



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:17 AM BST

PDB ID : 6BFZ
Title : Crystal structure of enolase from E. coli with a mixture of apo form, substrate, and product form
Authors : Erlandsen, H.; Wright, D.; Krucinska, J.
Deposited on : 2017-10-27
Resolution : 2.21 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

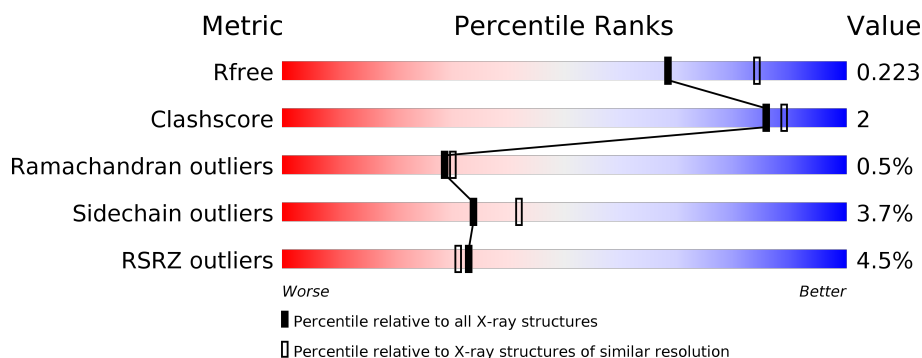
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 $\leq 5\%$. 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	449	<div> <div>0%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	449	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>..</div> </div> </div>
1	C	449	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>..</div> </div> </div>
1	D	449	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	E	449	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>..</div> </div> </div>
1	F	449	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>6%</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	PEP	E	602	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20287 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3246	2030	557	644	15			
1	B	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	E	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	F	438	Total	C	N	O	S	0	1	0
			3254	2036	559	644	15			
1	D	438	Total	C	N	O	S	0	1	0
			3253	2034	559	645	15			
1	C	429	Total	C	N	O	S	0	0	0
			3183	1996	544	628	15			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP B7MLA0
A	-16	SER	-	expression tag	UNP B7MLA0
A	-15	HIS	-	expression tag	UNP B7MLA0
A	-14	MET	-	expression tag	UNP B7MLA0
A	-13	ALA	-	expression tag	UNP B7MLA0
A	-12	SER	-	expression tag	UNP B7MLA0
A	-11	MET	-	expression tag	UNP B7MLA0
A	-10	THR	-	expression tag	UNP B7MLA0
A	-9	GLY	-	expression tag	UNP B7MLA0
A	-8	GLY	-	expression tag	UNP B7MLA0
A	-7	GLN	-	expression tag	UNP B7MLA0
A	-6	GLN	-	expression tag	UNP B7MLA0
A	-5	MET	-	expression tag	UNP B7MLA0
A	-4	GLY	-	expression tag	UNP B7MLA0
A	-3	ARG	-	expression tag	UNP B7MLA0
A	-2	GLY	-	expression tag	UNP B7MLA0
A	-1	SER	-	expression tag	UNP B7MLA0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP B7MLA0
B	-16	SER	-	expression tag	UNP B7MLA0
B	-15	HIS	-	expression tag	UNP B7MLA0
B	-14	MET	-	expression tag	UNP B7MLA0
B	-13	ALA	-	expression tag	UNP B7MLA0
B	-12	SER	-	expression tag	UNP B7MLA0
B	-11	MET	-	expression tag	UNP B7MLA0
B	-10	THR	-	expression tag	UNP B7MLA0
B	-9	GLY	-	expression tag	UNP B7MLA0
B	-8	GLY	-	expression tag	UNP B7MLA0
B	-7	GLN	-	expression tag	UNP B7MLA0
B	-6	GLN	-	expression tag	UNP B7MLA0
B	-5	MET	-	expression tag	UNP B7MLA0
B	-4	GLY	-	expression tag	UNP B7MLA0
B	-3	ARG	-	expression tag	UNP B7MLA0
B	-2	GLY	-	expression tag	UNP B7MLA0
B	-1	SER	-	expression tag	UNP B7MLA0
E	-17	GLY	-	expression tag	UNP B7MLA0
E	-16	SER	-	expression tag	UNP B7MLA0
E	-15	HIS	-	expression tag	UNP B7MLA0
E	-14	MET	-	expression tag	UNP B7MLA0
E	-13	ALA	-	expression tag	UNP B7MLA0
E	-12	SER	-	expression tag	UNP B7MLA0
E	-11	MET	-	expression tag	UNP B7MLA0
E	-10	THR	-	expression tag	UNP B7MLA0
E	-9	GLY	-	expression tag	UNP B7MLA0
E	-8	GLY	-	expression tag	UNP B7MLA0
E	-7	GLN	-	expression tag	UNP B7MLA0
E	-6	GLN	-	expression tag	UNP B7MLA0
E	-5	MET	-	expression tag	UNP B7MLA0
E	-4	GLY	-	expression tag	UNP B7MLA0
E	-3	ARG	-	expression tag	UNP B7MLA0
E	-2	GLY	-	expression tag	UNP B7MLA0
E	-1	SER	-	expression tag	UNP B7MLA0
F	-17	GLY	-	expression tag	UNP B7MLA0
F	-16	SER	-	expression tag	UNP B7MLA0
F	-15	HIS	-	expression tag	UNP B7MLA0
F	-14	MET	-	expression tag	UNP B7MLA0
F	-13	ALA	-	expression tag	UNP B7MLA0
F	-12	SER	-	expression tag	UNP B7MLA0
F	-11	MET	-	expression tag	UNP B7MLA0
F	-10	THR	-	expression tag	UNP B7MLA0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	expression tag	UNP B7MLA0
F	-8	GLY	-	expression tag	UNP B7MLA0
F	-7	GLN	-	expression tag	UNP B7MLA0
F	-6	GLN	-	expression tag	UNP B7MLA0
F	-5	MET	-	expression tag	UNP B7MLA0
F	-4	GLY	-	expression tag	UNP B7MLA0
F	-3	ARG	-	expression tag	UNP B7MLA0
F	-2	GLY	-	expression tag	UNP B7MLA0
F	-1	SER	-	expression tag	UNP B7MLA0
D	-17	GLY	-	expression tag	UNP B7MLA0
D	-16	SER	-	expression tag	UNP B7MLA0
D	-15	HIS	-	expression tag	UNP B7MLA0
D	-14	MET	-	expression tag	UNP B7MLA0
D	-13	ALA	-	expression tag	UNP B7MLA0
D	-12	SER	-	expression tag	UNP B7MLA0
D	-11	MET	-	expression tag	UNP B7MLA0
D	-10	THR	-	expression tag	UNP B7MLA0
D	-9	GLY	-	expression tag	UNP B7MLA0
D	-8	GLY	-	expression tag	UNP B7MLA0
D	-7	GLN	-	expression tag	UNP B7MLA0
D	-6	GLN	-	expression tag	UNP B7MLA0
D	-5	MET	-	expression tag	UNP B7MLA0
D	-4	GLY	-	expression tag	UNP B7MLA0
D	-3	ARG	-	expression tag	UNP B7MLA0
D	-2	GLY	-	expression tag	UNP B7MLA0
D	-1	SER	-	expression tag	UNP B7MLA0
C	-17	GLY	-	expression tag	UNP B7MLA0
C	-16	SER	-	expression tag	UNP B7MLA0
C	-15	HIS	-	expression tag	UNP B7MLA0
C	-14	MET	-	expression tag	UNP B7MLA0
C	-13	ALA	-	expression tag	UNP B7MLA0
C	-12	SER	-	expression tag	UNP B7MLA0
C	-11	MET	-	expression tag	UNP B7MLA0
C	-10	THR	-	expression tag	UNP B7MLA0
C	-9	GLY	-	expression tag	UNP B7MLA0
C	-8	GLY	-	expression tag	UNP B7MLA0
C	-7	GLN	-	expression tag	UNP B7MLA0
C	-6	GLN	-	expression tag	UNP B7MLA0
C	-5	MET	-	expression tag	UNP B7MLA0
C	-4	GLY	-	expression tag	UNP B7MLA0
C	-3	ARG	-	expression tag	UNP B7MLA0
C	-2	GLY	-	expression tag	UNP B7MLA0

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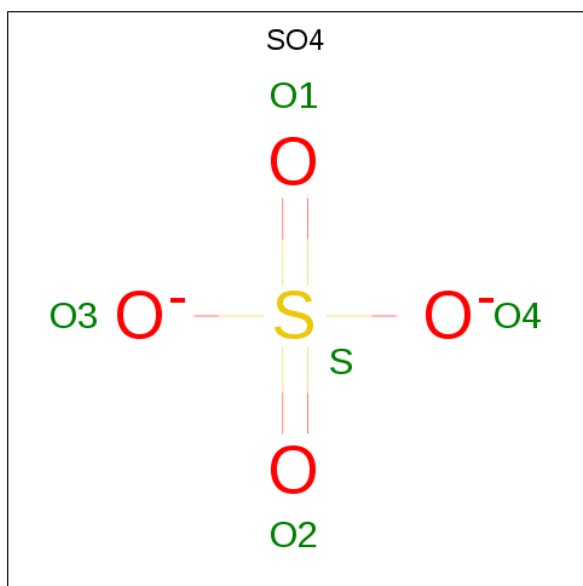
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP B7MLA0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



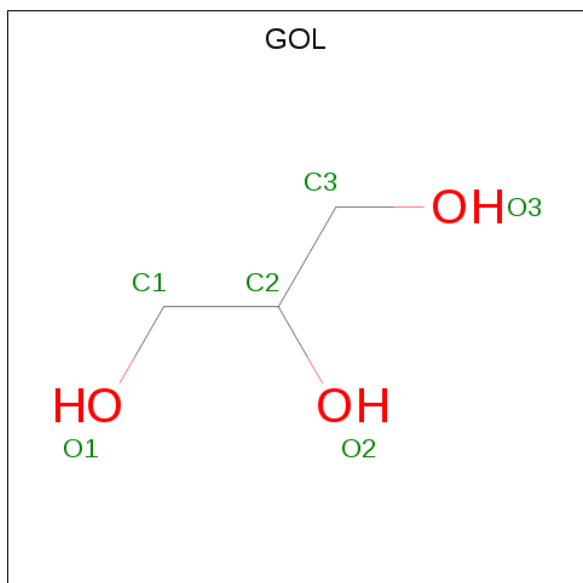
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



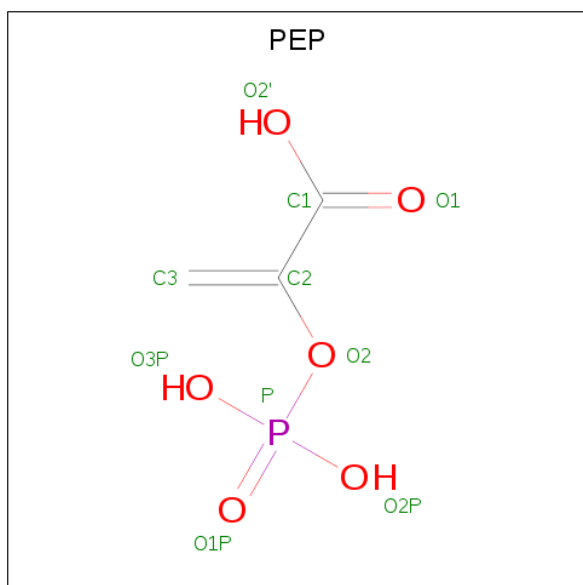
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

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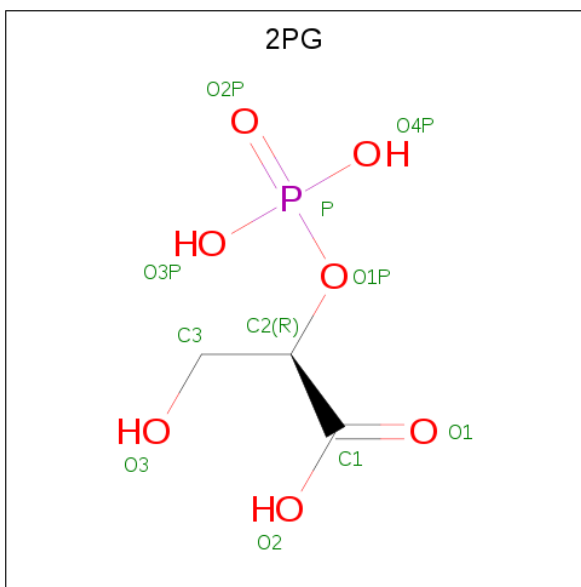
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



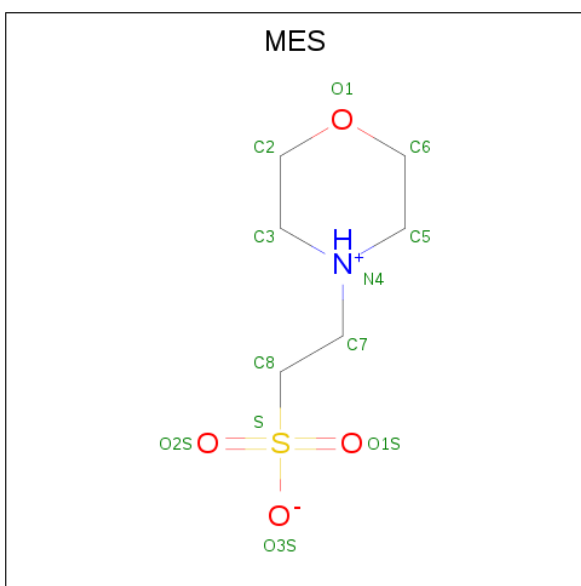
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 6 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	O	P	0	0
			11	3	7	1		
6	F	1	Total	C	O	P	0	0
			11	3	7	1		
6	D	1	Total	C	O	P	0	0
			11	3	7	1		
6	C	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

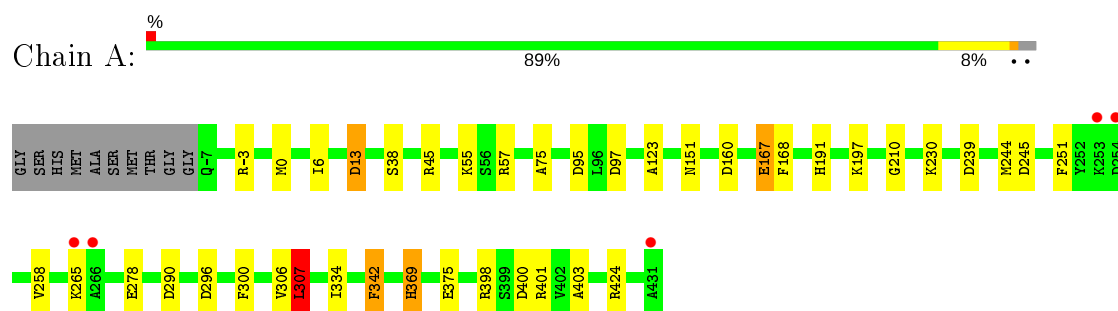
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	133	Total	O	0	0
			133	133		
8	B	110	Total	O	0	0
			110	110		
8	E	133	Total	O	0	0
			133	133		
8	F	97	Total	O	0	0
			97	97		
8	D	113	Total	O	0	0
			113	113		
8	C	90	Total	O	0	0
			90	90		

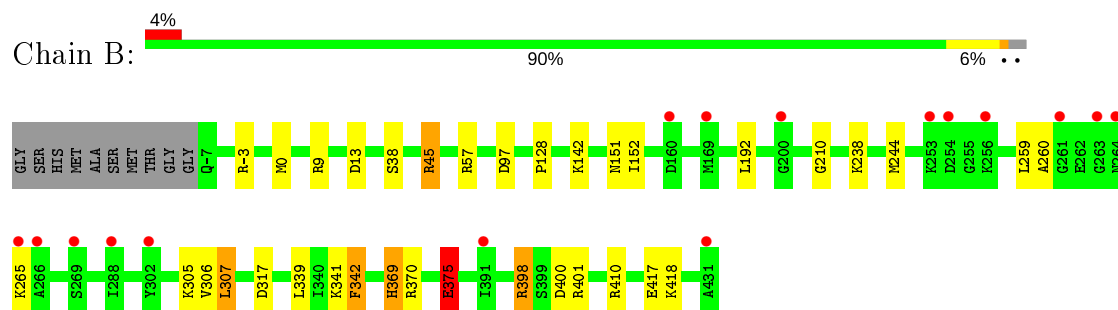
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

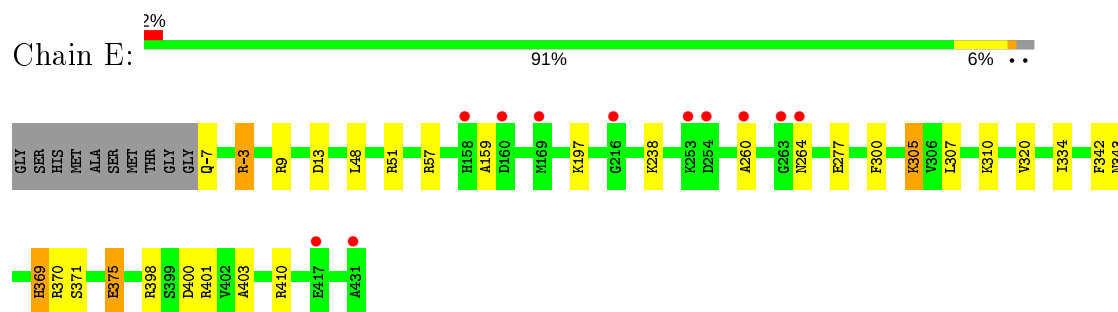
- Molecule 1: Enolase



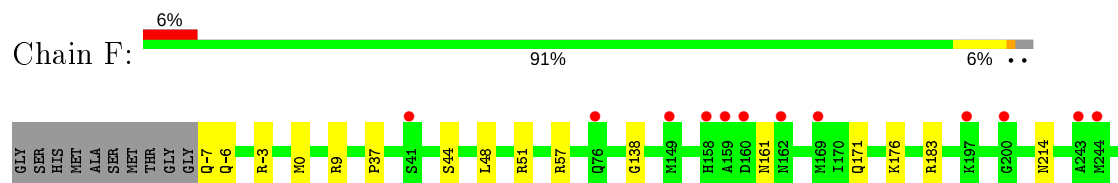
- Molecule 1: Enolase

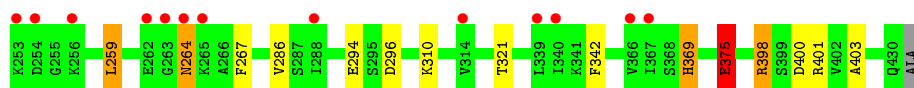


- Molecule 1: Enolase

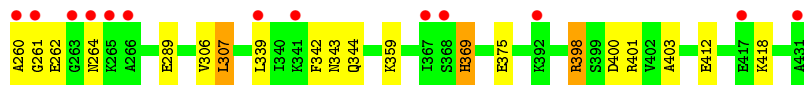
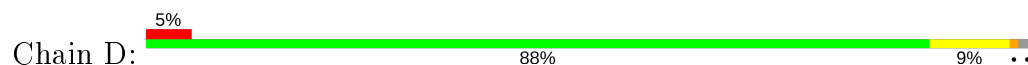


- Molecule 1: Enolase

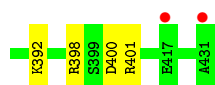
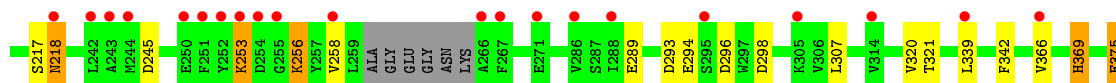
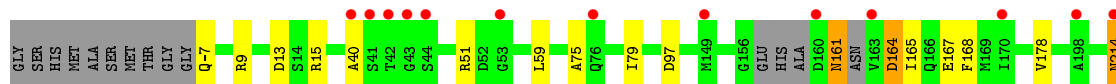
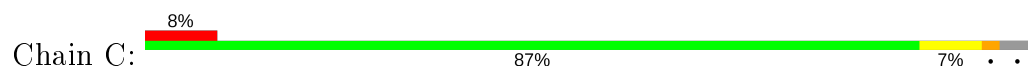




• Molecule 1: Enolase



• Molecule 1: Enolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.26 Å 143.29 Å 207.04 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 – 2.21 29.69 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.69-2.21) 99.4 (29.69-2.21)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.171 , 0.218 0.180 , 0.223	Depositor DCC
R_{free} test set	8374 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20287	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, MES, PEP, SO4, 2PG

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	0.90	1/3288 (0.0%)	0.96	13/4427 (0.3%)
1	B	0.90	2/3296 (0.1%)	0.95	11/4435 (0.2%)
1	C	0.93	0/3221	0.95	8/4330 (0.2%)
1	D	0.92	0/3294	0.93	10/4432 (0.2%)
1	E	0.90	1/3296 (0.0%)	0.92	9/4435 (0.2%)
1	F	0.88	0/3299	0.94	16/4439 (0.4%)
All	All	0.90	4/19694 (0.0%)	0.94	67/26498 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	SER	CB-OG	7.53	1.52	1.42
1	E	371	SER	CB-OG	-5.72	1.34	1.42
1	A	38	SER	CB-OG	5.20	1.49	1.42
1	B	417	GLU	CG-CD	5.15	1.59	1.51

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NE-CZ-NH1	11.78	126.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	A	45	ARG	NE-CZ-NH2	-10.15	115.23	120.30
1	B	45	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	D	13	ASP	CB-CG-OD1	8.41	125.87	118.30
1	E	51	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	375	GLU	CB-CA-C	-7.09	96.22	110.40
1	C	15	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	C	293	ASP	CB-CG-OD1	6.91	124.52	118.30
1	E	57	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	E	410	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	E	13	ASP	CB-CG-OD1	6.82	124.44	118.30
1	E	51	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	57	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	F	375	GLU	CB-CA-C	-6.78	96.83	110.40
1	A	290	ASP	CB-CG-OD1	6.62	124.26	118.30
1	F	183	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	F	57	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	D	375	GLU	CB-CA-C	-6.46	97.49	110.40
1	A	296	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	13	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	375	GLU	CB-CA-C	-6.26	97.88	110.40
1	E	9	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	51	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	290	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	F	0	MET	CG-SD-CE	6.10	109.96	100.20
1	F	296	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	B	13	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	57	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	E	375	GLU	CB-CA-C	-6.01	98.38	110.40
1	C	375	GLU	CB-CA-C	-6.01	98.38	110.40
1	B	398	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	97	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	D	51	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	F	296	ASP	CB-CG-OD1	5.87	123.58	118.30
1	F	375	GLU	CA-CB-CG	5.86	126.30	113.40
1	F	51	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	51	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	342	PHE	CB-CG-CD1	5.75	124.83	120.80
1	C	9	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	239	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	0	MET	CG-SD-CE	5.68	109.29	100.20
1	F	183	ARG	NE-CZ-NH1	5.65	123.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	398	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	51	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	82	ASP	CB-CG-OD1	5.55	123.30	118.30
1	D	13	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	F	51	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	183	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	9	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	410	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	57	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	E	410	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	398	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	307	LEU	CA-CB-CG	5.28	127.44	115.30
1	E	305	LYS	CA-CB-CG	5.25	124.94	113.40
1	C	296	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	95	ASP	CB-CG-OD1	5.21	122.99	118.30
1	F	57	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	398	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	13	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	370	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	342	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	F	9	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	F	-3	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	F	-7	GLN	CB-CA-C	5.02	120.44	110.40
1	D	207	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	40	ALA	Peptide
1	D	156	GLY	Peptide

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	3246	0	3257	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3254	0	3279	10	0
1	C	3183	0	3216	15	0
1	D	3253	0	3267	25	0
1	E	3254	0	3279	10	0
1	F	3254	0	3280	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	20	0	0	0	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	B	6	0	8	1	0
4	C	6	0	8	2	0
4	F	6	0	8	0	0
5	E	10	0	1	6	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
6	E	11	0	1	3	0
6	F	11	0	4	0	0
7	D	12	0	13	0	0
7	E	12	0	13	0	0
8	A	133	0	0	3	0
8	B	110	0	0	0	0
8	C	90	0	0	1	0
8	D	113	0	0	2	0
8	E	133	0	0	2	0
8	F	97	0	0	0	0
All	All	20287	0	19642	85	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 2.

All (85) 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:D:101[B]:ASN:HD22	1:D:101[B]:ASN:H	1.22	0.87
5:E:602:PEP:O2'	6:E:603:2PG:O2P	1.94	0.85
1:D:101[B]:ASN:ND2	8:D:601:HOH:O	2.17	0.77
1:E:-7:GLN:OE1	8:E:702:HOH:O	2.05	0.75
1:F:369:HIS:CD2	1:F:401:ARG:HH11	2.06	0.73
5:E:602:PEP:O1P	5:E:602:PEP:O2'	2.08	0.68
5:E:602:PEP:O1P	5:E:602:PEP:C1	2.41	0.68
1:D:306:VAL:HG12	1:D:307:LEU:HD13	1.77	0.67
1:D:155:GLY:O	1:D:163:VAL:O	2.13	0.66
1:E:369:HIS:CD2	1:E:401:ARG:HH11	2.14	0.65
1:D:369:HIS:CD2	1:D:401:ARG:HH11	2.14	0.65
1:B:369:HIS:CD2	1:B:401:ARG:HH11	2.16	0.64
1:C:75:ALA:O	1:C:79:ILE:HG12	1.99	0.63
1:D:403:ALA:HB2	1:C:375:GLU:HG3	1.81	0.62
1:E:403:ALA:HB2	1:F:375:GLU:HG3	1.81	0.61
1:A:403:ALA:HB2	1:B:375:GLU:HG3	1.83	0.60
1:D:158:HIS:O	1:D:160:ASP:N	2.35	0.60
1:C:167:GLU:OE1	1:C:392:LYS:CE	2.49	0.60
1:D:162:ASN:HD22	1:D:162:ASN:H	1.52	0.58
1:D:165:ILE:HD13	1:D:244:MET:HE3	1.86	0.58
1:B:-3:ARG:HD3	4:B:604:GOL:H2	1.86	0.57
1:A:369:HIS:CD2	1:A:401:ARG:HH11	2.23	0.56
1:C:245:ASP:HA	1:C:289:GLU:HB3	1.86	0.56
1:A:168:PHE:CE1	1:A:244:MET:HE2	2.41	0.56
1:F:369:HIS:HD2	1:F:401:ARG:HH11	1.53	0.55
1:D:260:ALA:HA	1:D:264:ASN:HD22	1.72	0.54
1:C:369:HIS:CD2	1:C:401:ARG:HH11	2.25	0.54
1:D:101[B]:ASN:ND2	1:D:101[B]:ASN:H	1.98	0.54
1:C:164:ASP:OD2	1:C:218:ASN:HA	2.08	0.53
1:F:44:SER:HB2	1:F:294:GLU:OE2	2.08	0.53
5:E:602:PEP:O2'	6:E:603:2PG:P	2.63	0.53
1:C:167:GLU:OE1	1:C:392:LYS:HE2	2.09	0.52
1:E:370:ARG:NE	5:E:602:PEP:O2P	2.40	0.52
1:E:-3:ARG:HH11	4:C:505:GOL:H32	1.75	0.51
6:E:603:2PG:O3	8:E:701:HOH:O	0.58	0.50
1:A:251:PHE:HB2	1:A:258:VAL:O	2.13	0.48
1:D:165:ILE:HD13	1:D:244:MET:CE	2.43	0.48
1:D:179:LYS:HE3	8:C:679:HOH:O	2.13	0.48
1:E:277:GLU:HG3	1:E:307:LEU:HD11	1.95	0.48
1:A:191:HIS:HE1	8:A:826:HOH:O	1.97	0.48
1:B:306:VAL:HG12	1:B:307:LEU:HD13	1.95	0.48
1:B:151:ASN:ND2	1:B:210:GLY:HA3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:HIS:HD2	1:E:401:ARG:HH11	1.62	0.47
1:C:164:ASP:N	1:C:164:ASP:OD1	2.47	0.47
1:F:321:THR:O	1:F:321:THR:HG22	2.14	0.47
1:B:259:LEU:N	1:B:259:LEU:HD12	2.30	0.46
1:C:165:ILE:HB	1:C:168:PHE:CE1	2.50	0.46
1:A:306:VAL:HG12	1:A:307:LEU:HD13	1.97	0.46
1:E:-3:ARG:HH11	4:C:505:GOL:C3	2.29	0.46
1:D:369:HIS:HD2	1:D:401:ARG:HH11	1.60	0.45
1:A:424:ARG:HD2	8:A:704:HOH:O	2.16	0.45
5:E:602:PEP:P	5:E:602:PEP:O2'	2.71	0.45
1:E:300:PHE:HB3	1:E:334:ILE:HG23	1.99	0.45
1:A:300:PHE:HB3	1:A:334:ILE:HG23	1.99	0.45
1:B:152:ILE:HG13	1:B:192:LEU:CD2	2.48	0.44
1:D:101[B]:ASN:HD22	1:D:101[B]:ASN:N	1.94	0.44
1:D:245:ASP:HA	1:D:289:GLU:HB3	2.00	0.44
1:F:259:LEU:HD22	1:F:267:PHE:CE1	2.53	0.44
1:A:123:ALA:HB2	1:C:-7:GLN:HB3	2.00	0.44
1:D:150:MET:O	1:D:169:MET:HA	2.17	0.43
1:D:259:LEU:O	1:D:264:ASN:HA	2.18	0.43
1:B:339:LEU:HD23	1:B:341:LYS:HE3	2.00	0.43
1:C:339:LEU:HD12	1:C:366:VAL:HB	2.00	0.43
1:D:260:ALA:HA	1:D:264:ASN:ND2	2.34	0.43
1:F:171:GLN:HE22	1:F:286:VAL:CG2	2.32	0.43
1:E:375:GLU:HG3	1:F:403:ALA:HB2	2.00	0.42
8:A:703:HOH:O	1:F:138:GLY:HA2	2.20	0.42
1:C:59:LEU:HD12	1:C:59:LEU:N	2.35	0.42
1:D:359:LYS:HE2	8:D:645:HOH:O	2.19	0.42
1:C:320:VAL:O	1:C:321:THR:C	2.57	0.42
1:F:264:ASN:HD22	1:F:264:ASN:HA	1.67	0.41
1:C:253:LYS:O	1:C:256:LYS:HB2	2.19	0.41
1:D:289:GLU:OE2	1:D:339:LEU:HD22	2.20	0.41
1:A:-3:ARG:HG2	1:A:0:MET:CE	2.50	0.41
1:A:151:ASN:ND2	1:A:210:GLY:HA3	2.36	0.41
1:A:6:ILE:HD12	1:A:75:ALA:HA	2.03	0.41
1:B:151:ASN:HD22	1:B:210:GLY:HA3	1.85	0.41
1:C:161:ASN:CG	1:C:214:ASN:HA	2.41	0.41
1:D:46:GLU:CD	1:D:344:GLN:HG2	2.41	0.41
1:A:167:GLU:HG3	1:A:245:ASP:HB3	2.03	0.41
1:D:165:ILE:HD12	1:D:218:ASN:HB3	2.03	0.41
1:F:369:HIS:CD2	1:F:401:ARG:NH1	2.83	0.41
1:D:177:THR:HB	1:D:412:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101[B]:ASN:ND2	1:D:101[B]:ASN:N	2.64	0.40
1:B:45:ARG:HD3	3:B:602:SO4:O2	2.21	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	437/449 (97%)	423 (97%)	13 (3%)	1 (0%)	47	54
1	B	437/449 (97%)	423 (97%)	12 (3%)	2 (0%)	29	30
1	C	421/449 (94%)	397 (94%)	21 (5%)	3 (1%)	22	21
1	D	435/449 (97%)	417 (96%)	15 (3%)	3 (1%)	22	21
1	E	437/449 (97%)	418 (96%)	15 (3%)	4 (1%)	17	15
1	F	437/449 (97%)	422 (97%)	14 (3%)	1 (0%)	47	54
All	All	2604/2694 (97%)	2500 (96%)	90 (4%)	14 (0%)	29	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	262	GLU
1	C	164	ASP
1	D	261	GLY
1	B	260	ALA
1	E	159	ALA
1	E	260	ALA
1	E	398	ARG
1	F	398	ARG
1	A	398	ARG
1	D	398	ARG

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Mol	Chain	Res	Type
1	C	398	ARG
1	B	398	ARG
1	E	320	VAL
1	C	258	VAL

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	329/337 (98%)	317 (96%)	12 (4%)	35	43
1	B	331/337 (98%)	317 (96%)	14 (4%)	30	36
1	C	325/337 (96%)	311 (96%)	14 (4%)	29	35
1	D	331/337 (98%)	322 (97%)	9 (3%)	44	55
1	E	331/337 (98%)	320 (97%)	11 (3%)	38	47
1	F	332/337 (98%)	319 (96%)	13 (4%)	32	40
All	All	1979/2022 (98%)	1906 (96%)	73 (4%)	34	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	55	LYS
1	A	160	ASP
1	A	167	GLU
1	A	197	LYS
1	A	230	LYS
1	A	265	LYS
1	A	278	GLU
1	A	307	LEU
1	A	342	PHE
1	A	369	HIS
1	A	400	ASP
1	B	97	ASP
1	B	128	PRO

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Mol	Chain	Res	Type
1	B	142	LYS
1	B	238	LYS
1	B	244	MET
1	B	265	LYS
1	B	305	LYS
1	B	307	LEU
1	B	317	ASP
1	B	342	PHE
1	B	369	HIS
1	B	375	GLU
1	B	400	ASP
1	B	418	LYS
1	E	-3	ARG
1	E	48	LEU
1	E	197	LYS
1	E	238	LYS
1	E	264	ASN
1	E	305	LYS
1	E	310	LYS
1	E	342	PHE
1	E	343	ASN
1	E	369	HIS
1	E	400	ASP
1	F	-6	GLN
1	F	37	PRO
1	F	48	LEU
1	F	161	ASN
1	F	176	LYS
1	F	214	ASN
1	F	259	LEU
1	F	264	ASN
1	F	310	LYS
1	F	342	PHE
1	F	369	HIS
1	F	375	GLU
1	F	400	ASP
1	D	161	ASN
1	D	162	ASN
1	D	253	LYS
1	D	307	LEU
1	D	342	PHE
1	D	343	ASN

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Mol	Chain	Res	Type
1	D	369	HIS
1	D	400	ASP
1	D	418	LYS
1	C	97	ASP
1	C	161	ASN
1	C	178	VAL
1	C	214	ASN
1	C	217	SER
1	C	218	ASN
1	C	253	LYS
1	C	256	LYS
1	C	294	GLU
1	C	298	ASP
1	C	307	LEU
1	C	342	PHE
1	C	369	HIS
1	C	400	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	154	ASN
1	A	162	ASN
1	A	171	GLN
1	A	264	ASN
1	A	274	HIS
1	A	303	GLN
1	A	369	HIS
1	B	151	ASN
1	B	154	ASN
1	B	171	GLN
1	B	303	GLN
1	B	369	HIS
1	E	154	ASN
1	E	171	GLN
1	E	214	ASN
1	E	264	ASN
1	E	274	HIS
1	E	303	GLN
1	E	369	HIS
1	F	154	ASN

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Mol	Chain	Res	Type
1	F	171	GLN
1	F	264	ASN
1	F	274	HIS
1	F	303	GLN
1	F	369	HIS
1	D	154	ASN
1	D	162	ASN
1	D	171	GLN
1	D	264	ASN
1	D	274	HIS
1	D	303	GLN
1	D	369	HIS
1	C	154	ASN
1	C	171	GLN
1	C	214	ASN
1	C	303	GLN
1	C	369	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	SO4	C	504	-	4,4,4	0.74	0	6,6,6	0.43	0
5	PEP	E	602	2,6	6,9,9	0.98	0	8,13,13	2.52	4 (50%)
6	2PG	D	501	2	7,10,10	2.04	3 (42%)	8,14,14	2.83	4 (50%)
7	MES	D	504	-	12,12,12	1.83	1 (8%)	14,16,16	2.27	6 (42%)
6	2PG	C	501	2	7,10,10	1.32	1 (14%)	8,14,14	2.11	3 (37%)
3	SO4	D	503	-	4,4,4	0.40	0	6,6,6	0.50	0
3	SO4	B	603	-	4,4,4	0.59	0	6,6,6	2.23	3 (50%)
3	SO4	C	503	-	4,4,4	0.62	0	6,6,6	0.53	0
3	SO4	E	604	-	4,4,4	0.69	0	6,6,6	0.55	0
3	SO4	F	503	-	4,4,4	0.43	0	6,6,6	0.56	0
3	SO4	B	602	-	4,4,4	0.31	0	6,6,6	1.46	1 (16%)
3	SO4	A	602	-	4,4,4	0.71	0	6,6,6	1.40	1 (16%)
4	GOL	C	505	-	5,5,5	0.56	0	5,5,5	1.44	1 (20%)
4	GOL	B	604	-	5,5,5	0.49	0	5,5,5	1.86	1 (20%)
6	2PG	E	603	2,5	7,10,10	1.67	1 (14%)	8,14,14	2.52	4 (50%)
3	SO4	E	605	-	4,4,4	0.40	0	6,6,6	0.46	0
6	2PG	F	501	2	7,10,10	2.19	1 (14%)	8,14,14	3.13	6 (75%)
3	SO4	A	603	-	4,4,4	0.28	0	6,6,6	0.50	0
3	SO4	A	604	-	4,4,4	0.45	0	6,6,6	0.48	0
3	SO4	F	504	-	4,4,4	0.84	0	6,6,6	0.44	0
4	GOL	F	505	-	5,5,5	0.55	0	5,5,5	1.02	0
3	SO4	A	605	-	4,4,4	0.63	0	6,6,6	0.16	0
7	MES	E	606	-	12,12,12	2.16	2 (16%)	14,16,16	2.45	7 (50%)

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
5	PEP	E	602	2,6	-	2/5/9/9	-
4	GOL	F	505	-	-	2/4/4/4	-
4	GOL	C	505	-	-	2/4/4/4	-
7	MES	D	504	-	-	0/6/14/14	0/1/1/1
6	2PG	D	501	2	-	0/7/11/11	-
6	2PG	C	501	2	-	1/7/11/11	-
4	GOL	B	604	-	-	2/4/4/4	-
7	MES	E	606	-	-	4/6/14/14	0/1/1/1
6	2PG	E	603	2,5	-	2/7/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2PG	F	501	2	-	2/7/11/11	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	606	MES	C8-S	-6.62	1.68	1.77
7	D	504	MES	C8-S	-5.17	1.70	1.77
6	F	501	2PG	O1P-C2	-5.16	1.39	1.45
6	D	501	2PG	O1P-C2	-3.84	1.40	1.45
6	E	603	2PG	O1P-C2	-3.32	1.41	1.45
6	D	501	2PG	P-O2P	2.63	1.59	1.50
6	C	501	2PG	O1P-C2	-2.31	1.42	1.45
6	D	501	2PG	P-O1P	2.16	1.63	1.59
7	E	606	MES	O1S-S	2.13	1.51	1.45

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	501	2PG	O4P-P-O2P	5.52	132.29	110.68
6	D	501	2PG	O3P-P-O2P	5.17	130.91	110.68
7	E	606	MES	C6-C5-N4	4.93	117.58	110.10
5	E	602	PEP	O2-C2-C3	-4.65	115.83	124.79
6	E	603	2PG	O1P-P-O2P	-4.60	91.63	109.39
7	D	504	MES	C2-C3-N4	4.25	116.55	110.10
6	C	501	2PG	O4P-P-O2P	4.23	127.26	110.68
7	D	504	MES	O2S-S-C8	4.07	111.81	106.92
6	F	501	2PG	O3-C3-C2	4.05	122.25	111.42
6	D	501	2PG	O1P-P-O2P	-3.94	94.17	109.39
6	F	501	2PG	O3P-P-O2P	-3.75	95.99	110.68
4	B	604	GOL	O1-C1-C2	-3.60	92.92	110.20
7	E	606	MES	O2S-S-C8	3.51	111.14	106.92
7	E	606	MES	O3S-S-O2S	-3.49	102.75	111.27
3	B	603	SO4	O4-S-O3	-3.49	94.18	109.06
6	E	603	2PG	O3-C3-C2	3.42	120.56	111.42
5	E	602	PEP	O2-P-O1P	-3.42	97.18	109.32
6	D	501	2PG	O3-C3-C2	3.26	120.13	111.42
7	E	606	MES	O3S-S-O1S	3.23	119.16	111.27
3	B	603	SO4	O4-S-O2	3.12	125.59	109.31
6	E	603	2PG	O3P-P-O2P	3.00	122.43	110.68
5	E	602	PEP	O3P-P-O1P	2.88	121.97	110.68
7	D	504	MES	C5-N4-C3	2.72	114.95	108.83
6	E	603	2PG	P-O1P-C2	-2.68	116.88	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	SO4	O4-S-O3	-2.67	97.65	109.06
3	A	602	SO4	O3-S-O2	-2.58	95.84	109.31
7	E	606	MES	C6-O1-C2	2.52	118.30	109.89
7	D	504	MES	O3S-S-C8	2.49	109.80	105.77
6	C	501	2PG	O3-C3-C2	2.48	118.06	111.42
7	D	504	MES	C6-O1-C2	2.44	118.03	109.89
4	C	505	GOL	O3-C3-C2	2.41	121.77	110.20
7	D	504	MES	O2S-S-O1S	-2.41	105.62	113.95
6	C	501	2PG	O4P-P-O1P	-2.37	95.36	105.99
6	F	501	2PG	O4P-P-O3P	2.29	116.38	107.64
6	D	501	2PG	O4P-P-O3P	-2.26	99.01	107.64
5	E	602	PEP	O2P-P-O2	-2.14	98.72	105.25
6	F	501	2PG	O1P-P-O2P	-2.14	101.14	109.39
7	E	606	MES	O1S-S-C8	-2.10	104.39	106.92
6	F	501	2PG	O4P-P-O1P	-2.08	96.67	105.99
7	E	606	MES	C7-N4-C5	2.07	116.52	111.23
3	B	603	SO4	O2-S-O1	-2.05	94.26	109.43

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	602	PEP	C1-C2-O2-P
5	E	602	PEP	C3-C2-O2-P
4	C	505	GOL	C1-C2-C3-O3
4	C	505	GOL	O2-C2-C3-O3
4	B	604	GOL	O1-C1-C2-C3
6	E	603	2PG	C1-C2-C3-O3
6	E	603	2PG	O1P-C2-C3-O3
6	F	501	2PG	C1-C2-C3-O3
7	E	606	MES	C8-C7-N4-C5
7	E	606	MES	C7-C8-S-O1S
7	E	606	MES	C7-C8-S-O2S
7	E	606	MES	C7-C8-S-O3S
4	F	505	GOL	O1-C1-C2-C3
6	F	501	2PG	O1P-C2-C3-O3
4	B	604	GOL	O1-C1-C2-O2
6	C	501	2PG	C1-C2-C3-O3
4	F	505	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	602	PEP	6	0
3	B	602	SO4	1	0
4	C	505	GOL	2	0
4	B	604	GOL	1	0
6	E	603	2PG	3	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	439/449 (97%)	-0.30	5 (1%) 80 79	25, 34, 56, 84	0
1	B	439/449 (97%)	-0.15	16 (3%) 42 40	24, 36, 65, 97	0
1	C	429/449 (95%)	0.26	36 (8%) 11 9	26, 40, 82, 107	0
1	D	438/449 (97%)	-0.04	24 (5%) 25 23	26, 37, 67, 103	0
1	E	439/449 (97%)	-0.16	11 (2%) 57 55	25, 34, 61, 104	0
1	F	438/449 (97%)	-0.03	25 (5%) 23 22	27, 37, 64, 104	0
All	All	2622/2694 (97%)	-0.07	117 (4%) 33 31	24, 36, 67, 107	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	431	ALA	7.0
1	E	263	GLY	6.7
1	D	157	GLU	5.7
1	C	266	ALA	5.6
1	C	253	LYS	5.2
1	C	42	THR	5.0
1	E	431	ALA	5.0
1	D	263	GLY	5.0
1	B	431	ALA	4.8
1	F	263	GLY	4.7
1	B	261	GLY	4.7
1	C	252	TYR	4.6
1	D	431	ALA	4.5
1	D	253	LYS	4.4
1	D	260	ALA	4.3
1	D	254	ASP	4.1
1	C	41	SER	4.1
1	E	158	HIS	4.1
1	A	254	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	253	LYS	3.9
1	B	254	ASP	3.9
1	F	254	ASP	3.9
1	F	158	HIS	3.8
1	D	264	ASN	3.7
1	F	253	LYS	3.7
1	D	339	LEU	3.6
1	C	40	ALA	3.6
1	D	259	LEU	3.5
1	C	255	GLY	3.5
1	C	254	ASP	3.5
1	D	163	VAL	3.5
1	E	254	ASP	3.4
1	C	288	ILE	3.4
1	D	266	ALA	3.3
1	C	267	PHE	3.3
1	C	170	ILE	3.2
1	F	265	LYS	3.2
1	F	200	GLY	3.2
1	A	253	LYS	3.1
1	C	214	ASN	3.0
1	D	265	LYS	3.0
1	C	43	GLY	3.0
1	C	243	ALA	2.9
1	C	366	VAL	2.9
1	A	431	ALA	2.9
1	F	314	VAL	2.8
1	C	149	MET	2.8
1	B	391	ILE	2.8
1	F	160	ASP	2.8
1	C	160	ASP	2.8
1	C	258	VAL	2.8
1	B	263	GLY	2.8
1	E	253	LYS	2.7
1	C	244	MET	2.7
1	F	243	ALA	2.7
1	D	160	ASP	2.7
1	B	266	ALA	2.7
1	E	264	ASN	2.7
1	D	162	ASN	2.7
1	D	341	LYS	2.7
1	D	392	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	258	VAL	2.6
1	F	76	GLN	2.6
1	C	251	PHE	2.6
1	D	261	GLY	2.5
1	C	250	GLU	2.5
1	D	170	ILE	2.5
1	B	264	ASN	2.5
1	F	41	SER	2.5
1	C	339	LEU	2.5
1	C	271	GLU	2.4
1	F	339	LEU	2.4
1	A	265	LYS	2.4
1	E	216	GLY	2.4
1	A	266	ALA	2.4
1	B	169	MET	2.4
1	C	242	LEU	2.4
1	C	295	SER	2.4
1	B	288	ILE	2.3
1	F	264	ASN	2.3
1	C	314	VAL	2.3
1	B	160	ASP	2.3
1	F	162	ASN	2.3
1	D	367	ILE	2.3
1	D	368	SER	2.3
1	C	218	ASN	2.3
1	E	169	MET	2.3
1	F	288	ILE	2.3
1	F	366	VAL	2.2
1	B	265	LYS	2.2
1	F	256	LYS	2.2
1	B	200	GLY	2.2
1	F	340	ILE	2.2
1	D	158	HIS	2.2
1	C	44	SER	2.2
1	E	160	ASP	2.2
1	E	417	GLU	2.2
1	F	159	ALA	2.2
1	C	198	ALA	2.1
1	C	305	LYS	2.1
1	F	169	MET	2.1
1	F	244	MET	2.1
1	B	256	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	76	GLN	2.1
1	C	163	VAL	2.1
1	B	269	SER	2.1
1	C	286	VAL	2.1
1	C	53	GLY	2.1
1	F	367	ILE	2.0
1	D	255	GLY	2.0
1	C	417	GLU	2.0
1	B	302	TYR	2.0
1	F	197	LYS	2.0
1	F	149	MET	2.0
1	D	417	GLU	2.0
1	E	260	ALA	2.0
1	F	262	GLU	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 monosaccharides 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, 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	B-factors(\AA^2)	Q<0.9
3	SO4	F	503	5/5	0.77	0.31	87,103,110,116	0
7	MES	D	504	12/12	0.81	0.25	62,68,91,92	0
4	GOL	F	505	6/6	0.85	0.23	42,51,61,76	0
7	MES	E	606	12/12	0.85	0.15	52,56,74,77	0
2	MG	C	502	1/1	0.86	0.06	50,50,50,50	0
4	GOL	B	604	6/6	0.86	0.20	51,55,57,72	0
4	GOL	C	505	6/6	0.87	0.19	41,49,60,73	0
3	SO4	F	504	5/5	0.93	0.11	52,53,60,77	0
3	SO4	D	503	5/5	0.93	0.27	88,91,98,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	E	605	5/5	0.93	0.22	92,94,105,108	0
2	MG	B	601	1/1	0.93	0.17	53,53,53,53	0
6	2PG	C	501	11/11	0.94	0.11	45,55,63,64	0
6	2PG	F	501	11/11	0.95	0.10	33,38,45,58	0
2	MG	A	601	1/1	0.95	0.10	54,54,54,54	0
3	SO4	E	604	5/5	0.95	0.14	62,63,64,77	0
6	2PG	E	603	11/11	0.96	0.11	17,25,28,36	11
2	MG	D	502	1/1	0.96	0.06	41,41,41,41	0
3	SO4	C	503	5/5	0.96	0.12	53,60,70,76	0
6	2PG	D	501	11/11	0.96	0.11	35,40,46,53	0
3	SO4	A	604	5/5	0.97	0.08	46,47,49,57	0
5	PEP	E	602	10/10	0.97	0.12	36,46,56,63	10
2	MG	E	601	1/1	0.97	0.08	35,35,35,35	0
3	SO4	A	605	5/5	0.97	0.12	52,56,60,68	0
3	SO4	B	603	5/5	0.97	0.10	39,45,48,55	0
3	SO4	A	602	5/5	0.97	0.09	41,46,53,55	0
3	SO4	C	504	5/5	0.98	0.10	51,51,59,64	0
3	SO4	B	602	5/5	0.98	0.10	44,49,52,54	0
2	MG	F	502	1/1	0.99	0.08	39,39,39,39	0
3	SO4	A	603	5/5	0.99	0.09	41,43,45,50	0

6.5 Other polymers

There are no such residues in this entry.