Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N6B
Title	:	Structure of endothelial nitric oxide synthase H373S single mutant heme domain complexed with 6,6'-(2,2'-(pyridine-3,5-diyl)bis(ethane-2,1-diyl))bis(4-methylpyridin-2-amine)
Authors	:	Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on	:	2010-05-25
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

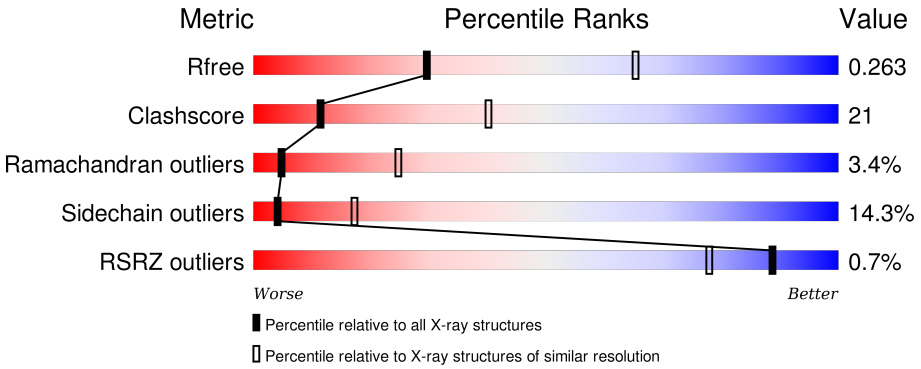
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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.

Mol	Chain	Length	Quality of chain
1	A	444	% 52% 33% 6% 9%
1	B	444	% 48% 33% 9% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	XFJ	A	800	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6600 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.

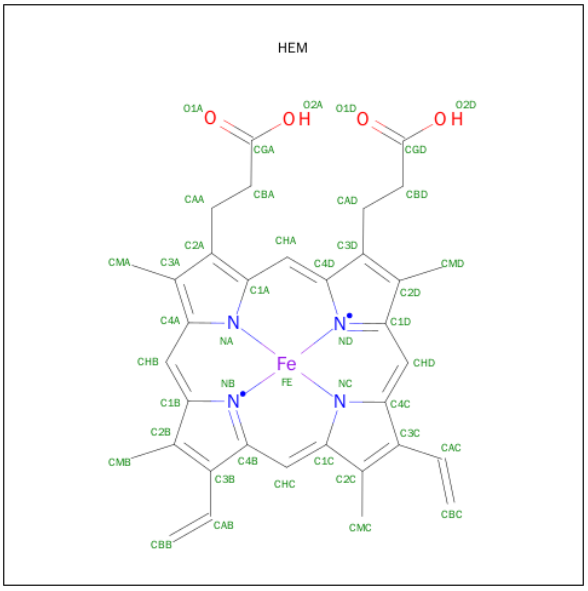
- Molecule 1 is a protein called Nitric oxide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3205	2038	562	589	16			
1	B	402	Total	C	N	O	S	0	1	0
			3206	2040	561	589	16			

There are 4 discrepancies between the modelled and reference sequences:

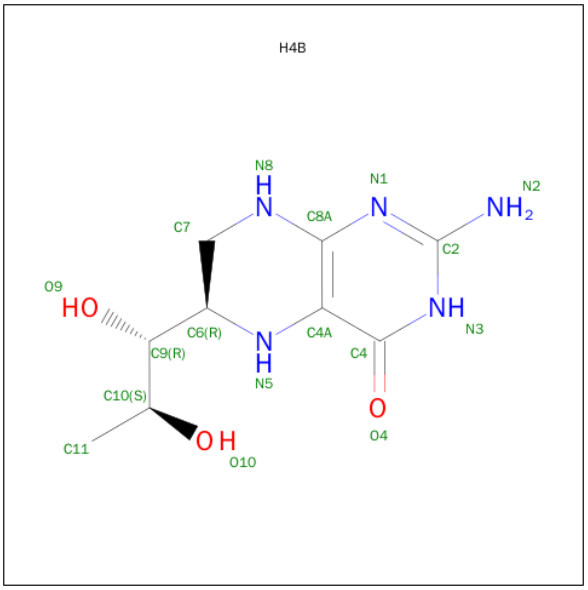
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29476
A	373	SER	HIS	ENGINEERED MUTATION	UNP P29476
B	100	ARG	CYS	SEE REMARK 999	UNP P29476
B	373	SER	HIS	ENGINEERED MUTATION	UNP P29476

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



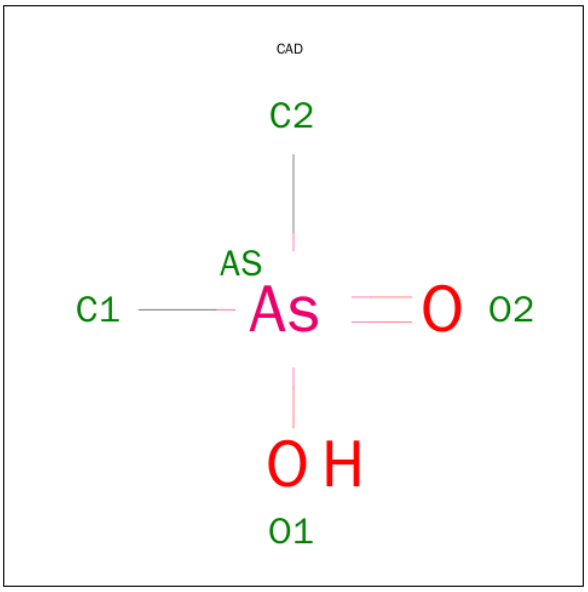
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



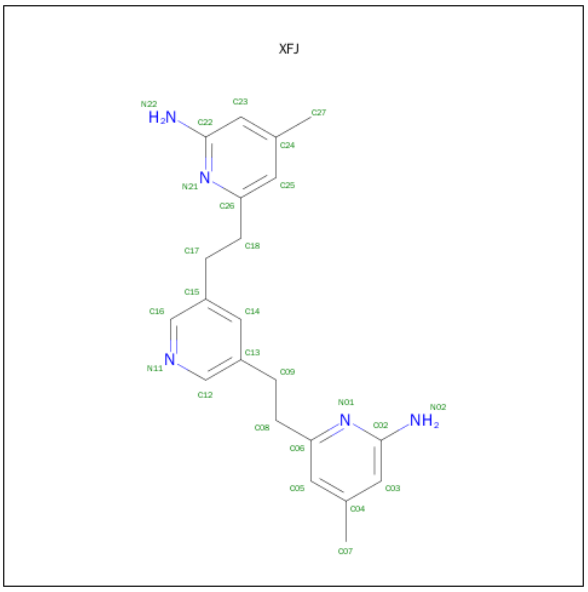
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total As C 3 1 2	0	0
4	B	1	Total As C 3 1 2	0	0

- Molecule 5 is 6,6'-(PYRIDINE-3,5-DIYLDIETHANE-2,1-DIYL)BIS(4-METHYLPYRIDIN-2-AMINE) (three-letter code: XFJ) (formula: $C_{21}H_{25}N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 26 21 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N 26 21 5	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

- Molecule 7 is water.

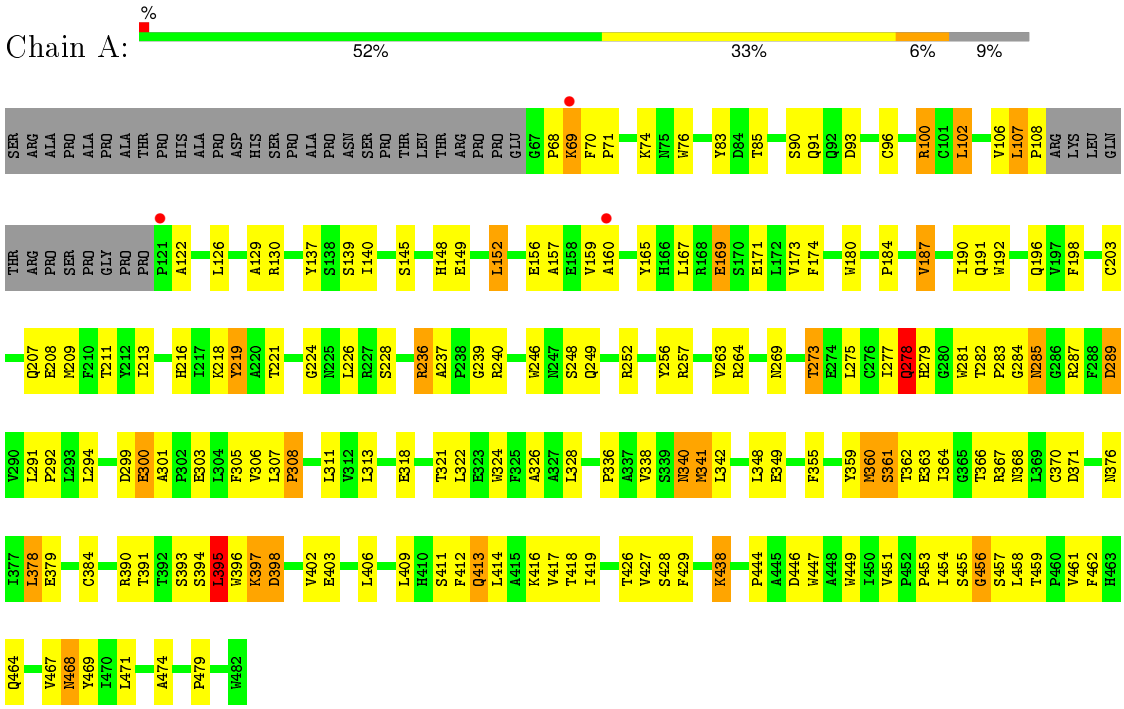
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total O 5 5	0	0
7	B	5	Total O 5 5	0	0

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.

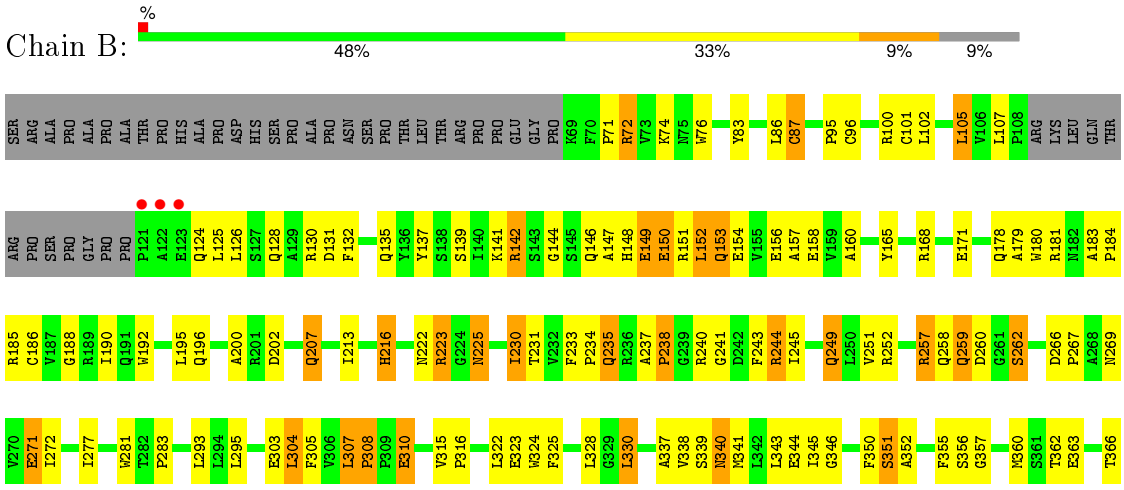
- Molecule 1: Nitric oxide synthase

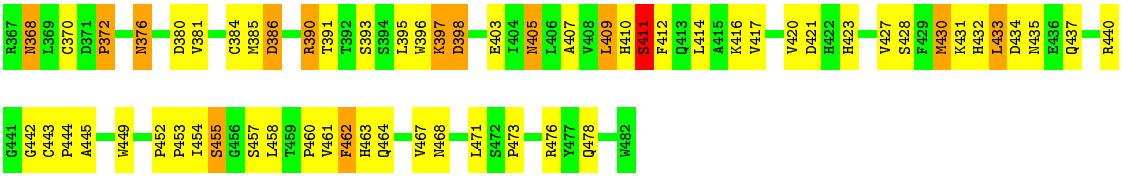
Chain A:



- Molecule 1: Nitric oxide synthase

Chain B:




R367
N368
L369
C370
D371
P372
N376
D380
V381
C384
M385
D386
R390
T391
T392
S393
S394
L395
W396
K397
D398
E403
I404
N405
L406
A407
V408
L409
H410
S411
F412
Q413
L414
A415
K416
V417
V420
D421
H422
H423
V427
S428
F429
M430
K431
H432
L433
D434
N435
E436
Q437
R440
G441
G442
C443
P444
A445
W449
P452
P453
I454
S455
G456
S457
L458
T459
P460
V461
F462
H463
Q464
V467
N468
L471
S472
P473
R476
Y477
Q478
W482

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.76Å 106.55Å 157.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 3.10 39.46 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.46-3.10) 99.1 (39.46-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.187 , 0.274 0.185 , 0.263	Depositor DCC
R_{free} test set	894 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 18280 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6600	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, ZN, XFJ, H4B, CAD

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	0.75	0/3294	0.82	1/4487 (0.0%)
1	B	0.73	0/3295	0.85	0/4488
All	All	0.74	0/6589	0.83	1/8975 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	395	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	ALA	Peptide

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	3205	0	3113	120	0
1	B	3206	0	3112	145	0
2	A	43	0	30	7	0
2	B	43	0	30	9	0
3	A	17	0	15	3	0
3	B	17	0	15	1	0
4	A	3	0	0	1	0
4	B	3	0	0	2	0
5	A	26	0	25	1	0
5	B	26	0	25	4	0
6	A	1	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
All	All	6600	0	6365	266	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 21.

All (266) 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:384:CYS:SG	4:A:950:CAD:AS	2.73	1.06
1:B:244:ARG:HG3	1:B:244:ARG:HH11	1.20	1.02
1:B:260:ASP:OD1	1:B:262:SER:HB2	1.63	0.99
1:B:409:LEU:HD11	1:B:421:ASP:HB3	1.47	0.95
1:A:236:ARG:HH11	1:A:236:ARG:HB2	1.29	0.94
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.36	0.90
1:B:244:ARG:NH1	1:B:244:ARG:HG3	1.83	0.88
1:B:384:CYS:SG	4:B:950:CAD:AS	2.94	0.86
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.62	0.82
1:B:328:LEU:HB3	1:B:330:LEU:HD23	1.59	0.82
1:B:152:LEU:O	1:B:156:GLU:HG2	1.77	0.82
1:B:328:LEU:HB3	1:B:330:LEU:CD2	2.10	0.82
1:B:431:LYS:HE3	1:B:435:ASN:OD1	1.82	0.80
1:B:244:ARG:CG	1:B:244:ARG:HH11	1.95	0.79
1:B:344:GLU:HG3	1:B:476:ARG:HH21	1.46	0.78
1:B:158:GLU:OE2	1:B:165:TYR:HA	1.83	0.77
1:A:196:GLN:HG2	1:A:219:TYR:OH	1.87	0.75
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.50	0.74
2:B:500:HEM:O1A	3:B:600:H4B:N3	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:THR:HA	1:B:405:ASN:HD21	1.54	0.73
1:A:203:CYS:HA	1:A:208:GLU:OE2	1.89	0.72
1:A:236:ARG:NH1	1:A:236:ARG:HB2	2.03	0.72
1:B:230:ILE:HD12	1:B:355:PHE:HB3	1.71	0.70
1:B:260:ASP:OD1	1:B:262:SER:CB	2.37	0.70
1:A:338:VAL:CG1	1:A:341:MET:HG3	2.21	0.69
1:A:96:CYS:HB3	1:B:96:CYS:HB3	1.73	0.69
1:A:398:ASP:OD1	1:A:398:ASP:N	2.19	0.69
1:A:303:GLU:HB2	1:A:305:PHE:CE1	2.28	0.69
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.76	0.68
1:B:150:GLU:O	1:B:153:GLN:HB2	1.94	0.68
1:A:273:THR:HG23	1:A:291:LEU:HD21	1.74	0.68
1:A:196:GLN:HG2	1:A:219:TYR:CZ	2.30	0.67
1:B:251:VAL:O	1:B:252:ARG:HG2	1.92	0.67
1:B:409:LEU:HD11	1:B:421:ASP:CB	2.22	0.67
1:B:156:GLU:O	1:B:160:ALA:HB2	1.95	0.66
1:A:322:LEU:HD13	1:A:324:TRP:CZ2	2.29	0.66
1:A:446:ASP:HB3	1:A:449:TRP:HB2	1.77	0.66
1:B:437:GLN:HA	1:B:442:GLY:H	1.61	0.65
1:A:277:ILE:HG12	1:A:283:PRO:HD3	1.78	0.65
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.79	0.65
1:B:233:PHE:HB3	1:B:234:PRO:HD2	1.79	0.65
1:A:218:LYS:HG2	1:A:311:LEU:HD11	1.78	0.65
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.32	0.65
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.78	0.64
1:A:409:LEU:O	1:A:413:GLN:HB2	1.97	0.64
1:A:207:GLN:HE21	1:A:211:THR:HG23	1.63	0.64
1:A:364:ILE:HA	1:A:368:ASN:HD22	1.63	0.64
1:A:213:ILE:O	1:A:216:HIS:HB3	1.97	0.63
1:B:186:CYS:HB2	2:B:500:HEM:ND	2.13	0.63
1:A:338:VAL:HG11	1:A:341:MET:HG3	1.80	0.63
1:B:337:ALA:CB	1:B:356:SER:HB3	2.29	0.63
1:A:426:THR:O	1:A:427:VAL:C	2.38	0.62
1:A:203:CYS:SG	1:A:208:GLU:HB3	2.40	0.61
1:A:303:GLU:HB2	1:A:305:PHE:HE1	1.62	0.61
1:B:340:ASN:HD22	1:B:340:ASN:H	1.47	0.61
1:B:396:TRP:CE2	1:B:397:LYS:HD2	2.35	0.61
1:A:370:CYS:SG	1:A:378:LEU:HD12	2.40	0.60
1:B:131:ASP:O	1:B:135:GLN:HG3	2.00	0.60
1:B:180:TRP:CZ3	1:B:192:TRP:HA	2.36	0.60
1:A:226:LEU:HD12	1:A:418:THR:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:THR:HG21	1:B:453:PRO:HB2	1.84	0.60
1:A:318:GLU:HG2	1:A:326:ALA:HB2	1.83	0.60
1:B:207:GLN:NE2	1:B:305:PHE:HE1	2.00	0.60
1:B:72:ARG:HH11	1:B:72:ARG:HB3	1.66	0.59
1:B:281:TRP:O	1:B:283:PRO:HD3	2.02	0.59
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.13	0.59
1:A:367:ARG:NE	1:A:371:ASP:OD2	2.36	0.59
1:B:407:ALA:O	1:B:411:SER:OG	2.21	0.58
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.67	0.58
2:A:500:HEM:O1A	3:A:600:H4B:N2	2.36	0.58
1:B:237:ALA:HB3	1:B:240:ARG:HG3	1.86	0.58
1:B:423:HIS:O	1:B:427:VAL:HG23	2.03	0.58
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.38	0.58
1:B:251:VAL:C	1:B:252:ARG:HG2	2.24	0.57
1:A:371:ASP:OD1	1:B:463:HIS:CE1	2.57	0.57
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.08	0.56
1:A:139:SER:HB3	1:A:174:PHE:CE1	2.40	0.56
1:B:216:HIS:HB2	1:B:231:THR:OG1	2.06	0.56
1:A:453:PRO:HB2	1:B:457:SER:HB3	1.87	0.55
1:A:252:ARG:HB3	1:A:269:ASN:ND2	2.22	0.55
1:A:221:THR:O	1:A:226:LEU:HD23	2.05	0.55
1:A:360:MET:O	1:A:362:THR:N	2.40	0.55
1:B:396:TRP:CZ2	1:B:397:LYS:HD2	2.43	0.54
1:B:444:PRO:HG3	1:B:471:LEU:HD12	1.89	0.54
1:B:412:PHE:HD2	1:B:417:VAL:CG1	2.20	0.54
1:A:236:ARG:CB	1:A:236:ARG:HH11	2.11	0.54
1:A:74:LYS:HD3	1:A:76:TRP:CE2	2.42	0.54
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.89	0.54
1:B:223:ARG:HH11	1:B:223:ARG:CG	2.21	0.54
1:A:360:MET:O	1:A:361:SER:C	2.46	0.53
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.20	0.53
2:A:500:HEM:O1A	3:A:600:H4B:N3	2.40	0.53
1:A:269:ASN:O	1:A:273:THR:OG1	2.25	0.53
1:A:378:LEU:HD21	1:A:397:LYS:HB3	1.91	0.53
1:B:381:VAL:O	1:B:381:VAL:HG12	2.08	0.53
1:B:126:LEU:O	1:B:130:ARG:HB2	2.09	0.53
1:B:363:GLU:OE1	5:B:800:XFJ:N01	2.43	0.52
1:B:428:SER:O	1:B:431:LYS:HB3	2.09	0.52
1:B:293:LEU:HB3	1:B:295:LEU:HD21	1.91	0.52
1:B:303:GLU:HB2	1:B:305:PHE:HE2	1.74	0.52
1:B:328:LEU:HB3	1:B:330:LEU:HD21	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:GLY:HA2	1:B:148:HIS:ND1	2.25	0.52
1:A:159:VAL:HG23	1:A:165:TYR:HB3	1.90	0.52
1:B:281:TRP:HB2	1:B:304:LEU:CD1	2.40	0.52
1:B:343:LEU:HB3	1:B:350:PHE:HB2	1.92	0.52
1:B:384:CYS:SG	4:B:950:CAD:C2	2.99	0.51
1:B:153:GLN:O	1:B:156:GLU:HB2	2.10	0.51
1:A:308:PRO:HB2	1:A:311:LEU:HB2	1.92	0.51
1:B:445:ALA:O	1:B:468:ASN:HB2	2.11	0.51
1:A:156:GLU:O	1:A:157:ALA:C	2.49	0.51
1:A:145:SER:O	1:A:149:GLU:HG2	2.11	0.50
1:B:179:ALA:HA	1:B:473:PRO:O	2.11	0.50
2:A:500:HEM:C1C	5:A:800:XFJ:H07B	2.46	0.50
1:B:225:ASN:HD22	1:B:225:ASN:C	2.15	0.50
1:A:224:GLY:O	1:A:417:VAL:HA	2.12	0.50
1:B:223:ARG:HH11	1:B:223:ARG:HG2	1.77	0.50
1:B:372:PRO:HA	1:B:376:ASN:CG	2.32	0.50
1:B:360:MET:HA	1:B:420:VAL:O	2.12	0.50
1:A:100:ARG:HH12	1:A:102:LEU:HD22	1.76	0.50
2:B:500:HEM:HBB2	2:B:500:HEM:CHC	2.30	0.49
1:A:137:TYR:HA	1:A:140:ILE:HG12	1.94	0.49
1:B:240:ARG:NH1	1:B:241:GLY:O	2.45	0.49
1:A:393:SER:HB2	1:B:409:LEU:HD22	1.95	0.49
1:B:357:GLY:H	5:B:800:XFJ:H07A	1.77	0.49
1:B:192:TRP:CD1	1:B:432:HIS:HE1	2.30	0.49
1:B:181:ARG:CZ	1:B:440:ARG:HD3	2.43	0.49
1:A:281:TRP:CG	1:A:292:PRO:HG3	2.48	0.49
1:B:237:ALA:HA	1:B:238:PRO:HD2	1.60	0.48
1:B:216:HIS:C	1:B:216:HIS:CD2	2.86	0.48
1:A:96:CYS:CB	1:B:96:CYS:HB3	2.41	0.48
1:A:355:PHE:CD1	2:A:500:HEM:CAC	2.95	0.48
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.48	0.48
1:B:230:ILE:O	1:B:230:ILE:HG23	2.14	0.48
2:A:500:HEM:HBC2	2:A:500:HEM:CMC	2.43	0.48
1:A:165:TYR:CE2	1:A:348:LEU:HD11	2.48	0.48
1:A:366:THR:O	1:A:370:CYS:HB2	2.14	0.48
1:A:96:CYS:HB3	1:B:96:CYS:CB	2.44	0.48
1:A:277:ILE:C	1:A:279:HIS:H	2.17	0.48
1:A:299:ASP:O	1:A:300:GLU:C	2.52	0.48
1:A:403:GLU:HA	1:A:403:GLU:OE1	2.13	0.48
1:B:310:GLU:H	1:B:310:GLU:CD	2.17	0.48
1:A:156:GLU:O	1:A:160:ALA:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASN:HB3	1:B:225:ASN:O	2.13	0.48
1:A:457:SER:HA	1:A:462:PHE:CG	2.49	0.48
1:B:455:SER:O	1:B:458:LEU:HB2	2.14	0.47
1:B:281:TRP:HB2	1:B:304:LEU:HD11	1.96	0.47
1:A:371:ASP:OD1	1:B:463:HIS:HE1	1.97	0.47
1:B:460:PRO:O	1:B:461:VAL:C	2.52	0.47
1:B:149:GLU:O	1:B:153:GLN:NE2	2.48	0.47
1:B:125:LEU:HA	1:B:128:GLN:OE1	2.14	0.47
1:B:243:PHE:O	1:B:351:SER:HB2	2.14	0.47
1:B:260:ASP:C	1:B:262:SER:H	2.18	0.47
1:A:396:TRP:CH2	1:A:397:LYS:HD3	2.49	0.47
1:B:196:GLN:NE2	1:B:196:GLN:HA	2.29	0.47
1:B:102:LEU:HB3	1:B:105:LEU:HG	1.97	0.47
1:B:366:THR:O	1:B:370:CYS:HB2	2.14	0.47
1:A:68:PRO:HG2	1:A:83:TYR:CE1	2.49	0.47
1:B:395:LEU:HD22	1:B:398:ASP:OD2	2.15	0.46
1:A:289:ASP:OD1	1:A:289:ASP:N	2.48	0.46
1:A:257:ARG:NH1	1:A:257:ARG:CG	2.78	0.46
1:A:456:GLY:O	1:A:459:THR:OG1	2.33	0.46
1:A:256:TYR:CZ	1:A:284:GLY:O	2.68	0.46
1:A:190:ILE:HG23	1:A:191:GLN:HG2	1.98	0.46
1:A:100:ARG:N	1:A:100:ARG:HD3	2.30	0.46
1:B:168:ARG:HB2	1:B:171:GLU:OE2	2.16	0.46
1:B:137:TYR:HB3	1:B:142:ARG:O	2.16	0.46
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.51	0.46
1:B:185:ARG:HD3	1:B:449:TRP:CE3	2.50	0.46
1:B:216:HIS:HB2	1:B:231:THR:HG1	1.79	0.46
1:A:438:LYS:CA	1:A:438:LYS:HE3	2.46	0.46
1:B:181:ARG:NH2	1:B:440:ARG:HD3	2.31	0.46
1:A:96:CYS:SG	1:B:101:CYS:HB2	2.56	0.45
1:B:186:CYS:HB2	2:B:500:HEM:C4D	2.51	0.45
1:B:328:LEU:CB	1:B:330:LEU:HD23	2.41	0.45
1:B:235:GLN:O	1:B:235:GLN:HG2	2.15	0.45
1:B:457:SER:HA	1:B:462:PHE:CG	2.51	0.45
1:B:416:LYS:HA	1:B:416:LYS:HD3	1.77	0.45
1:A:273:THR:HG23	1:A:291:LEU:CD2	2.43	0.45
1:A:70:PHE:HB3	1:A:71:PRO:CD	2.46	0.45
1:A:148:HIS:CD2	1:A:152:LEU:HD13	2.51	0.45
1:A:165:TYR:HE2	1:A:167:LEU:HD23	1.81	0.45
1:B:315:VAL:HG12	1:B:316:PRO:O	2.17	0.45
1:B:444:PRO:HA	1:B:467:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:HD2	1:A:69:LYS:N	2.32	0.45
1:B:267:PRO:C	1:B:269:ASN:H	2.19	0.45
1:A:467:VAL:HG12	1:A:469:TYR:HD1	1.82	0.45
1:A:184:PRO:HB2	1:A:468:ASN:HD21	1.82	0.45
1:A:169:GLU:O	1:A:173:VAL:HG23	2.17	0.45
1:B:384:CYS:C	1:B:386:ASP:H	2.21	0.44
1:A:209:MET:HE2	1:A:209:MET:HB3	1.89	0.44
1:A:198:PHE:HZ	1:A:219:TYR:CD1	2.35	0.44
1:A:180:TRP:CZ3	1:A:192:TRP:HA	2.52	0.44
1:A:467:VAL:HG12	1:A:469:TYR:CD1	2.52	0.44
1:B:430:MET:HE3	1:B:464:GLN:HB2	1.99	0.44
1:A:444:PRO:HA	1:A:467:VAL:O	2.17	0.44
1:A:471:LEU:O	1:A:474:ALA:HB2	2.18	0.44
1:B:433:LEU:O	1:B:434:ASP:C	2.55	0.44
1:B:363:GLU:O	1:B:368:ASN:HB2	2.17	0.44
1:A:394:SER:O	1:A:395:LEU:HB2	2.18	0.44
1:A:252:ARG:HB3	1:A:269:ASN:HD21	1.83	0.44
1:A:277:ILE:C	1:A:279:HIS:N	2.72	0.44
2:B:500:HEM:O2D	5:B:800:XFJ:H18A	2.18	0.44
1:A:139:SER:HB3	1:A:174:PHE:HE1	1.82	0.44
1:B:157:ALA:O	1:B:160:ALA:HB3	2.18	0.43
1:B:455:SER:HB3	1:B:458:LEU:CD2	2.48	0.43
1:A:275:LEU:HA	1:A:278:GLN:HE21	1.82	0.43
1:A:148:HIS:HD2	1:A:152:LEU:HD13	1.83	0.43
1:A:285:ASN:HA	1:A:285:ASN:HD22	1.64	0.43
1:B:178:GLN:HB3	1:B:473:PRO:HG2	2.01	0.43
1:A:236:ARG:HG2	1:A:237:ALA:N	2.33	0.43
1:A:219:TYR:C	1:A:219:TYR:CD2	2.92	0.43
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.54	0.43
1:B:71:PRO:O	1:B:83:TYR:HA	2.19	0.43
1:B:233:PHE:HB2	1:B:352:ALA:HB3	2.01	0.43
2:A:500:HEM:CGA	3:A:600:H4B:HN3	2.31	0.43
1:B:412:PHE:CD2	1:B:417:VAL:CG1	3.02	0.43
1:A:412:PHE:CG	1:A:419:ILE:HD12	2.54	0.43
1:A:203:CYS:HA	1:A:208:GLU:CD	2.39	0.42
1:B:325:PHE:O	1:B:328:LEU:HB2	2.18	0.42
1:B:457:SER:HA	1:B:462:PHE:CD1	2.54	0.42
1:A:455:SER:O	1:A:456:GLY:C	2.57	0.42
1:B:185:ARG:HD3	1:B:449:TRP:CD2	2.53	0.42
1:A:190:ILE:HD13	1:A:428:SER:O	2.20	0.42
1:B:86:LEU:O	1:B:87:CYS:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.54	0.42
1:B:195:LEU:HG	1:B:196:GLN:N	2.33	0.42
1:B:340:ASN:H	1:B:340:ASN:ND2	2.16	0.42
1:B:223:ARG:HH11	1:B:223:ARG:CB	2.33	0.42
1:B:390:ARG:HB3	1:B:390:ARG:HH11	1.84	0.42
1:B:188:GLY:HA3	2:B:500:HEM:C2B	2.55	0.42
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.49	0.42
1:B:223:ARG:NH1	1:B:223:ARG:HG2	2.35	0.42
1:B:74:LYS:HE2	1:B:76:TRP:CD2	2.55	0.42
1:A:398:ASP:O	1:A:402:VAL:HG23	2.20	0.41
1:B:430:MET:CE	1:B:464:GLN:HB2	2.50	0.41
1:A:137:TYR:CD1	1:A:140:ILE:HD11	2.54	0.41
1:A:187:VAL:HG22	1:A:429:PHE:HB2	2.01	0.41
1:B:245:ILE:HG21	1:B:339:SER:HB2	2.02	0.41
1:B:343:LEU:HD21	1:B:345:ILE:HD11	2.01	0.41
1:B:341:MET:C	1:B:478:GLN:HE21	2.24	0.41
1:A:248:SER:HA	1:A:340:ASN:HB3	2.02	0.41
1:A:461:VAL:O	1:A:464:GLN:HB3	2.20	0.41
1:B:266:ASP:HA	1:B:267:PRO:HD3	1.92	0.41
1:B:186:CYS:HB2	2:B:500:HEM:C1D	2.56	0.41
1:B:183:ALA:HA	1:B:184:PRO:HD3	1.81	0.41
2:B:500:HEM:C1C	5:B:800:XFJ:H07B	2.56	0.41
1:B:249:GLN:HB2	1:B:252:ARG:HD2	2.03	0.41
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.79	0.41
1:B:168:ARG:NH1	1:B:168:ARG:HG2	2.35	0.41
1:B:178:GLN:HE22	1:B:181:ARG:HH11	1.67	0.41
1:B:449:TRP:CD1	1:B:449:TRP:N	2.89	0.41
1:B:147:ALA:C	1:B:149:GLU:N	2.72	0.41
1:A:447:TRP:O	1:A:449:TRP:N	2.54	0.41
1:A:378:LEU:CD2	1:A:397:LYS:HB3	2.49	0.41
1:A:455:SER:HA	1:B:454:ILE:HG22	2.03	0.41
1:B:307:LEU:HD23	1:B:308:PRO:HD2	2.01	0.41
1:B:452:PRO:HA	1:B:453:PRO:HD2	1.60	0.41
1:A:342:LEU:HD11	1:A:349:GLU:HB3	2.02	0.41
1:A:307:LEU:HA	1:A:308:PRO:HD2	1.67	0.40
1:A:129:ALA:O	1:A:130:ARG:C	2.60	0.40
1:A:106:VAL:HG13	1:A:449:TRP:HZ2	1.87	0.40
1:B:403:GLU:OE1	1:B:403:GLU:HA	2.21	0.40
1:B:200:ALA:C	1:B:202:ASP:H	2.24	0.40
1:A:367:ARG:NH2	1:A:371:ASP:OD2	2.54	0.40
1:B:151:ARG:HD2	1:B:154:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PHE:HB2	1:B:346:GLY:HA2	2.02	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	400/444 (90%)	339 (85%)	51 (13%)	10 (2%)	7 32
1	B	399/444 (90%)	319 (80%)	63 (16%)	17 (4%)	3 19
All	All	799/888 (90%)	658 (82%)	114 (14%)	27 (3%)	5 25

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	257	ARG
1	A	90	SER
1	A	122	ALA
1	A	239	GLY
1	A	361	SER
1	B	142	ARG
1	B	258	GLN
1	B	259	GLN
1	A	278	GLN
1	A	363	GLU
1	A	456	GLY
1	A	479	PRO
1	B	190	ILE
1	B	380	ASP
1	B	385	MET
1	A	308	PRO
1	B	368	ASN

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Mol	Chain	Res	Type
1	B	410	HIS
1	B	411	SER
1	B	433	LEU
1	A	240	ARG
1	B	238	PRO
1	B	271	GLU
1	B	462	PHE
1	B	230	ILE
1	B	308	PRO
1	B	95	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	343/377 (91%)	295 (86%)	48 (14%)	4 18
1	B	343/377 (91%)	293 (85%)	50 (15%)	4 16
All	All	686/754 (91%)	588 (86%)	98 (14%)	4 17

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	85	THR
1	A	91	GLN
1	A	93	ASP
1	A	100	ARG
1	A	102	LEU
1	A	107	LEU
1	A	126	LEU
1	A	152	LEU
1	A	169	GLU
1	A	171	GLU
1	A	187	VAL
1	A	219	TYR

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Mol	Chain	Res	Type
1	A	228	SER
1	A	236	ARG
1	A	263	VAL
1	A	264	ARG
1	A	273	THR
1	A	278	GLN
1	A	282	THR
1	A	285	ASN
1	A	287	ARG
1	A	289	ASP
1	A	300	GLU
1	A	306	VAL
1	A	313	LEU
1	A	321	THR
1	A	328	LEU
1	A	340	ASN
1	A	341	MET
1	A	360	MET
1	A	376	ASN
1	A	378	LEU
1	A	379	GLU
1	A	390	ARG
1	A	391	THR
1	A	395	LEU
1	A	397	LYS
1	A	398	ASP
1	A	406	LEU
1	A	411	SER
1	A	413	GLN
1	A	414	LEU
1	A	416	LYS
1	A	438	LYS
1	A	454	ILE
1	A	458	LEU
1	A	468	ASN
1	B	72	ARG
1	B	87	CYS
1	B	100	ARG
1	B	105	LEU
1	B	107	LEU
1	B	124	GLN
1	B	139	SER

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Mol	Chain	Res	Type
1	B	141	LYS
1	B	146	GLN
1	B	149	GLU
1	B	150	GLU
1	B	152	LEU
1	B	153	GLN
1	B	207	GLN
1	B	213	ILE
1	B	216	HIS
1	B	223	ARG
1	B	225	ASN
1	B	235	GLN
1	B	244	ARG
1	B	249	GLN
1	B	257	ARG
1	B	259	GLN
1	B	262	SER
1	B	271	GLU
1	B	272	ILE
1	B	277	ILE
1	B	304	LEU
1	B	307	LEU
1	B	310	GLU
1	B	323	GLU
1	B	330	LEU
1	B	338	VAL
1	B	340	ASN
1	B	351	SER
1	B	372	PRO
1	B	376	ASN
1	B	386	ASP
1	B	390	ARG
1	B	391	THR
1	B	393	SER
1	B	397	LYS
1	B	398	ASP
1	B	405	ASN
1	B	409	LEU
1	B	411	SER
1	B	414	LEU
1	B	430	MET
1	B	443	CYS

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Mol	Chain	Res	Type
1	B	455	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	146	GLN
1	A	191	GLN
1	A	207	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	463	HIS
1	A	468	ASN
1	B	124	GLN
1	B	134	ASN
1	B	146	GLN
1	B	153	GLN
1	B	166	HIS
1	B	178	GLN
1	B	191	GLN
1	B	196	GLN
1	B	207	GLN
1	B	225	ASN
1	B	259	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	432	HIS
1	B	463	HIS
1	B	478	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)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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	A	500	1	30,50,50	2.49	7 (23%)	24,82,82	2.61	11 (45%)
3	H4B	A	600	-	13,18,18	0.68	0	11,26,26	2.25	4 (36%)
5	XFJ	A	800	-	28,28,28	0.55	0	38,38,38	1.98	13 (34%)
4	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	-	30,50,50	2.00	6 (20%)	24,82,82	2.67	12 (50%)
3	H4B	B	600	-	13,18,18	1.31	2 (15%)	11,26,26	3.10	6 (54%)
5	XFJ	B	800	-	28,28,28	0.78	0	38,38,38	1.69	7 (18%)
4	CAD	B	950	-	0,2,4	0.00	-	0,1,6	0.00	-

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	A	500	1	-	0/10/54/54	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
5	XFJ	A	800	-	-	0/10/10/10	0/3/3/3
4	CAD	A	950	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	-	-	0/10/54/54	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
5	XFJ	B	800	-	-	0/10/10/10	0/3/3/3
4	CAD	B	950	-	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3B-C4B	-9.38	1.43	1.51
2	B	500	HEM	C3B-C4B	-7.91	1.44	1.51
2	A	500	HEM	C3D-C4D	-5.50	1.44	1.51
2	A	500	HEM	C2C-C1C	-3.38	1.46	1.52
2	B	500	HEM	C2C-C1C	-2.89	1.47	1.52
2	B	500	HEM	C3D-C4D	-2.71	1.48	1.51
2	B	500	HEM	C2B-C1B	-2.63	1.43	1.51
2	A	500	HEM	C2D-C1D	-2.60	1.43	1.51
2	B	500	HEM	C2D-C1D	-2.12	1.44	1.51
2	B	500	HEM	C2A-C3A	-2.01	1.31	1.37
3	B	600	H4B	C2-N3	2.04	1.39	1.35
2	A	500	HEM	C4C-NC	2.44	1.39	1.36
2	A	500	HEM	FE-NB	2.53	2.10	1.97
3	B	600	H4B	C4-N3	2.91	1.38	1.33
2	A	500	HEM	FE-ND	3.29	2.14	1.97

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C3C-CAC-CBC	-6.90	113.87	124.46
2	B	500	HEM	CBA-CAA-C2A	-4.56	104.36	112.53
2	B	500	HEM	C3B-CAB-CBB	-4.17	118.06	124.46
2	A	500	HEM	C3B-CAB-CBB	-3.84	118.57	124.46
5	B	800	XFJ	C04-C05-C06	-3.67	117.98	120.28
3	B	600	H4B	N3-C2-N1	-3.62	119.60	125.53
2	B	500	HEM	C3C-CAC-CBC	-2.87	120.05	124.46
2	B	500	HEM	CAA-CBA-CGA	-2.77	107.66	112.75
5	A	800	XFJ	C04-C05-C06	-2.73	118.57	120.28
5	A	800	XFJ	C24-C25-C26	-2.65	118.62	120.28
5	A	800	XFJ	C18-C17-C15	-2.63	104.60	113.27
5	A	800	XFJ	C05-C06-N01	-2.61	120.02	122.96
5	B	800	XFJ	C18-C17-C15	-2.45	105.20	113.27
5	A	800	XFJ	C15-C14-C13	-2.40	118.14	121.25
2	A	500	HEM	CMA-C3A-C4A	-2.39	124.41	128.36
3	A	600	H4B	N3-C2-N1	-2.32	121.74	125.53
2	A	500	HEM	CAD-CBD-CGD	-2.28	103.72	113.02
2	B	500	HEM	CBD-CAD-C3D	-2.13	107.37	113.55
5	A	800	XFJ	C18-C26-C25	-2.09	118.19	121.13
5	B	800	XFJ	C15-C14-C13	-2.05	118.60	121.25
2	B	500	HEM	C2C-C1C-CHC	2.00	126.72	123.68
5	B	800	XFJ	C14-C13-C12	2.10	118.86	116.57
2	A	500	HEM	C3B-C4B-CHC	2.12	126.14	123.16
3	B	600	H4B	C2-N1-C8A	2.29	119.68	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	XFJ	C22-N21-C26	2.29	119.86	118.23
3	B	600	H4B	C4A-C8A-N8	2.39	121.25	118.43
2	A	500	HEM	C2D-C3D-C4D	2.40	105.57	101.50
5	A	800	XFJ	N22-C22-N21	2.46	120.98	116.50
2	A	500	HEM	CMB-C2B-C3B	2.61	123.04	116.53
5	A	800	XFJ	C08-C06-C05	2.62	124.81	121.13
3	A	600	H4B	C4A-C8A-N8	2.71	121.62	118.43
5	A	800	XFJ	C14-C13-C12	2.74	119.56	116.57
5	B	800	XFJ	C14-C15-C16	2.80	119.63	116.57
2	A	500	HEM	CMD-C2D-C3D	2.81	126.79	114.35
5	B	800	XFJ	C22-N21-C26	2.95	120.32	118.23
2	B	500	HEM	CMD-C2D-C3D	2.97	127.47	114.35
5	A	800	XFJ	C18-C26-N21	3.01	120.13	115.69
2	A	500	HEM	CAD-C3D-C2D	3.35	122.86	113.22
3	A	600	H4B	C4-N3-C2	3.54	120.86	115.94
5	A	800	XFJ	C14-C15-C16	3.60	120.50	116.57
2	B	500	HEM	CMC-C2C-C3C	3.64	125.62	116.53
2	B	500	HEM	C3B-C4B-CHC	3.77	128.47	123.16
2	B	500	HEM	CAD-C3D-C2D	4.25	125.45	113.22
2	B	500	HEM	CMB-C2B-C3B	4.26	127.17	116.53
2	A	500	HEM	CMC-C2C-C3C	4.30	127.27	116.53
3	B	600	H4B	N2-C2-N3	4.56	124.75	117.20
3	A	600	H4B	C4-C4A-C8A	4.64	118.77	114.56
3	B	600	H4B	C4-N3-C2	4.69	122.45	115.94
2	B	500	HEM	CAD-C3D-C4D	5.03	130.20	112.47
5	B	800	XFJ	C02-N01-C06	5.17	121.90	118.23
2	A	500	HEM	CAD-C3D-C4D	5.39	131.48	112.47
3	B	600	H4B	C4-C4A-C8A	5.74	119.75	114.56
5	A	800	XFJ	C02-N01-C06	6.21	122.64	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	7	0
3	A	600	H4B	3	0
5	A	800	XFJ	1	0
4	A	950	CAD	1	0
2	B	500	HEM	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	H4B	1	0
5	B	800	XFJ	4	0
4	B	950	CAD	2	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	404/444 (90%)	-0.31	3 (0%)	89	78	52, 77, 108, 120	0
1	B	402/444 (90%)	-0.41	3 (0%)	89	78	49, 77, 114, 145	0
All	All	806/888 (90%)	-0.36	6 (0%)	89	78	49, 77, 110, 145	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	123	GLU	4.6
1	B	122	ALA	3.1
1	A	69	LYS	2.8
1	B	121	PRO	2.7
1	A	121	PRO	2.7
1	A	160	ALA	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	XFJ	A	800	26/26	0.92	0.33	3.02	81,104,110,111	0
3	H4B	B	600	17/17	0.89	0.25	1.78	77,82,84,84	0
5	XFJ	B	800	26/26	0.91	0.28	1.34	57,89,105,106	0
2	HEM	B	500	43/43	0.98	0.20	0.78	46,51,65,74	0
2	HEM	A	500	43/43	0.98	0.21	0.73	51,57,63,69	0
3	H4B	A	600	17/17	0.95	0.21	0.67	71,73,77,79	0
6	ZN	A	900	1/1	0.99	0.12	-0.51	73,73,73,73	0
4	CAD	A	950	3/5	0.97	0.13	-0.86	103,103,106,106	0
4	CAD	B	950	3/5	0.98	0.09	-2.16	122,122,122,124	0

6.5 Other polymers (i)

There are no such residues in this entry.