



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 06:57 am GMT

PDB ID : 2E1Q  
Title : Crystal Structure of Human Xanthine Oxidoreductase mutant, Glu803Val  
Authors : Yamaguchi, Y.; Matsumura, T.; Ichida, K.; Okamoto, K.; Nishino, T.  
Deposited on : 2006-10-27  
Resolution : 2.60 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.

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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 : trunk28620  
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) : recalc28949



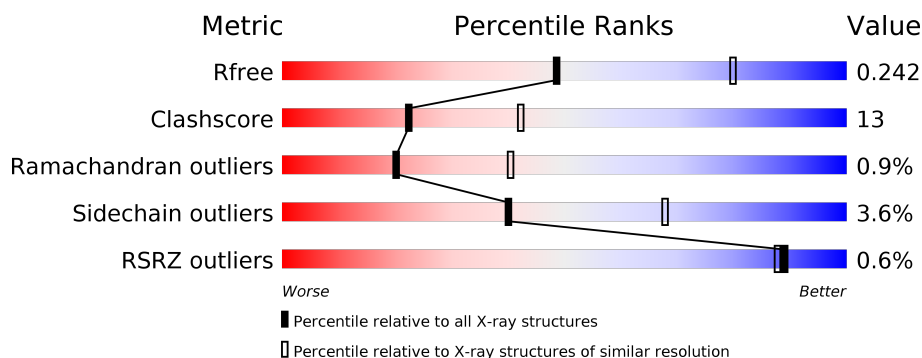
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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.

Mol	Chain	Length	Quality of chain
1	A	1333	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>
1	B	1333	<div> <div></div> <div>71%</div> <div>25%</div> <div>• •</div> </div>
1	C	1333	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>• •</div> </div> </div>
1	D	1333	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	A	7002	-	-	-	X
3	CA	B	7004	-	-	-	X
3	CA	C	7006	-	-	-	X
3	CA	D	7008	-	-	-	X
7	MOM	A	2005	-	-	X	-
7	MOM	B	3005	-	-	X	-
7	MOM	C	4005	-	-	X	-
7	MOM	D	5005	-	-	X	-
8	SAL	A	2006	-	-	-	X
8	SAL	B	3006	-	-	-	X
8	SAL	C	4006	-	-	-	X
8	SAL	D	5006	-	-	-	X



## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41721 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/oxidase.

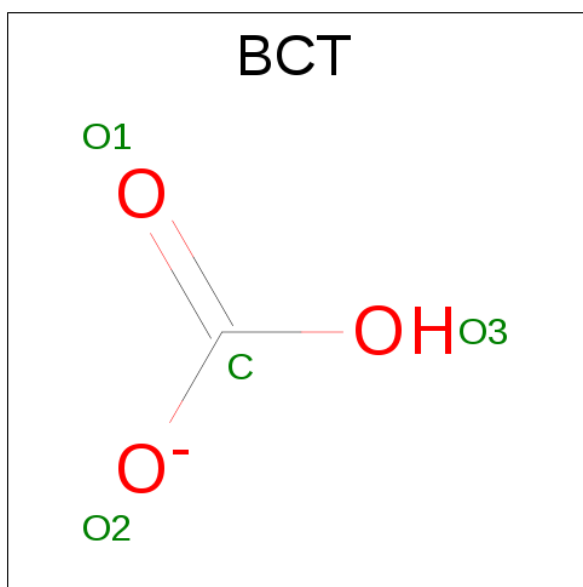
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	B	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	C	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	D	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP P47989
A	803	VAL	GLU	ENGINEERED	UNP P47989
B	1	MET	-	INITIATING METHIONINE	UNP P47989
B	803	VAL	GLU	ENGINEERED	UNP P47989
C	1	MET	-	INITIATING METHIONINE	UNP P47989
C	803	VAL	GLU	ENGINEERED	UNP P47989
D	1	MET	-	INITIATING METHIONINE	UNP P47989
D	803	VAL	GLU	ENGINEERED	UNP P47989

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).





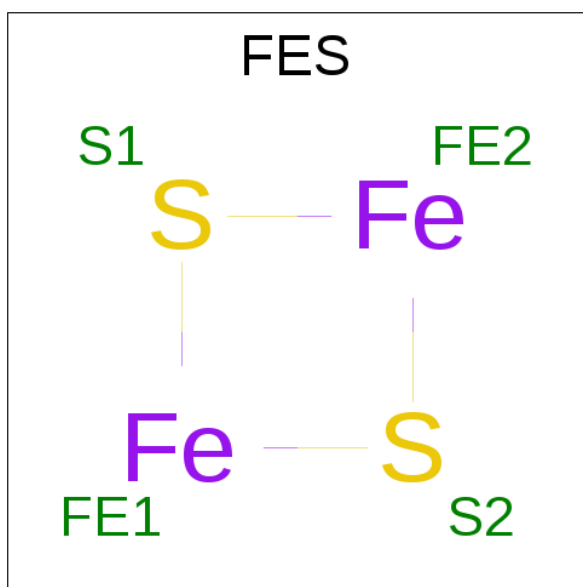
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		
2	C	1	Total	C	O	0	0
			4	1	3		
2	D	1	Total	C	O	0	0
			4	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		
3	D	2	Total	Ca	0	0
			2	2		
3	C	2	Total	Ca	0	0
			2	2		

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

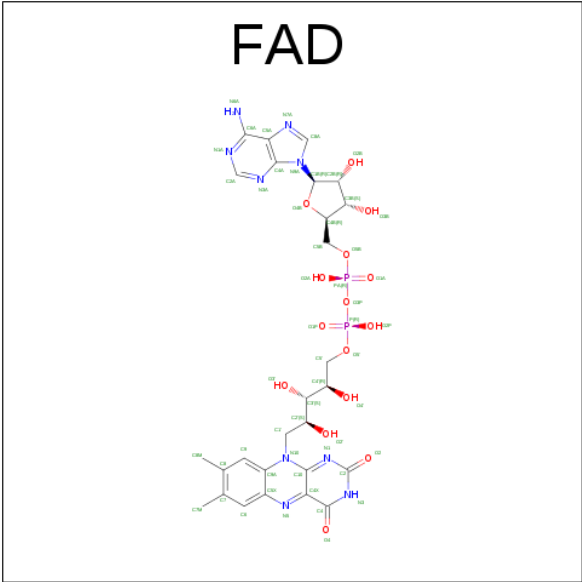




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

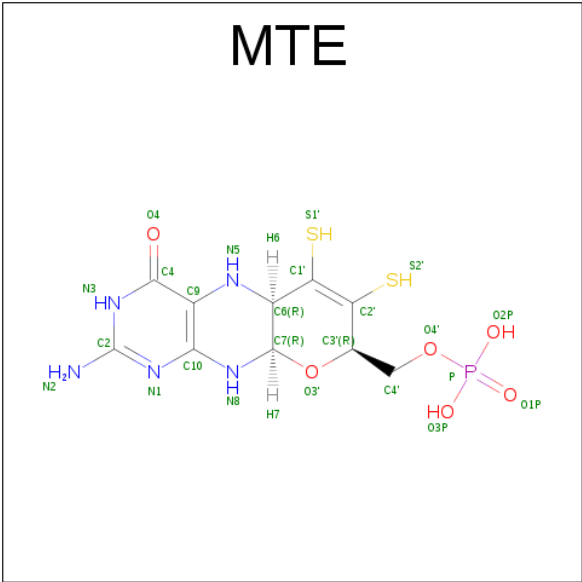
- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).





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

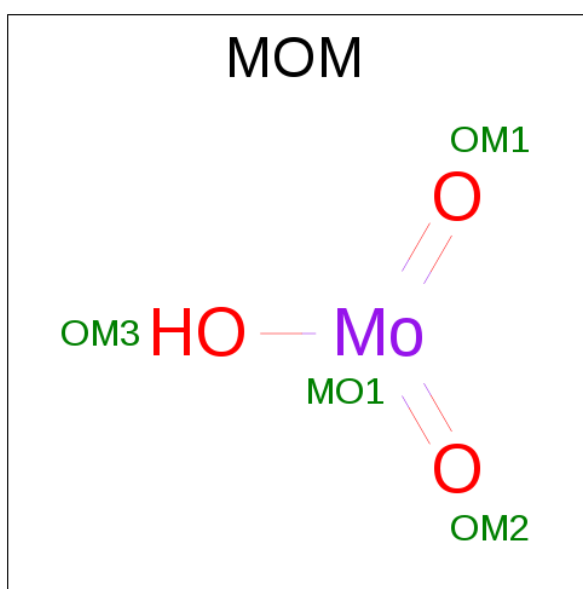
- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>PS<sub>2</sub>).





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

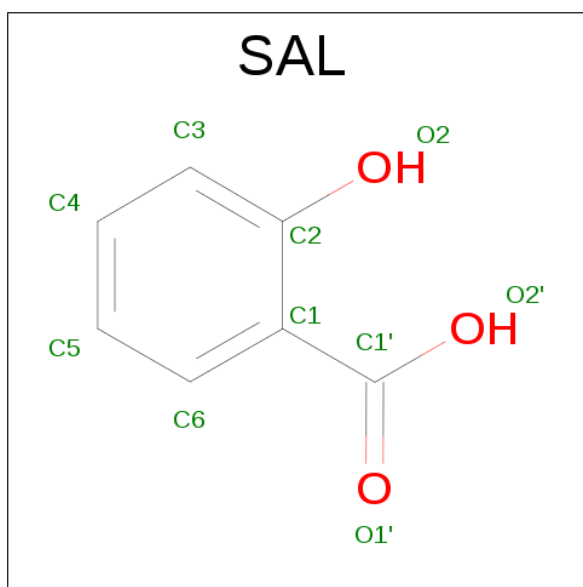
- Molecule 7 is HYDROXY(DIOXO)MOLYBDENUM (three-letter code: MOM) (formula:  $\text{HMoO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Mo	O		
			4	1	3	0	0
7	B	1	Total	Mo	O		
			4	1	3	0	0
7	C	1	Total	Mo	O		
			4	1	3	0	0
7	D	1	Total	Mo	O		
			4	1	3	0	0

- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula:  $\text{C}_7\text{H}_6\text{O}_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	7	3		
8	B	1	Total	C	O	0	0
			10	7	3		
8	C	1	Total	C	O	0	0
			10	7	3		
8	D	1	Total	C	O	0	0
			10	7	3		

- Molecule 9 is water.

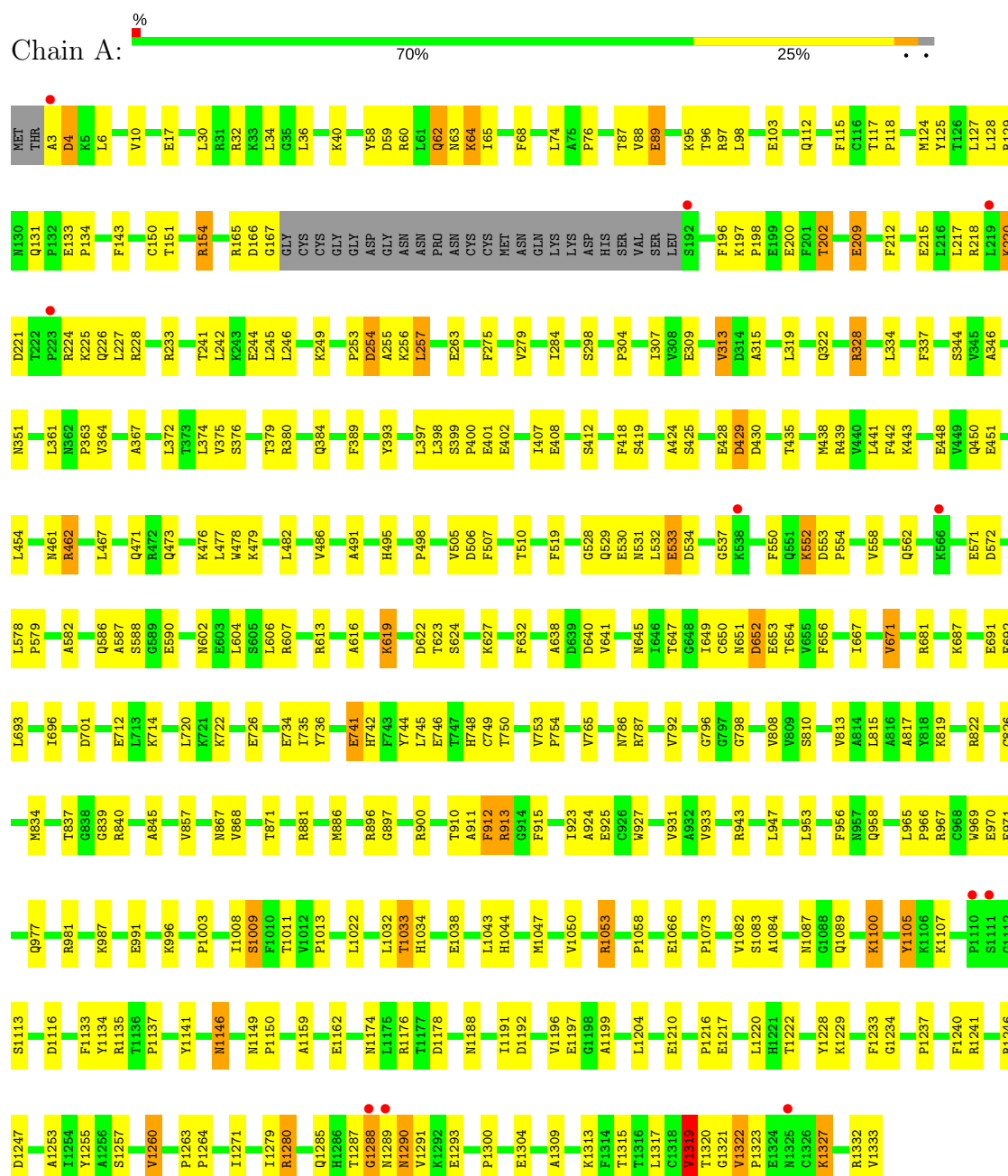
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	234	Total	O	0	0
			234	234		
9	B	245	Total	O	0	0
			245	245		
9	C	237	Total	O	0	0
			237	237		
9	D	233	Total	O	0	0
			233	233		



### 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.

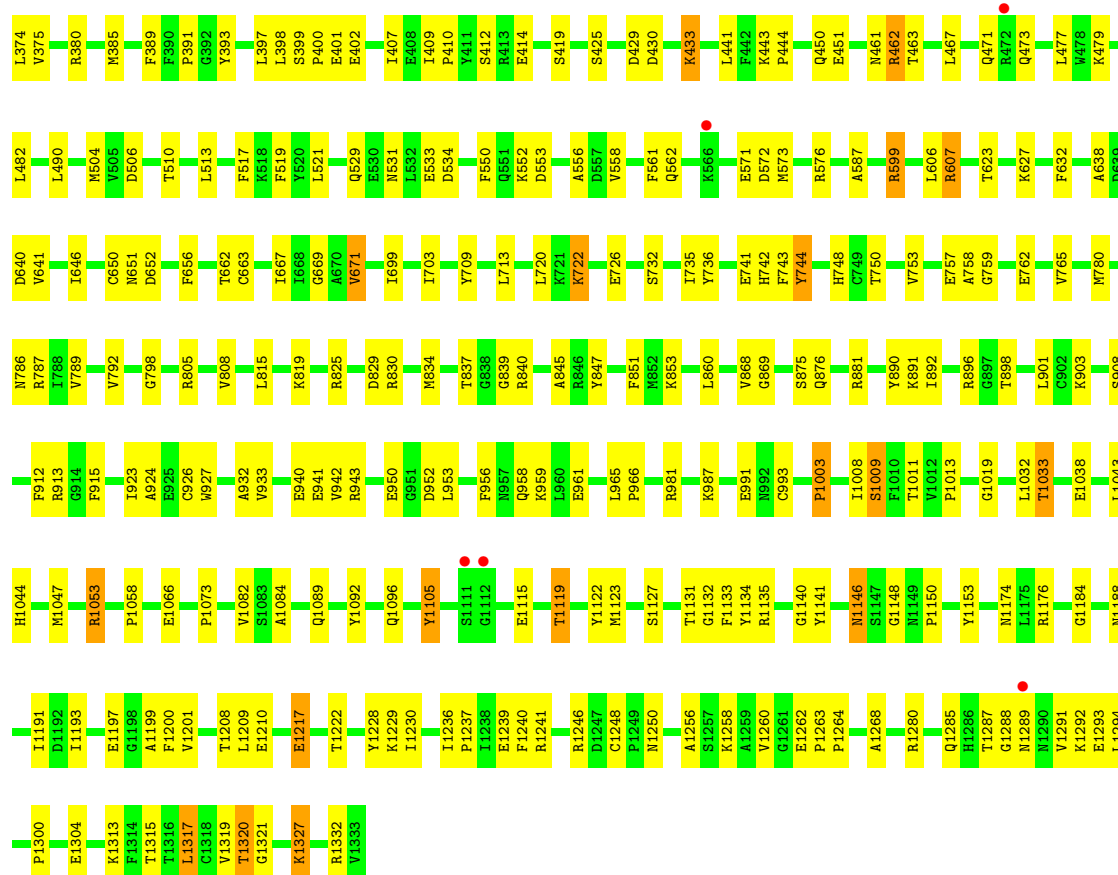
- Molecule 1: Xanthine dehydrogenase/oxidase



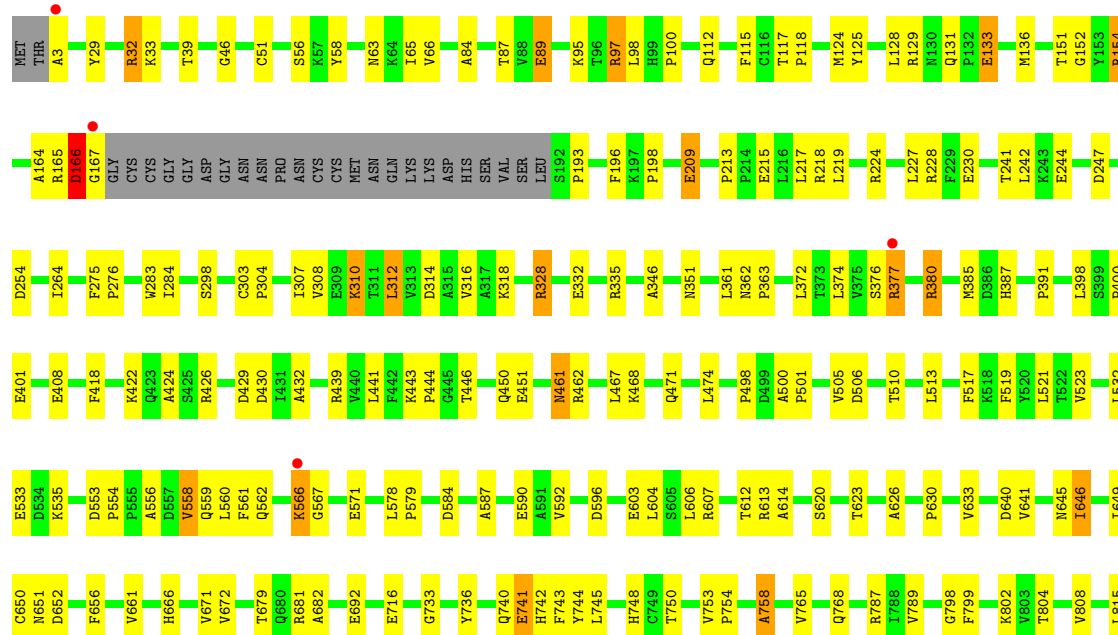
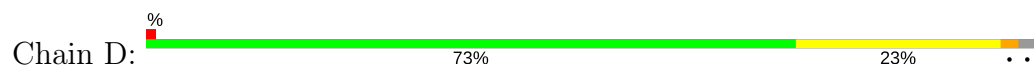








• Molecule 1: Xanthine dehydrogenase/oxidase





F1240	K1106	D952	A816
R1241	K1107	F956	A817
V1242	K1108	L965	X818
S1243	N1109	P966	X819
R1246	G1112	E970	R822
N1250	E1115	E971	P823
K1251	D1116	Y978	R830
K1252	V1117	K982	X834
A1253	V1118	N989	T837
H1254	T1119	K996	H841
Y1255	M1123	R997	H847
A1256	S1127	G998	V857
S1257	T1131	L999	L860
E1262	G1132	C1000	E861
P1263	F1133	I1001	
P1264	Y1134	I1002	
L1265	R1135	P1003	X867
I1271	Y1141	I1008	X868
D1277	S1142	S1009	D873
R1283	F1143	L1021	L878
H1286	N1146	L1022	X879
T1287	P1150	S1029	E880
G1288	V1163	H1034	R881
N1289	N1174	G1035	R896
N1290	I1193	T1037	C902
V1291	E1197	E1038	N905
K1292	G1198	M1039	T910
E1293	A1199	L1043	A911
P1300	F1200	H1044	X912
A1301	V1201	M1047	R913
T1302	L1204	V1050	G914
P1303	T1208	A1051	F915
T1315	L1209	S1052	A924
V1319	S1215	P1058	A927
T1320	P1216	T1059	E940
G1321	E1217	P1073	E941
V1322	T1222	A1079	X942
P1323	A1232	A1080	R943
P1324	P1237	S1081	R944
E1324	I1238	G1088	L947
P1325	E1239	X948	X949
X1325			
C1326			
K1327			
P1328			
V1331			
R1332			
V1333			



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.57Å 140.94Å 176.48Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.47 – 2.58	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.60) 94.0 (49.47-2.58)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.58Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.192 , 0.246 0.190 , 0.242	Depositor DCC
$R_{free}$ test set	3840 reflections (2.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l 0.014 for k,h,-l 0.146 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	41721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAL, CA, FES, MOM, BCT, 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	0.35	0/10303	0.62	0/13950
1	B	0.36	0/10303	0.63	1/13950 (0.0%)
1	C	0.36	0/10303	0.62	0/13950
1	D	0.36	0/10303	0.62	0/13950
All	All	0.36	0/41212	0.63	1/55800 (0.0%)

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
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1032	LEU	CA-CB-CG	5.62	128.22	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1105	TYR	Sidechain
1	C	1105	TYR	Sidechain



## 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	10088	0	10112	281	0
1	B	10088	0	10111	275	0
1	C	10088	0	10110	266	0
1	D	10088	0	10112	237	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	1	0
5	A	53	0	31	2	0
5	B	53	0	31	3	0
5	C	53	0	31	2	0
5	D	53	0	31	3	0
6	A	24	0	10	4	0
6	B	24	0	8	2	0
6	C	24	0	10	2	0
6	D	24	0	10	2	0
7	A	4	0	0	2	0
7	B	4	0	0	2	0
7	C	4	0	0	2	0
7	D	4	0	0	3	0
8	A	10	0	4	0	0
8	B	10	0	4	0	0
8	C	10	0	4	0	0
8	D	10	0	4	0	0
9	A	234	0	0	7	0
9	B	245	0	0	3	0
9	C	237	0	0	2	0
9	D	233	0	0	6	0
All	All	41721	0	40623	1063	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 13.

The worst 5 of 1063 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)
6:A:2004:MTE:N5	6:A:2004:MTE:C9	1.68	1.52
6:C:4004:MTE:C9	6:C:4004:MTE:N5	1.68	1.51
1:A:133:GLU:HG2	1:A:165:ARG:HB3	1.40	1.03
1:D:1320:THR:HG23	1:D:1321:GLY:H	1.26	1.00
1:A:3:ALA:HB1	1:A:228:ARG:H	1.28	0.99

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	1303/1333 (98%)	1225 (94%)	64 (5%)	14 (1%)	17	35
1	B	1303/1333 (98%)	1228 (94%)	65 (5%)	10 (1%)	22	44
1	C	1303/1333 (98%)	1228 (94%)	69 (5%)	6 (0%)	32	58
1	D	1303/1333 (98%)	1223 (94%)	64 (5%)	16 (1%)	15	32
All	All	5212/5332 (98%)	4904 (94%)	262 (5%)	46 (1%)	20	40

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1009	SER
1	A	1290	ASN
1	B	553	ASP
1	B	1009	SER
1	C	758	ALA



### 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	1104/1126 (98%)	1066 (97%)	38 (3%)	42	69
1	B	1104/1126 (98%)	1063 (96%)	41 (4%)	39	66
1	C	1104/1126 (98%)	1070 (97%)	34 (3%)	45	73
1	D	1104/1126 (98%)	1060 (96%)	44 (4%)	36	64
All	All	4416/4504 (98%)	4259 (96%)	157 (4%)	40	68

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1073	PRO
1	C	310	LYS
1	D	971	GLU
1	B	1135	ARG
1	C	62	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1325	ASN
1	C	473	GLN
1	D	1146	ASN
1	C	63	ASN
1	C	322	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	2001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	2002	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	A	2003	-	51,58,58	2.67	20 (39%)	54,89,89	3.14	21 (38%)
6	MTE	A	2004	7	21,26,26	7.24	12 (57%)	19,40,40	2.73	8 (42%)
7	MOM	A	2005	6	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	A	2006	-	7,10,10	1.99	3 (42%)	9,13,13	1.21	1 (11%)
2	BCT	A	6001	-	0,3,3	0.00	-	0,3,3	0.00	-
4	FES	B	2001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	B	2002	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	B	3003	-	51,58,58	2.70	23 (45%)	54,89,89	3.13	20 (37%)
6	MTE	B	3004	7	21,26,26	6.74	13 (61%)	19,40,40	2.98	8 (42%)
7	MOM	B	3005	6	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	B	3006	-	7,10,10	1.86	3 (42%)	9,13,13	1.19	1 (11%)
2	BCT	B	6002	-	0,3,3	0.00	-	0,3,3	0.00	-
4	FES	C	2001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	C	2002	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	C	4003	-	51,58,58	2.67	21 (41%)	54,89,89	3.13	21 (38%)
6	MTE	C	4004	7	21,26,26	7.11	13 (61%)	19,40,40	5.21	9 (47%)
7	MOM	C	4005	6	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	C	4006	-	7,10,10	1.92	3 (42%)	9,13,13	1.18	0
2	BCT	C	6003	-	0,3,3	0.00	-	0,3,3	0.00	-
4	FES	D	2001	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	D	2002	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	D	5003	-	51,58,58	2.59	20 (39%)	54,89,89	3.12	18 (33%)
6	MTE	D	5004	7	21,26,26	7.11	14 (66%)	19,40,40	5.39	8 (42%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MOM	D	5005	6	0,3,3	0.00	-	0,3,3	0.00	-
8	SAL	D	5006	-	7,10,10	1.99	3 (42%)	9,13,13	1.19	0
2	BCT	D	6004	-	0,3,3	0.00	-	0,3,3	0.00	-

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	2001	1	-	0/0/4/4	0/1/1/1
4	FES	A	2002	1	-	0/0/4/4	0/1/1/1
5	FAD	A	2003	-	-	0/28/50/50	0/6/6/6
6	MTE	A	2004	7	-	0/6/34/34	0/3/3/3
7	MOM	A	2005	6	-	0/0/0/0	0/0/0/0
8	SAL	A	2006	-	-	0/0/4/4	0/1/1/1
2	BCT	A	6001	-	-	0/0/0/0	0/0/0/0
4	FES	B	2001	1	-	0/0/4/4	0/1/1/1
4	FES	B	2002	1	-	0/0/4/4	0/1/1/1
5	FAD	B	3003	-	-	0/28/50/50	0/6/6/6
6	MTE	B	3004	7	-	0/6/34/34	0/3/3/3
7	MOM	B	3005	6	-	0/0/0/0	0/0/0/0
8	SAL	B	3006	-	-	0/0/4/4	0/1/1/1
2	BCT	B	6002	-	-	0/0/0/0	0/0/0/0
4	FES	C	2001	1	-	0/0/4/4	0/1/1/1
4	FES	C	2002	1	-	0/0/4/4	0/1/1/1
5	FAD	C	4003	-	-	0/28/50/50	0/6/6/6
6	MTE	C	4004	7	-	0/6/34/34	0/3/3/3
7	MOM	C	4005	6	-	0/0/0/0	0/0/0/0
8	SAL	C	4006	-	-	0/0/4/4	0/1/1/1
2	BCT	C	6003	-	-	0/0/0/0	0/0/0/0
4	FES	D	2001	1	-	0/0/4/4	0/1/1/1
4	FES	D	2002	1	-	0/0/4/4	0/1/1/1
5	FAD	D	5003	-	-	0/28/50/50	0/6/6/6
6	MTE	D	5004	7	-	0/6/34/34	0/3/3/3
7	MOM	D	5005	6	-	0/0/0/0	0/0/0/0
8	SAL	D	5006	-	-	0/0/4/4	0/1/1/1
2	BCT	D	6004	-	-	0/0/0/0	0/0/0/0

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



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3004	MTE	C4'-C3'	-14.33	1.31	1.52
6	D	5004	MTE	C4'-C3'	-12.12	1.34	1.52
6	C	4004	MTE	C4'-C3'	-11.36	1.35	1.52
6	C	4004	MTE	O4'-C4'	-8.28	1.11	1.44
6	D	5004	MTE	O4'-C4'	-8.07	1.12	1.44

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4003	FAD	N3A-C2A-N1A	-12.76	117.75	128.86
5	A	2003	FAD	N3A-C2A-N1A	-12.74	117.77	128.86
5	B	3003	FAD	N3A-C2A-N1A	-12.60	117.89	128.86
5	D	5003	FAD	N3A-C2A-N1A	-12.56	117.92	128.86
5	A	2003	FAD	C1'-N10-C10	-5.23	113.14	118.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2003	FAD	2	0
6	A	2004	MTE	4	0
7	A	2005	MOM	2	0
2	A	6001	BCT	1	0
5	B	3003	FAD	3	0
6	B	3004	MTE	2	0
7	B	3005	MOM	2	0
2	B	6002	BCT	1	0
5	C	4003	FAD	2	0
6	C	4004	MTE	2	0
7	C	4005	MOM	2	0
4	D	2002	FES	1	0
5	D	5003	FAD	3	0
6	D	5004	MTE	2	0
7	D	5005	MOM	3	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1307/1333 (98%)	-0.39	11 (0%) 86 83	10, 27, 56, 169	0
1	B	1307/1333 (98%)	-0.47	5 (0%) 92 91	10, 25, 52, 166	0
1	C	1307/1333 (98%)	-0.43	7 (0%) 90 89	9, 26, 54, 156	0
1	D	1307/1333 (98%)	-0.46	8 (0%) 89 88	8, 25, 55, 150	0
All	All	5228/5332 (98%)	-0.44	31 (0%) 89 88	8, 26, 55, 169	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1321	GLY	4.9
1	B	1325	ASN	4.7
1	C	1289	ASN	4.7
1	D	1325	ASN	4.4
1	B	566	LYS	4.1

### 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CA	B	7004	1/1	0.97	0.38	11.52	18,18,18,18	0
3	CA	A	7002	1/1	0.97	0.38	10.86	18,18,18,18	0
3	CA	C	7006	1/1	0.98	0.36	7.63	18,18,18,18	0
3	CA	D	7008	1/1	0.98	0.26	6.98	23,23,23,23	0
8	SAL	D	5006	10/10	0.92	0.20	3.43	41,42,42,43	0
8	SAL	B	3006	10/10	0.91	0.20	2.32	41,42,42,43	0
8	SAL	A	2006	10/10	0.93	0.18	2.17	36,37,37,38	0
8	SAL	C	4006	10/10	0.91	0.19	2.01	36,37,37,38	0
5	FAD	C	4003	53/53	0.96	0.17	1.87	26,36,47,49	0
5	FAD	D	5003	53/53	0.96	0.16	1.41	26,35,45,47	0
2	BCT	C	6003	4/4	0.94	0.19	1.33	17,18,19,19	0
3	CA	B	7003	1/1	0.91	0.20	1.31	20,20,20,20	0
5	FAD	B	3003	53/53	0.96	0.16	1.30	26,34,47,49	0
5	FAD	A	2003	53/53	0.97	0.15	0.92	26,36,46,48	0
3	CA	D	7007	1/1	0.96	0.18	0.61	20,20,20,20	0
3	CA	A	7001	1/1	0.95	0.18	0.59	20,20,20,20	0
2	BCT	A	6001	4/4	0.95	0.17	0.53	17,18,19,19	0
2	BCT	D	6004	4/4	0.94	0.17	-0.31	17,18,19,19	0
3	CA	C	7005	1/1	0.97	0.14	-0.80	20,20,20,20	0
7	MOM	A	2005	4/4	0.99	0.14	-0.91	28,29,30,31	0
7	MOM	C	4005	4/4	0.99	0.14	-1.21	28,29,30,31	0
4	FES	A	2001	4/4	0.96	0.12	-1.39	14,14,14,33	0
7	MOM	D	5005	4/4	0.99	0.14	-1.45	27,28,28,29	0
6	MTE	D	5004	24/24	0.94	0.13	-1.53	19,23,28,30	0
4	FES	C	2002	4/4	0.99	0.09	-1.73	14,14,14,14	0
4	FES	B	2002	4/4	0.99	0.09	-1.84	14,14,14,14	0
2	BCT	B	6002	4/4	0.97	0.12	-1.88	17,18,19,19	0
4	FES	D	2002	4/4	0.99	0.08	-1.94	14,14,14,14	0
7	MOM	B	3005	4/4	0.99	0.13	-1.96	27,28,28,29	0
6	MTE	C	4004	24/24	0.95	0.12	-2.09	20,24,28,30	0
6	MTE	B	3004	24/24	0.95	0.12	-2.15	19,23,28,30	0
6	MTE	A	2004	24/24	0.96	0.12	-2.19	20,24,28,30	0
4	FES	D	2001	4/4	0.99	0.09	-2.55	14,14,14,14	0
4	FES	A	2002	4/4	0.99	0.08	-2.65	14,14,14,14	0
4	FES	B	2001	4/4	0.99	0.10	-3.00	14,14,14,14	0
4	FES	C	2001	4/4	0.99	0.09	-3.15	14,14,14,14	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.