



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:11 am GMT

PDB ID : 1V97  
Title : Crystal Structure of Bovine Milk Xanthine Dehydrogenase FYX-051 bound form  
Authors : Okamoto, K.; Matsumoto, K.; Hille, R.; Eger, B.T.; Pai, E.F.; Nishino, T.  
Deposited on : 2004-01-21  
Resolution : 1.94 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

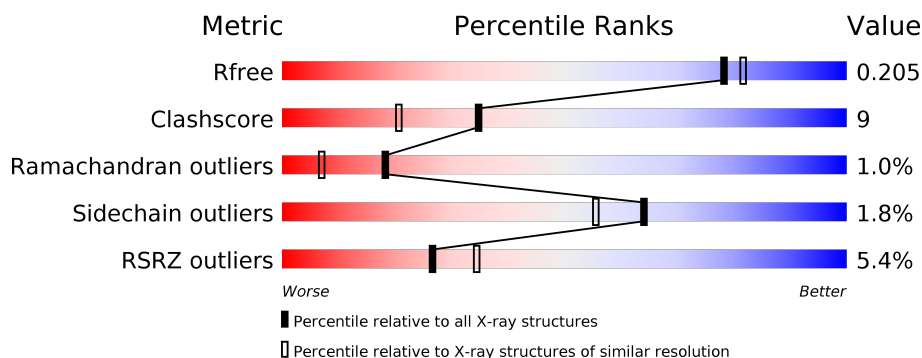
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	3233 (1.96-1.92)
Clashscore	112137	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

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	1332	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	1332	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MOS	A	3004	-	-	X	-
5	MOS	B	4004	-	-	X	-
7	FYX	A	3006	-	X	-	-
8	ACY	A	3007	-	-	X	-
8	ACY	B	4007	-	-	X	-
9	GOL	A	5001	-	X	-	X
9	GOL	A	5003	-	X	-	X
9	GOL	A	5005	-	X	-	X
9	GOL	A	5007	-	X	-	-
9	GOL	B	5002	-	X	-	X
9	GOL	B	5004	-	X	-	X
9	GOL	B	5006	-	X	-	-
9	GOL	B	5008	-	X	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 22481 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.

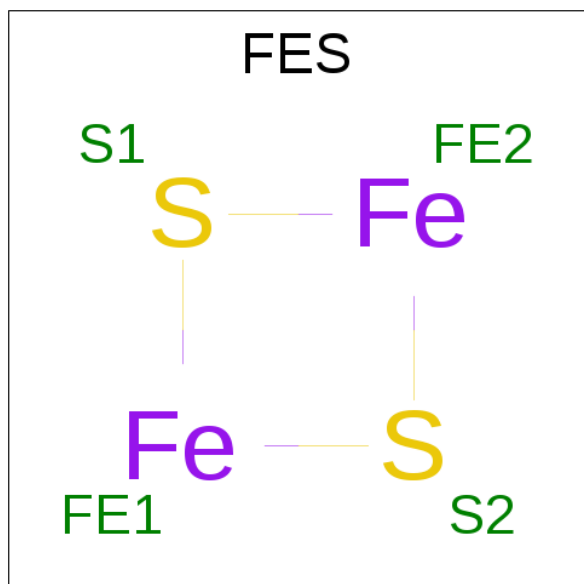
- Molecule 1 is a protein called Xanthine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1298	Total	C	N	O	S	0	0	0
			10071	6401	1727	1882	61			
1	B	1296	Total	C	N	O	S	0	0	0
			10054	6391	1724	1878	61			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

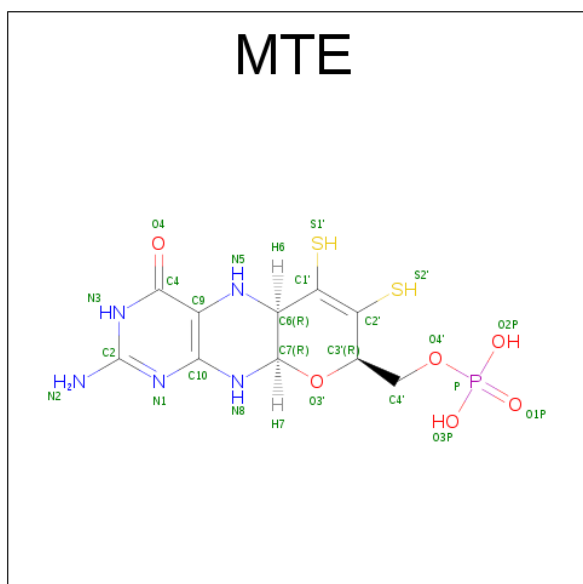
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



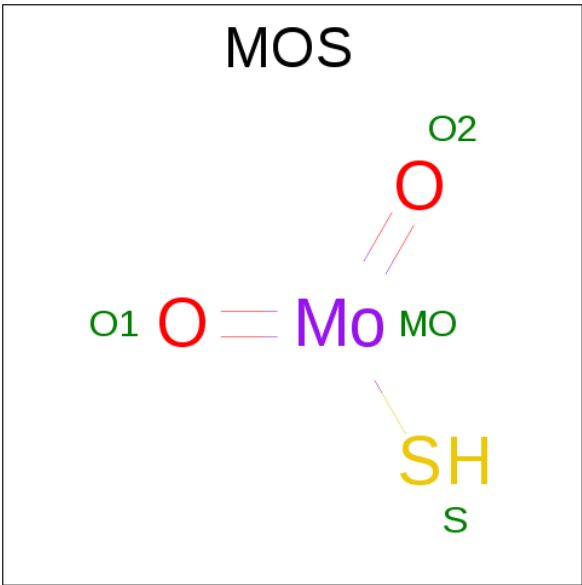
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0

- Molecule 4 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:  $C_{10}H_{14}N_5O_6PS_2$ ).



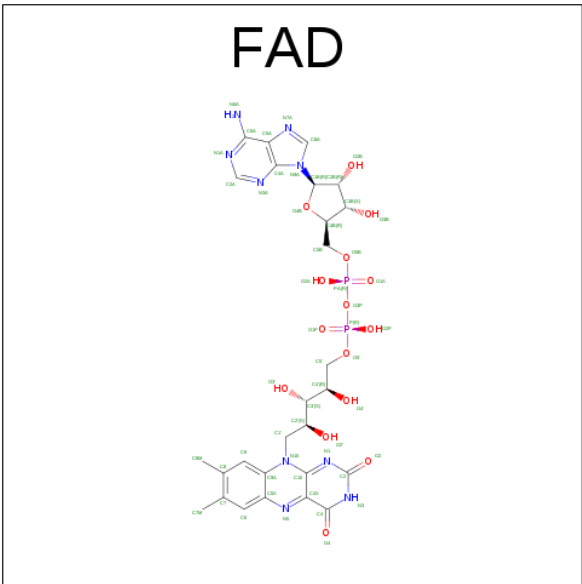
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 24 10 5 6 1 2	0	0
4	B	1	Total C N O P S 24 10 5 6 1 2	0	0

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $HMoO_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		

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



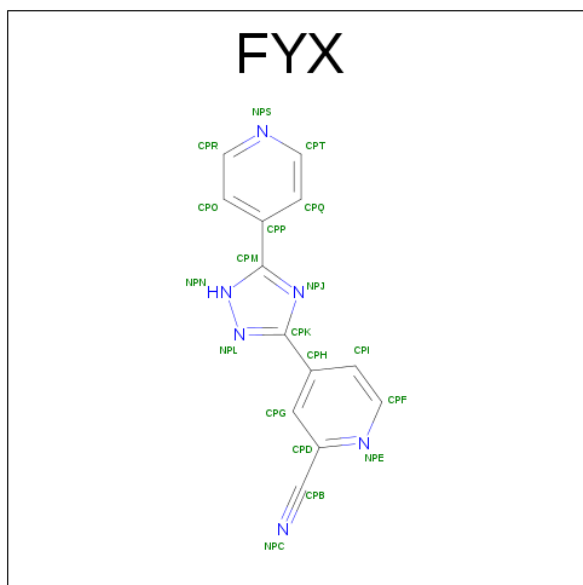
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0
			53	27	9	15	2	

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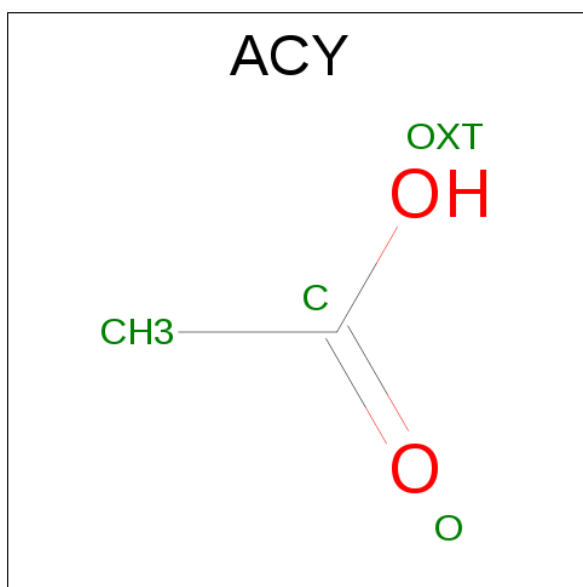
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 7 is 4-(5-PYRIDIN-4-YL-1H-1,2,4-TRIAZOL-3-YL)PYRIDINE-2-CARBONITRILE (three-letter code: FYX) (formula: C<sub>13</sub>H<sub>8</sub>N<sub>6</sub>).



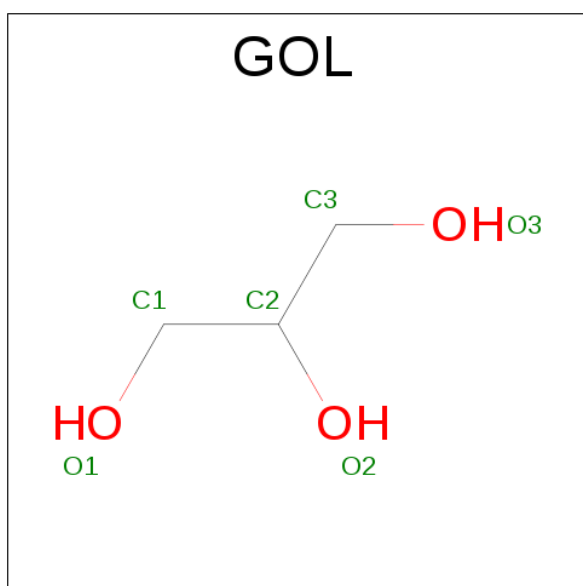
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	N	0	0
			19	13	6		
7	B	1	Total	C	N	0	0
			19	13	6		

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

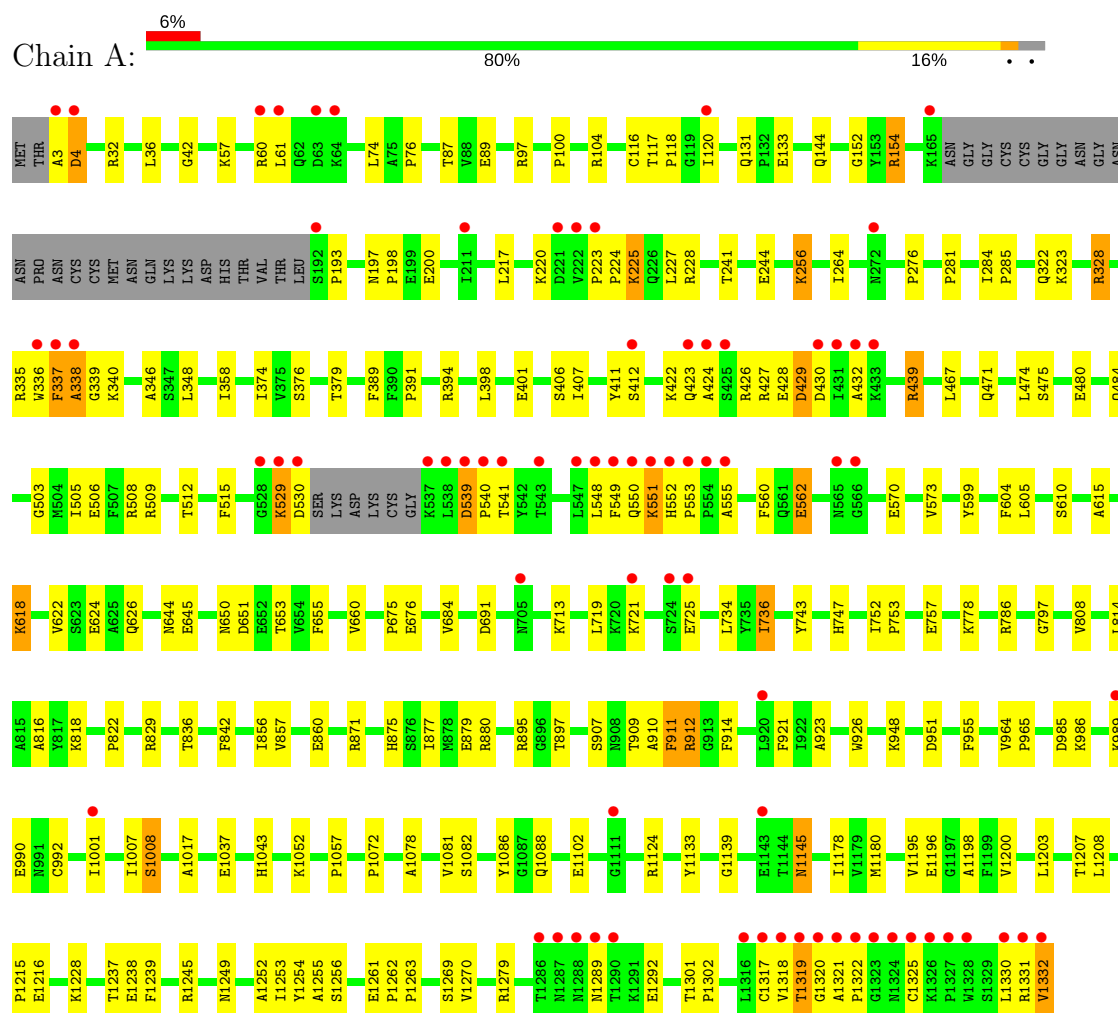
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1061	Total 1061	O 1061	0	0
10	B	1021	Total 1021	O 1021	0	0

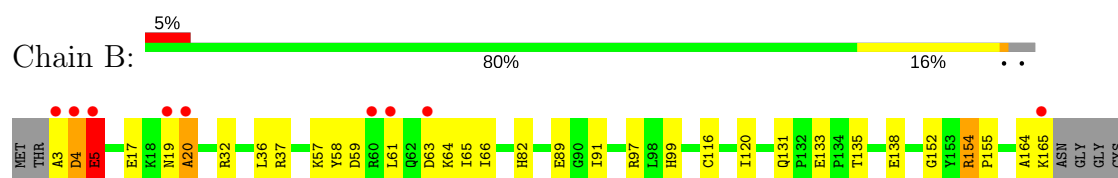
### 3 Residue-property plots

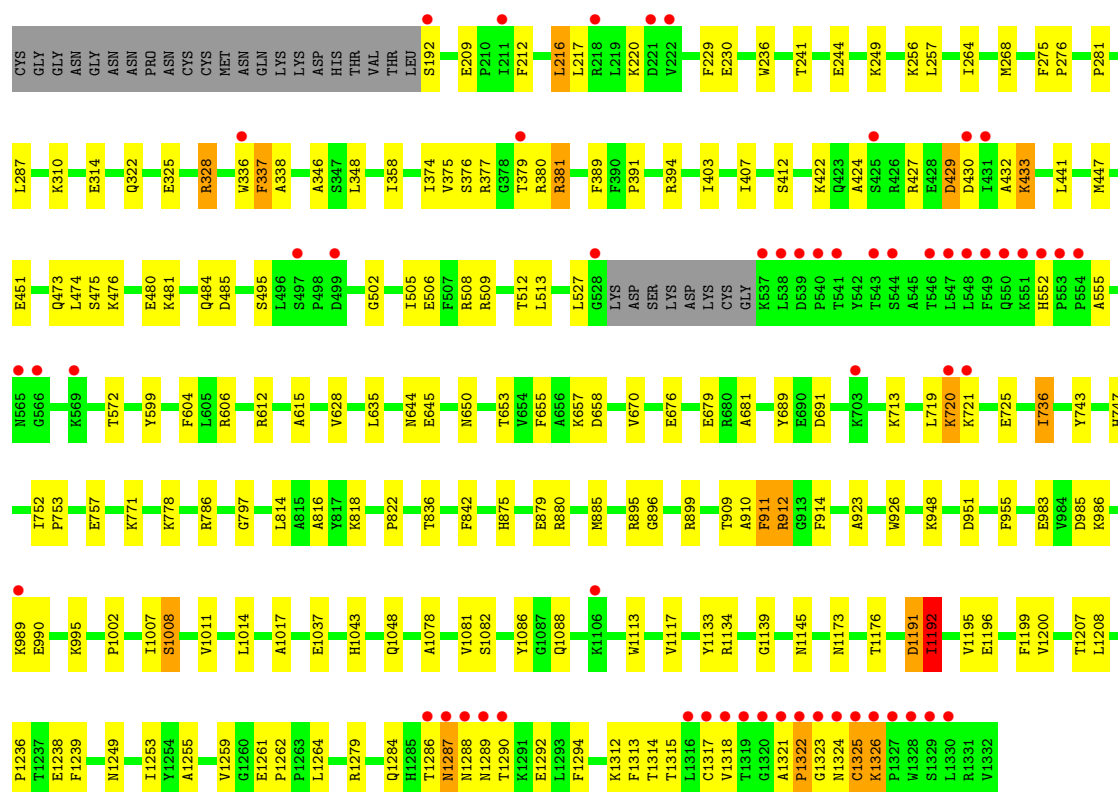
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



- Molecule 1: Xanthine dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.99Å 124.61Å 146.93Å 90.00° 90.99° 90.00°	Depositor
Resolution (Å)	40.00 – 1.94 30.49 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-1.94) 96.4 (30.49-1.94)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.10 (at 1.94Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.178 , 0.208 0.176 , 0.205	Depositor DCC
$R_{free}$ test set	6405 reflections (3.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22481	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MOS, CA, FES, FYX, ACY, 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	0.31	0/10292	0.60	0/13931
1	B	0.31	0/10275	0.62	4/13909 (0.0%)
All	All	0.31	0/20567	0.61	4/27840 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1192	ILE	N-CA-CB	-9.77	88.34	110.80
1	B	1191	ASP	N-CA-C	7.02	129.96	111.00
1	B	5	GLU	N-CA-C	6.78	129.29	111.00
1	B	1192	ILE	N-CA-C	-5.30	96.70	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	10071	0	10071	181	0
1	B	10054	0	10053	200	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	0	0	0
4	A	24	0	10	1	0
4	B	24	0	10	1	0
5	A	4	0	0	2	0
5	B	4	0	0	2	0
6	A	53	0	31	3	0
6	B	53	0	31	3	0
7	A	19	0	7	0	0
7	B	19	0	7	0	0
8	A	4	0	3	3	0
8	B	4	0	3	4	0
9	A	24	0	16	3	0
9	B	24	0	15	3	0
10	A	1061	0	0	16	0
10	B	1021	0	0	14	0
All	All	22481	0	20257	381	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 9.

All (381) 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:A:340:LYS:NZ	10:A:6066:HOH:O	1.60	1.25
1:A:3:ALA:HB1	1:A:228:ARG:H	1.17	1.06
1:B:1286:THR:HG22	1:B:1287:ASN:H	1.28	0.98
1:B:229:PHE:HA	10:B:5161:HOH:O	1.65	0.95
1:B:955:PHE:HA	1:B:1145:ASN:HD21	1.35	0.89
1:A:3:ALA:HB1	1:A:228:ARG:N	1.91	0.83
1:A:736:ILE:CG2	1:A:842:PHE:HB2	2.08	0.83
1:B:645:GLU:HG2	1:B:650:ASN:HD22	1.43	0.82
1:A:650:ASN:HD21	1:A:778:LYS:HE3	1.46	0.81
1:B:1289:ASN:HB3	1:B:1292:GLU:HB2	1.60	0.81
1:B:131:GLN:HE21	1:B:133:GLU:H	1.25	0.81
1:B:249:LYS:HD3	1:B:257:LEU:HD11	1.62	0.81
1:A:422:LYS:HE3	1:A:432:ALA:HB2	1.63	0.80
1:B:736:ILE:CG2	1:B:842:PHE:HB2	2.10	0.80
1:B:433:LYS:HE3	1:B:433:LYS:HA	1.64	0.80
1:A:719:LEU:HD11	1:A:895:ARG:HB2	1.65	0.79
1:A:1088:GLN:HE22	9:A:5007:GOL:C3	1.95	0.79
1:B:1253:ILE:HD12	9:B:5008:GOL:H12	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:GLN:HG2	1:A:1133:TYR:CD1	2.17	0.78
1:B:17:GLU:HG3	1:B:20:ALA:HB2	1.66	0.78
1:B:1321:ALA:HB1	1:B:1322:PRO:HD2	1.64	0.78
1:A:955:PHE:HA	1:A:1145:ASN:HD21	1.49	0.77
1:B:509:ARG:O	1:B:513:LEU:HD13	1.84	0.77
1:B:154:ARG:HD3	1:B:1196:GLU:OE2	1.84	0.76
1:B:19:ASN:O	1:B:20:ALA:HB3	1.85	0.75
1:A:154:ARG:HD3	1:A:1196:GLU:OE2	1.86	0.75
1:A:645:GLU:HG2	1:A:650:ASN:HD22	1.50	0.75
1:B:1088:GLN:HG2	1:B:1133:TYR:CD1	2.22	0.75
1:B:57:LYS:NZ	1:B:66:ILE:HD11	2.02	0.74
1:A:509:ARG:NH1	1:A:1317:CYS:HB2	2.05	0.72
1:A:131:GLN:HE21	1:A:133:GLU:H	1.36	0.71
1:B:3:ALA:HB3	1:B:19:ASN:C	2.11	0.71
1:A:358:ILE:HD11	10:A:6068:HOH:O	1.89	0.71
1:B:3:ALA:N	1:B:19:ASN:HA	2.05	0.70
1:B:995:LYS:NZ	1:B:1284:GLN:HE21	1.87	0.70
1:A:736:ILE:O	1:A:736:ILE:HG23	1.91	0.69
1:A:719:LEU:HD11	1:A:895:ARG:CB	2.23	0.69
1:B:1286:THR:HG22	1:B:1287:ASN:N	2.05	0.68
1:A:736:ILE:HG21	1:A:842:PHE:HB2	1.76	0.66
1:B:719:LEU:HD11	1:B:895:ARG:HB3	1.77	0.66
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.59	0.66
1:B:36:LEU:HD22	1:B:89:GLU:HG3	1.75	0.66
1:A:914:PHE:HA	8:A:3007:ACY:H1	1.77	0.66
1:A:505:ILE:O	1:A:509:ARG:HG3	1.96	0.65
1:A:1289:ASN:HD22	1:A:1292:GLU:HB2	1.59	0.65
1:A:328:ARG:HH11	1:A:328:ARG:HG2	1.61	0.65
1:B:555:ALA:HB3	1:B:1238:GLU:HG3	1.79	0.65
1:A:573:VAL:HG21	1:A:1052:LYS:HD2	1.76	0.65
1:B:495:SER:HA	1:B:509:ARG:NH1	2.12	0.65
1:B:57:LYS:HZ1	1:B:66:ILE:HD11	1.62	0.65
1:A:506:GLU:HG2	1:A:1319:THR:HB	1.77	0.64
5:B:4004:MOS:O2	5:B:4004:MOS:MO	1.68	0.64
1:A:753:PRO:HD3	1:A:816:ALA:HB1	1.79	0.64
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.79	0.64
1:B:17:GLU:CG	1:B:20:ALA:HB2	2.28	0.64
5:A:3004:MOS:O2	5:A:3004:MOS:MO	1.70	0.63
1:B:19:ASN:O	1:B:20:ALA:CB	2.45	0.63
1:B:650:ASN:HD21	1:B:778:LYS:HE3	1.63	0.63
1:A:541:THR:CG2	1:A:992:CYS:HB2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:PHE:H	8:B:4007:ACY:H3	1.64	0.63
1:A:336:TRP:HB3	1:A:427:ARG:O	1.99	0.63
1:A:335:ARG:NH2	1:A:549:PHE:HB3	2.14	0.62
1:A:1180:MET:HE1	1:A:1263:PRO:HB3	1.79	0.62
1:A:684:VAL:O	1:A:684:VAL:HG12	2.00	0.62
1:B:375:VAL:HG22	1:B:380:ARG:HG3	1.81	0.62
1:B:986:LYS:HA	1:B:989:LYS:NZ	2.14	0.62
1:A:217:LEU:O	1:A:220:LYS:HG2	2.00	0.62
1:A:474:LEU:O	1:A:475:SER:HB2	2.00	0.62
1:A:509:ARG:HG2	10:A:5250:HOH:O	1.99	0.62
1:B:422:LYS:HE3	1:B:432:ALA:HB2	1.82	0.61
1:B:736:ILE:HG21	1:B:842:PHE:HB2	1.82	0.61
1:A:1008:SER:HA	1:A:1081:VAL:HG11	1.83	0.61
1:B:495:SER:HA	1:B:509:ARG:HH12	1.64	0.61
1:A:264:ILE:HD11	6:A:3005:FAD:H3B	1.82	0.61
1:B:1286:THR:CG2	1:B:1287:ASN:H	2.08	0.61
1:B:914:PHE:HA	8:B:4007:ACY:H2	1.82	0.61
1:B:911:PHE:N	8:B:4007:ACY:H3	2.15	0.61
1:A:4:ASP:HB3	10:A:5500:HOH:O	2.00	0.60
1:B:325:GLU:HB2	1:B:412:SER:OG	2.01	0.60
1:B:3:ALA:HB3	1:B:20:ALA:N	2.15	0.60
1:A:376:SER:HB3	1:A:379:THR:OG1	2.01	0.60
1:B:736:ILE:O	1:B:736:ILE:HG23	2.02	0.60
1:B:441:LEU:HB3	1:B:451:GLU:HB2	1.84	0.60
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.84	0.60
1:B:61:LEU:HD23	1:B:61:LEU:O	2.02	0.59
1:A:338:ALA:HA	1:A:429:ASP:OD1	2.01	0.59
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.17	0.59
1:B:721:LYS:O	1:B:725:GLU:HG3	2.02	0.59
1:B:1008:SER:HA	1:B:1081:VAL:HG11	1.83	0.59
1:B:32:ARG:HH12	1:B:676:GLU:CD	2.06	0.59
1:B:336:TRP:HB3	1:B:427:ARG:O	2.02	0.59
1:B:1286:THR:HG22	1:B:1287:ASN:ND2	2.17	0.59
1:B:241:THR:OG1	1:B:244:GLU:HG3	2.03	0.59
1:B:474:LEU:O	1:B:475:SER:HB2	2.03	0.59
1:B:512:THR:OG1	1:B:513:LEU:HD12	2.03	0.59
1:B:328:ARG:HG2	10:B:5538:HOH:O	2.03	0.59
1:A:346:ALA:HB1	6:A:3005:FAD:H4'	1.84	0.58
1:B:880:ARG:HD2	1:B:914:PHE:HB3	1.84	0.58
1:B:995:LYS:HZ1	1:B:1284:GLN:HE21	1.50	0.58
1:A:1321:ALA:HB1	1:A:1325:CYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:720:LYS:HB2	1:B:720:LYS:NZ	2.20	0.57
1:B:747:HIS:CD2	1:B:836:THR:HG21	2.40	0.57
1:A:736:ILE:HG23	1:A:842:PHE:H	1.69	0.56
1:B:1249:ASN:O	1:B:1255:ALA:HA	2.06	0.56
1:A:818:LYS:HE2	10:A:5813:HOH:O	2.04	0.56
1:B:381:ARG:HH11	1:B:381:ARG:CG	2.19	0.56
1:A:1249:ASN:O	1:A:1255:ALA:HA	2.06	0.55
1:A:1330:LEU:HD23	10:A:5762:HOH:O	2.05	0.55
1:B:948:LYS:HG2	1:B:951:ASP:OD2	2.06	0.55
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.07	0.55
1:A:555:ALA:HB3	1:A:1238:GLU:HG3	1.88	0.55
1:B:4:ASP:CB	10:B:5161:HOH:O	2.54	0.55
1:B:909:THR:O	8:B:4007:ACY:H1	2.06	0.54
1:A:154:ARG:HD2	10:A:5244:HOH:O	2.07	0.54
1:B:1207:THR:OG1	1:B:1208:LEU:HD13	2.06	0.54
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.38	0.54
1:A:655:PHE:HE1	1:A:814:LEU:HD23	1.71	0.54
1:A:430:ASP:HB2	1:A:1228:LYS:HE2	1.90	0.54
1:B:986:LYS:HA	1:B:989:LYS:HZ1	1.72	0.54
1:A:340:LYS:HE3	10:A:6067:HOH:O	2.08	0.53
1:A:407:ILE:N	1:A:407:ILE:HD12	2.23	0.53
1:A:1203:LEU:HD13	1:A:1270:VAL:HG21	1.91	0.53
1:A:948:LYS:HG2	1:A:951:ASP:OD2	2.07	0.53
1:B:635:LEU:HD21	1:B:818:LYS:HG2	1.90	0.53
1:A:877:ILE:HD13	8:A:3007:ACY:H3	1.89	0.53
1:A:1001:ILE:CG1	1:A:1269:SER:HB3	2.39	0.53
1:B:875:HIS:O	1:B:879:GLU:HG3	2.09	0.53
1:A:1289:ASN:ND2	1:A:1292:GLU:HB2	2.22	0.52
1:B:1007:ILE:O	1:B:1008:SER:CB	2.57	0.52
1:B:612:ARG:NH1	1:B:689:TYR:HB2	2.23	0.52
1:B:604:PHE:HD2	9:B:5004:GOL:H11	1.74	0.52
1:A:747:HIS:CD2	1:A:836:THR:HG21	2.43	0.52
1:B:256:LYS:HG3	1:B:275:PHE:CD2	2.44	0.52
1:B:513:LEU:HD12	1:B:513:LEU:N	2.24	0.52
1:B:736:ILE:HG23	1:B:842:PHE:H	1.73	0.52
1:B:753:PRO:HD3	1:B:816:ALA:HB1	1.92	0.52
1:A:552:HIS:HB3	1:A:1237:THR:HG21	1.92	0.52
1:B:1007:ILE:O	1:B:1008:SER:HB3	2.08	0.52
1:B:5:GLU:HG3	10:B:5560:HOH:O	2.09	0.52
1:A:604:PHE:CD2	1:A:675:PRO:HG3	2.44	0.51
1:A:32:ARG:HH12	1:A:676:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:ASP:O	1:B:19:ASN:O	2.28	0.51
1:A:439:ARG:HB3	1:A:439:ARG:HH11	1.75	0.51
1:A:736:ILE:HG22	1:A:842:PHE:HB2	1.89	0.51
1:A:394:ARG:HD2	10:A:5374:HOH:O	2.09	0.51
1:A:719:LEU:HD13	1:A:860:GLU:OE2	2.10	0.51
1:A:1082:SER:HB2	4:A:3003:MTE:O3P	2.10	0.51
1:B:374:ILE:HB	1:B:381:ARG:HD3	1.91	0.51
1:A:1331:ARG:O	1:A:1332:VAL:HG12	2.11	0.51
1:A:622:VAL:O	1:A:626:GLN:HG3	2.10	0.51
1:A:624:GLU:HB2	1:A:684:VAL:HG12	1.91	0.51
1:B:381:ARG:HH11	1:B:381:ARG:HG2	1.75	0.51
1:A:541:THR:HG22	1:A:992:CYS:HB2	1.92	0.51
1:A:552:HIS:CG	1:A:553:PRO:HD2	2.46	0.51
1:A:1301:THR:HB	1:A:1302:PRO:HD2	1.93	0.50
1:A:875:HIS:O	1:A:879:GLU:HG3	2.10	0.50
1:B:1326:LYS:O	1:B:1326:LYS:HG3	2.11	0.50
1:B:310:LYS:O	1:B:314:GLU:HG3	2.10	0.50
1:B:57:LYS:HZ3	1:B:66:ILE:HD11	1.73	0.50
1:A:1007:ILE:O	1:A:1008:SER:CB	2.59	0.50
1:A:42:GLY:O	1:A:829:ARG:HD2	2.12	0.50
1:B:131:GLN:HE21	1:B:133:GLU:N	2.04	0.50
1:B:1314:THR:O	1:B:1318:VAL:HG13	2.11	0.50
1:A:323:LYS:HE2	1:A:411:TYR:HB3	1.92	0.50
1:A:358:ILE:HD11	10:A:5914:HOH:O	2.11	0.50
1:B:407:ILE:HD12	1:B:407:ILE:N	2.26	0.50
1:B:358:ILE:HD11	10:B:5893:HOH:O	2.12	0.50
1:B:338:ALA:HA	1:B:429:ASP:OD1	2.12	0.50
1:A:374:ILE:HD13	1:A:398:LEU:CD2	2.41	0.50
1:B:1289:ASN:CB	1:B:1292:GLU:HB2	2.37	0.50
1:A:1001:ILE:HG12	1:A:1269:SER:HB3	1.93	0.50
1:B:424:ALA:HB1	1:B:430:ASP:OD2	2.12	0.50
1:B:82:HIS:HA	1:B:216:LEU:HD21	1.94	0.50
1:B:3:ALA:O	1:B:19:ASN:O	2.30	0.49
1:A:509:ARG:HH11	1:A:1317:CYS:HB2	1.77	0.49
1:A:1319:THR:O	1:A:1319:THR:HG23	2.12	0.49
1:B:1191:ASP:O	1:B:1195:VAL:HG23	2.13	0.49
1:A:508:ARG:O	1:A:512:THR:HG23	2.13	0.49
1:A:406:SER:C	1:A:407:ILE:HD12	2.32	0.49
1:A:1007:ILE:O	1:A:1008:SER:HB3	2.12	0.49
1:B:192:SER:HB3	10:B:5427:HOH:O	2.13	0.49
1:B:508:ARG:O	1:B:512:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:LYS:HD3	1:A:1254:TYR:CZ	2.48	0.49
1:B:719:LEU:HD11	1:B:895:ARG:CB	2.42	0.49
1:B:1287:ASN:O	1:B:1288:ASN:HB2	2.12	0.49
1:B:64:LYS:HG2	1:B:65:ILE:N	2.28	0.49
1:B:1324:ASN:O	1:B:1326:LYS:N	2.46	0.48
1:B:1287:ASN:H	1:B:1287:ASN:HD22	1.62	0.48
1:B:757:GLU:HB3	1:B:786:ARG:HE	1.78	0.48
1:B:606:ARG:CZ	1:B:679:GLU:HG3	2.43	0.48
1:B:394:ARG:HD2	10:B:5793:HOH:O	2.13	0.48
1:A:985:ASP:O	1:A:989:LYS:HG3	2.13	0.48
1:A:1207:THR:O	1:A:1208:LEU:HD12	2.14	0.48
1:B:1011:VAL:HG23	1:B:1011:VAL:O	2.13	0.48
1:A:986:LYS:HA	1:A:989:LYS:NZ	2.29	0.48
1:A:467:LEU:O	1:A:471:GLN:HG2	2.13	0.47
1:B:281:PRO:HB2	1:B:287:LEU:CD1	2.43	0.47
1:B:1078:ALA:HB1	5:B:4004:MOS:O1	2.14	0.47
1:B:217:LEU:O	1:B:220:LYS:HG2	2.14	0.47
1:A:116:CYS:O	1:A:120:ILE:HG13	2.14	0.47
1:B:509:ARG:O	1:B:513:LEU:CD1	2.58	0.47
1:A:1052:LYS:HE2	10:A:5520:HOH:O	2.14	0.47
1:A:506:GLU:CD	1:A:506:GLU:H	2.18	0.47
1:A:736:ILE:O	1:A:736:ILE:CG2	2.61	0.47
1:A:911:PHE:O	1:A:912:ARG:C	2.52	0.47
1:A:964:VAL:HB	1:A:965:PRO:HD3	1.95	0.47
1:B:1088:GLN:HG2	1:B:1133:TYR:CE1	2.48	0.47
1:B:154:ARG:HD2	10:B:5205:HOH:O	2.15	0.47
1:A:856:ILE:N	1:A:856:ILE:HD12	2.29	0.47
1:A:923:ALA:HA	1:A:926:TRP:NE1	2.30	0.47
1:A:144:GLN:HB2	1:A:339:GLY:HA2	1.97	0.47
1:B:995:LYS:HZ3	1:B:1284:GLN:HE21	1.63	0.47
1:B:3:ALA:HB1	1:B:20:ALA:O	2.15	0.47
1:B:379:THR:HG22	1:B:380:ARG:N	2.30	0.47
1:A:1252:ALA:HB3	1:A:1256:SER:O	2.15	0.46
1:A:555:ALA:O	1:A:1238:GLU:HA	2.15	0.46
1:B:216:LEU:HD13	1:B:216:LEU:O	2.15	0.46
1:B:3:ALA:C	10:B:5161:HOH:O	2.54	0.46
1:B:1261:GLU:N	1:B:1262:PRO:CD	2.78	0.46
1:B:1315:THR:HG22	1:B:1315:THR:O	2.14	0.46
1:B:152:GLY:HA2	1:B:1200:VAL:HG21	1.97	0.46
1:B:212:PHE:CZ	1:B:216:LEU:HD12	2.50	0.46
1:A:548:LEU:HD12	1:A:548:LEU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:ARG:HD2	1:A:914:PHE:HB3	1.98	0.46
1:B:480:GLU:O	1:B:484:GLN:HG3	2.16	0.46
1:B:1082:SER:HB2	4:B:4003:MTE:O3P	2.15	0.46
1:B:513:LEU:HD22	1:B:1317:CYS:SG	2.56	0.46
1:B:1287:ASN:O	1:B:1288:ASN:CB	2.64	0.46
1:B:325:GLU:N	1:B:412:SER:OG	2.48	0.46
1:B:389:PHE:O	1:B:391:PRO:HD3	2.16	0.46
1:A:322:GLN:O	1:A:412:SER:HB3	2.16	0.46
1:A:752:ILE:CD1	1:A:822:PRO:HB3	2.45	0.46
1:B:264:ILE:HD11	6:B:4005:FAD:H3B	1.96	0.46
1:A:424:ALA:HB1	1:A:430:ASP:OD2	2.15	0.46
1:A:615:ALA:HB2	1:A:691:ASP:HA	1.97	0.46
1:B:1325:CYS:O	1:B:1326:LYS:HB3	2.15	0.46
1:B:713:LYS:HD2	1:B:895:ARG:NH1	2.30	0.46
1:A:225:LYS:HB2	1:A:225:LYS:NZ	2.30	0.45
1:A:1124:ARG:HD2	1:B:1134:ARG:HG3	1.98	0.45
1:B:911:PHE:O	1:B:912:ARG:C	2.55	0.45
1:B:403:ILE:C	1:B:403:ILE:HD12	2.37	0.45
1:B:506:GLU:HG3	10:B:5340:HOH:O	2.16	0.45
1:A:1215:PRO:HD2	1:A:1216:GLU:OE2	2.17	0.45
1:A:529:LYS:O	1:A:530:ASP:HB2	2.16	0.45
1:B:3:ALA:HB3	1:B:19:ASN:CA	2.47	0.45
1:B:923:ALA:HA	1:B:926:TRP:NE1	2.31	0.45
1:A:1261:GLU:N	1:A:1262:PRO:CD	2.80	0.45
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.16	0.45
1:B:375:VAL:HG12	1:B:376:SER:N	2.31	0.45
1:B:1207:THR:O	1:B:1208:LEU:HD12	2.17	0.45
1:B:381:ARG:CG	1:B:381:ARG:NH1	2.79	0.45
1:A:480:GLU:O	1:A:484:GLN:HG3	2.16	0.45
1:A:877:ILE:CD1	8:A:3007:ACY:H3	2.47	0.45
1:B:473:GLN:O	1:B:476:LYS:HB2	2.17	0.45
1:A:599:TYR:HA	1:B:599:TYR:HA	1.97	0.45
1:B:655:PHE:HE1	1:B:814:LEU:HD23	1.81	0.45
1:A:117:THR:HB	1:A:118:PRO:HD3	1.98	0.45
1:A:907:SER:N	9:A:5001:GOL:O3	2.38	0.45
1:A:650:ASN:ND2	1:A:778:LYS:HE3	2.25	0.45
1:B:376:SER:OG	1:B:379:THR:HB	2.17	0.45
1:A:1001:ILE:HD11	1:A:1269:SER:HB3	1.98	0.44
1:A:423:GLN:HB2	1:A:515:PHE:HZ	1.82	0.44
1:B:1279:ARG:HD3	10:B:5701:HOH:O	2.17	0.44
1:B:628:VAL:HG21	1:B:681:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:HB2	1:B:97:ARG:NH1	2.32	0.44
1:A:276:PRO:HG2	10:A:6037:HOH:O	2.17	0.44
1:B:116:CYS:O	1:B:120:ILE:HG13	2.17	0.44
1:B:257:LEU:O	6:B:4005:FAD:H2B	2.16	0.44
1:B:37:ARG:HG2	10:B:5115:HOH:O	2.17	0.44
1:B:4:ASP:HB3	10:B:5161:HOH:O	2.16	0.44
1:B:909:THR:OG1	1:B:910:ALA:N	2.49	0.44
1:A:1088:GLN:HG2	1:A:1133:TYR:CE1	2.49	0.44
1:B:164:ALA:O	1:B:165:LYS:HB3	2.17	0.44
1:A:509:ARG:HH12	1:A:1317:CYS:HA	1.82	0.44
1:B:986:LYS:O	1:B:990:GLU:HG3	2.18	0.44
1:A:337:PHE:C	1:A:337:PHE:CD2	2.91	0.44
1:A:734:LEU:HD21	1:A:921:PHE:CE2	2.53	0.44
1:B:955:PHE:HA	1:B:1145:ASN:ND2	2.17	0.44
1:B:572:THR:OG1	1:B:1048:GLN:HG2	2.18	0.44
1:A:725:GLU:HG3	1:A:857:VAL:HG11	2.00	0.44
1:A:757:GLU:HB3	1:A:786:ARG:HE	1.82	0.44
1:A:152:GLY:HA2	1:A:1200:VAL:HG21	2.00	0.44
1:B:322:GLN:O	1:B:412:SER:HB2	2.18	0.44
1:A:1017:ALA:HB1	1:A:1086:TYR:CD2	2.53	0.43
1:A:428:GLU:O	1:A:429:ASP:C	2.56	0.43
1:A:1198:ALA:HB3	1:A:1263:PRO:HB2	2.00	0.43
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.82	0.43
1:A:713:LYS:HD3	1:A:897:THR:HG22	2.00	0.43
1:A:1180:MET:HE3	1:A:1195:VAL:HG13	2.00	0.43
1:A:87:THR:HG1	1:A:89:GLU:HG2	1.83	0.43
1:B:91:ILE:O	1:B:99:HIS:HB2	2.18	0.43
1:A:1207:THR:OG1	1:A:1208:LEU:HD13	2.18	0.43
1:A:1245:ARG:HG2	10:A:5452:HOH:O	2.18	0.43
1:A:509:ARG:HH12	1:A:1317:CYS:CA	2.31	0.43
1:A:651:ASP:OD2	1:A:871:ARG:NH1	2.51	0.43
1:A:74:LEU:O	1:A:76:PRO:HD3	2.19	0.43
1:B:375:VAL:CG1	1:B:376:SER:N	2.82	0.43
1:B:1037:GLU:HB2	1:B:1043:HIS:CD2	2.53	0.43
1:A:549:PHE:HE1	1:A:551:LYS:HG2	1.84	0.43
1:B:328:ARG:HG2	1:B:328:ARG:NH1	2.32	0.43
1:B:670:VAL:HG11	1:B:681:ALA:HB3	2.00	0.43
1:B:752:ILE:CD1	1:B:822:PRO:HB3	2.48	0.43
1:B:985:ASP:O	1:B:989:LYS:HG3	2.18	0.43
1:A:624:GLU:HB3	1:A:684:VAL:HG11	2.00	0.43
1:B:1017:ALA:HB1	1:B:1086:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.88	0.43
1:A:618:LYS:HA	1:A:618:LYS:HE3	2.01	0.43
1:B:1113:TRP:O	1:B:1117:VAL:HG23	2.18	0.43
1:B:264:ILE:O	1:B:268:MET:HG2	2.19	0.43
1:B:346:ALA:HB1	6:B:4005:FAD:H4'	2.01	0.42
1:B:657:LYS:O	1:B:658:ASP:HB2	2.18	0.42
1:A:1078:ALA:HB1	5:A:3004:MOS:O1	2.19	0.42
1:B:1192:ILE:HA	1:B:1195:VAL:HB	2.01	0.42
1:A:97:ARG:CZ	1:A:97:ARG:HB2	2.50	0.42
1:B:555:ALA:O	1:B:1238:GLU:HA	2.20	0.42
1:B:1279:ARG:HG2	1:B:1294:PHE:HE2	1.84	0.42
1:A:225:LYS:C	1:A:225:LYS:HD3	2.40	0.42
1:A:909:THR:OG1	1:A:910:ALA:N	2.49	0.42
1:B:1011:VAL:CG2	1:B:1014:LEU:HD12	2.50	0.42
1:B:1312:LYS:HE3	1:B:1313:PHE:CZ	2.54	0.42
1:B:644:ASN:O	1:B:653:THR:HA	2.20	0.42
1:B:1176:THR:HG21	1:B:1199:PHE:CZ	2.55	0.42
1:B:505:ILE:HG22	1:B:506:GLU:N	2.34	0.42
1:B:899:ARG:HD2	1:B:899:ARG:HA	1.85	0.42
1:A:1253:ILE:HD12	9:A:5007:GOL:H12	2.01	0.42
1:A:610:SER:HB2	1:A:660:VAL:HG11	2.01	0.42
1:B:1259:VAL:O	1:B:1259:VAL:HG22	2.19	0.42
1:B:154:ARG:N	1:B:155:PRO:HD2	2.34	0.42
1:B:377:ARG:HG2	1:B:377:ARG:NH1	2.35	0.42
1:B:447:MET:HG2	1:B:527:LEU:HD13	2.02	0.42
1:A:197:ASN:O	1:A:200:GLU:HG2	2.20	0.42
1:B:1173:ASN:O	1:B:1236:PRO:HA	2.20	0.42
1:B:1253:ILE:HD12	9:B:5008:GOL:C1	2.42	0.42
1:B:1264:LEU:HD23	1:B:1264:LEU:C	2.40	0.42
1:B:880:ARG:HD2	1:B:914:PHE:O	2.20	0.42
1:A:503:GLY:C	1:A:505:ILE:HD12	2.40	0.42
1:A:540:PRO:O	1:A:541:THR:HB	2.18	0.42
1:A:651:ASP:OD1	1:A:871:ARG:HG3	2.20	0.42
1:A:570:GLU:CD	1:A:1057:PRO:HG3	2.40	0.41
1:A:1279:ARG:HD2	10:A:5671:HOH:O	2.20	0.41
1:A:549:PHE:CD1	1:A:549:PHE:C	2.93	0.41
1:B:58:TYR:CD2	1:B:220:LYS:HB2	2.54	0.41
1:A:100:PRO:O	1:A:104:ARG:HG3	2.20	0.41
1:A:1037:GLU:HB2	1:A:1043:HIS:CD2	2.55	0.41
1:B:1287:ASN:H	1:B:1287:ASN:ND2	2.17	0.41
1:A:736:ILE:HG22	1:A:842:PHE:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:CD2	1:B:337:PHE:C	2.94	0.41
1:B:655:PHE:CE1	1:B:814:LEU:HD23	2.56	0.41
1:A:1178:ILE:CG2	1:A:1180:MET:HE2	2.50	0.41
1:A:193:PRO:HG2	1:A:560:PHE:CE1	2.55	0.41
1:B:1289:ASN:O	1:B:1290:THR:HB	2.21	0.41
1:B:615:ALA:HB2	1:B:691:ASP:HA	2.02	0.41
1:B:3:ALA:HB1	1:B:230:GLU:O	2.20	0.41
1:B:481:LYS:HE2	1:B:485:ASP:OD1	2.21	0.41
1:A:193:PRO:HB3	1:A:562:GLU:HG2	2.01	0.41
1:A:721:LYS:HD2	1:A:721:LYS:C	2.41	0.41
1:A:505:ILE:HD12	1:A:505:ILE:N	2.36	0.41
1:A:857:VAL:HG12	1:A:857:VAL:O	2.20	0.41
1:A:256:LYS:HE3	6:A:3005:FAD:O3B	2.21	0.41
1:A:644:ASN:O	1:A:653:THR:HA	2.21	0.41
1:A:808:VAL:HG23	10:A:6039:HOH:O	2.21	0.41
1:B:509:ARG:HG2	1:B:509:ARG:HH11	1.86	0.41
1:A:401:GLU:HB2	10:A:6007:HOH:O	2.21	0.41
1:A:426:ARG:NH2	1:A:429:ASP:O	2.52	0.41
1:B:3:ALA:CB	1:B:230:GLU:O	2.69	0.41
1:B:885:MET:SD	1:B:896:GLY:HA3	2.61	0.41
1:A:284:ILE:HA	1:A:285:PRO:HD2	1.89	0.41
1:A:651:ASP:CG	1:A:871:ARG:HH11	2.24	0.41
1:A:509:ARG:NH1	1:A:1317:CYS:CB	2.80	0.40
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.36	0.40
1:B:229:PHE:HB2	1:B:236:TRP:HB3	2.03	0.40
1:B:59:ASP:O	1:B:63:ASP:N	2.53	0.40
1:A:389:PHE:O	1:A:391:PRO:HD3	2.21	0.40
1:B:502:GLY:HA3	10:B:5612:HOH:O	2.20	0.40
1:B:61:LEU:HD23	1:B:61:LEU:C	2.39	0.40
1:A:197:ASN:HA	1:A:198:PRO:HD3	1.92	0.40
1:A:605:LEU:C	1:A:605:LEU:HD23	2.41	0.40
1:B:513:LEU:CD1	1:B:513:LEU:N	2.84	0.40
1:A:986:LYS:O	1:A:990:GLU:HG3	2.21	0.40
1:B:275:PHE:HA	1:B:276:PRO:HD2	1.93	0.40
1:B:771:LYS:HA	1:B:771:LYS:HD3	1.87	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	1292/1332 (97%)	1235 (96%)	43 (3%)	14 (1%)	17	6
1	B	1290/1332 (97%)	1235 (96%)	42 (3%)	13 (1%)	18	7
All	All	2582/2664 (97%)	2470 (96%)	85 (3%)	27 (1%)	18	7

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	1008	SER
1	A	1322	PRO
1	B	4	ASP
1	B	5	GLU
1	B	1008	SER
1	B	1287	ASN
1	A	429	ASP
1	A	1319	THR
1	B	1139	GLY
1	A	61	LEU
1	A	338	ALA
1	A	539	ASP
1	A	912	ARG
1	A	1318	VAL
1	B	20	ALA
1	B	429	ASP
1	B	912	ARG
1	A	529	LYS
1	B	1322	PRO
1	B	1325	CYS
1	B	1326	LYS
1	A	797	GLY
1	A	1139	GLY
1	B	797	GLY

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Mol	Chain	Res	Type
1	A	1320	GLY
1	B	1323	GLY

### 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	1100/1128 (98%)	1078 (98%)	22 (2%)	60	51
1	B	1098/1128 (97%)	1081 (98%)	17 (2%)	70	63
All	All	2198/2256 (97%)	2159 (98%)	39 (2%)	64	55

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	154	ARG
1	A	225	LYS
1	A	256	LYS
1	A	281	PRO
1	A	328	ARG
1	A	337	PHE
1	A	348	LEU
1	A	439	ARG
1	A	539	ASP
1	A	550	GLN
1	A	551	LYS
1	A	562	GLU
1	A	618	LYS
1	A	736	ILE
1	A	743	TYR
1	A	911	PHE
1	A	1072	PRO
1	A	1102	GLU
1	A	1145	ASN
1	A	1239	PHE

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Mol	Chain	Res	Type
1	A	1332	VAL
1	B	154	ARG
1	B	209	GLU
1	B	216	LEU
1	B	328	ARG
1	B	337	PHE
1	B	348	LEU
1	B	381	ARG
1	B	433	LYS
1	B	552	HIS
1	B	720	LYS
1	B	736	ILE
1	B	743	TYR
1	B	911	PHE
1	B	983	GLU
1	B	1002	PRO
1	B	1192	ILE
1	B	1239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	251	GLN
1	A	351	ASN
1	A	473	GLN
1	A	556	ASN
1	A	567	GLN
1	A	650	ASN
1	A	976	GLN
1	A	1088	GLN
1	A	1145	ASN
1	A	1284	GLN
1	A	1289	ASN
1	B	62	GLN
1	B	131	GLN
1	B	146	ASN
1	B	272	ASN
1	B	351	ASN
1	B	473	GLN
1	B	552	HIS
1	B	565	ASN

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Mol	Chain	Res	Type
1	B	626	GLN
1	B	650	ASN
1	B	1145	ASN
1	B	1284	GLN
1	B	1287	ASN
1	B	1324	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 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\# Z  > 2$
3	FES	A	3001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	A	3002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	A	3003	5	21,26,26	5.90	11 (52%)	19,40,40	2.86	7 (36%)
5	MOS	A	3004	4,7	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	A	3005	-	51,58,58	2.09	11 (21%)	54,89,89	2.97	18 (33%)
7	FYX	A	3006	5	21,21,21	2.69	11 (52%)	26,28,28	4.42	14 (53%)
8	ACY	A	3007	-	1,3,3	1.15	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	GOL	A	5001	-	5,5,5	5.43	4 (80%)	5,5,5	6.08	3 (60%)
9	GOL	A	5003	1	5,5,5	5.43	4 (80%)	5,5,5	6.08	3 (60%)
9	GOL	A	5005	-	5,5,5	5.43	4 (80%)	5,5,5	6.08	3 (60%)
9	GOL	A	5007	1	5,5,5	5.44	4 (80%)	5,5,5	6.08	3 (60%)
3	FES	B	4001	1	0,4,4	0.00	-	0,4,4	0.00	-
3	FES	B	4002	1	0,4,4	0.00	-	0,4,4	0.00	-
4	MTE	B	4003	5	21,26,26	5.94	13 (61%)	19,40,40	2.89	7 (36%)
5	MOS	B	4004	4,7	0,3,3	0.00	-	0,3,3	0.00	-
6	FAD	B	4005	-	51,58,58	2.03	11 (21%)	54,89,89	3.10	16 (29%)
7	FYX	B	4006	5	21,21,21	2.68	9 (42%)	26,28,28	4.36	14 (53%)
8	ACY	B	4007	-	1,3,3	1.25	0	0,3,3	0.00	-
9	GOL	B	5002	-	5,5,5	5.44	4 (80%)	5,5,5	6.08	3 (60%)
9	GOL	B	5004	-	5,5,5	5.44	4 (80%)	5,5,5	6.08	3 (60%)
9	GOL	B	5006	-	5,5,5	5.44	4 (80%)	5,5,5	6.08	3 (60%)
9	GOL	B	5008	1	5,5,5	5.43	4 (80%)	5,5,5	6.08	3 (60%)

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	FES	A	3001	1	-	0/0/4/4	0/1/1/1
3	FES	A	3002	1	-	0/0/4/4	0/1/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/3/3/3
5	MOS	A	3004	4,7	-	0/0/0/0	0/0/0/0
6	FAD	A	3005	-	-	0/28/50/50	0/6/6/6
7	FYX	A	3006	5	-	0/8/10/10	0/3/3/3
8	ACY	A	3007	-	-	0/0/0/0	0/0/0/0
9	GOL	A	5001	-	-	0/4/4/4	0/0/0/0
9	GOL	A	5003	1	-	0/4/4/4	0/0/0/0
9	GOL	A	5005	-	-	0/4/4/4	0/0/0/0
9	GOL	A	5007	1	-	0/4/4/4	0/0/0/0
3	FES	B	4001	1	-	0/0/4/4	0/1/1/1
3	FES	B	4002	1	-	0/0/4/4	0/1/1/1
4	MTE	B	4003	5	-	0/6/34/34	0/3/3/3
5	MOS	B	4004	4,7	-	0/0/0/0	0/0/0/0
6	FAD	B	4005	-	-	0/28/50/50	0/6/6/6
7	FYX	B	4006	5	-	0/8/10/10	0/3/3/3
8	ACY	B	4007	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	B	5002	-	-	0/4/4/4	0/0/0/0
9	GOL	B	5004	-	-	0/4/4/4	0/0/0/0
9	GOL	B	5006	-	-	0/4/4/4	0/0/0/0
9	GOL	B	5008	1	-	0/4/4/4	0/0/0/0

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	5006	GOL	C3-C2	-10.32	1.14	1.52
9	B	5002	GOL	C3-C2	-10.31	1.14	1.52
9	B	5004	GOL	C3-C2	-10.30	1.14	1.52
9	A	5007	GOL	C3-C2	-10.30	1.14	1.52
9	B	5008	GOL	C3-C2	-10.30	1.14	1.52
9	A	5001	GOL	C3-C2	-10.30	1.14	1.52
9	A	5005	GOL	C3-C2	-10.30	1.14	1.52
9	A	5003	GOL	C3-C2	-10.29	1.14	1.52
4	B	4003	MTE	P-O4'	-6.59	1.39	1.60
4	A	3003	MTE	P-O4'	-6.39	1.39	1.60
7	A	3006	FYX	NPL-NPN	-5.58	1.27	1.37
7	B	4006	FYX	NPL-NPN	-5.50	1.27	1.37
7	A	3006	FYX	CPD-CPB	-4.97	1.40	1.45
7	B	4006	FYX	CPD-CPB	-4.93	1.40	1.45
4	B	4003	MTE	P-O3P	-4.50	1.36	1.54
4	A	3003	MTE	P-O3P	-4.50	1.36	1.54
9	B	5004	GOL	C1-C2	-4.15	1.36	1.52
9	A	5005	GOL	C1-C2	-4.13	1.37	1.52
9	B	5002	GOL	C1-C2	-4.13	1.37	1.52
9	A	5007	GOL	C1-C2	-4.13	1.37	1.52
9	A	5003	GOL	C1-C2	-4.13	1.37	1.52
9	B	5006	GOL	C1-C2	-4.12	1.37	1.52
9	A	5001	GOL	C1-C2	-4.12	1.37	1.52
9	B	5008	GOL	C1-C2	-4.11	1.37	1.52
9	B	5002	GOL	O2-C2	-3.51	1.33	1.43
9	A	5005	GOL	O2-C2	-3.51	1.33	1.43
9	B	5006	GOL	O2-C2	-3.51	1.33	1.43
9	B	5008	GOL	O2-C2	-3.51	1.33	1.43
9	A	5007	GOL	O2-C2	-3.50	1.33	1.43
9	A	5001	GOL	O2-C2	-3.50	1.33	1.43
9	B	5004	GOL	O2-C2	-3.49	1.33	1.43
9	A	5003	GOL	O2-C2	-3.48	1.33	1.43
7	B	4006	FYX	CPP-CPM	-3.45	1.39	1.48
7	A	3006	FYX	CPP-CPM	-3.35	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	4006	FYX	CPH-CPK	-3.22	1.40	1.48
7	A	3006	FYX	CPH-CPK	-3.11	1.40	1.48
4	B	4003	MTE	O4'-C4'	-2.63	1.34	1.44
4	A	3003	MTE	O4'-C4'	-2.13	1.36	1.44
4	B	4003	MTE	P-O2P	-2.06	1.46	1.54
4	B	4003	MTE	C4'-C3'	-2.05	1.49	1.52
4	A	3003	MTE	P-O2P	-2.03	1.46	1.54
7	A	3006	FYX	CPM-NPJ	2.03	1.38	1.35
7	A	3006	FYX	CPG-CPH	2.03	1.43	1.39
7	A	3006	FYX	CPQ-CPP	2.04	1.43	1.39
7	B	4006	FYX	CPG-CPD	2.17	1.41	1.39
6	A	3005	FAD	C6-C7	2.18	1.43	1.37
6	B	4005	FAD	C1'-N10	2.20	1.50	1.48
6	B	4005	FAD	C2A-N3A	2.22	1.35	1.32
6	B	4005	FAD	C6-C7	2.24	1.43	1.37
6	A	3005	FAD	C2A-N3A	2.31	1.36	1.32
4	A	3003	MTE	C2-N1	2.32	1.39	1.35
6	A	3005	FAD	PA-O1A	2.35	1.59	1.50
6	B	4005	FAD	P-O1P	2.35	1.59	1.50
7	A	3006	FYX	CPG-CPD	2.38	1.41	1.39
6	B	4005	FAD	PA-O1A	2.39	1.59	1.50
6	A	3005	FAD	C1'-N10	2.39	1.50	1.48
4	B	4003	MTE	O4-C4	2.43	1.30	1.24
6	A	3005	FAD	P-O1P	2.50	1.60	1.50
4	B	4003	MTE	C2-N1	2.52	1.39	1.35
7	B	4006	FYX	CPK-NPJ	2.57	1.39	1.35
6	A	3005	FAD	C4A-N3A	2.59	1.39	1.35
4	A	3003	MTE	O4-C4	2.65	1.31	1.24
6	B	4005	FAD	C4A-N3A	2.88	1.39	1.35
7	B	4006	FYX	CPK-NPL	3.22	1.37	1.33
6	B	4005	FAD	O4B-C1B	3.24	1.45	1.41
4	A	3003	MTE	C4-N3	3.38	1.39	1.33
7	A	3006	FYX	CPM-NPN	3.39	1.38	1.33
7	B	4006	FYX	CPM-NPN	3.39	1.38	1.33
4	B	4003	MTE	C4-N3	3.40	1.39	1.33
7	A	3006	FYX	CPK-NPL	3.44	1.38	1.33
9	A	5005	GOL	O1-C1	3.47	1.57	1.42
9	B	5006	GOL	O1-C1	3.49	1.57	1.42
9	B	5002	GOL	O1-C1	3.49	1.57	1.42
9	B	5004	GOL	O1-C1	3.49	1.57	1.42
9	A	5003	GOL	O1-C1	3.49	1.57	1.42
9	A	5001	GOL	O1-C1	3.49	1.57	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	5008	GOL	O1-C1	3.49	1.57	1.42
9	A	5007	GOL	O1-C1	3.51	1.57	1.42
6	A	3005	FAD	C4X-N5	3.54	1.38	1.33
6	B	4005	FAD	C4X-N5	3.58	1.38	1.33
6	A	3005	FAD	O4B-C1B	3.77	1.46	1.41
7	A	3006	FYX	CPB-NPC	3.79	1.23	1.14
7	B	4006	FYX	CPB-NPC	3.90	1.23	1.14
4	B	4003	MTE	C6-N5	4.37	1.51	1.45
4	A	3003	MTE	C4-C9	4.93	1.47	1.41
4	B	4003	MTE	C4-C9	4.93	1.47	1.41
6	A	3005	FAD	C9A-N10	5.31	1.45	1.38
6	B	4005	FAD	C9A-N10	5.34	1.45	1.38
6	B	4005	FAD	C4-N3	5.55	1.43	1.33
6	A	3005	FAD	C4-N3	5.63	1.43	1.33
4	B	4003	MTE	C9-N5	5.70	1.50	1.37
6	B	4005	FAD	C10-N1	6.93	1.43	1.33
6	A	3005	FAD	C10-N1	7.34	1.43	1.33
4	A	3003	MTE	C9-N5	8.00	1.55	1.37
4	B	4003	MTE	C9-C10	10.57	1.61	1.41
4	A	3003	MTE	C9-C10	10.61	1.61	1.41
4	A	3003	MTE	C7-C6	20.68	1.68	1.53
4	B	4003	MTE	C7-C6	21.06	1.69	1.53

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3005	FAD	N3A-C2A-N1A	-12.15	118.28	128.86
6	B	4005	FAD	N3A-C2A-N1A	-11.89	118.50	128.86
6	A	3005	FAD	C1'-N10-C10	-5.72	112.64	118.50
7	A	3006	FYX	CPI-CPF-NPE	-5.16	117.97	123.92
7	B	4006	FYX	CPI-CPF-NPE	-5.11	118.03	123.92
6	B	4005	FAD	C1'-N10-C10	-4.91	113.47	118.50
6	B	4005	FAD	O5'-C5'-C4'	-3.97	98.78	109.36
7	B	4006	FYX	CPG-CPD-NPE	-3.87	119.55	123.59
7	A	3006	FYX	CPG-CPD-NPE	-3.86	119.56	123.59
4	A	3003	MTE	N3-C2-N1	-3.72	119.42	125.45
4	B	4003	MTE	N3-C2-N1	-3.68	119.48	125.45
4	A	3003	MTE	O3'-C7-C6	-3.51	106.62	108.96
7	A	3006	FYX	CPO-CPR-NPS	-3.24	117.97	123.63
7	B	4006	FYX	CPO-CPR-NPS	-3.21	118.03	123.63
7	A	3006	FYX	CPQ-CPT-NPS	-2.87	118.61	123.63
7	B	4006	FYX	CPQ-CPT-NPS	-2.81	118.73	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4003	MTE	O3'-C7-C6	-2.79	107.10	108.96
6	A	3005	FAD	O3B-C3B-C4B	-2.48	103.84	111.09
6	B	4005	FAD	O3B-C3B-C4B	-2.38	104.12	111.09
6	B	4005	FAD	C9A-C5X-N5	-2.34	118.75	122.24
6	B	4005	FAD	C4X-C4-N3	-2.33	120.17	123.48
6	A	3005	FAD	C4X-C4-N3	-2.30	120.21	123.48
6	A	3005	FAD	C9A-C5X-N5	-2.25	118.89	122.24
6	A	3005	FAD	C8M-C8-C7	2.01	124.94	120.72
6	A	3005	FAD	O5'-P-O1P	2.03	117.45	109.25
7	B	4006	FYX	CPP-CPM-NPN	2.21	127.11	124.20
6	A	3005	FAD	C2A-N1A-C6A	2.26	122.73	118.77
6	A	3005	FAD	O5B-PA-O1A	2.30	118.51	109.25
6	A	3005	FAD	O2'-C2'-C1'	2.30	115.10	109.79
6	B	4005	FAD	C2A-N1A-C6A	2.32	122.82	118.77
9	A	5003	GOL	O1-C1-C2	2.48	122.58	110.07
7	A	3006	FYX	CPP-CPM-NPN	2.48	127.47	124.20
9	A	5001	GOL	O1-C1-C2	2.49	122.60	110.07
9	B	5008	GOL	O1-C1-C2	2.49	122.64	110.07
9	B	5002	GOL	O1-C1-C2	2.50	122.65	110.07
9	A	5007	GOL	O1-C1-C2	2.50	122.66	110.07
9	A	5005	GOL	O1-C1-C2	2.50	122.67	110.07
9	B	5006	GOL	O1-C1-C2	2.50	122.68	110.07
9	B	5004	GOL	O1-C1-C2	2.51	122.70	110.07
7	B	4006	FYX	CPH-CPK-NPL	2.64	127.68	124.20
6	B	4005	FAD	O2'-C2'-C1'	2.65	115.93	109.79
6	A	3005	FAD	O2B-C2B-C3B	2.66	120.36	111.83
6	B	4005	FAD	O3'-C3'-C4'	2.92	116.05	108.82
7	A	3006	FYX	CPH-CPK-NPL	2.99	128.13	124.20
7	A	3006	FYX	CPH-CPK-NPJ	3.02	127.40	123.75
6	A	3005	FAD	C4-C4X-N5	3.05	122.02	118.68
6	B	4005	FAD	C4-C4X-N5	3.05	122.02	118.68
7	A	3006	FYX	CPB-CPD-NPE	3.08	118.90	115.86
7	B	4006	FYX	CPB-CPD-NPE	3.09	118.91	115.86
7	B	4006	FYX	CPH-CPK-NPJ	3.35	127.80	123.75
7	A	3006	FYX	CPP-CPM-NPJ	3.50	127.98	123.75
6	A	3005	FAD	O2'-C2'-C3'	3.58	117.97	109.09
7	B	4006	FYX	CPP-CPM-NPJ	3.70	128.22	123.75
6	A	3005	FAD	O3'-C3'-C4'	3.77	118.16	108.82
7	B	4006	FYX	CPT-NPS-CPR	3.91	126.24	116.83
7	A	3006	FYX	CPT-NPS-CPR	3.94	126.32	116.83
6	B	4005	FAD	O2'-C2'-C3'	4.25	119.65	109.09
4	B	4003	MTE	N2-C2-N3	4.27	124.07	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3005	FAD	O4'-C4'-C3'	4.32	119.80	109.09
4	A	3003	MTE	N2-C2-N3	4.33	124.16	117.24
4	A	3003	MTE	P-O4'-C4'	4.36	130.31	118.30
6	B	4005	FAD	O2B-C2B-C3B	4.53	126.35	111.83
9	A	5003	GOL	O2-C2-C3	4.70	131.06	108.84
9	A	5001	GOL	O2-C2-C3	4.71	131.09	108.84
9	B	5004	GOL	O2-C2-C3	4.71	131.10	108.84
9	A	5005	GOL	O2-C2-C3	4.71	131.10	108.84
9	B	5002	GOL	O2-C2-C3	4.71	131.10	108.84
9	B	5008	GOL	O2-C2-C3	4.72	131.11	108.84
9	A	5007	GOL	O2-C2-C3	4.72	131.14	108.84
9	B	5006	GOL	O2-C2-C3	4.73	131.16	108.84
4	A	3003	MTE	N8-C10-N1	4.92	126.43	116.90
4	B	4003	MTE	C4-N3-C2	4.96	123.19	116.06
4	A	3003	MTE	C4-N3-C2	4.99	123.24	116.06
6	B	4005	FAD	O4'-C4'-C3'	5.11	121.77	109.09
4	B	4003	MTE	P-O4'-C4'	5.11	132.38	118.30
4	B	4003	MTE	N8-C10-N1	5.15	126.88	116.90
4	B	4003	MTE	C2-N1-C10	5.64	127.22	114.51
4	A	3003	MTE	C2-N1-C10	5.65	127.24	114.51
6	A	3005	FAD	C4X-N5-C5X	6.55	123.68	116.76
6	A	3005	FAD	C4-N3-C2	6.56	120.89	115.16
6	B	4005	FAD	C4-N3-C2	6.57	120.90	115.16
6	B	4005	FAD	C4X-N5-C5X	6.73	123.87	116.76
7	A	3006	FYX	CPM-NPN-NPL	6.83	110.70	104.71
7	B	4006	FYX	CPM-NPN-NPL	7.07	110.91	104.71
7	B	4006	FYX	CPK-NPL-NPN	7.08	110.92	104.71
7	A	3006	FYX	CPK-NPL-NPN	7.16	110.99	104.71
7	B	4006	FYX	CPF-NPE-CPD	7.72	124.93	116.18
7	A	3006	FYX	CPF-NPE-CPD	7.74	124.94	116.18
6	A	3005	FAD	C1'-N10-C9A	8.22	125.88	118.35
6	B	4005	FAD	C1'-N10-C9A	8.90	126.50	118.35
9	A	5005	GOL	O3-C3-C2	12.39	172.49	110.07
9	B	5004	GOL	O3-C3-C2	12.39	172.50	110.07
9	B	5006	GOL	O3-C3-C2	12.40	172.54	110.07
9	B	5002	GOL	O3-C3-C2	12.40	172.54	110.07
9	A	5007	GOL	O3-C3-C2	12.40	172.54	110.07
9	A	5001	GOL	O3-C3-C2	12.40	172.55	110.07
9	A	5003	GOL	O3-C3-C2	12.40	172.56	110.07
9	B	5008	GOL	O3-C3-C2	12.41	172.58	110.07
7	B	4006	FYX	CPK-NPJ-CPM	13.84	108.98	101.07
7	A	3006	FYX	CPK-NPJ-CPM	14.38	109.29	101.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3003	MTE	1	0
5	A	3004	MOS	2	0
6	A	3005	FAD	3	0
8	A	3007	ACY	3	0
9	A	5001	GOL	1	0
9	A	5007	GOL	2	0
4	B	4003	MTE	1	0
5	B	4004	MOS	2	0
6	B	4005	FAD	3	0
8	B	4007	ACY	4	0
9	B	5004	GOL	1	0
9	B	5008	GOL	2	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

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	1298/1332 (97%)	0.17	75 (5%) 24 31	9, 18, 39, 61	0
1	B	1296/1332 (97%)	0.17	66 (5%) 29 37	9, 19, 38, 61	0
All	All	2594/2664 (97%)	0.17	141 (5%) 26 34	9, 18, 39, 61	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1325	CYS	14.1
1	B	1321	ALA	13.9
1	B	3	ALA	13.0
1	B	1322	PRO	12.6
1	A	538	LEU	12.4
1	A	1321	ALA	11.8
1	A	1319	THR	11.3
1	B	1323	GLY	11.2
1	A	1325	CYS	11.0
1	A	1323	GLY	10.8
1	A	1320	GLY	10.5
1	B	1320	GLY	10.3
1	A	1322	PRO	9.7
1	A	1324	ASN	9.6
1	A	1318	VAL	9.3
1	B	1324	ASN	8.8
1	B	1319	THR	8.6
1	B	1287	ASN	8.0
1	B	1288	ASN	7.9
1	A	61	LEU	7.4
1	A	530	ASP	7.3
1	A	549	PHE	7.1
1	A	431	ILE	7.1
1	A	1332	VAL	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	1288	ASN	6.8
1	A	537	LYS	6.7
1	A	1287	ASN	6.6
1	B	540	PRO	6.5
1	B	1318	VAL	6.4
1	A	540	PRO	5.9
1	B	551	LYS	5.9
1	A	565	ASN	5.8
1	B	550	GLN	5.7
1	B	1326	LYS	5.7
1	A	550	GLN	5.5
1	B	538	LEU	5.5
1	B	4	ASP	5.4
1	A	539	ASP	5.4
1	A	553	PRO	5.2
1	B	552	HIS	5.2
1	B	537	LYS	5.0
1	B	431	ILE	5.0
1	A	552	HIS	5.0
1	B	60	ARG	4.8
1	A	551	LYS	4.7
1	A	1317	CYS	4.7
1	B	565	ASN	4.6
1	A	1286	THR	4.5
1	B	543	THR	4.4
1	B	553	PRO	4.3
1	B	547	LEU	4.3
1	B	61	LEU	4.2
1	B	1289	ASN	4.2
1	A	60	ARG	4.1
1	A	548	LEU	3.8
1	A	1290	THR	3.8
1	B	192	SER	3.8
1	B	528	GLY	3.8
1	B	1317	CYS	3.8
1	B	336	TRP	3.7
1	A	223	PRO	3.6
1	A	1326	LYS	3.6
1	A	192	SER	3.5
1	A	432	ALA	3.5
1	A	543	THR	3.5
1	B	165	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	539	ASP	3.5
1	B	541	THR	3.5
1	B	19	ASN	3.4
1	A	3	ALA	3.4
1	A	529	LYS	3.4
1	A	555	ALA	3.4
1	B	548	LEU	3.4
1	B	1330	LEU	3.4
1	A	1316	LEU	3.3
1	B	989	LYS	3.2
1	B	1286	THR	3.2
1	A	63	ASP	3.1
1	B	1316	LEU	3.1
1	A	1330	LEU	3.0
1	B	221	ASP	3.0
1	B	63	ASP	3.0
1	A	221	ASP	3.0
1	A	165	LYS	2.9
1	B	20	ALA	2.9
1	A	721	LYS	2.8
1	B	5	GLU	2.8
1	B	554	PRO	2.7
1	A	336	TRP	2.7
1	A	1289	ASN	2.7
1	A	989	LYS	2.7
1	B	720	LYS	2.7
1	A	554	PRO	2.7
1	A	424	ALA	2.7
1	A	425	SER	2.7
1	B	425	SER	2.7
1	B	1290	THR	2.7
1	B	566	GLY	2.6
1	A	433	LYS	2.6
1	B	499	ASP	2.6
1	B	1328	TRP	2.6
1	B	1329	SER	2.5
1	A	272	ASN	2.5
1	B	546	THR	2.5
1	A	1328	TRP	2.5
1	A	1143	GLU	2.5
1	A	423	GLN	2.4
1	B	1327	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	379	THR	2.4
1	A	724	SER	2.4
1	A	222	VAL	2.4
1	A	430	ASP	2.3
1	A	64	LYS	2.3
1	A	547	LEU	2.3
1	B	430	ASP	2.3
1	B	549	PHE	2.3
1	A	705	ASN	2.3
1	A	1111	GLY	2.3
1	A	566	GLY	2.2
1	A	4	ASP	2.2
1	B	569	LYS	2.2
1	B	703	LYS	2.2
1	A	541	THR	2.2
1	B	218	ARG	2.2
1	B	497	SER	2.2
1	B	211	ILE	2.2
1	A	528	GLY	2.1
1	A	337	PHE	2.1
1	A	412	SER	2.1
1	B	544	SER	2.1
1	B	721	LYS	2.1
1	A	120	ILE	2.1
1	A	338	ALA	2.1
1	B	222	VAL	2.1
1	A	1001	ILE	2.1
1	A	1327	PRO	2.1
1	B	1106	LYS	2.1
1	A	920	LEU	2.0
1	A	725	GLU	2.0
1	A	211	ILE	2.0
1	A	1331	ARG	2.0

## 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<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(Å <sup>2</sup> )	Q<0.9
9	GOL	B	5004	6/6	0.66	0.29	10.93	34,38,41,42	0
9	GOL	A	5003	6/6	0.76	0.23	5.65	29,34,35,37	0
9	GOL	A	5001	6/6	0.85	0.26	3.86	23,29,30,36	0
9	GOL	B	5002	6/6	0.90	0.23	3.47	24,29,31,31	0
9	GOL	A	5005	6/6	0.89	0.19	2.52	29,34,38,41	0
9	GOL	B	5006	6/6	0.85	0.19	1.71	31,35,37,40	0
7	FYX	B	4006	19/19	0.93	0.12	1.36	14,18,24,27	0
8	ACY	A	3007	4/4	0.97	0.13	1.33	4,9,13,13	0
7	FYX	A	3006	19/19	0.94	0.10	0.46	15,18,27,27	0
8	ACY	B	4007	4/4	0.97	0.11	0.23	7,13,13,16	0
4	MTE	B	4003	24/24	0.98	0.08	-0.17	9,11,15,16	0
4	MTE	A	3003	24/24	0.97	0.08	-0.25	8,12,15,17	0
6	FAD	A	3005	53/53	0.97	0.09	-0.61	12,16,20,24	0
6	FAD	B	4005	53/53	0.97	0.09	-0.73	12,17,21,23	0
3	FES	A	3001	4/4	0.99	0.06	-1.28	11,11,11,11	0
3	FES	B	4002	4/4	0.99	0.07	-1.29	11,12,12,12	0
3	FES	B	4001	4/4	0.99	0.07	-1.84	11,11,12,12	0
3	FES	A	3002	4/4	0.99	0.06	-1.95	11,11,12,12	0
2	CA	B	4008	1/1	1.00	0.05	-2.54	16,16,16,16	0
5	MOS	A	3004	4/4	1.00	0.05	-3.20	12,14,15,16	0
5	MOS	B	4004	4/4	1.00	0.05	-3.47	10,13,14,15	0
2	CA	A	3008	1/1	1.00	0.05	-4.02	12,12,12,12	0
9	GOL	B	5008	6/6	0.72	0.29	-	42,43,45,46	0
9	GOL	A	5007	6/6	0.73	0.27	-	40,42,43,45	0

## 6.5 Other polymers

There are no such residues in this entry.