wwPDB X-ray Structure Validation Summary Report (i)

Nov 3, 2016 – 02:00 PM EDT

PDB ID	:	5G5H
Title	:	Escherichia coli Periplamic Aldehyde Oxidase R440H mutant
Authors	:	Correia, M.A.S.; Otrelo-Cardoso, A.R.; Romao, M.J.; Santos-Silva, T.
Deposited on	:	2016-05-25
Resolution	:	2.30 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:

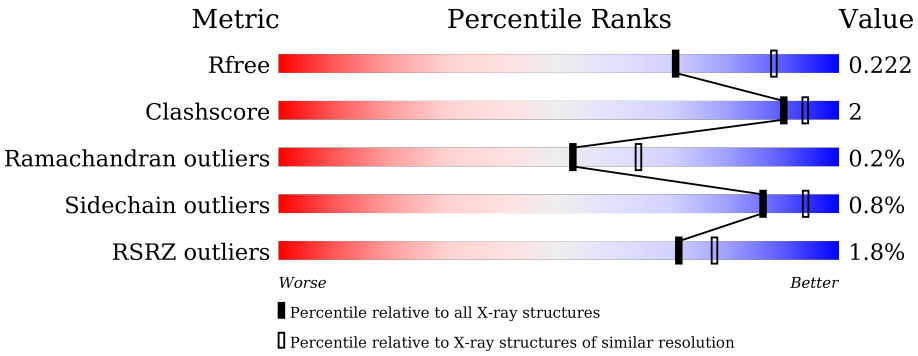
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	229	74% 24%
2	B	318	3% 95%
3	C	732	2% 95%

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
11	MCN	C	1732	-	-	X	-
12	MOS	C	1733	-	-	-	X
13	GOL	C	1744	-	-	-	X
13	GOL	C	1745	-	-	-	X
13	GOL	C	1746	-	-	-	X
6	ACT	C	1743	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 9954 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 PUTATIVE XANTHINE DEHYDROGENASE YAGT IRON-SULFUR-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1272	781	226	252	13			

- Molecule 2 is a protein called PUTATIVE XANTHINE DEHYDROGENASE YAGS FAD-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	316	Total	C	N	O	S	0	0	0
			2368	1490	432	438	8			

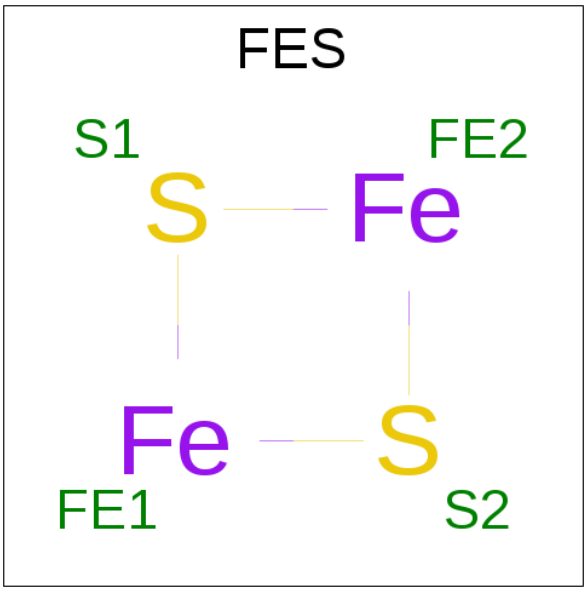
- Molecule 3 is a protein called PUTATIVE XANTHINE DEHYDROGENASE YAGR MOLYBDENUM-BINDING SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	729	Total	C	N	O	S	0	3	0
			5480	3422	977	1056	25			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	88	VAL	ALA	CLONING ARTIFACT	UNP P77489
C	391	GLY	ASP	CLONING ARTIFACT	UNP P77489
C	440	HIS	ARG	ENGINEERED MUTATION	UNP P77489

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

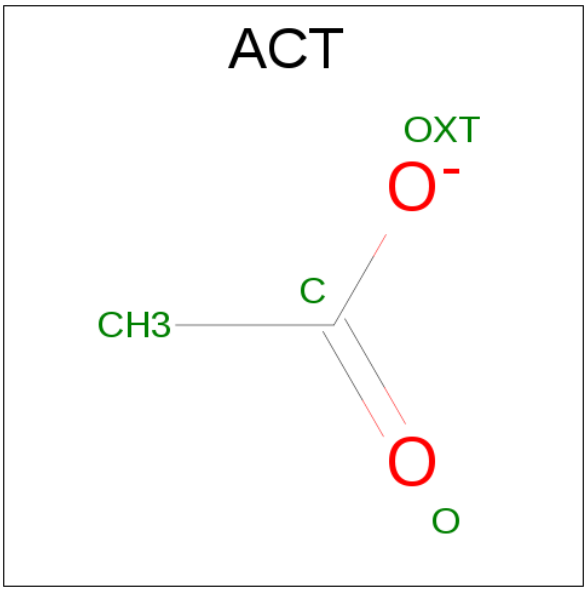


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total I 3 3	0	0
5	A	1	Total I 1 1	0	0
5	C	4	Total I 4 4	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

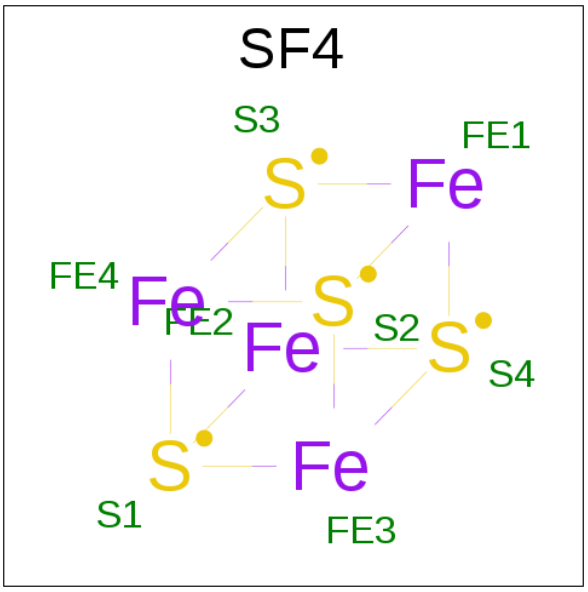


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

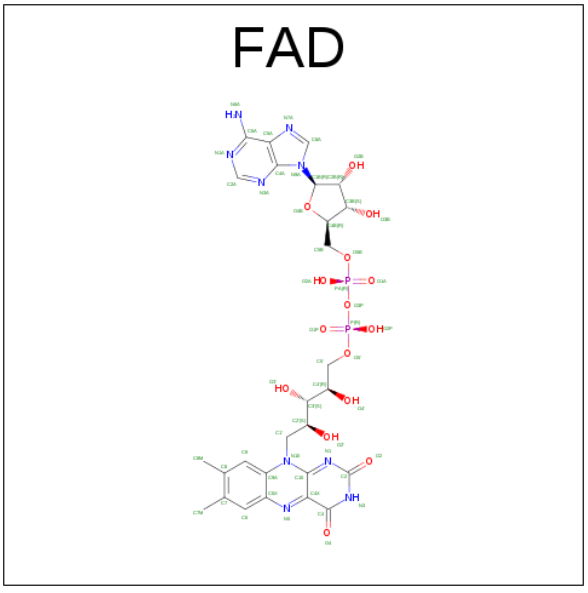
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	3	Total Cl 3 3	0	0
7	A	1	Total Cl 1 1	0	0
7	C	6	Total Cl 6 6	0	0

- Molecule 8 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



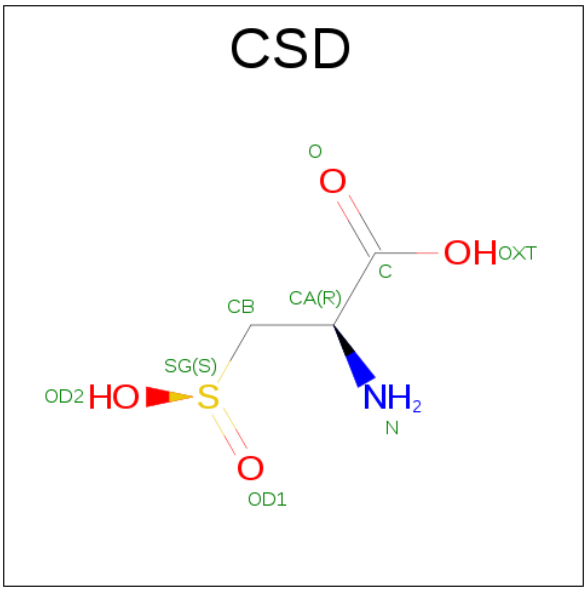
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	B	1	8	4	4	0	0

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



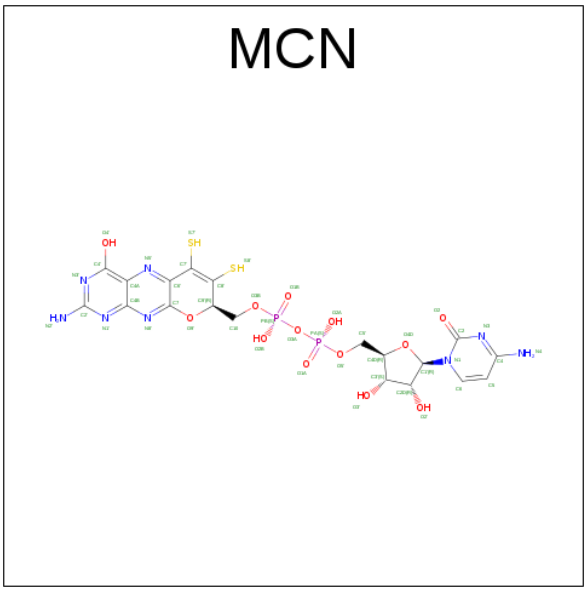
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	B	1	53	27	9	15	2	0	0

- Molecule 10 is 3-SULFINOALANINE (three-letter code: CSD) (formula: $C_3H_7NO_4S$).



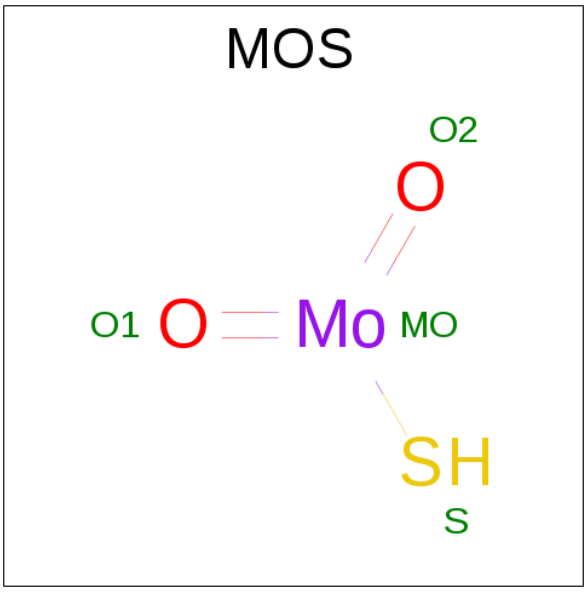
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
10	C	1	8	3	1	3	1	0	0

- Molecule 11 is PTERIN CYTOSINE DINUCLEOTIDE (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).



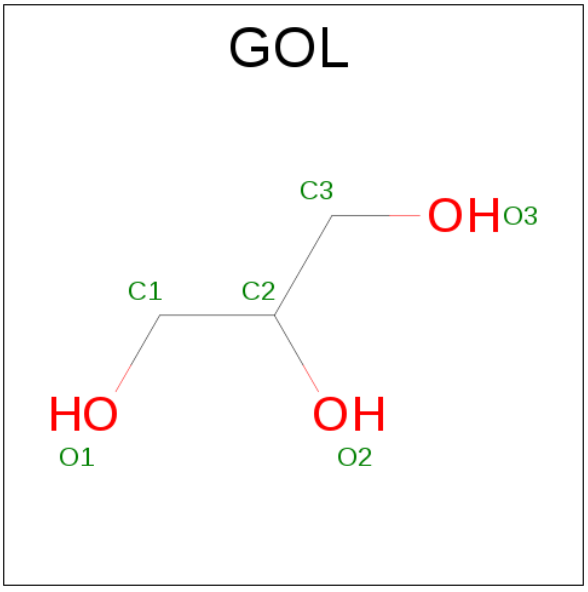
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
11	C	1	44	19	8	13	2	2	0	0

- Molecule 12 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total Mo O S 4 1 2 1	0	0

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C O 6 3 3	0	0
13	C	1	Total C O 6 3 3	0	0
13	C	1	Total C O 6 3 3	0	0

- Molecule 14 is water.

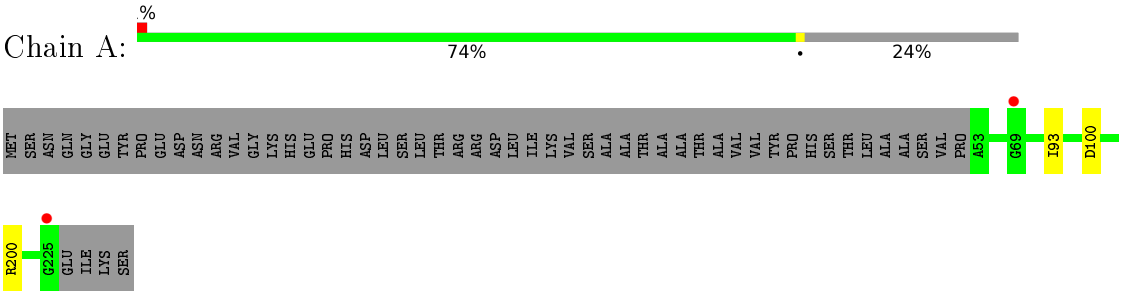
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	111	Total O 111 111	0	0
14	B	155	Total O 155 155	0	0
14	C	395	Total O 395 395	0	0

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.

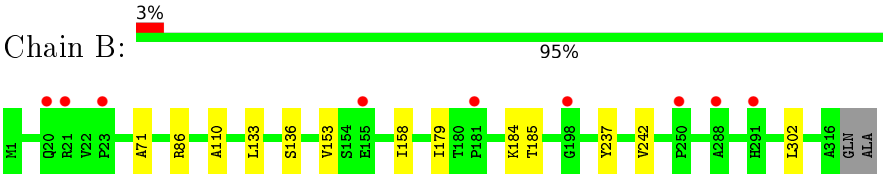
• Molecule 1: PUTATIVE XANTHINE DEHYDROGENASE YAGT IRON-SULFUR-BINDING SUBUNIT

Chain A:



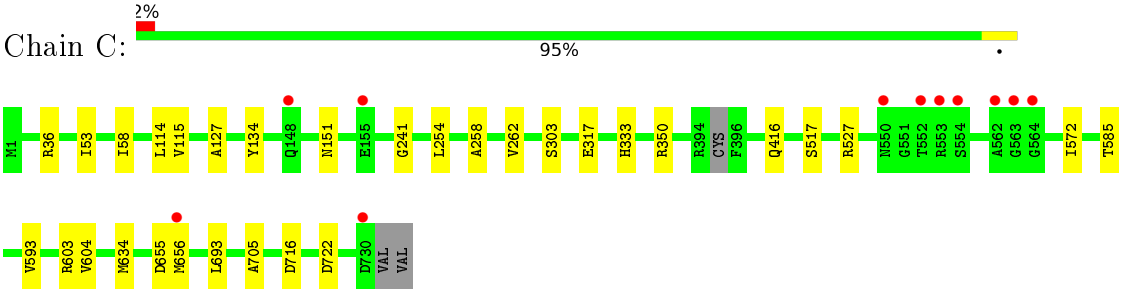
• Molecule 2: PUTATIVE XANTHINE DEHYDROGENASE YAGS FAD-BINDING SUBUNIT

Chain B:



• Molecule 3: PUTATIVE XANTHINE DEHYDROGENASE YAGR MOLYBDENUM-BINDING SUBUNIT

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	109.84Å 78.26Å 151.73Å 90.00° 99.93° 90.00°	Depositor
Resolution (Å)	48.27 – 2.30 48.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.27-2.30) 98.0 (48.27-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.164 , 0.220 0.173 , 0.222	Depositor DCC
R_{free} test set	2811 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9954	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, MCN, CL, MOS, CSD, SF4, FES, ACT, IOD, FAD

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	0.46	0/1288	0.74	2/1748 (0.1%)
2	B	0.43	0/2412	0.67	0/3281
3	C	0.47	0/5596	0.70	2/7599 (0.0%)
All	All	0.46	0/9296	0.70	4/12628 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	527	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	200	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	200	ARG	NE-CZ-NH1	5.20	122.90	120.30
3	C	603	ARG	NE-CZ-NH1	5.11	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1272	0	1263	1	0
2	B	2368	0	2413	5	0
3	C	5480	0	5429	15	0
4	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	3	0	0	0	0
5	C	4	0	0	1	0
6	A	4	0	3	0	0
6	C	8	0	6	0	0
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	C	6	0	0	0	0
8	B	8	0	0	0	0
9	B	53	0	31	0	0
10	C	8	0	5	0	0
11	C	44	0	11	22	0
12	C	4	0	0	0	0
13	C	18	0	24	1	0
14	A	111	0	0	0	0
14	B	155	0	0	0	0
14	C	395	0	0	0	0
All	All	9954	0	9185	42	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 2.

The worst 5 of 42 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)
11:C:1732:MCN:C1'	11:C:1732:MCN:C2D	1.79	1.60
11:C:1732:MCN:C3'	11:C:1732:MCN:C4D	1.76	1.59
11:C:1732:MCN:C4B	11:C:1732:MCN:C4A	1.78	1.58
11:C:1732:MCN:N3	11:C:1732:MCN:C2	1.70	1.50
11:C:1732:MCN:N5'	11:C:1732:MCN:C6'	1.86	1.38

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	171/229 (75%)	165 (96%)	6 (4%)	0	100	100
2	B	314/318 (99%)	308 (98%)	6 (2%)	0	100	100
3	C	728/732 (100%)	705 (97%)	21 (3%)	2 (0%)	46	57
All	All	1213/1279 (95%)	1178 (97%)	33 (3%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	241	GLY
3	C	350	ARG

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	139/186 (75%)	138 (99%)	1 (1%)	88	95
2	B	243/244 (100%)	240 (99%)	3 (1%)	78	89
3	C	566/566 (100%)	562 (99%)	4 (1%)	88	95
All	All	948/996 (95%)	940 (99%)	8 (1%)	86	94

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	237	TYR
3	C	716	ASP
3	C	416	GLN
2	B	184	LYS
3	C	151	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
2	B	126	ASN
3	C	42	HIS
3	C	281	HIS
3	C	550	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

Of 31 ligands modelled in this entry, 18 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
4	FES	A	1226	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	1227	1	0,4,4	0.00	-	0,4,4	0.00	-
6	ACT	A	1229	-	0,3,3	0.00	-	0,3,3	0.00	-
8	SF4	B	1317	2	0,12,12	0.00	-	0,24,24	0.00	-
9	FAD	B	1318	-	52,58,58	1.95	17 (32%)	52,89,89	2.81	18 (34%)
10	CSD	C	1731	3	2,7,8	1.07	0	2,8,10	2.38	1 (50%)
11	MCN	C	1732	12	34,48,48	9.62	23 (67%)	37,74,74	5.76	23 (62%)
12	MOS	C	1733	11,3	0,3,3	0.00	-	0,3,3	0.00	-
6	ACT	C	1742	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ACT	C	1743	-	0,3,3	0.00	-	0,3,3	0.00	-
13	GOL	C	1744	-	5,5,5	0.32	0	5,5,5	0.44	0
13	GOL	C	1745	-	5,5,5	0.37	0	5,5,5	0.46	0
13	GOL	C	1746	-	5,5,5	0.70	0	5,5,5	0.87	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
4	FES	A	1226	1	-	0/0/4/4	0/1/1/1
4	FES	A	1227	1	-	0/0/4/4	0/1/1/1
6	ACT	A	1229	-	-	0/0/0/0	0/0/0/0
8	SF4	B	1317	2	-	0/0/48/48	0/6/5/5
9	FAD	B	1318	-	-	0/30/50/50	0/6/6/6
10	CSD	C	1731	3	-	1/2/6/8	0/0/0/0
11	MCN	C	1732	12	-	0/18/54/54	0/5/5/5
12	MOS	C	1733	11,3	-	0/0/0/0	0/0/0/0
6	ACT	C	1742	-	-	0/0/0/0	0/0/0/0
6	ACT	C	1743	-	-	0/0/0/0	0/0/0/0
13	GOL	C	1744	-	-	0/4/4/4	0/0/0/0
13	GOL	C	1745	-	-	0/4/4/4	0/0/0/0
13	GOL	C	1746	-	-	0/4/4/4	0/0/0/0

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1732	MCN	O4D-C1'	-9.52	1.27	1.41
11	C	1732	MCN	C4B-N8'	-8.45	1.21	1.36
11	C	1732	MCN	C5'-C4D	-7.04	1.28	1.51
11	C	1732	MCN	O2'-C2D	-6.31	1.28	1.43
11	C	1732	MCN	O5'-C5'	-4.83	1.25	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	1732	MCN	C5-C4-N3	-17.36	99.77	121.79
9	B	1318	FAD	C4-C4X-C10	-10.16	113.44	119.94
11	C	1732	MCN	C5-C4-N4	-8.61	107.39	121.19
11	C	1732	MCN	N2'-C2'-N1'	-8.38	101.99	117.72
11	C	1732	MCN	O4'-C4'-C4A	-7.89	105.81	119.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	1731	CSD	CA-CB-SG-OD1

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1732	MCN	22	0
13	C	1745	GOL	1	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	173/229 (75%)	-0.02	2 (1%)	81	85	16, 25, 40, 54	0
2	B	316/318 (99%)	0.05	9 (2%)	56	66	18, 29, 45, 68	0
3	C	729/732 (99%)	-0.17	11 (1%)	76	81	14, 23, 42, 71	0
All	All	1218/1279 (95%)	-0.09	22 (1%)	71	78	14, 25, 43, 71	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	155	GLU	3.6
2	B	21	ARG	3.4
3	C	563	GLY	3.3
2	B	181	PRO	3.0
1	A	225	GLY	2.8

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

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

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, 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
13	GOL	C	1745	6/6	0.84	0.26	8.61	47,50,53,55	0
13	GOL	C	1744	6/6	0.88	0.18	6.67	41,44,46,46	0
6	ACT	C	1743	4/4	0.94	0.22	4.82	16,18,18,22	0
13	GOL	C	1746	6/6	0.90	0.19	3.95	43,45,47,47	0
12	MOS	C	1733	4/4	0.90	0.21	2.83	11,14,15,16	1
6	ACT	A	1229	4/4	0.72	0.19	0.86	46,47,48,49	0
10	CSD	C	1731	8/9	0.94	0.19	0.67	24,28,39,39	0
7	CL	A	1230	1/1	0.99	0.16	-0.07	10,10,10,10	0
9	FAD	B	1318	53/53	0.95	0.12	-0.24	15,18,24,25	0
4	FES	A	1226	4/4	0.96	0.11	-0.79	15,17,18,21	0
11	MCN	C	1732	44/44	0.98	0.10	-0.93	10,13,16,17	0
7	CL	B	1322	1/1	0.87	0.12	-1.08	50,50,50,50	0
5	IOD	C	1735	1/1	0.99	0.06	-1.60	29,29,29,29	1
5	IOD	C	1734	1/1	0.99	0.12	-1.65	33,33,33,33	1
7	CL	C	1739	1/1	0.98	0.05	-1.71	33,33,33,33	0
5	IOD	C	1737	1/1	0.99	0.05	-1.94	35,35,35,35	1
4	FES	A	1227	4/4	0.99	0.10	-2.03	13,14,15,17	0
5	IOD	A	1228	1/1	1.00	0.07	-3.69	25,25,25,25	1
5	IOD	B	1320	1/1	0.97	0.06	-3.79	54,54,54,54	1
8	SF4	B	1317	8/8	0.98	0.05	-3.90	25,27,30,30	0
5	IOD	C	1736	1/1	1.00	0.06	-4.62	37,37,37,37	1
7	CL	C	1748	1/1	0.95	0.12	-	26,26,26,26	0
5	IOD	B	1319	1/1	0.99	0.04	-	36,36,36,36	1
6	ACT	C	1742	4/4	0.79	0.22	-	51,54,55,56	0
7	CL	C	1747	1/1	0.95	0.07	-	48,48,48,48	0
7	CL	C	1740	1/1	0.94	0.10	-	37,37,37,37	0
7	CL	B	1324	1/1	0.97	0.04	-	37,37,37,37	0
7	CL	C	1741	1/1	0.99	0.13	-	22,22,22,22	0
5	IOD	B	1323	1/1	0.99	0.03	-	37,37,37,37	1
7	CL	B	1321	1/1	0.99	0.17	-	21,21,21,21	0
7	CL	C	1738	1/1	0.86	0.12	-	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.