



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:23 PM UTC

PDB ID : 6BFY / pdb_00006bfy
Title : Crystal structure of enolase from Escherichia coli with bound 2-phosphoglycerate substrate
Authors : Erlandsen, H.; Wright, D.; Krucinska, J.
Deposited on : 2017-10-27
Resolution : 1.81 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

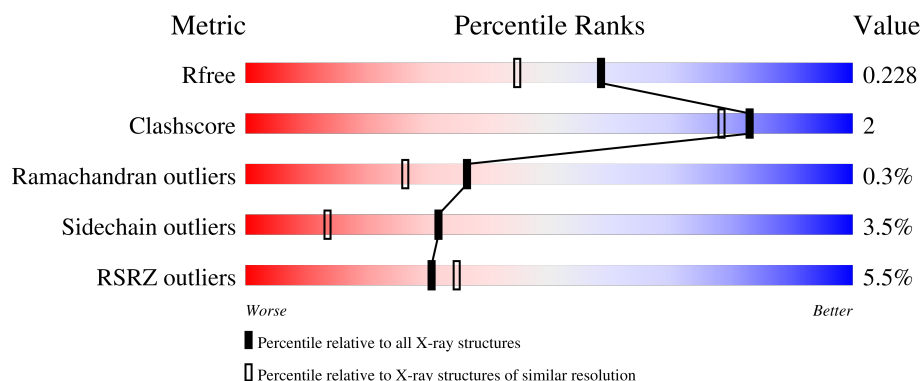
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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 of 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	4% 80% 16% ..
1	B	449	2% 81% 16% ..
1	C	449	2% 83% 13% ..
1	D	449	7% 85% 11% ..
1	E	449	3% 84% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	449	

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	GOL	D	806	-	X	-	-
5	GOL	F	505	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20818 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
			3254	2036	559	644	15			
1	B	438	Total	C	N	O	S	0	0	0
			3249	2033	558	643	15			
1	C	439	Total	C	N	O	S	0	0	0
			3254	2036	559	644	15			
1	F	438	Total	C	N	O	S	0	0	0
			3245	2031	557	642	15			
1	D	438	Total	C	N	O	S	0	0	0
			3249	2033	558	643	15			
1	E	438	Total	C	N	O	S	0	1	0
			3258	2039	560	644	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
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
C	-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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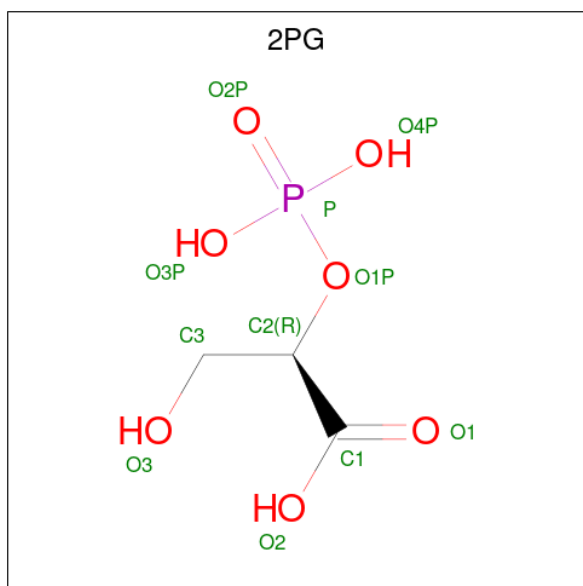
Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	GLY	-	expression tag	UNP B7MLA0
F	-8	GLY	-	expression tag	UNP B7MLA0
F	-7	GLN	-	expression tag	UNP B7MLA0
F	-6	GLN	-	expression tag	UNP B7MLA0
F	-5	MET	-	expression tag	UNP B7MLA0
F	-4	GLY	-	expression tag	UNP B7MLA0
F	-3	ARG	-	expression tag	UNP B7MLA0
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
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

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

- Molecule 2 is 2-PHOSPHOGLYCERIC ACID (CCD ID: 2PG) (formula: $C_3H_7O_7P$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

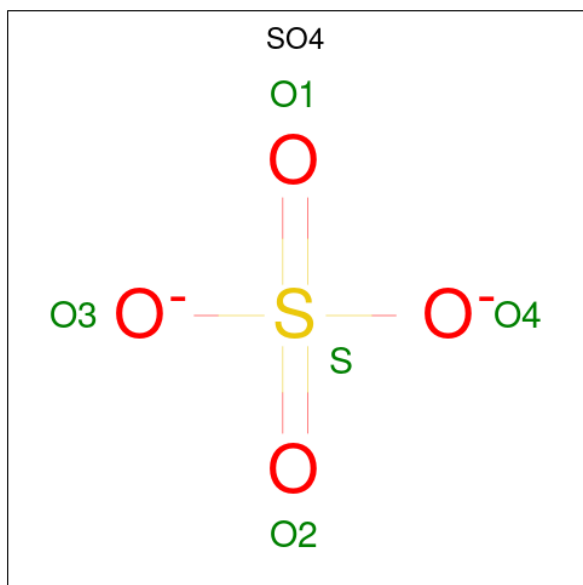
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

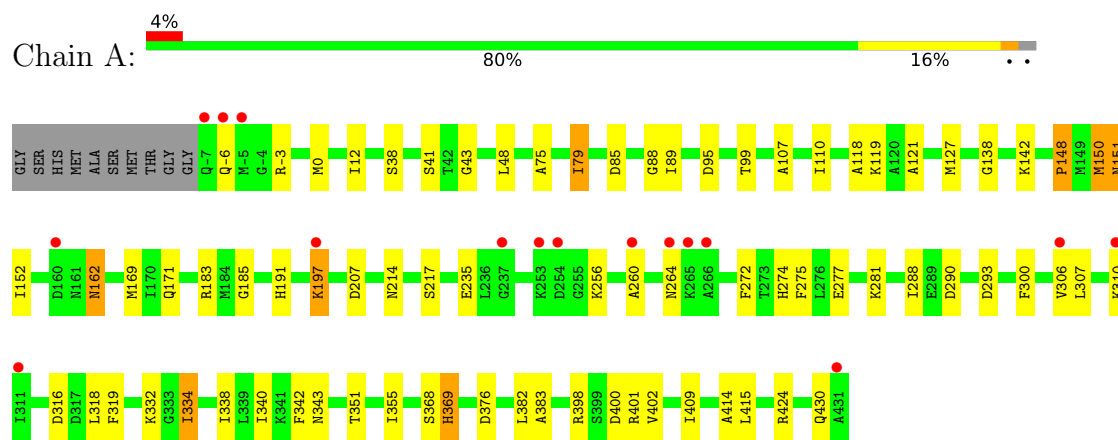
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total	O	0	0
			186	186		
6	B	209	Total	O	0	0
			209	209		
6	C	241	Total	O	0	0
			241	241		
6	F	123	Total	O	0	0
			123	123		
6	D	169	Total	O	0	0
			169	169		
6	E	175	Total	O	0	0
			175	175		

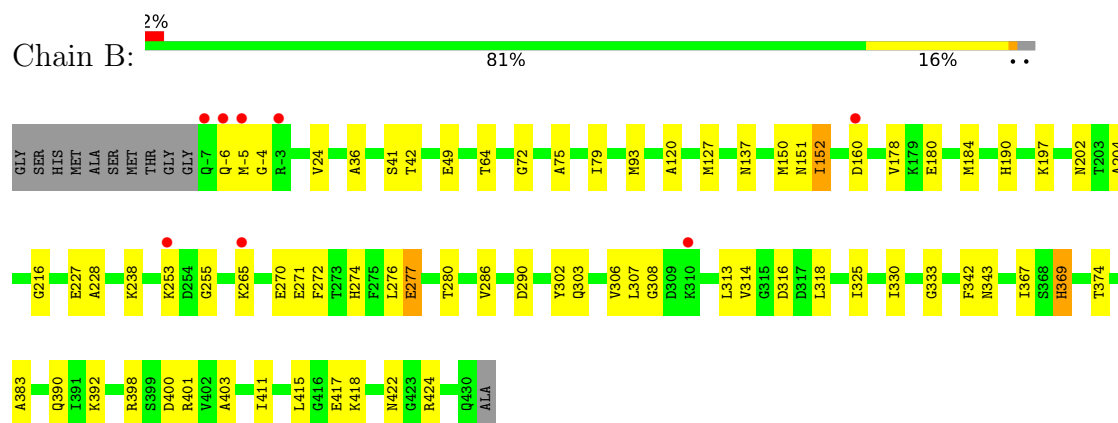
3 Residue-property plots [i](#)

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.

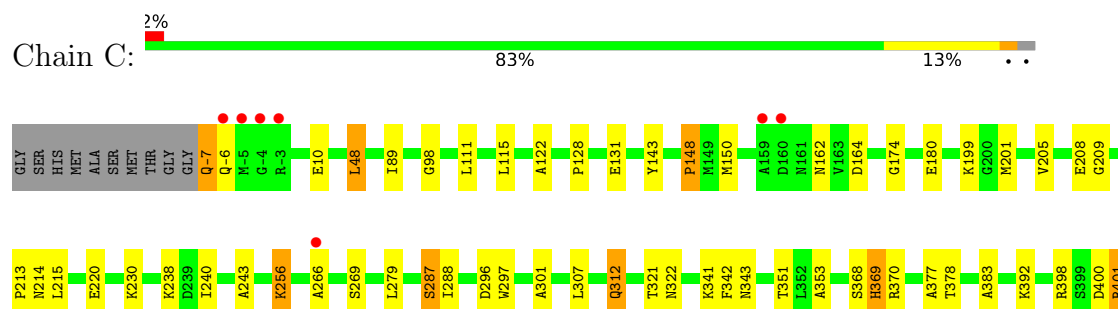
• Molecule 1: Enolase



• Molecule 1: Enolase

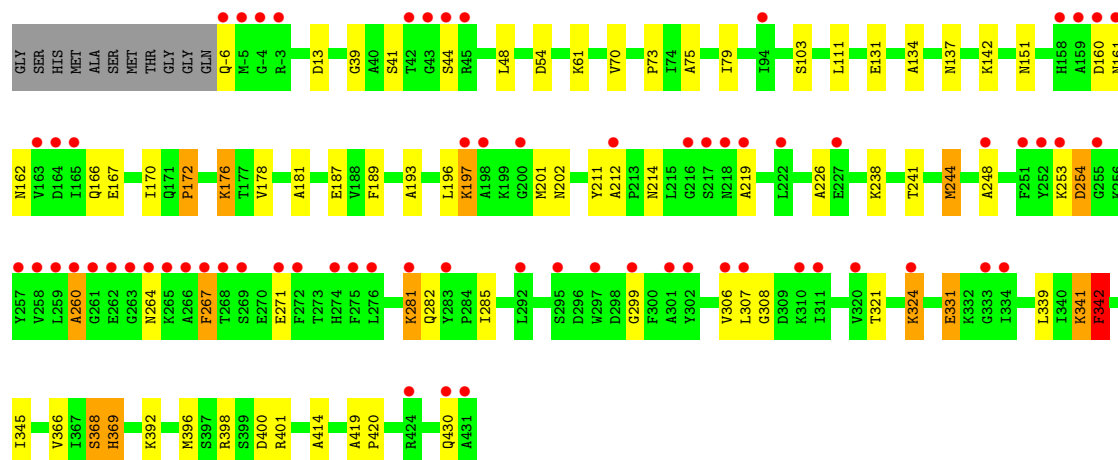
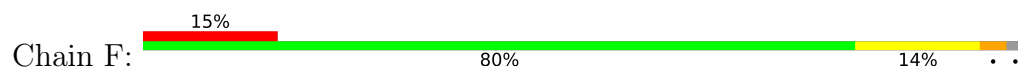


• Molecule 1: Enolase

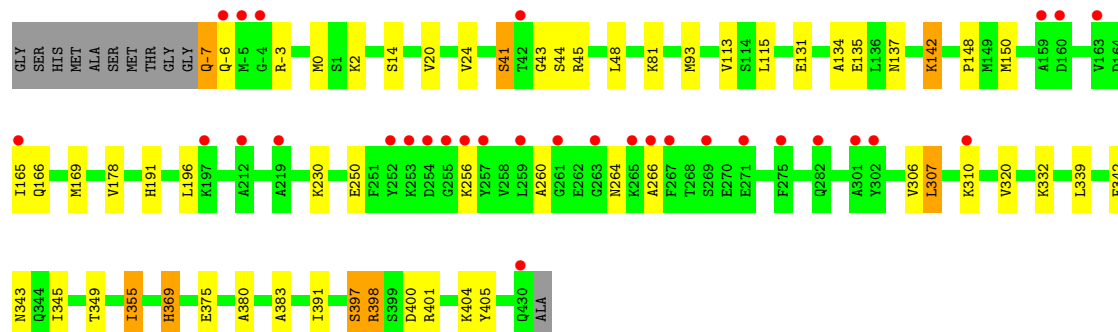
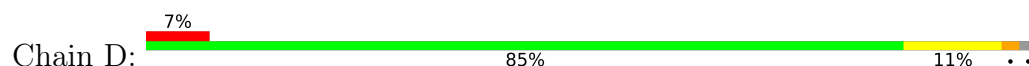




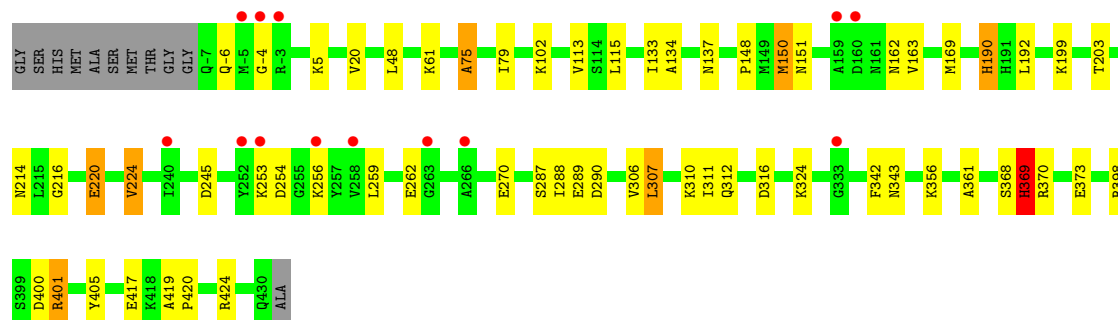
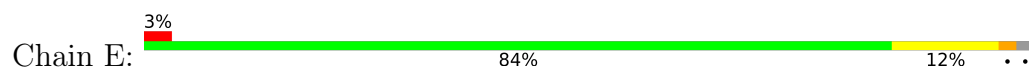
● Molecule 1: Enolase



● 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	105.94Å 142.40Å 206.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.61 – 1.81 78.61 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.61-1.81) 99.9 (78.61-1.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.166 , 0.232 0.195 , 0.228	Depositor DCC
R_{free} test set	14046 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20818	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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, 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	1.74	42/3296 (1.3%)	1.32	12/4435 (0.3%)
1	B	1.78	43/3291 (1.3%)	1.32	13/4428 (0.3%)
1	C	1.79	48/3296 (1.5%)	1.34	9/4435 (0.2%)
1	D	1.72	36/3291 (1.1%)	1.32	6/4428 (0.1%)
1	E	1.65	28/3300 (0.8%)	1.30	7/4439 (0.2%)
1	F	1.66	29/3287 (0.9%)	1.35	11/4423 (0.2%)
All	All	1.72	226/19761 (1.1%)	1.32	58/26588 (0.2%)

All (226) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405	TYR	N-CA	9.15	1.57	1.46
1	A	150	MET	N-CA	8.76	1.56	1.46
1	C	148	PRO	CA-C	8.75	1.63	1.52
1	C	288	ILE	CA-CB	8.72	1.66	1.54
1	B	392	LYS	C-O	8.71	1.33	1.24
1	C	115	LEU	N-CA	8.58	1.56	1.46
1	C	-6	GLN	CA-C	8.28	1.62	1.52
1	C	220	GLU	CA-C	8.23	1.63	1.52
1	C	404	LYS	CA-CB	-7.78	1.40	1.53
1	A	79	ILE	C-O	-7.76	1.16	1.24
1	C	164	ASP	N-CA	7.67	1.56	1.46
1	D	41	SER	CA-C	7.65	1.62	1.53
1	F	187	GLU	CA-C	7.50	1.62	1.52
1	C	89	ILE	C-O	7.39	1.32	1.24
1	D	115	LEU	N-CA	7.36	1.55	1.46
1	F	341	LYS	CA-C	-7.30	1.44	1.52
1	B	277	GLU	CA-C	-7.29	1.43	1.52
1	C	10	GLU	CA-C	7.25	1.61	1.52
1	E	75	ALA	N-CA	7.22	1.55	1.46
1	C	419	ALA	N-CA	7.21	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	ILE	CA-CB	-6.99	1.46	1.54
1	A	119	LYS	N-CA	6.94	1.54	1.46
1	D	196	LEU	CA-C	6.90	1.61	1.52
1	C	287	SER	CA-CB	6.83	1.65	1.53
1	F	267	PHE	C-O	6.82	1.32	1.23
1	C	-6	GLN	N-CA	6.80	1.54	1.46
1	C	351	THR	N-CA	-6.78	1.38	1.46
1	B	190	HIS	N-CA	6.75	1.54	1.46
1	C	312	GLN	N-CA	-6.75	1.37	1.46
1	A	118	ALA	CA-C	-6.70	1.44	1.52
1	A	89	ILE	C-O	6.66	1.31	1.24
1	A	12	ILE	C-O	6.61	1.30	1.24
1	B	314	VAL	C-N	-6.61	1.29	1.33
1	A	376	ASP	N-CA	6.60	1.54	1.46
1	A	183	ARG	N-CA	-6.58	1.38	1.46
1	B	150	MET	N-CA	6.56	1.54	1.46
1	B	303	GLN	N-CA	-6.55	1.38	1.46
1	C	213	PRO	N-CA	-6.51	1.39	1.47
1	B	180	GLU	C-O	-6.48	1.16	1.24
1	D	14	SER	C-O	-6.46	1.15	1.24
1	B	41	SER	N-CA	6.42	1.55	1.46
1	D	391	ILE	CA-C	6.40	1.60	1.52
1	E	311	ILE	C-O	6.39	1.30	1.24
1	D	131	GLU	N-CA	6.38	1.54	1.46
1	A	318	LEU	N-CA	6.34	1.53	1.46
1	B	238	LYS	CA-C	6.33	1.60	1.52
1	D	250	GLU	N-CA	6.29	1.54	1.46
1	E	224	VAL	N-CA	6.29	1.53	1.46
1	E	-6	GLN	CA-C	6.28	1.60	1.52
1	E	288	ILE	CA-CB	6.25	1.62	1.54
1	C	410	ARG	N-CA	6.21	1.53	1.46
1	E	287	SER	CA-CB	6.17	1.64	1.53
1	D	339	LEU	C-O	6.13	1.31	1.24
1	D	165	ILE	C-O	6.12	1.31	1.24
1	A	402	VAL	N-CA	6.10	1.54	1.46
1	A	272	PHE	N-CA	6.07	1.53	1.46
1	E	419	ALA	C-O	6.07	1.31	1.24
1	C	296	ASP	C-O	6.05	1.31	1.23
1	D	355	ILE	CA-C	6.03	1.60	1.52
1	C	174	GLY	N-CA	6.02	1.54	1.45
1	D	349	THR	N-CA	6.02	1.53	1.46
1	F	170	ILE	CA-C	6.02	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	113	VAL	C-O	-6.00	1.17	1.24
1	A	110	ILE	N-CA	-6.00	1.39	1.46
1	B	227	GLU	C-O	5.99	1.30	1.24
1	B	314	VAL	C-O	-5.97	1.17	1.24
1	F	70	VAL	C-O	5.97	1.30	1.24
1	E	405	TYR	N-CA	5.96	1.53	1.46
1	F	241	THR	CA-CB	5.94	1.64	1.54
1	D	134	ALA	CA-C	5.94	1.60	1.52
1	D	-6	GLN	N-CA	5.90	1.53	1.46
1	C	301	ALA	C-O	5.89	1.30	1.24
1	A	340	ILE	CA-C	5.89	1.59	1.52
1	F	212	ALA	CA-C	5.88	1.59	1.53
1	C	353	ALA	CA-CB	5.87	1.62	1.53
1	B	24	VAL	N-CA	-5.87	1.39	1.46
1	B	272	PHE	N-CA	5.84	1.53	1.46
1	C	240	ILE	CA-C	-5.84	1.45	1.52
1	F	-6	GLN	CD-NE2	5.83	1.45	1.33
1	A	121	ALA	N-CA	-5.82	1.39	1.46
1	A	148	PRO	N-CA	-5.80	1.40	1.47
1	B	178	VAL	CA-C	5.79	1.61	1.52
1	C	238	LYS	C-O	-5.79	1.17	1.24
1	C	122	ALA	N-CA	5.78	1.53	1.46
1	B	120	ALA	CA-C	-5.78	1.45	1.52
1	C	370	ARG	N-CA	-5.76	1.39	1.45
1	B	72	GLY	N-CA	5.74	1.52	1.44
1	B	93	MET	C-O	5.74	1.30	1.24
1	D	-7	GLN	CA-C	5.74	1.65	1.52
1	D	383	ALA	N-CA	5.73	1.53	1.46
1	F	420	PRO	C-O	5.72	1.30	1.23
1	D	93	MET	N-CA	5.72	1.53	1.46
1	E	420	PRO	C-O	5.72	1.30	1.23
1	A	207	ASP	C-O	-5.71	1.16	1.24
1	A	351	THR	C-O	-5.71	1.17	1.24
1	C	287	SER	CA-C	-5.70	1.45	1.52
1	C	378	THR	CA-CB	5.69	1.62	1.53
1	F	414	ALA	CA-CB	5.69	1.62	1.53
1	A	88	GLY	N-CA	5.68	1.53	1.45
1	A	171	GLN	CA-CB	-5.68	1.46	1.53
1	B	422	ASN	C-O	-5.67	1.16	1.24
1	F	172	PRO	CA-C	5.67	1.58	1.52
1	D	355	ILE	N-CA	5.66	1.53	1.46
1	B	36	ALA	C-O	5.65	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	39	GLY	C-O	5.65	1.32	1.23
1	D	24	VAL	N-CA	5.64	1.53	1.46
1	B	49	GLU	N-CA	5.64	1.53	1.46
1	F	73	PRO	C-O	5.63	1.30	1.24
1	B	152	ILE	N-CA	-5.63	1.39	1.46
1	B	415	LEU	N-CA	5.62	1.53	1.46
1	F	134	ALA	CA-C	5.61	1.60	1.52
1	C	411	ILE	CA-CB	-5.61	1.47	1.54
1	A	338	ILE	CA-C	5.61	1.59	1.52
1	C	401	ARG	CA-CB	5.59	1.62	1.53
1	B	383	ALA	C-O	-5.56	1.17	1.24
1	B	417	GLU	C-O	-5.56	1.16	1.24
1	A	383	ALA	C-N	-5.56	1.26	1.33
1	B	286	VAL	N-CA	-5.54	1.39	1.46
1	C	269	SER	C-O	5.53	1.30	1.24
1	A	185	GLY	C-O	5.53	1.30	1.23
1	C	430	GLN	N-CA	5.53	1.53	1.46
1	D	81	LYS	C-O	-5.53	1.17	1.23
1	E	5	LYS	N-CA	5.52	1.52	1.46
1	B	333	GLY	CA-C	5.51	1.57	1.51
1	A	162	ASN	CA-C	5.50	1.60	1.52
1	E	102	LYS	CA-C	-5.50	1.46	1.53
1	F	189	PHE	C-O	5.48	1.30	1.24
1	F	281	LYS	N-CA	5.48	1.53	1.46
1	B	79	ILE	C-O	-5.46	1.18	1.24
1	E	61	LYS	CA-C	5.46	1.60	1.52
1	D	142	LYS	N-CA	5.44	1.52	1.46
1	D	2	LYS	CA-C	5.43	1.59	1.52
1	A	275	PHE	N-CA	5.43	1.52	1.46
1	C	243	ALA	CA-C	-5.43	1.45	1.52
1	F	396	MET	CA-CB	5.42	1.59	1.53
1	E	245	ASP	CA-C	-5.42	1.46	1.52
1	F	271	GLU	C-O	5.42	1.30	1.24
1	F	151	ASN	C-O	5.41	1.30	1.23
1	B	75	ALA	CA-C	-5.41	1.45	1.52
1	E	259	LEU	CA-C	5.41	1.60	1.52
1	C	230	LYS	CA-CB	5.41	1.61	1.53
1	D	230	LYS	CA-C	5.40	1.59	1.52
1	C	405	TYR	N-CA	5.39	1.52	1.46
1	B	184	MET	C-O	-5.39	1.17	1.24
1	E	113	VAL	C-O	-5.38	1.17	1.24
1	D	380	ALA	CA-CB	-5.37	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	GLU	C-O	-5.36	1.17	1.24
1	B	418	LYS	C-O	-5.36	1.17	1.24
1	B	374	THR	C-O	-5.36	1.16	1.23
1	E	190	HIS	N-CA	5.36	1.52	1.46
1	C	279	LEU	N-CA	5.34	1.52	1.46
1	C	377	ALA	C-O	5.33	1.31	1.23
1	A	430	GLN	CA-C	5.33	1.59	1.52
1	B	390	GLN	C-O	5.31	1.30	1.23
1	E	405	TYR	C-O	5.31	1.30	1.24
1	B	403	ALA	C-O	5.30	1.30	1.24
1	A	355	ILE	N-CA	5.30	1.52	1.46
1	F	366	VAL	C-O	5.30	1.30	1.24
1	F	414	ALA	C-O	-5.30	1.18	1.24
1	A	382	LEU	CA-C	-5.29	1.46	1.52
1	D	256	LYS	C-O	5.28	1.30	1.23
1	D	48	LEU	CA-CB	5.28	1.61	1.53
1	C	341	LYS	C-O	5.27	1.30	1.24
1	B	374	THR	N-CA	-5.27	1.38	1.46
1	A	409	ILE	N-CA	5.26	1.52	1.46
1	F	299	GLY	C-O	5.25	1.30	1.23
1	E	137	ASN	N-CA	5.25	1.52	1.46
1	E	20	VAL	N-CA	-5.25	1.39	1.46
1	A	107	ALA	C-O	5.24	1.30	1.24
1	B	422	ASN	N-CA	5.21	1.52	1.46
1	F	324	LYS	C-O	-5.21	1.18	1.24
1	F	331	GLU	N-CA	5.20	1.52	1.46
1	B	318	LEU	N-CA	5.19	1.52	1.46
1	A	38	SER	CA-CB	-5.18	1.45	1.53
1	C	199	LYS	C-O	-5.18	1.16	1.23
1	D	404	LYS	C-N	-5.17	1.27	1.33
1	C	420	PRO	C-O	5.16	1.29	1.23
1	A	217	SER	N-CA	5.16	1.52	1.46
1	B	216	GLY	C-O	-5.16	1.17	1.24
1	C	98	GLY	N-CA	5.16	1.53	1.45
1	D	320	VAL	CA-C	5.15	1.59	1.52
1	A	235	GLU	N-CA	5.15	1.52	1.46
1	E	312	GLN	C-O	5.15	1.30	1.24
1	D	45	ARG	N-CA	5.15	1.52	1.46
1	C	418	LYS	N-CA	5.14	1.53	1.46
1	A	99	THR	CA-C	-5.13	1.46	1.52
1	D	134	ALA	N-CA	-5.13	1.40	1.46
1	A	293	ASP	C-O	5.13	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	378	THR	N-CA	5.12	1.52	1.46
1	B	367	ILE	N-CA	5.12	1.52	1.46
1	E	115	LEU	N-CA	5.11	1.52	1.46
1	C	383	ALA	N-CA	5.11	1.52	1.46
1	B	270	GLU	CA-CB	5.11	1.61	1.53
1	A	414	ALA	N-CA	5.10	1.52	1.46
1	F	248	ALA	C-O	-5.10	1.17	1.24
1	C	297	TRP	C-O	5.09	1.30	1.24
1	B	325	ILE	C-O	-5.09	1.17	1.23
1	E	361	ALA	CA-C	5.09	1.59	1.52
1	C	111	LEU	N-CA	5.08	1.52	1.46
1	A	334	ILE	N-CA	5.08	1.52	1.46
1	A	41	SER	N-CA	5.08	1.53	1.46
1	C	208	GLU	N-CA	5.08	1.52	1.46
1	D	135	GLU	C-O	-5.07	1.18	1.24
1	E	133	ILE	N-CA	5.07	1.52	1.46
1	E	163	VAL	CA-C	5.06	1.58	1.52
1	D	-7	GLN	CA-CB	5.06	1.63	1.53
1	A	288	ILE	C-O	-5.06	1.18	1.24
1	A	414	ALA	C-O	-5.05	1.18	1.24
1	E	289	GLU	CA-CB	5.05	1.62	1.53
1	E	262	GLU	CA-C	5.05	1.59	1.52
1	C	392	LYS	CA-CB	5.05	1.61	1.53
1	D	44	SER	N-CA	5.05	1.52	1.46
1	F	61	LYS	N-CA	5.04	1.51	1.46
1	B	255	GLY	C-O	-5.04	1.17	1.24
1	F	131	GLU	C-O	-5.04	1.18	1.24
1	D	397	SER	N-CA	-5.04	1.39	1.45
1	A	85	ASP	C-O	5.03	1.30	1.23
1	F	419	ALA	C-O	-5.03	1.18	1.24
1	E	401	ARG	CA-C	-5.02	1.47	1.52
1	D	20	VAL	N-CA	5.02	1.52	1.46
1	F	308	GLY	N-CA	5.02	1.52	1.45
1	B	313	LEU	C-O	-5.01	1.18	1.24
1	A	0	MET	C-O	5.01	1.30	1.23
1	E	220	GLU	CA-C	5.01	1.59	1.52
1	A	415	LEU	C-O	-5.00	1.17	1.24
1	C	128	PRO	C-O	5.00	1.29	1.23

All (58) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-7	GLN	CB-CA-C	9.51	128.16	110.10
1	F	219	ALA	N-CA-C	8.08	122.84	112.34
1	F	430	GLN	N-CA-C	7.64	123.54	113.30
1	C	-7	GLN	CB-CA-C	7.32	124.01	110.10
1	D	-6	GLN	N-CA-C	7.30	120.42	108.52
1	B	308	GLY	N-CA-C	7.20	123.20	113.99
1	B	271	GLU	CG-CD-OE1	6.81	134.06	118.40
1	A	332	LYS	N-CA-C	6.77	121.14	113.02
1	B	330	ILE	N-CA-C	-6.53	104.12	110.72
1	B	127	MET	N-CA-C	6.51	115.81	108.25
1	D	43	GLY	N-CA-C	-6.33	104.65	111.93
1	E	192	LEU	N-CA-C	6.31	118.24	111.36
1	F	260	ALA	N-CA-C	6.26	118.91	111.71
1	C	-6	GLN	N-CA-C	6.23	119.98	109.76
1	F	196	LEU	N-CA-C	6.14	117.97	111.28
1	F	226	ALA	N-CA-C	6.11	118.45	111.11
1	E	369	HIS	N-CA-C	6.05	117.70	110.19
1	C	368	SER	N-CA-C	5.99	118.97	109.50
1	A	-6	GLN	N-CA-C	5.97	119.38	109.46
1	C	48	LEU	N-CA-C	5.97	118.37	109.59
1	A	306	VAL	N-CA-C	5.91	117.44	111.00
1	E	368	SER	N-CA-C	5.87	118.78	109.50
1	A	424	ARG	NE-CZ-NH1	-5.86	115.64	121.50
1	C	378	THR	N-CA-C	5.84	118.39	111.33
1	F	368	SER	N-CA-C	5.81	118.88	109.40
1	F	345	ILE	CB-CA-C	5.79	116.86	111.30
1	D	345	ILE	CB-CA-C	5.78	116.85	111.30
1	A	138	GLY	N-CA-C	-5.72	106.86	115.32
1	E	134	ALA	N-CA-C	5.67	117.46	111.28
1	B	424	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	B	-4	GLY	N-CA-C	5.59	118.47	112.33
1	B	64	THR	N-CA-C	5.52	117.30	111.28
1	A	319	PHE	N-CA-C	5.51	120.28	113.50
1	E	419	ALA	CA-C-N	-5.45	114.16	119.78
1	E	419	ALA	C-N-CA	-5.45	114.16	119.78
1	E	150	MET	N-CA-C	5.42	117.47	108.20
1	A	95	ASP	N-CA-C	5.40	117.16	111.28
1	A	127	MET	O-C-N	5.36	125.56	121.65
1	A	43	GLY	N-CA-C	-5.35	105.24	112.14
1	D	375	GLU	CA-C-N	5.30	128.63	121.05
1	D	375	GLU	C-N-CA	5.30	128.63	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	322	ASN	CB-CA-C	5.27	118.58	110.62
1	A	151	ASN	N-CA-CB	-5.24	103.01	110.46
1	F	342	PHE	N-CA-C	5.24	117.73	111.71
1	A	-3	ARG	N-CA-C	-5.23	105.76	111.82
1	B	228	ALA	N-CA-C	5.14	116.57	111.07
1	C	205	VAL	N-CA-C	5.08	116.62	108.89
1	B	151	ASN	N-CA-CB	-5.08	103.25	110.46
1	B	42	THR	CA-C-N	5.08	124.92	120.10
1	B	42	THR	C-N-CA	5.08	124.92	120.10
1	C	209	GLY	CA-C-N	5.04	126.80	121.45
1	C	209	GLY	C-N-CA	5.04	126.80	121.45
1	F	306	VAL	N-CA-C	5.04	115.27	110.53
1	B	271	GLU	CB-CA-C	5.04	120.34	110.67
1	F	212	ALA	CA-C-N	5.03	124.93	119.85
1	F	212	ALA	C-N-CA	5.03	124.93	119.85
1	A	368	SER	N-CA-C	5.02	117.43	109.50
1	B	271	GLU	CG-CD-OE2	-5.01	106.88	118.40

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	3254	0	3278	15	0
1	B	3249	0	3273	12	0
1	C	3254	0	3278	15	0
1	D	3249	0	3273	14	0
1	E	3258	0	3285	14	0
1	F	3245	0	3270	27	0
2	A	11	0	4	0	0
2	B	11	0	4	0	0
2	C	11	0	4	0	0
2	D	11	0	4	0	0
2	E	11	0	4	0	0
2	F	11	0	4	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	25	0	0	0	0
4	B	25	0	0	1	0
4	C	25	0	0	0	0
4	D	10	0	0	0	0
4	E	20	0	0	1	0
4	F	5	0	0	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	6	0	0
6	A	186	0	0	1	0
6	B	209	0	0	1	0
6	C	241	0	0	1	0
6	D	169	0	0	3	0
6	E	175	0	0	1	0
6	F	123	0	0	1	0
All	All	20818	0	19703	95	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 (95) 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:C:201:MET:HE1	1:C:215:LEU:HD23	1.20	1.20
1:C:201:MET:CE	1:C:215:LEU:HD23	1.78	1.13
1:F:167:GLU:OE1	1:F:392:LYS:HE2	1.60	1.01
1:C:201:MET:HE1	1:C:215:LEU:CD2	1.95	0.96
1:A:197:LYS:HA	1:A:197:LYS:HE2	1.59	0.85
1:A:369:HIS:CD2	1:A:401:ARG:HH11	2.07	0.73
1:F:369:HIS:CD2	1:F:401:ARG:HH11	2.07	0.71
1:B:369:HIS:CD2	1:B:401:ARG:HH11	2.08	0.70
1:C:201:MET:HE2	1:C:215:LEU:HD23	1.71	0.69
1:C:369:HIS:CD2	1:C:401:ARG:HH11	2.12	0.68
1:B:274:HIS:HD2	1:B:277:GLU:OE1	1.77	0.67
1:A:197:LYS:HE3	1:B:160:ASP:OD2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-3:ARG:HA	1:D:0:MET:HE3	1.77	0.66
1:D:-3:ARG:HG2	1:D:0:MET:HE3	1.79	0.65
1:A:274:HIS:HD2	1:A:277:GLU:OE1	1.81	0.62
1:E:369:HIS:CD2	1:E:401:ARG:HH11	2.17	0.62
1:B:202:ASN:ND2	1:B:204:ALA:H	1.98	0.62
1:D:306:VAL:HG12	1:D:307:LEU:HD13	1.82	0.60
1:D:369:HIS:CD2	1:D:401:ARG:HH11	2.19	0.59
1:F:137:ASN:ND2	6:F:602:HOH:O	2.34	0.58
1:D:260:ALA:HA	1:D:264:ASN:HD22	1.67	0.58
1:F:75:ALA:O	1:F:79:ILE:HG12	2.03	0.58
1:A:197:LYS:HA	1:A:197:LYS:CE	2.33	0.57
1:D:137:ASN:ND2	6:D:902:HOH:O	2.38	0.56
1:A:369:HIS:HD2	1:A:401:ARG:HH11	1.54	0.56
1:B:369:HIS:HD2	1:B:401:ARG:HH11	1.52	0.56
1:F:244:MET:SD	1:F:285:ILE:HD13	2.46	0.56
1:E:270:GLU:HG3	6:E:752:HOH:O	2.07	0.53
1:F:162:ASN:OD1	1:F:214:ASN:HA	2.09	0.53
1:A:191:HIS:HE1	6:A:770:HOH:O	1.90	0.53
1:A:300:PHE:HB3	1:A:334:ILE:HG23	1.91	0.52
1:F:172:PRO:HG2	1:F:181:ALA:HB1	1.91	0.52
1:D:148:PRO:HG2	1:D:150:MET:HE3	1.90	0.52
1:D:142:LYS:HG2	6:D:969:HOH:O	2.10	0.51
1:F:369:HIS:HD2	1:F:401:ARG:HH11	1.56	0.51
1:D:191:HIS:HE1	6:D:1049:HOH:O	1.94	0.50
1:E:216:GLY:N	1:E:220:GLU:OE1	2.42	0.49
1:C:148:PRO:HG2	1:C:150:MET:HE3	1.95	0.49
1:A:75:ALA:O	1:A:79:ILE:HG12	2.12	0.49
1:E:306:VAL:HG12	1:E:307:LEU:HD13	1.95	0.49
1:E:190:HIS:NE2	4:E:507:SO4:O4	2.44	0.49
1:F:167:GLU:OE1	1:F:392:LYS:CE	2.47	0.48
1:B:302:TYR:O	1:B:306:VAL:HG23	2.13	0.48
1:C:201:MET:CE	1:C:215:LEU:CD2	2.67	0.48
1:C:201:MET:HE2	1:C:214:ASN:O	2.13	0.48
1:F:48:LEU:HD23	1:F:103:SER:HA	1.96	0.48
1:E:151:ASN:HA	1:E:169:MET:HG2	1.97	0.47
1:F:260:ALA:HA	1:F:264:ASN:HD22	1.79	0.47
1:E:75:ALA:O	1:E:79:ILE:HG12	2.15	0.47
1:A:260:ALA:HA	1:A:264:ASN:OD1	2.14	0.46
1:D:150:MET:O	1:D:169:MET:HA	2.16	0.46
1:E:369:HIS:HD2	1:E:401:ARG:HH11	1.64	0.46
1:F:162:ASN:N	1:F:214:ASN:HD22	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ALA:HA	1:D:264:ASN:ND2	2.30	0.46
1:F:253:LYS:O	1:F:254:ASP:C	2.59	0.45
1:B:369:HIS:CD2	1:B:401:ARG:NH1	2.83	0.45
1:F:193:ALA:HB2	1:F:211:TYR:OH	2.17	0.45
1:F:54:ASP:OD1	1:F:54:ASP:C	2.58	0.45
1:C:162:ASN:H	1:C:214:ASN:HD22	1.65	0.45
1:E:370:ARG:O	1:E:373:GLU:HG2	2.16	0.45
1:F:339:LEU:HG	1:F:368:SER:HB2	1.99	0.44
1:F:161:ASN:HA	1:F:214:ASN:HD21	1.83	0.44
1:F:162:ASN:H	1:F:214:ASN:HD22	1.65	0.44
1:E:290:ASP:OD2	1:E:316:ASP:HB3	2.17	0.44
1:E:148:PRO:HG2	1:E:150:MET:HE3	2.00	0.44
1:F:111:LEU:HD21	1:F:342:PHE:CD1	2.53	0.44
1:C:256:LYS:HD3	1:C:266:ALA:HB1	2.00	0.43
1:F:176:LYS:HE3	1:F:176:LYS:HA	1.98	0.43
1:F:160:ASP:OD2	1:E:203:THR:OG1	2.32	0.43
1:F:392:LYS:NZ	2:F:501:2PG:O2	2.51	0.43
1:A:152:ILE:HD13	1:A:152:ILE:HG21	1.84	0.43
1:D:397:SER:O	1:D:398:ARG:HB2	2.18	0.43
1:D:41:SER:OG	1:D:166:GLN:OE1	2.37	0.42
1:C:287:SER:HA	1:C:312:GLN:O	2.19	0.42
1:E:162:ASN:H	1:E:214:ASN:HD22	1.68	0.42
1:A:162:ASN:H	1:A:214:ASN:HD22	1.67	0.42
1:C:256:LYS:CD	1:C:266:ALA:HB1	2.49	0.42
1:B:290:ASP:OD2	1:B:316:ASP:HB3	2.20	0.41
1:D:355:ILE:HD13	1:D:355:ILE:HG21	1.85	0.41
1:A:290:ASP:OD2	1:A:316:ASP:HB3	2.19	0.41
1:B:137:ASN:ND2	6:B:615:HOH:O	2.52	0.41
1:C:321:THR:HG22	1:C:321:THR:O	2.21	0.41
1:F:339:LEU:HD23	1:F:341:LYS:HE3	2.02	0.41
1:B:276:LEU:O	1:B:280:THR:HG23	2.21	0.41
1:B:152:ILE:HD13	1:B:152:ILE:HG21	1.83	0.41
1:C:214:ASN:ND2	6:C:617:HOH:O	2.52	0.41
1:F:197:LYS:NZ	1:F:201:MET:O	2.50	0.41
1:F:321:THR:O	1:F:321:THR:HG22	2.21	0.41
1:C:131:GLU:HG3	1:C:143:TYR:OH	2.22	0.40
1:F:13:ASP:OD1	1:F:13:ASP:C	2.63	0.40
1:A:148:PRO:HG2	1:A:150:MET:HE3	2.03	0.40
1:B:202:ASN:HB2	4:B:507:SO4:O3	2.21	0.40
1:F:41:SER:OG	1:F:166:GLN:OE1	2.40	0.40
1:A:151:ASN:CA	1:A:169:MET:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:LYS:HE2	1:E:224:VAL:HG12	2.03	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%)	425 (97%)	11 (2%)	1 (0%)	43	33
1	B	436/449 (97%)	418 (96%)	17 (4%)	1 (0%)	43	33
1	C	437/449 (97%)	426 (98%)	10 (2%)	1 (0%)	43	33
1	D	436/449 (97%)	419 (96%)	15 (3%)	2 (0%)	24	14
1	E	437/449 (97%)	422 (97%)	13 (3%)	2 (0%)	24	14
1	F	436/449 (97%)	424 (97%)	10 (2%)	2 (0%)	24	14
All	All	2619/2694 (97%)	2534 (97%)	76 (3%)	9 (0%)	36	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	254	ASP
1	D	266	ALA
1	E	-4	GLY
1	B	398	ARG
1	C	398	ARG
1	D	398	ARG
1	E	398	ARG
1	A	398	ARG
1	F	398	ARG

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	331/337 (98%)	320 (97%)	11 (3%)	33	15
1	B	331/337 (98%)	321 (97%)	10 (3%)	36	17
1	C	331/337 (98%)	323 (98%)	8 (2%)	43	27
1	D	331/337 (98%)	322 (97%)	9 (3%)	39	22
1	E	332/337 (98%)	318 (96%)	14 (4%)	26	10
1	F	330/337 (98%)	313 (95%)	17 (5%)	21	6
All	All	1986/2022 (98%)	1917 (96%)	69 (4%)	32	13

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	142	LYS
1	A	197	LYS
1	A	256	LYS
1	A	281	LYS
1	A	307	LEU
1	A	310	LYS
1	A	342	PHE
1	A	343	ASN
1	A	369	HIS
1	A	400	ASP
1	B	-6	GLN
1	B	-5	MET
1	B	197	LYS
1	B	253	LYS
1	B	265	LYS
1	B	307	LEU
1	B	342	PHE
1	B	343	ASN
1	B	369	HIS
1	B	400	ASP
1	C	-7	GLN

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Mol	Chain	Res	Type
1	C	48	LEU
1	C	256	LYS
1	C	307	LEU
1	C	342	PHE
1	C	343	ASN
1	C	369	HIS
1	C	400	ASP
1	F	44	SER
1	F	142	LYS
1	F	176	LYS
1	F	178	VAL
1	F	197	LYS
1	F	202	ASN
1	F	238	LYS
1	F	244	MET
1	F	267	PHE
1	F	281	LYS
1	F	282	GLN
1	F	307	LEU
1	F	324	LYS
1	F	331	GLU
1	F	342	PHE
1	F	369	HIS
1	F	400	ASP
1	D	-7	GLN
1	D	178	VAL
1	D	307	LEU
1	D	310	LYS
1	D	332	LYS
1	D	342	PHE
1	D	343	ASN
1	D	369	HIS
1	D	400	ASP
1	E	48	LEU
1	E	253	LYS
1	E	254	ASP
1	E	256	LYS
1	E	307	LEU
1	E	310	LYS
1	E	324	LYS
1	E	342	PHE
1	E	343	ASN

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Mol	Chain	Res	Type
1	E	356	LYS
1	E	369	HIS
1	E	400	ASP
1	E	417	GLU
1	E	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-7	GLN
1	A	-6	GLN
1	A	137	ASN
1	A	151	ASN
1	A	154	ASN
1	A	166	GLN
1	A	171	GLN
1	A	191	HIS
1	A	214	ASN
1	A	274	HIS
1	A	369	HIS
1	B	-6	GLN
1	B	202	ASN
1	B	274	HIS
1	B	282	GLN
1	B	369	HIS
1	C	-6	GLN
1	C	154	ASN
1	C	171	GLN
1	C	214	ASN
1	C	369	HIS
1	F	166	GLN
1	F	171	GLN
1	F	214	ASN
1	F	264	ASN
1	F	369	HIS
1	D	137	ASN
1	D	154	ASN
1	D	166	GLN
1	D	171	GLN
1	D	191	HIS
1	D	202	ASN
1	D	264	ASN

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Mol	Chain	Res	Type
1	D	303	GLN
1	D	369	HIS
1	E	17	ASN
1	E	154	ASN
1	E	158	HIS
1	E	171	GLN
1	E	214	ASN
1	E	282	GLN
1	E	303	GLN
1	E	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 43 ligands modelled in this entry, 12 are monoatomic - leaving 31 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	508	-	4,4,4	0.62	0	6,6,6	0.49	0
4	SO4	D	805	-	4,4,4	0.87	0	6,6,6	0.82	0
4	SO4	C	507	-	4,4,4	0.63	0	6,6,6	0.66	0
4	SO4	D	801	-	4,4,4	0.59	0	6,6,6	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	C	505	-	4,4,4	0.46	0	6,6,6	0.77	0
2	2PG	A	501	3	9,10,10	2.47	3 (33%)	12,14,14	1.95	3 (25%)
5	GOL	E	508	-	5,5,5	0.37	0	5,5,5	1.95	1 (20%)
4	SO4	C	508	-	4,4,4	0.69	0	6,6,6	0.74	0
2	2PG	C	501	3	9,10,10	1.74	4 (44%)	12,14,14	1.56	2 (16%)
4	SO4	E	506	-	4,4,4	0.60	0	6,6,6	0.58	0
4	SO4	E	507	-	4,4,4	0.72	0	6,6,6	0.91	0
5	GOL	F	505	-	5,5,5	1.58	1 (20%)	5,5,5	2.93	4 (80%)
4	SO4	B	506	-	4,4,4	0.54	0	6,6,6	0.64	0
5	GOL	D	806	-	5,5,5	0.93	0	5,5,5	2.82	4 (80%)
4	SO4	E	505	-	4,4,4	0.63	0	6,6,6	1.25	1 (16%)
4	SO4	B	505	-	4,4,4	0.67	0	6,6,6	0.59	0
4	SO4	A	504	-	4,4,4	1.14	1 (25%)	6,6,6	0.58	0
2	2PG	F	501	3	9,10,10	1.93	4 (44%)	12,14,14	1.60	3 (25%)
4	SO4	A	505	-	4,4,4	0.55	0	6,6,6	0.62	0
4	SO4	A	507	-	4,4,4	0.69	0	6,6,6	1.12	1 (16%)
4	SO4	F	504	-	4,4,4	0.51	0	6,6,6	1.16	0
4	SO4	B	507	-	4,4,4	0.66	0	6,6,6	0.64	0
4	SO4	C	504	-	4,4,4	0.80	0	6,6,6	1.37	1 (16%)
2	2PG	E	502	3	9,10,10	1.26	1 (11%)	12,14,14	1.73	3 (25%)
4	SO4	C	506	-	4,4,4	0.26	0	6,6,6	1.46	1 (16%)
4	SO4	B	508	-	4,4,4	0.84	0	6,6,6	1.52	2 (33%)
4	SO4	E	501	-	4,4,4	0.72	0	6,6,6	1.21	0
2	2PG	B	501	3	9,10,10	1.75	2 (22%)	12,14,14	2.02	4 (33%)
4	SO4	A	506	-	4,4,4	0.80	0	6,6,6	0.73	0
2	2PG	D	802	3	9,10,10	1.52	3 (33%)	12,14,14	1.24	1 (8%)
4	SO4	B	504	-	4,4,4	0.70	0	6,6,6	0.51	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	2PG	A	501	3	-	0/11/11/11	-
2	2PG	F	501	3	-	0/11/11/11	-
5	GOL	E	508	-	-	4/4/4/4	-
2	2PG	C	501	3	-	2/11/11/11	-
2	2PG	E	502	3	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2PG	B	501	3	-	2/11/11/11	-
5	GOL	F	505	-	-	2/4/4/4	-
2	2PG	D	802	3	-	2/11/11/11	-
5	GOL	D	806	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	2PG	P-O1P	5.30	1.68	1.59
2	B	501	2PG	P-O1P	3.73	1.66	1.59
2	A	501	2PG	O1-C1	3.53	1.32	1.22
2	F	501	2PG	P-O2P	3.44	1.61	1.50
2	A	501	2PG	C2-C1	3.20	1.56	1.52
2	B	501	2PG	C2-C1	2.92	1.55	1.52
2	D	802	2PG	P-O4P	-2.77	1.44	1.54
2	C	501	2PG	P-O3P	-2.70	1.44	1.54
2	C	501	2PG	P-O1P	2.65	1.64	1.59
2	E	502	2PG	O1-C1	2.64	1.29	1.22
2	F	501	2PG	P-O1P	2.45	1.63	1.59
2	C	501	2PG	C2-C1	2.38	1.55	1.52
5	F	505	GOL	O2-C2	-2.28	1.36	1.43
4	A	504	SO4	O1-S	2.27	1.58	1.44
2	D	802	2PG	O1-C1	2.26	1.28	1.22
2	F	501	2PG	O1-C1	2.14	1.28	1.22
2	F	501	2PG	C2-C1	2.09	1.54	1.52
2	C	501	2PG	P-O4P	-2.09	1.47	1.54
2	D	802	2PG	C2-C1	2.01	1.54	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	2PG	P-O1P-C2	-4.72	112.20	123.04
2	B	501	2PG	O1-C1-C2	-4.40	113.35	122.85
5	D	806	GOL	O3-C3-C2	-4.36	90.73	110.38
5	F	505	GOL	O2-C2-C1	-3.85	93.25	109.18
2	C	501	2PG	P-O1P-C2	-3.68	114.58	123.04
2	E	502	2PG	P-O1P-C2	-3.51	114.99	123.04
2	A	501	2PG	O1P-P-O2P	-3.32	97.48	109.33
5	E	508	GOL	O2-C2-C1	-3.10	96.34	109.18
5	F	505	GOL	O2-C2-C3	3.08	121.91	109.18
5	D	806	GOL	O2-C2-C3	-3.08	96.45	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	505	GOL	C3-C2-C1	3.08	123.07	111.80
2	A	501	2PG	O4P-P-O2P	2.87	122.02	110.83
2	F	501	2PG	O1P-P-O2P	-2.83	99.26	109.33
2	B	501	2PG	O2-C1-C2	2.81	120.02	112.71
2	B	501	2PG	P-O1P-C2	-2.81	116.60	123.04
2	E	502	2PG	O1P-C2-C1	2.74	117.37	111.66
4	C	506	SO4	O3-S-O2	-2.69	95.51	109.56
2	E	502	2PG	O3-C3-C2	2.59	118.31	111.73
4	E	505	SO4	O3-S-O1	-2.58	96.08	109.56
2	C	501	2PG	O4P-P-O3P	2.56	117.40	107.80
4	B	508	SO4	O3-S-O1	-2.42	96.91	109.56
4	A	507	SO4	O4-S-O1	-2.42	96.93	109.56
5	D	806	GOL	O2-C2-C1	2.37	118.97	109.18
2	B	501	2PG	O3P-P-O2P	2.36	120.01	110.83
5	D	806	GOL	O1-C1-C2	2.32	120.81	110.38
5	F	505	GOL	O1-C1-C2	-2.30	100.01	110.38
4	B	508	SO4	O4-S-O3	2.18	120.57	108.54
2	F	501	2PG	O2-C1-C2	2.18	118.38	112.71
4	C	504	SO4	O4-S-O1	-2.08	98.67	109.56
2	F	501	2PG	O3-C3-C2	2.05	116.96	111.73
2	D	802	2PG	P-O1P-C2	-2.00	118.44	123.04

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	802	2PG	O1-C1-C2-C3
5	D	806	GOL	C1-C2-C3-O3
5	E	508	GOL	O1-C1-C2-C3
5	E	508	GOL	C1-C2-C3-O3
5	F	505	GOL	C1-C2-C3-O3
5	E	508	GOL	O1-C1-C2-O2
5	E	508	GOL	O2-C2-C3-O3
2	B	501	2PG	O1-C1-C2-C3
2	C	501	2PG	O1-C1-C2-C3
2	C	501	2PG	O2-C1-C2-C3
2	D	802	2PG	O2-C1-C2-C3
5	F	505	GOL	O2-C2-C3-O3
5	D	806	GOL	O2-C2-C3-O3
2	B	501	2PG	O2-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	507	SO4	1	0
2	F	501	2PG	1	0
4	B	507	SO4	1	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%)	0.32	16 (3%) 46 53	13, 23, 42, 63	0
1	B	438/449 (97%)	0.20	8 (1%) 67 73	14, 21, 39, 66	0
1	C	439/449 (97%)	0.09	8 (1%) 67 73	12, 20, 38, 54	0
1	D	438/449 (97%)	0.43	31 (7%) 22 25	13, 22, 47, 67	0
1	E	438/449 (97%)	0.37	13 (2%) 52 59	13, 25, 46, 68	1 (0%)
1	F	438/449 (97%)	0.98	68 (15%) 5 5	15, 29, 56, 82	0
All	All	2630/2694 (97%)	0.40	144 (5%) 30 35	12, 23, 46, 82	1 (0%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	258	VAL	7.6
1	F	431	ALA	6.6
1	C	431	ALA	6.0
1	F	266	ALA	5.6
1	D	-5	MET	5.3
1	D	263	GLY	5.2
1	F	263	GLY	5.2
1	F	260	ALA	5.0
1	F	159	ALA	4.9
1	F	257	TYR	4.8
1	B	-5	MET	4.6
1	C	160	ASP	4.6
1	E	160	ASP	4.6
1	A	431	ALA	4.6
1	F	163	VAL	4.6
1	F	253	LYS	4.5
1	D	160	ASP	4.4
1	F	272	PHE	4.4
1	B	253	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	164	ASP	4.3
1	F	261	GLY	4.3
1	F	259	LEU	4.2
1	F	160	ASP	4.1
1	D	266	ALA	3.9
1	F	165	ILE	3.9
1	A	310	LYS	3.8
1	F	274	HIS	3.8
1	B	160	ASP	3.7
1	E	-5	MET	3.7
1	A	160	ASP	3.7
1	F	334	ILE	3.6
1	A	266	ALA	3.5
1	F	283	TYR	3.5
1	B	-3	ARG	3.5
1	F	265	LYS	3.5
1	F	297	TRP	3.4
1	F	-4	GLY	3.4
1	F	-6	GLN	3.4
1	F	212	ALA	3.4
1	F	219	ALA	3.4
1	F	252	TYR	3.4
1	D	271	GLU	3.4
1	D	253	LYS	3.3
1	F	262	GLU	3.3
1	F	302	TYR	3.3
1	D	302	TYR	3.3
1	A	260	ALA	3.1
1	F	306	VAL	3.1
1	D	255	GLY	3.1
1	A	306	VAL	3.1
1	D	159	ALA	3.1
1	E	258	VAL	3.0
1	F	267	PHE	3.0
1	D	165	ILE	3.0
1	A	-5	MET	3.0
1	C	-5	MET	3.0
1	D	275	PHE	3.0
1	F	158	HIS	3.0
1	F	268	THR	3.0
1	A	253	LYS	2.9
1	A	197	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	430	GLN	2.8
1	F	251	PHE	2.8
1	F	275	PHE	2.7
1	D	269	SER	2.7
1	D	163	VAL	2.7
1	D	256	LYS	2.7
1	F	43	GLY	2.7
1	F	-5	MET	2.7
1	F	-3	ARG	2.7
1	F	255	GLY	2.7
1	F	269	SER	2.7
1	F	320	VAL	2.7
1	B	-6	GLN	2.6
1	F	299	GLY	2.6
1	F	217	SER	2.6
1	F	222	LEU	2.5
1	F	311	ILE	2.5
1	E	159	ALA	2.5
1	D	-4	GLY	2.5
1	E	-4	GLY	2.5
1	F	281	LYS	2.5
1	D	257	TYR	2.4
1	D	259	LEU	2.4
1	E	240	ILE	2.4
1	C	-4	GLY	2.4
1	D	261	GLY	2.4
1	A	-6	GLN	2.4
1	D	-6	GLN	2.4
1	D	301	ALA	2.4
1	C	-6	GLN	2.4
1	F	44	SER	2.4
1	E	253	LYS	2.4
1	A	237	GLY	2.3
1	F	42	THR	2.3
1	D	267	PHE	2.3
1	E	252	TYR	2.3
1	F	198	ALA	2.3
1	C	159	ALA	2.3
1	E	266	ALA	2.3
1	F	424	ARG	2.3
1	E	263	GLY	2.3
1	A	254	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	-7	GLN	2.3
1	F	292	LEU	2.3
1	D	42	THR	2.3
1	D	219	ALA	2.2
1	F	295	SER	2.2
1	A	311	ILE	2.2
1	D	254	ASP	2.2
1	F	161	ASN	2.2
1	F	264	ASN	2.2
1	E	256	LYS	2.2
1	F	200	GLY	2.2
1	F	248	ALA	2.2
1	F	324	LYS	2.2
1	F	45	ARG	2.2
1	D	282	GLN	2.2
1	F	333	GLY	2.2
1	C	266	ALA	2.2
1	F	310	LYS	2.2
1	D	212	ALA	2.2
1	A	265	LYS	2.2
1	C	-3	ARG	2.2
1	D	197	LYS	2.2
1	F	271	GLU	2.1
1	A	-7	GLN	2.1
1	F	197	LYS	2.1
1	D	310	LYS	2.1
1	F	301	ALA	2.1
1	D	252	TYR	2.1
1	F	216	GLY	2.1
1	F	227	GLU	2.1
1	F	218	ASN	2.1
1	B	265	LYS	2.1
1	D	265	LYS	2.1
1	D	430	GLN	2.1
1	F	307	LEU	2.1
1	F	276	LEU	2.0
1	B	310	LYS	2.0
1	F	94	ILE	2.0
1	A	264	ASN	2.0
1	E	333	GLY	2.0
1	E	-3	ARG	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	SO4	A	507	5/5	0.59	0.19	54,57,95,102	0
4	SO4	D	805	5/5	0.65	0.27	68,78,115,131	0
4	SO4	C	507	5/5	0.70	0.21	53,53,70,87	0
4	SO4	B	504	5/5	0.73	0.14	51,61,92,110	0
4	SO4	F	504	5/5	0.81	0.13	48,59,65,70	0
5	GOL	F	505	6/6	0.81	0.22	29,33,39,73	0
4	SO4	E	507	5/5	0.83	0.14	52,52,56,85	0
4	SO4	A	508	5/5	0.83	0.14	33,65,70,97	0
5	GOL	E	508	6/6	0.86	0.13	32,39,49,49	0
4	SO4	E	505	5/5	0.87	0.12	43,44,47,66	0
5	GOL	D	806	6/6	0.88	0.15	27,34,39,66	0
4	SO4	C	506	5/5	0.89	0.13	40,41,60,67	0
3	MG	F	503	1/1	0.89	0.13	48,48,48,48	0
4	SO4	C	504	5/5	0.89	0.10	38,41,44,49	0
4	SO4	C	508	5/5	0.90	0.11	27,58,65,71	0
4	SO4	B	507	5/5	0.91	0.10	26,60,61,70	0
4	SO4	A	506	5/5	0.91	0.10	40,44,45,58	0
4	SO4	A	505	5/5	0.92	0.10	43,44,51,55	0
3	MG	C	502	1/1	0.93	0.11	19,19,19,19	0
4	SO4	B	505	5/5	0.93	0.09	40,42,48,57	0
4	SO4	A	504	5/5	0.94	0.11	38,40,42,44	0
4	SO4	E	506	5/5	0.94	0.09	39,44,52,60	0
4	SO4	E	501	5/5	0.94	0.08	36,39,47,64	0
4	SO4	B	506	5/5	0.95	0.08	36,39,41,48	0
3	MG	D	803	1/1	0.95	0.17	28,28,28,28	0
4	SO4	B	508	5/5	0.95	0.13	34,39,43,49	0
4	SO4	D	801	5/5	0.95	0.09	35,37,44,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	804	1/1	0.95	0.13	36,36,36,36	0
3	MG	A	502	1/1	0.95	0.09	29,29,29,29	0
2	2PG	F	501	11/11	0.96	0.08	25,29,36,37	0
3	MG	B	502	1/1	0.96	0.07	27,27,27,27	0
2	2PG	A	501	11/11	0.97	0.06	16,19,22,23	0
2	2PG	D	802	11/11	0.97	0.07	18,23,28,29	0
2	2PG	E	502	11/11	0.97	0.06	18,20,26,29	0
3	MG	E	504	1/1	0.97	0.05	34,34,34,34	0
3	MG	A	503	1/1	0.98	0.10	33,33,33,33	0
2	2PG	B	501	11/11	0.98	0.05	16,17,19,19	0
4	SO4	C	505	5/5	0.98	0.07	32,34,44,46	0
3	MG	B	503	1/1	0.98	0.05	28,28,28,28	0
3	MG	E	503	1/1	0.98	0.06	25,25,25,25	0
2	2PG	C	501	11/11	0.98	0.04	14,16,21,21	0
3	MG	C	503	1/1	0.98	0.05	27,27,27,27	0
3	MG	F	502	1/1	0.98	0.07	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.