



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:47 am GMT

PDB ID : 1JRP  
Title : Crystal Structure of Xanthine Dehydrogenase inhibited by alloxanthine from Rhodobacter capsulatus  
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.  
Deposited on : 2001-08-14  
Resolution : 3.00 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](mailto: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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

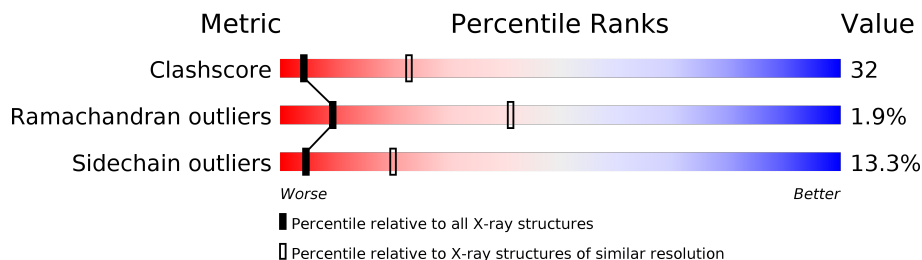
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	462	
1	C	462	
1	E	462	
1	G	462	
2	B	777	
2	D	777	
2	F	777	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	H	777	<div>44% 43% 8% . .</div>

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
4	FES	E	3002	-	-	X	-
4	FES	G	3001	-	-	X	-
5	MTE	F	3003	-	-	X	-
5	MTE	H	3003	-	-	X	-
6	MOS	B	3004	-	-	X	-
6	MOS	D	3004	-	-	X	-
6	MOS	F	3004	-	-	X	-
6	MOS	H	3004	-	-	X	-
8	141	B	4000	-	-	X	-
8	141	D	4000	-	-	X	-
8	141	F	4000	-	-	X	-
8	141	H	4000	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36748 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 xanthine dehydrogenase, chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			

- Molecule 2 is a protein called xanthine dehydrogenase, chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

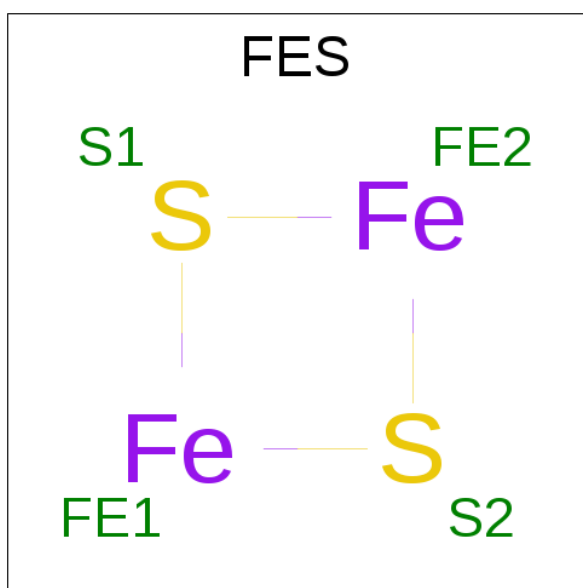
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	CONFLICT	EMBL 13397863
D	772	ARG	GLY	CONFLICT	EMBL 13397863
F	772	ARG	GLY	CONFLICT	EMBL 13397863
H	772	ARG	GLY	CONFLICT	EMBL 13397863

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

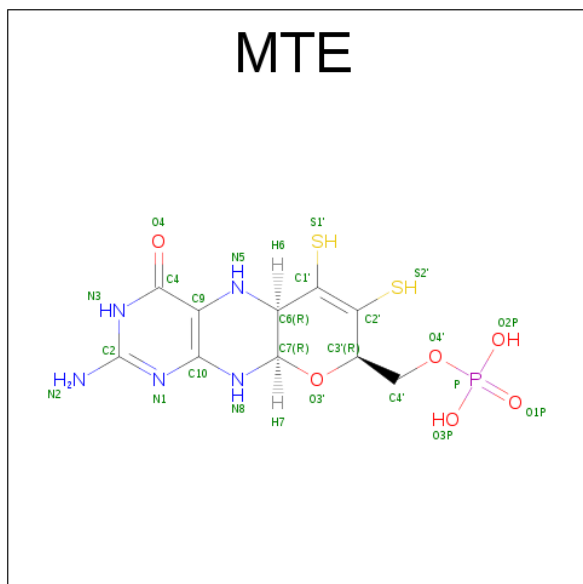
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



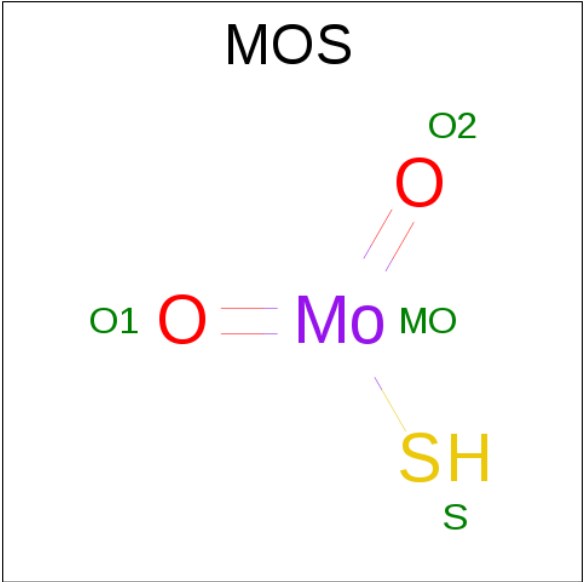
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0
4	C	1	Total Fe S 4 2 2	0	0
4	C	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	G	1	Total Fe S 4 2 2	0	0
4	G	1	Total Fe S 4 2 2	0	0

- Molecule 5 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula:  $C_{10}H_{14}N_5O_6PS_2$ ).



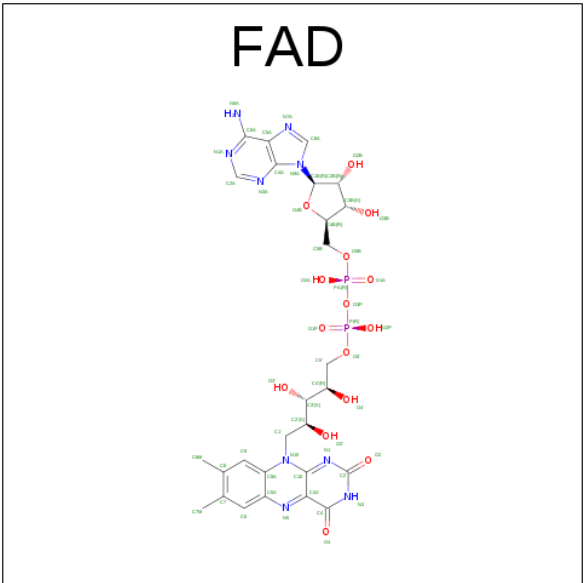
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	F	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	H	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 6 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $HMoO_2S$ ).



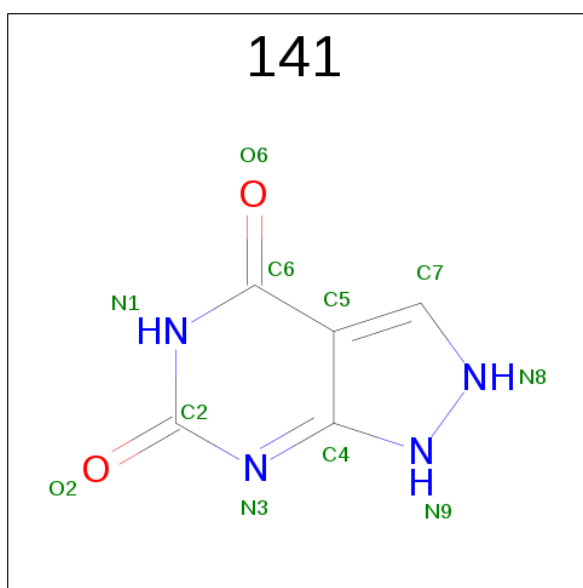
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	Mo	O	S	0	0
			3	1	1	1		
6	D	1	Total	Mo	O	S	0	0
			3	1	1	1		
6	F	1	Total	Mo	O	S	0	0
			3	1	1	1		
6	H	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
7	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 8 is OXYPURINOL (three-letter code: 141) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>).



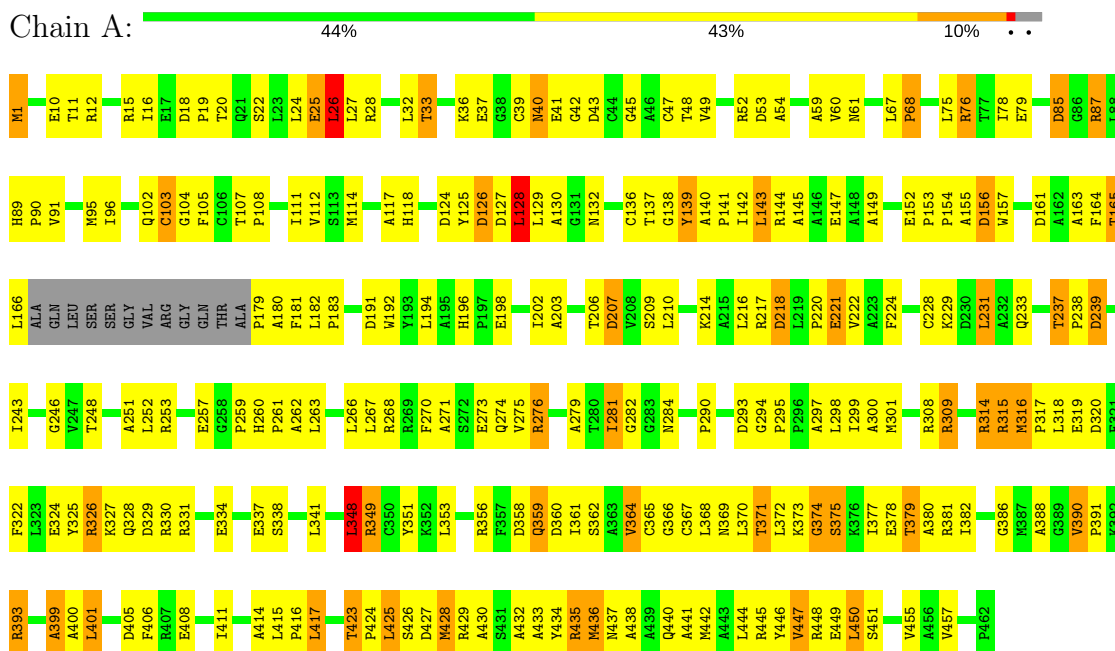
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	5	4	2		
8	D	1	Total	C	N	O	0	0
			11	5	4	2		
8	F	1	Total	C	N	O	0	0
			11	5	4	2		
8	H	1	Total	C	N	O	0	0
			11	5	4	2		

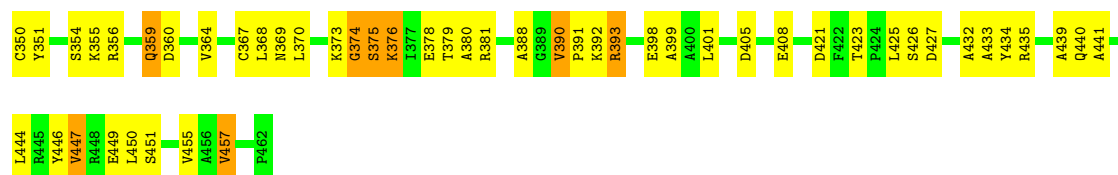
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

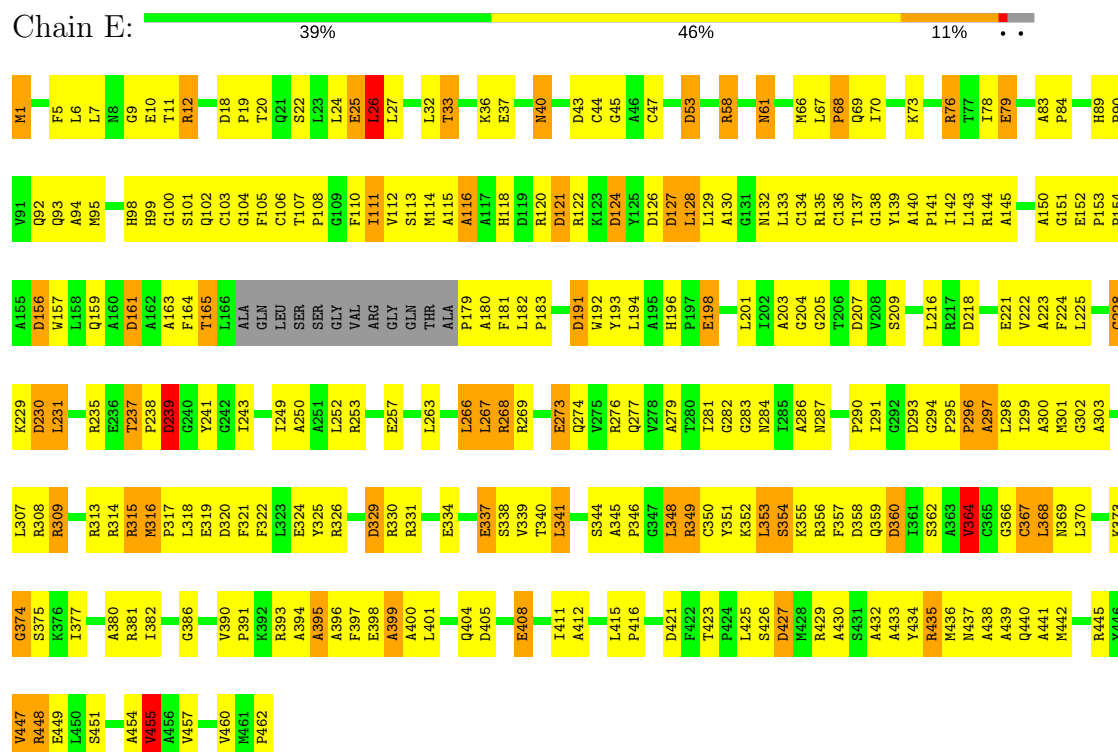
Note EDS was not executed.

- Molecule 1: xanthine dehydrogenase, chain A

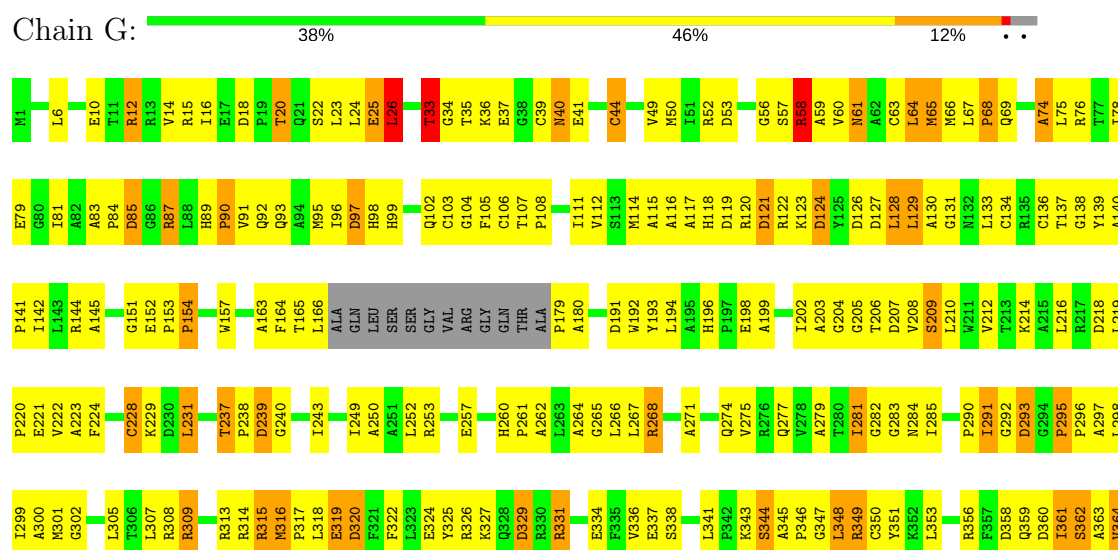


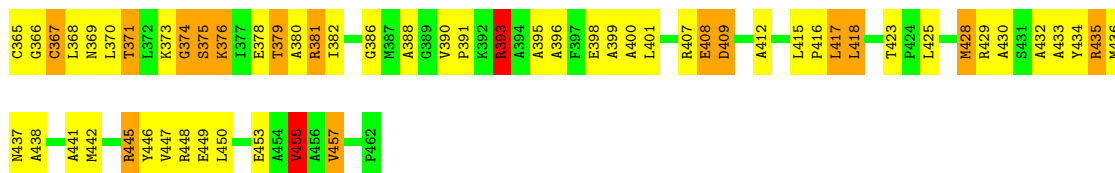


• Molecule 1: xanthine dehydrogenase, chain A



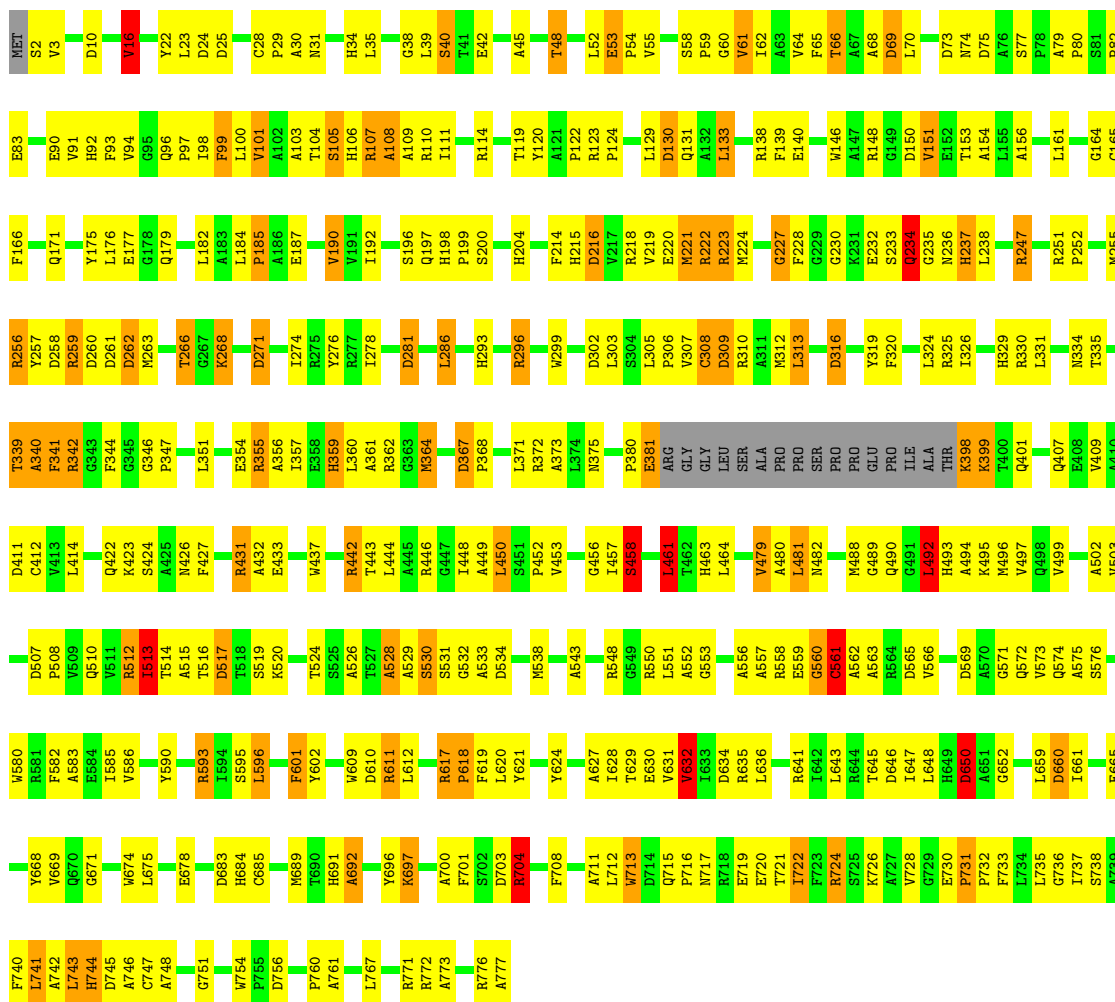
• Molecule 1: xanthine dehydrogenase, chain A





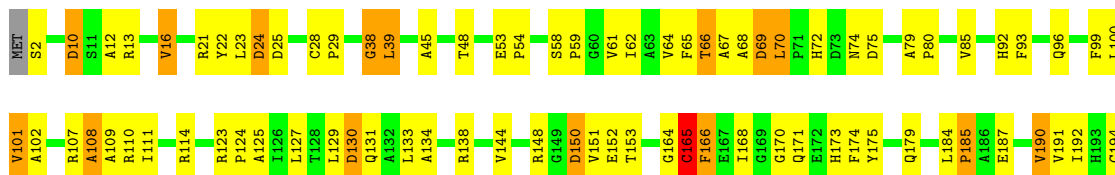
- Molecule 2: xanthine dehydrogenase, chain B

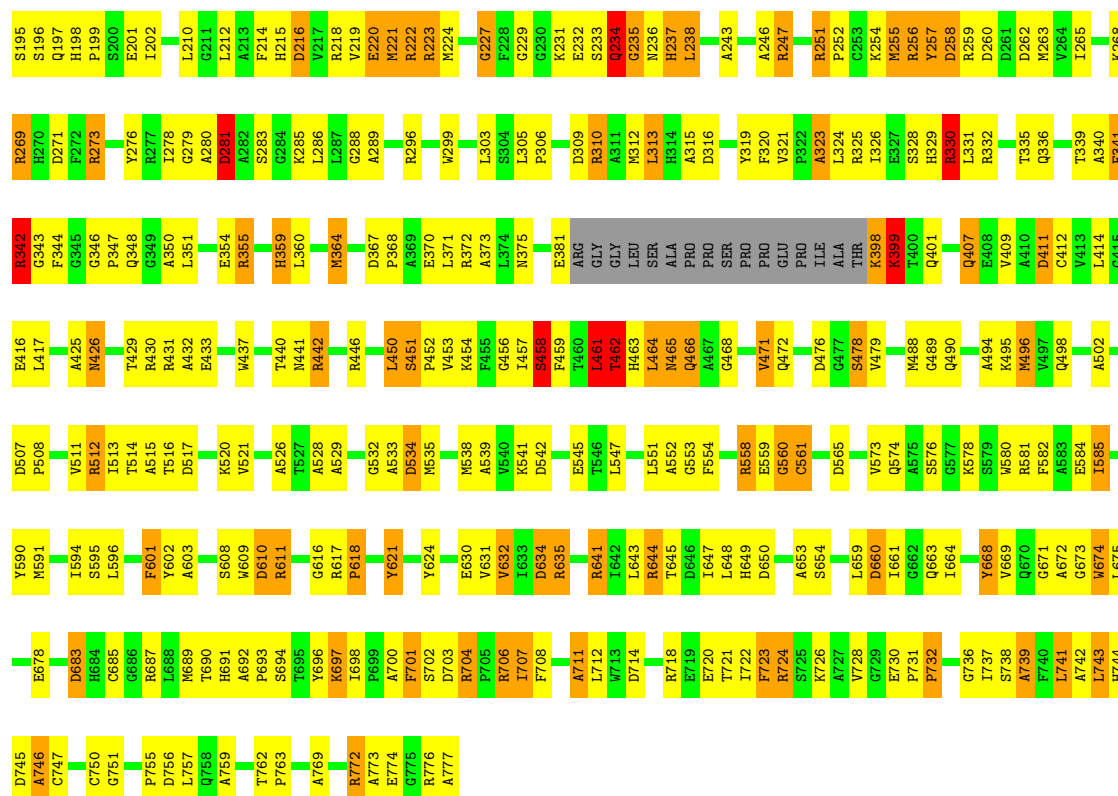
Chain B:



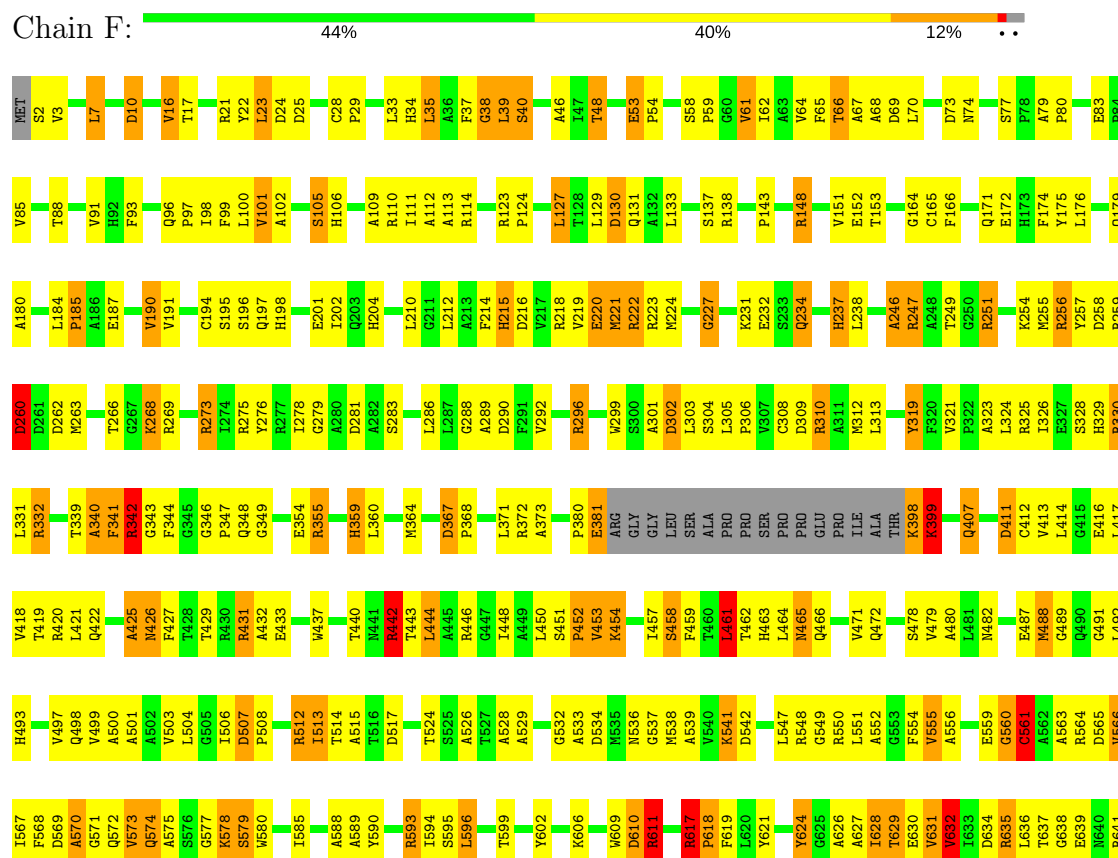
- Molecule 2: xanthine dehydrogenase, chain B

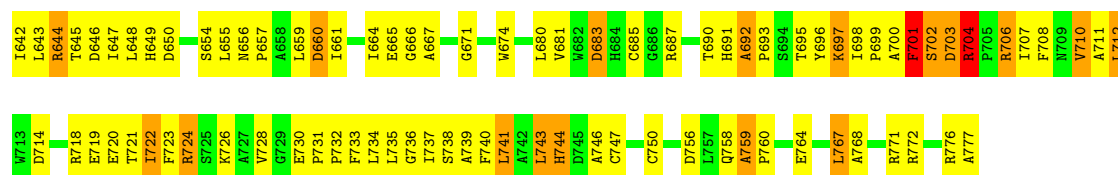
Chain D:





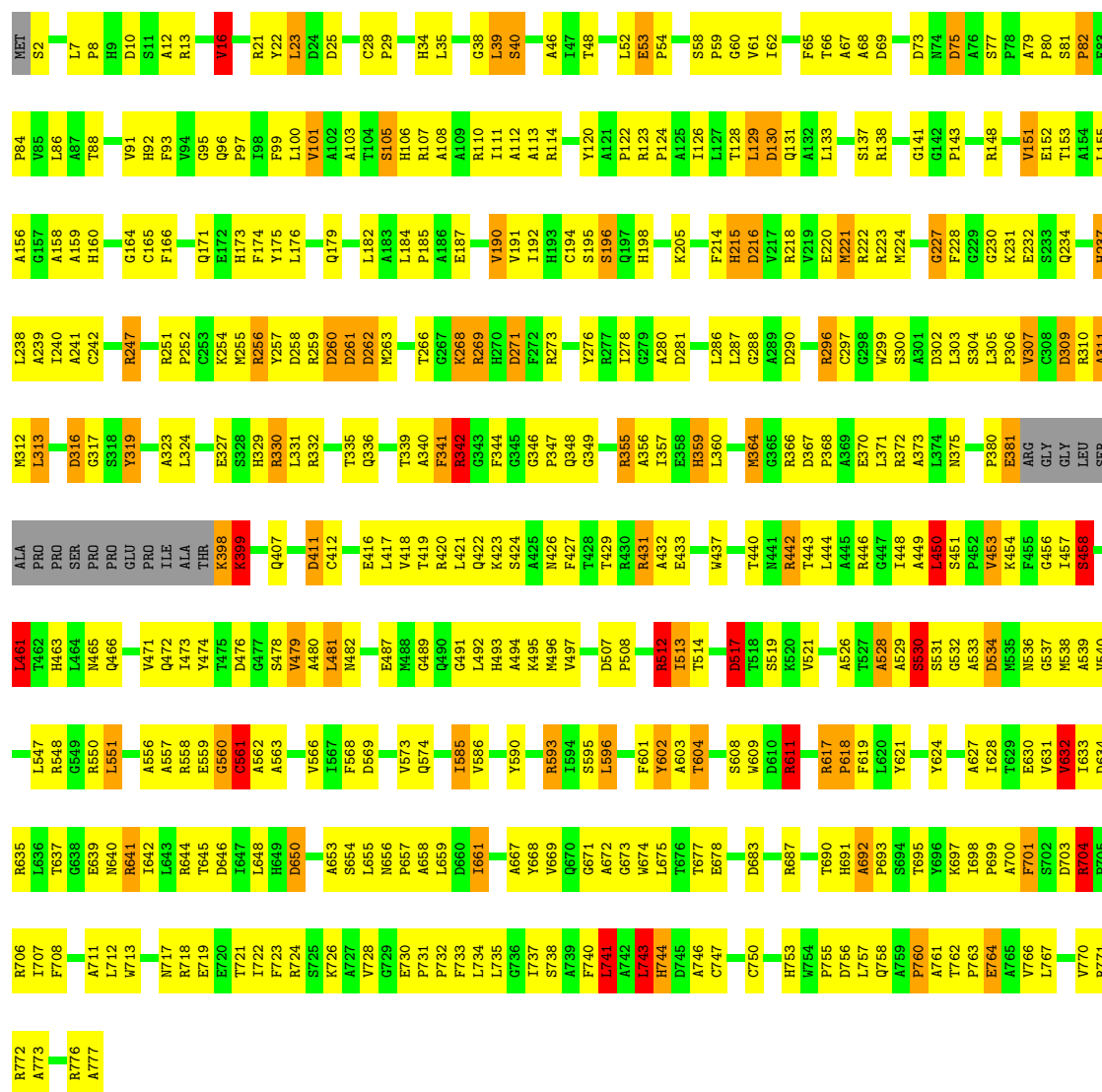
Chain F:





- Molecule 2: xanthine dehydrogenase, chain B

Chain H:  44% 43% 8% 5%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.62Å 140.73Å 157.66Å 109.59° 105.84° 101.25°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (30.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.193 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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: 141, MOS, CA, FES, FAD, MTE

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	1.17	3/3431 (0.1%)	1.34	28/4647 (0.6%)
1	C	1.44	15/3431 (0.4%)	1.37	31/4647 (0.7%)
1	E	1.23	6/3431 (0.2%)	1.40	35/4647 (0.8%)
1	G	1.16	4/3431 (0.1%)	1.38	29/4647 (0.6%)
2	B	1.41	22/5845 (0.4%)	1.46	65/7942 (0.8%)
2	D	1.50	37/5845 (0.6%)	1.49	78/7942 (1.0%)
2	F	1.39	18/5845 (0.3%)	1.48	70/7942 (0.9%)
2	H	1.34	20/5845 (0.3%)	1.43	54/7942 (0.7%)
All	All	1.35	125/37104 (0.3%)	1.43	390/50356 (0.8%)

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	674	TRP	CB-CG	-8.75	1.34	1.50
2	F	220	GLU	CD-OE2	8.40	1.34	1.25
1	C	116	ALA	CA-CB	-8.12	1.35	1.52
2	D	759	ALA	CA-CB	-7.75	1.36	1.52
1	C	103	CYS	CB-SG	-7.70	1.69	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	704	ARG	NE-CZ-NH1	-12.32	114.14	120.30
2	D	542	ASP	CB-CG-OD2	12.01	129.11	118.30
2	D	635	ARG	NE-CZ-NH2	-11.81	114.39	120.30
2	D	273	ARG	NE-CZ-NH1	-11.38	114.61	120.30
2	B	660	ASP	CB-CG-OD2	11.14	128.33	118.30

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	3370	0	3368	249	0
1	C	3370	0	3368	158	0
1	E	3370	0	3370	293	1
1	G	3370	0	3370	299	1
2	B	5717	0	5630	326	0
2	D	5717	0	5631	309	0
2	F	5717	0	5631	368	0
2	H	5717	0	5630	409	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	0	1	0
4	C	8	0	0	0	0
4	E	8	0	0	4	0
4	G	8	0	0	3	0
5	B	24	0	10	4	0
5	D	24	0	10	4	0
5	F	24	0	11	7	0
5	H	24	0	10	7	0
6	B	3	0	0	4	0
6	D	3	0	0	7	0
6	F	3	0	0	8	0
6	H	3	0	0	5	0
7	A	53	0	31	10	0
7	C	53	0	30	3	0
7	E	53	0	30	11	0
7	G	53	0	31	8	0
8	B	11	0	3	9	0
8	D	11	0	3	5	0
8	F	11	0	3	5	0
8	H	11	0	3	4	0
All	All	36748	0	36173	2352	1

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 32.

The worst 5 of 2352 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:D:689:MET:SD	2:D:689:MET:CE	2.04	1.46
1:E:381:ARG:HH21	1:E:393:ARG:NH2	1.30	1.28
1:A:425:LEU:CD1	2:F:579:SER:HB3	1.62	1.27
2:D:496:MET:HA	2:D:496:MET:HE2	1.18	1.17
1:A:425:LEU:HD12	2:F:579:SER:HB3	1.22	1.14

All (1) 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:E:235:ARG:CD	1:G:152:GLU:OE2[1_655]	2.08	0.12

## 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	446/462 (96%)	385 (86%)	53 (12%)	8 (2%)	10	43
1	C	446/462 (96%)	408 (92%)	31 (7%)	7 (2%)	11	46
1	E	446/462 (96%)	370 (83%)	63 (14%)	13 (3%)	5	28
1	G	446/462 (96%)	375 (84%)	58 (13%)	13 (3%)	5	28
2	B	756/777 (97%)	696 (92%)	47 (6%)	13 (2%)	11	44
2	D	756/777 (97%)	697 (92%)	46 (6%)	13 (2%)	11	44
2	F	756/777 (97%)	688 (91%)	57 (8%)	11 (2%)	12	48
2	H	756/777 (97%)	678 (90%)	67 (9%)	11 (2%)	12	48
All	All	4808/4956 (97%)	4297 (89%)	422 (9%)	89 (2%)	9	41

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ALA
2	B	281	ASP
2	B	399	LYS
2	B	458	SER
2	B	561	CYS

### 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	339/347 (98%)	294 (87%)	45 (13%)	4	20
1	C	339/347 (98%)	295 (87%)	44 (13%)	5	21
1	E	339/347 (98%)	289 (85%)	50 (15%)	3	17
1	G	339/347 (98%)	291 (86%)	48 (14%)	4	18
2	B	571/584 (98%)	499 (87%)	72 (13%)	5	23
2	D	571/584 (98%)	493 (86%)	78 (14%)	4	19
2	F	571/584 (98%)	495 (87%)	76 (13%)	4	20
2	H	571/584 (98%)	500 (88%)	71 (12%)	5	23
All	All	3640/3724 (98%)	3156 (87%)	484 (13%)	4	20

5 of 484 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	574	GLN
1	E	291	ILE
2	H	359	HIS
2	D	634	ASP
1	E	33	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	744	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	196	HIS
2	H	359	HIS
1	E	40	ASN
1	E	93	GLN

### 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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
7	FAD	A	3005	-	51,58,58	1.76	8 (15%)	54,89,89	3.24	24 (44%)
5	MTE	B	3003	6	21,26,26	5.05	12 (57%)	19,40,40	5.67	10 (52%)
6	MOS	B	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	B	4000	6	10,12,12	2.54	4 (40%)	4,17,17	11.21	3 (75%)
4	FES	C	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	C	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
7	FAD	C	3005	-	51,58,58	1.80	12 (23%)	54,89,89	3.23	26 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MTE	D	3003	6	21,26,26	5.27	10 (47%)	19,40,40	7.44	9 (47%)
6	MOS	D	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	D	4000	6	10,12,12	2.56	4 (40%)	4,17,17	9.45	2 (50%)
4	FES	E	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	E	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
7	FAD	E	3005	-	51,58,58	1.71	12 (23%)	54,89,89	2.97	24 (44%)
5	MTE	F	3003	6	21,26,26	5.35	13 (61%)	19,40,40	6.63	11 (57%)
6	MOS	F	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	F	4000	6	10,12,12	3.06	6 (60%)	4,17,17	11.79	2 (50%)
4	FES	G	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	G	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
7	FAD	G	3005	-	51,58,58	1.67	10 (19%)	54,89,89	3.02	25 (46%)
5	MTE	H	3003	6	21,26,26	5.94	10 (47%)	19,40,40	6.02	10 (52%)
6	MOS	H	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	H	4000	6	10,12,12	2.58	3 (30%)	4,17,17	11.48	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
4	FES	A	3001	1	-	0/0/4/4	0/1/1/1
4	FES	A	3002	1	-	0/0/4/4	0/1/1/1
7	FAD	A	3005	-	-	0/28/50/50	0/6/6/6
5	MTE	B	3003	6	-	0/6/34/34	0/3/3/3
6	MOS	B	3004	8,5	-	0/0/0/0	0/0/0/0
8	141	B	4000	6	-	0/0/0/0	0/2/2/2
4	FES	C	3001	1	-	0/0/4/4	0/1/1/1
4	FES	C	3002	1	-	0/0/4/4	0/1/1/1
7	FAD	C	3005	-	-	0/28/50/50	0/6/6/6
5	MTE	D	3003	6	-	0/6/34/34	0/3/3/3
6	MOS	D	3004	8,5	-	0/0/0/0	0/0/0/0
8	141	D	4000	6	-	0/0/0/0	0/2/2/2
4	FES	E	3001	1	-	0/0/4/4	0/1/1/1
4	FES	E	3002	1	-	0/0/4/4	0/1/1/1
7	FAD	E	3005	-	-	0/28/50/50	0/6/6/6
5	MTE	F	3003	6	-	0/6/34/34	0/3/3/3
6	MOS	F	3004	8,5	-	0/0/0/0	0/0/0/0
8	141	F	4000	6	-	0/0/0/0	0/2/2/2
4	FES	G	3001	1	-	0/0/4/4	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	G	3002	1	-	0/0/4/4	0/1/1/1
7	FAD	G	3005	-	-	0/28/50/50	0/6/6/6
5	MTE	H	3003	6	-	0/6/34/34	0/3/3/3
6	MOS	H	3004	8,5	-	0/0/0/0	0/0/0/0
8	141	H	4000	6	-	0/0/0/0	0/2/2/2

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3003	MTE	P-O4'	-7.28	1.36	1.60
5	D	3003	MTE	P-O4'	-6.91	1.38	1.60
5	D	3003	MTE	C4'-C3'	-6.56	1.42	1.52
5	H	3003	MTE	C4'-C3'	-6.32	1.42	1.52
5	B	3003	MTE	P-O4'	-6.24	1.40	1.60

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3003	MTE	O3'-C7-C6	-29.62	89.21	108.96
5	F	3003	MTE	O3'-C7-C6	-24.82	92.41	108.96
5	H	3003	MTE	O3'-C7-C6	-23.00	93.63	108.96
5	B	3003	MTE	O3'-C7-C6	-20.63	95.20	108.96
8	H	4000	141	C5-C6-N1	-18.86	111.14	124.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3002	FES	1	0
7	A	3005	FAD	10	0
5	B	3003	MTE	4	0
6	B	3004	MOS	4	0
8	B	4000	141	9	0
7	C	3005	FAD	3	0
5	D	3003	MTE	4	0
6	D	3004	MOS	7	0
8	D	4000	141	5	0
4	E	3001	FES	1	0
4	E	3002	FES	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	3005	FAD	11	0
5	F	3003	MTE	7	0
6	F	3004	MOS	8	0
8	F	4000	141	5	0
4	G	3001	FES	2	0
4	G	3002	FES	1	0
7	G	3005	FAD	8	0
5	H	3003	MTE	7	0
6	H	3004	MOS	5	0
8	H	4000	141	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.