



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 26, 2017 – 02:44 PM EDT

PDB ID : 3LSH
Title : Pyranose 2-oxidase T169A, monoclinic
Authors : Divne, C.; Tan, T.C.; Spadiut, O.
Deposited on : unknown
Resolution : 1.90 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

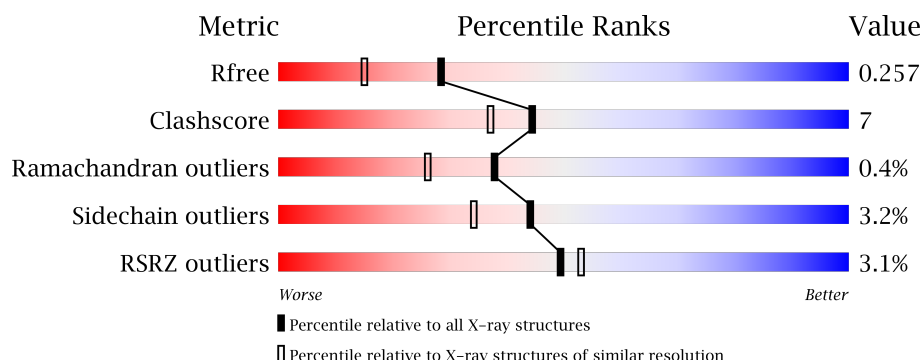
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	623	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
1	C	623	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	623	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20177 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.

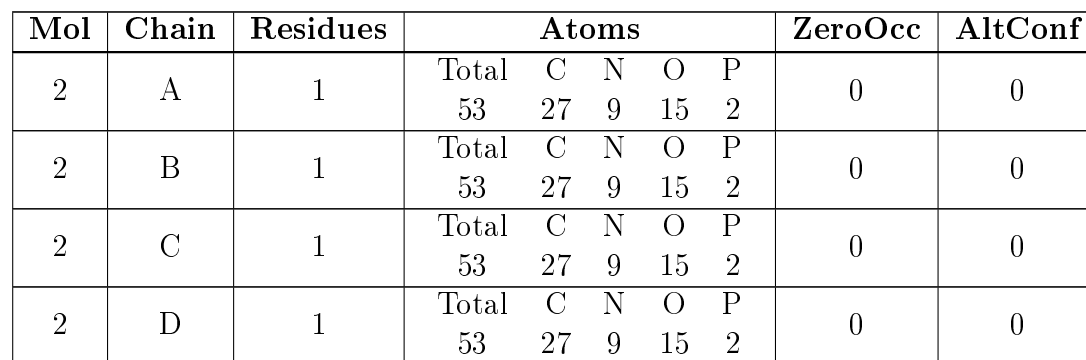
- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4540	2867	777	871	25			
1	B	576	Total	C	N	O	S	0	0	0
			4540	2867	777	871	25			
1	C	575	Total	C	N	O	S	0	0	0
			4531	2862	776	869	24			
1	D	574	Total	C	N	O	S	0	0	0
			4524	2858	775	867	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ALA	THR	ENGINEERED	UNP Q7ZA32
B	169	ALA	THR	ENGINEERED	UNP Q7ZA32
C	169	ALA	THR	ENGINEERED	UNP Q7ZA32
D	169	ALA	THR	ENGINEERED	UNP Q7ZA32

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

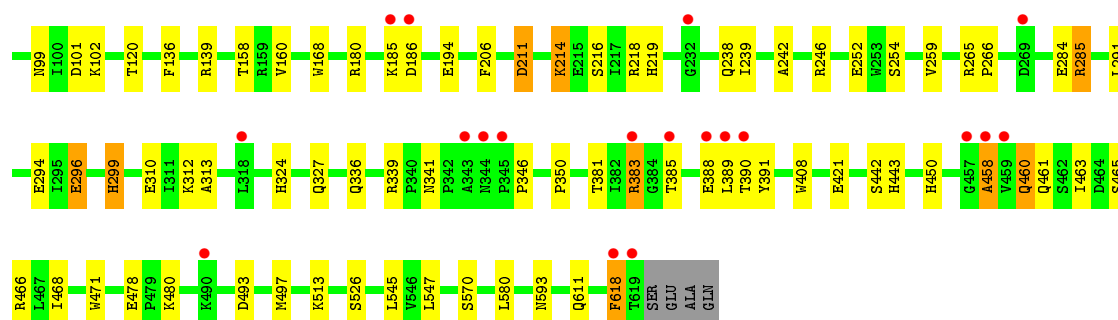


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- Chemical structure of MES (2-(2-methyl-5-sulfinylphenyl)propanoic acid) with atom labels:
- O1: Oxygen atom of the phenyl ring.
 - C2, C3, C5, C6, C7, C8: Carbon atoms of the phenyl ring and the propyl chain.
 - N4: Nitrogen atom of the amine group.
 - S: Sulfur atom of the sulfinyl group.
 - O2S, O1S, O3S: Oxygen atoms of the sulfinyl group.

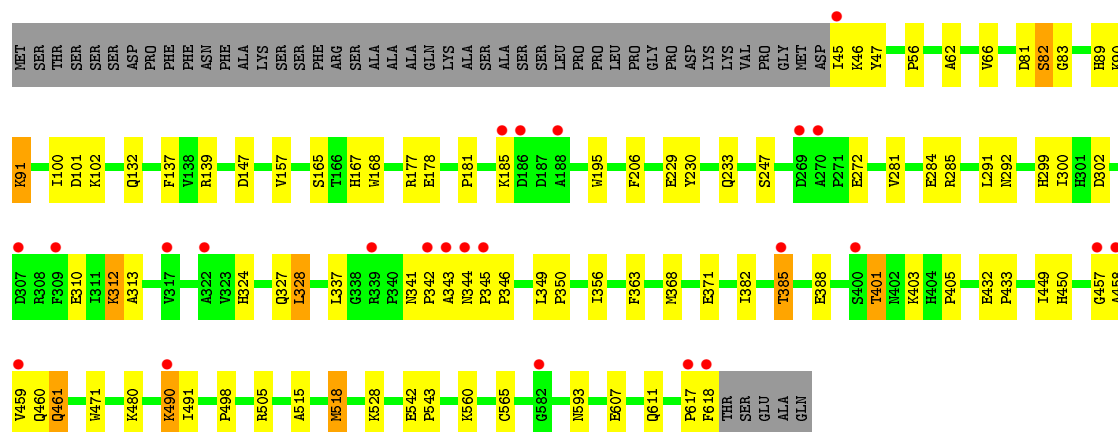
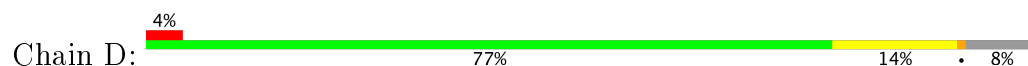
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	450	Total	O	0	0
			450	450		
4	B	554	Total	O	0	0
			554	554		
4	C	472	Total	O	0	0
			472	472		
4	D	342	Total	O	0	0
			342	342		



• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.40Å 102.73Å 137.82Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	28.50 – 1.90 28.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.50-1.90) 98.8 (28.46-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.195 , 0.246 0.212 , 0.257	Depositor DCC
R_{free} test set	3217 reflections (1.50%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l 0.008 for k,h,-l 0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20177	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.07	5/4656 (0.1%)	0.98	12/6330 (0.2%)
1	B	1.15	12/4656 (0.3%)	1.02	15/6330 (0.2%)
1	C	1.03	5/4647 (0.1%)	0.94	9/6319 (0.1%)
1	D	0.92	1/4640 (0.0%)	0.90	6/6309 (0.1%)
All	All	1.05	23/18599 (0.1%)	0.96	42/25288 (0.2%)

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	1
1	C	0	1
1	D	0	1
All	All	0	3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	296	GLU	CG-CD	9.41	1.66	1.51
1	B	310	GLU	CG-CD	7.83	1.63	1.51
1	B	564	CYS	CB-SG	-6.71	1.70	1.82
1	B	478	GLU	CD-OE1	6.53	1.32	1.25
1	A	421	GLU	CB-CG	5.85	1.63	1.52

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	NE-CZ-NH2	-9.30	115.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	ASP	CB-CG-OD1	-9.24	109.99	118.30
1	C	139	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	B	211	ASP	CB-CG-OD1	8.18	125.67	118.30
1	C	139	ARG	NE-CZ-NH1	8.12	124.36	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	GLN	Peptide
1	C	458	ALA	Peptide
1	D	458	ALA	Peptide

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	4540	0	4386	66	0
1	B	4540	0	4386	57	0
1	C	4531	0	4380	68	0
1	D	4524	0	4373	79	0
2	A	53	0	30	2	0
2	B	53	0	29	2	0
2	C	53	0	29	2	0
2	D	53	0	28	4	0
3	C	12	0	12	1	0
4	A	450	0	0	15	0
4	B	554	0	0	12	0
4	C	472	0	0	18	0
4	D	342	0	0	14	0
All	All	20177	0	17653	269	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 7.

The worst 5 of 269 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ARG:HB3	1:C:383:ARG:NH1	1.29	1.41
1:C:383:ARG:CB	1:C:383:ARG:HH11	1.45	1.28
1:C:285:ARG:HD3	4:C:2746:HOH:O	1.30	1.23
1:B:458:ALA:HB2	4:B:2756:HOH:O	1.33	1.22
1:C:383:ARG:CB	1:C:383:ARG:NH1	2.03	1.16

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	574/623 (92%)	549 (96%)	22 (4%)	3 (0%)	32	20
1	B	574/623 (92%)	555 (97%)	16 (3%)	3 (0%)	32	20
1	C	573/623 (92%)	554 (97%)	17 (3%)	2 (0%)	44	34
1	D	572/623 (92%)	548 (96%)	22 (4%)	2 (0%)	44	34
All	All	2293/2492 (92%)	2206 (96%)	77 (3%)	10 (0%)	38	26

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	389	LEU
1	B	82	SER
1	C	186	ASP
1	D	82	SER

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	503/541 (93%)	491 (98%)	12 (2%)	54	47
1	B	503/541 (93%)	487 (97%)	16 (3%)	44	34
1	C	502/541 (93%)	483 (96%)	19 (4%)	38	27
1	D	501/541 (93%)	483 (96%)	18 (4%)	40	29
All	All	2009/2164 (93%)	1944 (97%)	65 (3%)	44	34

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	91	LYS
1	C	336	GLN
1	D	460	GLN
1	C	101	ASP
1	C	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	324	HIS
1	B	611	GLN
1	D	461	GLN
1	B	341	ASN
1	B	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	FAD	A	801	-	51,58,58	1.70	11 (21%)	54,89,89	3.26	12 (22%)
2	FAD	B	801	-	51,58,58	1.37	7 (13%)	54,89,89	2.29	12 (22%)
2	FAD	C	801	-	51,58,58	1.27	4 (7%)	54,89,89	3.59	15 (27%)
3	MES	C	903	-	12,12,12	1.65	1 (8%)	14,16,16	9.32	10 (71%)
2	FAD	D	801	-	51,58,58	1.45	6 (11%)	54,89,89	2.98	18 (33%)

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	FAD	A	801	-	-	0/28/50/50	0/6/6/6
2	FAD	B	801	-	-	0/28/50/50	0/6/6/6
2	FAD	C	801	-	-	0/28/50/50	0/6/6/6
3	MES	C	903	-	-	0/6/14/14	0/1/1/1
2	FAD	D	801	-	-	0/28/50/50	0/6/6/6

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	MES	C8-S	-5.25	1.69	1.77
2	A	801	FAD	O4B-C4B	-3.83	1.36	1.45
2	B	801	FAD	O3B-C3B	-3.17	1.35	1.43
2	B	801	FAD	C9A-N10	-2.97	1.34	1.38
2	C	801	FAD	C2B-C1B	-2.89	1.49	1.53

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	903	MES	O2S-S-C8	-24.54	85.72	106.79
3	C	903	MES	O1S-S-C8	-18.71	90.72	106.79
3	C	903	MES	O3S-S-C8	-12.95	90.12	106.06
2	C	801	FAD	C4X-C4-N3	-11.28	107.42	123.48
2	D	801	FAD	N3A-C2A-N1A	-11.17	119.13	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	2	0
2	B	801	FAD	2	0
2	C	801	FAD	2	0
3	C	903	MES	1	0
2	D	801	FAD	4	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, 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	576/623 (92%)	-0.03	18 (3%) 49 53	15, 22, 44, 71	0
1	B	576/623 (92%)	-0.09	10 (1%) 70 73	14, 21, 38, 58	0
1	C	575/623 (92%)	0.08	19 (3%) 47 50	17, 27, 48, 72	0
1	D	574/623 (92%)	0.25	24 (4%) 37 40	19, 34, 56, 74	0
All	All	2301/2492 (92%)	0.05	71 (3%) 49 53	14, 26, 49, 74	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	LEU	7.7
1	D	618	PHE	6.5
1	A	459	VAL	6.2
1	C	619	THR	6.1
1	B	459	VAL	6.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MES	C	903	12/12	0.95	0.12	1.37	40,41,43,47	0
2	FAD	D	801	53/53	0.96	0.11	-0.31	23,28,32,34	0
2	FAD	B	801	53/53	0.98	0.10	-0.52	12,15,20,21	0
2	FAD	A	801	53/53	0.98	0.10	-0.53	12,17,21,22	0
2	FAD	C	801	53/53	0.98	0.10	-0.69	17,22,25,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.