	0.41
1:A:386:LEU:HD21	1:A:405:LYS:HD2	2.02	0.41
1:A:474:MET:HE3	1:A:474:MET:HB3	1.95	0.41
1:A:163:VAL:CG1	1:A:167:ILE:HD11	2.39	0.41
1:A:244:ARG:NH2	1:A:250:ASP:OD2	2.54	0.41
1:A:244:ARG:HB2	1:A:357:GLU:O	2.19	0.41
1:A:331:GLU:C	1:A:333:PHE:H	2.28	0.41
1:A:477:TYR:HD2	1:A:479:LEU:CD2	2.24	0.41
1:A:173:TYR:CE1	1:A:356:LEU:HG	2.55	0.41
1:A:188:TRP:O	1:A:189:ARG:C	2.63	0.41
1:A:128:THR:HA	1:A:129:PRO:HD2	1.88	0.41
1:A:153:ILE:HB	1:A:154:GLU:OE1	2.20	0.41
1:A:257:GLN:CB	1:A:345:ALA:O	2.58	0.41
1:A:488:GLU:O	1:A:491:LYS:HG3	2.19	0.41
1:A:78:TYR:CG	1:A:91:HIS:HB3	2.55	0.41
1:A:147:SER:O	1:A:148:PHE:C	2.64	0.41
1:A:206:PHE:HB2	1:A:239:THR:HB	2.03	0.41
1:A:213:THR:CB	1:A:216:GLU:HB2	2.49	0.41
1:A:290:LYS:HA	1:A:291:PRO:HD3	1.58	0.41
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.76	0.41
1:A:333:PHE:HA	1:A:336:LEU:HD23	2.03	0.41
1:A:132:GLU:C	1:A:135:PRO:HD2	2.45	0.41
1:A:154:GLU:H	1:A:154:GLU:CD	2.24	0.41
1:A:221:ILE:CD1	1:A:303:LEU:HD21	2.50	0.41
1:A:417:LEU:O	1:A:421:GLN:CD	2.64	0.41
1:A:429:ASP:CG	1:A:432:THR:OG1	2.64	0.41
1:A:140:PHE:CD1	1:A:140:PHE:C	2.98	0.41
1:A:188:TRP:O	1:A:191:ALA:N	2.52	0.41
1:A:245:SER:OG	1:A:249:HIS:HB2	2.21	0.41
1:A:330:TYR:O	1:A:331:GLU:C	2.63	0.41
1:A:114:MET:CE	1:A:457:TRP:CZ2	3.03	0.40
1:A:370:THR:HG23	1:A:430:HIS:CE1	2.55	0.40
1:A:389:VAL:O	1:A:389:VAL:HG12	2.20	0.40
1:A:389:VAL:HG11	1:A:412:ILE:HG13	2.02	0.40
1:A:182:PHE:CD2	1:A:182:PHE:C	2.99	0.40
1:A:330:TYR:CB	1:A:332:TRP:HE1	2.32	0.40
1:A:437:PHE:CE1	1:A:458:LEU:HD13	2.57	0.40
1:A:442:GLN:HG2	1:A:442:GLN:H	1.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:TRP:O	1:A:190:ASN:N	2.54	0.40
1:A:198:ILE:HB	1:A:440:HIS:HB2	2.02	0.40
1:A:399:THR:O	1:A:401:ALA:N	2.55	0.40
1:A:140:PHE:CE2	1:A:353:VAL:HG22	2.56	0.40
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.36	0.40
1:A:289:TRP:CG	1:A:300:PRO:HG3	2.56	0.40
1:A:462:VAL:O	1:A:463:SER:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:ND2	1:A:471:HIS:O[11_554]	1.97	0.23

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	410/422 (97%)	255 (62%)	109 (27%)	46 (11%)	0 2

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	TRP
1	A	94	LEU
1	A	127	PRO
1	A	148	PHE
1	A	197	ARG
1	A	262	ALA
1	A	268	ASP
1	A	293	TYR
1	A	386	LEU

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Mol	Chain	Res	Type
1	A	395	LEU
1	A	423	GLN
1	A	85	GLY
1	A	153	ILE
1	A	207	ASP
1	A	208	ALA
1	A	243	GLN
1	A	269	GLY
1	A	270	THR
1	A	273	GLY
1	A	289	TRP
1	A	331	GLU
1	A	400	LEU
1	A	452	PRO
1	A	129	PRO
1	A	397	THR
1	A	409	VAL
1	A	465	SER
1	A	97	LYS
1	A	144	TYR
1	A	165	LYS
1	A	329	LYS
1	A	420	PHE
1	A	464	GLY
1	A	79	VAL
1	A	121	ARG
1	A	183	ALA
1	A	212	SER
1	A	373	GLY
1	A	408	ALA
1	A	416	VAL
1	A	218	PHE
1	A	354	GLY
1	A	385	ILE
1	A	271	ILE
1	A	469	VAL
1	A	263	GLY

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	362/370 (98%)	221 (61%)	141 (39%)	0 0

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	79	VAL
1	A	81	ILE
1	A	83	ASN
1	A	89	ILE
1	A	90	LEU
1	A	94	LEU
1	A	97	LYS
1	A	100	SER
1	A	110	LEU
1	A	112	SER
1	A	113	ILE
1	A	114	MET
1	A	115	ASN
1	A	119	LEU
1	A	121	ARG
1	A	125	ASP
1	A	126	LYS
1	A	132	GLU
1	A	134	LEU
1	A	139	GLU
1	A	144	TYR
1	A	147	SER
1	A	148	PHE
1	A	149	LYS
1	A	161	GLU
1	A	163	VAL
1	A	164	THR
1	A	166	GLU
1	A	169	THR
1	A	170	THR
1	A	172	THR
1	A	175	LEU
1	A	177	LEU

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Mol	Chain	Res	Type
1	A	181	ILE
1	A	186	MET
1	A	189	ARG
1	A	193	ARG
1	A	195	ILE
1	A	198	ILE
1	A	201	SER
1	A	203	LEU
1	A	205	VAL
1	A	213	THR
1	A	215	GLN
1	A	219	GLN
1	A	220	HIS
1	A	221	ILE
1	A	223	ARG
1	A	226	LEU
1	A	233	ASN
1	A	234	ILE
1	A	239	THR
1	A	248	LYS
1	A	253	LEU
1	A	256	SER
1	A	258	LEU
1	A	264	TYR
1	A	265	GLN
1	A	266	MET
1	A	270	THR
1	A	271	ILE
1	A	277	THR
1	A	278	LEU
1	A	281	THR
1	A	285	ILE
1	A	290	LYS
1	A	292	ARG
1	A	295	ARG
1	A	296	PHE
1	A	297	ASP
1	A	298	VAL
1	A	301	LEU
1	A	303	LEU
1	A	308	GLN
1	A	311	GLU

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Mol	Chain	Res	Type
1	A	312	VAL
1	A	318	ASP
1	A	321	LEU
1	A	324	THR
1	A	326	GLU
1	A	329	LYS
1	A	330	TYR
1	A	331	GLU
1	A	333	PHE
1	A	334	GLN
1	A	335	GLU
1	A	336	LEU
1	A	338	LEU
1	A	346	VAL
1	A	348	ASN
1	A	368	MET
1	A	370	THR
1	A	372	ILE
1	A	374	VAL
1	A	376	ASP
1	A	379	ASP
1	A	380	THR
1	A	381	GLN
1	A	385	ILE
1	A	387	GLU
1	A	392	ARG
1	A	393	MET
1	A	395	LEU
1	A	396	GLU
1	A	397	THR
1	A	399	THR
1	A	400	LEU
1	A	402	SER
1	A	403	LEU
1	A	405	LYS
1	A	406	ASP
1	A	410	THR
1	A	411	GLU
1	A	413	ASN
1	A	416	VAL
1	A	417	LEU
1	A	422	LYS

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Mol	Chain	Res	Type
1	A	425	VAL
1	A	432	THR
1	A	435	GLU
1	A	438	MET
1	A	442	GLN
1	A	448	ARG
1	A	456	ILE
1	A	459	VAL
1	A	463	SER
1	A	465	SER
1	A	466	ILE
1	A	467	THR
1	A	473	GLU
1	A	474	MET
1	A	475	LEU
1	A	476	ASN
1	A	479	LEU
1	A	480	SER
1	A	487	ILE
1	A	491	LYS
1	A	494	ILE
1	A	496	GLN
1	A	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	95	HIS
1	A	96	HIS
1	A	115	ASN
1	A	174	GLN
1	A	215	GLN
1	A	219	GLN
1	A	220	HIS
1	A	231	ASN
1	A	233	ASN
1	A	243	GLN
1	A	304	GLN
1	A	381	GLN
1	A	398	HIS
1	A	423	GLN

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Mol	Chain	Res	Type
1	A	430	HIS
1	A	431	HIS
1	A	471	HIS
1	A	476	ASN
1	A	493	HIS
1	A	496	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
4	HBI	A	1501	-	15,18,18	3.17	2 (13%)	14,26,26	2.15	6 (42%)
2	FC1	A	1499	-	17,19,19	1.46	4 (23%)	19,25,25	2.58	6 (31%)
3	HEM	A	1500	1	50,50,50	1.66	10 (20%)	67,82,82	0.96	3 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HBI	A	1501	-	-	0/4/17/17	0/2/2/2
2	FC1	A	1499	-	-	3/7/7/7	0/2/2/2
3	HEM	A	1500	1	-	6/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	HBI	C6-N5	11.34	1.46	1.28
3	A	1500	HEM	CBC-CAC	5.07	1.54	1.30
3	A	1500	HEM	CBB-CAB	5.01	1.54	1.30
4	A	1501	HBI	C4A-C8A	3.57	1.48	1.40
3	A	1500	HEM	CAC-C3C	3.40	1.56	1.47
2	A	1499	FC1	C1-C2	3.00	1.50	1.45
3	A	1500	HEM	CAB-C3B	2.57	1.54	1.47
3	A	1500	HEM	CMC-C2C	2.53	1.56	1.50
3	A	1500	HEM	FE-NB	2.52	2.02	1.94
3	A	1500	HEM	O2A-CGA	-2.50	1.22	1.30
3	A	1500	HEM	FE-NA	2.46	2.03	1.95
3	A	1500	HEM	FE-NC	2.11	2.02	1.95
3	A	1500	HEM	CMD-C2D	2.09	1.55	1.50
2	A	1499	FC1	C12-C9	2.05	1.42	1.38
2	A	1499	FC1	C9-C4	2.02	1.42	1.38
2	A	1499	FC1	C4-C1	2.02	1.43	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1499	FC1	C1-C3-S7	-6.34	116.85	123.82
2	A	1499	FC1	O6-C2-C5	-5.51	119.13	125.47
2	A	1499	FC1	C4-C1-C2	-5.27	115.29	123.13
4	A	1501	HBI	C2-N1-C8A	4.26	120.88	113.36
4	A	1501	HBI	O4-C4-C4A	-4.19	115.48	126.53
2	A	1499	FC1	C8-C3-S7	3.35	123.01	116.43
2	A	1499	FC1	O6-C2-C1	2.97	116.37	113.56
4	A	1501	HBI	C4A-C4-N3	2.87	120.57	113.25
3	A	1500	HEM	CBB-CAB-C3B	-2.84	113.32	127.53
4	A	1501	HBI	C4A-N5-C6	2.53	121.51	116.08
3	A	1500	HEM	O1A-CGA-CBA	-2.44	115.37	123.09
2	A	1499	FC1	C1-C2-C5	2.08	124.49	121.45
4	A	1501	HBI	O4-C4-N3	2.04	123.95	120.11
3	A	1500	HEM	CAA-CBA-CGA	2.03	119.05	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1501	HBI	C2-N3-C4	-2.02	121.44	125.11

There are no chirality outliers.

All (9) torsion outliers are listed below:

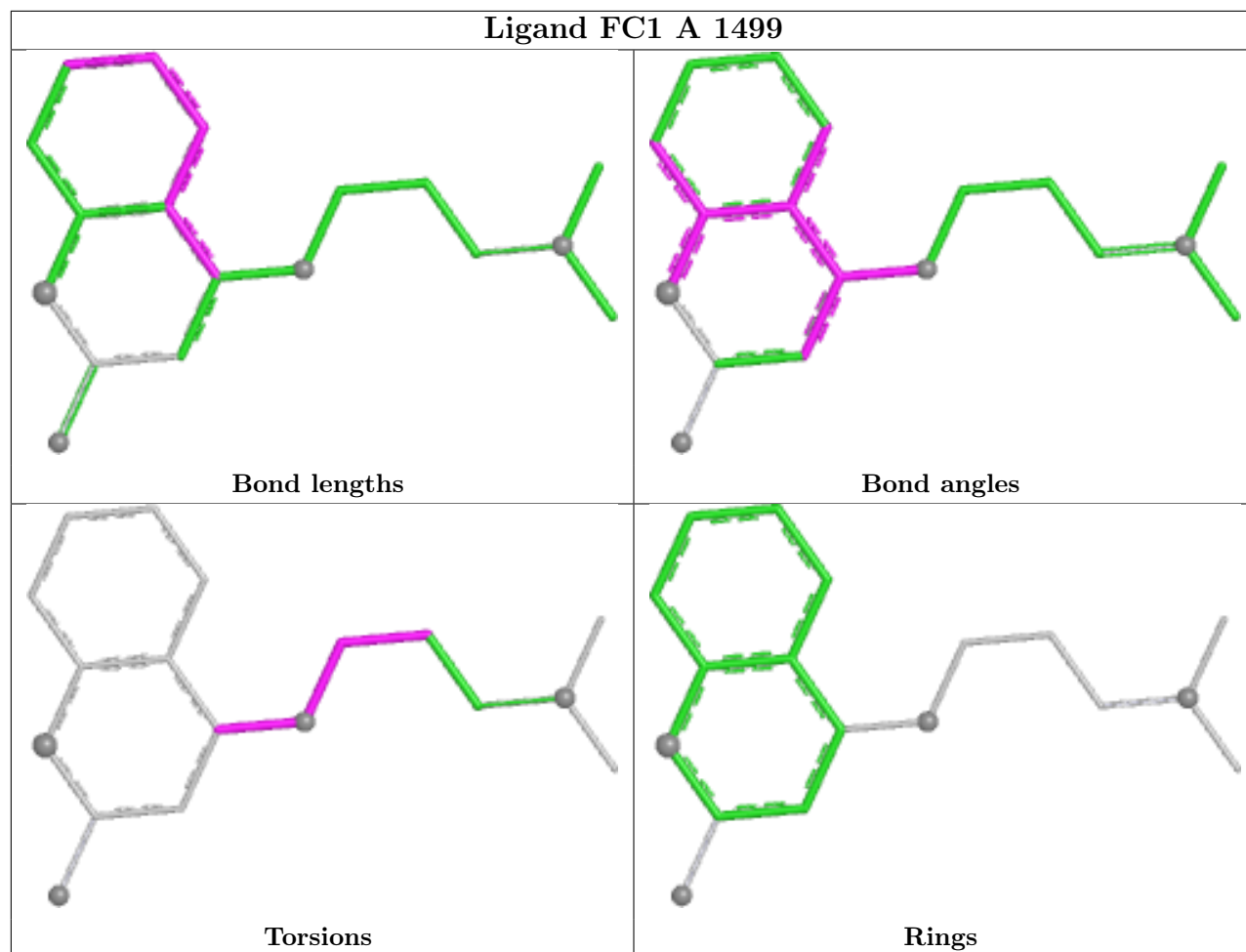
Mol	Chain	Res	Type	Atoms
3	A	1500	HEM	C2B-C3B-CAB-CBB
3	A	1500	HEM	C4B-C3B-CAB-CBB
2	A	1499	FC1	O6-C11-C14-C15
3	A	1500	HEM	C2A-CAA-CBA-CGA
3	A	1500	HEM	CAA-CBA-CGA-O2A
3	A	1500	HEM	CAA-CBA-CGA-O1A
2	A	1499	FC1	C1-C2-O6-C11
2	A	1499	FC1	C14-C11-O6-C2
3	A	1500	HEM	CAD-CBD-CGD-O2D

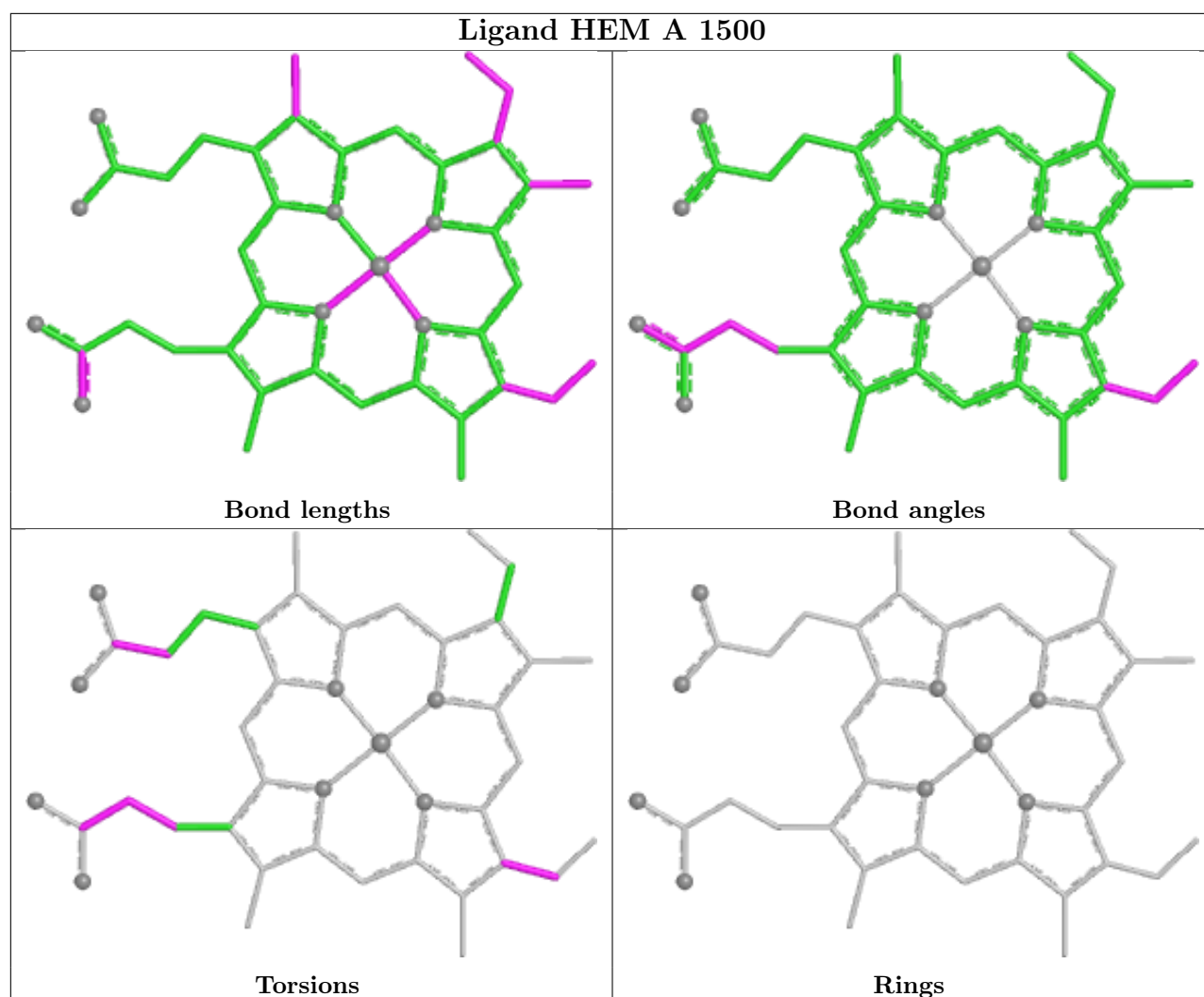
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	HBI	1	0
2	A	1499	FC1	2	0
3	A	1500	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.