



wwPDB X-ray Structure Validation Summary Report (i)

Sep 5, 2014 – 04:02 AM EDT

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)

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

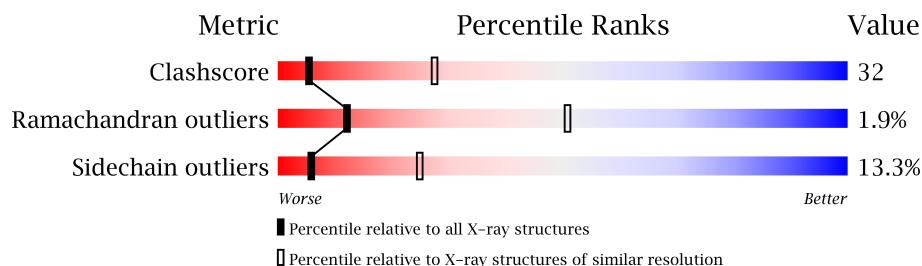
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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	
2	H	777	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36748 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

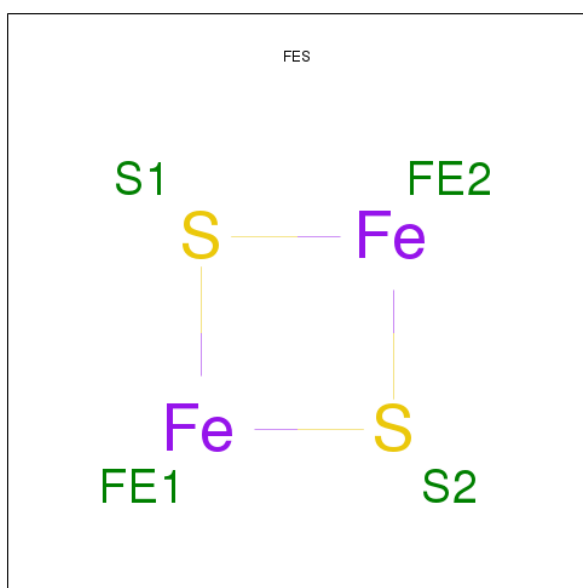
There are 4 discrepancies between the modelled and reference sequences:

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).

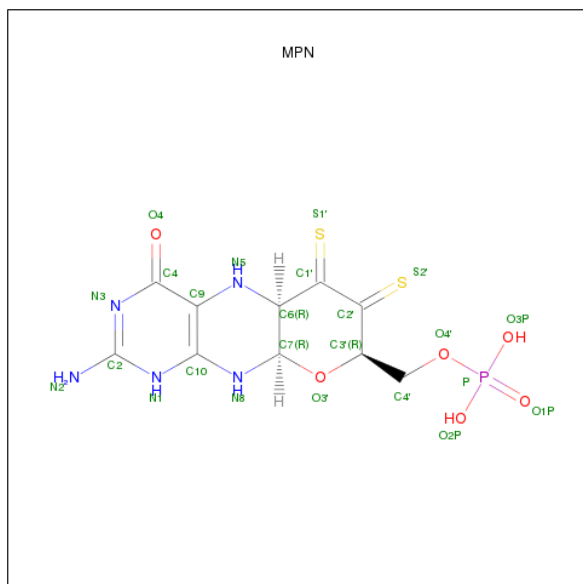
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



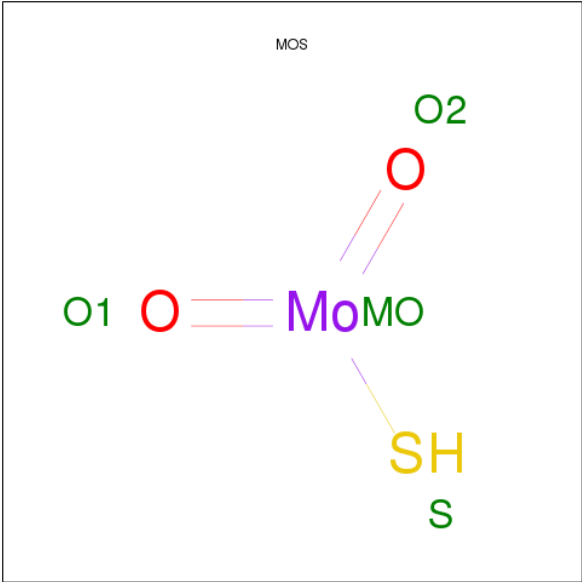
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0
4	C	1	Total Fe S 4 2 2	0	0
4	C	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	G	1	Total Fe S 4 2 2	0	0
4	G	1	Total Fe S 4 2 2	0	0

- Molecule 5 is PHOSPHORIC ACID MONO-(2-AMINO-4-OXO-5,6-DITHIOXO-1,5,6,7,8A, 9,10,10A-OCTAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL)ESTER (three-letter code: MPN) (formula: $C_{10}H_{12}N_5O_6PS_2$).



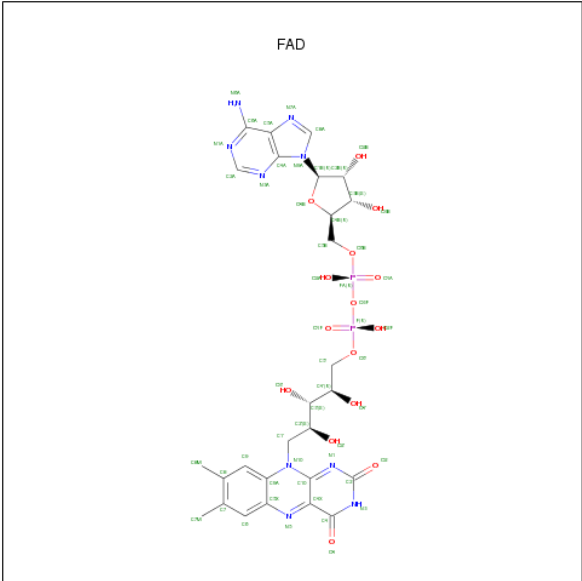
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	F	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
5	H	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

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



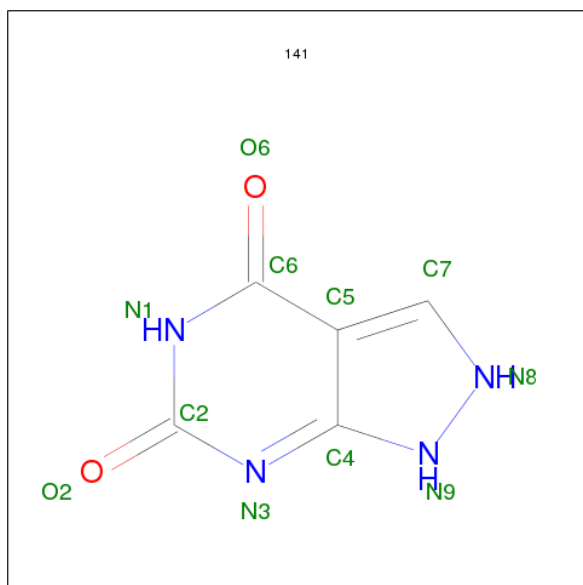
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	Mo	O	S	0	0
			3	1	1	1		
6	D	1	Total	Mo	O	S	0	0
			3	1	1	1		
6	F	1	Total	Mo	O	S	0	0
			3	1	1	1		
6	H	1	Total	Mo	O	S	0	0
			3	1	1	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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: $C_5H_4N_4O_2$).



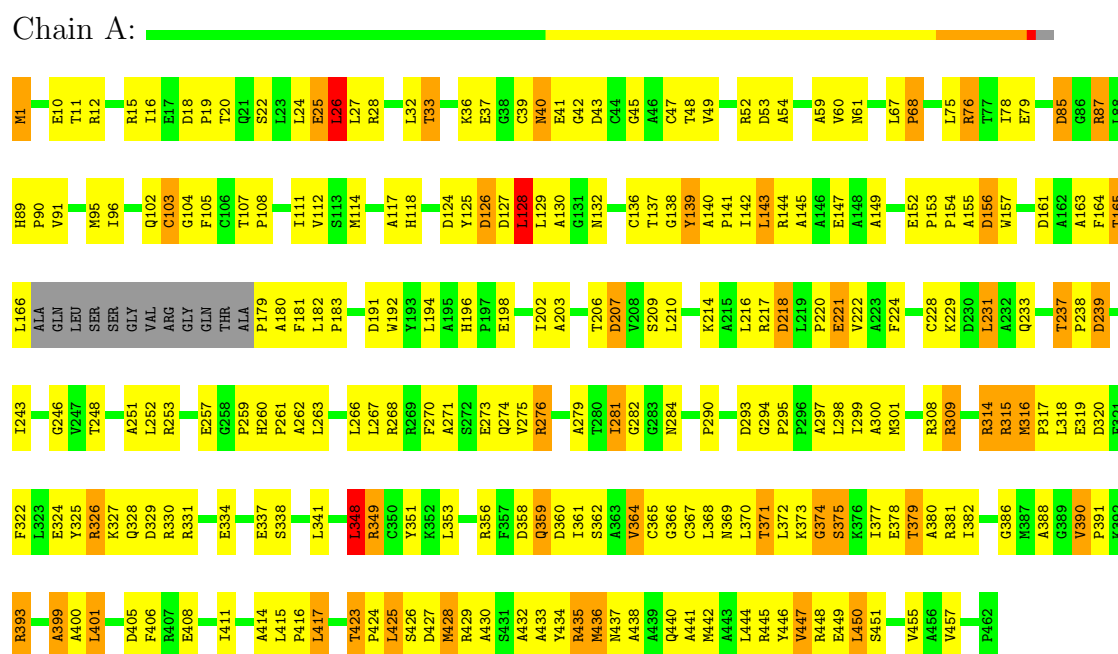
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			11	5	4	2		
8	D	1	Total	C	N	O	0	0
			11	5	4	2		
8	F	1	Total	C	N	O	0	0
			11	5	4	2		
8	H	1	Total	C	N	O	0	0
			11	5	4	2		

3 Residue-property plots

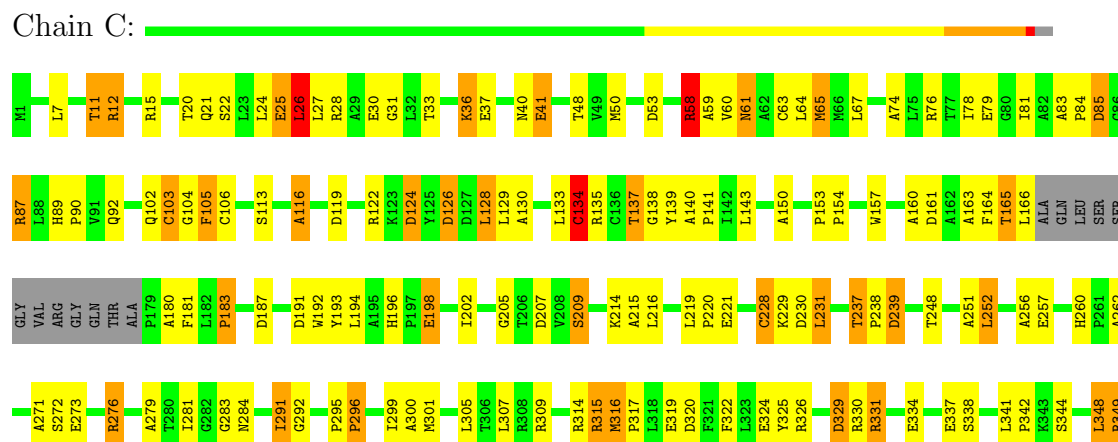
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

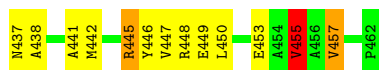
Note EDS was not executed.

- Molecule 1: xanthine dehydrogenase, chain A



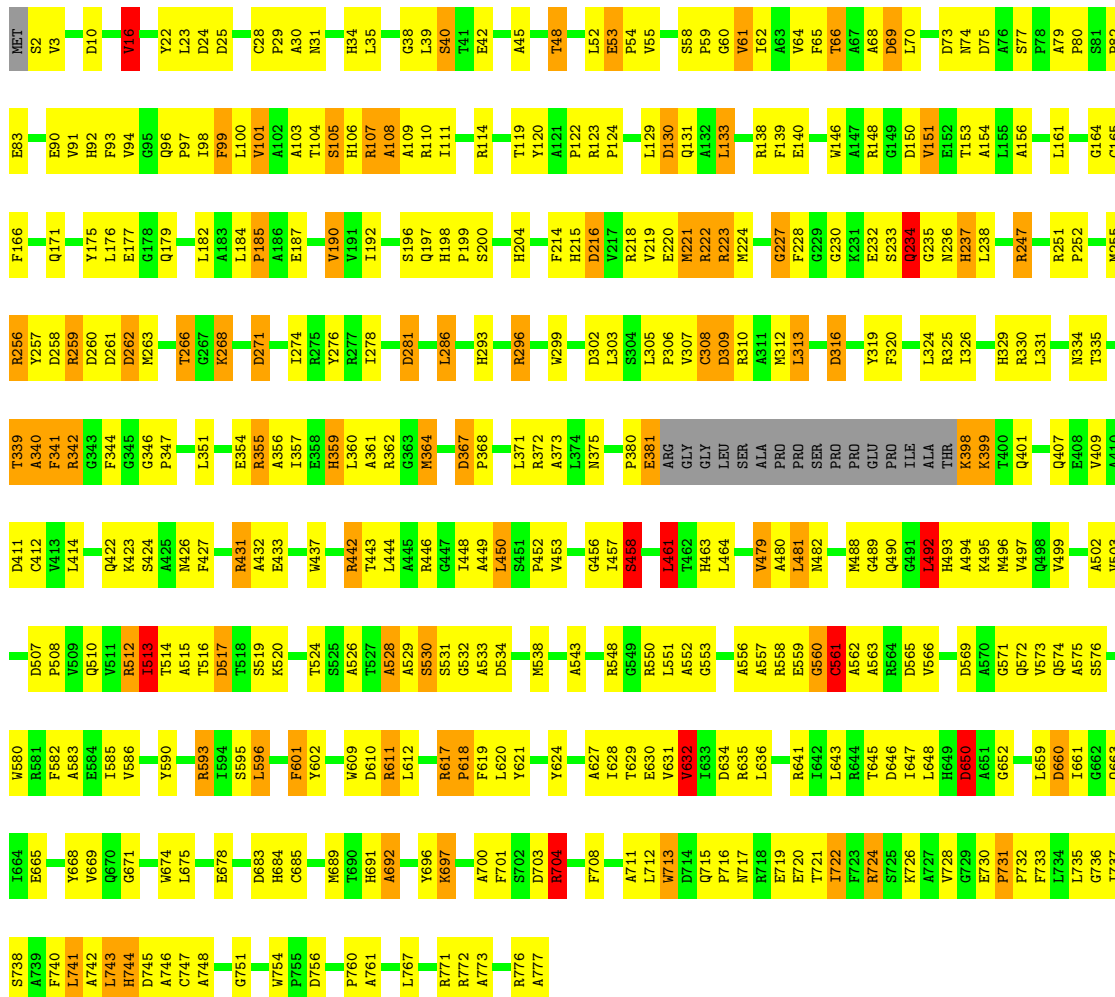
- Molecule 1: xanthine dehydrogenase, chain A





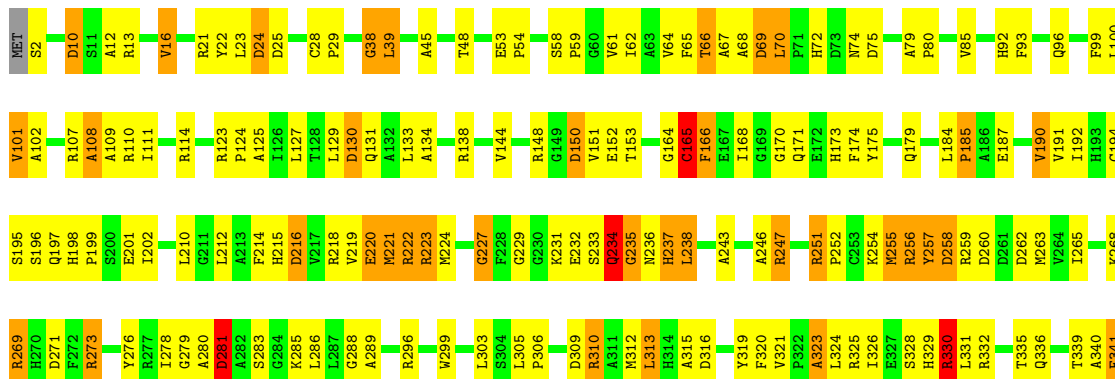
• Molecule 2: xanthine dehydrogenase, chain B

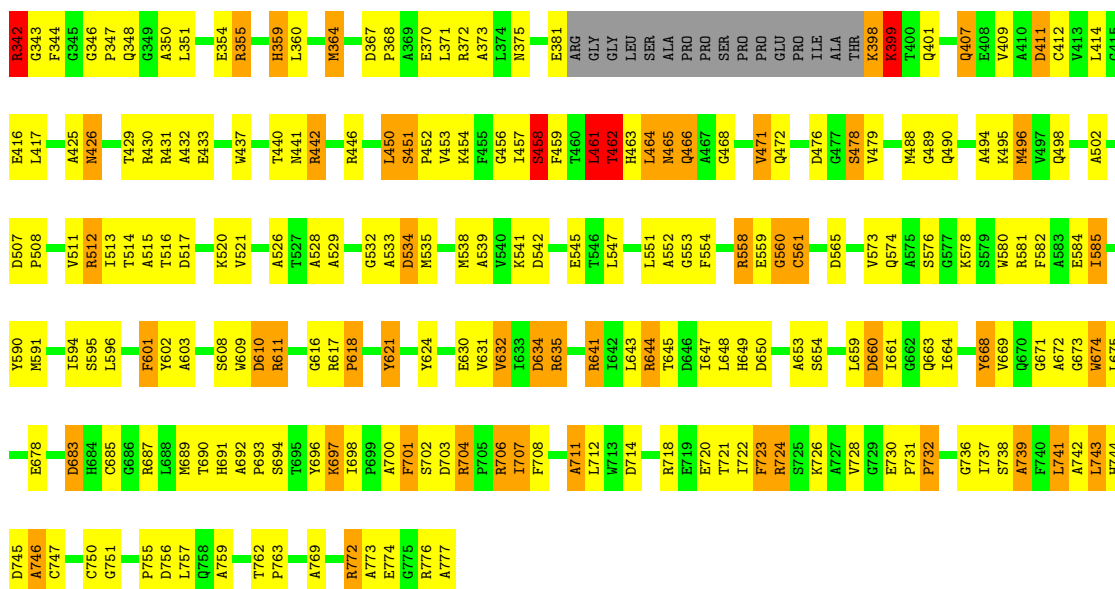
Chain B:



• Molecule 2: xanthine dehydrogenase, chain B

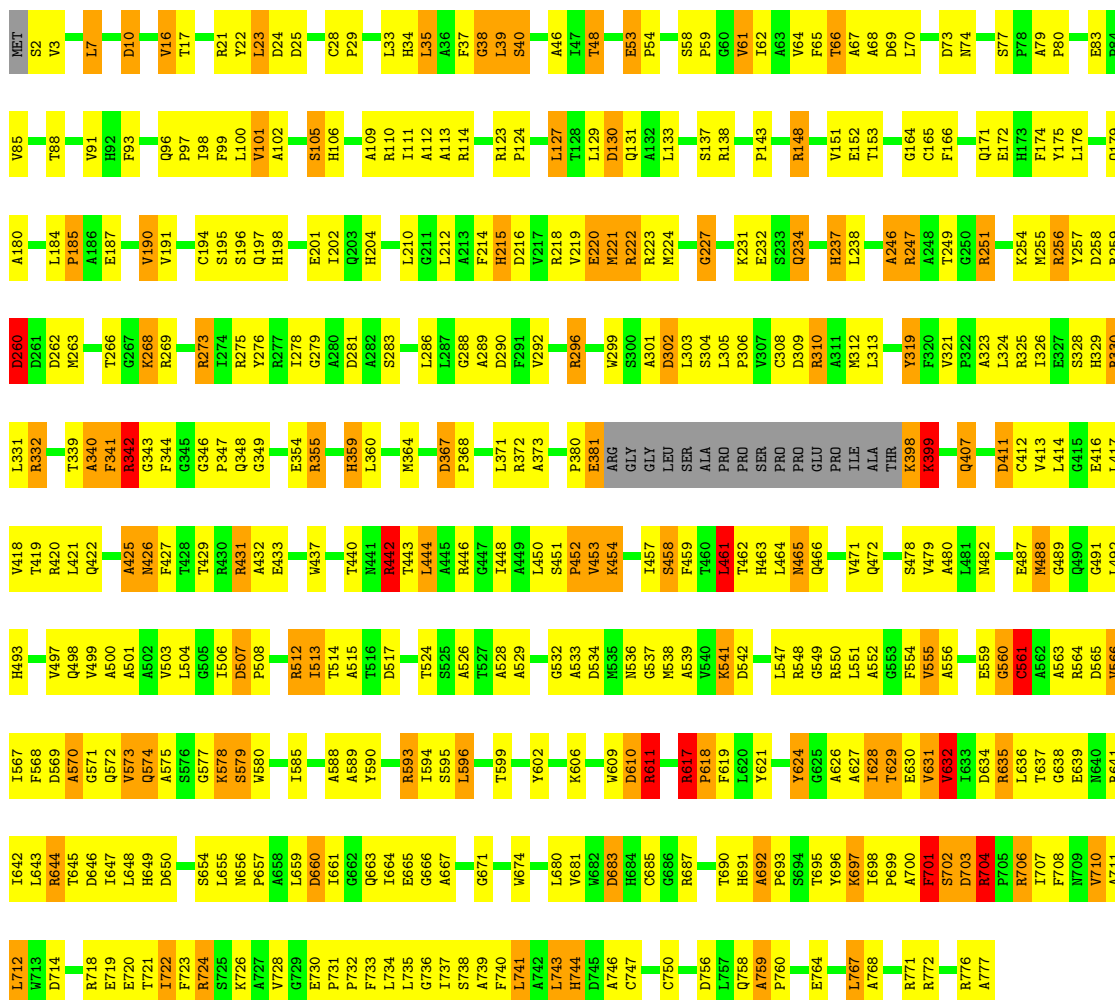
Chain D:





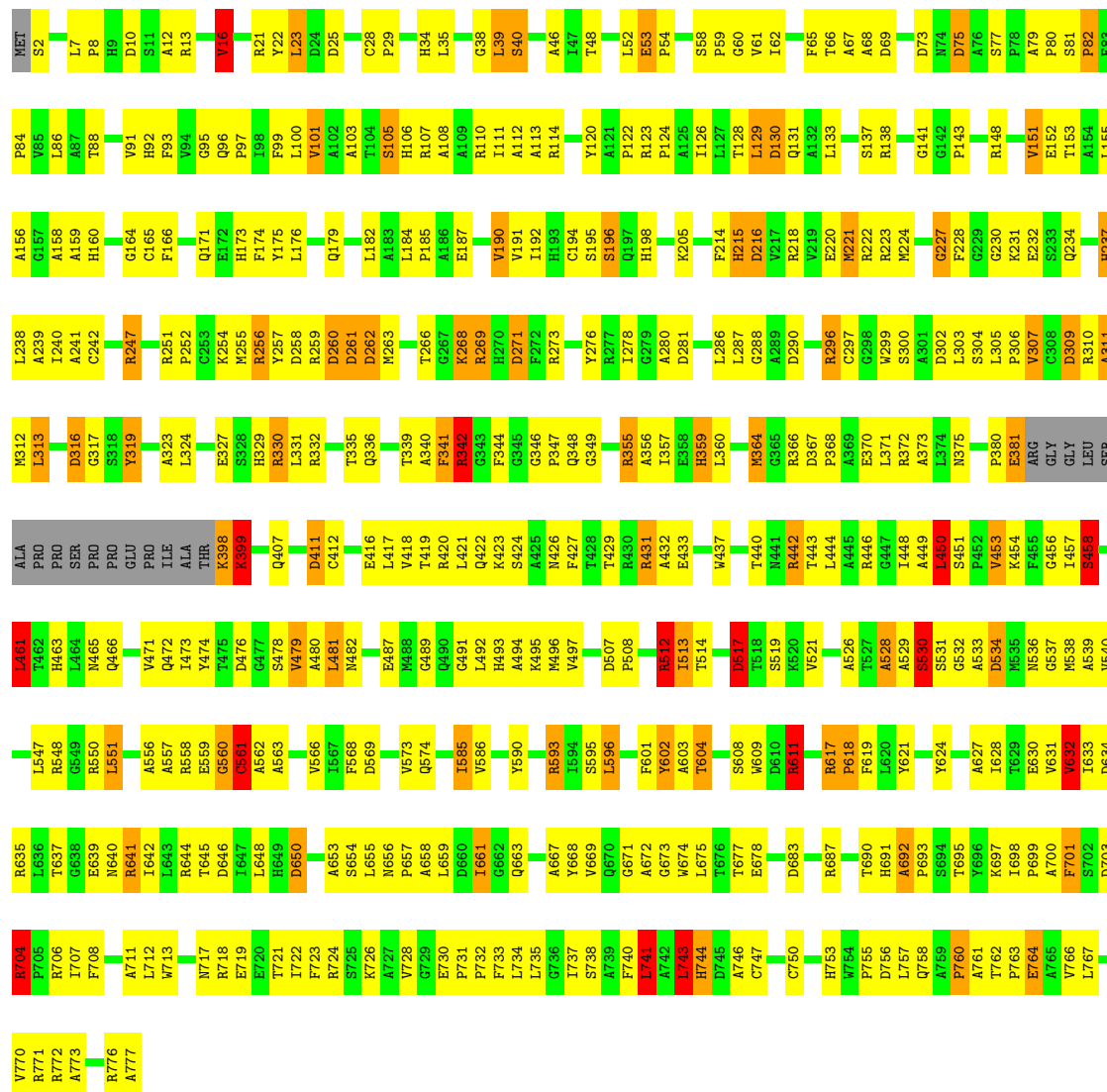
• Molecule 2: xanthine dehydrogenase, chain B

Chain F:



• Molecule 2: xanthine dehydrogenase, chain B

Chain H:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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, MPN, FES, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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	327	0
2	D	5717	0	5631	309	0
2	F	5717	0	5631	369	0
2	H	5717	0	5630	410	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	5	0
5	D	24	0	10	4	0
5	F	24	0	10	7	0
5	H	24	0	10	8	0
6	B	3	0	0	4	0
6	D	3	0	0	7	0
6	F	3	0	0	7	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	2	9	0
8	D	11	0	2	5	0
8	F	11	0	2	5	0
8	H	11	0	2	4	0
All	All	36748	0	36168	2354	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 32.

The worst 5 of 2354 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	13	53
1	C	446/462 (96%)	408 (92%)	31 (7%)	7 (2%)	14	56
1	E	446/462 (96%)	370 (83%)	63 (14%)	13 (3%)	7	35
1	G	446/462 (96%)	375 (84%)	58 (13%)	13 (3%)	7	35
2	B	756/777 (97%)	696 (92%)	47 (6%)	13 (2%)	14	54
2	D	756/777 (97%)	697 (92%)	46 (6%)	13 (2%)	14	54
2	F	756/777 (97%)	688 (91%)	57 (8%)	11 (2%)	15	58
2	H	756/777 (97%)	678 (90%)	67 (9%)	11 (2%)	15	58
All	All	4808/4956 (97%)	4297 (89%)	422 (9%)	89 (2%)	12	51

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 ⓘ

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%)	6	25
1	C	339/347 (98%)	295 (87%)	44 (13%)	6	26
1	E	339/347 (98%)	289 (85%)	50 (15%)	4	21
1	G	339/347 (98%)	291 (86%)	48 (14%)	5	22
2	B	571/584 (98%)	499 (87%)	72 (13%)	7	27
2	D	571/584 (98%)	493 (86%)	78 (14%)	5	24
2	F	571/584 (98%)	495 (87%)	76 (13%)	6	25
2	H	571/584 (98%)	500 (88%)	71 (12%)	7	28
All	All	3640/3724 (98%)	3156 (87%)	484 (13%)	6	25

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 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	744	HIS
1	E	196	HIS
2	H	426	ASN

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Mol	Chain	Res	Type
1	E	40	ASN
1	E	93	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 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	-	58,58,58	1.57	8 (13%)	85,89,89	2.89	30 (35%)
5	MPN	B	3003	6	26,26,26	5.84	14 (53%)	35,40,40	4.24	17 (48%)
6	MOS	B	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	B	4000	6	12,12,12	2.94	6 (50%)	8,17,17	8.30	3 (37%)
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	-	58,58,58	1.63	10 (17%)	85,89,89	2.92	38 (44%)
5	MPN	D	3003	6	26,26,26	6.47	14 (53%)	35,40,40	5.40	19 (54%)
6	MOS	D	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	141	D	4000	6	12,12,12	3.52	4 (33%)	8,17,17	7.89	3 (37%)
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	-	58,58,58	1.48	10 (17%)	85,89,89	2.82	36 (42%)
5	MPN	F	3003	6	26,26,26	6.18	16 (61%)	35,40,40	4.75	21 (60%)
6	MOS	F	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	F	4000	6	12,12,12	4.37	6 (50%)	8,17,17	7.55	3 (37%)
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	-	58,58,58	1.51	10 (17%)	85,89,89	2.59	31 (36%)
5	MPN	H	3003	6	26,26,26	6.96	14 (53%)	35,40,40	4.61	17 (48%)
6	MOS	H	3004	8,5	0,2,3	0.00	-	0,1,3	0.00	-
8	141	H	4000	6	12,12,12	2.78	4 (33%)	8,17,17	5.99	5 (62%)

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	-	-	0/34/50/50	0/6/6/6
5	MPN	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	-	-	0/34/50/50	0/6/6/6
5	MPN	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	-	-	0/34/50/50	0/6/6/6
5	MPN	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
4	FES	G	3002	1	-	0/0/4/4	0/1/1/1
7	FAD	G	3005	-	-	0/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPN	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 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	3003	MPN	C9-C10	25.13	1.61	1.40
5	D	3003	MPN	C9-C10	24.71	1.61	1.40
5	F	3003	MPN	C9-C10	20.92	1.58	1.40
5	B	3003	MPN	C9-C10	20.12	1.57	1.40
5	H	3003	MPN	C7-C6	15.69	1.66	1.53

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	3003	MPN	O3'-C7-C6	-25.17	89.21	108.99
8	B	4000	141	C7-N8-N9	-22.86	102.73	109.22
8	D	4000	141	C7-N8-N9	-22.10	102.95	109.22
5	F	3003	MPN	O3'-C7-C6	-21.10	92.41	108.99
8	F	4000	141	C7-N8-N9	-20.69	103.35	109.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.