



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 11:33 AM GMT

PDB ID : 1H29
Title : SULFATE RESPIRATION IN DESULFOVIBRIO VULGARIS HILDENBOROUGH: STRUCTURE OF THE 16-HEME CYTOCHROME C HMCA AT 2.5 Å RESOLUTION AND A VIEW OF ITS ROLE IN TRANSMEMBRANE ELECTRON TRANSFER
Authors : Matias, P.M.; Coelho, A.V.; Valente, F.M.A.; Placido, D.; Legall, J.; Xavier, A.V.; Pereira, I.A.C.; Carrondo, M.A.
Deposited on : 2002-08-01
Resolution : 2.51 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

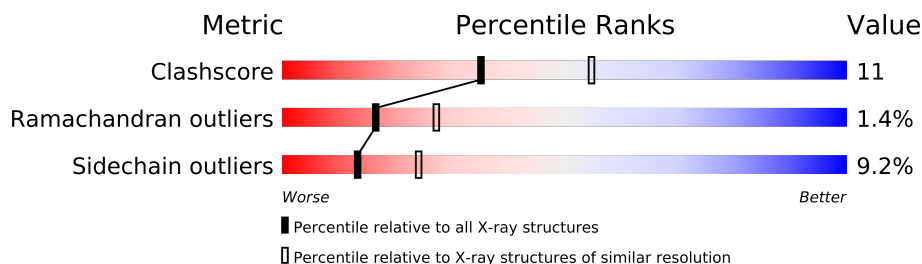
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
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 2.51 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	
1	C	514	
1	D	514	

2 Entry composition i

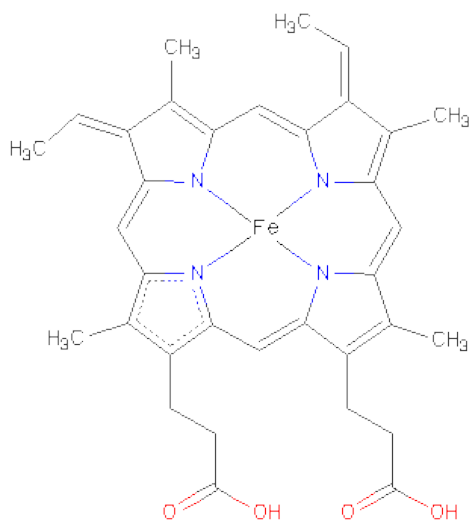
There are 3 unique types of molecules in this entry. The entry contains 18287 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HIGH-MOLECULAR-WEIGHTCYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	38	0	0
			3783	2323	717	699	44			
1	B	499	Total	C	N	O	S	75	0	0
			3763	2312	712	695	44			
1	C	501	Total	C	N	O	S	90	0	0
			3777	2320	714	699	44			
1	D	492	Total	C	N	O	S	70	0	0
			3715	2284	699	688	44			

- 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	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	126	Total 126	O 126	0	0
3	C	136	Total 136	O 136	0	0
3	D	112	Total 112	O 112	0	0

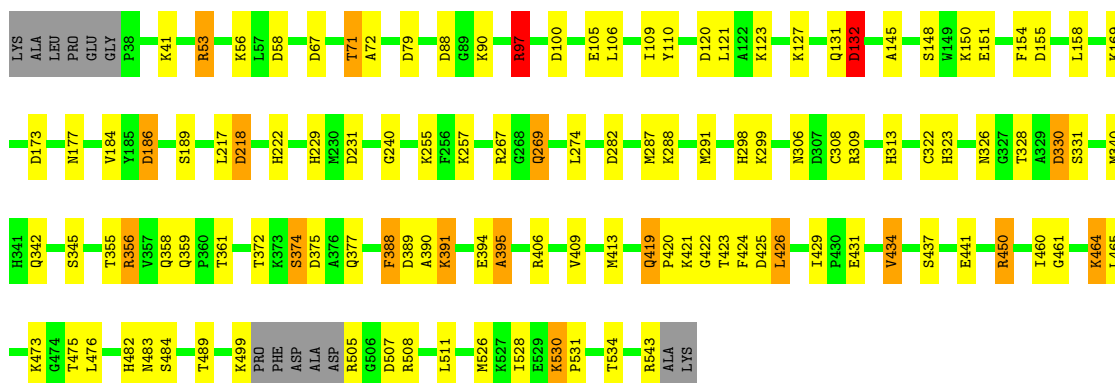
3 Residue-property plots

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.

Note EDS was not executed.

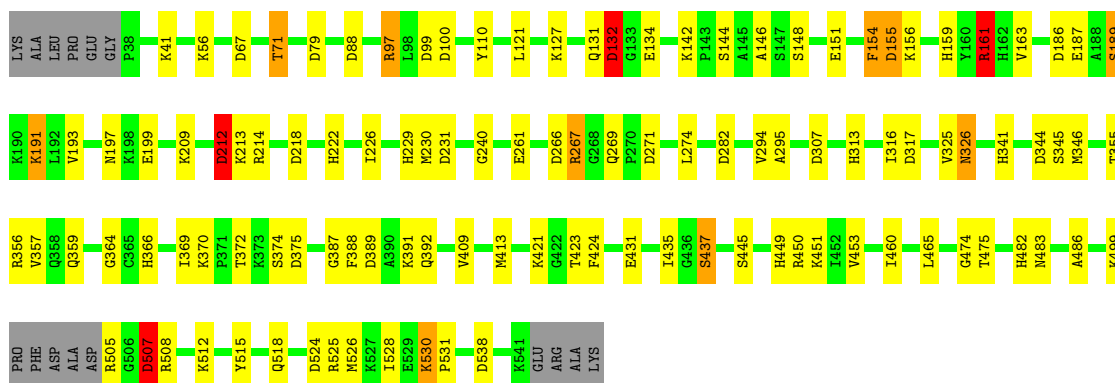
• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

Chain A:



• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

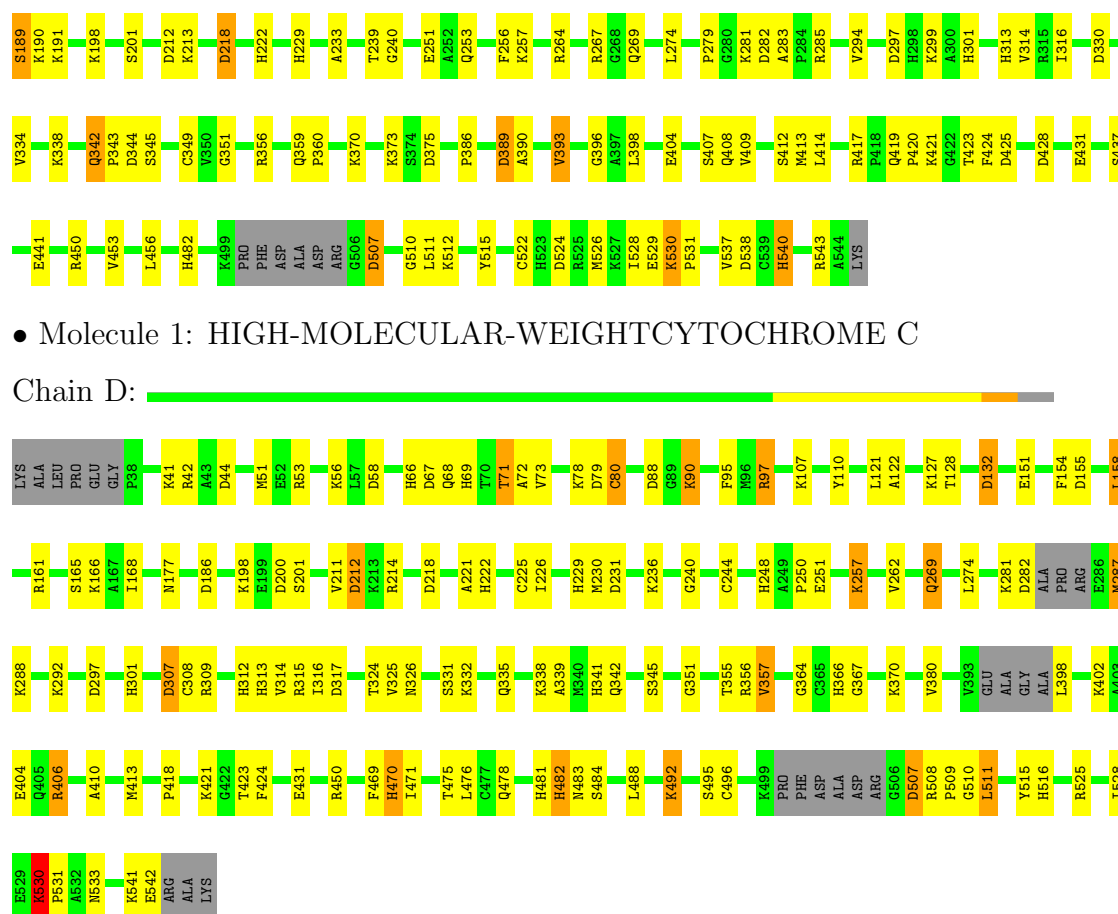
Chain B:



• Molecule 1: HIGH-MOLECULAR-WEIGHTCYTOCHROME C

Chain C:





• Molecule 1: HIGH-MOLECULAR-WEIGHT CYTOCHROME C

Chain D: 

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	220.39Å 220.39Å 102.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.51	Depositor
% Data completeness (in resolution range)	92.1 (30.00-2.51)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18287	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC

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	0.59	0/3864	0.83	17/5201 (0.3%)
1	B	0.59	1/3844 (0.0%)	0.83	21/5175 (0.4%)
1	C	0.57	0/3858	0.85	19/5194 (0.4%)
1	D	0.53	0/3793	0.83	15/5103 (0.3%)
All	All	0.57	1/15359 (0.0%)	0.84	72/20673 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	D	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	SER	CB-OG	7.80	1.52	1.42

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	ASP	CB-CG-OD2	10.44	127.69	118.30
1	A	132	ASP	CB-CG-OD2	8.26	125.73	118.30
1	D	79	ASP	CB-CG-OD2	8.20	125.68	118.30
1	C	97	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	C	428	ASP	CB-CG-OD2	7.37	124.93	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	GLN	Peptide
1	A	217	LEU	Peptide
1	B	131	GLN	Peptide
1	B	154	PHE	Peptide
1	D	470	HIS	Peptide

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	3783	0	3716	68	0
1	B	3763	0	3697	67	0
1	C	3777	0	3708	80	0
1	D	3715	0	3644	81	0
2	A	688	0	480	38	0
2	B	688	0	480	36	0
2	C	688	0	480	39	0
2	D	688	0	480	44	0
3	A	123	0	0	1	0
3	B	126	0	0	2	0
3	C	136	0	0	3	0
3	D	112	0	0	1	0
All	All	18287	0	16685	357	0

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 11.

The worst 5 of 357 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:530:LYS:HB3	1:D:531:PRO:CD	1.85	1.07
1:B:530:LYS:HB2	1:B:531:PRO:HD3	1.34	1.06
1:D:530:LYS:HB3	1:D:531:PRO:HD3	1.29	1.06
1:C:522:CYS:SG	1:C:526:MET:HE2	1.97	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:530:LYS:CB	1:B:531:PRO:HD3	1.89	1.03

There are no symmetry-related clashes.

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	497/514 (97%)	463 (93%)	25 (5%)	9 (2%)	13	20
1	B	495/514 (96%)	460 (93%)	28 (6%)	7 (1%)	16	27
1	C	497/514 (97%)	468 (94%)	24 (5%)	5 (1%)	22	38
1	D	484/514 (94%)	451 (93%)	26 (5%)	7 (1%)	16	27
All	All	1973/2056 (96%)	1842 (93%)	103 (5%)	28 (1%)	16	27

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	218	ASP
1	A	390	ALA
1	A	395	ALA
1	B	132	ASP

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	405/414 (98%)	363 (90%)	42 (10%)	10	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	403/414 (97%)	368 (91%)	35 (9%)	15	27
1	C	404/414 (98%)	374 (93%)	30 (7%)	20	35
1	D	400/414 (97%)	359 (90%)	41 (10%)	10	19
All	All	1612/1656 (97%)	1464 (91%)	148 (9%)	13	24

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	C	161	ARG
1	D	398	LEU
1	B	437	SER
1	B	508	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	483	ASN
1	C	358	GLN
1	D	443	GLN
1	C	68	GLN
1	C	377	GLN

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 ⓘ

64 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$
2	HEC	A	1101	1	50,50,50	2.92	17 (34%)	56,82,82	1.48	10 (17%)
2	HEC	A	1102	1	50,50,50	2.76	16 (32%)	56,82,82	1.54	9 (16%)
2	HEC	A	1103	1	50,50,50	2.78	17 (34%)	56,82,82	1.80	13 (23%)
2	HEC	A	1104	1	50,50,50	2.72	14 (28%)	56,82,82	1.47	6 (10%)
2	HEC	A	1105	1	50,50,50	2.78	14 (28%)	56,82,82	1.52	11 (19%)
2	HEC	A	1106	1	50,50,50	2.72	16 (32%)	56,82,82	1.52	12 (21%)
2	HEC	A	1107	1	50,50,50	2.76	15 (30%)	56,82,82	1.89	14 (25%)
2	HEC	A	1108	1	50,50,50	2.82	15 (30%)	56,82,82	1.67	15 (26%)
2	HEC	A	1109	1	50,50,50	2.91	15 (30%)	56,82,82	1.52	10 (17%)
2	HEC	A	1110	1	50,50,50	2.76	16 (32%)	56,82,82	1.49	11 (19%)
2	HEC	A	1111	1	50,50,50	2.89	16 (32%)	56,82,82	1.42	7 (12%)
2	HEC	A	1112	1	50,50,50	2.79	16 (32%)	56,82,82	1.37	10 (17%)
2	HEC	A	1113	1	50,50,50	2.82	15 (30%)	56,82,82	1.45	8 (14%)
2	HEC	A	1114	1	50,50,50	2.97	16 (32%)	56,82,82	1.51	9 (16%)
2	HEC	A	1115	1	50,50,50	2.86	16 (32%)	56,82,82	1.62	11 (19%)
2	HEC	A	1116	1	50,50,50	2.71	15 (30%)	56,82,82	1.65	12 (21%)
2	HEC	B	1101	1	50,50,50	2.83	15 (30%)	56,82,82	1.65	12 (21%)
2	HEC	B	1102	1	50,50,50	2.73	15 (30%)	56,82,82	1.46	10 (17%)
2	HEC	B	1103	1	50,50,50	2.86	16 (32%)	56,82,82	1.63	12 (21%)
2	HEC	B	1104	1	50,50,50	2.89	15 (30%)	56,82,82	1.52	8 (14%)
2	HEC	B	1105	1	50,50,50	2.95	18 (36%)	56,82,82	1.42	8 (14%)
2	HEC	B	1106	1	50,50,50	2.79	15 (30%)	56,82,82	1.52	12 (21%)
2	HEC	B	1107	1	50,50,50	2.73	14 (28%)	56,82,82	1.60	12 (21%)
2	HEC	B	1108	1	50,50,50	2.78	17 (34%)	56,82,82	1.49	7 (12%)
2	HEC	B	1109	1	50,50,50	2.91	18 (36%)	56,82,82	1.23	7 (12%)
2	HEC	B	1110	1	50,50,50	2.78	15 (30%)	56,82,82	1.79	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	B	1111	1	50,50,50	2.83	16 (32%)	56,82,82	1.39	8 (14%)
2	HEC	B	1112	1	50,50,50	2.66	14 (28%)	56,82,82	1.71	14 (25%)
2	HEC	B	1113	1	50,50,50	2.81	16 (32%)	56,82,82	1.71	9 (16%)
2	HEC	B	1114	1	50,50,50	2.96	17 (34%)	56,82,82	1.42	8 (14%)
2	HEC	B	1115	1	50,50,50	2.91	16 (32%)	56,82,82	1.43	9 (16%)
2	HEC	B	1116	1	50,50,50	2.82	15 (30%)	56,82,82	1.65	11 (19%)
2	HEC	C	1101	1	50,50,50	2.67	14 (28%)	56,82,82	1.50	11 (19%)
2	HEC	C	1102	1	50,50,50	2.81	16 (32%)	56,82,82	1.50	10 (17%)
2	HEC	C	1103	1	50,50,50	2.76	16 (32%)	56,82,82	1.71	9 (16%)
2	HEC	C	1104	1	50,50,50	2.86	15 (30%)	56,82,82	1.45	11 (19%)
2	HEC	C	1105	1	50,50,50	2.80	15 (30%)	56,82,82	1.48	10 (17%)
2	HEC	C	1106	1	50,50,50	2.78	16 (32%)	56,82,82	1.68	15 (26%)
2	HEC	C	1107	1	50,50,50	2.73	13 (26%)	56,82,82	1.71	13 (23%)
2	HEC	C	1108	1	50,50,50	2.76	15 (30%)	56,82,82	1.43	11 (19%)
2	HEC	C	1109	1	50,50,50	2.73	16 (32%)	56,82,82	1.49	10 (17%)
2	HEC	C	1110	1	50,50,50	2.77	15 (30%)	56,82,82	1.65	12 (21%)
2	HEC	C	1111	1	50,50,50	2.77	15 (30%)	56,82,82	1.31	7 (12%)
2	HEC	C	1112	1	50,50,50	2.71	15 (30%)	56,82,82	1.39	7 (12%)
2	HEC	C	1113	1	50,50,50	2.79	14 (28%)	56,82,82	1.70	14 (25%)
2	HEC	C	1114	1	50,50,50	2.89	16 (32%)	56,82,82	1.47	7 (12%)
2	HEC	C	1115	1	50,50,50	2.91	15 (30%)	56,82,82	1.91	16 (28%)
2	HEC	C	1116	1	50,50,50	2.73	14 (28%)	56,82,82	1.66	13 (23%)
2	HEC	D	1101	1	50,50,50	2.91	15 (30%)	56,82,82	1.48	7 (12%)
2	HEC	D	1102	1	50,50,50	2.84	17 (34%)	56,82,82	1.53	9 (16%)
2	HEC	D	1103	1	50,50,50	2.83	15 (30%)	56,82,82	1.79	15 (26%)
2	HEC	D	1104	1	50,50,50	2.81	15 (30%)	56,82,82	1.54	9 (16%)
2	HEC	D	1105	1	50,50,50	2.95	16 (32%)	56,82,82	1.45	8 (14%)
2	HEC	D	1106	1	50,50,50	2.80	16 (32%)	56,82,82	1.42	10 (17%)
2	HEC	D	1107	1	50,50,50	2.89	15 (30%)	56,82,82	1.51	10 (17%)
2	HEC	D	1108	1	50,50,50	2.88	16 (32%)	56,82,82	1.64	11 (19%)
2	HEC	D	1109	1	50,50,50	2.92	16 (32%)	56,82,82	1.37	11 (19%)
2	HEC	D	1110	1	50,50,50	2.94	17 (34%)	56,82,82	1.49	12 (21%)
2	HEC	D	1111	1	50,50,50	2.80	15 (30%)	56,82,82	1.51	10 (17%)
2	HEC	D	1112	1	50,50,50	2.78	14 (28%)	56,82,82	1.48	8 (14%)
2	HEC	D	1113	1	50,50,50	2.70	13 (26%)	56,82,82	1.63	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEC	D	1114	1	50,50,50	2.82	17 (34%)	56,82,82	1.64	12 (21%)
2	HEC	D	1115	1	50,50,50	2.91	15 (30%)	56,82,82	1.53	8 (14%)
2	HEC	D	1116	1	50,50,50	2.72	14 (28%)	56,82,82	1.67	8 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	1101	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1107	1	-	1/10/54/54	0/0/8/8
2	HEC	A	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	A	1116	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1101	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1107	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	B	1116	1	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	C	1101	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1107	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	C	1116	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1101	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1102	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1103	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1104	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1105	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1106	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1107	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1108	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1109	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1110	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1111	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1112	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1113	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1114	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1115	1	-	0/10/54/54	0/0/8/8
2	HEC	D	1116	1	-	0/10/54/54	0/0/8/8

The worst 5 of 987 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1103	HEC	C3C-CAC	10.72	1.57	1.35
2	D	1105	HEC	C3C-CAC	10.70	1.57	1.35
2	A	1101	HEC	C3C-CAC	10.60	1.57	1.35
2	B	1110	HEC	C3C-CAC	10.57	1.57	1.35
2	A	1107	HEC	C3C-CAC	10.56	1.57	1.35

The worst 5 of 664 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1103	HEC	CBD-CAD-C3D	-7.45	99.57	112.69
2	C	1103	HEC	CBD-CAD-C3D	-6.70	100.89	112.69
2	B	1113	HEC	CBD-CAD-C3D	-6.03	102.07	112.69
2	A	1116	HEC	CBD-CAD-C3D	-6.03	102.07	112.69
2	C	1116	HEC	CBD-CAD-C3D	-5.84	102.40	112.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1107	HEC	C1A-C2A-CAA-CBA

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.