



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 05:43 PM GMT

PDB ID : 3VRD
Title : Crystal structure of flavocytochrome c from *Thermochromatium tepidum*
Authors : Hirano, Y.; Kimura, Y.; Suzuki, H.; Miki, K.; Wang, Z.-Y.
Deposited on : 2012-04-09
Resolution : 1.50 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

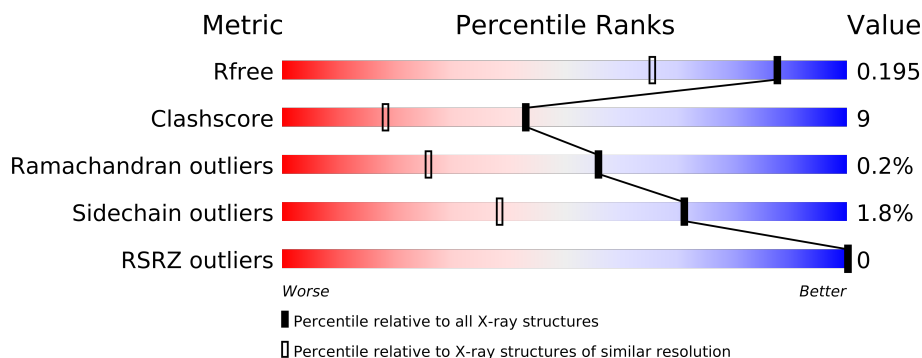
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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.

Mol	Chain	Length	Quality of chain
1	A	174	
2	B	401	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NO3	B	503	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5107 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.

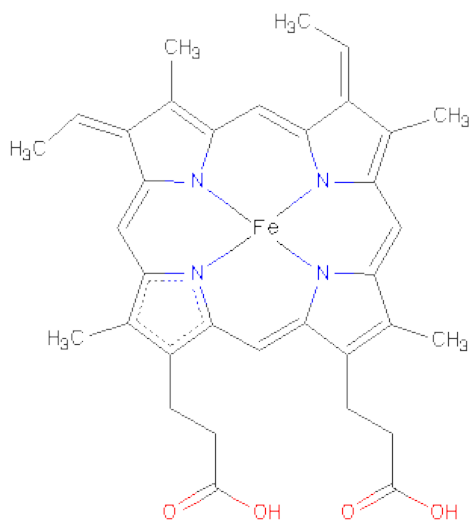
- Molecule 1 is a protein called Flavocytochrome c heme subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	1	0
			1370	863	233	263	11			

- Molecule 2 is a protein called Flavocytochrome c flavin subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	400	Total	C	N	O	S	0	0	0
			3015	1912	512	579	12			

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



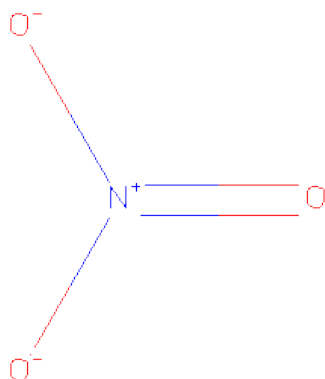
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	1
			47	36	1	4	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



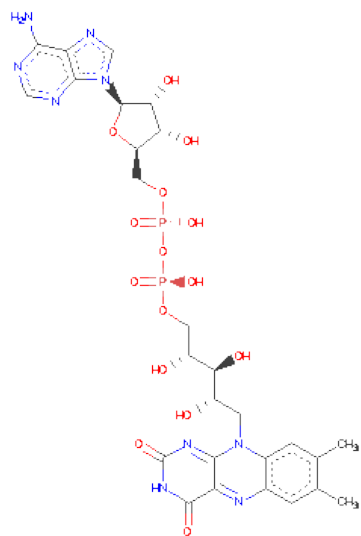
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	B	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total	O	0	0
			186	186		
7	B	367	Total	O	0	0
			367	367		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

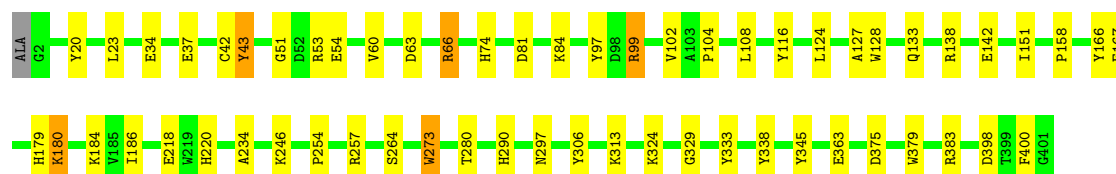
- Molecule 1: Flavocytochrome c heme subunit

Chain A: 



- Molecule 2: Flavocytochrome c flavin subunit

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	140.62Å 140.62Å 57.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.50 35.15 – 1.50	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-1.50) 93.4 (35.15-1.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.160 , 0.195 0.160 , 0.195	Depositor DCC
R_{free} test set	4208 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	8.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.5	EDS
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 84163 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5107	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NO3, FAD, CSS, 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	1.35	4/1402 (0.3%)	1.80	15/1881 (0.8%)
2	B	1.45	14/3073 (0.5%)	1.29	18/4184 (0.4%)
All	All	1.42	18/4475 (0.4%)	1.47	33/6065 (0.5%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	GLU	CD-OE1	7.17	1.33	1.25
2	B	43	TYR	CG-CD2	7.05	1.48	1.39
2	B	379	TRP	CD2-CE2	6.68	1.49	1.41
2	B	329	GLY	N-CA	6.42	1.55	1.46
2	B	166	TYR	CE1-CZ	6.27	1.46	1.38
2	B	363	GLU	CD-OE2	-6.09	1.19	1.25
2	B	383	ARG	CZ-NH2	6.08	1.41	1.33
2	B	167	GLU	CD-OE1	5.52	1.31	1.25
2	B	97	TYR	CE2-CZ	5.49	1.45	1.38
1	A	130	ARG	CZ-NH2	-5.43	1.25	1.33
2	B	264	SER	CB-OG	-5.33	1.35	1.42
2	B	43	TYR	CD1-CE1	5.15	1.47	1.39
2	B	97	TYR	CG-CD1	5.15	1.45	1.39
1	A	5	GLU	CG-CD	5.09	1.59	1.51
2	B	363	GLU	CG-CD	5.08	1.59	1.51
2	B	273	TRP	CE2-CZ2	5.08	1.48	1.39
1	A	42	GLU	CD-OE2	5.02	1.31	1.25
2	B	51	GLY	N-CA	5.01	1.53	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH1	34.69	137.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH2	-30.22	105.19	120.30
1	A	130	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	A	140	ARG	CD-NE-CZ	14.66	144.13	123.60
1	A	130	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	A	141	ARG	NE-CZ-NH2	-11.44	114.58	120.30
2	B	66	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	A	137	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	140	ARG	CB-CG-CD	8.80	134.48	111.60
2	B	138	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	154	LEU	CB-CG-CD1	-8.13	97.18	111.00
2	B	53	ARG	NE-CZ-NH2	-8.09	116.25	120.30
2	B	338	TYR	CB-CG-CD1	-7.59	116.45	121.00
1	A	135	ASP	CB-CG-OD2	-7.50	111.55	118.30
2	B	63	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	7	LEU	CB-CG-CD1	-6.55	99.86	111.00
2	B	124	LEU	CB-CG-CD2	6.12	121.41	111.00
1	A	163	LEU	CB-CG-CD1	-5.94	100.91	111.00
2	B	375	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	59	LYS	CD-CE-NZ	-5.87	98.20	111.70
2	B	23	LEU	CB-CG-CD2	5.85	120.94	111.00
2	B	142	GLU	OE1-CD-OE2	-5.81	116.33	123.30
2	B	54	GLU	OE1-CD-OE2	-5.72	116.44	123.30
2	B	54	GLU	CG-CD-OE1	5.71	129.73	118.30
2	B	63	ASP	CB-CG-OD2	-5.68	113.18	118.30
2	B	398	ASP	CB-CG-OD1	-5.62	113.24	118.30
2	B	99	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	B	383	ARG	NE-CZ-NH1	5.29	122.95	120.30
2	B	66	ARG	NH1-CZ-NH2	5.25	125.17	119.40
2	B	363	GLU	OE1-CD-OE2	5.21	129.56	123.30
1	A	154	LEU	CB-CG-CD2	-5.08	102.36	111.00
2	B	116	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	104	CYS	CA-CB-SG	-5.01	104.99	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1370	0	1341	49	0
2	B	3015	0	2959	27	0
3	A	90	0	40	15	0
4	A	12	0	16	0	0
4	B	6	0	8	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	B	53	0	30	3	0
7	A	186	0	0	10	0
7	B	367	0	0	5	0
All	All	5107	0	4394	78	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 9.

All (78) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:42:CYS:SG	6:B:501:FAD:C8M	2.03	1.45
1:A:11:CYS:SG	3:A:201:HEC:CAB	2.06	1.44
1:A:14:CYS:SG	3:A:201:HEC:CAC	2.09	1.39
1:A:148:ALA:HB1	1:A:152:LYS:NZ	1.34	1.38
1:A:11:CYS:SG	3:A:201:HEC:CBB	2.30	1.20
2:B:184:LYS:HE2	7:B:967:HOH:O	1.42	1.19
1:A:14:CYS:SG	3:A:201:HEC:CBC	2.48	1.02
1:A:148:ALA:HB1	1:A:152:LYS:HZ2	1.23	1.01
1:A:148:ALA:HB1	1:A:152:LYS:HZ3	1.24	1.01
1:A:11:CYS:SG	3:A:201:HEC:HBB3	2.07	0.94
3:A:202[A]:HEC:O1D	7:A:455:HOH:O	1.86	0.92
1:A:140:ARG:HD3	7:A:330:HOH:O	1.70	0.91
1:A:14:CYS:SG	3:A:201:HEC:HAC	2.13	0.87
1:A:11:CYS:SG	3:A:201:HEC:HAB	2.16	0.86
1:A:140:ARG:CD	7:A:330:HOH:O	2.22	0.85
2:B:99:ARG:HH11	2:B:290:HIS:HE1	1.23	0.85
1:A:148:ALA:CB	1:A:152:LYS:NZ	2.31	0.83
1:A:97:HIS:HE1	1:A:102:GLU:OE1	1.65	0.79
1:A:14:CYS:SG	3:A:201:HEC:HBC3	2.28	0.73
2:B:99:ARG:HH11	2:B:290:HIS:CE1	2.08	0.71
1:A:14:CYS:SG	3:A:201:HEC:C3C	2.81	0.68
1:A:154:LEU:HD11	1:A:166:LEU:HD11	1.77	0.67
1:A:11:CYS:SG	3:A:201:HEC:C3B	2.85	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:42:CYS:SG	6:B:501:FAD:C8	2.84	0.64
1:A:140:ARG:HD2	7:A:330:HOH:O	1.95	0.62
2:B:42:CYS:SG	6:B:501:FAD:HM81	2.32	0.62
2:B:151:ILE:HD13	2:B:186:ILE:HB	1.80	0.62
2:B:297:ASN:ND2	7:B:694:HOH:O	2.27	0.60
1:A:148:ALA:CB	1:A:152:LYS:HZ3	2.06	0.59
2:B:66:ARG:NH2	7:B:828:HOH:O	2.12	0.59
1:A:148:ALA:HB1	1:A:152:LYS:HZ1	1.55	0.57
3:A:202[A]:HEC:CGD	7:A:455:HOH:O	2.48	0.57
1:A:67:GLN:NE2	7:A:425:HOH:O	2.39	0.56
1:A:75:GLN:HG2	7:A:459:HOH:O	2.06	0.55
1:A:97:HIS:CE1	1:A:102:GLU:OE1	2.55	0.54
2:B:81:ASP:OD2	2:B:84:LYS:HG3	2.07	0.54
1:A:71:GLU:HB3	7:A:419:HOH:O	2.08	0.54
1:A:148:ALA:CB	1:A:152:LYS:HZ2	2.05	0.54
2:B:102:VAL:HG12	2:B:104:PRO:HD3	1.90	0.54
2:B:280:THR:O	2:B:290:HIS:HD2	1.92	0.53
1:A:154:LEU:CD1	1:A:166:LEU:HD11	2.38	0.53
1:A:154:LEU:C	1:A:154:LEU:HD23	2.30	0.52
2:B:20:TYR:CZ	2:B:313:LYS:HE2	2.43	0.52
2:B:273:TRP:HB2	2:B:297:ASN:ND2	2.25	0.51
1:A:97:HIS:HD2	1:A:170:TYR:OH	1.94	0.51
1:A:9:ASN:HB3	2:B:313:LYS:HD3	1.95	0.48
2:B:60:VAL:HG11	2:B:400:PHE:CG	2.48	0.47
1:A:85:PHE:CE1	1:A:87:LYS:HD2	2.49	0.47
1:A:2:PRO:HB2	1:A:7:LEU:HG	1.97	0.46
1:A:146:LYS:HD3	1:A:146:LYS:HA	1.73	0.46
2:B:34:GLU:O	2:B:74:HIS:HA	2.16	0.45
3:A:201:HEC:HMC1	3:A:201:HEC:HBC3	1.98	0.44
1:A:11:CYS:CB	3:A:201:HEC:CAB	2.92	0.44
1:A:74[A]:LYS:NZ	7:A:395:HOH:O	2.52	0.43
2:B:66:ARG:NE	7:B:828:HOH:O	2.47	0.43
2:B:37:GLU:HA	2:B:74:HIS:CE1	2.53	0.43
1:A:97:HIS:CD2	1:A:101:CYS:HB2	2.53	0.42
2:B:179:HIS:C	2:B:180:LYS:HG2	2.40	0.42
2:B:108:LEU:HB3	2:B:254:PRO:HG2	2.02	0.42
2:B:127:ALA:HA	2:B:133:GLN:HB3	2.03	0.41
2:B:234:ALA:O	2:B:246:LYS:NZ	2.54	0.41
2:B:99:ARG:HD3	2:B:290:HIS:HE1	1.86	0.41
2:B:324:LYS:HG3	7:B:774:HOH:O	2.20	0.41
1:A:149:SER:O	1:A:153:GLU:HG3	2.20	0.41
2:B:218:GLU:OE1	2:B:220:HIS:HE1	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:78:TYR:HE2	7:A:429:HOH:O	2.04	0.40
1:A:14:CYS:CB	3:A:201:HEC:C3C	2.99	0.40
2:B:99:ARG:HD3	2:B:290:HIS:CE1	2.57	0.40
1:A:153:GLU:HA	1:A:156:LYS:HE2	2.04	0.40
1:A:130:ARG:HG2	1:A:167:PHE:CE2	2.56	0.40

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	173/174 (99%)	171 (99%)	1 (1%)	1 (1%)	33	9
2	B	396/401 (99%)	388 (98%)	8 (2%)	0	100	100
All	All	569/575 (99%)	559 (98%)	9 (2%)	1 (0%)	56	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ILE

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	142/141 (101%)	142 (100%)	0	100	100
2	B	310/310 (100%)	302 (97%)	8 (3%)	59	21
All	All	452/451 (100%)	444 (98%)	8 (2%)	71	38

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	43	TYR
2	B	128	TRP
2	B	158	PRO
2	B	180	LYS
2	B	257	ARG
2	B	306	TYR
2	B	333	TYR
2	B	345	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	174	GLN
2	B	220	HIS
2	B	290	HIS
2	B	335	ASN
2	B	397	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues 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	CSS	B	161	2	5,6,7	6.63	2 (40%)	4,6,8	1.23	0
2	CSS	B	337	2	5,6,7	7.34	2 (40%)	4,6,8	3.41	2 (50%)

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	CSS	B	161	2	-	0/2/5/7	0/0/0/0
2	CSS	B	337	2	-	0/2/5/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	337	CSS	O-C	16.16	1.22	1.11
2	B	161	CSS	O-C	14.16	1.21	1.11
2	B	161	CSS	CA-C	3.89	1.55	1.48
2	B	337	CSS	CA-C	2.87	1.53	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	CSS	C-CA-N	-5.84	107.99	113.83
2	B	337	CSS	CA-CB-SG	-2.91	104.23	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 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	HEC	A	201	1	50,50,50	2.00	11 (22%)	56,82,82	2.83	25 (44%)
3	HEC	A	202[A]	-	2,3,50	1.59	1 (50%)	1,3,82	0.72	0
3	HEC	A	202[B]	-	2,3,50	0.16	0	1,3,82	0.66	0
4	GOL	A	203	-	5,5,5	1.37	0	5,5,5	0.78	0
4	GOL	A	204	-	5,5,5	0.63	0	5,5,5	0.77	0
5	NO3	A	205	-	3,3,3	2.02	1 (33%)	3,3,3	0.33	0
6	FAD	B	501	-	58,58,58	1.79	9 (15%)	85,89,89	2.12	20 (23%)
4	GOL	B	502	-	5,5,5	0.87	0	5,5,5	0.52	0
5	NO3	B	503	-	3,3,3	1.79	1 (33%)	3,3,3	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	A	201	1	-	0/10/54/54	0/0/8/8
3	HEC	A	202[A]	-	-	0/0/0/54	0/0/0/8
3	HEC	A	202[B]	-	-	0/0/0/54	0/0/0/8
4	GOL	A	203	-	-	0/4/4/4	0/0/0/0
4	GOL	A	204	-	-	0/4/4/4	0/0/0/0
5	NO3	A	205	-	-	0/0/0/0	0/0/0/0
6	FAD	B	501	-	-	0/34/50/50	0/1/6/6
4	GOL	B	502	-	-	0/4/4/4	0/0/0/0
5	NO3	B	503	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	HEC	C1C-C2C	6.40	1.48	1.40
6	B	501	FAD	C1'-N10	5.67	1.54	1.48
6	B	501	FAD	C6-C5X	-5.47	1.35	1.41
3	A	201	HEC	C3B-CAB	4.90	1.45	1.35
6	B	501	FAD	C9A-N10	4.59	1.45	1.38
6	B	501	FAD	C1'-C2'	-4.58	1.47	1.51
3	A	201	HEC	C3C-CAC	4.12	1.44	1.35
3	A	201	HEC	C3C-C4C	3.75	1.46	1.41
3	A	201	HEC	C1B-C2B	3.57	1.44	1.40
6	B	501	FAD	C7M-C7	2.94	1.57	1.51
3	A	201	HEC	C1D-C2D	2.83	1.43	1.40
3	A	201	HEC	C2A-C3A	2.75	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	FAD	C4X-N5	-2.74	1.30	1.36
5	A	205	NO3	O2-N	2.63	1.39	1.25
3	A	201	HEC	C1A-CHA	2.63	1.46	1.38
3	A	201	HEC	FE-NA	2.57	2.03	1.92
6	B	501	FAD	P-O3P	2.53	1.64	1.59
3	A	201	HEC	CBA-CGA	2.39	1.56	1.50
3	A	201	HEC	FE-NC	2.37	2.02	1.92
5	B	503	NO3	O2-N	2.30	1.37	1.25
6	B	501	FAD	C8A-N7A	2.22	1.39	1.34
3	A	202[A]	HEC	O1D-CGD	2.08	1.26	1.22
6	B	501	FAD	O2-C2	2.05	1.27	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	501	FAD	N3A-C2A-N1A	-9.43	120.83	128.71
3	A	201	HEC	C3B-C2B-C1B	-7.98	101.76	107.07
3	A	201	HEC	C2B-C1B-NB	6.13	114.04	109.41
3	A	201	HEC	C1A-CHA-C4D	-5.96	119.63	127.47
3	A	201	HEC	C4C-CHD-C1D	-5.55	120.17	127.47
6	B	501	FAD	C9A-N10-C10	-5.47	116.40	121.77
3	A	201	HEC	CMB-C2B-C3B	5.42	131.71	125.72
6	B	501	FAD	O4B-C1B-N9A	-5.09	103.70	108.44
6	B	501	FAD	C8A-N9A-C4A	4.97	110.69	106.90
6	B	501	FAD	C2A-N1A-C6A	4.92	127.65	118.77
3	A	201	HEC	C4B-CHC-C1C	-4.57	121.45	127.47
3	A	201	HEC	C1A-C2A-C3A	-4.51	103.13	106.69
3	A	201	HEC	C4A-CHB-C1B	-4.44	121.63	127.47
6	B	501	FAD	C2'-C1'-N10	4.29	118.14	112.45
3	A	201	HEC	C2B-C1B-CHB	-4.15	118.14	126.00
6	B	501	FAD	O4B-C1B-C2B	-4.11	100.47	106.77
6	B	501	FAD	C4X-N5-C5X	3.97	121.15	116.69
3	A	201	HEC	CBD-CAD-C3D	-3.94	105.75	112.69
3	A	201	HEC	CMC-C2C-C3C	3.83	129.95	125.72
6	B	501	FAD	C5X-C9A-N10	3.80	120.54	116.80
3	A	201	HEC	CBA-CAA-C2A	-3.77	105.30	112.35
3	A	201	HEC	CBC-CAC-C3C	-3.51	118.56	128.44
3	A	201	HEC	C2A-C1A-NA	3.22	112.05	109.64
3	A	201	HEC	CMC-C2C-C1C	-2.96	124.06	128.62
3	A	201	HEC	CAA-C2A-C1A	2.82	129.76	124.67
3	A	201	HEC	C4B-NB-C1B	-2.76	103.13	106.76
3	A	201	HEC	O2D-CGD-CBD	2.67	123.64	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	HEC	CMD-C2D-C1D	-2.64	124.55	128.62
3	A	201	HEC	C1D-C2D-C3D	2.57	108.78	107.00
6	B	501	FAD	C6-C5X-C9A	2.51	122.50	119.02
6	B	501	FAD	C5A-C4A-N9A	-2.50	103.56	107.16
3	A	201	HEC	C4B-C3B-C2B	2.42	108.22	106.68
6	B	501	FAD	C4X-C10-N10	-2.39	119.32	120.51
6	B	501	FAD	C7M-C7-C8	-2.37	115.27	120.74
6	B	501	FAD	C4X-C10-N1	2.35	125.08	122.73
3	A	201	HEC	O1D-CGD-CBD	-2.26	115.25	123.03
6	B	501	FAD	N3A-C4A-N9A	2.22	129.44	125.43
6	B	501	FAD	C4-N3-C2	-2.20	120.87	125.39
3	A	201	HEC	CHC-C1C-NC	2.19	128.23	124.58
3	A	201	HEC	C3D-C4D-CHA	-2.19	121.86	126.00
6	B	501	FAD	C1'-N10-C10	2.18	122.26	119.17
3	A	201	HEC	C2C-C1C-CHC	-2.08	122.06	126.00
6	B	501	FAD	O5B-C5B-C4B	-2.06	101.38	108.94
6	B	501	FAD	C4A-C5A-N7A	2.05	111.28	109.52
6	B	501	FAD	C10-C4X-N5	2.05	122.94	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	174/174 (100%)	-0.37	0 100 100	6, 12, 27, 38	0
2	B	400/401 (99%)	-0.52	0 100 100	5, 10, 20, 34	0
All	All	574/575 (99%)	-0.47	0 100 100	5, 10, 24, 38	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CSS	B	337	7/8	0.04	-1.86	5,6,9,11	0
2	CSS	B	161	7/8	0.04	-2.13	6,6,8,10	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NO3	B	503	4/4	0.18	10.79	22,25,29,32	0
3	HEC	A	202[A]	4/43	0.07	0.74	14,15,16,17	4
6	FAD	B	501	53/53	0.07	0.60	4,5,8,9	0
3	HEC	A	201	43/43	0.07	0.55	5,6,8,11	0
3	HEC	A	202[B]	4/43	0.07	0.45	12,13,13,16	4
5	NO3	A	205	4/4	0.09	0.02	18,24,24,30	0
4	GOL	A	204	6/6	0.06	-0.02	9,11,12,14	0
4	GOL	B	502	6/6	0.06	-0.07	8,10,10,10	0
4	GOL	A	203	6/6	0.05	-0.98	7,7,9,9	0

6.5 Other polymers ⓘ

There are no such residues in this entry.