Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:45 AM GMT

PDB ID	:	2BHJ
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

http://wwpdb.org/validation/2016/XrayValidationReportHelp

with specific help available everywhere you see the ⓘ symbol.

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

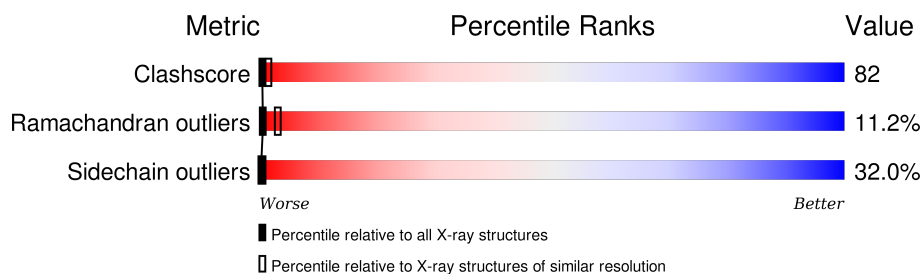|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

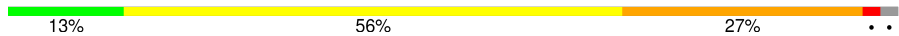The reported resolution of this entry is 3.20 Å.

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	Percentile Ranks	Value
Clashscore		82
Ramachandran outliers		11.2%
Sidechain outliers		32.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	422	13% 56% 27% • •

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
1	A	414	Total 3381	C 2165	N 583	O 613	S 20	0	0	0

- Molecule 2 is THIOCOUMARIN (three-letter code: FC1) (formula: $C_{14}H_{17}NO_2S$).
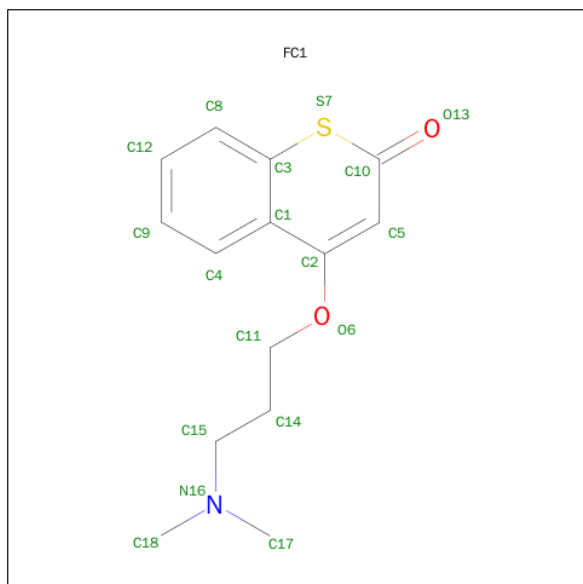
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 18	C 14	N 1	O 2	S 1	0	0

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

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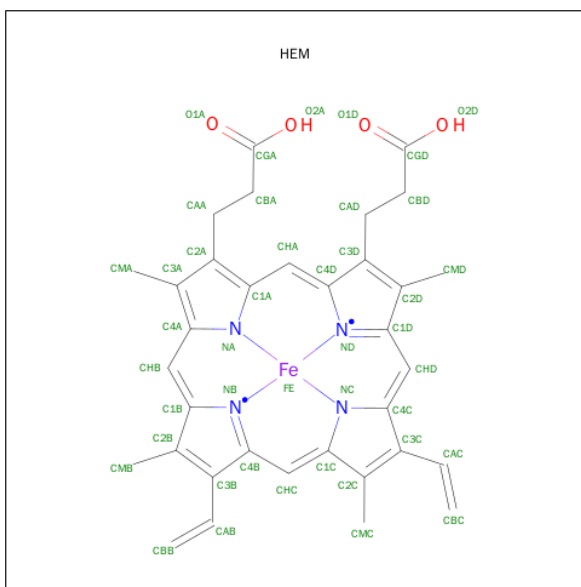
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0

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

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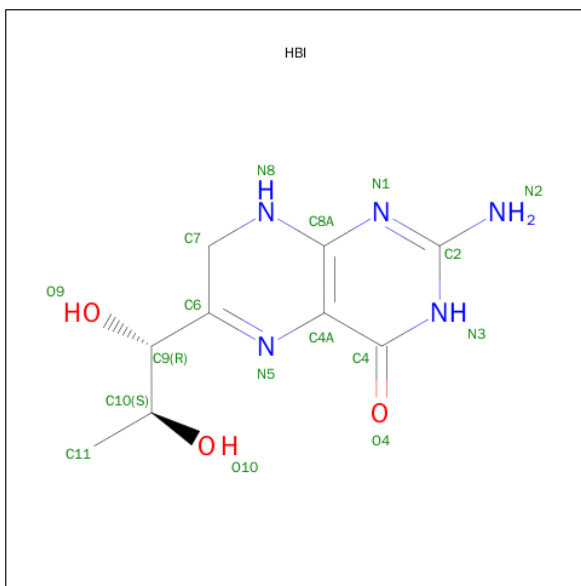
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	17	9	5	3	0	0

- Molecule 5 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: NITRIC OXIDE SYNTHASE

Chain A: 13% 56% 27%
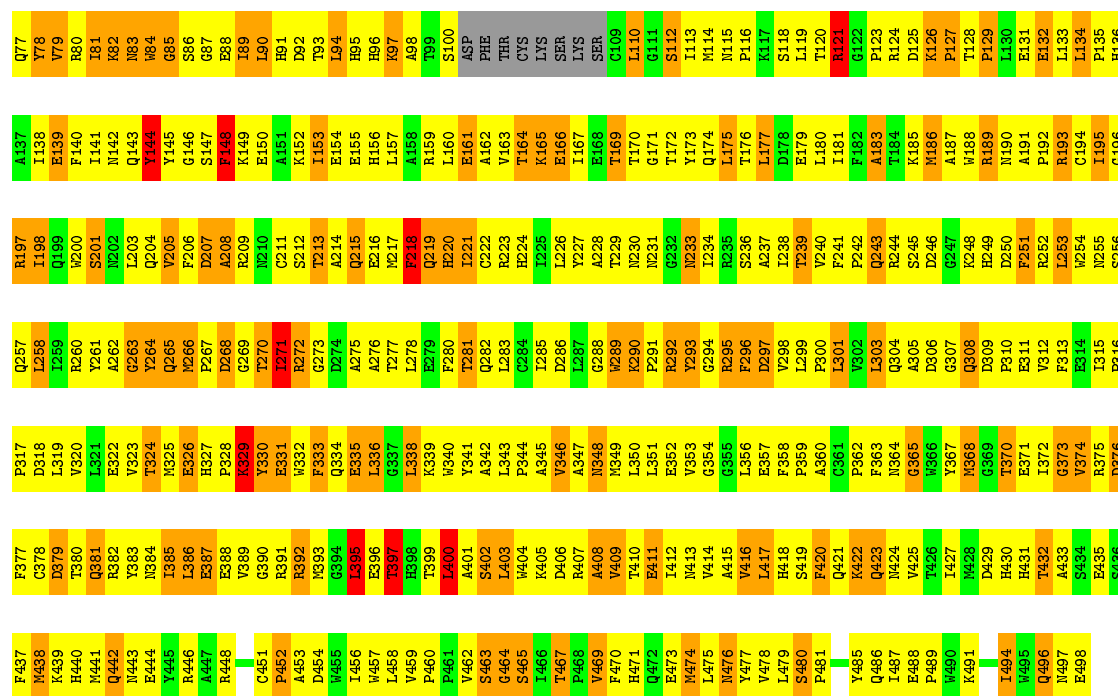
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 (Å²)	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, HBI, 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	0.38	0/3479	0.69	2/4727 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	365	GLY	N-CA-C	-5.39	99.62	113.10
1	A	368	MET	N-CA-C	-5.28	96.75	111.00

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	557	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	557	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 82.

All (557) 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: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: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:308:GLN:H	1:A:308:GLN:CD	1.70	0.95
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:NE2	1:A:381:GLN:H	1.67	0.92
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.05	0.91
1:A:148:PHE:H	1:A:148:PHE:HD1	1.14	0.91
1:A:236:SER:HA	1:A:364:ASN:ND2	1.86	0.91
1:A:381:GLN:HE21	1:A:381:GLN:H	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:N	1:A:381:GLN:HE21	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: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:333:PHE:HE2	1:A:415:ALA:CB	1.88	0.86
1:A:257:GLN:HB2	1:A:345:ALA:O	1.76	0.85
1:A:255:ASN:O	1:A:347:ALA:HB3	1.76	0.85
1:A:327:HIS:ND1	1:A:328:PRO:HD2	1.92	0.85
1:A:263:GLY:H	1:A:281:THR:HG21	1.42	0.85
1:A:134:LEU:O	1:A:138:ILE:HG12	1.76	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:389:VAL:O	1:A:393:MET:HB2	1.79	0.83
1:A:265:GLN:O	1:A:265:GLN:HG3	1.78	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:N	1:A:295:ARG:HD3	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:O	1:A:78:TYR:CD1	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:393:MET:HG2	1:A:395:LEU:CD2	2.13	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:399:THR:HG22	1:A:399:THR:O	1.81	0.79
1:A:332:TRP:HE3	1:A:392:ARG:NH1	1.80	0.78
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:332:TRP:CZ3	1:A:392:ARG:HB2	2.20	0.75
1:A:323:VAL:CG2	1:A:425:VAL:HG21	2.15	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:440:HIS:O	1:A:443:ASN:HB2	1.89	0.73
1:A:407:ARG:HH11	1:A:407:ARG:HG3	1.53	0.73
1:A:134:LEU:HD13	1:A:138:ILE:HD11	1.68	0.73
1:A:308:GLN:H	1:A:308:GLN:NE2	1.87	0.72
1:A:163:VAL:HG12	1:A:167:ILE:CD1	2.18	0.72
1:A:438:MET:CE	1:A:469:VAL:HG12	2.19	0.72
1:A:410:THR:O	1:A:414:VAL:HG23	1.89	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:393:MET:HE1	1:A:411:GLU:HG2	1.72	0.70
1:A:488:GLU:HB2	1:A:491:LYS:CG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:373:GLY:O	1:A:377:PHE:HB2	1.92	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
1:A:422:LYS:C	1:A:424:ASN:H	1.95	0.68
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:272:ARG:NH1	1:A:295:ARG:HD2	2.09	0.67
1:A:195:ILE:HG22	1:A:437:PHE:HB2	1.76	0.67
1:A:148:PHE:N	1:A:148:PHE:CD1	2.58	0.67
1:A:422:LYS:O	1:A:424:ASN:N	2.26	0.67
1:A:480:SER:HA	1:A:481:PRO:C	2.14	0.67
1:A:418:HIS:HA	1:A:421:GLN:OE1	1.94	0.67
1:A:393:MET:CE	1:A:411:GLU:HG2	2.26	0.66
1:A:325:MET:SD	1:A:416:VAL:HA	2.34	0.66
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.76	0.66
1:A:114:MET:HE2	1:A:457:TRP:HZ2	1.61	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:257:GLN:HE22	2:A:1499:FC1:H141	1.60	0.65
1:A:306:ASP:CB	1:A:308:GLN:HE22	2.09	0.65
1:A:478:VAL:C	1:A:479:LEU:HD23	2.17	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:326:GLU:HB2	1:A:334:GLN:CD	2.18	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:372:ILE:HA	1:A:376:ASP:OD2	1.97	0.64
1:A:218:PHE:CD2	1:A:313:PHE:CD1	2.86	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:HA	1:A:282:GLN:OE1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:O	1:A:197:ARG:HD3	1.98	0.63
1:A:291:PRO:C	1:A:293:TYR:H	2.00	0.63
1:A:204:GLN:HB2	1:A:237:ALA:HB2	1.81	0.63
1:A:402:SER:O	1:A:403:LEU:HB2	1.99	0.63
1:A:180:LEU:HD23	1:A:180:LEU:O	1.99	0.63
1:A:206:PHE:HB2	1:A:239:THR:HA	1.81	0.62
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: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:77:GLN:HE21	1:A:78:TYR:HB3	1.65	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:385:ILE:CG1	1:A:386:LEU:H	2.12	0.62
1:A:417:LEU:HD21	1:A:429:ASP:HB3	1.80	0.61
1:A:285:ILE:CG1	1:A:291:PRO:HG3	2.31	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:306:ASP:HB3	1:A:308:GLN:HE22	1.65	0.61
1:A:228:ALA:HB1	1:A:343:LEU:HD11	1.83	0.61
1:A:110:LEU:H	1:A:110:LEU:HD12	1.64	0.61
1:A:309:ASP:OD2	1:A:497:ASN:HB2	2.00	0.60
1:A:242:PRO:HG2	1:A:251:PHE:CE1	2.34	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:261:TYR:HD1	1:A:296:PHE:C	2.04	0.60
1:A:253:LEU:HG	1:A:347:ALA:HB1	1.82	0.60
1:A:304:GLN:O	1:A:304:GLN:HG3	2.00	0.60
1:A:382:ARG:HH11	1:A:382:ARG:HG3	1.66	0.60
1:A:81:ILE:HD11	1:A:90:LEU:HD12	1.82	0.60
1:A:126:LYS:O	1:A:127:PRO:O	2.20	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:333:PHE:CE2	1:A:415:ALA:CB	2.77	0.60
1:A:251:PHE:O	1:A:252:ARG:HG2	2.01	0.60
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.04	0.59
1:A:306:ASP:CA	1:A:308:GLN:HE22	2.14	0.59
1:A:188:TRP:CH2	1:A:200:TRP:HA	2.37	0.59
1:A:323:VAL:HG22	1:A:425:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:HB3	1:A:233:ASN:O	2.02	0.59
1:A:180:LEU:HD11	1:A:240:VAL:HG11	1.83	0.59
1:A:215:GLN:HG3	1:A:219:GLN:HE21	1.67	0.59
1:A:192:PRO:HA	1:A:452:PRO:O	2.03	0.59
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:266:MET:HG3	1:A:267:PRO:HD2	1.84	0.58
1:A:124:ARG:NH1	1:A:357:GLU:OE1	2.36	0.58
1:A:116:PRO:HB2	1:A:118:SER:OG	2.03	0.58
1:A:272:ARG:CZ	1:A:295:ARG:HD2	2.33	0.58
1:A:260:ARG:HE	1:A:277:THR:HG21	1.67	0.58
1:A:175:LEU:N	1:A:175:LEU:HD12	2.17	0.58
1:A:344:PRO:HD2	1:A:365:GLY:O	2.03	0.58
1:A:233:ASN:C	1:A:233:ASN:HD22	2.06	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:246:ASP:OD1	1:A:248:LYS:HB3	2.04	0.57
1:A:390:GLY:O	1:A:393:MET:HB3	2.03	0.57
1:A:297:ASP:OD1	1:A:297:ASP:N	2.37	0.57
1:A:420:PHE:CD2	1:A:427:ILE:HB	2.40	0.57
1:A:204:GLN:HG3	1:A:227:TYR:CZ	2.40	0.57
1:A:96:HIS:C	1:A:98:ALA:H	2.08	0.57
1:A:328:PRO:O	1:A:329:LYS:HD2	2.04	0.57
1:A:79:VAL:HG23	1:A:95:HIS:NE2	2.20	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: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: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: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:271:ILE:HD13	1:A:278:LEU:HD11	1.87	0.56
1:A:261:TYR:CE2	1:A:341:TYR:HD1	2.23	0.56
1:A:257:GLN:HG2	1:A:260:ARG:HG3	1.87	0.56
1:A:243:GLN:NE2	1:A:356:LEU:HD22	2.20	0.56
1:A:478:VAL:O	1:A:479:LEU:HD23	2.05	0.56
1:A:430:HIS:CD2	1:A:431:HIS:CD2	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:O	1:A:198:ILE:HG13	2.03	0.56
1:A:453:ALA:O	1:A:476:ASN:HB3	2.04	0.56
1:A:431:HIS:O	1:A:435:GLU:HG2	2.04	0.56
1:A:180:LEU:CD2	1:A:240:VAL:HG21	2.35	0.56
1:A:144:TYR:HE2	1:A:179:GLU:CG	2.16	0.56
1:A:80:ARG:HG3	1:A:91:HIS:HD2	1.71	0.56
1:A:330:TYR:HD2	1:A:332:TRP:CZ2	2.24	0.56
1:A:251:PHE:CD1	1:A:305:ALA:O	2.58	0.56
1:A:132:GLU:O	1:A:135:PRO:HD2	2.06	0.56
1:A:419:SER:O	1:A:422:LYS:HB3	2.06	0.56
1:A:204:GLN:NE2	1:A:206:PHE:HE1	2.04	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:330:TYR:HB3	1:A:332:TRP:CE2	2.41	0.56
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:93:THR:O	1:A:95:HIS:N	2.39	0.55
1:A:382:ARG:NH1	1:A:382:ARG:HG3	2.22	0.55
1:A:370:THR:O	1:A:374:VAL:HG13	2.07	0.55
1:A:261:TYR:CE2	1:A:341:TYR:CD1	2.95	0.55
1:A:308:GLN:N	1:A:308:GLN:CD	2.48	0.55
1:A:176:THR:O	1:A:179:GLU:N	2.37	0.55
1:A:189:ARG:HD3	1:A:444:GLU:OE2	2.07	0.55
1:A:386:LEU:CD1	1:A:409:VAL:HG23	2.37	0.55
1:A:203:LEU:HD11	1:A:238:ILE:HG22	1.89	0.55
1:A:285:ILE:HG13	1:A:291:PRO:HG3	1.89	0.54
1:A:379:ASP:HB3	1:A:381:GLN:NE2	2.22	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: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:161:GLU:HG3	1:A:162:ALA:N	2.22	0.54
1:A:153:ILE:HD12	1:A:153:ILE:H	1.73	0.54
1:A:120:THR:CG2	1:A:121:ARG:H	2.05	0.54
1:A:82:LYS:CB	1:A:89:ILE:HG23	2.38	0.54
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.21	0.54
1:A:120:THR:O	1:A:121:ARG:HD3	2.07	0.54
1:A:437:PHE:HD2	1:A:438:MET:HE3	1.72	0.53
1:A:134:LEU:HD23	1:A:167:ILE:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:N	1:A:268:ASP:OD2	2.40	0.53
1:A:395:LEU:HD13	1:A:395:LEU:H	1.72	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: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:496:GLN:HE21	1:A:496:GLN:C	2.12	0.53
1:A:233:ASN:ND2	1:A:233:ASN:C	2.61	0.53
1:A:330:TYR:HB3	1:A:332:TRP:HE1	1.69	0.53
1:A:480:SER:HA	1:A:481:PRO:O	2.09	0.53
1:A:165:LYS:O	1:A:169:THR:HG23	2.09	0.53
1:A:77:GLN:HE21	1:A:78:TYR:CB	2.22	0.53
1:A:253:LEU:H	1:A:253:LEU:CD2	2.21	0.53
1:A:252:ARG:NH1	1:A:486:GLN:HB3	2.24	0.53
1:A:86:SER:OG	1:A:88:GLU:HB2	2.09	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: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: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:268:ASP:C	1:A:270:THR:H	2.12	0.52
1:A:330:TYR:O	1:A:332:TRP:N	2.43	0.52
1:A:114:MET:CE	1:A:457:TRP:HZ2	2.21	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:221:ILE:O	1:A:224:HIS:HB3	2.10	0.52
1:A:294:GLY:C	1:A:295:ARG:HD3	2.30	0.51
1:A:217:MET:SD	1:A:241:PHE:CE2	3.03	0.51
1:A:173:TYR:C	1:A:174:GLN:HE21	2.14	0.51
1:A:95:HIS:O	1:A:98:ALA:HB2	2.09	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
1:A:404:TRP:CD2	1:A:405:LYS:HG2	2.45	0.51
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.92	0.51
1:A:187:ALA:HB2	1:A:481:PRO:HB2	1.91	0.51
1:A:386:LEU:HD11	1:A:409:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ALA:O	1:A:418:HIS:HB3	2.11	0.51
1:A:324:THR:H	1:A:423:GLN:HE22	1.58	0.51
1:A:249:HIS:CA	1:A:306:ASP:O	2.57	0.51
1:A:470:PHE:HD1	1:A:471:HIS:HD2	1.54	0.51
1:A:140:PHE:O	1:A:143:GLN:N	2.43	0.51
1:A:134:LEU:O	1:A:138:ILE:CG1	2.56	0.51
1:A:189:ARG:HE	1:A:444:GLU:CD	2.14	0.51
1:A:308:GLN:N	1:A:308:GLN:NE2	2.57	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:H	1.76	0.51
1:A:351:LEU:HD12	1:A:352:GLU:N	2.26	0.51
1:A:296:PHE:CE1	1:A:339:LYS:N	2.79	0.50
1:A:175:LEU:HA	1:A:179:GLU:OE1	2.10	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:84:TRP:O	1:A:85:GLY:C	2.50	0.50
1:A:377:PHE:O	1:A:384:ASN:N	2.44	0.50
1:A:218:PHE:HE1	1:A:222:CYS:SG	2.32	0.50
1:A:371:GLU:OE1	1:A:375:ARG:HG3	2.10	0.50
1:A:309:ASP:OD1	1:A:496:GLN:HG3	2.12	0.50
1:A:82:LYS:HD3	1:A:84:TRP:CZ3	2.46	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:372:ILE:HG22	1:A:416:VAL:HG21	1.94	0.50
1:A:316:PRO:CB	1:A:319:LEU:HD12	2.41	0.50
1:A:325:MET:HB2	1:A:338:LEU:HB3	1.94	0.50
1:A:306:ASP:H	1:A:308:GLN:CD	2.14	0.50
1:A:253:LEU:O	1:A:253:LEU:HD23	2.12	0.49
1:A:330:TYR:CD1	1:A:330:TYR:N	2.80	0.49
1:A:217:MET:O	1:A:220:HIS:HB2	2.12	0.49
1:A:165:LYS:O	1:A:169:THR:CG2	2.60	0.49
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.93	0.49
1:A:346:VAL:HG21	1:A:363:PHE:CZ	2.48	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:186:MET:HE3	1:A:189:ARG:HH11	1.76	0.49
1:A:322:GLU:CD	1:A:339:LYS:HE3	2.33	0.49
1:A:306:ASP:HB3	1:A:308:GLN:NE2	2.27	0.49
1:A:144:TYR:HE1	1:A:148:PHE:HZ	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:HG2	1:A:173:TYR:HB2	1.94	0.49
1:A:437:PHE:HE2	1:A:441:MET:CE	2.26	0.49
1:A:404:TRP:CZ2	1:A:405:LYS:HD3	2.47	0.49
1:A:144:TYR:C	1:A:146:GLY:H	2.16	0.49
1:A:138:ILE:O	1:A:142:ASN:ND2	2.41	0.49
1:A:221:ILE:HD13	1:A:301:LEU:HD22	1.93	0.48
1:A:352:GLU:O	1:A:481:PRO:HB3	2.12	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:276:ALA:HB2	1:A:382:ARG:CD	2.43	0.48
1:A:81:ILE:HG13	1:A:90:LEU:O	2.12	0.48
1:A:422:LYS:HG2	1:A:423:GLN:N	2.28	0.48
1:A:264:TYR:CD1	1:A:264:TYR:N	2.80	0.48
1:A:422:LYS:C	1:A:424:ASN:N	2.65	0.48
1:A:200:TRP:N	1:A:200:TRP:CD1	2.81	0.48
1:A:333:PHE:CE2	1:A:415:ALA:HB1	2.49	0.48
1:A:268:ASP:O	1:A:270:THR:N	2.47	0.48
1:A:399:THR:O	1:A:400:LEU:C	2.51	0.48
1:A:407:ARG:HG3	1:A:407:ARG:NH1	2.24	0.48
1:A:229:THR:HG22	1:A:231:ASN:N	2.29	0.48
1:A:371:GLU:HA	1:A:375:ARG:CG	2.43	0.48
1:A:92:ASP:OD2	1:A:95:HIS:HB3	2.13	0.48
1:A:418:HIS:O	1:A:419:SER:C	2.52	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: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:188:TRP:CH2	3:A:1500:HEM:HMC1	2.50	0.47
1:A:439:LYS:HA	1:A:442:GLN:HG3	1.97	0.47
1:A:129:PRO:O	1:A:132:GLU:N	2.46	0.47
1:A:330:TYR:HD2	1:A:332:TRP:HZ2	1.62	0.47
1:A:338:LEU:HG	1:A:377:PHE:CE1	2.49	0.47
1:A:391:ARG:C	1:A:393:MET:H	2.17	0.47
1:A:289:TRP:HB2	1:A:312:VAL:HG11	1.95	0.47
1:A:133:LEU:C	1:A:135:PRO:HD2	2.34	0.47
1:A:193:ARG:NH1	1:A:485:TYR:OH	2.47	0.47
1:A:144:TYR:C	1:A:144:TYR:CD1	2.89	0.47
1:A:494:ILE:HD12	1:A:494:ILE:O	2.15	0.47
1:A:393:MET:O	1:A:395:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:HE1	1:A:474:MET:HE2	1.97	0.47
1:A:265:GLN:HB3	1:A:278:LEU:HD21	1.96	0.47
1:A:395:LEU:CD1	1:A:395:LEU:H	2.29	0.46
1:A:306:ASP:C	1:A:308:GLN:HE22	2.19	0.46
1:A:189:ARG:HG3	1:A:200:TRP:CE3	2.50	0.46
1:A:462:VAL:O	1:A:463:SER:CB	2.63	0.46
1:A:206:PHE:HB2	1:A:239:THR:CB	2.45	0.46
1:A:350:LEU:HB2	1:A:486:GLN:CD	2.36	0.46
1:A:188:TRP:CZ3	1:A:200:TRP:CA	2.89	0.46
1:A:291:PRO:C	1:A:293:TYR:N	2.69	0.46
1:A:206:PHE:CD2	1:A:239:THR:HG22	2.50	0.46
1:A:176:THR:HG23	1:A:179:GLU:CD	2.36	0.46
1:A:258:LEU:HD22	1:A:345:ALA:HB1	1.97	0.46
1:A:176:THR:O	1:A:177:LEU:C	2.53	0.46
1:A:252:ARG:HH12	1:A:486:GLN:CB	2.28	0.46
1:A:181:ILE:HG13	1:A:205:VAL:HG21	1.96	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:296:PHE:HE2	1:A:383:TYR:CE2	2.34	0.46
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.97	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:457:TRP:HA	4:A:1501:HBI:N1	2.31	0.45
1:A:288:GLY:O	1:A:289:TRP:C	2.54	0.45
1:A:403:LEU:HD23	1:A:403:LEU:N	2.30	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
1:A:252:ARG:NH2	1:A:489:PRO:HG3	2.32	0.45
1:A:81:ILE:CD1	1:A:90:LEU:HD12	2.45	0.45
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.50	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:188:TRP:CZ2	3:A:1500:HEM:HMC1	2.51	0.45
1:A:144:TYR:C	1:A:146:GLY:N	2.70	0.45
1:A:173:TYR:C	1:A:174:GLN:NE2	2.70	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:217:MET:CE	1:A:303:LEU:HB3	2.47	0.45
1:A:186:MET:O	1:A:189:ARG:N	2.50	0.45
1:A:294:GLY:HA3	1:A:297:ASP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:ASN:OD1	1:A:280:PHE:CZ	2.69	0.45
1:A:157:LEU:O	1:A:160:LEU:HB2	2.16	0.45
1:A:295:ARG:HH11	1:A:295:ARG:H	1.65	0.45
1:A:195:ILE:HA	1:A:437:PHE:HD1	1.80	0.45
1:A:437:PHE:HE2	1:A:441:MET:HE2	1.82	0.45
1:A:275:ALA:HB1	1:A:278:LEU:HD12	1.98	0.45
1:A:303:LEU:O	1:A:310:PRO:HA	2.17	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: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:198:ILE:O	1:A:198:ILE:CG1	2.66	0.44
1:A:144:TYR:C	1:A:144:TYR:HD1	2.20	0.44
1:A:92:ASP:O	1:A:95:HIS:CD2	2.70	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:188:TRP:C	1:A:190:ASN:N	2.68	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:437:PHE:CZ	1:A:458:LEU:CD1	3.01	0.44
1:A:298:VAL:HG11	1:A:315:ILE:HD12	1.99	0.44
1:A:327:HIS:C	1:A:329:LYS:H	2.21	0.44
1:A:85:GLY:HA2	1:A:381:GLN:HB3	2.00	0.44
1:A:89:ILE:H	1:A:89:ILE:HD12	1.83	0.44
1:A:266:MET:SD	1:A:272:ARG:CG	3.04	0.44
1:A:388:GLU:C	1:A:390:GLY:N	2.69	0.44
1:A:454:ASP:OD1	1:A:454:ASP:C	2.56	0.44
1:A:395:LEU:N	1:A:395:LEU:CD1	2.81	0.44
1:A:417:LEU:HB3	1:A:421:GLN:HE22	1.83	0.44
1:A:206:PHE:HB2	1:A:239:THR:CA	2.47	0.44
1:A:163:VAL:C	1:A:167:ILE:HD12	2.39	0.44
1:A:283:LEU:O	1:A:286:ASP:N	2.51	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: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:213:THR:HB	1:A:216:GLU:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ILE:HG13	1:A:494:ILE:H	1.43	0.43
1:A:411:GLU:OE1	1:A:411:GLU:HA	2.18	0.43
1:A:218:PHE:CD1	1:A:218:PHE:C	2.90	0.43
1:A:144:TYR:O	1:A:146:GLY:N	2.51	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:340:TRP:CZ3	1:A:383:TYR:CE1	3.06	0.43
1:A:217:MET:CG	1:A:241:PHE:CE2	3.01	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:458:LEU:O	1:A:469:VAL:HG21	2.19	0.43
1:A:285:ILE:HD11	1:A:291:PRO:HG3	2.00	0.43
1:A:429:ASP:OD2	1:A:432:THR:OG1	2.37	0.43
1:A:217:MET:O	1:A:220:HIS:N	2.51	0.43
1:A:197:ARG:NH2	1:A:451:CYS:SG	2.91	0.43
1:A:159:ARG:O	1:A:162:ALA:HB3	2.19	0.43
1:A:385:ILE:HG13	1:A:386:LEU:N	2.18	0.43
1:A:451:CYS:O	1:A:453:ALA:N	2.51	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:131:GLU:O	1:A:135:PRO:HG3	2.19	0.43
1:A:78:TYR:O	1:A:79:VAL:C	2.57	0.43
1:A:245:SER:OG	1:A:246:ASP:N	2.43	0.42
1:A:430:HIS:O	1:A:431:HIS:C	2.56	0.42
1:A:114:MET:HE2	1:A:457:TRP:CZ2	2.48	0.42
1:A:306:ASP:CB	1:A:308:GLN:NE2	2.79	0.42
1:A:175:LEU:HD11	1:A:356:LEU:HD13	2.01	0.42
1:A:397:THR:CG2	1:A:397:THR:O	2.67	0.42
1:A:437:PHE:C	1:A:437:PHE:CD2	2.91	0.42
1:A:453:ALA:HB3	1:A:474:MET:HB2	2.00	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:407:ARG:CG	1:A:407:ARG:NH1	2.82	0.42
1:A:152:LYS:HD2	1:A:155:GLU:OE2	2.19	0.42
1:A:338:LEU:HD21	1:A:385:ILE:HG21	2.02	0.42
1:A:180:LEU:O	1:A:183:ALA:HB3	2.20	0.42
1:A:261:TYR:CD1	1:A:296:PHE:HA	2.55	0.42
1:A:420:PHE:O	1:A:421:GLN:C	2.58	0.42
1:A:348:ASN:O	1:A:349:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:VAL:O	1:A:378:CYS:HB2	2.20	0.42
1:A:200:TRP:CG	1:A:201:SER:N	2.88	0.42
1:A:140:PHE:CE2	1:A:353:VAL:CG2	3.02	0.42
1:A:175:LEU:H	1:A:175:LEU:CD1	2.24	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:419:SER:O	1:A:420:PHE:C	2.57	0.42
1:A:217:MET:HE1	1:A:304:GLN:N	2.35	0.42
1:A:370:THR:HG22	1:A:374:VAL:HG12	2.02	0.42
1:A:301:LEU:H	1:A:301:LEU:HD12	1.85	0.42
1:A:244:ARG:NH1	1:A:357:GLU:OE2	2.51	0.42
1:A:144:TYR:CE2	1:A:179:GLU:HA	2.55	0.42
1:A:112:SER:HA	1:A:456:ILE:HD12	2.02	0.42
1:A:324:THR:H	1:A:423:GLN:NE2	2.17	0.41
1:A:474:MET:HB3	1:A:474:MET:HE2	1.72	0.41
1:A:299:LEU:HD22	1:A:300:PRO:HD2	2.02	0.41
1:A:213:THR:HG1	1:A:216:GLU:HB2	1.85	0.41
1:A:383:TYR:O	1:A:384:ASN:HB3	2.21	0.41
1:A:257:GLN:OE1	1:A:260:ARG:NH1	2.44	0.41
1:A:217:MET:HE1	1:A:303:LEU:HB3	2.02	0.41
1:A:446:ARG:HG3	1:A:446:ARG:NH1	2.35	0.41
1:A:136:HIS:O	1:A:139:GLU:HB2	2.20	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:189:ARG:HG3	1:A:200:TRP:CD2	2.55	0.41
1:A:131:GLU:O	1:A:135:PRO:CD	2.68	0.41
1:A:215:GLN:O	1:A:219:GLN:CG	2.66	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:140:PHE:O	1:A:141:ILE:C	2.58	0.41
1:A:163:VAL:CG1	1:A:167:ILE:HD11	2.39	0.41
1:A:477:TYR:HD2	1:A:479:LEU:CD2	2.24	0.41
1:A:388:GLU:C	1:A:390:GLY:H	2.23	0.41
1:A:173:TYR:CE1	1:A:356:LEU:HG	2.55	0.41
1:A:268:ASP:C	1:A:270:THR:N	2.73	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: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:333:PHE:HA	1:A:336:LEU:HD23	2.03	0.41
1:A:206:PHE:HB2	1:A:239:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LEU:HA	1:A:299:LEU:HD23	1.76	0.41
1:A:78:TYR:CG	1:A:91:HIS:HB3	2.55	0.41
1:A:290:LYS:HA	1:A:291:PRO:HD3	1.58	0.41
1:A:213:THR:CB	1:A:216:GLU:HB2	2.49	0.41
1:A:415:ALA:O	1:A:416:VAL:C	2.58	0.41
1:A:221:ILE:CD1	1:A:303:LEU:HD21	2.50	0.41
1:A:441:MET:O	1:A:442:GLN:C	2.59	0.41
1:A:245:SER:OG	1:A:249:HIS:HB2	2.21	0.41
1:A:188:TRP:O	1:A:191:ALA:N	2.52	0.41
1:A:163:VAL:O	1:A:164:THR:C	2.58	0.41
1:A:114:MET:CE	1:A:457:TRP:CZ2	3.03	0.40
1:A:389:VAL:HG11	1:A:412:ILE:HG13	2.02	0.40
1:A:389:VAL:HG12	1:A:389:VAL:O	2.20	0.40
1:A:408:ALA:O	1:A:409:VAL:C	2.59	0.40
1:A:370:THR:HG23	1:A:430:HIS:CE1	2.55	0.40
1:A:330:TYR:CB	1:A:332:TRP:HE1	2.32	0.40
1:A:442:GLN:HG2	1:A:442:GLN:H	1.48	0.40
1:A:437:PHE:CE1	1:A:458:LEU:HD13	2.57	0.40
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:289:TRP:CG	1:A:300:PRO:HG3	2.56	0.40
1:A:215:GLN:HG3	1:A:219:GLN:NE2	2.36	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	3

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
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

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Mol	Chain	Res	Type
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 (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	362/370 (98%)	246 (68%)	116 (32%)	0	0

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	81	ILE
1	A	82	LYS
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	115	ASN
1	A	121	ARG
1	A	125	ASP

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Mol	Chain	Res	Type
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	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
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	205	VAL
1	A	213	THR
1	A	215	GLN
1	A	218	PHE
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	251	PHE
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	271	ILE

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Mol	Chain	Res	Type
1	A	272	ARG
1	A	281	THR
1	A	290	LYS
1	A	292	ARG
1	A	295	ARG
1	A	296	PHE
1	A	297	ASP
1	A	301	LEU
1	A	303	LEU
1	A	308	GLN
1	A	311	GLU
1	A	318	ASP
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	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	374	VAL
1	A	376	ASP
1	A	379	ASP
1	A	380	THR
1	A	381	GLN
1	A	387	GLU
1	A	392	ARG
1	A	395	LEU
1	A	396	GLU
1	A	397	THR
1	A	400	LEU
1	A	402	SER
1	A	403	LEU
1	A	406	ASP
1	A	411	GLU
1	A	413	ASN
1	A	417	LEU

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Mol	Chain	Res	Type
1	A	422	LYS
1	A	432	THR
1	A	438	MET
1	A	442	GLN
1	A	448	ARG
1	A	463	SER
1	A	465	SER
1	A	467	THR
1	A	473	GLU
1	A	474	MET
1	A	475	LEU
1	A	476	ASN
1	A	480	SER
1	A	487	ILE
1	A	494	ILE
1	A	496	GLN
1	A	498	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	95	HIS
1	A	96	HIS
1	A	174	GLN
1	A	215	GLN
1	A	219	GLN
1	A	231	ASN
1	A	233	ASN
1	A	243	GLN
1	A	381	GLN
1	A	398	HIS
1	A	423	GLN
1	A	430	HIS
1	A	431	HIS
1	A	471	HIS
1	A	476	ASN
1	A	486	GLN
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 carbohydrates 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	#$|Z| > 2$
2	FC1	A	1499	-	17,19,19	2.49	7 (41%)	19,25,25	1.85	4 (21%)
3	HEM	A	1500	1	30,50,50	2.66	7 (23%)	24,82,82	3.09	14 (58%)
4	HBI	A	1501	-	14,18,18	3.88	3 (21%)	9,26,26	2.46	5 (55%)

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	FC1	A	1499	-	-	0/7/7/7	0/1/2/2
3	HEM	A	1500	1	-	0/10/54/54	0/0/8/8
4	HBI	A	1501	-	-	0/4/17/17	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1500	HEM	C3B-C4B	-7.65	1.45	1.51
3	A	1500	HEM	C2D-C3D	-6.49	1.35	1.54
3	A	1500	HEM	C3D-C4D	-5.42	1.44	1.51
3	A	1500	HEM	C2C-C1C	-2.54	1.47	1.52
2	A	1499	FC1	C8-C3	2.21	1.42	1.40
2	A	1499	FC1	C12-C8	2.27	1.41	1.36
4	A	1501	HBI	C4-N3	2.30	1.37	1.33
2	A	1499	FC1	C9-C4	2.48	1.42	1.36
2	A	1499	FC1	C10-S7	2.55	1.77	1.73
4	A	1501	HBI	C4A-C8A	2.60	1.48	1.41
3	A	1500	HEM	C3C-CAC	2.74	1.56	1.51
2	A	1499	FC1	C2-C1	2.75	1.50	1.42
2	A	1499	FC1	C3-S7	3.25	1.77	1.72
3	A	1500	HEM	CBB-CAB	4.36	1.54	1.29
3	A	1500	HEM	CBC-CAC	4.41	1.54	1.29
2	A	1499	FC1	C5-C10	7.45	1.49	1.37
4	A	1501	HBI	C6-N5	13.69	1.46	1.28

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1500	HEM	C3B-CAB-CBB	-7.26	113.32	124.46
3	A	1500	HEM	C3C-CAC-CBC	-4.09	118.19	124.46
2	A	1499	FC1	C1-C3-S7	-3.33	116.85	120.77
2	A	1499	FC1	C4-C1-C2	-3.00	115.29	122.53
4	A	1501	HBI	N3-C2-N1	-2.98	120.64	125.53
3	A	1500	HEM	CBA-CAA-C2A	-2.93	107.28	112.53
3	A	1500	HEM	CAA-C2A-C1A	-2.72	124.06	127.01
3	A	1500	HEM	CMA-C3A-C4A	-2.63	124.02	128.36
3	A	1500	HEM	CBD-CAD-C3D	-2.24	107.03	113.55
4	A	1501	HBI	C4A-C4-N3	-2.21	120.57	123.59
3	A	1500	HEM	C3B-C4B-CHC	2.59	126.81	123.16
4	A	1501	HBI	C2-N1-C8A	2.82	120.88	114.54
3	A	1500	HEM	CMD-C2D-C3D	3.02	127.69	114.35
3	A	1500	HEM	C2D-C3D-C4D	3.27	107.05	101.50
2	A	1499	FC1	C10-C5-C2	3.42	125.57	119.09
3	A	1500	HEM	CAA-CBA-CGA	3.44	119.05	112.75
4	A	1501	HBI	C4-C4A-C8A	3.53	116.88	114.52
3	A	1500	HEM	CAD-C3D-C4D	3.89	126.19	112.47
4	A	1501	HBI	C4-N3-C2	3.96	121.44	115.94
3	A	1500	HEM	CMB-C2B-C3B	4.42	127.57	116.53
2	A	1499	FC1	C8-C3-S7	4.66	123.01	117.57
3	A	1500	HEM	CAD-C3D-C2D	4.71	126.75	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1500	HEM	CMC-C2C-C3C	5.52	130.32	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.