Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N6C
Title	:	Structure of endothelial nitric oxide synthase H373S single mutant heme domain complexed with 4-(2-(6-(2-(6-amino-4-methylpyridin-2-yl)ethyl)pyridin-2-yl)ethyl)-6-methylpyridin-2-amine
Authors	:	Delker, S.L.; Li, H.; Poulos, T.L.
Deposited on	:	2010-05-25
Resolution	:	3.06 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:

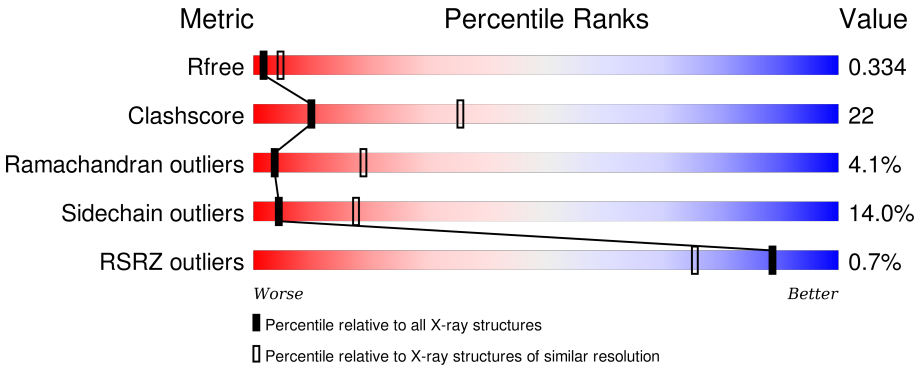
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

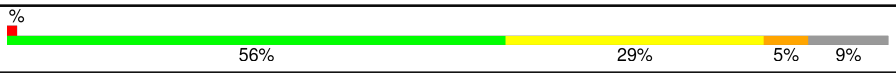
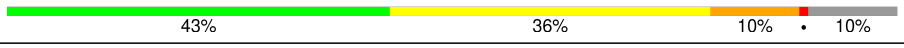
The reported resolution of this entry is 3.06 Å.

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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	
1	B	444	

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
4	ACT	A	860	-	-	-	X
4	ACT	B	850	-	-	-	X
4	ACT	B	860	-	-	-	X
7	XFM	A	800	-	-	-	X
7	XFM	B	800	-	-	-	X
8	ZN	B	900	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6621 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.

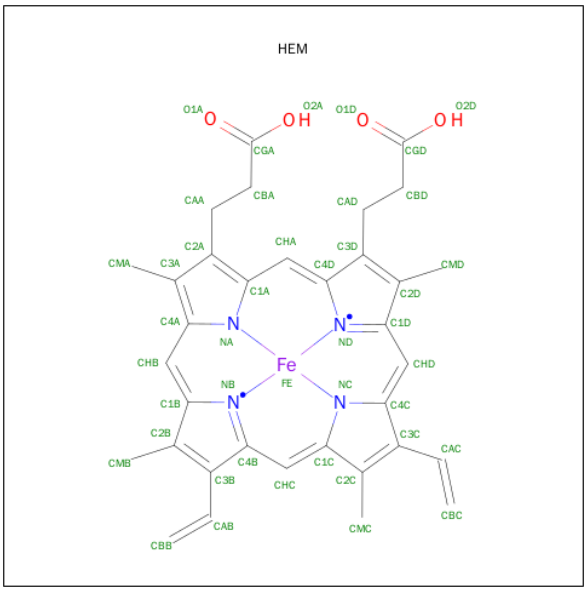
- Molecule 1 is a protein called Nitric oxide synthase.

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	401	Total	C	N	O	S	0	0	0
			3187	2026	559	586	16			

There are 4 discrepancies between the modelled and reference sequences:

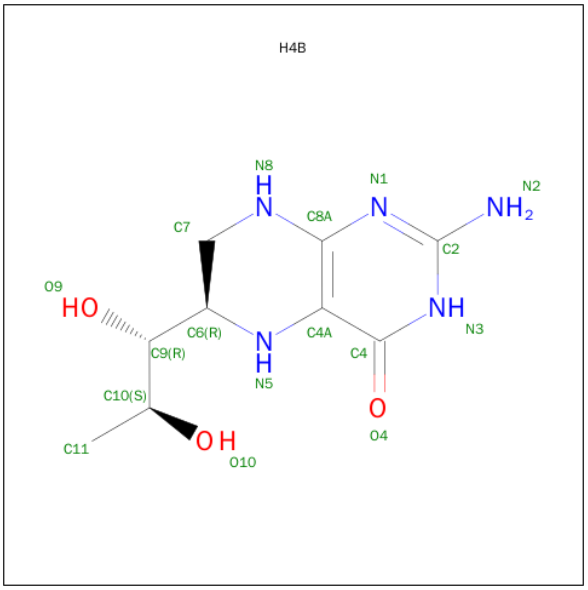
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29476
A	373	SER	HIS	ENGINEERED MUTATION	UNP P29476
B	100	ARG	CYS	SEE REMARK 999	UNP P29476
B	373	SER	HIS	ENGINEERED MUTATION	UNP P29476

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



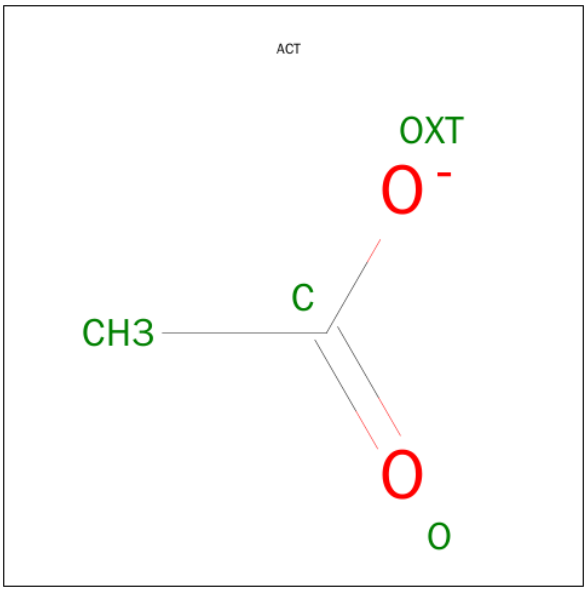
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



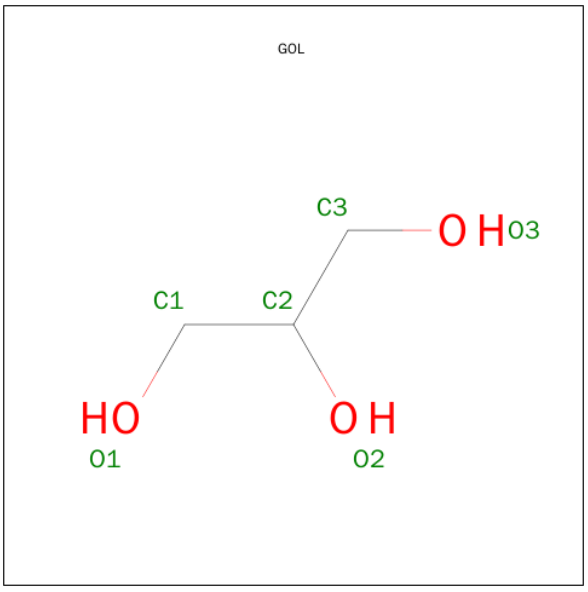
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

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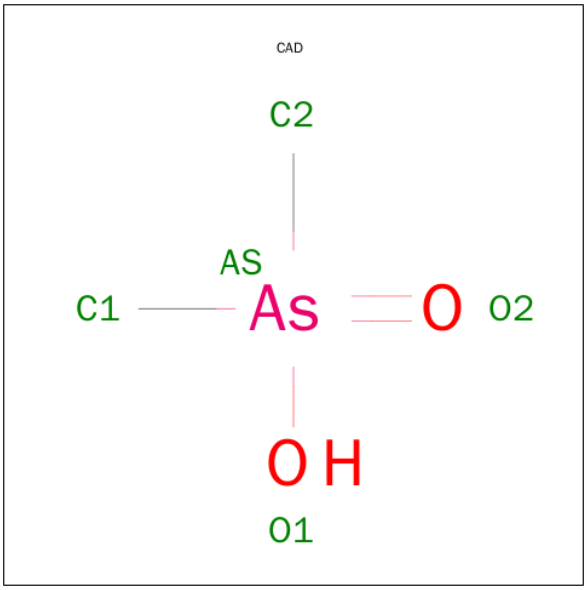
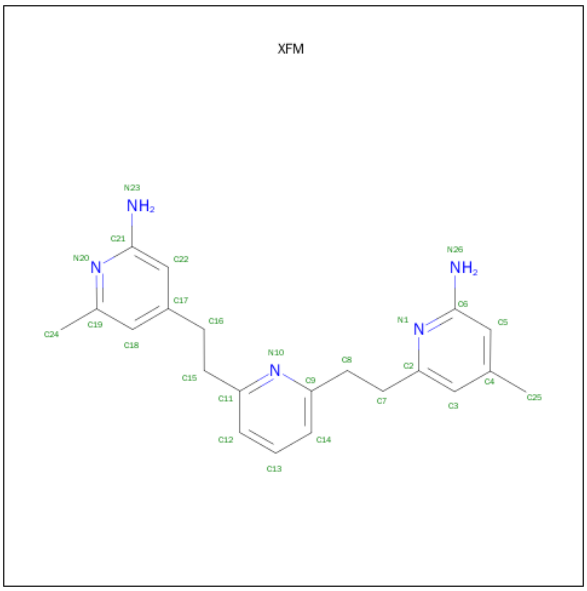
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



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

- Molecule 7 is 6-(2-{6-[2-(2-AMINO-6-METHYLPYRIDIN-4-YL)ETHYL]PYRIDIN-2-YL} ETHYL)-4-METHYLPYRIDIN-2-AMINE (three-letter code: XFM) (formula: $C_{21}H_{25}N_5$).



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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Zn 1 1	0	0

- Molecule 9 is water.

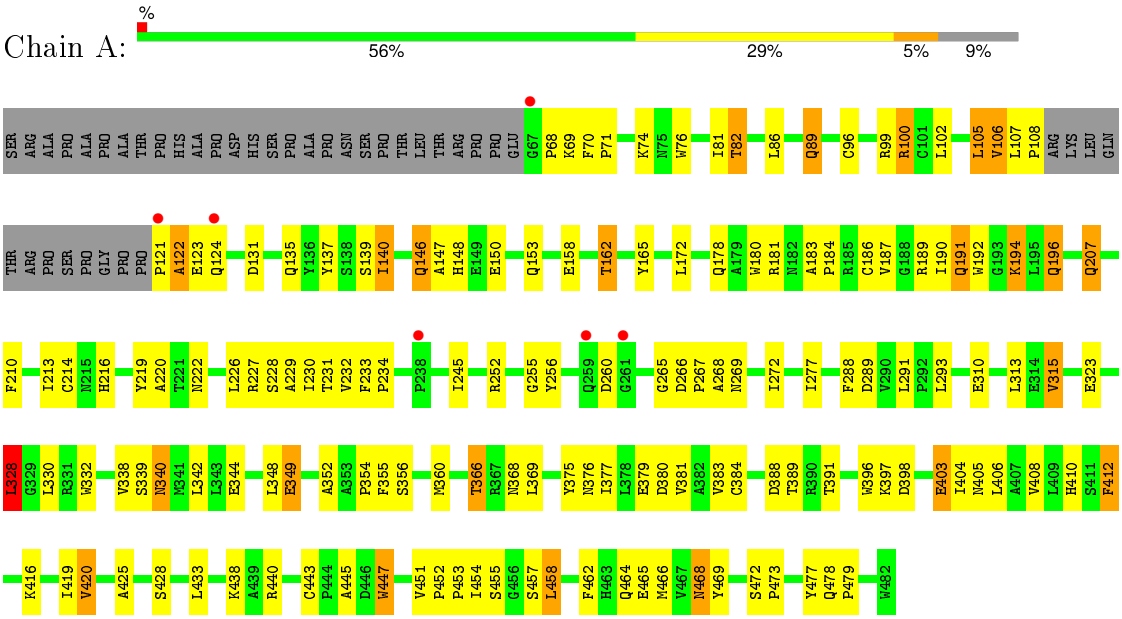
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	13	Total O 13 13	0	0
9	B	13	Total O 13 13	0	0

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.

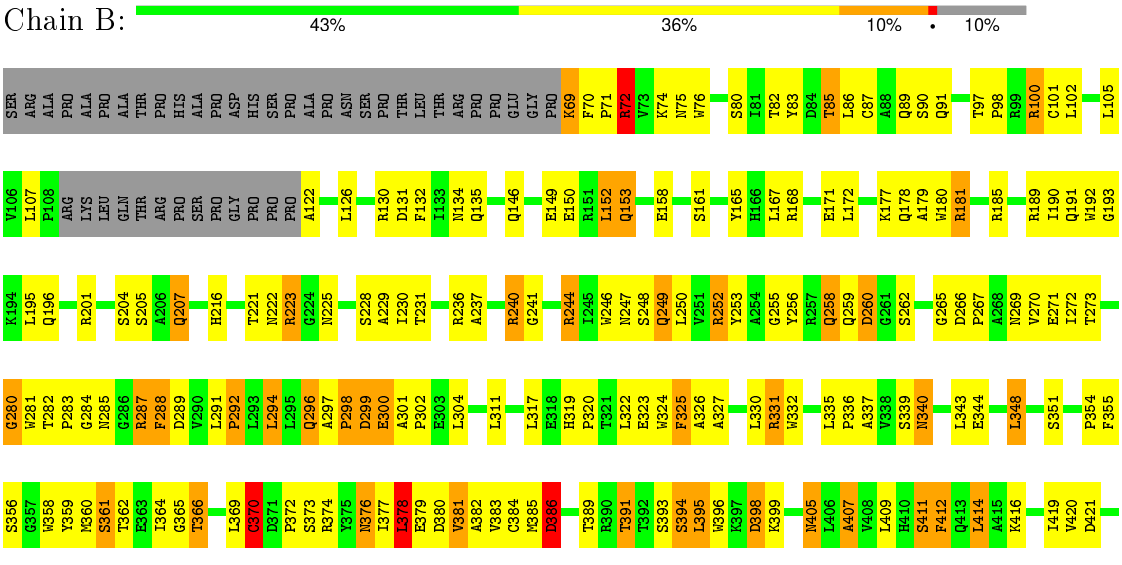
- Molecule 1: Nitric oxide synthase

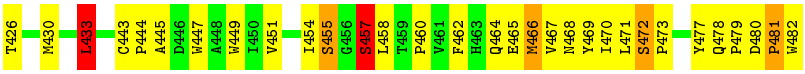
Chain A:



- Molecule 1: Nitric oxide synthase

Chain B:




T426
N430
L433
C443
P444
A445
D446
W447
A448
W449
T450
V451
I454
S455
G456
S457
L458
T459
P460
V461
F462
H463
Q464
E465
N466
V467
N468
Y469
I470
L471
S472
P473
Y477
Q478
P479
D480
P481
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	58.14Å 105.69Å 159.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.80 – 3.06 39.80 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.80-3.06) 97.5 (39.80-3.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.97 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.233 , 0.332 0.233 , 0.334	Depositor DCC
R_{free} test set	917 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.982	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 18649 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6621	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: GOL, ZN, XFM, H4B, ACT, HEM, 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	0.56	0/3294	0.71	0/4487
1	B	0.59	0/3274	0.71	1/4459 (0.0%)
All	All	0.58	0/6568	0.71	1/8946 (0.0%)

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	B	72	ARG	NE-CZ-NH1	5.68	123.14	120.30

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	3205	0	3113	122	0
1	B	3187	0	3097	173	0
2	A	43	0	30	8	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	3	0	0	1	0
6	B	3	0	0	1	0
7	A	26	0	25	4	0
7	B	26	0	25	2	0
8	B	1	0	0	2	0
9	A	13	0	0	0	0
9	B	13	0	0	1	0
All	All	6621	0	6375	287	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 22.

All (287) 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:B:244:ARG:HG3	1:B:244:ARG:HH11	0.95	1.10
1:B:100:ARG:HH11	1:B:100:ARG:HG2	1.21	1.02
1:B:252:ARG:HB3	1:B:269:ASN:ND2	1.77	1.00
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.28	0.98
1:A:384:CYS:SG	6:A:950:CAD:AS	2.84	0.95
1:B:244:ARG:NH1	1:B:244:ARG:HG3	1.75	0.95
1:B:355:PHE:CD1	2:B:500:HEM:HAC	2.02	0.94
1:B:100:ARG:CG	1:B:100:ARG:HH11	1.81	0.94
1:B:385:MET:O	1:B:386:ASP:HB2	1.64	0.92
1:B:299:ASP:O	1:B:300:GLU:HG2	1.69	0.92
1:A:181:ARG:NH2	1:A:440:ARG:HG3	1.86	0.91
1:A:477:TYR:HE1	7:A:800:XFM:H18	1.39	0.88
1:A:404:ILE:O	1:A:408:VAL:HG23	1.74	0.88
1:A:181:ARG:HH21	1:A:440:ARG:HG3	1.39	0.86
1:B:222:ASN:HB3	1:B:225:ASN:O	1.76	0.85
1:B:168:ARG:HB2	1:B:171:GLU:HG3	1.57	0.84
1:A:100:ARG:NH1	1:A:100:ARG:HG2	1.90	0.81
1:B:240:ARG:HD2	1:B:241:GLY:O	1.80	0.81
1:A:477:TYR:CE1	7:A:800:XFM:H18	2.17	0.79
1:A:455:SER:HA	1:B:454:ILE:HG22	1.65	0.78
1:B:69:LYS:N	1:B:69:LYS:HE2	1.98	0.78
1:B:284:GLY:HA3	1:B:289:ASP:OD2	1.84	0.77
1:A:181:ARG:HD2	1:A:192:TRP:CZ2	2.19	0.77
1:A:355:PHE:CD1	2:A:500:HEM:HAC	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:CYS:SG	8:B:900:ZN:ZN	1.74	0.75
1:B:150:GLU:HA	1:B:153:GLN:HB2	1.68	0.74
1:B:362:THR:HA	1:B:405:ASN:HD21	1.52	0.74
1:A:194:LYS:HA	1:A:194:LYS:HE3	1.70	0.74
1:B:471:LEU:O	1:B:472:SER:HB2	1.86	0.73
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.71	0.72
1:B:478:GLN:HB2	1:B:479:PRO:HD2	1.71	0.72
1:B:100:ARG:NH1	1:B:100:ARG:HG2	2.00	0.72
1:B:249:GLN:HA	1:B:337:ALA:O	1.89	0.72
1:B:365:GLY:HA2	1:B:369:LEU:HD12	1.72	0.71
1:B:101:CYS:HG	8:B:900:ZN:ZN	1.03	0.71
1:A:328:LEU:HB3	1:A:330:LEU:HG	1.73	0.71
1:B:165:TYR:CE2	1:B:348:LEU:HD11	2.26	0.71
1:B:249:GLN:HB2	1:B:252:ARG:HD2	1.74	0.70
1:B:180:TRP:CZ3	1:B:192:TRP:HA	2.26	0.70
1:A:106:VAL:HG21	1:B:76:TRP:NE1	2.06	0.70
1:A:366:THR:OG1	1:A:405:ASN:ND2	2.21	0.70
1:B:291:LEU:HB3	1:B:292:PRO:HD2	1.74	0.69
1:B:370:CYS:HA	1:B:377:ILE:H	1.56	0.69
1:B:244:ARG:CG	1:B:244:ARG:HH11	1.88	0.69
1:A:457:SER:HA	1:A:462:PHE:CD1	2.27	0.69
1:B:370:CYS:HB2	1:B:378:LEU:HD22	1.73	0.69
1:B:179:ALA:HA	1:B:473:PRO:O	1.93	0.67
1:B:280:GLY:O	1:B:304:LEU:HD22	1.94	0.67
1:A:369:LEU:O	1:A:377:ILE:HG12	1.94	0.66
1:A:420:VAL:HG22	1:A:425:ALA:HB2	1.77	0.66
1:B:395:LEU:HD22	1:B:398:ASP:OD1	1.95	0.66
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.30	0.66
1:A:455:SER:HB3	1:A:458:LEU:HB2	1.77	0.66
1:A:181:ARG:NH2	1:A:440:ARG:CG	2.59	0.66
1:B:189:ARG:O	1:B:192:TRP:HD1	1.78	0.65
1:B:472:SER:HA	1:B:473:PRO:C	2.15	0.65
1:A:230:ILE:HG13	1:A:355:PHE:HB3	1.77	0.65
1:B:255:GLY:O	1:B:273:THR:HG21	1.96	0.64
1:B:455:SER:O	1:B:458:LEU:HB2	1.96	0.64
1:A:196:GLN:HE21	1:A:196:GLN:HA	1.61	0.64
1:A:355:PHE:CG	2:A:500:HEM:HAC	2.32	0.64
1:B:319:HIS:HD2	1:B:407:ALA:HB2	1.64	0.63
1:A:181:ARG:HD2	1:A:192:TRP:CH2	2.34	0.63
1:A:377:ILE:O	1:A:381:VAL:HG23	1.99	0.63
1:A:100:ARG:CG	1:A:100:ARG:HH11	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TRP:HB2	1:B:294:LEU:HB3	1.80	0.62
1:B:185:ARG:HG2	1:B:449:TRP:CD2	2.35	0.62
1:A:420:VAL:CG2	1:A:425:ALA:HB2	2.29	0.62
1:B:72:ARG:HB2	1:B:83:TYR:CE2	2.35	0.61
1:B:389:THR:O	1:B:389:THR:HG22	2.00	0.61
1:B:132:PHE:O	1:B:135:GLN:HB2	2.01	0.61
1:B:102:LEU:HG	1:B:105:LEU:HD23	1.83	0.60
1:A:403:GLU:OE1	1:A:406:LEU:HD23	2.00	0.60
1:B:165:TYR:CZ	1:B:348:LEU:HD11	2.36	0.60
1:B:379:GLU:O	1:B:383:VAL:HG23	2.02	0.59
1:B:444:PRO:HA	1:B:467:VAL:O	2.02	0.59
1:B:258:GLN:O	1:B:260:ASP:N	2.35	0.59
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.50	0.59
1:B:185:ARG:HG2	1:B:449:TRP:CG	2.37	0.59
1:A:102:LEU:HD21	1:B:71:PRO:HB3	1.85	0.59
1:B:370:CYS:HB3	1:B:378:LEU:HD13	1.84	0.58
1:A:377:ILE:HD11	1:A:404:ILE:HG21	1.84	0.58
1:A:468:ASN:HD22	1:A:469:TYR:H	1.52	0.58
1:A:196:GLN:NE2	1:A:196:GLN:HA	2.18	0.58
1:B:407:ALA:O	1:B:411:SER:OG	2.21	0.58
1:A:189:ARG:O	1:A:192:TRP:HB3	2.04	0.58
1:B:267:PRO:HA	1:B:270:VAL:HG23	1.86	0.58
1:B:389:THR:HG23	1:B:396:TRP:CZ2	2.38	0.58
1:B:75:ASN:HB3	1:B:80:SER:HB2	1.85	0.57
1:B:252:ARG:HB3	1:B:269:ASN:HD22	1.69	0.57
1:B:299:ASP:O	1:B:300:GLU:CG	2.50	0.57
1:A:158:GLU:OE1	1:A:165:TYR:HA	2.05	0.57
1:B:343:LEU:HD12	1:B:344:GLU:N	2.20	0.57
1:A:465:GLU:HG2	1:B:105:LEU:HA	1.86	0.56
1:A:207:GLN:HE21	1:A:207:GLN:C	2.09	0.56
1:A:340:ASN:HD22	1:A:340:ASN:H	1.52	0.56
1:B:337:ALA:HA	1:B:356:SER:HB3	1.87	0.56
1:B:216:HIS:CE1	1:B:231:THR:H	2.24	0.56
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.88	0.55
1:B:180:TRP:CG	2:B:500:HEM:HBC2	2.41	0.55
1:B:256:TYR:O	1:B:258:GLN:HG3	2.06	0.55
1:A:472:SER:HA	1:A:473:PRO:C	2.25	0.55
1:A:403:GLU:OE2	1:B:399:LYS:HE3	2.06	0.55
1:B:481:PRO:HD2	1:B:482:TRP:CZ3	2.42	0.55
1:B:270:VAL:O	1:B:273:THR:HG22	2.07	0.54
1:B:246:TRP:HE1	1:B:296:GLN:NE2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PRO:O	1:A:70:PHE:N	2.41	0.54
1:B:359:TYR:CD2	1:B:364:ILE:HD11	2.43	0.54
1:B:230:ILE:O	1:B:230:ILE:HG23	2.08	0.54
1:B:412:PHE:HB3	1:B:419:ILE:HG21	1.90	0.54
1:B:281:TRP:CZ3	1:B:283:PRO:HA	2.43	0.53
1:A:191:GLN:HE22	1:A:194:LYS:HD2	1.72	0.53
1:A:86:LEU:O	1:A:89:GLN:HB2	2.09	0.53
1:B:252:ARG:HB3	1:B:269:ASN:HD21	1.69	0.52
1:A:137:TYR:C	1:A:139:SER:H	2.13	0.52
1:B:324:TRP:CE3	1:B:325:PHE:HA	2.43	0.52
1:A:181:ARG:HD2	1:A:192:TRP:CE2	2.44	0.52
1:B:322:LEU:HD22	1:B:324:TRP:HE1	1.74	0.52
1:B:89:GLN:O	1:B:91:GLN:HG2	2.10	0.52
1:A:338:VAL:HG23	7:A:800:XFM:H3	1.92	0.52
2:A:500:HEM:HBA2	7:A:800:XFM:H8	1.92	0.52
1:B:177:LYS:HG3	1:B:195:LEU:HD23	1.92	0.51
1:B:447:TRP:CH2	1:B:451:VAL:HG21	2.45	0.51
1:B:231:THR:O	1:B:354:PRO:HD2	2.11	0.51
1:B:322:LEU:HD13	1:B:324:TRP:CZ2	2.46	0.51
1:B:291:LEU:HB3	1:B:292:PRO:CD	2.40	0.51
1:A:398:ASP:OD2	1:B:455:SER:CB	2.59	0.51
1:B:478:GLN:CB	1:B:479:PRO:HD2	2.40	0.50
1:B:122:ALA:N	9:B:1019:HOH:O	2.44	0.50
1:A:256:TYR:OH	1:A:289:ASP:OD2	2.28	0.50
1:A:252:ARG:CB	1:A:291:LEU:HD12	2.41	0.50
1:B:189:ARG:C	1:B:191:GLN:H	2.15	0.50
1:A:190:ILE:HG21	1:A:428:SER:HB2	1.93	0.50
1:B:480:ASP:O	1:B:482:TRP:N	2.45	0.50
1:A:339:SER:HB3	1:A:354:PRO:HB3	1.93	0.50
1:A:410:HIS:CG	1:A:410:HIS:O	2.65	0.49
1:B:325:PHE:C	1:B:325:PHE:CD1	2.86	0.49
1:B:317:LEU:HG	1:B:331:ARG:HA	1.94	0.49
1:B:389:THR:HA	1:B:396:TRP:NE1	2.28	0.49
1:B:391:THR:HG23	1:B:394:SER:HB3	1.95	0.49
1:B:389:THR:O	1:B:389:THR:CG2	2.60	0.49
1:B:361:SER:HB3	1:B:409:LEU:HD21	1.93	0.49
1:A:245:ILE:CD1	1:A:354:PRO:HG3	2.42	0.48
1:A:213:ILE:O	1:A:216:HIS:HB3	2.12	0.48
1:B:332:TRP:CD1	1:B:364:ILE:HG12	2.48	0.48
1:B:90:SER:OG	1:B:470:ILE:O	2.23	0.48
1:A:379:GLU:O	1:A:383:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:PRO:C	1:B:374:ARG:H	2.17	0.48
1:B:180:TRP:HB2	2:B:500:HEM:HBC2	1.94	0.48
1:A:477:TYR:OH	2:A:500:HEM:O2D	2.29	0.48
1:A:468:ASN:HD22	1:A:469:TYR:N	2.11	0.48
1:A:342:LEU:HD21	1:A:349:GLU:HG3	1.95	0.48
1:A:377:ILE:HD12	1:A:381:VAL:HG21	1.96	0.48
1:A:403:GLU:OE1	1:A:403:GLU:HA	2.13	0.48
1:A:228:SER:O	1:A:229:ALA:HB2	2.13	0.48
1:B:247:ASN:O	1:B:339:SER:OG	2.20	0.48
1:B:464:GLN:HG3	1:B:465:GLU:O	2.14	0.48
1:B:102:LEU:HG	1:B:105:LEU:CD2	2.44	0.47
1:B:74:LYS:HD3	1:B:76:TRP:CE2	2.49	0.47
1:B:266:ASP:OD2	1:B:374:ARG:NH2	2.43	0.47
1:A:396:TRP:CZ2	1:A:397:LYS:HE2	2.50	0.47
1:B:370:CYS:CB	1:B:378:LEU:HD13	2.44	0.47
1:B:86:LEU:HB3	1:B:469:TYR:OH	2.14	0.47
1:B:265:GLY:HA2	1:B:287:ARG:O	2.15	0.47
1:B:177:LYS:HE2	1:B:193:GLY:O	2.14	0.47
1:B:189:ARG:O	1:B:191:GLN:N	2.47	0.47
1:B:319:HIS:CD2	1:B:407:ALA:HB2	2.48	0.47
1:A:388:ASP:OD2	1:A:391:THR:HG22	2.15	0.47
1:B:237:ALA:H	1:B:240:ARG:NH1	2.13	0.47
1:A:106:VAL:CG2	1:B:76:TRP:NE1	2.78	0.47
1:B:467:VAL:HG12	1:B:469:TYR:HD1	1.78	0.47
1:A:369:LEU:HA	1:A:375:TYR:HB2	1.97	0.46
1:B:250:LEU:HB2	1:B:337:ALA:HB3	1.98	0.46
1:A:180:TRP:CG	2:A:500:HEM:HBC2	2.50	0.46
1:B:260:ASP:HB2	1:B:262:SER:OG	2.16	0.46
1:A:180:TRP:HB2	2:A:500:HEM:HBC2	1.97	0.46
1:A:252:ARG:HB3	1:A:291:LEU:HD12	1.97	0.46
1:B:223:ARG:HB2	1:B:223:ARG:HH11	1.80	0.46
1:A:445:ALA:HB1	1:A:466:MET:SD	2.55	0.46
1:A:478:GLN:HA	1:A:479:PRO:HD3	1.88	0.46
1:B:445:ALA:C	1:B:468:ASN:HB2	2.36	0.46
1:A:355:PHE:CD1	2:A:500:HEM:CAC	2.95	0.46
1:A:465:GLU:CD	1:B:105:LEU:HD13	2.37	0.46
1:A:146:GLN:NE2	1:A:147:ALA:H	2.14	0.46
1:A:186:CYS:HB2	2:A:500:HEM:C4D	2.52	0.45
1:A:377:ILE:HD11	1:A:404:ILE:CG2	2.45	0.45
1:B:221:THR:O	1:B:222:ASN:C	2.54	0.45
1:B:240:ARG:HD3	1:B:298:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:PHE:CZ	1:A:214:CYS:SG	3.09	0.45
1:A:332:TRP:CZ2	1:A:368:ASN:ND2	2.84	0.45
1:B:360:MET:HA	1:B:420:VAL:O	2.16	0.45
1:B:131:ASP:HA	1:B:134:ASN:HD22	1.80	0.45
1:A:233:PHE:HB3	1:A:234:PRO:CD	2.47	0.45
1:B:447:TRP:HD1	1:B:466:MET:HG3	1.82	0.45
1:A:220:ALA:O	1:A:226:LEU:HA	2.16	0.45
1:B:246:TRP:HB2	1:B:294:LEU:CB	2.47	0.45
1:B:294:LEU:HD23	1:B:302:PRO:HB2	1.99	0.45
1:B:335:LEU:HA	1:B:336:PRO:HD3	1.89	0.45
1:A:172:LEU:HD21	1:A:232:VAL:HG21	1.98	0.45
1:A:107:LEU:HA	1:A:108:PRO:HD3	1.75	0.45
1:B:207:GLN:HE21	1:B:207:GLN:HA	1.82	0.45
1:B:167:LEU:O	1:B:201:ARG:NH1	2.36	0.45
1:B:100:ARG:NH1	1:B:102:LEU:HD13	2.32	0.45
1:A:150:GLU:HA	1:A:153:GLN:HB2	1.97	0.45
1:B:248:SER:HA	1:B:340:ASN:HB3	1.99	0.45
1:A:266:ASP:CB	1:A:375:TYR:HE1	2.30	0.45
1:A:219:TYR:O	1:A:227:ARG:NH2	2.47	0.45
1:A:123:GLU:HB2	1:A:124:GLN:OE1	2.17	0.45
1:B:382:ALA:HA	1:B:385:MET:HB2	1.99	0.44
1:A:288:PHE:CE1	1:A:375:TYR:HE2	2.34	0.44
1:A:102:LEU:O	1:A:105:LEU:HB2	2.16	0.44
1:B:253:TYR:CD1	1:B:288:PHE:HB3	2.52	0.44
1:A:121:PRO:O	1:A:122:ALA:CB	2.65	0.44
1:B:358:TRP:H	2:B:500:HEM:HAB	1.82	0.44
1:A:81:ILE:HG22	1:A:82:THR:N	2.33	0.44
1:B:380:ASP:O	1:B:381:VAL:C	2.56	0.44
1:A:137:TYR:CD1	1:A:148:HIS:HB2	2.53	0.44
1:B:216:HIS:HE1	1:B:231:THR:H	1.67	0.43
1:A:219:TYR:CZ	1:A:227:ARG:HD2	2.52	0.43
1:B:382:ALA:O	1:B:386:ASP:N	2.48	0.43
1:B:391:THR:HG23	1:B:394:SER:CB	2.49	0.43
1:B:467:VAL:HG12	1:B:469:TYR:CD1	2.53	0.43
1:B:288:PHE:CD2	1:B:288:PHE:N	2.86	0.43
1:B:70:PHE:CD1	1:B:85:THR:HA	2.54	0.43
1:B:430:MET:CE	1:B:460:PRO:HB2	2.48	0.43
1:B:72:ARG:HB2	1:B:83:TYR:HE2	1.82	0.43
1:A:389:THR:HG22	1:A:396:TRP:CD2	2.54	0.43
1:B:477:TYR:CD1	7:B:800:XFM:H24A	2.54	0.43
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HG21	1:A:412:PHE:CZ	2.54	0.43
1:B:130:ARG:HG2	1:B:152:LEU:HD21	2.01	0.43
1:B:181:ARG:HG3	1:B:192:TRP:CD2	2.54	0.42
1:B:360:MET:O	1:B:362:THR:N	2.52	0.42
1:A:438:LYS:HA	1:A:438:LYS:HD2	1.74	0.42
1:B:178:GLN:HG2	1:B:473:PRO:HD2	2.01	0.42
1:A:135:GLN:O	1:A:139:SER:HB3	2.18	0.42
1:A:344:GLU:HG2	1:A:348:LEU:O	2.19	0.42
1:A:452:PRO:HA	1:A:453:PRO:HD3	1.69	0.42
1:B:457:SER:HA	1:B:462:PHE:CD1	2.53	0.42
1:A:100:ARG:O	1:A:100:ARG:NH1	2.52	0.42
1:B:189:ARG:C	1:B:191:GLN:N	2.73	0.42
1:A:266:ASP:O	1:A:268:ALA:N	2.53	0.42
1:A:74:LYS:HG3	1:A:81:ILE:HD13	2.00	0.42
1:A:96:CYS:SG	1:B:101:CYS:SG	3.17	0.42
1:A:398:ASP:OD2	1:B:455:SER:OG	2.33	0.42
1:A:81:ILE:O	1:A:82:THR:HG23	2.19	0.42
1:B:325:PHE:HD1	1:B:326:ALA:HA	1.84	0.42
1:B:414:LEU:C	1:B:416:LYS:H	2.21	0.42
1:B:325:PHE:HD1	1:B:326:ALA:N	2.17	0.42
1:B:317:LEU:HD23	1:B:317:LEU:HA	1.78	0.42
1:B:158:GLU:OE2	1:B:165:TYR:HA	2.19	0.42
1:B:447:TRP:CZ2	1:B:451:VAL:HG21	2.54	0.42
1:A:222:ASN:HB2	1:A:227:ARG:HH21	1.85	0.42
1:B:196:GLN:HB3	1:B:229:ALA:HB2	2.02	0.42
1:A:360:MET:HA	1:A:420:VAL:O	2.19	0.42
1:B:301:ALA:HA	1:B:302:PRO:HD2	1.80	0.42
1:A:146:GLN:OE1	1:A:146:GLN:N	2.45	0.42
1:B:433:LEU:HD22	1:B:433:LEU:HA	1.91	0.42
1:A:196:GLN:HE21	1:A:196:GLN:CA	2.29	0.42
1:A:158:GLU:O	1:A:162:THR:HG23	2.20	0.41
1:B:381:VAL:O	1:B:385:MET:HG3	2.20	0.41
1:B:366:THR:OG1	1:B:405:ASN:OD1	2.28	0.41
1:B:178:GLN:HB3	1:B:473:PRO:HD2	2.02	0.41
1:A:184:PRO:CB	1:A:468:ASN:HD21	2.34	0.41
1:A:375:TYR:O	1:A:376:ASN:C	2.59	0.41
1:A:131:ASP:O	1:A:135:GLN:NE2	2.49	0.41
1:A:447:TRP:O	1:A:451:VAL:HG23	2.20	0.41
1:B:165:TYR:O	1:B:348:LEU:HD21	2.21	0.41
1:B:319:HIS:CD2	1:B:320:PRO:HD2	2.56	0.41
1:A:412:PHE:N	1:A:412:PHE:HD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:HA2	1:A:265:GLY:HA3	2.01	0.41
1:B:149:GLU:O	1:B:153:GLN:N	2.53	0.41
1:B:70:PHE:CE1	1:B:85:THR:HG22	2.56	0.41
1:A:433:LEU:HD23	1:A:443:CYS:HB3	2.04	0.41
1:A:184:PRO:HB3	1:A:468:ASN:ND2	2.36	0.40
1:B:249:GLN:O	1:B:250:LEU:C	2.59	0.40
2:B:500:HEM:HBD2	7:B:800:XFM:C13	2.51	0.40
1:B:471:LEU:HB3	1:B:472:SER:H	1.70	0.40
1:A:342:LEU:HD23	1:A:342:LEU:C	2.42	0.40
1:B:384:CYS:SG	6:B:950:CAD:AS	3.40	0.40
1:A:464:GLN:HE21	1:A:465:GLU:N	2.19	0.40
1:B:412:PHE:CD2	1:B:419:ILE:HB	2.56	0.40
1:A:137:TYR:O	1:A:140:ILE:HG13	2.21	0.40
1:B:97:THR:O	1:B:98:PRO:C	2.57	0.40
1:A:340:ASN:O	1:A:478:GLN:HG2	2.22	0.40
1:A:252:ARG:HB2	1:A:291:LEU:HD12	2.02	0.40
1:A:245:ILE:HG13	1:A:352:ALA:HB1	2.04	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%)	329 (82%)	62 (16%)	9 (2%)	8 32
1	B	397/444 (89%)	302 (76%)	71 (18%)	24 (6%)	2 10
All	All	797/888 (90%)	631 (79%)	133 (17%)	33 (4%)	3 19

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS

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Mol	Chain	Res	Type
1	A	122	ALA
1	B	249	GLN
1	B	259	GLN
1	B	300	GLU
1	B	361	SER
1	B	378	LEU
1	B	386	ASP
1	A	260	ASP
1	B	260	ASP
1	B	285	ASN
1	B	299	ASP
1	B	370	CYS
1	B	373	SER
1	B	381	VAL
1	B	457	SER
1	B	472	SER
1	A	76	TRP
1	B	292	PRO
1	B	325	PHE
1	B	327	ALA
1	B	407	ALA
1	B	481	PRO
1	B	190	ILE
1	B	376	ASN
1	A	267	PRO
1	A	328	LEU
1	A	447	TRP
1	B	433	LEU
1	A	419	ILE
1	B	280	GLY
1	B	298	PRO
1	A	71	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%)	306 (89%)	37 (11%)	8 29
1	B	341/377 (90%)	282 (83%)	59 (17%)	2 10
All	All	684/754 (91%)	588 (86%)	96 (14%)	4 17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	THR
1	A	89	GLN
1	A	99	ARG
1	A	100	ARG
1	A	105	LEU
1	A	106	VAL
1	A	140	ILE
1	A	146	GLN
1	A	162	THR
1	A	178	GLN
1	A	187	VAL
1	A	191	GLN
1	A	194	LYS
1	A	196	GLN
1	A	207	GLN
1	A	231	THR
1	A	269	ASN
1	A	272	ILE
1	A	277	ILE
1	A	293	LEU
1	A	310	GLU
1	A	313	LEU
1	A	315	VAL
1	A	323	GLU
1	A	328	LEU
1	A	340	ASN
1	A	349	GLU
1	A	356	SER
1	A	366	THR
1	A	380	ASP
1	A	403	GLU
1	A	412	PHE
1	A	416	LYS
1	A	420	VAL
1	A	454	ILE

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Mol	Chain	Res	Type
1	A	458	LEU
1	A	468	ASN
1	B	69	LYS
1	B	72	ARG
1	B	82	THR
1	B	85	THR
1	B	87	CYS
1	B	100	ARG
1	B	107	LEU
1	B	126	LEU
1	B	146	GLN
1	B	152	LEU
1	B	153	GLN
1	B	161	SER
1	B	172	LEU
1	B	181	ARG
1	B	204	SER
1	B	205	SER
1	B	207	GLN
1	B	223	ARG
1	B	228	SER
1	B	236	ARG
1	B	240	ARG
1	B	244	ARG
1	B	252	ARG
1	B	258	GLN
1	B	271	GLU
1	B	272	ILE
1	B	282	THR
1	B	287	ARG
1	B	288	PHE
1	B	294	LEU
1	B	296	GLN
1	B	311	LEU
1	B	323	GLU
1	B	330	LEU
1	B	331	ARG
1	B	340	ASN
1	B	348	LEU
1	B	351	SER
1	B	366	THR
1	B	370	CYS

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Mol	Chain	Res	Type
1	B	376	ASN
1	B	378	LEU
1	B	386	ASP
1	B	391	THR
1	B	393	SER
1	B	394	SER
1	B	395	LEU
1	B	398	ASP
1	B	405	ASN
1	B	411	SER
1	B	412	PHE
1	B	414	LEU
1	B	421	ASP
1	B	426	THR
1	B	433	LEU
1	B	443	CYS
1	B	455	SER
1	B	457	SER
1	B	466	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	191	GLN
1	A	196	GLN
1	A	278	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	464	GLN
1	A	468	ASN
1	B	191	GLN
1	B	207	GLN
1	B	225	ASN
1	B	269	ASN
1	B	296	GLN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN
1	B	478	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	2.11	6 (20%)	24,82,82	2.47	9 (37%)
3	H4B	A	600	-	13,18,18	0.76	0	11,26,26	2.48	4 (36%)
7	XFM	A	800	-	28,28,28	0.53	0	37,38,38	1.92	10 (27%)
4	ACT	A	860	-	1,3,3	1.75	0	0,3,3	0.00	-
5	GOL	A	880	-	5,5,5	0.38	0	5,5,5	0.15	0
6	CAD	A	950	-	0,2,4	0.00	-	0,1,6	0.00	-
2	HEM	B	500	-	30,50,50	2.15	6 (20%)	24,82,82	2.31	8 (33%)
3	H4B	B	600	-	13,18,18	0.84	0	11,26,26	2.37	4 (36%)
7	XFM	B	800	-	28,28,28	0.52	0	37,38,38	1.91	10 (27%)
4	ACT	B	850	-	1,3,3	2.43	1 (100%)	0,3,3	0.00	-
4	ACT	B	860	-	1,3,3	1.15	0	0,3,3	0.00	-
5	GOL	B	880	-	5,5,5	0.30	0	5,5,5	0.27	0
6	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
7	XFM	A	800	-	-	0/10/10/10	0/3/3/3
4	ACT	A	860	-	-	0/0/0/0	0/0/0/0
5	GOL	A	880	-	-	0/4/4/4	0/0/0/0
6	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
7	XFM	B	800	-	-	0/10/10/10	0/3/3/3
4	ACT	B	850	-	-	0/0/0/0	0/0/0/0
4	ACT	B	860	-	-	0/0/0/0	0/0/0/0
5	GOL	B	880	-	-	0/4/4/4	0/0/0/0
6	CAD	B	950	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C4B	-7.91	1.44	1.51
2	A	500	HEM	C3B-C4B	-6.90	1.45	1.51
2	A	500	HEM	C3D-C4D	-5.00	1.45	1.51
2	B	500	HEM	C3D-C4D	-4.45	1.45	1.51
2	A	500	HEM	C2C-C1C	-4.02	1.44	1.52
2	B	500	HEM	C2C-C1C	-3.88	1.45	1.52
2	B	500	HEM	C2D-C1D	-2.42	1.43	1.51
2	A	500	HEM	C2B-C1B	-2.38	1.44	1.51
2	B	500	HEM	C2B-C1B	-2.15	1.44	1.51
2	B	500	HEM	C3C-CAC	2.16	1.55	1.51
2	A	500	HEM	FE-ND	2.24	2.09	1.97
4	B	850	ACT	CH3-C	2.43	1.52	1.48
2	A	500	HEM	FE-NB	2.49	2.10	1.97

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	CBA-CAA-C2A	-4.27	104.88	112.53
2	A	500	HEM	C3C-CAC-CBC	-3.68	118.82	124.46
7	B	800	XFM	C3-C2-N1	-3.47	119.04	122.96
3	B	600	H4B	N3-C2-N1	-3.29	120.14	125.53
7	A	800	XFM	C3-C2-N1	-3.09	119.47	122.96
3	A	600	H4B	N3-C2-N1	-3.07	120.50	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	CMA-C3A-C4A	-2.91	123.55	128.36
2	A	500	HEM	CBA-CAA-C2A	-2.70	107.69	112.53
2	B	500	HEM	C3B-CAB-CBB	-2.68	120.34	124.46
2	B	500	HEM	CAA-CBA-CGA	-2.29	108.54	112.75
7	B	800	XFM	C7-C8-C9	-2.25	108.19	112.53
7	A	800	XFM	C12-C11-N10	-2.22	119.69	122.41
7	B	800	XFM	C14-C9-N10	-2.07	119.88	122.41
7	A	800	XFM	C24-C19-N20	2.10	119.85	116.59
7	A	800	XFM	N26-C6-N1	2.25	120.60	116.50
7	B	800	XFM	C11-N10-C9	2.38	121.05	118.12
3	A	600	H4B	C2-N1-C8A	2.41	119.96	114.54
7	B	800	XFM	C24-C19-N20	2.47	120.41	116.59
7	A	800	XFM	C11-N10-C9	2.62	121.34	118.12
3	B	600	H4B	C2-N1-C8A	2.64	120.47	114.54
2	B	500	HEM	CMD-C2D-C3D	2.75	126.52	114.35
7	B	800	XFM	C8-C9-N10	2.76	119.77	115.69
2	A	500	HEM	CMD-C2D-C3D	2.81	126.80	114.35
7	A	800	XFM	C21-N20-C19	3.01	121.39	118.12
7	B	800	XFM	C15-C11-N10	3.15	120.34	115.69
7	B	800	XFM	C21-N20-C19	3.17	121.57	118.12
2	A	500	HEM	C3B-C4B-CHC	3.35	127.88	123.16
7	A	800	XFM	C8-C9-N10	3.44	120.77	115.69
3	B	600	H4B	C4-N3-C2	3.65	121.00	115.94
7	A	800	XFM	C7-C2-N1	3.73	121.20	115.69
2	B	500	HEM	CMB-C2B-C3B	3.95	126.39	116.53
2	B	500	HEM	CAD-C3D-C2D	4.02	124.76	113.22
3	A	600	H4B	C4-N3-C2	4.02	121.51	115.94
2	B	500	HEM	CMC-C2C-C3C	4.02	126.56	116.53
7	B	800	XFM	C7-C2-N1	4.13	121.80	115.69
2	A	500	HEM	CMC-C2C-C3C	4.17	126.93	116.53
2	A	500	HEM	CMB-C2B-C3B	4.23	127.10	116.53
2	A	500	HEM	CAD-C3D-C4D	4.25	127.47	112.47
7	A	800	XFM	C15-C11-N10	4.28	122.02	115.69
7	A	800	XFM	C6-N1-C2	4.78	121.63	118.23
3	B	600	H4B	C4-C4A-C8A	4.82	118.92	114.56
2	A	500	HEM	CAD-C3D-C2D	5.06	127.77	113.22
2	B	500	HEM	CAD-C3D-C4D	5.13	130.56	112.47
3	A	600	H4B	C4-C4A-C8A	5.20	119.27	114.56
7	B	800	XFM	C6-N1-C2	5.40	122.06	118.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	8	0
7	A	800	XFM	4	0
6	A	950	CAD	1	0
2	B	500	HEM	5	0
7	B	800	XFM	2	0
6	B	950	CAD	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

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%)	-0.34	6 (1%) 76 55	39, 55, 77, 92	0
1	B	401/444 (90%)	-0.40	0 100 100	45, 56, 71, 84	0
All	All	805/888 (90%)	-0.37	6 (0%) 89 75	39, 56, 73, 92	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	238	PRO	3.2
1	A	121	PRO	2.5
1	A	124	GLN	2.3
1	A	261	GLY	2.3
1	A	67	GLY	2.1
1	A	259	GLN	2.1

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
4	ACT	B	860	4/4	0.88	0.31	4.37	58,59,59,60	0
7	XFM	A	800	26/26	0.92	0.30	3.56	61,74,85,85	0
4	ACT	B	850	4/4	0.89	0.27	2.85	41,41,42,42	0
4	ACT	A	860	4/4	0.87	0.32	2.77	66,66,67,67	0
7	XFM	B	800	26/26	0.90	0.27	2.55	68,78,83,83	0
3	H4B	A	600	17/17	0.88	0.27	1.83	94,96,97,97	0
2	HEM	A	500	43/43	0.96	0.21	1.28	44,48,57,59	0
2	HEM	B	500	43/43	0.96	0.20	1.24	45,48,59,62	0
3	H4B	B	600	17/17	0.91	0.23	0.96	82,85,86,86	0
6	CAD	A	950	3/5	0.87	0.19	0.41	120,120,120,121	0
6	CAD	B	950	3/5	0.94	0.16	-0.57	118,118,118,118	0
8	ZN	B	900	1/1	0.98	0.10	-0.89	58,58,58,58	0
5	GOL	A	880	6/6	0.91	0.39	-	69,71,72,72	0
5	GOL	B	880	6/6	0.87	0.31	-	54,55,57,57	0

6.5 Other polymers

There are no such residues in this entry.