



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:39 AM GMT

PDB ID : 3ML1  
Title : Crystal Structure of the Periplasmic Nitrate Reductase from *Cupriavidus necator*  
Authors : Coelho, C.; Trincao, J.; Romao, M.J.  
Deposited on : 2010-04-16  
Resolution : 1.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 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

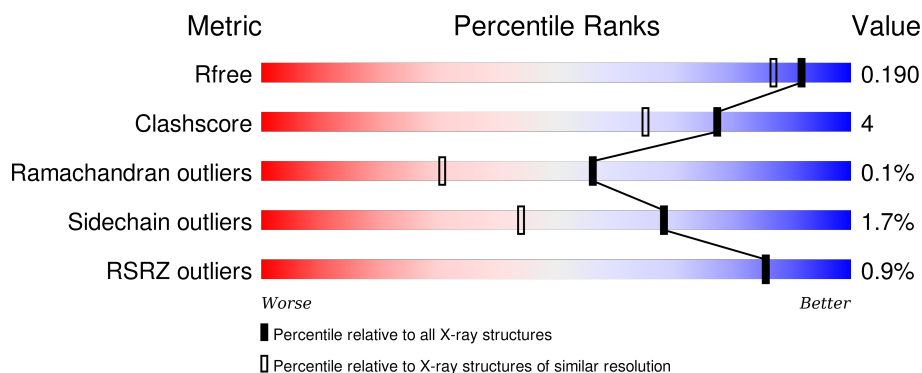
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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  $\geq 3$ , 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	802	<div> <div></div> <div>89%10%</div> </div>
2	B	135	<div> <div></div> <div>67%13%19%</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8129 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.

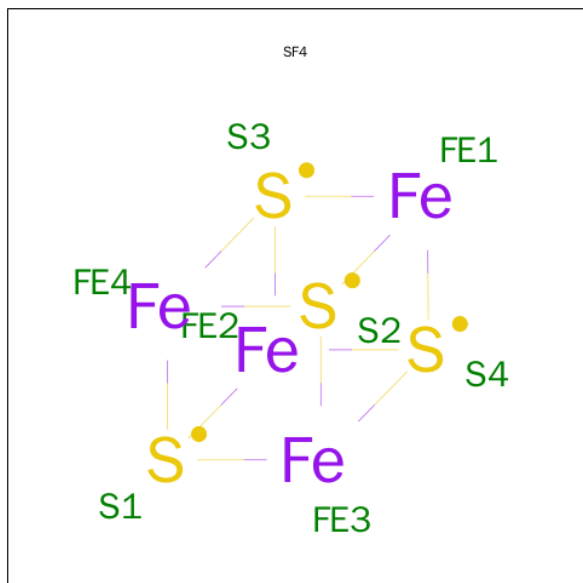
- Molecule 1 is a protein called Periplasmic nitrate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	799	6391	4087	1120	1150	34	0	9	0

- Molecule 2 is a protein called Diheme cytochrome c napB.

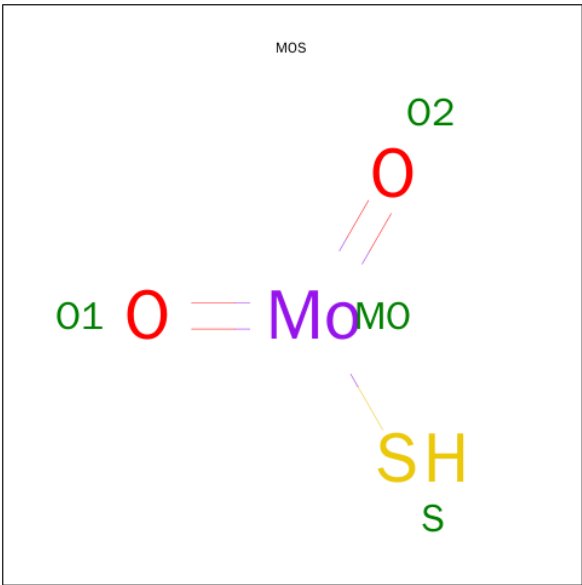
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	109	876	554	155	159	8	0	2	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



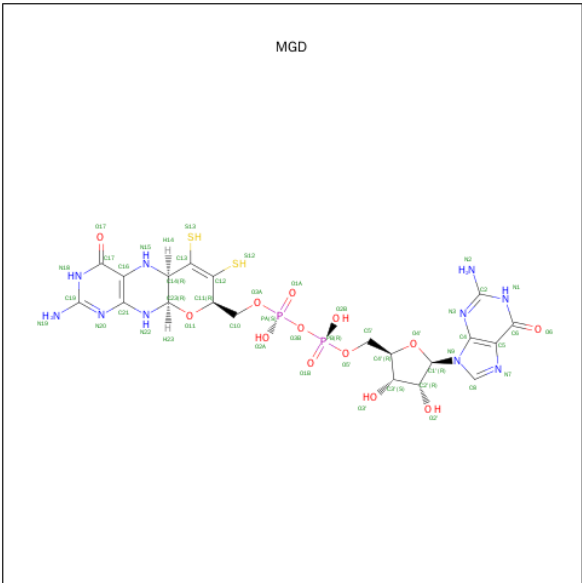
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	8	4	4	0	0

- Molecule 4 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO<sub>2</sub>S).

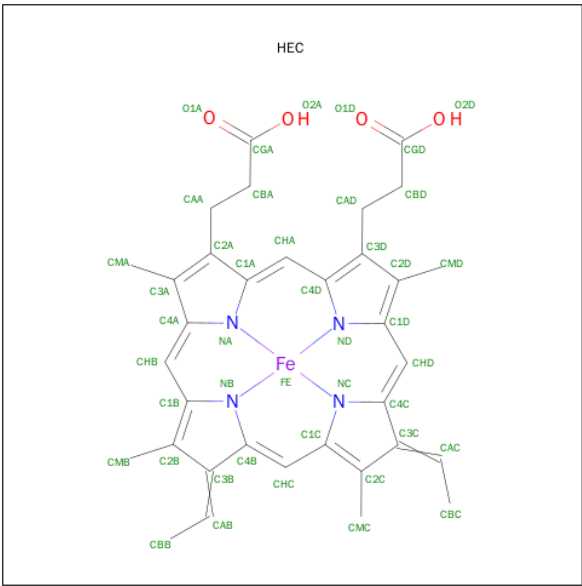


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Mo	S	0	0
			2	1	1		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



- Molecule 6 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

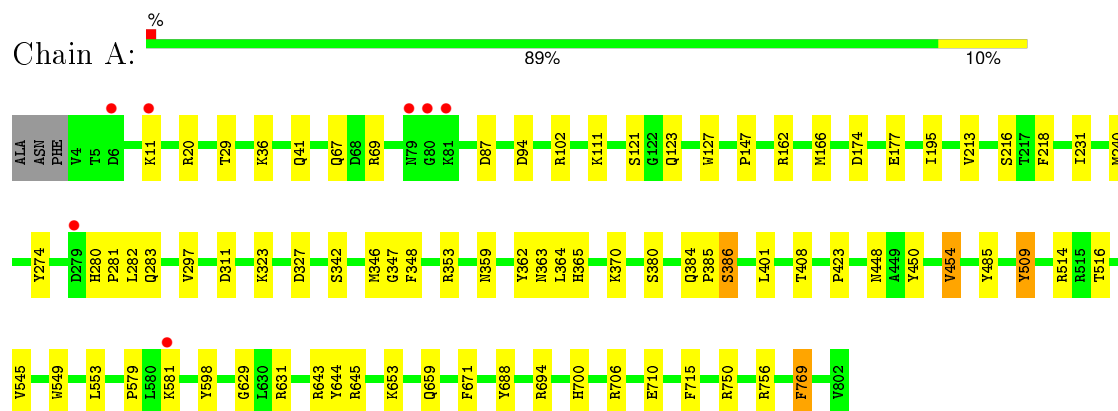
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	572	Total	O	0	0
			572	572		
7	B	100	Total	O	0	0
			100	100		

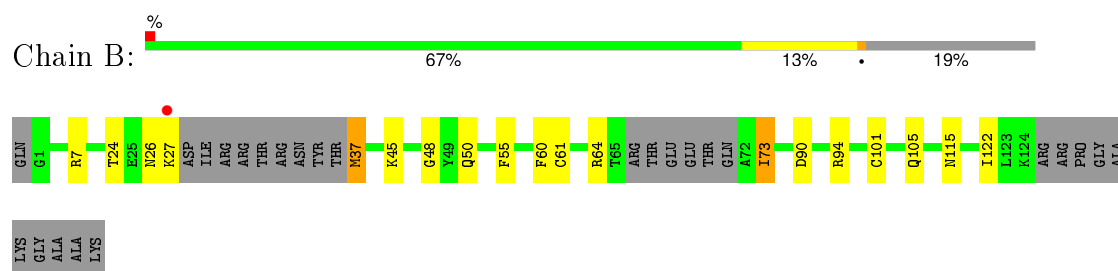
### 3 Residue-property plots [i](#)

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: Periplasmic nitrate reductase



- Molecule 2: Diheme cytochrome c napB



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.20Å 82.38Å 96.84Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	35.48 – 1.60 37.89 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (35.48-1.60) 97.0 (37.89-1.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.157 , 0.190 0.157 , 0.190	Depositor DCC
$R_{free}$ test set	7068 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.8	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 170001 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8129	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: MOS, SF4, HEC, MGD

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	1.29	7/6594 (0.1%)	1.12	25/8940 (0.3%)
2	B	1.21	3/903 (0.3%)	1.13	4/1227 (0.3%)
All	All	1.28	10/7497 (0.1%)	1.12	29/10167 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	TYR	CD1-CE1	6.52	1.49	1.39
1	A	485	TYR	CE1-CZ	6.43	1.47	1.38
1	A	218	PHE	CE2-CZ	6.36	1.49	1.37
2	B	48	GLY	N-CA	6.27	1.55	1.46
1	A	769	PHE	CG-CD2	5.96	1.47	1.38
1	A	177	GLU	CB-CG	5.77	1.63	1.52
2	B	55	PHE	CE2-CZ	5.46	1.47	1.37
1	A	213	VAL	CB-CG2	5.34	1.64	1.52
2	B	115	ASN	CB-CG	-5.17	1.39	1.51
1	A	450	TYR	CD2-CE2	5.15	1.47	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	MET	CG-SD-CE	-10.59	83.26	100.20
1	A	69	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	311	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	750	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	87[A]	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	87[B]	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	688	TYR	CB-CG-CD2	-6.85	116.89	121.00
1	A	348	PHE	CB-CG-CD2	-6.71	116.10	120.80
1	A	694	ARG	NE-CZ-NH1	6.68	123.64	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	64	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	364	LEU	CB-CG-CD1	-6.38	100.15	111.00
1	A	756	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	B	94	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	B	90	ASP	CB-CG-OD2	6.22	123.89	118.30
1	A	645	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	401	LEU	CB-CG-CD1	-6.15	100.55	111.00
1	A	509	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	A	644	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	A	750	ARG	NE-CZ-NH1	6.05	123.32	120.30
2	B	7	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	69	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	706	ARG	CG-CD-NE	-5.73	99.77	111.80
1	A	645	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	380	SER	N-CA-CB	-5.54	102.19	110.50
1	A	694	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	94	ASP	CB-CG-OD1	5.34	123.10	118.30
1	A	195	ILE	CG1-CB-CG2	5.32	123.11	111.40
1	A	102	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	353	ARG	NE-CZ-NH2	-5.09	117.76	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	6391	0	6295	40	0
2	B	876	0	865	12	0
3	A	8	0	0	0	0
4	A	2	0	0	0	0
5	A	94	0	44	2	0
6	B	86	0	62	10	0
7	A	572	0	0	3	0
7	B	100	0	0	2	0
All	All	8129	0	7266	53	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 4.

All (53) 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)
2:B:101:CYS:SG	6:B:1129:HEC:HAC	1.93	1.09
1:A:162:ARG:HE	1:A:359:ASN:HD21	1.18	0.91
1:A:274:TYR:H	1:A:283:GLN:HE22	1.19	0.90
1:A:20:ARG:HH12	1:A:123:GLN:HE21	1.21	0.84
2:B:61:CYS:SG	6:B:1128:HEC:HAC	2.19	0.81
1:A:280:HIS:HD2	1:A:282:LEU:H	1.28	0.81
1:A:363:ASN:HD21	1:A:671:PHE:H	1.39	0.71
2:B:61:CYS:SG	6:B:1128:HEC:C3C	2.79	0.70
2:B:101:CYS:SG	6:B:1129:HEC:C3C	2.82	0.68
6:B:1129:HEC:O1D	7:B:141:HOH:O	2.13	0.66
1:A:365:HIS:HD2	1:A:370:LYS:O	1.78	0.66
1:A:111:LYS:NZ	1:A:448:ASN:HD21	1.93	0.65
1:A:20:ARG:NH1	1:A:123:GLN:HE21	1.95	0.64
1:A:20:ARG:HH12	1:A:123:GLN:NE2	1.95	0.64
2:B:101:CYS:SG	6:B:1129:HEC:CBC	2.86	0.64
1:A:342:SER:OG	1:A:365:HIS:HE1	1.81	0.63
2:B:61:CYS:SG	6:B:1128:HEC:CBC	2.89	0.61
1:A:408:THR:HG23	7:A:1082:HOH:O	2.02	0.59
1:A:123:GLN:HG3	1:A:384:GLN:HE21	1.66	0.59
1:A:280:HIS:CD2	1:A:281:PRO:HD2	2.39	0.57
1:A:29:THR:OG1	1:A:41[B]:GLN:CG	2.54	0.56
1:A:41[A]:GLN:NE2	2:B:37:MET:HB3	2.21	0.55
1:A:347:GLY:HA3	5:A:1804:MGD:N3	2.22	0.54
1:A:710:GLU:HA	2:B:105:GLN:HE22	1.73	0.54
1:A:365:HIS:CD2	1:A:370:LYS:O	2.63	0.51
1:A:700:HIS:O	1:A:769:PHE:HA	2.11	0.50
1:A:111:LYS:HZ2	1:A:448:ASN:HD21	1.60	0.49
1:A:280:HIS:HE1	7:A:920:HOH:O	1.96	0.48
1:A:423:PRO:HG2	1:A:553:LEU:HG	1.94	0.48
1:A:280:HIS:CD2	1:A:282:LEU:H	2.19	0.48
1:A:29:THR:OG1	1:A:41[B]:GLN:HG3	2.14	0.47
1:A:516:THR:O	1:A:629:GLY:HA2	2.15	0.47
2:B:73:ILE:HD11	6:B:1129:HEC:CGA	2.46	0.46
6:B:1128:HEC:HMC1	6:B:1128:HEC:HBC3	1.98	0.46
1:A:386:SER:HB2	1:A:509:TYR:CD1	2.51	0.45
1:A:166[A]:MET:HG2	1:A:643:ARG:HH22	1.81	0.45
1:A:579:PRO:HG2	1:A:581:LYS:HG2	1.98	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG22	7:A:1308:HOH:O	2.16	0.45
6:B:1128:HEC:HMB1	6:B:1128:HEC:HBB3	1.99	0.44
2:B:24:THR:HB	2:B:45:LYS:HG2	1.99	0.44
1:A:274:TYR:H	1:A:283:GLN:NE2	2.00	0.44
1:A:653:LYS:H	1:A:659:GLN:NE2	2.15	0.43
2:B:26:ASN:OD1	2:B:45:LYS:HE2	2.18	0.43
1:A:36:LYS:CG	7:B:325:HOH:O	2.66	0.43
1:A:346:MET:HG2	5:A:1804:MGD:H101	2.01	0.42
1:A:514:ARG:O	1:A:631:ARG:HA	2.20	0.42
1:A:323:LYS:HE2	1:A:327:ASP:OD2	2.19	0.41
1:A:385:PRO:HB2	1:A:509:TYR:CD2	2.56	0.41
1:A:29:THR:OG1	1:A:41[B]:GLN:HG2	2.19	0.41
1:A:216:SER:O	1:A:231:ILE:HA	2.20	0.41
2:B:50[B]:GLN:H	2:B:50[B]:GLN:CD	2.18	0.41
1:A:545:VAL:HG13	1:A:549:TRP:CD2	2.56	0.40
1:A:121:SER:CB	1:A:454:VAL:HB	2.52	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	806/802 (100%)	775 (96%)	30 (4%)	1 (0%)	56	31
2	B	105/135 (78%)	102 (97%)	3 (3%)	0	100	100
All	All	911/937 (97%)	877 (96%)	33 (4%)	1 (0%)	56	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	PRO

### 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	670/665 (101%)	662 (99%)	8 (1%)	78	60
2	B	99/118 (84%)	94 (95%)	5 (5%)	29	7
All	All	769/783 (98%)	756 (98%)	13 (2%)	68	44

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	67	GLN
1	A	127	TRP
1	A	174	ASP
1	A	386	SER
1	A	454	VAL
1	A	598	TYR
1	A	715	PHE
2	B	27	LYS
2	B	37	MET
2	B	60	PHE
2	B	73	ILE
2	B	122	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	280	HIS
1	A	283	GLN
1	A	359	ASN
1	A	363	ASN
1	A	365	HIS
1	A	384	GLN
1	A	438	GLN
1	A	448	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	459	GLN
1	A	535	GLN
1	A	574	GLN
1	A	659	GLN
1	A	717	ASN
2	B	100	GLN
2	B	105	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 ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SF4	A	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
4	MOS	A	1802	1,5	0,1,3	0.00	-	0,0,3	0.00	-
5	MGD	A	1803	4	38,52,52	1.76	6 (15%)	43,81,81	2.52	13 (30%)
5	MGD	A	1804	4	38,52,52	1.19	5 (13%)	43,81,81	2.51	13 (30%)
6	HEC	B	1128	2	24,50,50	2.06	10 (41%)	19,82,82	2.86	8 (42%)
6	HEC	B	1129	2	24,50,50	2.59	9 (37%)	19,82,82	3.55	10 (52%)

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	SF4	A	1801	1	-	0/0/48/48	0/6/5/5
4	MOS	A	1802	1,5	-	0/0/0/0	0/0/0/0
5	MGD	A	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	A	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	B	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	B	1129	2	-	0/6/54/54	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1129	HEC	C3B-C2B	-7.69	1.32	1.40
6	B	1129	HEC	C3C-C2C	-5.22	1.35	1.40
6	B	1128	HEC	C3B-C2B	-4.36	1.36	1.40
6	B	1128	HEC	C3C-C2C	-3.36	1.37	1.40
6	B	1128	HEC	C2A-C3A	-2.10	1.31	1.37
6	B	1129	HEC	C4D-CHA	-2.09	1.34	1.39
6	B	1129	HEC	CBB-CAB	2.14	1.58	1.49
5	A	1804	MGD	C19-N20	2.15	1.39	1.35
5	A	1803	MGD	O2'-C2'	2.17	1.48	1.43
6	B	1128	HEC	C4C-NC	2.26	1.39	1.36
6	B	1128	HEC	CMD-C2D	2.26	1.56	1.51
6	B	1128	HEC	CAA-C2A	2.33	1.56	1.52
5	A	1804	MGD	C17-N18	2.40	1.37	1.33
5	A	1803	MGD	C19-N18	2.58	1.40	1.35
6	B	1129	HEC	C4B-NB	2.59	1.40	1.36
5	A	1804	MGD	C6-C5	2.61	1.46	1.41
6	B	1129	HEC	C1A-NA	2.62	1.40	1.36
6	B	1128	HEC	CMB-C2B	2.68	1.57	1.51
6	B	1128	HEC	CMA-C3A	2.78	1.57	1.51
5	A	1804	MGD	C5-C4	2.83	1.46	1.40
6	B	1129	HEC	CAA-C2A	3.12	1.58	1.52
6	B	1128	HEC	C3D-C2D	3.22	1.47	1.37
6	B	1128	HEC	CAD-C3D	3.32	1.57	1.52
5	A	1804	MGD	C14-N15	3.33	1.50	1.45
6	B	1129	HEC	C3D-C2D	3.55	1.48	1.37
5	A	1803	MGD	C2-N2	3.86	1.42	1.34
6	B	1129	HEC	CMB-C2B	3.97	1.60	1.51
5	A	1803	MGD	C16-C21	4.03	1.49	1.41
5	A	1803	MGD	C6-N1	4.06	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1803	MGD	C23-C14	5.02	1.57	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1128	HEC	CBB-CAB-C3B	-8.56	108.32	127.35
5	A	1803	MGD	C5-C6-N1	-8.09	112.53	123.59
6	B	1129	HEC	CBB-CAB-C3B	-7.26	111.21	127.35
5	A	1803	MGD	C4'-O4'-C1'	-6.64	102.42	109.72
6	B	1129	HEC	CMB-C2B-C1B	-6.11	118.26	128.36
5	A	1804	MGD	C5-C6-N1	-5.93	115.48	123.59
5	A	1804	MGD	C6-C5-C4	-5.15	114.74	120.90
6	B	1129	HEC	CAA-C2A-C1A	-5.02	121.56	127.01
5	A	1804	MGD	C2'-C1'-N9	-4.94	106.74	114.29
6	B	1129	HEC	CBA-CAA-C2A	-4.81	103.91	112.53
5	A	1804	MGD	C21-N22-C23	-4.67	114.51	123.67
6	B	1129	HEC	CMC-C2C-C1C	-4.55	120.83	128.36
5	A	1803	MGD	C1'-N9-C4	-4.27	120.49	126.94
6	B	1129	HEC	CAD-C3D-C4D	-4.23	122.41	127.01
6	B	1128	HEC	CBD-CAD-C3D	-4.23	104.95	112.53
5	A	1804	MGD	C4'-O4'-C1'	-4.20	105.11	109.72
6	B	1129	HEC	CBD-CAD-C3D	-4.19	105.02	112.53
6	B	1128	HEC	CBC-CAC-C3C	-4.03	118.40	127.35
6	B	1129	HEC	CBC-CAC-C3C	-3.99	118.49	127.35
5	A	1804	MGD	C4-C5-N7	-3.68	106.10	109.48
5	A	1803	MGD	C4-C5-N7	-3.28	106.46	109.48
6	B	1128	HEC	CMC-C2C-C1C	-3.13	123.19	128.36
5	A	1803	MGD	N18-C19-N20	-2.96	120.69	125.53
6	B	1129	HEC	C3B-C4B-NB	-2.50	106.23	110.94
5	A	1804	MGD	N18-C19-N20	-2.47	121.49	125.53
5	A	1803	MGD	PA-O3B-PB	-2.47	125.81	132.73
6	B	1128	HEC	CAA-C2A-C1A	-2.44	124.36	127.01
6	B	1128	HEC	CAD-CBD-CGD	-2.29	108.54	112.75
6	B	1128	HEC	CMB-C2B-C1B	-2.15	124.81	128.36
6	B	1128	HEC	C4C-C3C-C2C	2.33	108.86	106.35
5	A	1804	MGD	C19-N20-C21	2.52	120.19	114.54
5	A	1803	MGD	N19-C19-N20	2.69	121.65	117.20
5	A	1803	MGD	O11-C23-C14	2.98	111.00	108.96
5	A	1803	MGD	N22-C21-N20	3.04	121.45	116.62
5	A	1804	MGD	N19-C19-N18	3.15	122.42	117.20
6	B	1129	HEC	C4C-C3C-C2C	3.22	109.82	106.35
5	A	1803	MGD	O4'-C4'-C3'	3.23	111.65	105.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1803	MGD	C19-N20-C21	3.30	121.97	114.54
5	A	1804	MGD	C17-C16-C21	3.64	117.86	114.56
5	A	1804	MGD	C17-N18-C19	3.71	121.09	115.94
5	A	1803	MGD	C17-N18-C19	3.82	121.25	115.94
5	A	1804	MGD	C16-C21-N22	4.73	123.29	118.34
5	A	1803	MGD	C6-N1-C2	5.39	123.42	115.94
5	A	1804	MGD	C6-N1-C2	6.11	124.42	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1804	MGD	2	0
6	B	1128	HEC	5	0
6	B	1129	HEC	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	799/802 (99%)	-0.54	7 (0%) 85 85	6, 13, 27, 43	0
2	B	109/135 (80%)	-0.30	1 (0%) 85 85	8, 18, 37, 47	0
All	All	908/937 (96%)	-0.51	8 (0%) 85 85	6, 13, 28, 47	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASP	2.8
1	A	581	LYS	2.6
2	B	27	LYS	2.5
1	A	80	GLY	2.4
1	A	11	LYS	2.3
1	A	81	LYS	2.2
1	A	279[A]	ASP	2.0
1	A	79	ASN	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
6	HEC	B	1128	43/43	0.98	0.08	0.63	9,13,27,29	0
5	MGD	A	1804	47/47	0.99	0.09	0.31	5,8,10,11	0
5	MGD	A	1803	47/47	0.99	0.08	0.28	7,9,11,12	0
6	HEC	B	1129	43/43	0.99	0.06	-0.27	6,9,18,22	0
3	SF4	A	1801	8/8	1.00	0.06	-1.34	8,9,9,9	0
4	MOS	A	1802	2/4	1.00	0.05	-2.53	10,10,10,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.