wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 02:32 am BST

PDB ID	:	2QJI
Title	:	M. jannaschii ADH synthase complexed with dihydroxyacetone phosphate and glycerol
Authors	:	Ealick, S.E.; Morar, M.
Deposited on	:	2007-07-07
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

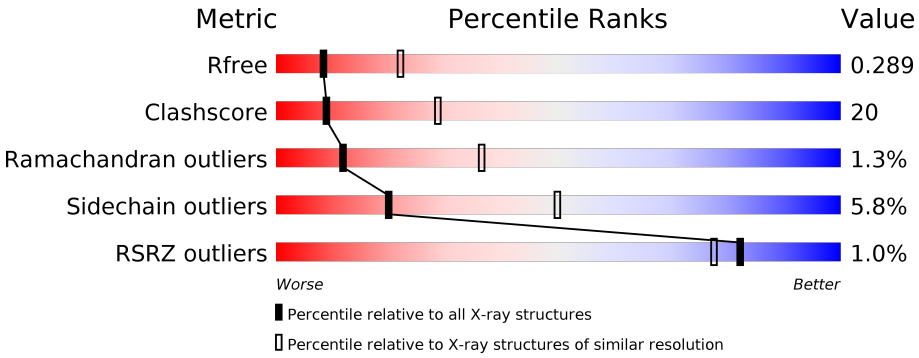
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. 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 <=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	273	65% 31%
1	B	273	% 65% 31%
1	C	273	% 66% 30%
1	D	273	% 67% 29%
1	E	273	% 65% 28% 5%
1	F	273	64% 31%

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Mol	Chain	Length	Quality of chain
1	G	273	64% 30%
1	H	273	68% 27%
1	I	273	63% 32%
1	J	273	2% 67% 28%
1	K	273	66% 30%
1	L	273	70% 26%
1	M	273	2% 62% 34%
1	N	273	4% 63% 33%
1	O	273	% 70% 27%
1	P	273	71% 25%
1	Q	273	% 67% 27% 5%
1	R	273	% 68% 29%
1	S	273	2% 64% 32%
1	T	273	% 66% 27% 5%

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	GOL	C	500	-	-	X	X
3	GOL	D	500	-	-	X	X
3	GOL	I	500	-	-	X	-
3	GOL	J	500	-	-	X	X
3	GOL	M	500	-	-	X	-
3	GOL	O	500	-	-	X	-
3	GOL	P	500	-	-	X	-
3	GOL	R	500	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41213 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 Putative aldolase MJ0400.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2042	1278	365	388	11			
1	B	271	Total	C	N	O	S	0	0	0
			2034	1273	364	386	11			
1	C	271	Total	C	N	O	S	0	0	0
			2029	1272	362	384	11			
1	D	271	Total	C	N	O	S	0	0	0
			2038	1276	365	386	11			
1	E	271	Total	C	N	O	S	0	0	0
			2051	1285	368	387	11			
1	F	271	Total	C	N	O	S	0	0	0
			2045	1282	365	387	11			
1	G	271	Total	C	N	O	S	0	0	0
			2044	1279	368	386	11			
1	H	271	Total	C	N	O	S	0	0	0
			2036	1276	363	386	11			
1	I	271	Total	C	N	O	S	0	0	0
			2038	1276	365	386	11			
1	J	271	Total	C	N	O	S	0	0	0
			2032	1273	362	386	11			
1	K	271	Total	C	N	O	S	0	0	0
			2032	1273	362	386	11			
1	L	271	Total	C	N	O	S	0	0	0
			2034	1273	364	386	11			
1	M	271	Total	C	N	O	S	0	0	0
			2038	1276	365	386	11			
1	N	271	Total	C	N	O	S	0	0	0
			2032	1273	362	386	11			
1	O	271	Total	C	N	O	S	0	0	0
			2028	1270	361	386	11			
1	P	271	Total	C	N	O	S	0	0	0
			2044	1279	368	386	11			

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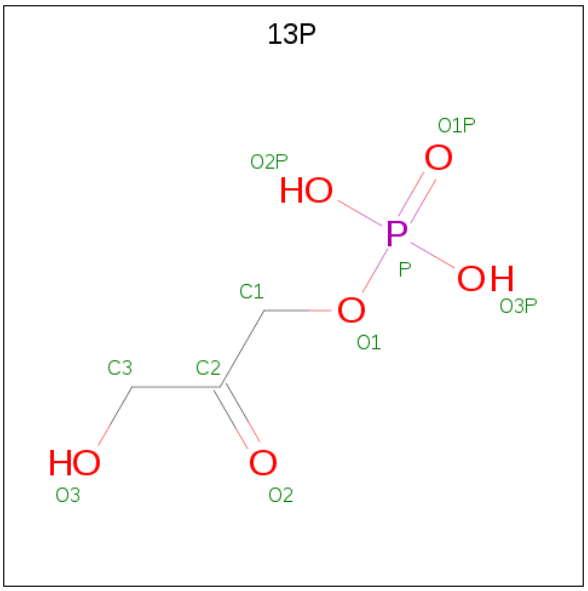
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	271	Total	C	N	O	S	0	0	0
			2032	1273	362	386	11			
1	R	271	Total	C	N	O	S	0	0	0
			2038	1276	365	386	11			
1	S	271	Total	C	N	O	S	0	0	0
			2038	1276	365	386	11			
1	T	269	Total	C	N	O	S	0	0	0
			2021	1267	359	384	11			

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	3	5	1		
2	B	1	Total	C	O	P	0	0
			9	3	5	1		
2	C	1	Total	C	O	P	0	0
			9	3	5	1		
2	D	1	Total	C	O	P	0	0
			9	3	5	1		
2	E	1	Total	C	O	P	0	0
			9	3	5	1		
2	F	1	Total	C	O	P	0	0
			9	3	5	1		
2	G	1	Total	C	O	P	0	0
			9	3	5	1		

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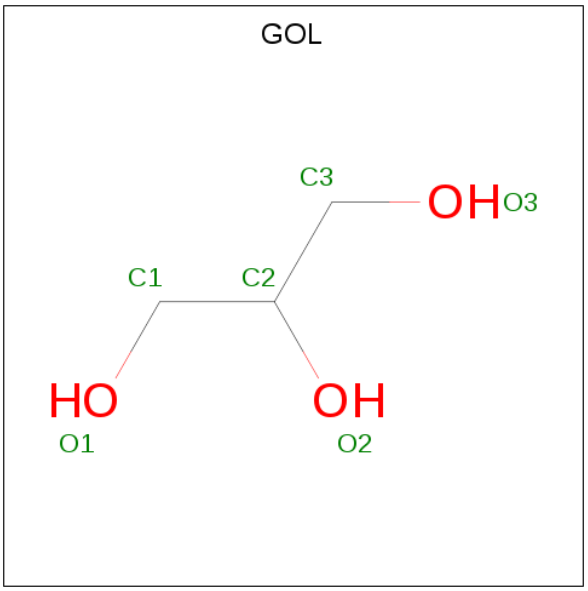
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	H	1	Total	C	O	P	0	0
			9	3	5	1		
2	I	1	Total	C	O	P	0	0
			9	3	5	1		
2	J	1	Total	C	O	P	0	0
			9	3	5	1		
2	K	1	Total	C	O	P	0	0
			9	3	5	1		
2	L	1	Total	C	O	P	0	0
			9	3	5	1		
2	M	1	Total	C	O	P	0	0
			9	3	5	1		
2	N	1	Total	C	O	P	0	0
			9	3	5	1		
2	O	1	Total	C	O	P	0	0
			9	3	5	1		
2	P	1	Total	C	O	P	0	0
			9	3	5	1		
2	Q	1	Total	C	O	P	0	0
			9	3	5	1		
2	R	1	Total	C	O	P	0	0
			9	3	5	1		
2	S	1	Total	C	O	P	0	0
			9	3	5	1		
2	T	1	Total	C	O	P	0	0
			9	3	5	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	G	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	I	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	K	1	Total C O 6 3 3	0	0
3	L	1	Total C O 6 3 3	0	0
3	M	1	Total C O 6 3 3	0	0
3	N	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	1	Total C O 6 3 3	0	0
3	P	1	Total C O 6 3 3	0	0
3	Q	1	Total C O 6 3 3	0	0
3	R	1	Total C O 6 3 3	0	0
3	S	1	Total C O 6 3 3	0	0
3	T	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	15	Total O 15 15	0	0
4	C	7	Total O 7 7	0	0
4	D	6	Total O 6 6	0	0
4	E	12	Total O 12 12	0	0
4	F	5	Total O 5 5	0	0
4	G	6	Total O 6 6	0	0
4	H	12	Total O 12 12	0	0
4	I	10	Total O 10 10	0	0
4	J	8	Total O 8 8	0	0
4	K	12	Total O 12 12	0	0
4	L	10	Total O 10 10	0	0
4	M	9	Total O 9 9	0	0

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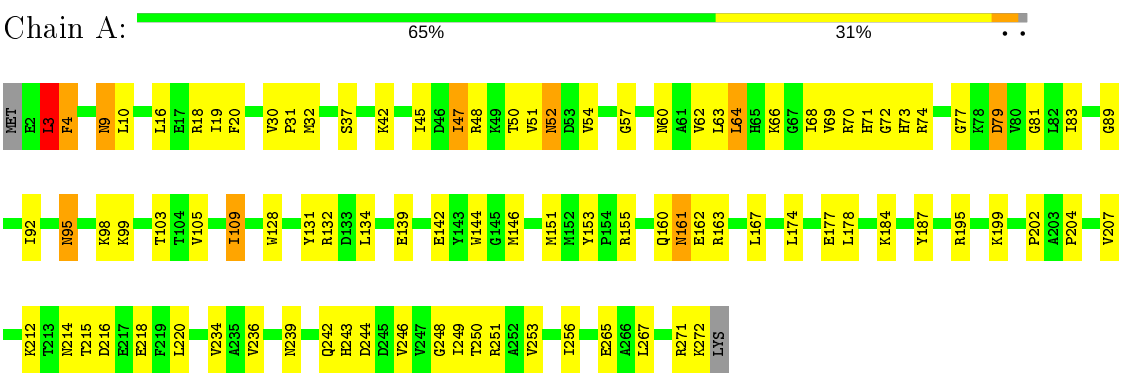
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	6	Total O 6 6	0	0
4	O	10	Total O 10 10	0	0
4	P	5	Total O 5 5	0	0
4	Q	16	Total O 16 16	0	0
4	R	12	Total O 12 12	0	0
4	S	8	Total O 8 8	0	0
4	T	8	Total O 8 8	0	0

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 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.

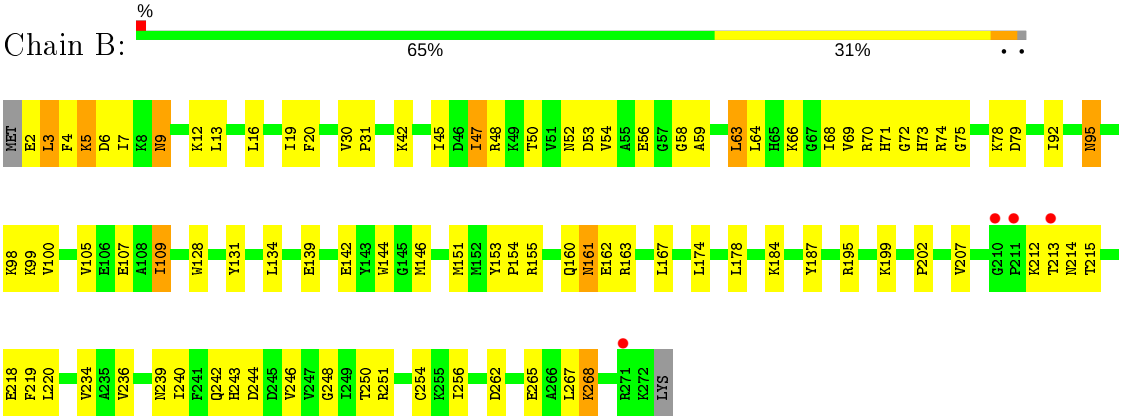
- Molecule 1: Putative aldolase MJ0400

Chain A:



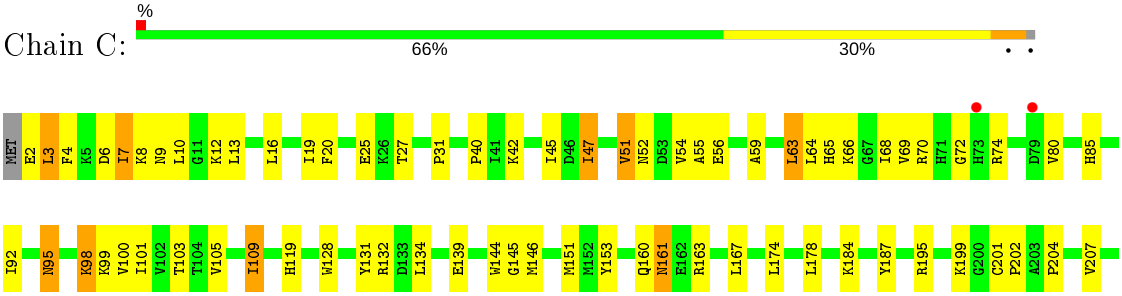
- Molecule 1: Putative aldolase MJ0400

Chain B:



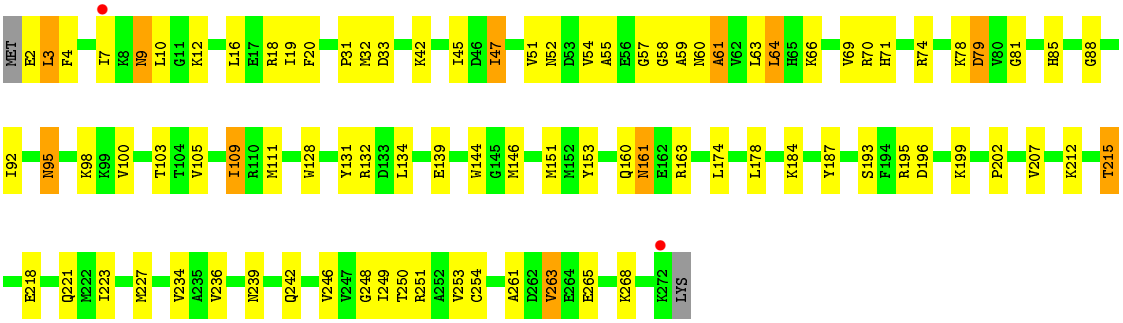
- Molecule 1: Putative aldolase MJ0400

Chain C:



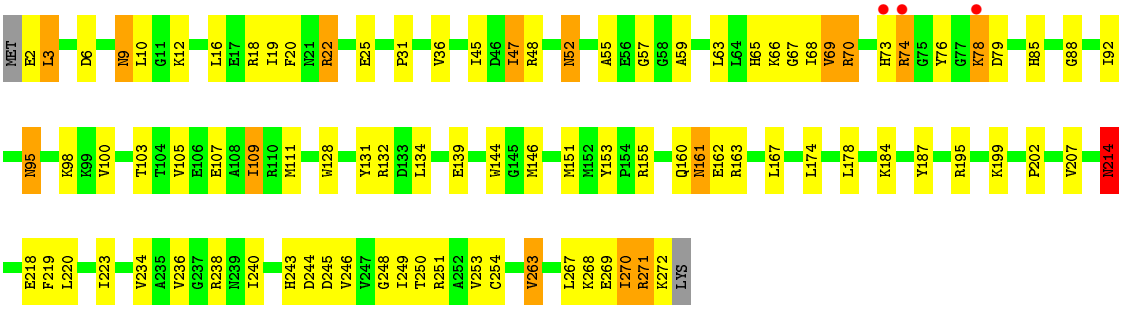
• Molecule 1: Putative aldolase MJ0400

Chain D:



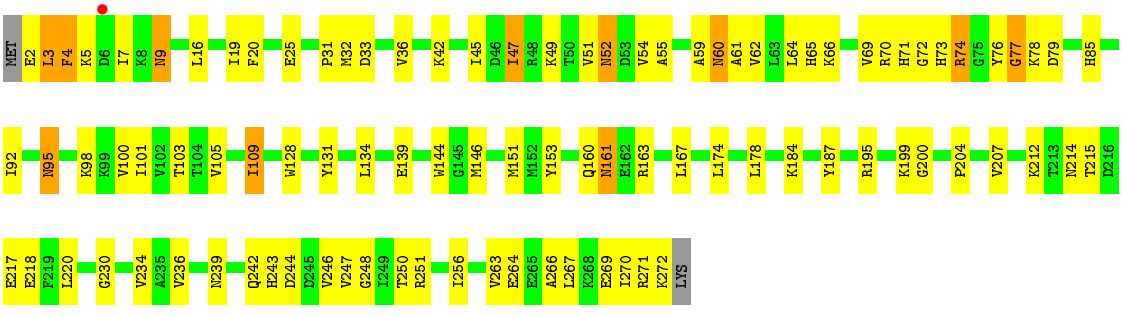
• Molecule 1: Putative aldolase MJ0400

Chain E:



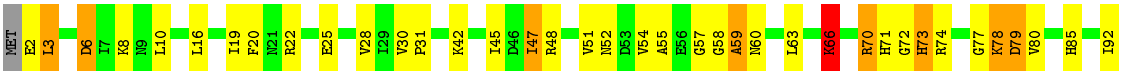
• Molecule 1: Putative aldolase MJ0400

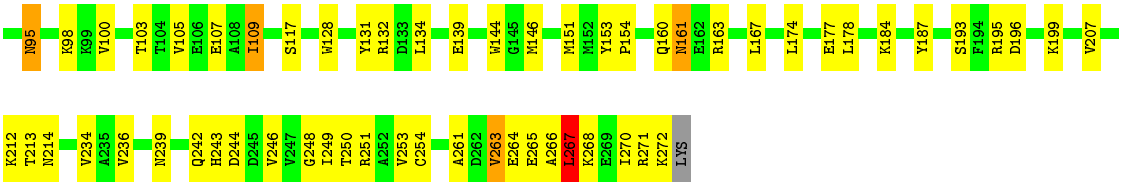
Chain F:



• Molecule 1: Putative aldolase MJ0400

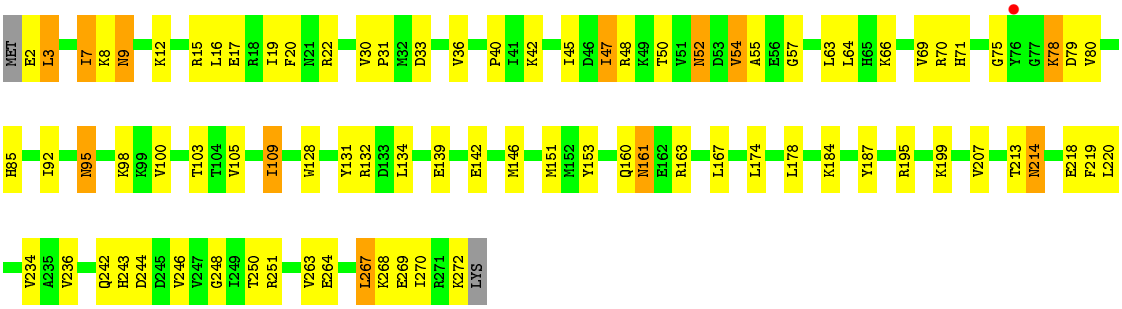
Chain G:





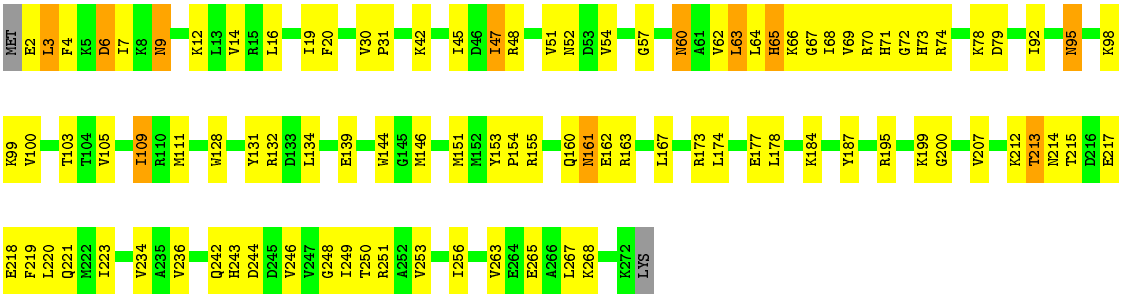
• Molecule 1: Putative aldolase MJ0400

Chain H:



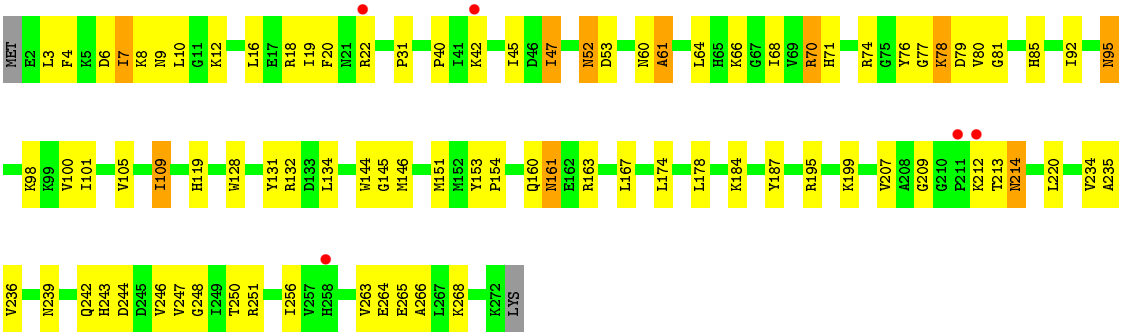
• Molecule 1: Putative aldolase MJ0400

Chain I:



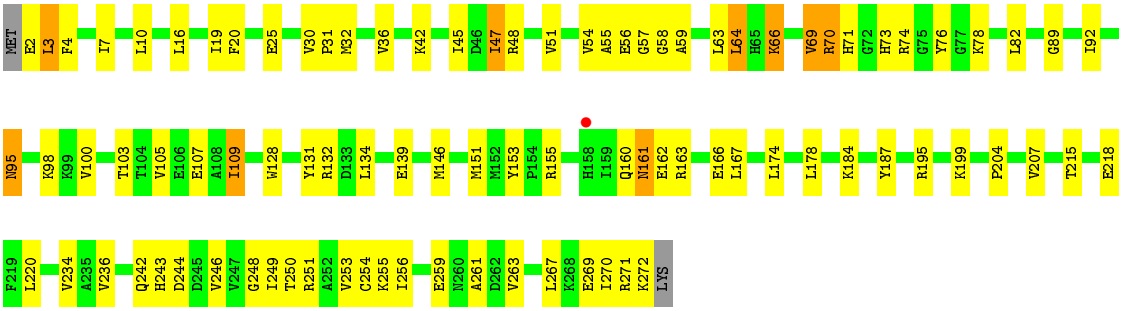
• Molecule 1: Putative aldolase MJ0400

Chain J:

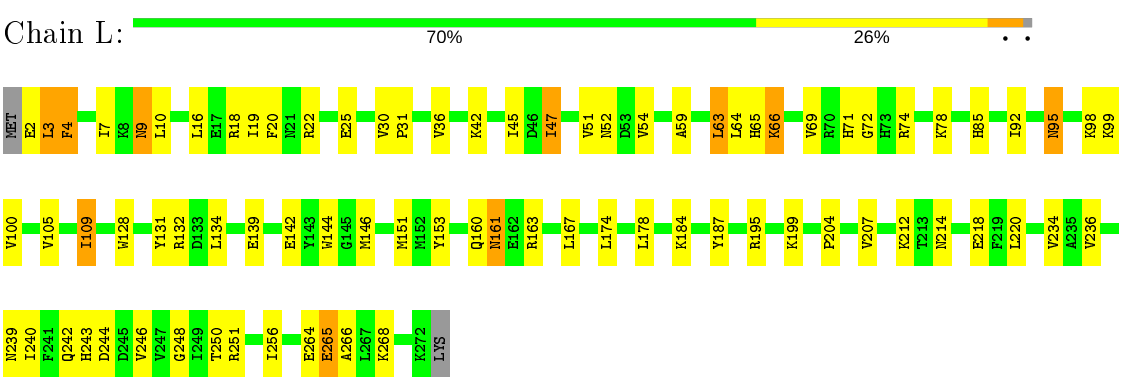


• Molecule 1: Putative aldolase MJ0400

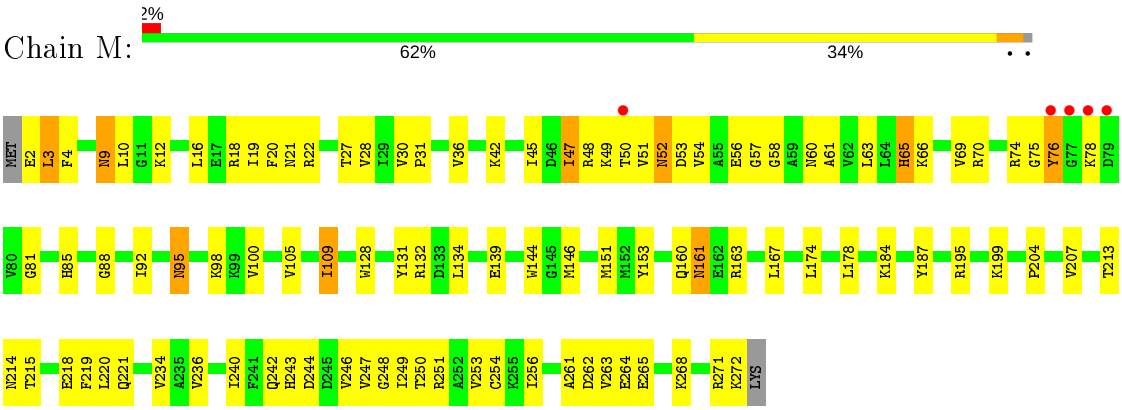
Chain K:



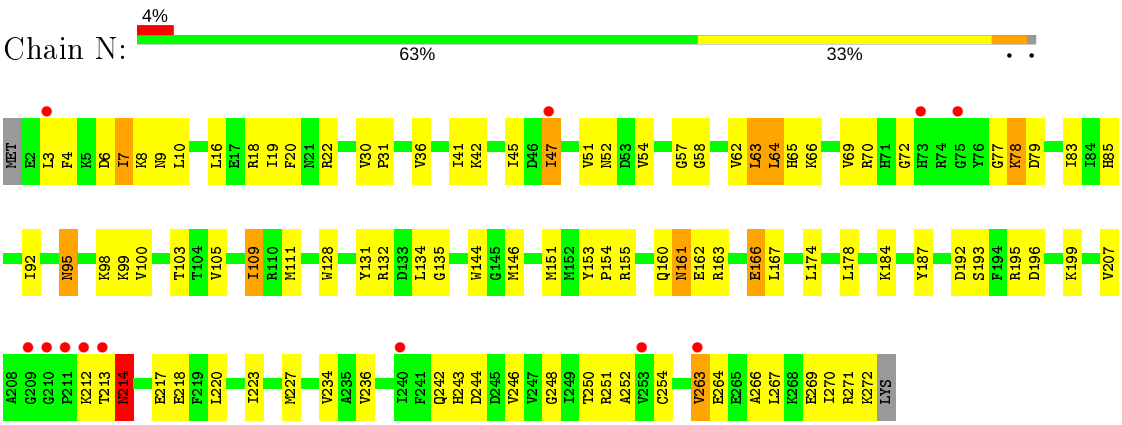
- Molecule 1: Putative aldolase MJ0400



- Molecule 1: Putative aldolase MJ0400

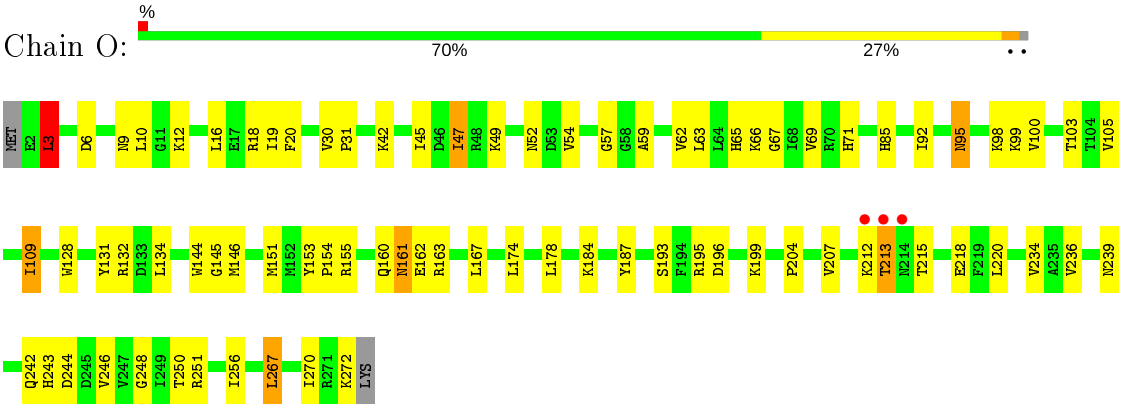


- Molecule 1: Putative aldolase MJ0400



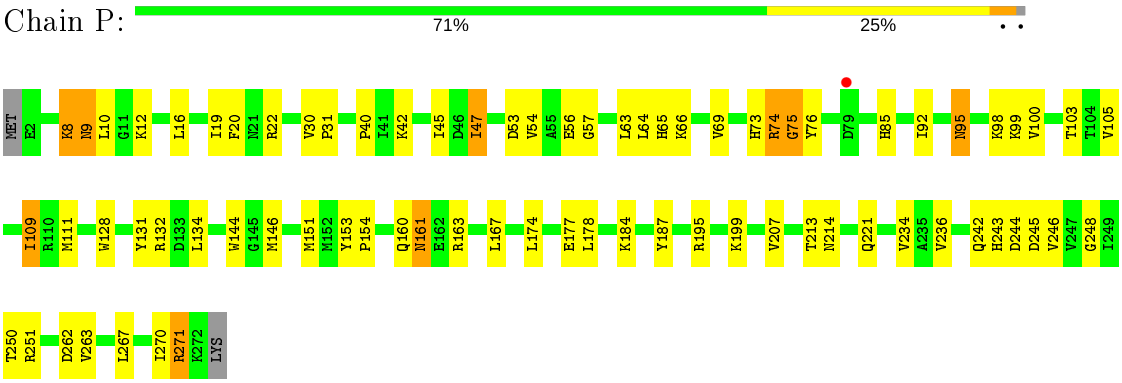
- Molecule 1: Putative aldolase MJ0400

Chain O:



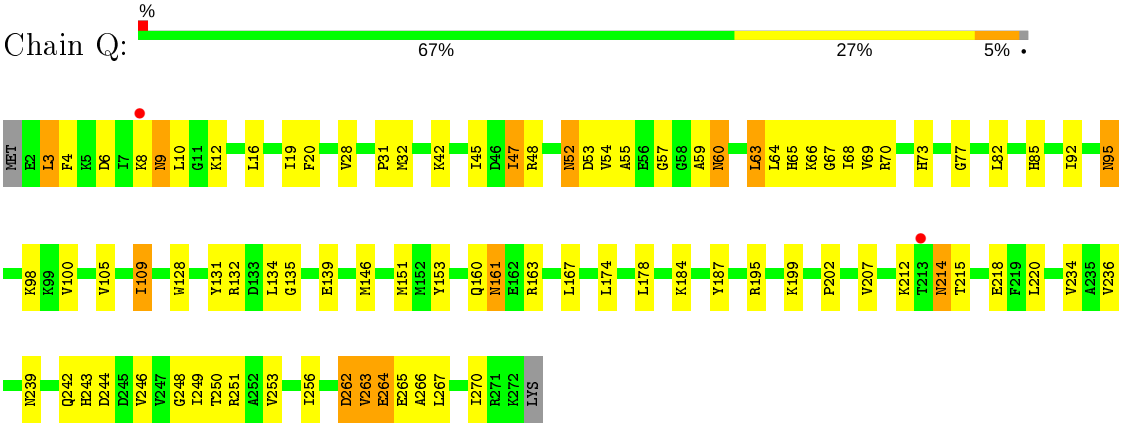
- Molecule 1: Putative aldolase MJ0400

Chain P:



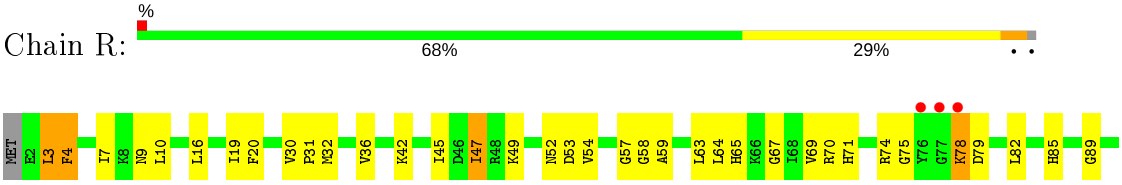
- Molecule 1: Putative aldolase MJ0400

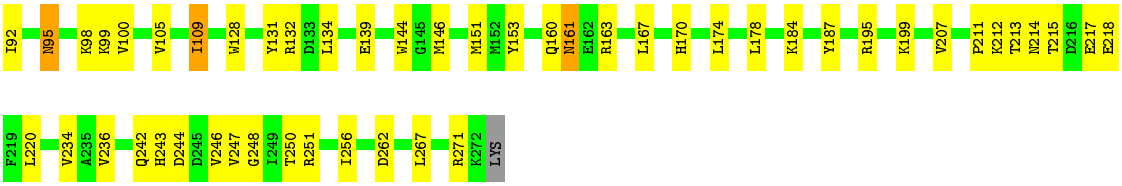
Chain Q:



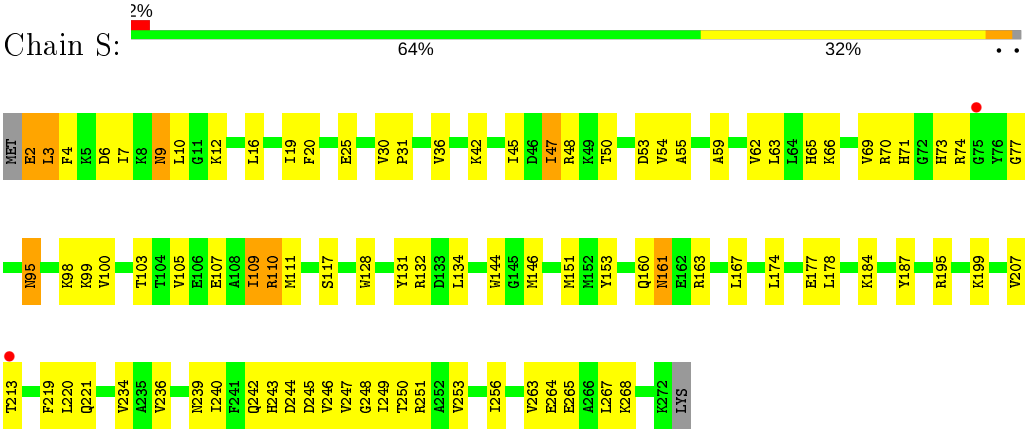
- Molecule 1: Putative aldolase MJ0400

Chain R:

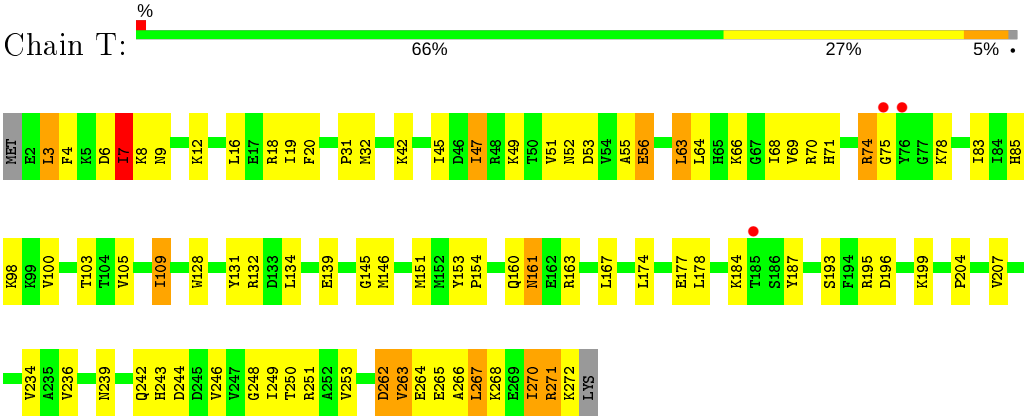




• Molecule 1: Putative aldolase MJ0400



• Molecule 1: Putative aldolase MJ0400



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	94.14Å 103.54Å 153.99Å 90.05° 87.97° 82.04°	Depositor
Resolution (Å)	41.19 – 2.80 47.81 – 2.38	Depositor EDS
% Data completeness (in resolution range)	88.3 (41.19-2.80) 87.2 (47.81-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.37Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.244 , 0.296 0.237 , 0.289	Depositor DCC
R_{free} test set	14868 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 22.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	41213	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 13P

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	0.42	0/2074	0.62	0/2806
1	B	0.38	0/2066	0.59	0/2797
1	C	0.37	0/2061	0.58	0/2790
1	D	0.37	0/2070	0.60	0/2801
1	E	0.45	0/2084	1.14	9/2819 (0.3%)
1	F	0.39	0/2078	0.66	2/2812 (0.1%)
1	G	0.42	0/2076	0.63	1/2808 (0.0%)
1	H	0.43	0/2068	0.62	0/2798
1	I	0.41	0/2070	0.64	2/2801 (0.1%)
1	J	0.37	0/2064	0.61	2/2794 (0.1%)
1	K	0.44	2/2064 (0.1%)	0.62	0/2794
1	L	0.39	0/2066	0.62	0/2797
1	M	0.38	0/2070	0.60	0/2801
1	N	0.42	1/2064 (0.0%)	0.67	3/2794 (0.1%)
1	O	0.38	0/2060	1.03	4/2790 (0.1%)
1	P	0.42	0/2076	0.61	0/2808
1	Q	0.40	0/2064	0.63	1/2794 (0.0%)
1	R	0.42	0/2070	0.66	2/2801 (0.1%)
1	S	0.42	0/2070	1.00	3/2801 (0.1%)
1	T	0.37	0/2052	0.59	0/2775
All	All	0.40	3/41367 (0.0%)	0.70	29/55981 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	166	GLU	CG-CD	6.07	1.61	1.51
1	N	166	GLU	CD-OE2	5.48	1.31	1.25
1	K	166	GLU	CB-CG	-5.08	1.42	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	18	ARG	NE-CZ-NH2	-29.62	105.49	120.30
1	S	110	ARG	NE-CZ-NH1	-28.80	105.90	120.30
1	O	18	ARG	NE-CZ-NH1	28.17	134.38	120.30
1	S	110	ARG	NE-CZ-NH2	27.27	133.94	120.30
1	E	238	ARG	NE-CZ-NH1	-26.27	107.17	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2042	0	2041	89	0
1	B	2034	0	2026	88	0
1	C	2029	0	2024	104	0
1	D	2038	0	2037	85	0
1	E	2051	0	2055	113	0
1	F	2045	0	2044	96	0
1	G	2044	0	2048	112	0
1	H	2036	0	2037	83	0
1	I	2038	0	2037	88	0
1	J	2032	0	2026	88	0
1	K	2032	0	2026	91	0
1	L	2034	0	2026	76	0
1	M	2038	0	2037	97	0
1	N	2032	0	2026	104	0
1	O	2028	0	2015	84	0
1	P	2044	0	2048	82	0
1	Q	2032	0	2026	83	0
1	R	2038	0	2037	86	0
1	S	2038	0	2037	91	0
1	T	2021	0	2016	92	0
2	A	9	0	5	3	0
2	B	9	0	5	2	0
2	C	9	0	5	2	0
2	D	9	0	5	3	0
2	E	9	0	5	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	9	0	5	2	0
2	G	9	0	5	3	0
2	H	9	0	5	2	0
2	I	9	0	5	2	0
2	J	9	0	5	2	0
2	K	9	0	5	2	0
2	L	9	0	5	2	0
2	M	9	0	5	2	0
2	N	9	0	5	2	0
2	O	9	0	5	2	0
2	P	9	0	5	2	0
2	Q	9	0	5	2	0
2	R	9	0	5	3	0
2	S	9	0	5	2	0
2	T	9	0	5	2	0
3	A	6	0	8	3	0
3	B	6	0	8	1	0
3	C	6	0	8	7	0
3	D	6	0	8	4	0
3	E	6	0	8	2	0
3	F	6	0	8	3	0
3	G	6	0	8	1	0
3	H	6	0	8	2	0
3	I	6	0	8	4	0
3	J	6	0	8	4	0
3	K	6	0	8	1	0
3	L	6	0	8	3	0
3	M	6	0	8	5	0
3	N	6	0	8	3	0
3	O	6	0	8	6	0
3	P	6	0	8	4	0
3	Q	6	0	8	1	0
3	R	6	0	8	8	0
3	S	6	0	8	3	0
3	T	6	0	8	2	0
4	A	10	0	0	0	0
4	B	15	0	0	1	0
4	C	7	0	0	3	0
4	D	6	0	0	1	0
4	E	12	0	0	5	0
4	F	5	0	0	4	0
4	G	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	12	0	0	0	0
4	I	10	0	0	1	0
4	J	8	0	0	3	0
4	K	12	0	0	3	0
4	L	10	0	0	1	0
4	M	9	0	0	3	0
4	N	6	0	0	2	0
4	O	10	0	0	2	0
4	P	5	0	0	0	0
4	Q	16	0	0	1	0
4	R	12	0	0	4	0
4	S	8	0	0	2	0
4	T	8	0	0	3	0
All	All	41213	0	40929	1666	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 20.

The worst 5 of 1666 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:H:30:VAL:HG21	1:H:54:VAL:HG11	1.38	1.05
1:D:212:LYS:HD2	1:D:239:ASN:HA	1.37	1.05
1:E:74:ARG:HH11	1:E:74:ARG:HG3	1.12	1.04
1:B:9:ASN:ND2	1:B:12:LYS:H	1.55	1.03
1:M:265:GLU:HA	1:M:268:LYS:HD3	1.37	1.02

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	269/273 (98%)	253 (94%)	12 (4%)	4 (2%)	10 33
1	B	269/273 (98%)	248 (92%)	18 (7%)	3 (1%)	14 41
1	C	269/273 (98%)	251 (93%)	13 (5%)	5 (2%)	8 26
1	D	269/273 (98%)	251 (93%)	14 (5%)	4 (2%)	10 33
1	E	269/273 (98%)	251 (93%)	14 (5%)	4 (2%)	10 33
1	F	269/273 (98%)	251 (93%)	13 (5%)	5 (2%)	8 26
1	G	269/273 (98%)	246 (91%)	15 (6%)	8 (3%)	4 15
1	H	269/273 (98%)	258 (96%)	11 (4%)	0	100 100
1	I	269/273 (98%)	254 (94%)	14 (5%)	1 (0%)	34 66
1	J	269/273 (98%)	251 (93%)	15 (6%)	3 (1%)	14 41
1	K	269/273 (98%)	248 (92%)	18 (7%)	3 (1%)	14 41
1	L	269/273 (98%)	248 (92%)	17 (6%)	4 (2%)	10 33
1	M	269/273 (98%)	246 (91%)	21 (8%)	2 (1%)	22 53
1	N	269/273 (98%)	251 (93%)	12 (4%)	6 (2%)	6 22
1	O	269/273 (98%)	250 (93%)	17 (6%)	2 (1%)	22 53
1	P	269/273 (98%)	255 (95%)	13 (5%)	1 (0%)	34 66
1	Q	269/273 (98%)	249 (93%)	17 (6%)	3 (1%)	14 41
1	R	269/273 (98%)	251 (93%)	16 (6%)	2 (1%)	22 53
1	S	269/273 (98%)	259 (96%)	9 (3%)	1 (0%)	34 66
1	T	265/273 (97%)	248 (94%)	10 (4%)	7 (3%)	5 18
All	All	5376/5460 (98%)	5019 (93%)	289 (5%)	68 (1%)	12 36

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	C	74	ARG
1	E	268	LYS
1	F	3	LEU
1	F	77	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	214/220 (97%)	199 (93%)	15 (7%)	15	40
1	B	212/220 (96%)	198 (93%)	14 (7%)	16	44
1	C	211/220 (96%)	202 (96%)	9 (4%)	29	62
1	D	213/220 (97%)	201 (94%)	12 (6%)	21	51
1	E	215/220 (98%)	198 (92%)	17 (8%)	12	34
1	F	214/220 (97%)	202 (94%)	12 (6%)	21	51
1	G	214/220 (97%)	200 (94%)	14 (6%)	17	44
1	H	213/220 (97%)	196 (92%)	17 (8%)	12	34
1	I	213/220 (97%)	200 (94%)	13 (6%)	18	48
1	J	212/220 (96%)	203 (96%)	9 (4%)	30	63
1	K	212/220 (96%)	202 (95%)	10 (5%)	26	59
1	L	212/220 (96%)	200 (94%)	12 (6%)	20	50
1	M	213/220 (97%)	201 (94%)	12 (6%)	21	51
1	N	212/220 (96%)	199 (94%)	13 (6%)	18	48
1	O	211/220 (96%)	202 (96%)	9 (4%)	29	62
1	P	214/220 (97%)	202 (94%)	12 (6%)	21	51
1	Q	212/220 (96%)	198 (93%)	14 (7%)	16	44
1	R	213/220 (97%)	201 (94%)	12 (6%)	21	51
1	S	213/220 (97%)	204 (96%)	9 (4%)	30	63
1	T	211/220 (96%)	200 (95%)	11 (5%)	23	55
All	All	4254/4400 (97%)	4008 (94%)	246 (6%)	20	50

5 of 246 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	6	ASP
1	K	95	ASN
1	S	3	LEU
1	I	52	ASN
1	J	52	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 117 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	95	ASN
1	K	214	ASN
1	S	71	HIS
1	I	161	ASN
1	J	214	ASN

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	$\#\|Z\| > 2$
3	GOL	L	500	-	5,5,5	0.22	0	5,5,5	0.85	0
3	GOL	E	500	-	5,5,5	0.33	0	5,5,5	0.67	0
3	GOL	I	500	-	5,5,5	0.26	0	5,5,5	0.65	0
3	GOL	J	500	-	5,5,5	0.30	0	5,5,5	0.42	0
2	13P	Q	501	1	8,8,9	1.53	1 (12%)	10,10,12	1.25	2 (20%)
3	GOL	B	500	-	5,5,5	0.26	0	5,5,5	0.42	0
3	GOL	P	500	-	5,5,5	0.20	0	5,5,5	0.45	0
2	13P	B	501	1	8,8,9	1.51	1 (12%)	10,10,12	1.24	2 (20%)
2	13P	M	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.26	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	13P	N	501	1	8,8,9	1.52	1 (12%)	10,10,12	1.26	2 (20%)
3	GOL	T	500	-	5,5,5	0.25	0	5,5,5	0.65	0
2	13P	J	501	1	8,8,9	1.51	1 (12%)	10,10,12	1.27	2 (20%)
2	13P	H	501	1	8,8,9	1.50	1 (12%)	10,10,12	1.26	2 (20%)
3	GOL	M	500	-	5,5,5	0.21	0	5,5,5	0.50	0
2	13P	S	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.25	2 (20%)
2	13P	T	501	1	8,8,9	1.48	1 (12%)	10,10,12	1.24	2 (20%)
2	13P	R	501	1	8,8,9	1.55	1 (12%)	10,10,12	1.25	2 (20%)
3	GOL	R	500	-	5,5,5	0.30	0	5,5,5	0.41	0
2	13P	E	501	1	8,8,9	1.51	1 (12%)	10,10,12	1.25	2 (20%)
2	13P	F	501	1	8,8,9	1.48	1 (12%)	10,10,12	1.26	2 (20%)
2	13P	G	501	1	8,8,9	1.51	1 (12%)	10,10,12	1.26	2 (20%)
2	13P	A	501	1	8,8,9	1.52	1 (12%)	10,10,12	1.24	2 (20%)
3	GOL	K	500	-	5,5,5	0.25	0	5,5,5	0.45	0
2	13P	I	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.25	2 (20%)
2	13P	K	501	1	8,8,9	1.50	1 (12%)	10,10,12	1.24	2 (20%)
3	GOL	C	500	-	5,5,5	0.27	0	5,5,5	0.48	0
2	13P	L	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.24	2 (20%)
2	13P	P	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.25	2 (20%)
3	GOL	H	500	-	5,5,5	0.29	0	5,5,5	0.76	0
3	GOL	A	500	-	5,5,5	0.36	0	5,5,5	0.28	0
2	13P	C	501	1	8,8,9	1.50	1 (12%)	10,10,12	1.26	2 (20%)
2	13P	D	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.26	2 (20%)
2	13P	O	501	1	8,8,9	1.49	1 (12%)	10,10,12	1.25	2 (20%)
3	GOL	G	500	-	5,5,5	0.28	0	5,5,5	0.75	0
3	GOL	S	500	-	5,5,5	0.29	0	5,5,5	0.43	0
3	GOL	O	500	-	5,5,5	0.21	0	5,5,5	0.37	0
3	GOL	F	500	-	5,5,5	0.21	0	5,5,5	0.50	0
3	GOL	D	500	-	5,5,5	0.27	0	5,5,5	0.49	0
3	GOL	N	500	-	5,5,5	0.21	0	5,5,5	0.46	0
3	GOL	Q	500	-	5,5,5	0.25	0	5,5,5	0.73	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
3	GOL	L	500	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	500	-	-	0/4/4/4	-
3	GOL	I	500	-	-	0/4/4/4	-
3	GOL	J	500	-	-	0/4/4/4	-
2	13P	Q	501	1	-	3/6/6/8	-
3	GOL	B	500	-	-	0/4/4/4	-
3	GOL	P	500	-	-	0/4/4/4	-
2	13P	B	501	1	-	2/6/6/8	-
2	13P	M	501	1	-	3/6/6/8	-
2	13P	N	501	1	-	3/6/6/8	-
3	GOL	T	500	-	-	0/4/4/4	-
2	13P	J	501	1	-	3/6/6/8	-
2	13P	H	501	1	-	2/6/6/8	-
3	GOL	M	500	-	-	0/4/4/4	-
2	13P	S	501	1	-	2/6/6/8	-
2	13P	T	501	1	-	3/6/6/8	-
2	13P	R	501	1	-	3/6/6/8	-
3	GOL	R	500	-	-	0/4/4/4	-
2	13P	E	501	1	-	3/6/6/8	-
2	13P	F	501	1	-	3/6/6/8	-
2	13P	G	501	1	-	3/6/6/8	-
2	13P	A	501	1	-	3/6/6/8	-
3	GOL	K	500	-	-	0/4/4/4	-
2	13P	I	501	1	-	3/6/6/8	-
2	13P	K	501	1	-	3/6/6/8	-
3	GOL	C	500	-	-	0/4/4/4	-
2	13P	L	501	1	-	3/6/6/8	-
2	13P	P	501	1	-	3/6/6/8	-
3	GOL	H	500	-	-	0/4/4/4	-
3	GOL	A	500	-	-	0/4/4/4	-
2	13P	C	501	1	-	3/6/6/8	-
2	13P	D	501	1	-	2/6/6/8	-
2	13P	O	501	1	-	3/6/6/8	-
3	GOL	G	500	-	-	0/4/4/4	-
3	GOL	S	500	-	-	0/4/4/4	-
3	GOL	O	500	-	-	0/4/4/4	-
3	GOL	F	500	-	-	0/4/4/4	-
3	GOL	D	500	-	-	0/4/4/4	-
3	GOL	N	500	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	Q	500	-	-	0/4/4/4	-

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	501	13P	P-O1P	3.41	1.61	1.50
2	B	501	13P	P-O1P	3.39	1.61	1.50
2	Q	501	13P	P-O1P	3.35	1.61	1.50
2	L	501	13P	P-O1P	3.35	1.61	1.50
2	G	501	13P	P-O1P	3.35	1.61	1.50

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	501	13P	C1-C2-C3	2.79	120.04	113.95
2	D	501	13P	C1-C2-C3	2.73	119.91	113.95
2	F	501	13P	C1-C2-C3	2.73	119.90	113.95
2	K	501	13P	C1-C2-C3	2.72	119.88	113.95
2	C	501	13P	C1-C2-C3	2.71	119.86	113.95

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Q	501	13P	C1-C2-C3-O3
2	B	501	13P	C1-C2-C3-O3
2	M	501	13P	C1-C2-C3-O3
2	N	501	13P	C1-C2-C3-O3
2	J	501	13P	C1-C2-C3-O3

There are no ring outliers.

40 monomers are involved in 111 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	500	GOL	3	0
3	E	500	GOL	2	0
3	I	500	GOL	4	0
3	J	500	GOL	4	0
2	Q	501	13P	2	0
3	B	500	GOL	1	0
3	P	500	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	13P	2	0
2	M	501	13P	2	0
2	N	501	13P	2	0
3	T	500	GOL	2	0
2	J	501	13P	2	0
2	H	501	13P	2	0
3	M	500	GOL	5	0
2	S	501	13P	2	0
2	T	501	13P	2	0
2	R	501	13P	3	0
3	R	500	GOL	8	0
2	E	501	13P	2	0
2	F	501	13P	2	0
2	G	501	13P	3	0
2	A	501	13P	3	0
3	K	500	GOL	1	0
2	I	501	13P	2	0
2	K	501	13P	2	0
3	C	500	GOL	7	0
2	L	501	13P	2	0
2	P	501	13P	2	0
3	H	500	GOL	2	0
3	A	500	GOL	3	0
2	C	501	13P	2	0
2	D	501	13P	3	0
2	O	501	13P	2	0
3	G	500	GOL	1	0
3	S	500	GOL	3	0
3	O	500	GOL	6	0
3	F	500	GOL	3	0
3	D	500	GOL	4	0
3	N	500	GOL	3	0
3	Q	500	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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	271/273 (99%)	-0.47	0 100 100	9, 47, 97, 170	0
1	B	271/273 (99%)	-0.44	4 (1%) 73 68	15, 52, 113, 178	0
1	C	271/273 (99%)	-0.37	2 (0%) 87 84	17, 55, 115, 167	0
1	D	271/273 (99%)	-0.44	2 (0%) 87 84	17, 53, 112, 166	0
1	E	271/273 (99%)	-0.46	3 (1%) 80 75	17, 48, 104, 181	0
1	F	271/273 (99%)	-0.42	1 (0%) 92 91	19, 52, 107, 158	0
1	G	271/273 (99%)	-0.48	0 100 100	12, 46, 106, 137	0
1	H	271/273 (99%)	-0.50	1 (0%) 92 91	15, 44, 103, 157	0
1	I	271/273 (99%)	-0.45	0 100 100	16, 50, 110, 149	0
1	J	271/273 (99%)	-0.33	5 (1%) 68 61	16, 54, 115, 196	0
1	K	271/273 (99%)	-0.42	1 (0%) 92 91	17, 50, 111, 200	0
1	L	271/273 (99%)	-0.49	0 100 100	16, 50, 106, 163	0
1	M	271/273 (99%)	-0.29	5 (1%) 68 61	7, 55, 120, 160	0
1	N	271/273 (99%)	-0.18	12 (4%) 34 24	23, 65, 130, 201	0
1	O	271/273 (99%)	-0.35	3 (1%) 80 75	8, 59, 113, 173	0
1	P	271/273 (99%)	-0.50	1 (0%) 92 91	16, 45, 91, 162	0
1	Q	271/273 (99%)	-0.40	2 (0%) 87 84	17, 49, 107, 202	0
1	R	271/273 (99%)	-0.38	3 (1%) 80 75	8, 49, 109, 202	0
1	S	271/273 (99%)	-0.35	6 (2%) 62 52	19, 51, 109, 202	0
1	T	269/273 (98%)	-0.32	4 (1%) 73 68	18, 57, 122, 161	0
All	All	5418/5460 (99%)	-0.40	55 (1%) 82 77	7, 52, 113, 202	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	211	PRO	11.8
1	M	79	ASP	10.4
1	S	210	GLY	10.0
1	R	76	TYR	9.7
1	K	158	HIS	8.6

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	GOL	J	500	6/6	0.55	0.56	57,58,58,61	0
3	GOL	D	500	6/6	0.70	0.68	57,58,58,61	0
3	GOL	C	500	6/6	0.75	0.61	57,58,58,61	0
2	13P	T	501	9/10	0.81	0.24	57,59,63,64	0
2	13P	F	501	9/10	0.83	0.33	57,59,63,64	0
3	GOL	N	500	6/6	0.83	0.41	57,58,58,61	0
2	13P	R	501	9/10	0.84	0.37	57,59,63,64	0
3	GOL	H	500	6/6	0.85	0.19	57,58,58,61	0
2	13P	S	501	9/10	0.85	0.33	57,59,63,64	0
3	GOL	P	500	6/6	0.85	0.22	57,58,58,61	0
3	GOL	M	500	6/6	0.86	0.49	57,58,58,61	0
3	GOL	I	500	6/6	0.86	0.66	57,58,58,61	0
3	GOL	B	500	6/6	0.86	0.34	57,58,58,61	0
2	13P	O	501	9/10	0.86	0.21	57,59,63,64	0
3	GOL	O	500	6/6	0.86	0.35	57,58,58,61	0
3	GOL	F	500	6/6	0.86	0.37	57,58,58,61	0
3	GOL	E	500	6/6	0.86	0.45	57,58,58,61	0
2	13P	N	501	9/10	0.86	0.26	57,59,63,64	0
2	13P	I	501	9/10	0.87	0.23	57,59,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	T	500	6/6	0.87	0.47	57,58,58,61	0
3	GOL	Q	500	6/6	0.87	0.72	57,58,58,61	0
3	GOL	G	500	6/6	0.89	0.37	57,58,58,61	0
3	GOL	R	500	6/6	0.89	0.41	57,58,58,61	0
3	GOL	S	500	6/6	0.90	0.41	57,58,58,61	0
2	13P	E	501	9/10	0.90	0.30	57,59,63,64	0
2	13P	K	501	9/10	0.90	0.27	57,59,63,64	0
2	13P	J	501	9/10	0.91	0.25	57,59,63,64	0
3	GOL	K	500	6/6	0.91	0.23	57,58,58,61	0
2	13P	C	501	9/10	0.91	0.23	57,59,63,64	0
2	13P	D	501	9/10	0.91	0.34	57,59,63,64	0
2	13P	Q	501	9/10	0.92	0.18	57,59,63,64	0
3	GOL	L	500	6/6	0.92	0.35	57,58,58,61	0
2	13P	L	501	9/10	0.92	0.24	57,59,63,64	0
3	GOL	A	500	6/6	0.92	0.41	57,58,58,61	0
2	13P	H	501	9/10	0.93	0.20	57,59,63,64	0
2	13P	M	501	9/10	0.93	0.16	57,59,63,64	0
2	13P	A	501	9/10	0.93	0.32	57,59,63,64	0
2	13P	P	501	9/10	0.93	0.16	57,59,63,64	0
2	13P	B	501	9/10	0.93	0.30	57,59,63,64	0
2	13P	G	501	9/10	0.94	0.18	57,59,63,64	0

6.5 Other polymers (i)

There are no such residues in this entry.