



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:10 AM GMT

PDB ID : 3EAH
Title : Structure of inhibited human eNOS oxygenase domain
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stuehr, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-25
Resolution : 2.44 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

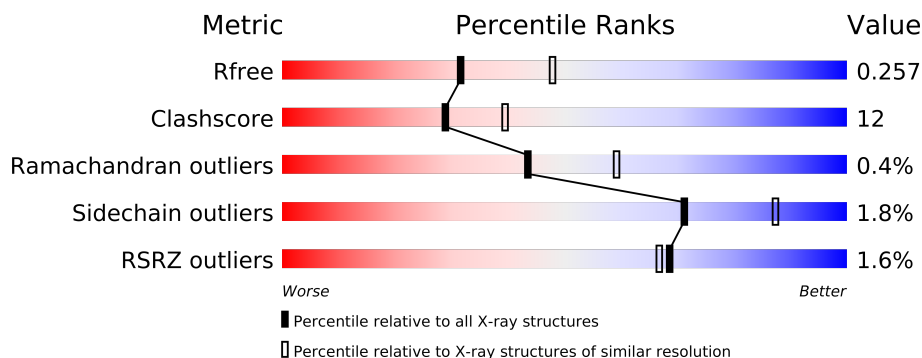
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.44 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}	66092	2989 (2.48-2.40)
Clashscore	79885	3698 (2.48-2.40)
Ramachandran outliers	78287	3639 (2.48-2.40)
Sidechain outliers	78261	3640 (2.48-2.40)
RSRZ outliers	66119	2993 (2.48-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	427	
1	B	427	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	327	A	864	-	X
4	327	B	1864	-	X
5	MPD	A	1866	-	X
5	MPD	A	1867	-	X
5	MPD	A	866	-	X
5	MPD	B	867	-	X
6	CL	B	865	-	X

2 Entry composition i

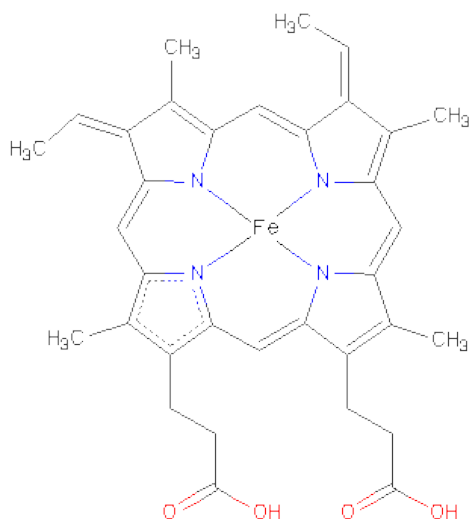
There are 7 unique types of molecules in this entry. The entry contains 6620 atoms, of which 0 are hydrogen and 0 are deuterium.

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, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3157	2015	553	573	16			
1	B	401	Total	C	N	O	S	0	0	0
			3171	2025	554	576	16			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

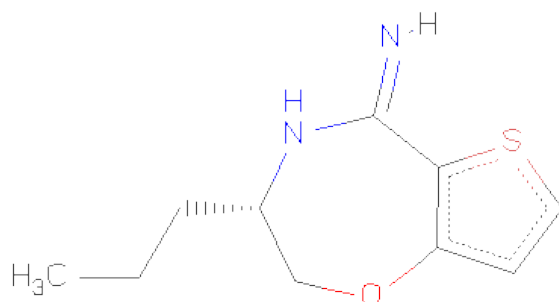


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

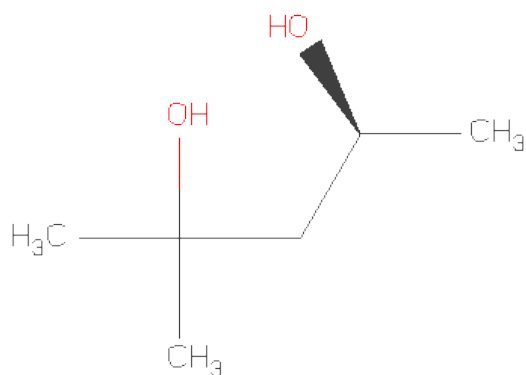
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (3S,5E)-3-PROPYL-3,4-DIHYDROTHIENO[2,3-F][1,4]OXAZEPIN-5(2H)-IMINE (three-letter code: 327) (formula: C₁₀H₁₄N₂OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			14	10	2	1	1		
4	B	1	Total	C	N	O	S	0	0
			14	10	2	1	1		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

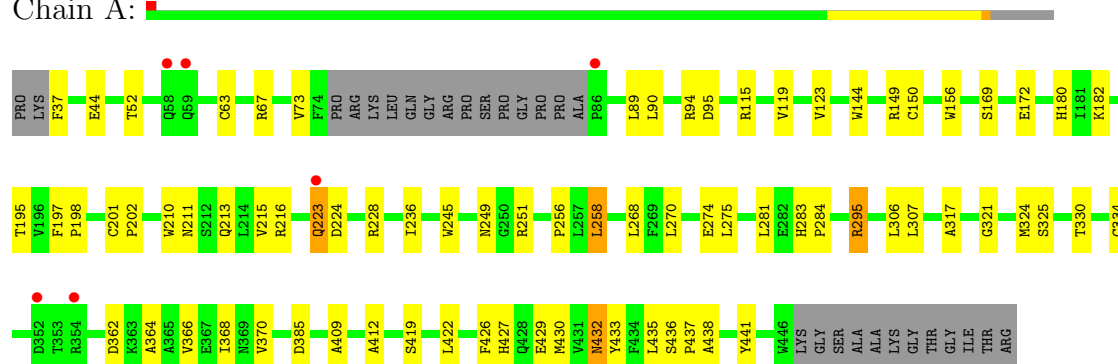
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	78	Total	O	0	0
			78	78		
7	B	65	Total	O	0	0
			65	65		

3 Residue-property plots

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.

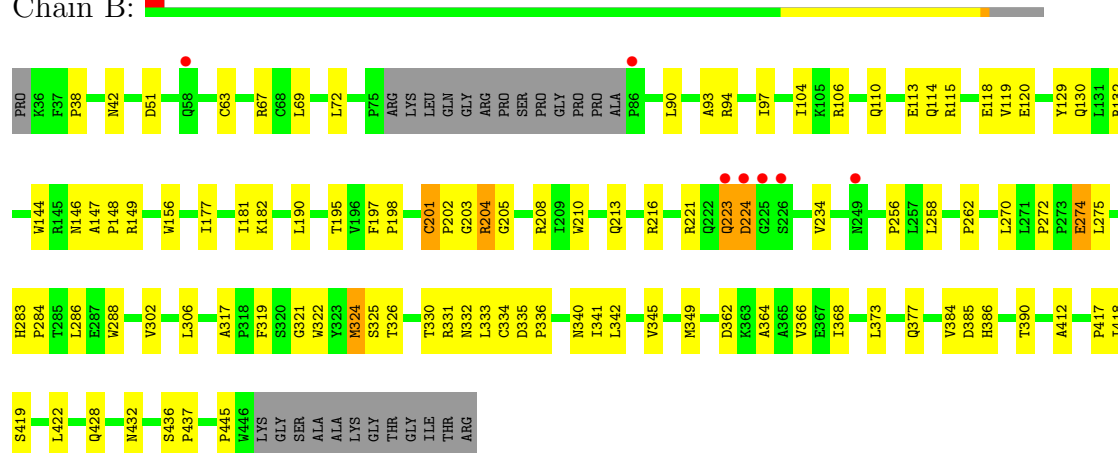
- Molecule 1: Nitric oxide synthase, endothelial

Chain A:



- Molecule 1: Nitric oxide synthase, endothelial

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.09Å 90.15Å 156.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.44 25.00 – 2.44	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.00-2.44) 95.4 (25.00-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.258 0.211 , 0.257	Depositor DCC
R_{free} test set	1803 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36307 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6620	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 327, ZN, HEC, MPD, CL

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	0.37	0/3248	0.64	1/4430 (0.0%)
1	B	0.37	0/3263	0.63	1/4451 (0.0%)
All	All	0.37	0/6511	0.63	2/8881 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	MET	N-CA-C	-5.53	96.07	111.00
1	B	324	MET	N-CA-C	-5.26	96.80	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3157	0	3042	73	0
1	B	3171	0	3057	88	1
2	A	43	0	32	7	0
2	B	43	0	32	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	13	6	0
4	B	14	0	13	5	0
5	A	24	0	42	5	0
5	B	8	0	14	0	0
6	A	1	0	0	2	0
6	B	1	0	0	3	0
7	A	78	0	0	0	1
7	B	65	0	0	1	0
All	All	6620	0	6245	158	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (158) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:221:ARG:HE	1:B:234:VAL:HG11	1.18	1.04
1:B:221:ARG:NE	1:B:234:VAL:HG11	1.83	0.92
1:A:258:LEU:HD13	1:A:268:LEU:HD23	1.50	0.92
1:A:432:ASN:HD22	1:A:433:TYR:N	1.77	0.83
1:A:258:LEU:HD13	1:A:268:LEU:CD2	2.09	0.82
1:A:210:TRP:HB2	1:A:258:LEU:HB3	1.63	0.81
1:B:144:TRP:HB2	2:B:1861:HEC:HBC3	1.67	0.77
1:B:272:PRO:HD2	1:B:275:LEU:HD12	1.67	0.75
1:A:90:LEU:HD23	1:A:94:ARG:NH2	2.05	0.72
6:B:865:CL:CL	4:B:1864:327:H10B	2.28	0.71
1:A:223:GLN:OE1	1:A:223:GLN:HA	1.89	0.71
1:B:334:CYS:SG	1:B:342:LEU:HD13	2.31	0.70
4:A:864:327:H10B	6:A:1865:CL:CL	2.30	0.69
1:A:432:ASN:HD22	1:A:432:ASN:C	1.97	0.67
1:B:110:GLN:HE21	1:B:114:GLN:HE21	1.41	0.67
1:B:336:PRO:HA	1:B:340:ASN:HB2	1.78	0.66
1:B:256:PRO:HB3	1:B:270:LEU:HD23	1.77	0.66
1:B:144:TRP:CZ3	1:B:156:TRP:HA	2.32	0.65
1:B:342:LEU:HB2	7:B:1867:HOH:O	1.98	0.64
1:B:144:TRP:CE3	1:B:156:TRP:HA	2.33	0.63
1:A:119:VAL:O	1:A:123:VAL:HG23	1.98	0.63
1:B:210:TRP:HB2	1:B:258:LEU:HB3	1.80	0.63
1:A:211:ASN:HA	1:A:236:ILE:CD1	2.29	0.63
1:A:213:GLN:CD	4:A:864:327:H10	2.19	0.63
1:A:366:VAL:O	1:A:370:VAL:HG23	1.99	0.63
1:A:37:PHE:CD2	1:A:52:THR:HA	2.34	0.62
1:A:144:TRP:HB2	2:A:861:HEC:HBC3	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:LEU:HB3	1:B:72:LEU:HD12	1.81	0.62
1:B:331:ARG:NH1	1:B:335:ASP:OD2	2.33	0.61
1:A:429:GLU:OE2	1:B:72:LEU:HD23	2.00	0.61
1:A:182:LYS:HG3	1:A:275:LEU:HD22	1.83	0.60
1:B:325:SER:OG	1:B:385:ASP:HA	2.02	0.60
1:B:208:ARG:NH2	1:B:445:PRO:HD3	2.17	0.60
1:A:211:ASN:HA	1:A:236:ILE:HD12	1.84	0.59
1:A:364:ALA:O	1:A:368:ILE:HG13	2.02	0.59
1:A:213:GLN:NE2	4:A:864:327:H10	2.18	0.59
1:A:37:PHE:HD2	1:A:52:THR:HA	1.68	0.59
1:A:215:VAL:O	1:A:216:ARG:HG2	2.03	0.58
1:B:190:LEU:HD12	1:B:322:TRP:HB3	1.84	0.58
1:B:221:ARG:HE	1:B:234:VAL:CG1	2.04	0.58
1:A:441:TYR:OH	2:A:861:HEC:O2D	2.19	0.56
1:B:90:LEU:HD23	1:B:94:ARG:NH2	2.21	0.56
1:B:182:LYS:HG3	1:B:275:LEU:HD21	1.86	0.56
1:B:213:GLN:CD	1:B:216:ARG:HD3	2.26	0.55
1:A:426:PHE:O	5:A:866:MPD:H12	2.05	0.55
1:A:37:PHE:CD2	1:A:52:THR:HG22	2.41	0.55
1:A:213:GLN:HB2	1:A:216:ARG:CG	2.37	0.55
1:A:169:SER:OG	1:A:172:GLU:HG3	2.07	0.54
1:A:281:LEU:HG	1:A:295:ARG:HA	1.89	0.54
1:A:412:ALA:HB1	5:A:1867:MPD:H52	1.90	0.54
1:B:272:PRO:O	1:B:275:LEU:HB2	2.08	0.53
1:A:144:TRP:CE3	1:A:156:TRP:HA	2.43	0.53
1:B:256:PRO:HB3	1:B:270:LEU:CD2	2.37	0.53
1:B:221:ARG:CZ	1:B:234:VAL:HG11	2.38	0.53
1:B:216:ARG:HH11	1:B:216:ARG:HG3	1.73	0.53
1:A:429:GLU:CD	1:B:72:LEU:HD23	2.29	0.53
1:A:321:GLY:N	4:A:864:327:H5	2.22	0.53
1:A:144:TRP:CZ3	1:A:156:TRP:HA	2.43	0.53
1:B:42:ASN:HD22	1:B:428:GLN:NE2	2.07	0.53
1:A:213:GLN:HB2	1:A:216:ARG:HG2	1.90	0.53
1:A:330:THR:O	1:A:334:CYS:HB2	2.09	0.52
1:B:213:GLN:HB2	1:B:216:ARG:HD3	1.90	0.52
1:A:245:TRP:HB2	1:A:268:LEU:HD13	1.91	0.52
1:A:63:CYS:HB3	1:B:63:CYS:CB	2.40	0.52
1:B:221:ARG:NE	1:B:234:VAL:CG1	2.66	0.52
1:B:321:GLY:N	4:B:1864:327:H5	2.25	0.51
1:A:73:VAL:CG2	5:A:1867:MPD:HM2	2.41	0.51
1:B:203:GLY:O	1:B:204:ARG:HB2	2.09	0.51
1:B:90:LEU:O	1:B:94:ARG:HG3	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:364:ALA:O	1:B:368:ILE:HG13	2.10	0.51
4:A:864:327:C10	6:A:1865:CL:CL	2.96	0.51
1:B:330:THR:HG21	1:B:418:ILE:HG23	1.92	0.51
1:B:213:GLN:OE1	4:B:1864:327:H10	2.12	0.50
1:A:149:ARG:HB2	2:A:861:HEC:HAD2	1.93	0.50
1:B:115:ARG:O	1:B:119:VAL:HG13	2.12	0.50
1:B:286:LEU:HD13	1:B:288:TRP:CZ2	2.47	0.50
1:B:190:LEU:HD12	1:B:322:TRP:CB	2.42	0.49
1:A:436:SER:HA	1:A:437:PRO:C	2.33	0.49
1:B:283:HIS:CG	1:B:284:PRO:HD2	2.47	0.49
1:B:419:SER:HB3	1:B:422:LEU:HD12	1.94	0.48
1:A:195:THR:O	1:A:317:ALA:HA	2.14	0.48
1:B:144:TRP:CH2	2:B:1861:HEC:HMC3	2.48	0.48
1:B:223:GLN:O	1:B:224:ASP:HB3	2.14	0.48
1:A:274:GLU:N	1:A:274:GLU:CD	2.67	0.48
1:A:429:GLU:OE2	1:B:72:LEU:CD2	2.60	0.48
1:B:146:ASN:O	1:B:148:PRO:HD3	2.14	0.48
1:A:306:LEU:HD23	1:A:306:LEU:C	2.35	0.47
1:B:345:VAL:O	1:B:349:MET:HG3	2.14	0.47
1:B:130:GLN:N	1:B:130:GLN:OE1	2.47	0.47
1:B:38:PRO:HD2	1:B:51:ASP:O	2.14	0.47
1:A:258:LEU:HD13	1:A:268:LEU:HD21	1.96	0.47
5:A:866:MPD:H53	1:B:412:ALA:HB1	1.97	0.47
1:B:216:ARG:NH1	1:B:216:ARG:HG3	2.30	0.46
6:B:865:CL:CL	4:B:1864:327:C10	2.97	0.46
1:A:274:GLU:H	1:A:274:GLU:CD	2.18	0.46
1:A:432:ASN:ND2	1:A:432:ASN:C	2.68	0.46
1:A:197:PHE:HB3	1:A:198:PRO:HD2	1.98	0.46
1:A:325:SER:OG	1:A:385:ASP:HA	2.15	0.46
1:A:44:GLU:HG3	1:B:336:PRO:HG2	1.96	0.46
1:A:228:ARG:NH1	1:A:251:ARG:HG3	2.30	0.46
1:A:409:ALA:HB3	1:A:430:MET:HB3	1.97	0.46
1:B:90:LEU:HD11	1:B:120:GLU:HA	1.98	0.45
1:B:118:GLU:OE1	1:B:132:ARG:NH2	2.48	0.45
1:A:256:PRO:HB3	1:A:270:LEU:CD2	2.47	0.45
1:B:213:GLN:HB2	1:B:216:ARG:HG2	1.99	0.45
1:B:213:GLN:CD	4:B:1864:327:H10	2.36	0.45
1:A:63:CYS:HB3	1:B:63:CYS:HB3	1.99	0.45
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.52	0.45
1:B:93:ALA:O	1:B:97:ILE:HG12	2.17	0.45
1:A:213:GLN:NE2	4:A:864:327:C10	2.80	0.44
1:A:144:TRP:CH2	2:A:861:HEC:HMC3	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:CYS:HA	1:B:202:PRO:HD3	1.84	0.44
1:B:149:ARG:HB2	2:B:1861:HEC:HAD2	2.00	0.44
1:B:182:LYS:CG	1:B:275:LEU:HD21	2.48	0.44
1:A:435:LEU:O	1:A:438:ALA:HB2	2.18	0.44
1:B:177:ILE:O	1:B:181:ILE:HG13	2.18	0.44
1:B:330:THR:O	1:B:334:CYS:HB2	2.18	0.43
1:B:386:HIS:O	1:B:390:THR:HG23	2.17	0.43
1:A:89:LEU:O	1:A:89:LEU:HD12	2.18	0.43
1:A:412:ALA:HB1	5:A:1867:MPD:C5	2.48	0.43
2:A:861:HEC:HHC	2:A:861:HEC:HBB3	2.00	0.43
1:B:283:HIS:ND1	1:B:284:PRO:HD2	2.34	0.43
1:A:362:ASP:O	1:A:366:VAL:HG23	2.18	0.43
1:B:373:LEU:O	1:B:377:GLN:HG3	2.19	0.43
1:A:144:TRP:HB2	2:A:861:HEC:CBC	2.47	0.43
1:B:340:ASN:CG	1:B:340:ASN:O	2.57	0.43
1:B:274:GLU:HG3	1:B:274:GLU:H	1.46	0.43
1:B:333:LEU:O	1:B:341:ILE:HG12	2.19	0.43
1:A:201:CYS:HA	1:A:202:PRO:HD3	1.89	0.42
1:A:63:CYS:CB	1:B:63:CYS:HB3	2.49	0.42
1:B:330:THR:HG21	1:B:417:PRO:HB2	2.01	0.42
1:A:150:CYS:HB2	2:A:861:HEC:ND	2.34	0.42
1:B:306:LEU:HD23	1:B:306:LEU:C	2.40	0.42
1:B:324:MET:HA	1:B:384:VAL:O	2.20	0.42
1:B:223:GLN:O	1:B:224:ASP:CB	2.67	0.42
1:B:436:SER:HA	1:B:437:PRO:C	2.40	0.42
1:B:332:ASN:ND2	6:B:865:CL:CL	2.85	0.42
1:B:104:ILE:HD12	1:B:106:ARG:HG3	2.02	0.42
1:B:326:THR:HB	1:B:417:PRO:HG2	2.01	0.41
1:A:180:HIS:ND1	1:A:195:THR:OG1	2.44	0.41
1:B:197:PHE:HB3	1:B:198:PRO:HD2	2.02	0.41
1:A:228:ARG:HD3	1:A:249:ASN:O	2.19	0.41
1:A:306:LEU:HD23	1:A:307:LEU:N	2.35	0.41
1:A:182:LYS:HG3	1:A:275:LEU:CD2	2.50	0.41
1:B:129:TYR:C	1:B:130:GLN:OE1	2.59	0.41
1:A:197:PHE:HB3	1:A:198:PRO:CD	2.50	0.41
1:A:427:HIS:HE1	1:B:331:ARG:NH1	2.19	0.41
1:A:211:ASN:HA	1:A:236:ILE:HD11	1.99	0.41
1:B:362:ASP:O	1:B:366:VAL:HG23	2.20	0.41
2:B:1861:HEC:HBC2	2:B:1861:HEC:HMC1	2.02	0.41
1:B:147:ALA:HA	1:B:148:PRO:HD3	1.89	0.41
1:A:256:PRO:HB3	1:A:270:LEU:HD23	2.03	0.41
1:B:302:VAL:HB	1:B:319:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:205:GLY:O	1:B:262:PRO:HB3	2.21	0.41
1:B:69:LEU:HB3	1:B:72:LEU:CD1	2.50	0.41
1:A:419:SER:HB3	1:A:422:LEU:HD12	2.03	0.40
1:B:195:THR:O	1:B:317:ALA:HA	2.21	0.40
1:A:63:CYS:HB3	1:B:63:CYS:HB2	2.04	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	Distance(Å)	Clash(Å)
1:B:113:GLU:OE2	7:A:1906:HOH:O[3_545]	1.89	0.31

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	395/427 (92%)	377 (95%)	17 (4%)	1 (0%)	50	66
1	B	397/427 (93%)	371 (94%)	24 (6%)	2 (0%)	38	51
All	All	792/854 (93%)	748 (94%)	41 (5%)	3 (0%)	43	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
1	B	224	ASP
1	B	204	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/359 (92%)	325 (98%)	7 (2%)	66	84
1	B	334/359 (93%)	329 (98%)	5 (2%)	76	90
All	All	666/718 (93%)	654 (98%)	12 (2%)	71	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	95	ASP
1	A	115	ARG
1	A	223	GLN
1	A	258	LEU
1	A	295	ARG
1	A	432	ASN
1	B	67	ARG
1	B	201	CYS
1	B	223	GLN
1	B	274	GLU
1	B	432	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	432	ASN
1	B	99	GLN
1	B	110	GLN
1	B	223	GLN
1	B	428	GLN
1	B	432	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 11 ligands modelled in this entry, 3 are 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$
5	MPD	A	1866	-	7,7,7	0.51	0	10,10,10	0.55	0
5	MPD	A	1867	-	7,7,7	0.39	0	10,10,10	0.44	0
2	HEC	A	861	1	50,50,50	2.98	13 (26%)	56,82,82	2.31	21 (37%)
4	327	A	864	-	15,15,15	2.18	3 (20%)	13,20,20	5.22	5 (38%)
5	MPD	A	866	-	7,7,7	0.60	0	10,10,10	0.48	0
2	HEC	B	1861	1	50,50,50	2.99	14 (28%)	56,82,82	2.39	19 (33%)
4	327	B	1864	-	15,15,15	2.25	3 (20%)	13,20,20	5.20	5 (38%)
5	MPD	B	867	-	7,7,7	0.58	0	10,10,10	0.37	0

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
5	MPD	A	1866	-	-	0/5/5/5	0/0/0/0
5	MPD	A	1867	-	-	0/5/5/5	0/0/0/0
2	HEC	A	861	1	-	0/10/54/54	0/0/8/8
4	327	A	864	-	-	0/3/16/16	0/0/2/2
5	MPD	A	866	-	-	0/5/5/5	0/0/0/0
2	HEC	B	1861	1	-	0/10/54/54	0/0/8/8
4	327	B	1864	-	-	0/3/16/16	0/0/2/2
5	MPD	B	867	-	-	0/5/5/5	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	861	HEC	C3B-CAB	9.66	1.55	1.35
2	B	1861	HEC	C3B-CAB	9.29	1.54	1.35
2	A	861	HEC	C3C-CAC	9.06	1.54	1.35
2	B	1861	HEC	C3C-CAC	8.93	1.53	1.35
2	B	1861	HEC	C1D-C2D	8.81	1.51	1.40
2	A	861	HEC	C1D-C2D	8.31	1.50	1.40
4	B	1864	327	C7-C1	6.82	1.59	1.50
4	A	864	327	C7-C1	6.59	1.59	1.50
2	B	1861	HEC	C1C-C2C	6.46	1.48	1.40
2	A	861	HEC	C1C-C2C	6.10	1.47	1.40
2	A	861	HEC	C1B-C2B	5.19	1.46	1.40
2	B	1861	HEC	C1B-C2B	5.14	1.46	1.40
2	A	861	HEC	C3B-C4B	4.86	1.47	1.41
2	B	1861	HEC	C4D-C3D	4.52	1.51	1.43
2	A	861	HEC	C4D-C3D	4.47	1.51	1.43
2	B	1861	HEC	C3B-C4B	4.15	1.46	1.41
2	B	1861	HEC	FE-NC	3.91	2.09	1.92
2	B	1861	HEC	C3C-C4C	3.78	1.46	1.41
2	A	861	HEC	C3C-C4C	3.66	1.46	1.41
2	A	861	HEC	FE-ND	3.62	2.08	1.92
4	B	1864	327	C1-N1	3.62	1.54	1.47
2	B	1861	HEC	FE-ND	3.22	2.06	1.92
4	A	864	327	C1-N1	3.11	1.53	1.47
2	A	861	HEC	FE-NC	3.08	2.05	1.92
2	A	861	HEC	C3B-C2B	-2.90	1.35	1.41
2	B	1861	HEC	C3B-C2B	-2.75	1.35	1.41
2	B	1861	HEC	C4A-NA	2.67	1.40	1.37
2	A	861	HEC	C4A-NA	2.46	1.40	1.37
2	B	1861	HEC	CAA-C2A	2.26	1.57	1.52
2	B	1861	HEC	C3C-C2C	-2.25	1.36	1.41
4	A	864	327	C8-C1	-2.24	1.48	1.53
4	B	1864	327	C4-C2	2.16	1.50	1.47
2	A	861	HEC	CAA-C2A	2.06	1.56	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1864	327	C9-C8-C1	-17.32	96.62	114.58
4	A	864	327	C9-C8-C1	-17.21	96.73	114.58
2	B	1861	HEC	CBD-CAD-C3D	-10.77	93.73	112.69
2	A	861	HEC	CBD-CAD-C3D	-9.77	95.47	112.69
4	A	864	327	C7-C1-N1	-5.13	103.46	111.84
4	B	1864	327	C7-C1-N1	-4.70	104.18	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1861	HEC	C2B-C1B-NB	4.63	112.91	109.41
2	A	861	HEC	C2B-C1B-NB	4.49	112.80	109.41
2	A	861	HEC	C2C-C1C-NC	3.95	112.39	109.41
2	B	1861	HEC	C2C-C1C-NC	3.93	112.38	109.41
2	B	1861	HEC	O1D-CGD-CBD	-3.72	110.24	123.03
2	A	861	HEC	O1D-CGD-CBD	-3.63	110.55	123.03
2	A	861	HEC	C2D-C1D-ND	3.61	112.14	109.41
4	A	864	327	O1-C7-C1	-3.54	104.53	112.36
4	B	1864	327	O1-C7-C1	-3.39	104.87	112.36
2	B	1861	HEC	C2D-C1D-ND	3.29	111.90	109.41
2	A	861	HEC	C4D-C3D-C2D	-3.29	103.52	106.92
2	B	1861	HEC	C4D-C3D-C2D	-3.26	103.54	106.92
2	A	861	HEC	C4A-CHB-C1B	-3.26	123.18	127.47
4	A	864	327	C1-N1-C2	-3.08	117.12	126.03
2	B	1861	HEC	CAD-CBD-CGD	2.91	122.81	113.47
4	B	1864	327	C1-N1-C2	-2.85	117.78	126.03
2	A	861	HEC	CMC-C2C-C3C	2.84	128.85	125.72
2	A	861	HEC	C4B-NB-C1B	-2.82	103.05	106.76
2	B	1861	HEC	C4B-NB-C1B	-2.81	103.06	106.76
2	B	1861	HEC	C3B-C2B-C1B	-2.73	105.25	107.07
2	A	861	HEC	C1A-CHA-C4D	2.71	131.03	127.47
2	B	1861	HEC	C4A-CHB-C1B	-2.67	123.96	127.47
2	B	1861	HEC	C4C-NC-C1C	-2.58	103.36	106.76
2	B	1861	HEC	CBB-CAB-C3B	-2.57	121.20	128.44
2	A	861	HEC	CAD-CBD-CGD	2.56	121.68	113.47
2	B	1861	HEC	CMC-C2C-C3C	2.55	128.54	125.72
4	B	1864	327	C7-O1-C3	2.55	122.74	116.25
2	A	861	HEC	C4C-NC-C1C	-2.51	103.46	106.76
2	A	861	HEC	C3B-C2B-C1B	-2.49	105.41	107.07
2	B	1861	HEC	CMB-C2B-C3B	2.45	128.43	125.72
2	A	861	HEC	CMD-C2D-C1D	-2.42	124.89	128.62
2	B	1861	HEC	CMD-C2D-C1D	-2.41	124.91	128.62
2	A	861	HEC	CBB-CAB-C3B	-2.40	121.70	128.44
2	A	861	HEC	CMB-C2B-C3B	2.32	128.28	125.72
4	A	864	327	C7-O1-C3	2.27	122.04	116.25
2	B	1861	HEC	C3D-C4D-ND	2.25	112.86	109.73
2	B	1861	HEC	C3C-C2C-C1C	-2.25	105.57	107.07
2	B	1861	HEC	O2D-CGD-CBD	2.22	122.07	114.22
2	A	861	HEC	C3C-C2C-C1C	-2.19	105.61	107.07
2	A	861	HEC	C3D-C4D-ND	2.17	112.75	109.73
2	A	861	HEC	O2D-CGD-CBD	2.13	121.75	114.22
2	B	1861	HEC	C2B-C1B-CHB	-2.12	121.98	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	861	HEC	C2B-C1B-CHB	-2.09	122.04	126.00
2	A	861	HEC	CMC-C2C-C1C	-2.02	125.52	128.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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	399/427 (93%)	-0.25	6 (1%) 70 69	24, 36, 54, 66	0
1	B	401/427 (93%)	-0.18	7 (1%) 67 65	23, 40, 58, 70	0
All	All	800/854 (93%)	-0.22	13 (1%) 68 67	23, 38, 56, 70	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	GLN	4.3
1	B	58	GLN	3.4
1	A	223	GLN	3.3
1	B	249	ASN	3.3
1	A	59	GLN	3.3
1	B	223	GLN	2.9
1	A	354	ARG	2.8
1	B	225	GLY	2.7
1	A	86	PRO	2.7
1	B	224	ASP	2.6
1	A	352	ASP	2.3
1	B	226	SER	2.1
1	B	86	PRO	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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MPD	A	866	8/8	0.46	13.44	66,67,69,71	0
5	MPD	A	1867	8/8	0.30	12.48	52,53,54,54	0
5	MPD	A	1866	8/8	0.27	6.95	54,56,57,58	0
4	327	B	1864	14/14	0.21	4.79	43,45,50,53	0
5	MPD	B	867	8/8	0.24	4.67	54,56,56,58	0
4	327	A	864	14/14	0.23	2.88	42,46,49,53	0
6	CL	B	865	1/1	0.20	2.47	71,71,71,71	0
2	HEC	B	1861	43/43	0.15	1.22	30,34,51,59	0
2	HEC	A	861	43/43	0.16	0.89	33,35,48,53	0
6	CL	A	1865	1/1	0.13	-0.50	52,52,52,52	0
3	ZN	A	862	1/1	0.03	-2.37	39,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.