wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:23 PM GMT

PDB ID	:	1OGY
Title	:	CRYSTAL STRUCTURE OF THE HETERODIMERIC NITRATE REDUCTASE FROM RHODOBACTER SPHAEROIDES
Authors	:	Arnoux, P.; Sabaty, M.; Alric, J.; Frangioni, B.; Guigliarelli, B.; Adriano, J.-M.; Pignol, D.
Deposited on	:	2003-05-19
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

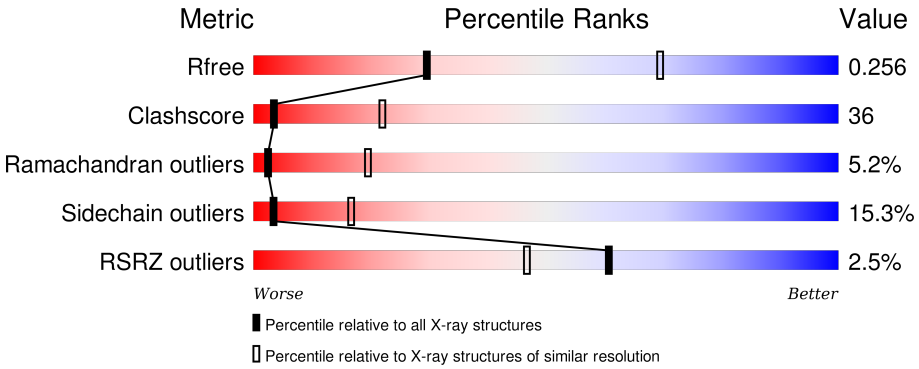
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	802	49% 39% 11%
1	C	802	46% 41% 11%
1	E	802	48% 40% 10%
1	G	802	46% 41% 11%
1	I	802	7% 44% 42% 12%

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Mol	Chain	Length	Quality of chain
1	K	802	2% 45% 41% 11%
1	M	802	% 48% 38% 11%
1	O	802	5% 44% 42% 12%
2	B	130	% 38% 43% 15%
2	D	130	2% 40% 42% 15%
2	F	130	2% 38% 45% 14%
2	H	130	2% 38% 45% 14%
2	J	130	4% 41% 38% 16%
2	L	130	3% 34% 46% 15%
2	N	130	2% 35% 44% 17%
2	P	130	3% 35% 45% 15%

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
6	HEC	D	1129	-	-	X	-
6	HEC	L	1129	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59336 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
1	A	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	C	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	E	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	G	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	I	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	K	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	M	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			
1	O	790	Total	C	N	O	S	0	0	1
			6251	3961	1114	1144	32			

- Molecule 2 is a protein called DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	D	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	F	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	H	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	J	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	L	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			

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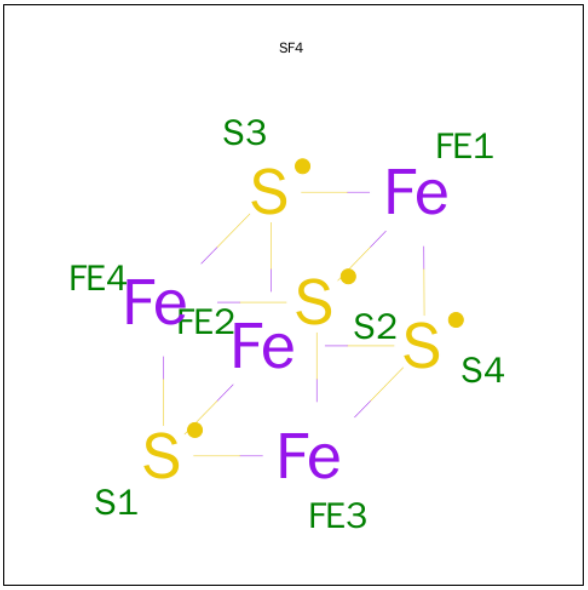
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			
2	P	127	Total	C	N	O	S	0	0	1
			977	603	180	185	9			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

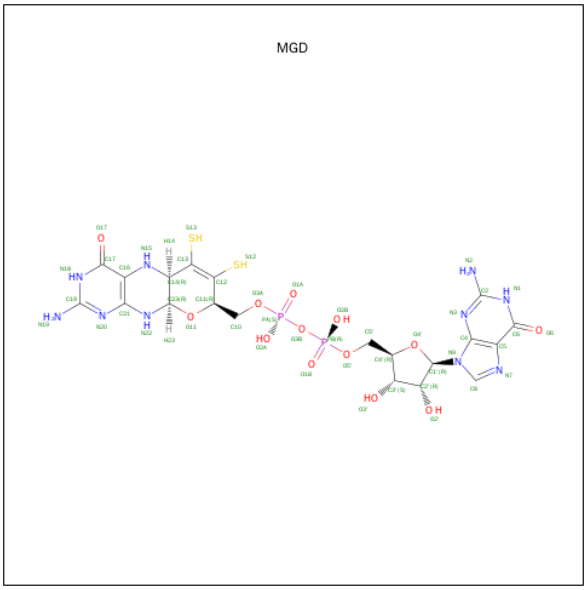


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	E	1	Total	Fe	S	0	0
			8	4	4		
3	G	1	Total	Fe	S	0	0
			8	4	4		
3	I	1	Total	Fe	S	0	0
			8	4	4		
3	K	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mo 1 1	0	0
4	K	1	Total Mo 1 1	0	0
4	E	1	Total Mo 1 1	0	0
4	I	1	Total Mo 1 1	0	0
4	C	1	Total Mo 1 1	0	0
4	A	1	Total Mo 1 1	0	0
4	O	1	Total Mo 1 1	0	0
4	M	1	Total Mo 1 1	0	0

- 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: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	A	1	Total C N O P S 47 20 10 13 2 2	0	0
5	C	1	Total C N O P S 47 20 10 13 2 2	0	0

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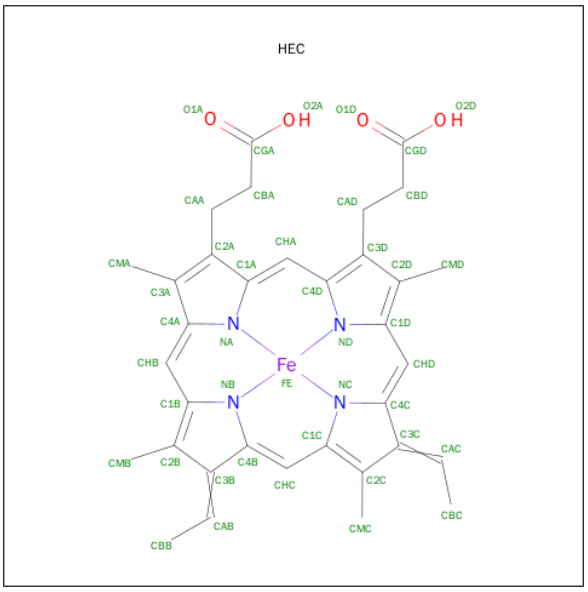
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	G	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	I	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	K	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	M	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	O	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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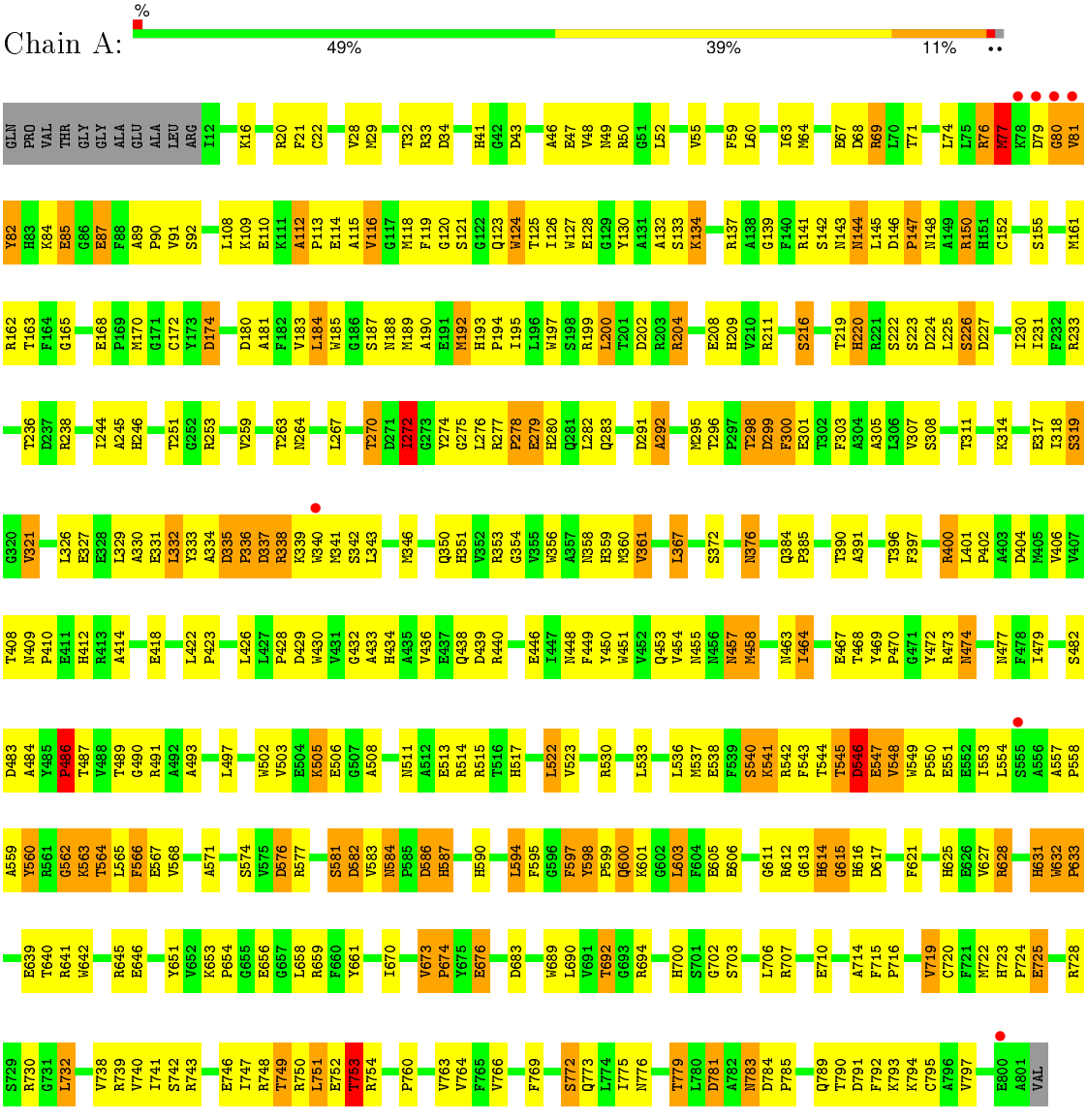
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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.

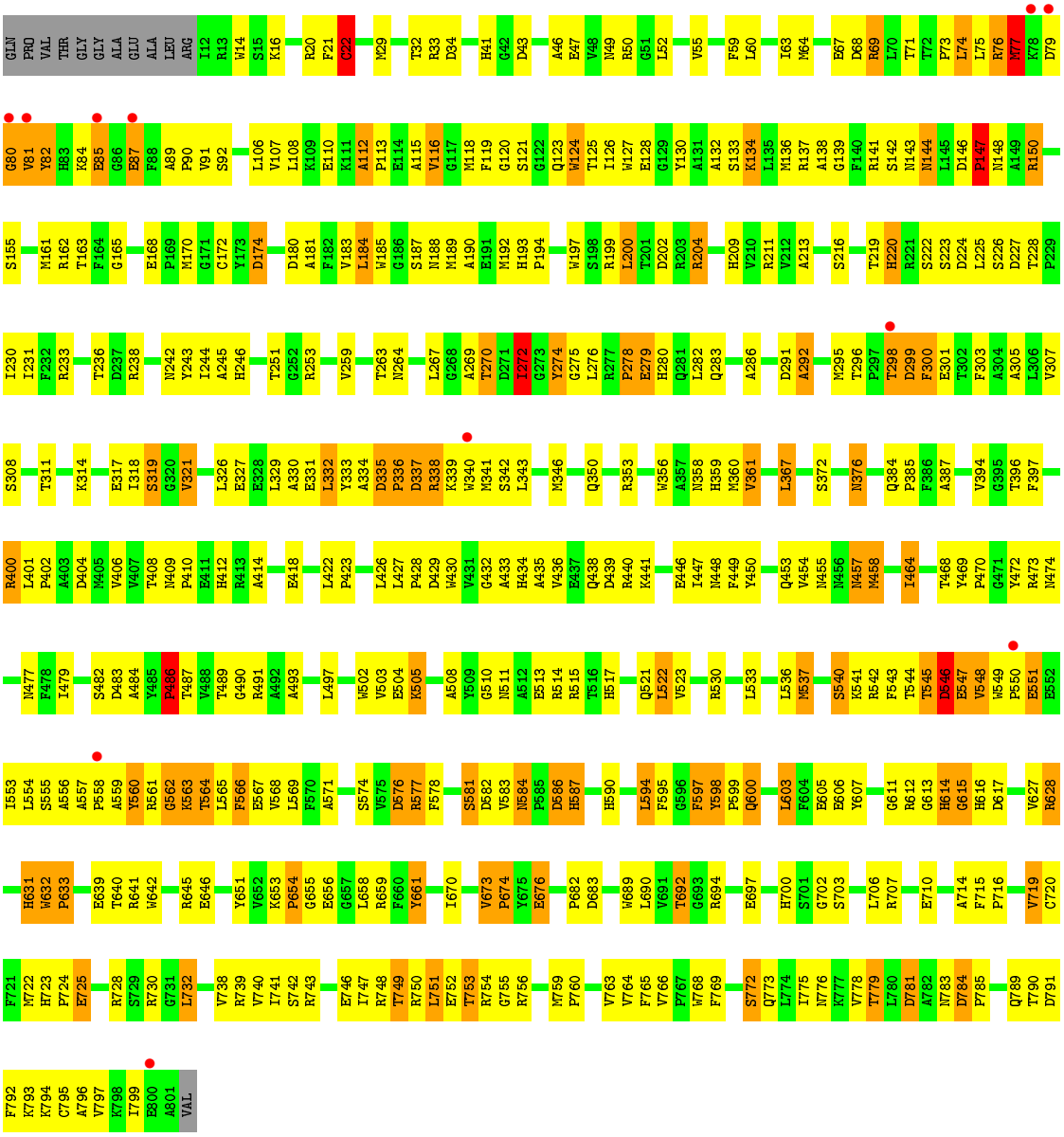
- Molecule 1: PERIPLASMIC NITRATE REDUCTASE

Chain A:



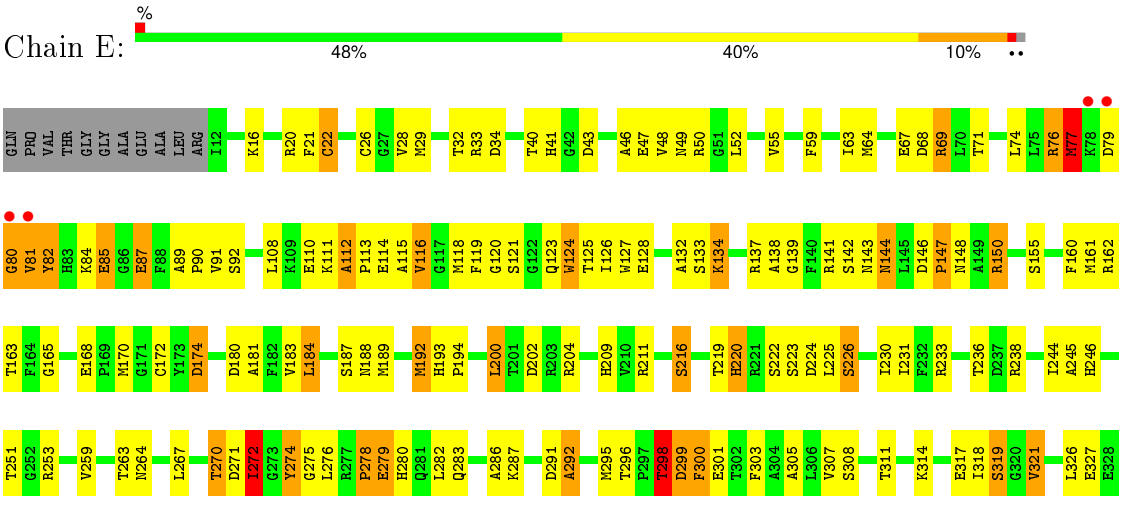
- Molecule 1: PERIPLASMIC NITRATE REDUCTASE

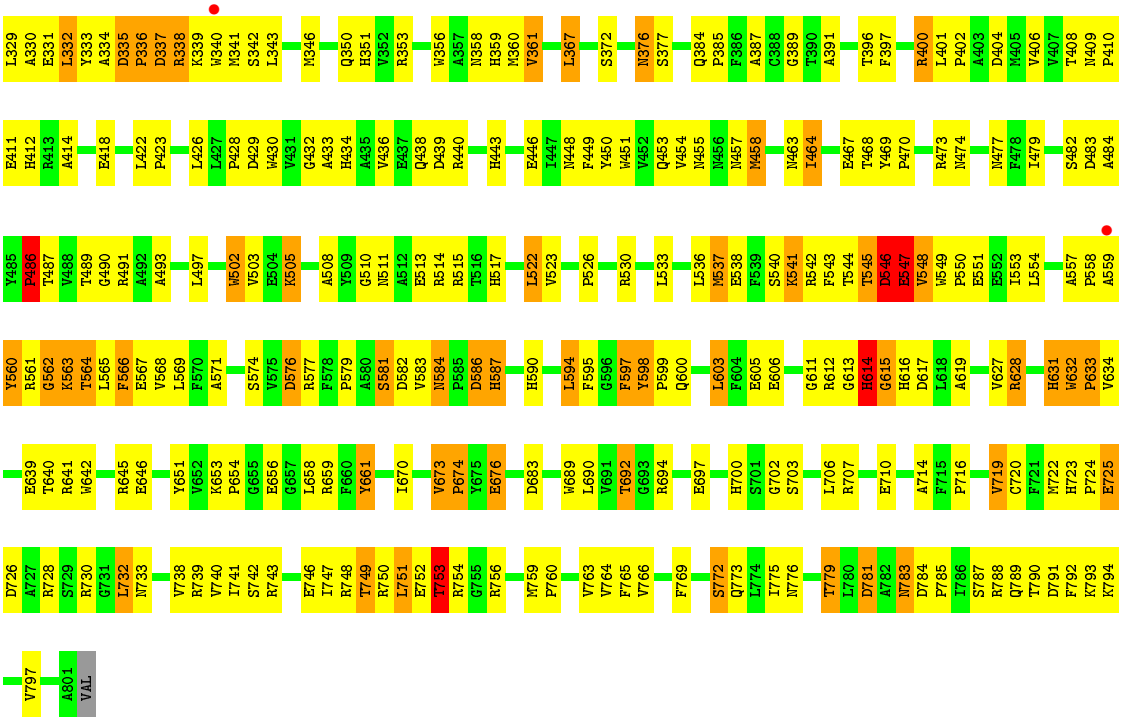
Chain C:



• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

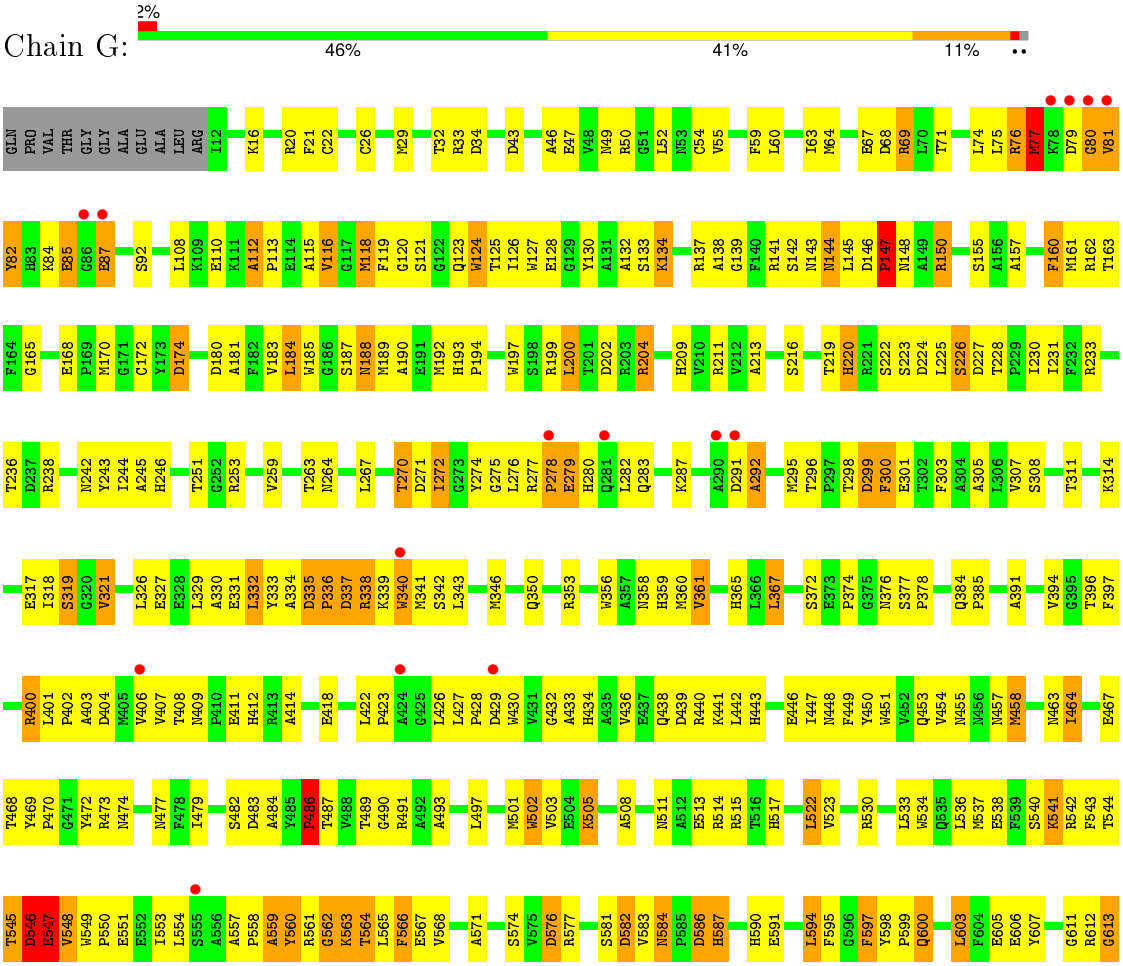
Chain E:

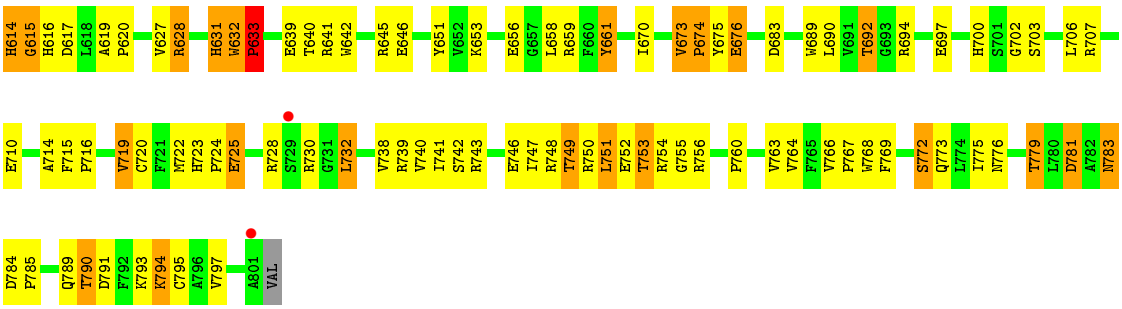




• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

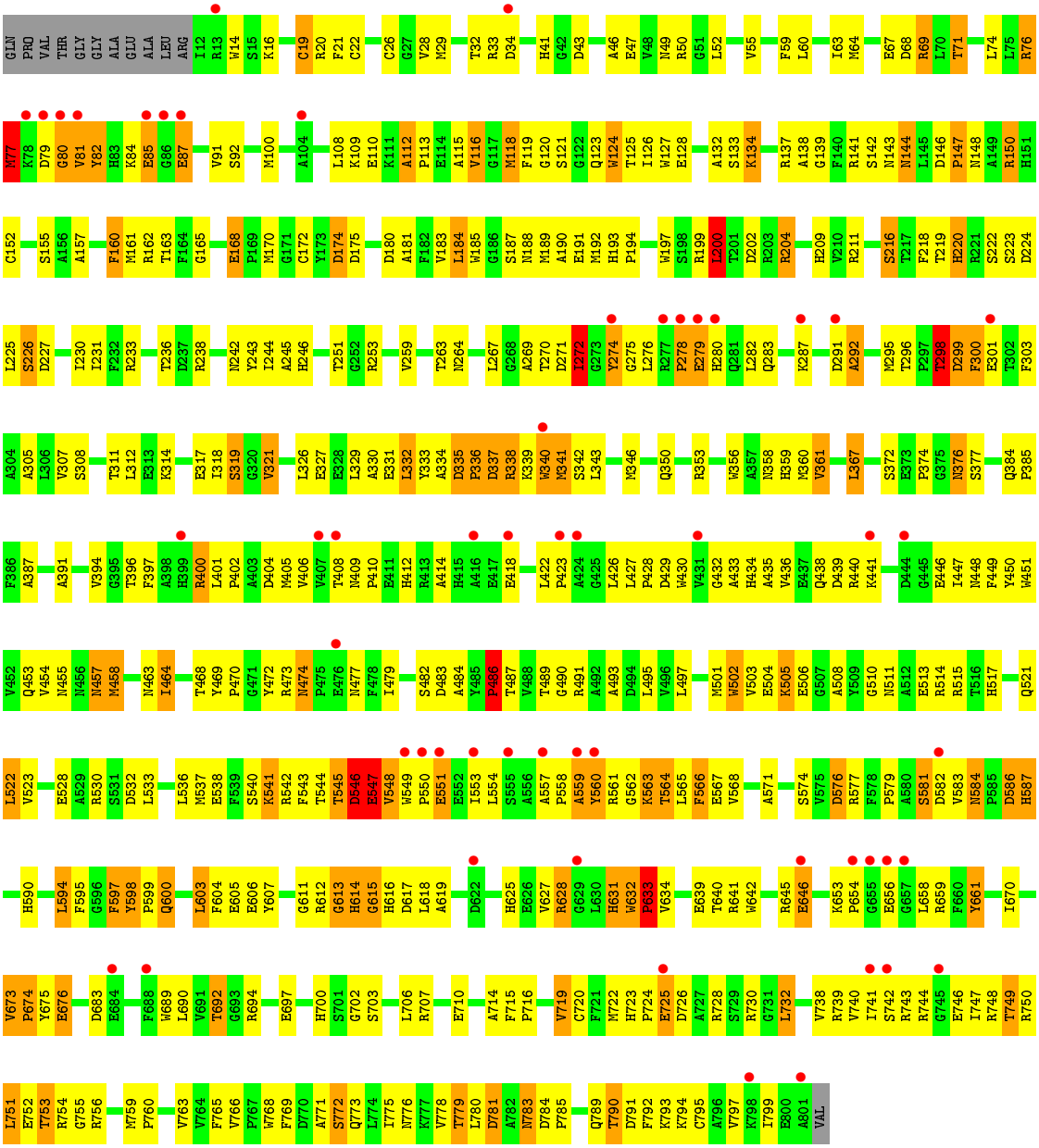
Chain G:





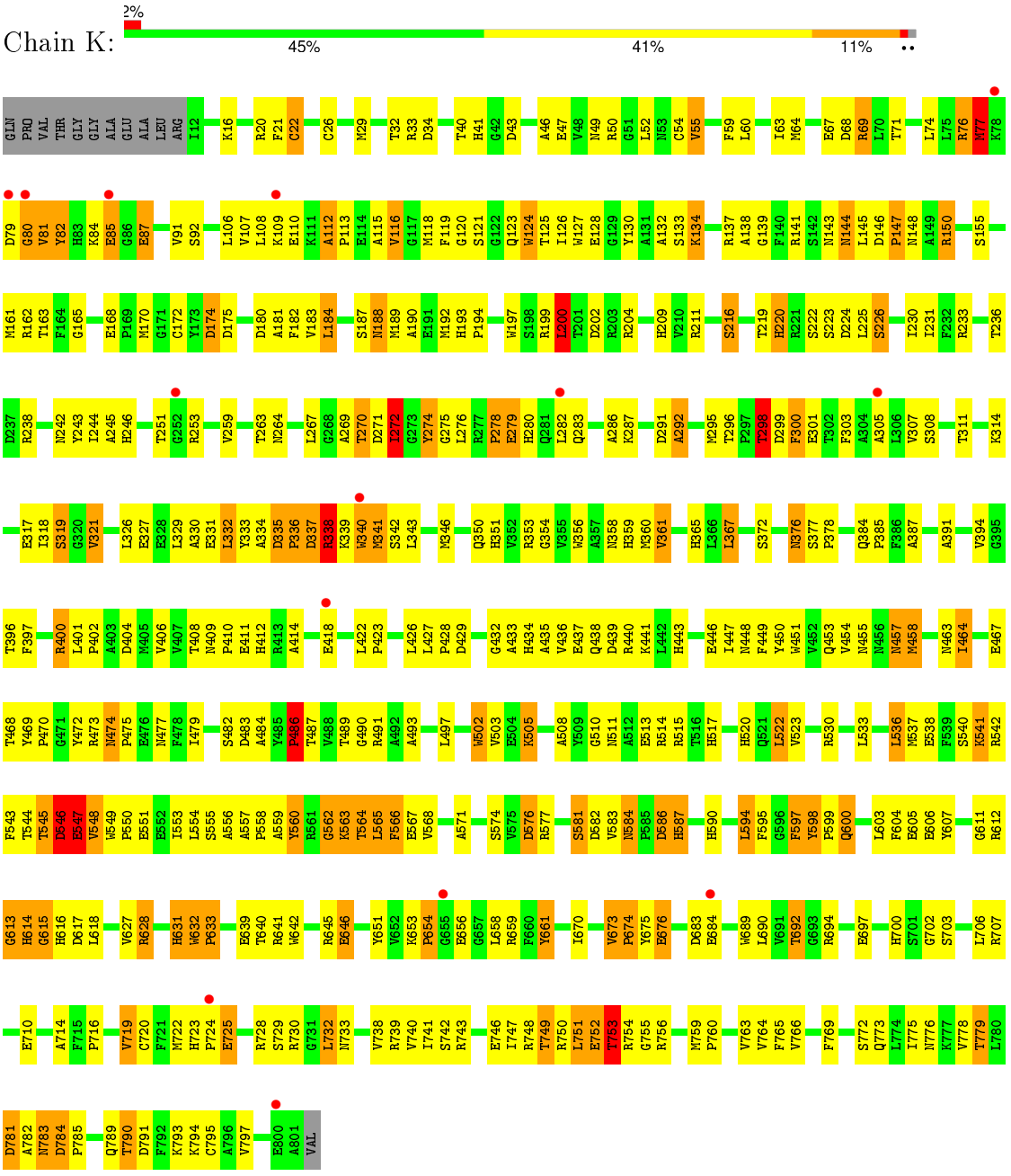
• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

Chain I:



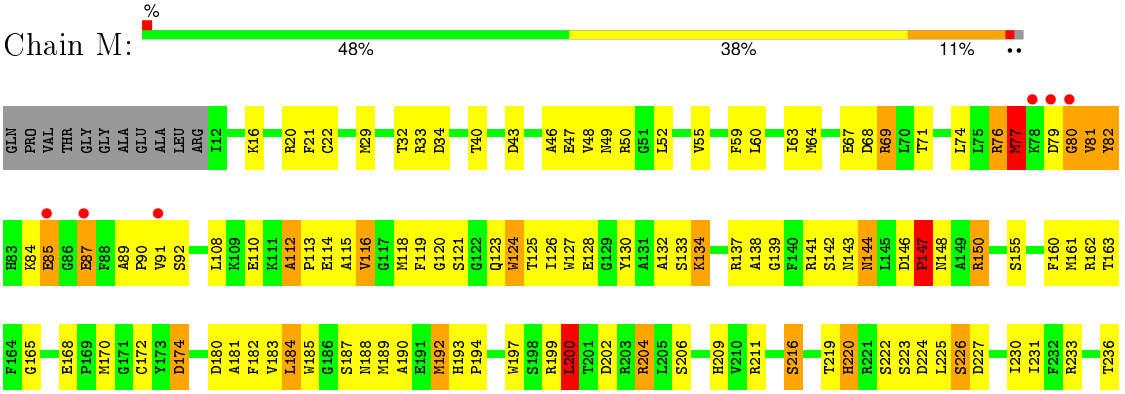
• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

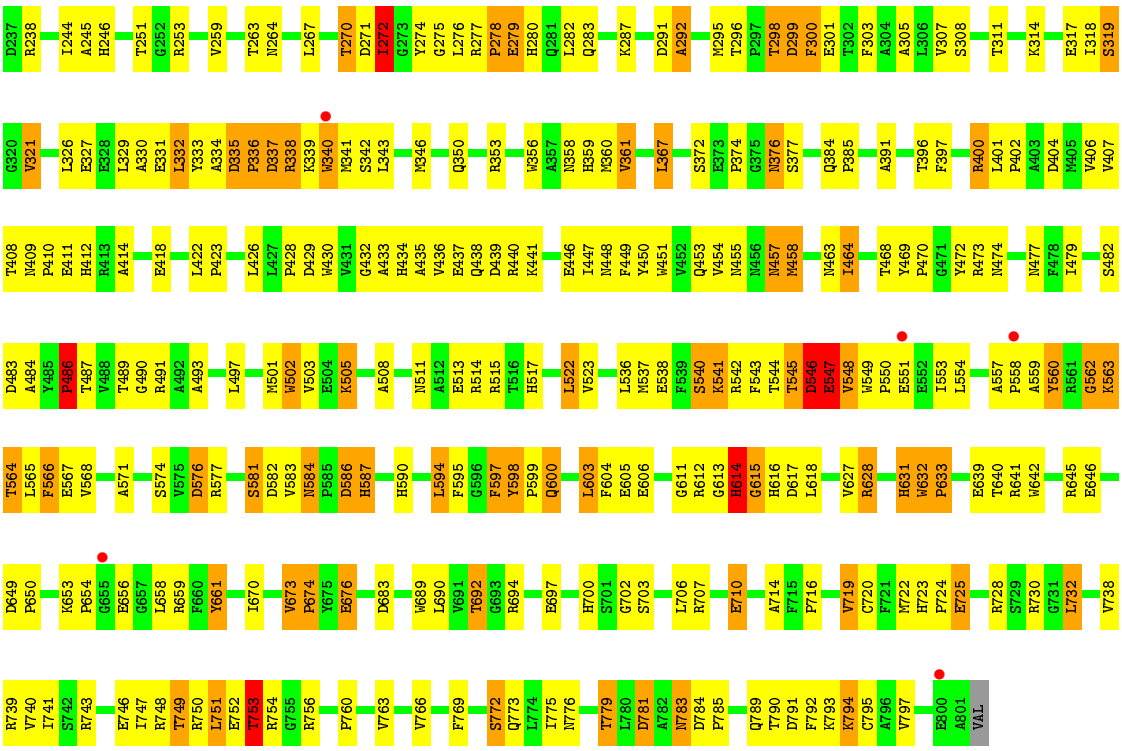
Chain K:



• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

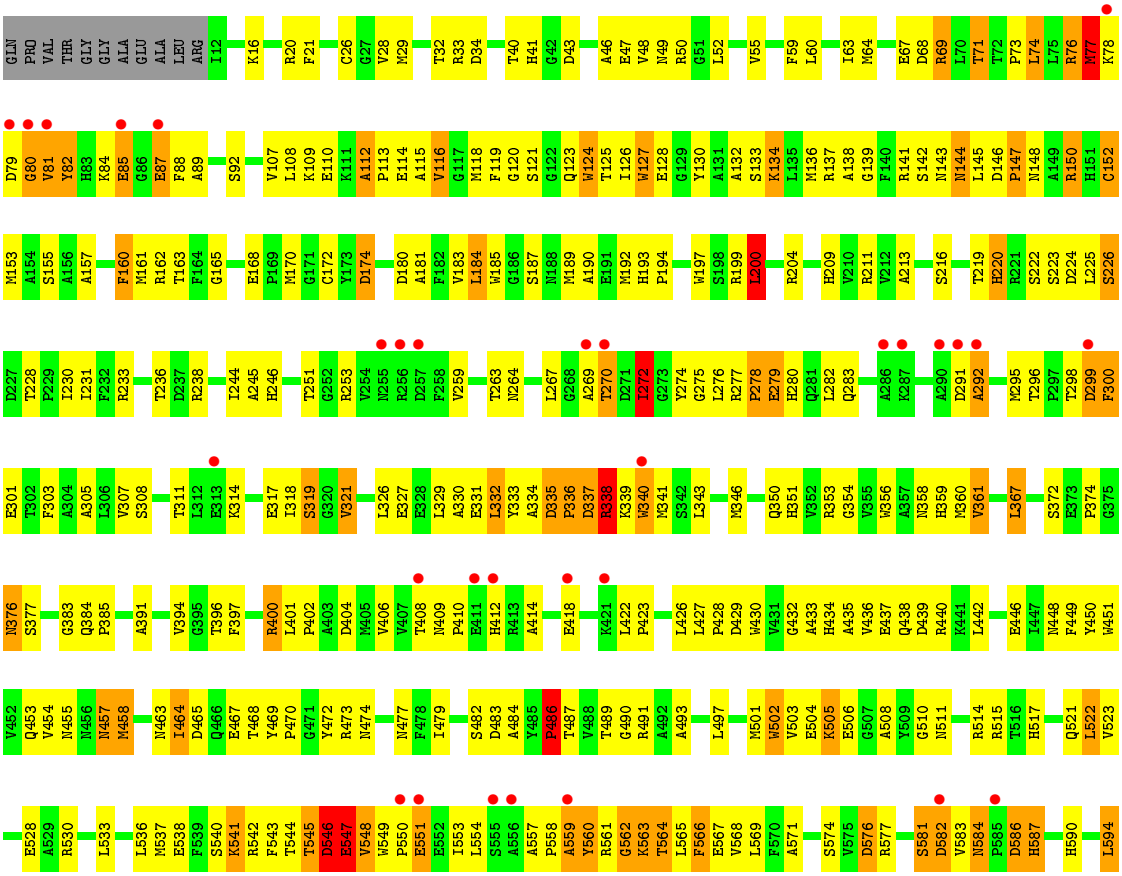
Chain M:

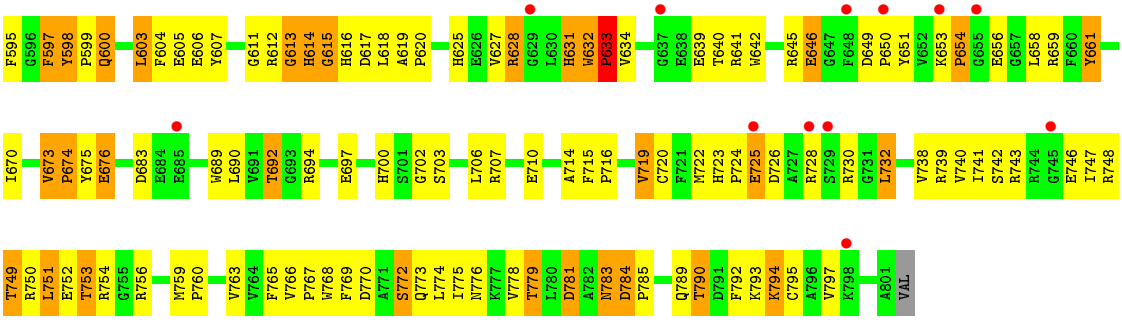




• Molecule 1: PERIPLASMIC NITRATE REDUCTASE

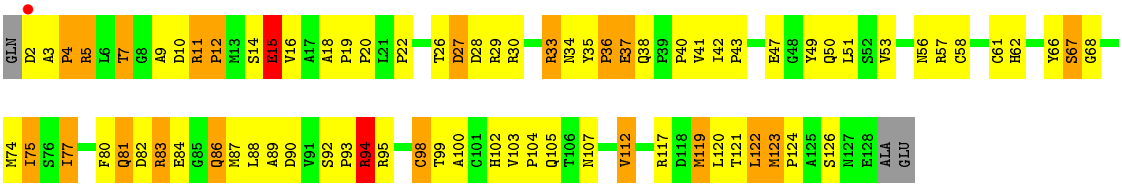
Chain O:





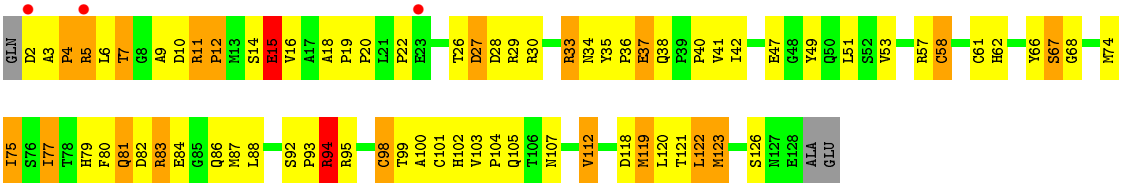
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain B:



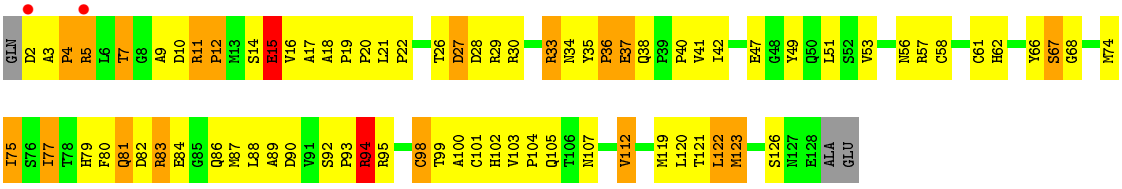
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain D:



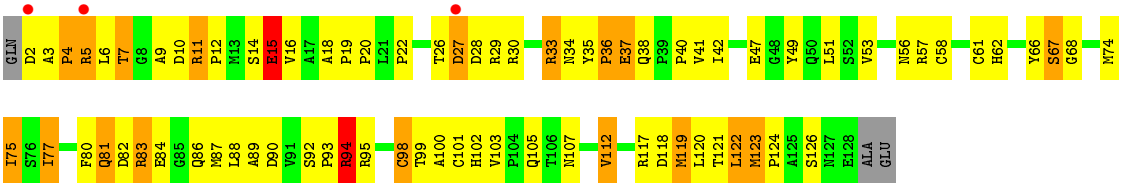
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain F:



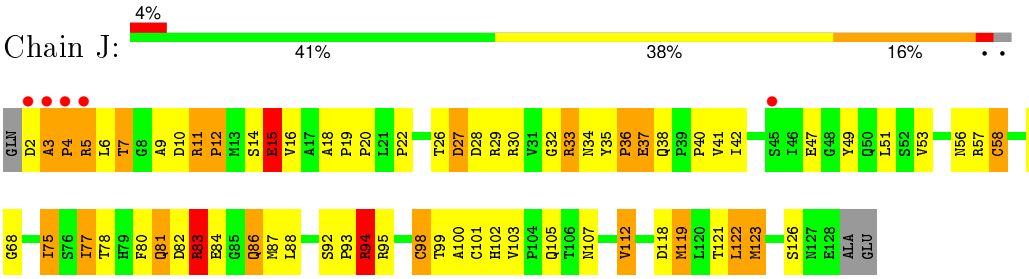
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain H:



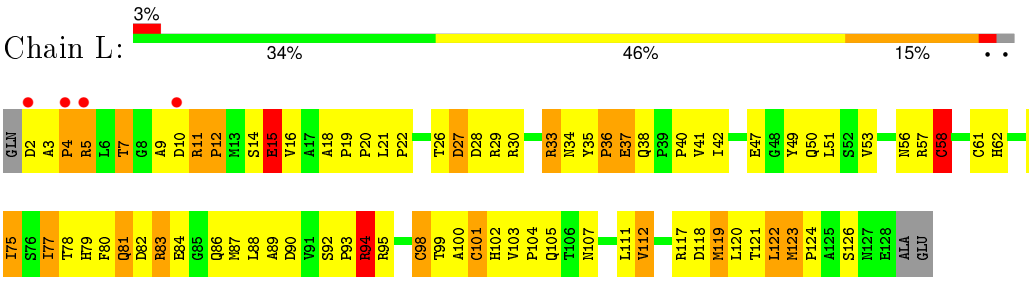
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain J:



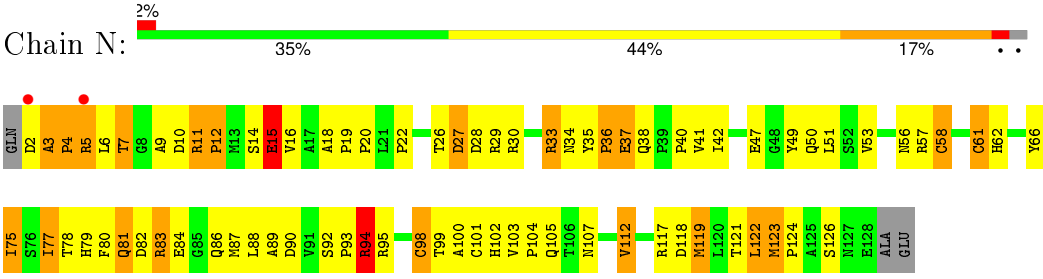
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain L:



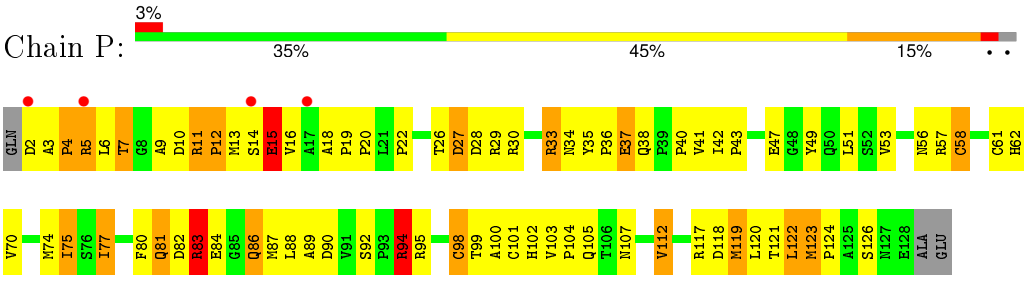
• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain N:



• Molecule 2: DIHEME CYTOCHROME C NAPB MOLECULE: NITRATE REDUCTASE

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	123.00Å 225.20Å 154.60Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 29.94 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-3.20) 97.0 (29.94-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.269 0.240 , 0.256	Depositor DCC
R_{free} test set	1348 reflections (1.02%)	DCC
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.7	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 134459 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	59336	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: SF4, HEC, MO, 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	0.70	2/6433 (0.0%)	0.89	13/8741 (0.1%)
1	C	0.67	1/6433 (0.0%)	0.90	13/8741 (0.1%)
1	E	0.70	3/6433 (0.0%)	0.89	13/8741 (0.1%)
1	G	0.70	1/6433 (0.0%)	0.92	12/8741 (0.1%)
1	I	0.82	2/6433 (0.0%)	0.92	13/8741 (0.1%)
1	K	0.68	2/6433 (0.0%)	0.91	16/8741 (0.2%)
1	M	0.66	1/6433 (0.0%)	0.89	13/8741 (0.1%)
1	O	0.76	1/6433 (0.0%)	0.92	16/8741 (0.2%)
2	B	0.74	0/1001	0.94	1/1368 (0.1%)
2	D	0.72	0/1001	0.93	1/1368 (0.1%)
2	F	0.75	0/1001	0.94	1/1368 (0.1%)
2	H	0.76	0/1001	0.95	1/1368 (0.1%)
2	J	0.73	0/1001	0.96	2/1368 (0.1%)
2	L	0.75	2/1001 (0.2%)	0.95	1/1368 (0.1%)
2	N	0.78	1/1001 (0.1%)	0.95	1/1368 (0.1%)
2	P	0.73	0/1001	0.94	2/1368 (0.1%)
All	All	0.72	16/59472 (0.0%)	0.91	119/80872 (0.1%)

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	22	CYS	CB-SG	-9.02	1.67	1.82
1	G	54	CYS	CB-SG	-7.57	1.69	1.82
1	K	22	CYS	CB-SG	-7.20	1.70	1.82
1	I	19	CYS	CB-SG	7.16	1.94	1.82
1	O	152	CYS	CB-SG	6.88	1.94	1.82

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	632	TRP	C-N-CD	-24.39	66.94	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	632	TRP	C-N-CD	-22.20	71.75	120.60
1	O	632	TRP	C-N-CD	-21.86	72.50	120.60
1	I	632	TRP	C-N-CD	-21.10	74.19	120.60
1	E	632	TRP	C-N-CD	-17.95	81.12	120.60

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	6251	0	5967	418	2
1	C	6251	0	5966	441	3
1	E	6251	0	5968	421	1
1	G	6251	0	5966	430	0
1	I	6251	0	5967	466	0
1	K	6251	0	5966	449	3
1	M	6251	0	5966	427	1
1	O	6251	0	5967	470	0
2	B	977	0	937	92	0
2	D	977	0	941	107	0
2	F	977	0	941	95	0
2	H	977	0	941	113	0
2	J	977	0	941	103	0
2	L	977	0	941	107	0
2	N	977	0	941	111	0
2	P	977	0	941	114	0
3	A	8	0	0	0	0
3	C	8	0	0	1	0
3	E	8	0	0	1	0
3	G	8	0	0	0	0
3	I	8	0	0	0	0
3	K	8	0	0	1	0
3	M	8	0	0	0	0
3	O	8	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	A	94	0	44	15	0
5	C	94	0	44	14	0
5	E	94	0	44	15	0
5	G	94	0	44	13	0
5	I	94	0	44	13	0
5	K	94	0	44	15	0
5	M	94	0	44	15	0
5	O	94	0	44	15	0
6	B	86	0	60	15	0
6	D	86	0	64	33	0
6	F	86	0	64	23	0
6	H	86	0	64	27	0
6	J	86	0	64	27	0
6	L	86	0	64	26	0
6	N	86	0	64	30	0
6	P	86	0	64	25	0
All	All	59336	0	56117	4193	5

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 36.

The worst 5 of 4193 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:N:58:CYS:SG	6:N:1128:HEC:HAB	1.34	1.64
2:F:98:CYS:SG	6:F:1129:HEC:HAB	1.39	1.61
2:J:98:CYS:SG	6:J:1129:HEC:HAB	1.38	1.61
2:H:58:CYS:SG	6:H:1128:HEC:HAB	1.41	1.60
2:D:98:CYS:SG	6:D:1129:HEC:HAB	1.45	1.57

All (5) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:CG	1:C:655:GLY:O[2_556]	1.82	0.38
1:C:577:ARG:CB	1:K:287:LYS:NZ[2_545]	1.90	0.30
1:C:577:ARG:CG	1:K:287:LYS:NZ[2_545]	1.97	0.23
1:E:411:GLU:OE2	1:M:410:PRO:CG[1_556]	2.06	0.14
1:A:410:PRO:CB	1:K:411:GLU:OE2[1_556]	2.15	0.05

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	788/802 (98%)	669 (85%)	85 (11%)	34 (4%)	3 25
1	C	788/802 (98%)	658 (84%)	94 (12%)	36 (5%)	3 23
1	E	788/802 (98%)	671 (85%)	82 (10%)	35 (4%)	3 24
1	G	788/802 (98%)	666 (84%)	90 (11%)	32 (4%)	3 27
1	I	788/802 (98%)	656 (83%)	99 (13%)	33 (4%)	3 26
1	K	788/802 (98%)	665 (84%)	89 (11%)	34 (4%)	3 25
1	M	788/802 (98%)	665 (84%)	87 (11%)	36 (5%)	3 23
1	O	788/802 (98%)	662 (84%)	92 (12%)	34 (4%)	3 25
2	B	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	1 4
2	D	125/130 (96%)	100 (80%)	13 (10%)	12 (10%)	1 5
2	F	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	1 4
2	H	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	1 4
2	J	125/130 (96%)	100 (80%)	11 (9%)	14 (11%)	0 3
2	L	125/130 (96%)	98 (78%)	14 (11%)	13 (10%)	1 4
2	N	125/130 (96%)	97 (78%)	14 (11%)	14 (11%)	0 3
2	P	125/130 (96%)	99 (79%)	14 (11%)	12 (10%)	1 5
All	All	7304/7456 (98%)	6100 (84%)	826 (11%)	378 (5%)	2 19

5 of 378 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	CYS
1	A	81	VAL
1	A	85	GLU
1	A	274	TYR
1	A	275	GLY

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	641/651 (98%)	546 (85%)	95 (15%)	4	18
1	C	641/651 (98%)	548 (86%)	93 (14%)	4	19
1	E	641/651 (98%)	546 (85%)	95 (15%)	4	18
1	G	641/651 (98%)	543 (85%)	98 (15%)	3	17
1	I	641/651 (98%)	542 (85%)	99 (15%)	3	16
1	K	641/651 (98%)	547 (85%)	94 (15%)	4	18
1	M	641/651 (98%)	543 (85%)	98 (15%)	3	17
1	O	641/651 (98%)	543 (85%)	98 (15%)	3	17
2	B	108/113 (96%)	89 (82%)	19 (18%)	2	11
2	D	108/113 (96%)	90 (83%)	18 (17%)	3	13
2	F	108/113 (96%)	91 (84%)	17 (16%)	3	15
2	H	108/113 (96%)	91 (84%)	17 (16%)	3	15
2	J	108/113 (96%)	89 (82%)	19 (18%)	2	11
2	L	108/113 (96%)	90 (83%)	18 (17%)	3	13
2	N	108/113 (96%)	90 (83%)	18 (17%)	3	13
2	P	108/113 (96%)	88 (82%)	20 (18%)	2	10
All	All	5992/6112 (98%)	5076 (85%)	916 (15%)	3	17

5 of 916 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	628	ARG

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Mol	Chain	Res	Type
1	I	464	ILE
1	O	361	VAL
1	G	732	LEU
1	I	116	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 197 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	700	HIS
1	I	457	ASN
1	O	457	ASN
1	G	733	ASN
1	I	144	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 8 are monoatomic - leaving 40 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	SF4	A	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	A	1803	4	38,52,52	2.67	16 (42%)	43,81,81	2.54	12 (27%)
5	MGD	A	1804	4	38,52,52	2.27	13 (34%)	43,81,81	2.52	17 (39%)
6	HEC	B	1128	2	24,50,50	2.95	6 (25%)	19,82,82	3.24	8 (42%)
6	HEC	B	1129	2	24,50,50	2.41	3 (12%)	19,82,82	2.69	9 (47%)
3	SF4	C	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	C	1803	4	38,52,52	2.47	16 (42%)	43,81,81	2.48	13 (30%)
5	MGD	C	1804	4	38,52,52	2.35	14 (36%)	43,81,81	2.49	15 (34%)
6	HEC	D	1128	2	24,50,50	2.52	8 (33%)	19,82,82	3.38	11 (57%)
6	HEC	D	1129	2	24,50,50	2.48	5 (20%)	19,82,82	2.82	11 (57%)
3	SF4	E	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	E	1803	4	38,52,52	2.45	17 (44%)	43,81,81	2.47	14 (32%)
5	MGD	E	1804	4	38,52,52	2.37	14 (36%)	43,81,81	2.48	20 (46%)
6	HEC	F	1128	2	24,50,50	2.38	4 (16%)	19,82,82	2.70	8 (42%)
6	HEC	F	1129	2	24,50,50	2.11	4 (16%)	19,82,82	3.00	10 (52%)
3	SF4	G	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	G	1803	4	38,52,52	2.60	17 (44%)	43,81,81	2.56	13 (30%)
5	MGD	G	1804	4	38,52,52	2.47	15 (39%)	43,81,81	2.56	16 (37%)
6	HEC	H	1128	2	24,50,50	2.65	5 (20%)	19,82,82	2.94	9 (47%)
6	HEC	H	1129	2	24,50,50	2.62	4 (16%)	19,82,82	2.79	9 (47%)
3	SF4	I	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	I	1803	4	38,52,52	3.33	18 (47%)	43,81,81	2.63	17 (39%)
5	MGD	I	1804	4	38,52,52	2.66	14 (36%)	43,81,81	2.55	15 (34%)
6	HEC	J	1128	2	24,50,50	2.84	7 (29%)	19,82,82	3.19	6 (31%)
6	HEC	J	1129	2	24,50,50	2.42	6 (25%)	19,82,82	3.32	11 (57%)
3	SF4	K	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	K	1803	4	38,52,52	2.42	17 (44%)	43,81,81	2.44	14 (32%)
5	MGD	K	1804	4	38,52,52	2.38	13 (34%)	43,81,81	2.54	17 (39%)
6	HEC	L	1128	2	24,50,50	2.38	9 (37%)	19,82,82	2.83	9 (47%)
6	HEC	L	1129	2	24,50,50	2.51	3 (12%)	19,82,82	3.02	11 (57%)
3	SF4	M	1801	1	0,12,12	0.00	-	0,24,24	0.00	-
5	MGD	M	1803	4	38,52,52	2.44	14 (36%)	43,81,81	2.40	13 (30%)
5	MGD	M	1804	4	38,52,52	2.38	13 (34%)	43,81,81	2.41	15 (34%)
6	HEC	N	1128	2	24,50,50	2.70	9 (37%)	19,82,82	3.27	11 (57%)
6	HEC	N	1129	2	24,50,50	2.69	5 (20%)	19,82,82	2.80	10 (52%)
3	SF4	O	1801	1	0,12,12	0.00	-	0,24,24	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MGD	O	1803	4	38,52,52	3.22	17 (44%)	43,81,81	2.48	14 (32%)
5	MGD	O	1804	4	38,52,52	2.65	17 (44%)	43,81,81	2.50	16 (37%)
6	HEC	P	1128	2	24,50,50	2.17	8 (33%)	19,82,82	2.78	6 (31%)
6	HEC	P	1129	2	24,50,50	1.97	6 (25%)	19,82,82	2.88	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
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
3	SF4	C	1801	1	-	0/0/48/48	0/6/5/5
5	MGD	C	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	C	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	D	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	D	1129	2	-	0/6/54/54	0/0/8/8
3	SF4	E	1801	1	-	0/0/48/48	0/6/5/5
5	MGD	E	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	E	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	F	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	F	1129	2	-	0/6/54/54	0/0/8/8
3	SF4	G	1801	1	-	0/0/48/48	0/6/5/5
5	MGD	G	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	G	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	H	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	H	1129	2	-	0/6/54/54	0/0/8/8
3	SF4	I	1801	1	-	0/0/48/48	0/6/5/5
5	MGD	I	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	I	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	J	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	J	1129	2	-	0/6/54/54	0/0/8/8
3	SF4	K	1801	1	-	0/0/48/48	0/6/5/5
5	MGD	K	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	K	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	L	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	L	1129	2	-	0/6/54/54	0/0/8/8
3	SF4	M	1801	1	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MGD	M	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	M	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	N	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	N	1129	2	-	0/6/54/54	0/0/8/8
3	SF4	O	1801	1	-	0/0/48/48	0/6/5/5
5	MGD	O	1803	4	-	0/18/66/66	0/6/6/6
5	MGD	O	1804	4	-	0/18/66/66	0/6/6/6
6	HEC	P	1128	2	-	0/6/54/54	0/0/8/8
6	HEC	P	1129	2	-	0/6/54/54	0/0/8/8

The worst 5 of 337 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	1129	HEC	C3B-C2B	-10.06	1.30	1.40
6	H	1129	HEC	C3B-C2B	-9.82	1.30	1.40
6	N	1128	HEC	C3B-C2B	-9.21	1.31	1.40
6	B	1128	HEC	C3B-C2B	-9.19	1.31	1.40
6	J	1128	HEC	C3B-C2B	-9.06	1.31	1.40

The worst 5 of 390 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1128	HEC	CBD-CAD-C3D	-7.60	98.91	112.53
6	N	1128	HEC	CBB-CAB-C3B	-7.34	111.05	127.35
6	L	1128	HEC	CBB-CAB-C3B	-7.20	111.34	127.35
6	D	1128	HEC	CBC-CAC-C3C	-7.10	111.58	127.35
5	G	1803	MGD	C5-C6-N1	-7.10	113.89	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

35 monomers are involved in 324 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1803	MGD	7	0
5	A	1804	MGD	8	0
6	B	1128	HEC	3	0
6	B	1129	HEC	12	0
3	C	1801	SF4	1	0
5	C	1803	MGD	8	0
5	C	1804	MGD	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1128	HEC	11	0
6	D	1129	HEC	22	0
3	E	1801	SF4	1	0
5	E	1803	MGD	8	0
5	E	1804	MGD	7	0
6	F	1128	HEC	12	0
6	F	1129	HEC	11	0
5	G	1803	MGD	7	0
5	G	1804	MGD	6	0
6	H	1128	HEC	13	0
6	H	1129	HEC	14	0
5	I	1803	MGD	7	0
5	I	1804	MGD	6	0
6	J	1128	HEC	11	0
6	J	1129	HEC	16	0
3	K	1801	SF4	1	0
5	K	1803	MGD	8	0
5	K	1804	MGD	7	0
6	L	1128	HEC	9	0
6	L	1129	HEC	17	0
5	M	1803	MGD	8	0
5	M	1804	MGD	7	0
6	N	1128	HEC	11	0
6	N	1129	HEC	19	0
5	O	1803	MGD	7	0
5	O	1804	MGD	8	0
6	P	1128	HEC	10	0
6	P	1129	HEC	15	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

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	790/802 (98%)	-0.30	7 (0%) 85 78	10, 24, 60, 88	0
1	C	790/802 (98%)	-0.16	11 (1%) 78 65	12, 38, 70, 92	0
1	E	790/802 (98%)	-0.27	6 (0%) 87 80	10, 30, 63, 88	0
1	G	790/802 (98%)	-0.03	17 (2%) 65 50	12, 44, 73, 92	0
1	I	790/802 (98%)	0.51	54 (6%) 20 11	23, 58, 77, 92	0
1	K	790/802 (98%)	-0.10	14 (1%) 71 58	17, 43, 70, 90	0
1	M	790/802 (98%)	-0.12	11 (1%) 78 65	13, 42, 70, 91	0
1	O	790/802 (98%)	0.37	43 (5%) 29 17	25, 53, 76, 95	0
2	B	127/130 (97%)	-0.20	1 (0%) 87 80	10, 33, 70, 83	0
2	D	127/130 (97%)	-0.04	3 (2%) 62 47	14, 38, 75, 87	0
2	F	127/130 (97%)	-0.14	2 (1%) 74 62	11, 34, 70, 85	0
2	H	127/130 (97%)	-0.06	3 (2%) 62 47	11, 39, 76, 86	0
2	J	127/130 (97%)	0.15	5 (3%) 43 28	18, 47, 82, 93	0
2	L	127/130 (97%)	-0.09	4 (3%) 52 38	15, 38, 75, 96	0
2	N	127/130 (97%)	-0.09	2 (1%) 74 62	12, 39, 75, 90	0
2	P	127/130 (97%)	0.01	4 (3%) 52 38	19, 44, 76, 89	0
All	All	7336/7456 (98%)	-0.02	187 (2%) 61 47	10, 43, 73, 96	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	79	ASP	7.1
2	J	2	ASP	7.1
1	E	79	ASP	6.6
2	L	2	ASP	6.4
1	M	78	LYS	6.3

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^{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
6	HEC	L	1129	43/43	0.92	0.25	2.40	10,29,44,46	0
6	HEC	D	1129	43/43	0.94	0.22	1.69	14,19,48,55	0
6	HEC	H	1129	43/43	0.92	0.24	1.47	13,19,42,46	0
6	HEC	J	1129	43/43	0.93	0.25	1.33	32,43,47,50	0
6	HEC	F	1129	43/43	0.94	0.21	1.28	10,19,38,43	0
6	HEC	F	1128	43/43	0.93	0.25	0.91	14,23,47,56	0
6	HEC	N	1129	43/43	0.94	0.21	0.91	18,27,41,44	0
6	HEC	D	1128	43/43	0.93	0.24	0.91	20,29,44,52	0
6	HEC	N	1128	43/43	0.93	0.25	0.87	25,31,43,51	0
6	HEC	P	1129	43/43	0.92	0.22	0.83	23,40,42,43	0
6	HEC	P	1128	43/43	0.92	0.26	0.80	27,37,49,54	0
6	HEC	B	1129	43/43	0.96	0.18	0.54	10,16,36,41	0
6	HEC	H	1128	43/43	0.93	0.25	0.52	15,24,38,45	0
5	MGD	C	1804	47/47	0.95	0.19	0.52	21,27,39,40	0
5	MGD	K	1804	47/47	0.94	0.21	0.39	24,36,39,42	0
6	HEC	J	1128	43/43	0.92	0.27	0.39	31,37,50,56	0
5	MGD	E	1804	47/47	0.95	0.18	0.23	10,12,20,24	0
6	HEC	L	1128	43/43	0.93	0.23	0.03	27,35,44,51	0
6	HEC	B	1128	43/43	0.95	0.20	0.01	12,15,38,45	0
5	MGD	C	1803	47/47	0.96	0.18	-0.14	19,26,32,34	0
5	MGD	A	1803	47/47	0.96	0.16	-0.20	10,12,16,17	0
5	MGD	I	1804	47/47	0.90	0.21	-0.21	47,53,61,64	0
5	MGD	A	1804	47/47	0.96	0.16	-0.26	10,10,12,18	0
5	MGD	G	1804	47/47	0.95	0.17	-0.32	28,35,39,42	0
5	MGD	O	1804	47/47	0.93	0.20	-0.34	46,50,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MGD	K	1803	47/47	0.97	0.17	-0.42	31,34,36,40	0
5	MGD	M	1803	47/47	0.97	0.16	-0.57	23,28,34,36	0
5	MGD	M	1804	47/47	0.97	0.16	-0.63	23,26,30,34	0
5	MGD	O	1803	47/47	0.93	0.18	-0.67	37,45,56,57	0
5	MGD	I	1803	47/47	0.92	0.20	-0.73	34,49,58,61	0
5	MGD	E	1803	47/47	0.97	0.15	-0.78	10,17,21,22	0
5	MGD	G	1803	47/47	0.97	0.15	-1.22	23,26,36,37	0
3	SF4	A	1801	8/8	0.99	0.10	-1.31	10,10,10,12	0
3	SF4	K	1801	8/8	0.99	0.11	-1.65	10,10,11,12	0
3	SF4	G	1801	8/8	0.99	0.09	-1.74	10,10,12,12	0
3	SF4	C	1801	8/8	0.99	0.09	-1.75	10,10,11,12	0
3	SF4	E	1801	8/8	0.99	0.09	-1.81	10,10,11,12	0
3	SF4	I	1801	8/8	0.98	0.11	-1.88	34,37,37,39	0
3	SF4	O	1801	8/8	0.98	0.10	-1.95	29,30,33,33	0
4	MO	G	1802	1/1	0.99	0.09	-2.19	35,35,35,35	0
4	MO	O	1802	1/1	0.96	0.08	-2.44	62,62,62,62	0
3	SF4	M	1801	8/8	0.99	0.09	-2.63	10,10,12,12	0
4	MO	K	1802	1/1	0.99	0.09	-3.04	40,40,40,40	0
4	MO	M	1802	1/1	0.99	0.07	-3.21	39,39,39,39	0
4	MO	C	1802	1/1	0.98	0.07	-3.50	38,38,38,38	0
4	MO	I	1802	1/1	0.93	0.05	-3.63	66,66,66,66	0
4	MO	E	1802	1/1	0.98	0.06	-4.53	28,28,28,28	0
4	MO	A	1802	1/1	0.99	0.07	-5.02	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.