



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2016 – 03:58 PM EDT

PDB ID : 4MLA
Title : Structure of maize cytokinin oxidase/dehydrogenase 2 (ZmCKO2)
Authors : Morera, S.; Kopečný, D.; Briozzo, P.; Koncitikova, R.
Deposited on : 2013-09-06
Resolution : 2.04 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

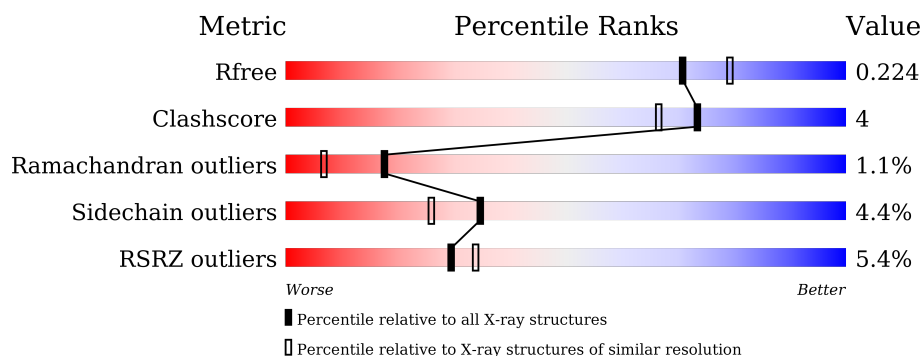
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	501	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• 5%</div> </div> </div>
1	B	501	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>• 8%</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
3	IPA	A	602	-	-	-	X
3	IPA	A	603	-	-	-	X
3	IPA	A	604	-	-	-	X
3	IPA	A	610	-	-	-	X
3	IPA	A	611	-	-	-	X
3	IPA	A	612	-	-	-	X
3	IPA	A	615	-	-	-	X
3	IPA	A	616	-	-	-	X
3	IPA	A	620	-	-	-	X
3	IPA	A	621	-	-	-	X
3	IPA	A	622	-	-	-	X
3	IPA	B	601	-	-	-	X
3	IPA	B	604	-	-	-	X
3	IPA	B	609	-	-	-	X
3	IPA	B	611	-	-	-	X
3	IPA	B	612	-	-	-	X
3	IPA	B	616	-	-	-	X
4	EDO	A	605	-	-	-	X
4	EDO	A	607	-	-	-	X
4	EDO	A	608	-	-	-	X
4	EDO	A	623	-	-	-	X
4	EDO	A	624	-	-	-	X
4	EDO	B	605	-	-	-	X
5	GOL	A	609	-	-	-	X
5	GOL	B	603	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8004 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.

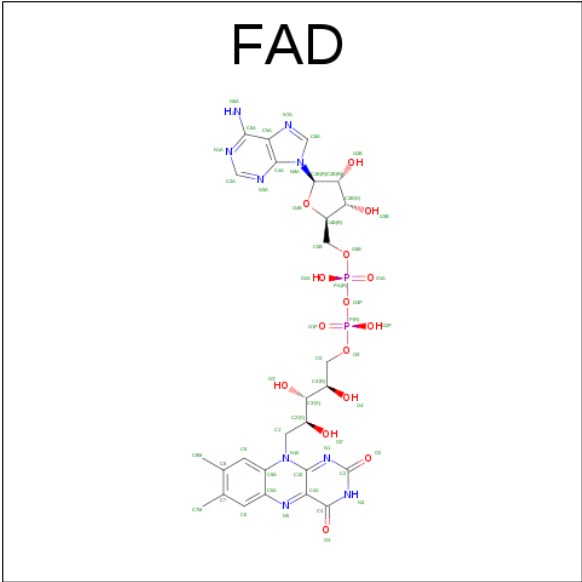
- Molecule 1 is a protein called Cytokinin oxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3760	2392	662	692	14			
1	B	460	Total	C	N	O	S	0	0	0
			3619	2303	634	668	14			

There are 8 discrepancies between the modelled and reference sequences:

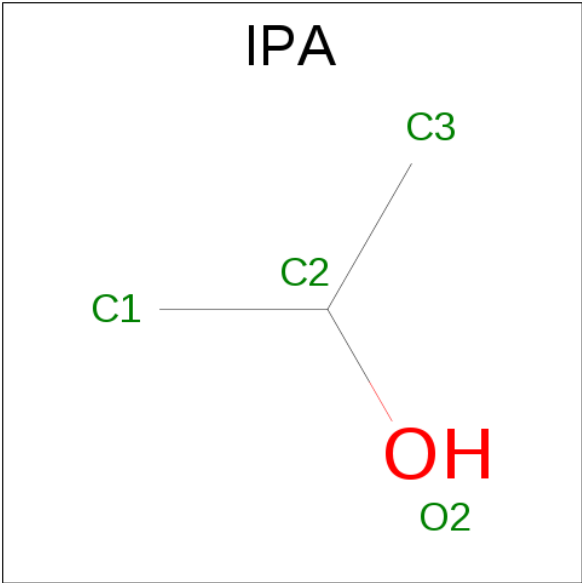
Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	EXPRESSION TAG	UNP Q709Q5
A	17	GLY	-	EXPRESSION TAG	UNP Q709Q5
A	18	HIS	-	EXPRESSION TAG	UNP Q709Q5
A	19	MET	-	EXPRESSION TAG	UNP Q709Q5
B	16	ALA	-	EXPRESSION TAG	UNP Q709Q5
B	17	GLY	-	EXPRESSION TAG	UNP Q709Q5
B	18	HIS	-	EXPRESSION TAG	UNP Q709Q5
B	19	MET	-	EXPRESSION TAG	UNP Q709Q5

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



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

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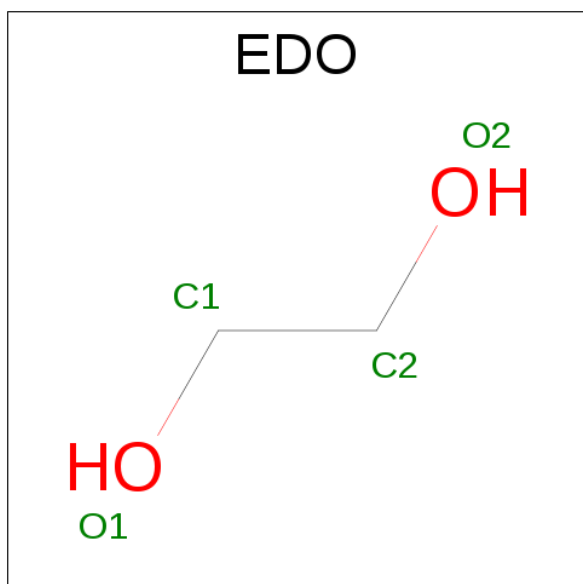
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



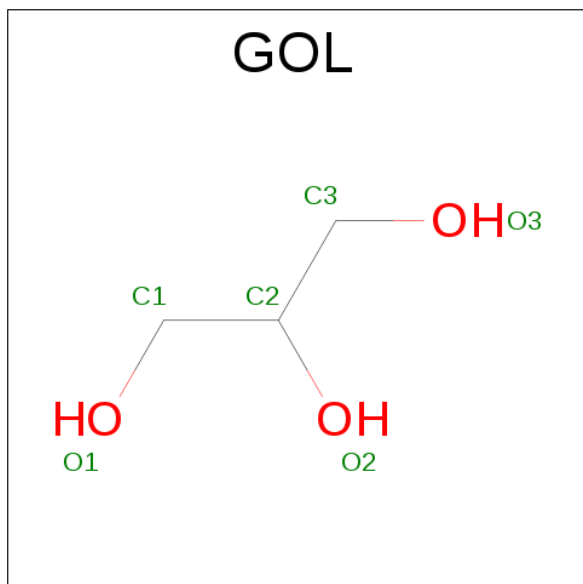
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

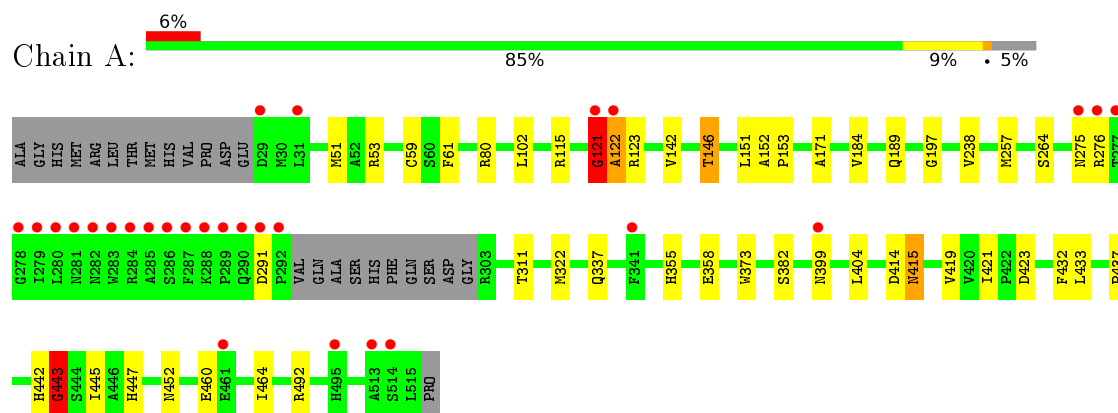
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	178	Total	O	0	0
			178	178		

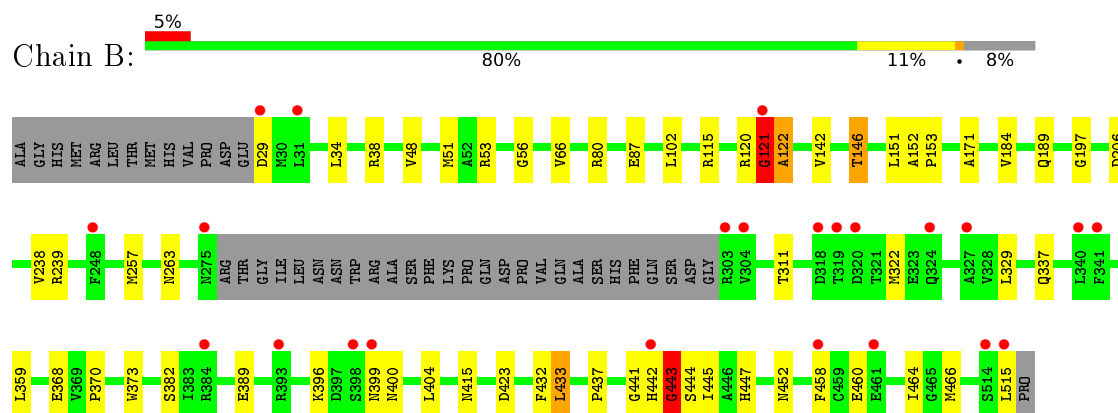
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: Cytokinin oxidase 2



• Molecule 1: Cytokinin oxidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.72Å 181.89Å 196.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.56 – 2.04 47.86 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.0 (23.56-2.04) 99.2 (47.86-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.193 , 0.222 0.198 , 0.224	Depositor DCC
R_{free} test set	4289 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	6 of 85770 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8004	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.78 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.1077e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, IPA, EDO, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/3853	0.68	2/5229 (0.0%)
1	B	0.49	0/3707	0.70	4/5030 (0.1%)
All	All	0.50	0/7560	0.69	6/10259 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	GLY	C-N-CA	6.11	136.98	121.70
1	B	121	GLY	C-N-CA	5.82	136.25	121.70
1	B	443	GLY	C-N-CA	5.80	136.21	121.70
1	A	121	GLY	C-N-CA	5.26	134.86	121.70
1	B	87	GLU	N-CA-C	5.15	124.92	111.00
1	B	87	GLU	C-N-CA	5.07	132.95	122.30

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	3760	0	3687	30	0
1	B	3619	0	3549	31	0
2	A	53	0	29	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	29	1	0
3	A	68	0	134	4	0
3	B	48	0	95	9	0
4	A	20	0	30	3	0
4	B	4	0	6	0	0
5	A	6	0	8	2	0
5	B	12	0	16	0	0
6	A	183	0	0	1	0
6	B	178	0	0	1	0
All	All	8004	0	7583	63	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 4.

All (63) 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:121:GLY:HA3	1:A:122:ALA:CB	2.00	0.91
1:B:121:GLY:HA3	1:B:122:ALA:CB	2.08	0.84
1:A:432:PHE:HB3	5:A:609:GOL:H11	1.61	0.82
1:A:121:GLY:HA3	1:A:122:ALA:HB2	1.64	0.79
1:B:121:GLY:HA3	1:B:122:ALA:HB2	1.74	0.68
1:A:146:THR:HG23	1:A:151:LEU:O	1.94	0.68
1:B:466:MET:H	3:B:607:IPA:H13	1.59	0.67
1:A:189:GLN:HE21	3:A:603:IPA:H32	1.60	0.67
1:B:146:THR:HG23	1:B:151:LEU:O	1.96	0.66
1:A:121:GLY:HA3	1:A:122:ALA:HB3	1.78	0.65
1:A:189:GLN:HG2	3:A:603:IPA:H13	1.80	0.64
1:B:189:GLN:HE21	3:B:611:IPA:H2	1.63	0.62
1:B:51:MET:HE1	1:B:115:ARG:HG3	1.82	0.61
1:A:414:ASP:HA	4:A:605:EDO:H22	1.82	0.61
1:B:121:GLY:HA3	1:B:122:ALA:HB3	1.83	0.61
1:A:452:ASN:OD1	5:A:609:GOL:H2	2.02	0.60
1:A:146:THR:CG2	1:A:152:ALA:HA	2.32	0.59
1:A:146:THR:HG21	1:A:153:PRO:HD3	1.87	0.57
1:B:437:PRO:HD2	1:B:443:GLY:O	2.04	0.57
1:B:452:ASN:OD1	3:B:613:IPA:H13	2.05	0.56
1:B:415:ASN:HA	3:B:612:IPA:H32	1.87	0.56
1:A:437:PRO:HD2	1:A:443:GLY:O	2.06	0.56
1:B:146:THR:CG2	1:B:152:ALA:HA	2.35	0.56
1:B:238:VAL:HG13	1:B:311:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:THR:HG21	1:B:153:PRO:HD3	1.89	0.53
1:A:51:MET:HE1	1:A:115:ARG:HG3	1.90	0.53
1:B:466:MET:N	3:B:607:IPA:H13	2.23	0.53
1:B:404:LEU:HD13	1:B:433:LEU:HD22	1.91	0.52
1:B:432:PHE:HB3	3:B:613:IPA:H12	1.90	0.52
1:A:355:HIS:HD2	1:A:358:GLU:OE1	1.93	0.52
1:A:146:THR:HG23	1:A:152:ALA:HA	1.93	0.51
1:B:382:SER:HB3	1:B:464:ILE:HG13	1.93	0.51
1:A:404:LEU:HD13	1:A:433:LEU:HD22	1.93	0.50
1:B:53:ARG:HD3	6:B:726:HOH:O	2.12	0.50
1:B:460:GLU:HA	3:B:607:IPA:H2	1.93	0.50
1:B:146:THR:HG23	1:B:152:ALA:HA	1.94	0.48
1:A:142:VAL:O	1:A:146:THR:HB	2.13	0.48
1:B:433:LEU:HD11	3:B:609:IPA:H2	1.95	0.48
1:A:382:SER:HB3	1:A:464:ILE:HG13	1.96	0.47
1:A:121:GLY:CA	1:A:122:ALA:CB	2.83	0.47
2:A:601:FAD:C4	3:A:610:IPA:H32	2.46	0.46
1:A:460:GLU:HA	3:A:614:IPA:H2	1.98	0.45
2:B:602:FAD:C4	3:B:609:IPA:H32	2.46	0.45
1:A:80:ARG:HG3	1:A:197:GLY:HA3	1.97	0.45
1:B:441:GLY:O	1:B:444:SER:HB3	2.17	0.45
1:A:415:ASN:H	4:A:605:EDO:H21	1.81	0.45
1:A:442:HIS:O	1:A:447:HIS:CD2	2.70	0.45
1:B:442:HIS:O	1:B:447:HIS:HD2	2.00	0.44
1:B:442:HIS:O	1:B:447:HIS:CD2	2.71	0.44
1:B:146:THR:HG21	1:B:152:ALA:HA	1.99	0.43
1:B:48:VAL:HG12	1:B:66:VAL:HG23	2.00	0.43
1:A:419:VAL:HG12	1:A:421:ILE:HG23	2.00	0.43
1:A:238:VAL:HG13	1:A:311:THR:HB	2.00	0.42
1:A:415:ASN:H	4:A:605:EDO:C2	2.32	0.42
1:B:80:ARG:HG3	1:B:197:GLY:HA3	2.01	0.42
1:A:146:THR:HG21	1:A:152:ALA:HA	2.00	0.42
1:B:102:LEU:HD13	1:B:373:TRP:HB2	2.03	0.41
1:A:102:LEU:HD13	1:A:373:TRP:HB2	2.02	0.41
1:B:56:GLY:O	1:B:370:PRO:HA	2.20	0.41
1:A:59:CYS:HB3	1:A:61:PHE:CE2	2.56	0.40
1:B:389:GLU:HG2	1:B:458:PHE:CD1	2.56	0.40
1:B:142:VAL:O	1:B:146:THR:HB	2.21	0.40
1:A:53:ARG:HD3	6:A:706:HOH:O	2.20	0.40

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	473/501 (94%)	452 (96%)	15 (3%)	6 (1%)	15	5
1	B	456/501 (91%)	433 (95%)	19 (4%)	4 (1%)	21	10
All	All	929/1002 (93%)	885 (95%)	34 (4%)	10 (1%)	17	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA
1	B	122	ALA
1	A	121	GLY
1	A	171	ALA
1	B	121	GLY
1	A	123	ARG
1	A	264	SER
1	B	171	ALA
1	A	443	GLY
1	B	443	GLY

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	405/425 (95%)	392 (97%)	13 (3%)	46	38
1	B	390/425 (92%)	368 (94%)	22 (6%)	26	16
All	All	795/850 (94%)	760 (96%)	35 (4%)	35	26

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	THR
1	A	184	VAL
1	A	257	MET
1	A	275	ASN
1	A	276	ARG
1	A	291	ASP
1	A	322	MET
1	A	337	GLN
1	A	399	ASN
1	A	415	ASN
1	A	423	ASP
1	A	445	ILE
1	A	492	ARG
1	B	29	ASP
1	B	34	LEU
1	B	38	ARG
1	B	120	ARG
1	B	146	THR
1	B	184	VAL
1	B	206	ASP
1	B	239	ARG
1	B	257	MET
1	B	263	ASN
1	B	322	MET
1	B	329	LEU
1	B	337	GLN
1	B	359	LEU
1	B	368	GLU
1	B	396	LYS
1	B	399	ASN
1	B	400	ASN
1	B	423	ASP
1	B	433	LEU
1	B	445	ILE
1	B	515	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	188	ASN

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Mol	Chain	Res	Type
1	A	189	GLN
1	A	281	ASN
1	A	282	ASN
1	A	337	GLN
1	A	355	HIS
1	A	415	ASN
1	A	447	HIS
1	A	468	GLN
1	A	476	GLN
1	B	68	HIS
1	B	188	ASN
1	B	189	GLN
1	B	447	HIS
1	B	468	GLN
1	B	476	GLN
1	B	478	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

40 ligands are modelled in this entry.

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
2	FAD	A	601	1	52,58,58	1.14	5 (9%)	52,89,89	2.42	7 (13%)
3	IPA	A	602	-	3,3,3	0.85	0	3,3,3	0.56	0
3	IPA	A	603	-	3,3,3	0.45	0	3,3,3	0.49	0
3	IPA	A	604	-	3,3,3	0.56	0	3,3,3	0.49	0
4	EDO	A	605	-	3,3,3	0.65	0	2,2,2	0.10	0
3	IPA	A	606	-	3,3,3	0.58	0	3,3,3	0.79	0
4	EDO	A	607	-	3,3,3	0.59	0	2,2,2	0.45	0
4	EDO	A	608	-	3,3,3	0.64	0	2,2,2	0.37	0
5	GOL	A	609	-	5,5,5	0.12	0	5,5,5	0.30	0
3	IPA	A	610	-	3,3,3	0.47	0	3,3,3	0.59	0
3	IPA	A	611	-	3,3,3	0.81	0	3,3,3	0.63	0
3	IPA	A	612	-	3,3,3	0.70	0	3,3,3	0.78	0
3	IPA	A	613	-	3,3,3	0.70	0	3,3,3	0.53	0
3	IPA	A	614	-	3,3,3	0.83	0	3,3,3	0.41	0
3	IPA	A	615	-	3,3,3	0.76	0	3,3,3	0.55	0
3	IPA	A	616	-	3,3,3	0.61	0	3,3,3	0.56	0
3	IPA	A	617	-	3,3,3	0.48	0	3,3,3	0.57	0
3	IPA	A	618	-	3,3,3	0.65	0	3,3,3	0.47	0
3	IPA	A	619	-	3,3,3	0.74	0	3,3,3	0.49	0
3	IPA	A	620	-	3,3,3	0.45	0	3,3,3	0.70	0
3	IPA	A	621	-	3,3,3	0.69	0	3,3,3	0.68	0
3	IPA	A	622	-	3,3,3	0.76	0	3,3,3	0.52	0
4	EDO	A	623	-	3,3,3	0.70	0	2,2,2	0.26	0
4	EDO	A	624	-	3,3,3	0.58	0	2,2,2	0.56	0
3	IPA	B	601	-	3,3,3	1.11	0	3,3,3	0.90	0
2	FAD	B	602	1	52,58,58	1.06	5 (9%)	52,89,89	2.42	7 (13%)
5	GOL	B	603	-	5,5,5	0.19	0	5,5,5	0.44	0
3	IPA	B	604	-	3,3,3	0.66	0	3,3,3	0.58	0
4	EDO	B	605	-	3,3,3	0.65	0	2,2,2	0.37	0
3	IPA	B	606	-	3,3,3	0.67	0	3,3,3	0.54	0
3	IPA	B	607	-	3,3,3	0.65	0	3,3,3	0.30	0
3	IPA	B	608	-	3,3,3	0.60	0	3,3,3	0.50	0
3	IPA	B	609	-	3,3,3	0.43	0	3,3,3	0.55	0
3	IPA	B	610	-	3,3,3	0.65	0	3,3,3	0.57	0
3	IPA	B	611	-	3,3,3	0.66	0	3,3,3	0.59	0
3	IPA	B	612	-	3,3,3	0.58	0	3,3,3	0.82	0
3	IPA	B	613	-	3,3,3	0.77	0	3,3,3	0.51	0
3	IPA	B	614	-	3,3,3	0.78	0	3,3,3	0.60	0
5	GOL	B	615	-	5,5,5	0.13	0	5,5,5	0.19	0
3	IPA	B	616	-	3,3,3	0.66	0	3,3,3	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	1	-	0/30/50/50	0/6/6/6
3	IPA	A	602	-	-	0/0/0/0	0/0/0/0
3	IPA	A	603	-	-	0/0/0/0	0/0/0/0
3	IPA	A	604	-	-	0/0/0/0	0/0/0/0
4	EDO	A	605	-	-	0/1/1/1	0/0/0/0
3	IPA	A	606	-	-	0/0/0/0	0/0/0/0
4	EDO	A	607	-	-	0/1/1/1	0/0/0/0
4	EDO	A	608	-	-	0/1/1/1	0/0/0/0
5	GOL	A	609	-	-	0/4/4/4	0/0/0/0
3	IPA	A	610	-	-	0/0/0/0	0/0/0/0
3	IPA	A	611	-	-	0/0/0/0	0/0/0/0
3	IPA	A	612	-	-	0/0/0/0	0/0/0/0
3	IPA	A	613	-	-	0/0/0/0	0/0/0/0
3	IPA	A	614	-	-	0/0/0/0	0/0/0/0
3	IPA	A	615	-	-	0/0/0/0	0/0/0/0
3	IPA	A	616	-	-	0/0/0/0	0/0/0/0
3	IPA	A	617	-	-	0/0/0/0	0/0/0/0
3	IPA	A	618	-	-	0/0/0/0	0/0/0/0
3	IPA	A	619	-	-	0/0/0/0	0/0/0/0
3	IPA	A	620	-	-	0/0/0/0	0/0/0/0
3	IPA	A	621	-	-	0/0/0/0	0/0/0/0
3	IPA	A	622	-	-	0/0/0/0	0/0/0/0
4	EDO	A	623	-	-	0/1/1/1	0/0/0/0
4	EDO	A	624	-	-	0/1/1/1	0/0/0/0
3	IPA	B	601	-	-	0/0/0/0	0/0/0/0
2	FAD	B	602	1	-	0/30/50/50	0/6/6/6
5	GOL	B	603	-	-	0/4/4/4	0/0/0/0
3	IPA	B	604	-	-	0/0/0/0	0/0/0/0
4	EDO	B	605	-	-	0/1/1/1	0/0/0/0
3	IPA	B	606	-	-	0/0/0/0	0/0/0/0
3	IPA	B	607	-	-	0/0/0/0	0/0/0/0
3	IPA	B	608	-	-	0/0/0/0	0/0/0/0
3	IPA	B	609	-	-	0/0/0/0	0/0/0/0
3	IPA	B	610	-	-	0/0/0/0	0/0/0/0
3	IPA	B	611	-	-	0/0/0/0	0/0/0/0
3	IPA	B	612	-	-	0/0/0/0	0/0/0/0
3	IPA	B	613	-	-	0/0/0/0	0/0/0/0
3	IPA	B	614	-	-	0/0/0/0	0/0/0/0
5	GOL	B	615	-	-	0/4/4/4	0/0/0/0
3	IPA	B	616	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	FAD	C4-C4X	2.64	1.46	1.41
2	B	602	FAD	C4X-C10	2.65	1.45	1.40
2	B	602	FAD	C9A-N10	2.88	1.42	1.38
2	A	601	FAD	C4X-C10	2.90	1.46	1.40
2	A	601	FAD	C9A-N10	2.95	1.43	1.38
2	B	602	FAD	C5X-N5	3.02	1.40	1.35
2	A	601	FAD	C4-N3	3.07	1.38	1.33
2	B	602	FAD	C4-N3	3.23	1.38	1.33
2	A	601	FAD	C5X-N5	3.34	1.40	1.35
2	A	601	FAD	C4-C4X	3.52	1.48	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-C4-N3	-7.06	114.29	123.52
2	B	602	FAD	C4X-C4-N3	-6.82	114.60	123.52
2	B	602	FAD	N3-C2-N1	-4.92	119.41	127.69
2	B	602	FAD	C4X-C10-N10	-4.79	117.04	120.52
2	A	601	FAD	C4X-C10-N10	-4.78	117.04	120.52
2	A	601	FAD	N3-C2-N1	-4.59	119.96	127.69
2	B	602	FAD	C4-C4X-C10	-3.97	117.40	119.94
2	A	601	FAD	C4-C4X-C10	-3.85	117.48	119.94
2	A	601	FAD	O2P-P-O5'	-2.75	95.12	108.24
2	B	602	FAD	O2P-P-O5'	-2.72	95.29	108.24
2	B	602	FAD	O5'-P-O1P	2.70	120.27	109.21
2	A	601	FAD	O5'-P-O1P	2.90	121.10	109.21
2	A	601	FAD	C4-N3-C2	12.72	125.78	115.16
2	B	602	FAD	C4-N3-C2	12.85	125.88	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	1	0
3	A	603	IPA	2	0
4	A	605	EDO	3	0
5	A	609	GOL	2	0
3	A	610	IPA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	614	IPA	1	0
2	B	602	FAD	1	0
3	B	607	IPA	3	0
3	B	609	IPA	2	0
3	B	611	IPA	1	0
3	B	612	IPA	1	0
3	B	613	IPA	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	477/501 (95%)	-0.02	28 (5%)	26	29	25, 37, 78, 116	0
1	B	460/501 (91%)	0.02	23 (5%)	32	37	26, 40, 73, 106	0
All	All	937/1002 (93%)	-0.00	51 (5%)	29	34	25, 39, 75, 116	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	281	ASN	7.9
1	A	285	ALA	7.4
1	A	291	ASP	7.1
1	A	279	ILE	6.5
1	A	283	TRP	6.4
1	A	289	PRO	6.1
1	A	286	SER	6.0
1	A	277	THR	5.7
1	B	341	PHE	5.3
1	B	514	SER	5.3
1	A	290	GLN	5.2
1	A	399	ASN	5.0
1	A	284	ARG	5.0
1	A	287	PHE	4.5
1	A	292	PRO	4.5
1	A	280	LEU	4.4
1	A	282	ASN	4.3
1	B	399	ASN	4.3
1	A	513	ALA	4.1
1	A	276	ARG	4.1
1	A	288	LYS	4.0
1	A	278	GLY	3.9
1	B	461	GLU	3.6
1	B	515	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	514	SER	3.4
1	B	320	ASP	3.4
1	B	324	GLN	3.2
1	A	341	PHE	3.1
1	A	31	LEU	3.0
1	B	340	LEU	2.9
1	A	461	GLU	2.9
1	A	121	GLY	2.8
1	B	31	LEU	2.8
1	B	248	PHE	2.6
1	B	442	HIS	2.6
1	B	121	GLY	2.5
1	A	495	HIS	2.4
1	B	303	ARG	2.4
1	B	318	ASP	2.4
1	B	327	ALA	2.4
1	B	458	PHE	2.4
1	B	319	THR	2.3
1	A	122	ALA	2.3
1	B	275	ASN	2.3
1	B	398	SER	2.3
1	B	393	ARG	2.2
1	B	384	ARG	2.2
1	A	29	ASP	2.2
1	B	29	ASP	2.2
1	B	304	VAL	2.1
1	A	275	ASN	2.0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	IPA	A	604	4/4	0.87	0.25	20.21	48,49,50,53	0
3	IPA	A	622	4/4	0.84	0.21	17.94	53,56,57,58	0
5	GOL	A	609	6/6	0.94	0.18	15.98	61,62,63,65	0
4	EDO	A	623	4/4	0.64	0.40	13.13	60,61,61,62	0
3	IPA	A	615	4/4	0.78	0.27	12.89	65,65,66,67	0
3	IPA	B	601	4/4	0.97	0.22	11.87	31,34,34,39	0
3	IPA	B	609	4/4	0.95	0.30	11.47	54,58,59,60	0
4	EDO	A	605	4/4	0.66	0.34	10.33	59,61,63,64	0
3	IPA	A	603	4/4	0.94	0.27	10.26	63,64,65,66	0
3	IPA	A	620	4/4	0.91	0.23	8.72	57,57,57,60	0
3	IPA	B	616	4/4	0.92	0.36	8.71	68,68,69,69	0
5	GOL	B	603	6/6	0.81	0.26	8.43	59,62,64,65	0
3	IPA	A	621	4/4	0.86	0.25	7.39	61,61,61,62	0
3	IPA	B	604	4/4	0.92	0.32	6.97	57,60,60,61	0
3	IPA	A	611	4/4	0.97	0.21	6.91	35,37,37,40	0
3	IPA	A	612	4/4	0.87	0.30	6.77	43,44,45,50	0
4	EDO	A	608	4/4	0.80	0.21	6.17	61,62,62,63	0
3	IPA	A	610	4/4	0.97	0.24	5.60	54,56,57,58	0
3	IPA	A	616	4/4	0.94	0.33	5.17	61,61,61,62	0
4	EDO	A	624	4/4	0.59	0.20	4.64	58,59,63,63	0
4	EDO	A	607	4/4	0.84	0.25	4.48	62,65,65,66	0
3	IPA	B	612	4/4	0.92	0.19	4.29	42,42,46,49	0
4	EDO	B	605	4/4	0.88	0.16	3.98	61,61,61,62	0
3	IPA	B	611	4/4	0.95	0.18	3.72	45,49,49,50	0
3	IPA	A	602	4/4	0.97	0.18	3.24	38,38,40,43	0
3	IPA	B	613	4/4	0.87	0.14	1.80	48,51,52,53	0
5	GOL	B	615	6/6	0.87	0.18	1.70	70,72,74,74	0
3	IPA	B	607	4/4	0.74	0.23	0.96	48,53,53,57	0
2	FAD	B	602	53/53	0.97	0.13	0.73	21,30,37,39	0
3	IPA	A	606	4/4	0.92	0.20	0.36	48,50,50,54	0
3	IPA	A	619	4/4	0.73	0.20	0.25	71,71,72,73	0
2	FAD	A	601	53/53	0.97	0.10	0.16	23,30,33,37	0
3	IPA	A	614	4/4	0.86	0.15	-0.00	44,45,47,49	0
3	IPA	B	608	4/4	0.72	0.17	-0.08	79,80,81,81	0
3	IPA	A	617	4/4	0.92	0.15	-0.15	47,51,53,55	0
3	IPA	B	610	4/4	0.96	0.17	-	51,55,56,57	0
3	IPA	A	613	4/4	0.93	0.21	-	59,60,61,63	0
3	IPA	B	606	4/4	0.85	0.23	-	63,65,66,67	0
3	IPA	A	618	4/4	0.96	0.10	-	50,50,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	IPA	B	614	4/4	0.89	0.17	-	56,58,58,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.