



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2016 – 05:08 AM EDT

PDB ID : 4XYD
Title : Nitric oxide reductase from *Roseobacter denitrificans* (RdNOR)
Authors : Crow, A.
Deposited on : 2015-02-02
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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) : rb-20027790

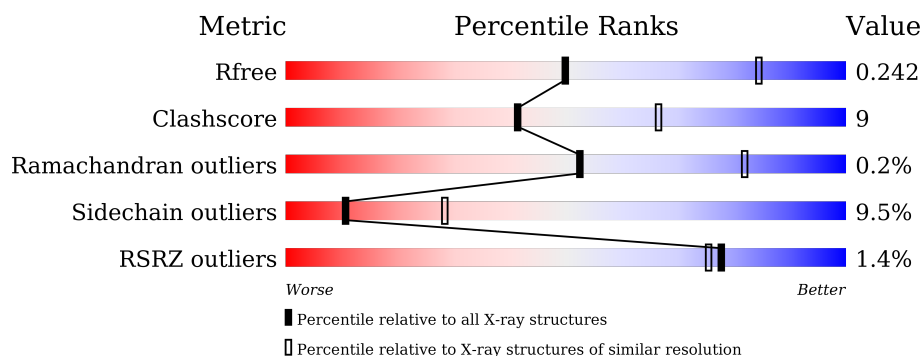
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 $\leq 5\%$. 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	456	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>..</div> </div> </div>
2	B	150	<div> <div></div> <div> <div>75%</div> <div>20%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4876 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.

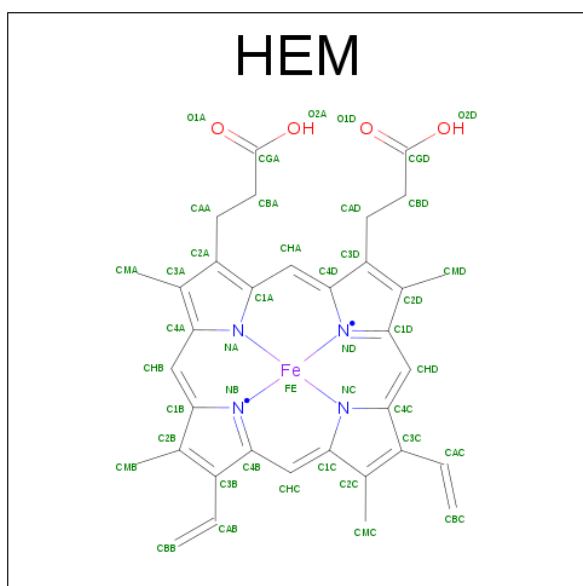
- Molecule 1 is a protein called Nitric-oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3563	2405	559	579	20			

- Molecule 2 is a protein called NorC-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	2	0
			1163	737	200	219	7			

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



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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------|---------|---------|
| 4 | A | 1 | Total O
2 2 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | A | 1 | Total Ca
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 6 | A | 1 | Total Fe
1 1 | 0 | 0 |

- # HEC
-
- The chemical structure of HEC (Hydroxyethylchlorin) is a complex macrocyclic molecule. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including hydroxyl groups (OH) and carboxylic acid groups (COOH). The side chains are labeled with green text: C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, C1AR, C2AR, C3AR, C4AR, C1AS, C2AS, C3AS, C4AS, C1AT, C2AT, C3AT, C4AT, C1AU, C2AU, C3AU, C4AU, C1AV, C2AV, C3AV, C4AV, C1AW, C2AW, C3AW, C4AW, C1AX, C2AX, C3AX, C4AX, C1AY, C2AY, C3AY, C4AY, C1AZ, C2AZ, C3AZ, C4AZ, C1BA, C2BA, C3BA, C4BA, C1BB, C2BB, C3BB, C4BB, C1BC, C2BC, C3BC, C4BC, C1BD, C2BD, C3BD, C4BD, C1BE, C2BE, C3BE, C4BE, C1BF, C2BF, C3BF, C4BF, C1BG, C2BG, C3BG, C4BG, C1BH, C2BH, C3BH, C4BH, C1BI, C2BI, C3BI, C4BI, C1BJ, C2BJ, C3BJ, C4BJ, C1BK, C2BK, C3BK, C4BK, C1BL, C2BL, C3BL, C4BL, C1BM, C2BM, C3BM, C4BM, C1BN, C2BN, C3BN, C4BN, C1BO, C2BO, C3BO, C4BO, C1BP, C2BP, C3BP, C4BP, C1BQ, C2BQ, C3BQ, C4BQ, C1BR, C2BR, C3BR, C4BR, C1BS, C2BS, C3BS, C4BS, C1BT, C2BT, C3BT, C4BT, C1BU, C2BU, C3BU, C4BU, C1BV, C2BV, C3BV, C4BV, C1BW, C2BW, C3BW, C4BW, C1BX, C2BX, C3BX, C4BX, C1BY, C2BY, C3BY, C4BY, C1BZ, C2BZ, C3BZ, C4BZ, C1CA, C2CA, C3CA, C4CA, C1CB, C2CB, C3CB, C4CB, C1CC, C2CC, C3CC, C4CC, C1CD, C2CD, C3CD, C4CD, C1CE, C2CE, C3CE, C4CE, C1CF, C2CF, C3CF, C4CF, C1CG, C2CG, C3CG, C4CG, C1CH, C2CH, C3CH, C4CH, C1CI, C2CI, C3CI, C4CI, C1CJ, C2CJ, C3CJ, C4CJ, C1CK, C2CK, C3CK, C4CK, C1CL, C2CL, C3CL, C4CL, C1CM, C2CM, C3CM, C4CM, C1CN, C2CN, C3CN, C4CN, C1CO, C2CO, C3CO, C4CO, C1CP, C2CP, C3CP, C4CP, C1CQ, C2CQ, C3CQ, C4CQ, C1CR, C2CR, C3CR, C4CR, C1CS, C2CS, C3CS, C4CS, C1CT, C2CT, C3CT, C4CT, C1CU, C2CU, C3CU, C4CU, C1CV, C2CV, C3CV, C4CV, C1CW, C2CW, C3CW, C4CW, C1CX, C2CX, C3CX, C4CX, C1CY, C2CY, C3CY, C4CY, C1CZ, C2CZ, C3CZ, C4CZ, C1DA, C2DA, C3DA, C4DA, C1DB, C2DB, C3DB, C4DB, C1DC, C2DC, C3DC, C4DC, C1DD, C2DD, C3DD, C4DD, C1DE, C2DE, C3DE, C4DE, C1DF, C2DF, C3DF, C4DF, C1DG, C2DG, C3DG, C4DG, C1DH, C2DH, C3DH, C4DH, C1DI, C2DI, C3DI, C4DI, C1DJ, C2DJ, C3DJ, C4DJ, C1DK, C2DK, C3DK, C4DK, C1DL, C2DL, C3DL, C4DL, C1DM, C2DM, C3DM, C4DM, C1DN, C2DN, C3DN, C4DN, C1DO, C2DO, C3DO, C4DO, C1DP, C2DP, C3DP, C4DP, C1DQ, C2DQ, C3DQ, C4DQ, C1DR, C2DR, C3DR, C4DR, C1DS, C2DS, C3DS, C4DS, C1DT, C2DT, C3DT, C4DT, C1DU, C2DU, C3DU, C4DU, C1DV, C2DV, C3DV, C4DV, C1DW, C2DW, C3DW, C4DW, C1DX, C2DX, C3DX, C4DX, C1DY, C2DY, C3DY, C4DY, C1DZ, C2DZ, C3DZ, C4DZ, C1EA, C2EA, C3EA, C4EA, C1EB, C2EB, C3EB, C4EB, C1EC, C2EC, C3EC, C4EC, C1ED, C2ED, C3ED, C4ED, C1EE, C2EE, C3EE, C4EE, C1EF, C2EF, C3EF, C4EF, C1EG, C2EG, C3EG, C4EG, C1EH, C2EH, C3EH, C4EH, C1EI, C2EI, C3EI, C4EI, C1EJ, C2EJ, C3EJ, C4EJ, C1EK, C2EK, C3EK, C4EK, C1EL, C2EL, C3EL, C4EL, C1EM, C2EM, C3EM, C4EM, C1EN, C2EN, C3EN, C4EN, C1EO, C2EO, C3EO, C4EO, C1EP, C2EP, C3EP, C4EP, C1EQ, C2EQ, C3EQ, C4EQ, C1ER, C2ER, C3ER, C4ER, C1ES, C2ES, C3ES, C4ES, C1ET, C2ET, C3ET, C4ET, C1EU, C2EU, C3EU, C4EU, C1EV, C2EV, C3EV, C4EV, C1EW, C2EW, C3EW, C4EW, C1EX, C2EX, C3EX, C4EX, C1EY, C2EY, C3EY, C4EY, C1EZ, C2EZ, C3EZ, C4EZ, C1FA, C2FA, C3FA, C4FA, C1FB, C2FB, C3FB, C4FB, C1FC, C2FC, C3FC, C4FC, C1FD, C2FD, C3FD, C4FD, C1FE, C2FE, C3FE, C4FE, C1FF, C2FF, C3FF, C4FF, C1FG, C2FG, C3FG, C4FG, C1FH, C2FH, C3FH, C4FH, C1FI, C2FI, C3FI, C4FI, C1FJ, C2FJ, C3FJ, C4FJ, C1FK, C2FK, C3FK, C4FK, C1FL, C2FL, C3FL, C4FL, C1FM, C2FM, C3FM, C4FM, C1FN, C2FN, C3FN, C4FN, C1FO, C2FO, C3FO, C4FO, C1FP, C2FP, C3FP, C4FP, C1FQ, C2FQ, C3FQ, C4FQ, C1FR, C2FR, C3FR, C4FR, C1FS, C2FS, C3FS, C4FS, C1FT, C2FT, C3FT, C4FT, C1FU, C2FU, C3FU, C4FU, C1FV, C2FV, C3FV, C4FV, C1FW, C2FW, C3FW, C4FW, C1FX, C2FX, C3FX, C4FX, C1FY, C2FY, C3FY, C4FY, C1FZ, C2FZ, C3FZ, C4FZ, C1GA, C2GA, C3GA, C4GA, C1GB, C2GB, C3GB, C4GB, C1GC, C2GC, C3GC, C4GC, C1GD, C2GD, C3GD, C4GD, C1GE, C2GE, C3GE, C4GE, C1GF, C2GF, C3GF, C4GF, C1GG, C2GG, C3GG, C4GG, C1GH, C2GH, C3GH, C4GH, C1GI, C2GI, C3GI, C4GI, C1GJ, C2GJ, C3GJ, C4GJ, C1GK, C2GK, C3GK, C4GK, C1GL, C2GL, C3GL, C4GL, C1GM, C2GM, C3GM, C4GM, C1GN, C2GN, C3GN, C4GN, C1GO, C2GO, C3GO, C4GO, C1GP, C2GP, C3GP, C4GP, C1GQ, C2GQ, C3GQ, C4GQ, C1GR, C2GR, C3GR, C4GR, C1GS, C2GS, C3GS, C4GS, C1GT, C2GT, C3GT, C4GT, C1GU, C2GU, C3GU, C4GU, C1GV, C2GV, C3GV, C4GV, C1GW, C2GW, C3GW, C4GW, C1GX, C2GX, C3GX, C4GX, C1GY, C2GY, C3GY, C4GY, C1GZ, C2GZ, C3GZ, C4GZ, C1HA, C2HA, C3HA, C4HA, C1HB, C2HB, C3HB, C4HB, C1HC, C2HC, C3HC, C4HC, C1HD, C2HD, C3HD, C4HD, C1HE, C2HE, C3HE, C4HE, C1HF, C2HF, C3HF, C4HF, C1HG, C2HG, C3HG, C4HG, C1HH, C2HH, C3HH, C4HH, C1HI, C2HI, C3HI, C4HI, C1HJ, C2HJ, C3HJ, C4HJ, C1HK, C2HK, C3HK, C4HK, C1HL, C2HL, C3HL, C4HL, C1HM, C2HM, C3HM, C4HM, C1HN, C2HN, C3HN, C4HN, C1HO, C2HO, C3HO, C4HO, C1HP, C2HP, C3HP, C4HP, C1HQ, C2HQ, C3HQ, C4HQ, C1HR, C2HR, C3HR, C4HR, C1HS, C2HS, C3HS, C4HS, C1HT, C2HT, C3HT, C4HT, C1HU, C2HU, C3HU, C4HU, C1HV, C2HV, C3HV, C4HV, C1HW, C2HW, C3HW, C4HW, C1HX, C2HX, C3HX, C4HX, C1HY, C2HY, C3HY, C4HY, C1HZ, C2HZ, C3HZ, C4HZ, C1IA, C2IA, C3IA, C4IA, C1IB, C2IB, C3IB, C4IB, C1IC, C2IC, C3IC, C4IC, C1ID, C2ID, C3ID, C4ID, C1IE, C2IE, C3IE, C4IE, C1IF, C2IF, C3IF, C4IF, C1IG, C2IG, C3IG, C4IG, C1IH, C2IH, C3IH, C4IH, C1II, C2II, C

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	12	Total 12	O 12	0	0
9	B	4	Total 4	O 4	0	0

- Molecule 1: Nitric-oxide reductase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.22Å 98.83Å 126.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.36 – 2.85 45.37 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.1 (53.36-2.85) 97.1 (45.37-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.188 , 0.243 0.193 , 0.242	Depositor DCC
R_{free} test set	1285 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4876	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 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE, HEC, HEM, UNL, CU

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	0.47	0/3679	0.65	1/5015 (0.0%)
2	B	0.47	0/1196	0.64	0/1627
All	All	0.47	0/4875	0.65	1/6642 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LEU	CA-CB-CG	6.03	129.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3563	0	3594	64	0
2	B	1163	0	1084	21	0
3	A	86	0	60	14	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	B	43	0	30	5	0
8	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	12	0	0	0	0
9	B	4	0	0	0	0
All	All	4876	0	4768	82	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 9.

All (82) 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:94:MET:O	1:A:98:THR:HG22	1.75	0.86
1:A:142:MET:CE	1:A:165:LEU:HB3	2.08	0.83
1:A:57:LEU:HD13	3:A:501:HEM:HBC2	1.65	0.79
1:A:142:MET:HE3	1:A:165:LEU:HB3	1.62	0.78
1:A:409:GLN:HE21	2:B:114:ARG:HH22	1.32	0.77
1:A:57:LEU:HD13	3:A:501:HEM:CBC	2.22	0.70
1:A:113:ASN:HD22	1:A:115:LEU:H	1.40	0.68
1:A:409:GLN:NE2	2:B:114:ARG:HH22	1.92	0.68
1:A:113:ASN:ND2	1:A:115:LEU:H	1.92	0.67
1:A:445:ILE:HD13	1:A:445:ILE:H	1.61	0.66
1:A:115:LEU:HA	1:A:128:VAL:HG13	1.78	0.66
1:A:377:ALA:O	1:A:381:THR:HG23	1.99	0.63
1:A:343:TYR:HE2	3:A:504:HEM:HBB2	1.64	0.62
1:A:57:LEU:CD1	3:A:501:HEM:CBC	2.78	0.62
1:A:381:THR:HA	1:A:384:THR:HG23	1.83	0.61
1:A:380:MET:CE	3:A:501:HEM:HMC3	2.30	0.61
1:A:124:LEU:HA	1:A:126:GLN:HE22	1.67	0.60
1:A:142:MET:HE1	1:A:165:LEU:HB3	1.84	0.59
2:B:8:SER:O	2:B:12:ASN:ND2	2.36	0.59
1:A:343:TYR:HE2	3:A:504:HEM:CBB	2.16	0.59
1:A:409:GLN:HE21	2:B:114:ARG:NH2	1.97	0.59
2:B:49[A]:GLU:OE1	2:B:49[A]:GLU:HA	2.03	0.59
2:B:113:ARG:NH1	7:B:201:HEC:O2D	2.38	0.57
2:B:113:ARG:NH1	7:B:201:HEC:CGD	2.68	0.57
1:A:113:ASN:ND2	1:A:116:LEU:H	2.04	0.56
1:A:337:LEU:HB2	1:A:384:THR:HG21	1.88	0.55
1:A:190:TRP:CE2	1:A:246:HIS:HB3	2.42	0.55
7:B:201:HEC:HMB1	7:B:201:HEC:HBB3	1.88	0.54
1:A:380:MET:O	1:A:384:THR:HG22	2.08	0.54
1:A:380:MET:HE1	3:A:501:HEM:HMC3	1.88	0.53
2:B:54:LYS:O	2:B:57:TRP:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CE2	1:A:40:LEU:HD22	2.43	0.53
1:A:257:GLN:O	1:A:261:SER:HB2	2.09	0.53
2:B:118:ASN:ND2	2:B:120:GLY:H	2.06	0.52
1:A:219:VAL:HG13	1:A:223:ILE:HD12	1.92	0.52
1:A:113:ASN:HD22	1:A:115:LEU:N	2.08	0.51
1:A:297:TRP:HB3	1:A:349:ALA:HB2	1.92	0.51
1:A:2:LYS:HB3	1:A:3:TYR:CE1	2.46	0.51
1:A:189:TRP:CH2	1:A:193:VAL:HG21	2.46	0.51
1:A:214:LEU:HD21	1:A:221:ARG:NH1	2.26	0.51
1:A:209:LEU:HD21	1:A:302:ALA:HB2	1.93	0.50
1:A:328:THR:HG23	1:A:330:ILE:H	1.76	0.50
1:A:167:GLY:C	1:A:200:THR:HG21	2.32	0.50
1:A:235:ALA:HA	1:A:270:PRO:HG3	1.94	0.50
1:A:55:ASN:ND2	1:A:105:TYR:OH	2.45	0.49
1:A:301:CYS:SG	1:A:346:LEU:HB2	2.53	0.49
1:A:331:THR:HG23	3:A:504:HEM:HBD1	1.94	0.49
1:A:70:TYR:OH	1:A:90:GLN:NE2	2.43	0.49
2:B:144:TRP:CG	2:B:145:PRO:HA	2.47	0.49
2:B:113:ARG:NH1	7:B:201:HEC:O1D	2.46	0.48
2:B:52:HIS:HE1	2:B:124:GLU:OE2	1.97	0.47
2:B:41:THR:HG22	2:B:139:ILE:HG12	1.96	0.47
1:A:213:MET:HA	1:A:213:MET:CE	2.45	0.47
2:B:102:TRP:HZ2	7:B:201:HEC:HBD1	1.80	0.47
1:A:380:MET:HE1	3:A:501:HEM:CMC	2.46	0.46
1:A:380:MET:HE3	3:A:501:HEM:HMC3	1.96	0.46
1:A:212:LEU:HD13	1:A:298:SER:OG	2.15	0.46
1:A:201:TRP:HB3	1:A:343:TYR:CE1	2.52	0.45
3:A:504:HEM:HBC2	3:A:504:HEM:HHD	1.99	0.45
2:B:75:PHE:CZ	2:B:114:ARG:HG2	2.52	0.45
2:B:118:ASN:HD22	2:B:120:GLY:H	1.66	0.44
1:A:396:HIS:O	1:A:400:VAL:HG22	2.18	0.44
1:A:101:VAL:HG23	1:A:130:VAL:HG21	1.99	0.44
1:A:343:TYR:CE2	3:A:504:HEM:CBB	2.99	0.44
1:A:261:SER:OG	1:A:318:LEU:HA	2.17	0.44
1:A:445:ILE:CD1	1:A:445:ILE:H	2.29	0.44
1:A:191:TYR:O	1:A:195:LEU:HB2	2.18	0.43
1:A:40:LEU:HG	1:A:43:ILE:HD12	2.00	0.43
2:B:34:ARG:HA	2:B:37:VAL:HG12	2.00	0.43
1:A:297:TRP:CH2	1:A:348:LEU:HD23	2.53	0.43
2:B:6:THR:O	2:B:9:MET:HB3	2.19	0.43
1:A:126:GLN:HE21	1:A:131:LYS:HE3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HD11	3:A:501:HEM:HBC1	2.01	0.42
1:A:314:PHE:O	1:A:317:THR:HG22	2.20	0.42
2:B:145:PRO:HB2	2:B:146:PRO:HD2	2.01	0.42
1:A:241:LEU:HD12	1:A:263:PHE:CZ	2.55	0.41
1:A:402:GLY:HA2	2:B:147:ASN:HD21	1.86	0.41
1:A:257:GLN:HE22	2:B:142:GLN:HG3	1.86	0.41
1:A:30:LEU:HD22	1:A:46:PHE:CE1	2.56	0.40
1:A:155:THR:O	1:A:158:THR:HG22	2.22	0.40
1:A:188:TYR:O	1:A:191:TYR:HB2	2.22	0.40
1:A:197:VAL:HG13	3:A:504:HEM:HBB2	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	443/456 (97%)	413 (93%)	29 (6%)	1 (0%)	52	82
2	B	145/150 (97%)	143 (99%)	2 (1%)	0	100	100
All	All	588/606 (97%)	556 (95%)	31 (5%)	1 (0%)	52	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ARG

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	365/374 (98%)	329 (90%)	36 (10%)	10	27
2	B	121/124 (98%)	111 (92%)	10 (8%)	14	36
All	All	486/498 (98%)	440 (90%)	46 (10%)	11	28

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	43	ILE
1	A	60	TRP
1	A	75	GLU
1	A	96	LEU
1	A	98	THR
1	A	99	LEU
1	A	113	ASN
1	A	121	ARG
1	A	126	GLN
1	A	128	VAL
1	A	154	LYS
1	A	158	THR
1	A	197	VAL
1	A	230	LEU
1	A	236	LEU
1	A	245	HIS
1	A	257	GLN
1	A	261	SER
1	A	264	SER
1	A	268	VAL
1	A	281	MET
1	A	312	TRP
1	A	315	LEU
1	A	316	HIS
1	A	328	THR
1	A	348	LEU
1	A	358	LEU
1	A	360	LYS
1	A	361	ARG
1	A	381	THR
1	A	384	THR
1	A	401	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	422	SER
1	A	424	ILE
1	A	445	ILE
2	B	9	MET
2	B	19	LEU
2	B	28	LEU
2	B	39	THR
2	B	46	LEU
2	B	63	VAL
2	B	88	VAL
2	B	90	ASP
2	B	111	GLU
2	B	118	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	55	ASN
1	A	90	GLN
1	A	108	ASN
1	A	113	ASN
1	A	126	GLN
1	A	257	GLN
1	A	316	HIS
1	A	409	GLN
2	B	12	ASN
2	B	118	ASN

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 7 ligands modelled in this entry, 1 is unknown and 3 are monoatomic - leaving 3 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	$\# Z > 2$
3	HEM	A	501	1,5	24,50,50	0.91	1 (4%)	16,82,82	2.81	6 (37%)
3	HEM	A	504	1,5,4	24,50,50	0.78	1 (4%)	16,82,82	1.61	5 (31%)
7	HEC	B	201	2	24,50,50	2.37	10 (41%)	19,82,82	3.01	7 (36%)

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
3	HEM	A	501	1,5	-	0/6/54/54	0/0/8/8
3	HEM	A	504	1,5,4	-	0/6/54/54	0/0/8/8
7	HEC	B	201	2	-	0/6/54/54	0/0/8/8

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	HEM	C3B-C2B	-3.00	1.36	1.40
3	A	504	HEM	C1B-NB	-2.03	1.34	1.36
7	B	201	HEC	C3B-C4B	2.20	1.47	1.43
7	B	201	HEC	C1C-CHC	2.35	1.46	1.40
7	B	201	HEC	C3C-C4C	2.41	1.47	1.43
7	B	201	HEC	C1B-CHB	2.47	1.46	1.40
7	B	201	HEC	C1D-CHD	2.48	1.46	1.40
7	B	201	HEC	C4D-CHA	2.78	1.47	1.40
7	B	201	HEC	C3D-C2D	3.07	1.46	1.37
7	B	201	HEC	C2A-C3A	3.16	1.47	1.37
7	B	201	HEC	C3C-C2C	5.25	1.46	1.40
7	B	201	HEC	C3B-C2B	6.14	1.47	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	201	HEC	CBD-CAD-C3D	-7.18	99.87	112.49
7	B	201	HEC	CBA-CAA-C2A	-6.99	100.21	112.47
3	A	501	HEM	CBD-CAD-C3D	-6.60	100.90	112.47
7	B	201	HEC	CBB-CAB-C3B	-5.77	114.72	127.34
3	A	501	HEM	C3C-CAC-CBC	-5.14	116.06	126.40
3	A	504	HEM	CBA-CAA-C2A	-2.87	107.45	112.49
3	A	501	HEM	CBA-CAA-C2A	-2.74	107.68	112.49
3	A	504	HEM	C3C-CAC-CBC	-2.57	121.23	126.40
3	A	504	HEM	CMA-C3A-C4A	-2.49	124.07	128.31
3	A	501	HEM	C3B-CAB-CBB	-2.42	121.54	126.40
3	A	504	HEM	C3C-C4C-NC	-2.39	106.43	110.94
3	A	501	HEM	C3B-C4B-NB	-2.27	106.28	109.21
3	A	504	HEM	C3B-CAB-CBB	-2.00	122.37	126.40
7	B	201	HEC	CMB-C2B-C1B	2.09	131.87	128.31
7	B	201	HEC	CMA-C3A-C2A	2.12	129.68	125.24
7	B	201	HEC	CMB-C2B-C3B	2.46	128.52	125.67
7	B	201	HEC	CMC-C2C-C3C	3.12	129.29	125.67
3	A	501	HEM	CAD-CBD-CGD	4.75	122.03	112.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	HEM	8	0
3	A	504	HEM	6	0
7	B	201	HEC	5	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	445/456 (97%)	-0.32	8 (1%) 71 68	35, 55, 78, 123	0
2	B	145/150 (96%)	-0.18	0 100 100	39, 57, 85, 131	0
All	All	590/606 (97%)	-0.28	8 (1%) 78 75	35, 55, 82, 131	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	404	TYR	3.5
1	A	401	GLN	3.2
1	A	400	VAL	2.7
1	A	403	ASP	2.7
1	A	82	HIS	2.3
1	A	407	ASP	2.0
1	A	402	GLY	2.0
1	A	4	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	HEM	A	504	43/43	0.96	0.17	0.10	48,55,62,65	0
3	HEM	A	501	43/43	0.98	0.17	-0.01	33,37,53,58	0
4	UNL	A	502	2/-	0.96	0.16	-0.22	43,43,43,51	0
7	HEC	B	201	43/43	0.98	0.15	-0.26	38,41,55,64	0
8	CU	B	202	1/1	0.98	0.07	-2.13	92,92,92,92	0
6	FE	A	505	1/1	0.99	0.06	-4.70	56,56,56,56	0
5	CA	A	503	1/1	0.97	0.09	-4.91	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.