



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:16 AM UTC

PDB ID : 7B2N / pdb_00007b2n
Title : Crystal structure of Chlamydomonas reinhardtii chloroplastic Fructose biphosphate aldolase
Authors : Le Moigne, T.; Lemaire, S.D.; Henri, J.
Deposited on : 2020-11-27
Resolution : 2.36 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

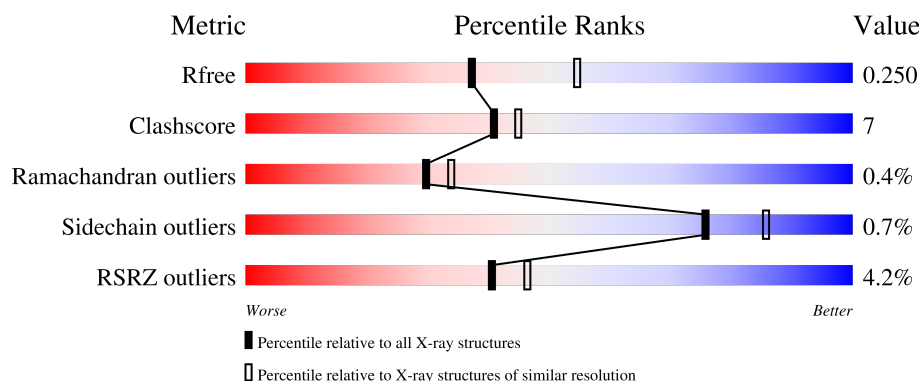
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	359	 3% 81% 11% 8%
1	B	359	 % 84% 8% 8%
1	C	359	 2% 82% 10% 8%
1	D	359	 3% 78% 13% 8%
1	E	359	 6% 77% 16% 7%

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Mol	Chain	Length	Quality of chain
1	F	359	4% 79% 13% 8%
1	G	359	4% 79% 13% 8%
1	H	359	8% 70% 22% 8%

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
2	SO4	D	404	-	-	X	-
2	SO4	F	405	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21458 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 Fructose-bisphosphate aldolase 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	3	0
			2566	1613	450	488	15			
1	B	332	Total	C	N	O	S	0	1	0
			2548	1603	448	482	15			
1	C	332	Total	C	N	O	S	0	2	0
			2560	1610	449	485	16			
1	D	329	Total	C	N	O	S	0	0	0
			2520	1588	441	476	15			
1	E	333	Total	C	N	O	S	0	0	0
			2545	1602	445	482	16			
1	F	331	Total	C	N	O	S	0	0	0
			2532	1594	443	480	15			
1	G	330	Total	C	N	O	S	0	0	0
			2524	1590	442	477	15			
1	H	330	Total	C	N	O	S	0	0	0
			2528	1592	442	479	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP Q42690
A	20	HIS	-	expression tag	UNP Q42690
A	21	HIS	-	expression tag	UNP Q42690
A	22	HIS	-	expression tag	UNP Q42690
A	23	HIS	-	expression tag	UNP Q42690
A	24	HIS	-	expression tag	UNP Q42690
A	25	HIS	-	expression tag	UNP Q42690
A	26	HIS	-	expression tag	UNP Q42690
A	27	MET	-	expression tag	UNP Q42690
B	19	MET	-	initiating methionine	UNP Q42690
B	20	HIS	-	expression tag	UNP Q42690
B	21	HIS	-	expression tag	UNP Q42690
B	22	HIS	-	expression tag	UNP Q42690

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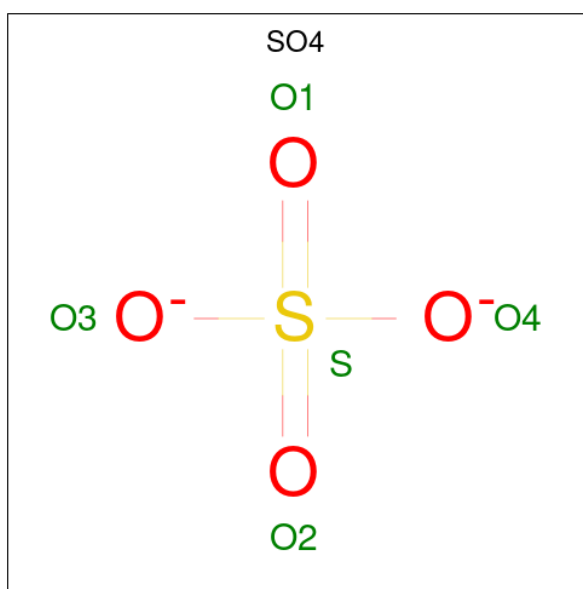
Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q42690
B	24	HIS	-	expression tag	UNP Q42690
B	25	HIS	-	expression tag	UNP Q42690
B	26	HIS	-	expression tag	UNP Q42690
B	27	MET	-	expression tag	UNP Q42690
C	19	MET	-	initiating methionine	UNP Q42690
C	20	HIS	-	expression tag	UNP Q42690
C	21	HIS	-	expression tag	UNP Q42690
C	22	HIS	-	expression tag	UNP Q42690
C	23	HIS	-	expression tag	UNP Q42690
C	24	HIS	-	expression tag	UNP Q42690
C	25	HIS	-	expression tag	UNP Q42690
C	26	HIS	-	expression tag	UNP Q42690
C	27	MET	-	expression tag	UNP Q42690
D	19	MET	-	initiating methionine	UNP Q42690
D	20	HIS	-	expression tag	UNP Q42690
D	21	HIS	-	expression tag	UNP Q42690
D	22	HIS	-	expression tag	UNP Q42690
D	23	HIS	-	expression tag	UNP Q42690
D	24	HIS	-	expression tag	UNP Q42690
D	25	HIS	-	expression tag	UNP Q42690
D	26	HIS	-	expression tag	UNP Q42690
D	27	MET	-	expression tag	UNP Q42690
E	19	MET	-	initiating methionine	UNP Q42690
E	20	HIS	-	expression tag	UNP Q42690
E	21	HIS	-	expression tag	UNP Q42690
E	22	HIS	-	expression tag	UNP Q42690
E	23	HIS	-	expression tag	UNP Q42690
E	24	HIS	-	expression tag	UNP Q42690
E	25	HIS	-	expression tag	UNP Q42690
E	26	HIS	-	expression tag	UNP Q42690
E	27	MET	-	expression tag	UNP Q42690
F	19	MET	-	initiating methionine	UNP Q42690
F	20	HIS	-	expression tag	UNP Q42690
F	21	HIS	-	expression tag	UNP Q42690
F	22	HIS	-	expression tag	UNP Q42690
F	23	HIS	-	expression tag	UNP Q42690
F	24	HIS	-	expression tag	UNP Q42690
F	25	HIS	-	expression tag	UNP Q42690
F	26	HIS	-	expression tag	UNP Q42690
F	27	MET	-	expression tag	UNP Q42690
G	19	MET	-	initiating methionine	UNP Q42690

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Chain	Residue	Modelled	Actual	Comment	Reference
G	20	HIS	-	expression tag	UNP Q42690
G	21	HIS	-	expression tag	UNP Q42690
G	22	HIS	-	expression tag	UNP Q42690
G	23	HIS	-	expression tag	UNP Q42690
G	24	HIS	-	expression tag	UNP Q42690
G	25	HIS	-	expression tag	UNP Q42690
G	26	HIS	-	expression tag	UNP Q42690
G	27	MET	-	expression tag	UNP Q42690
H	19	MET	-	initiating methionine	UNP Q42690
H	20	HIS	-	expression tag	UNP Q42690
H	21	HIS	-	expression tag	UNP Q42690
H	22	HIS	-	expression tag	UNP Q42690
H	23	HIS	-	expression tag	UNP Q42690
H	24	HIS	-	expression tag	UNP Q42690
H	25	HIS	-	expression tag	UNP Q42690
H	26	HIS	-	expression tag	UNP Q42690
H	27	MET	-	expression tag	UNP Q42690

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

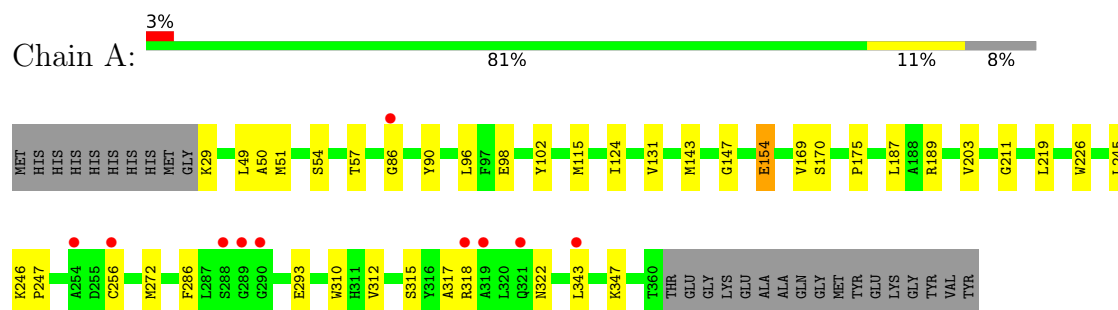
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	170	Total	O	0	0
			170	170		
4	C	152	Total	O	0	0
			152	152		
4	D	114	Total	O	0	0
			114	114		
4	E	86	Total	O	0	0
			86	86		
4	F	138	Total	O	0	0
			138	138		
4	G	87	Total	O	0	0
			87	87		
4	H	102	Total	O	0	0
			102	102		

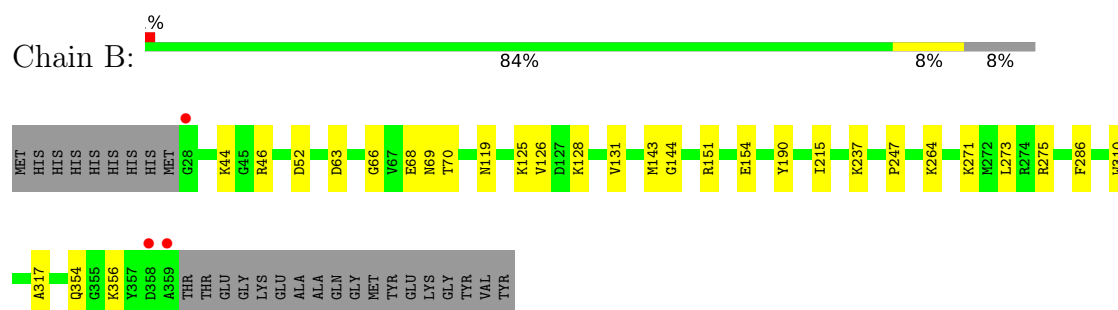
3 Residue-property plots [i](#)

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.

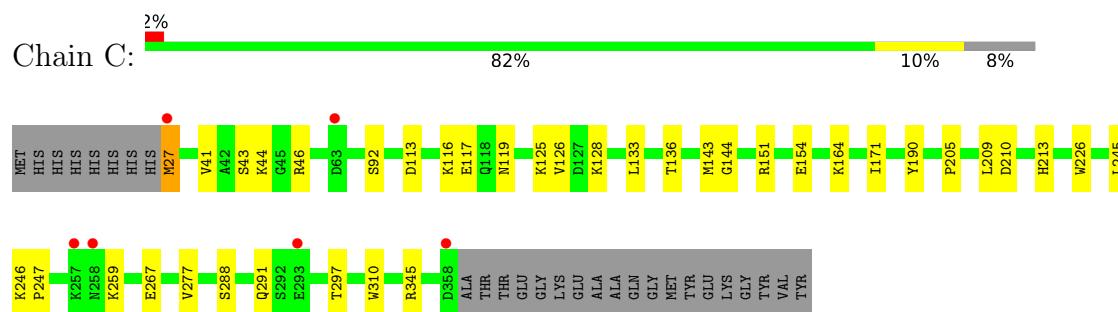
- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic



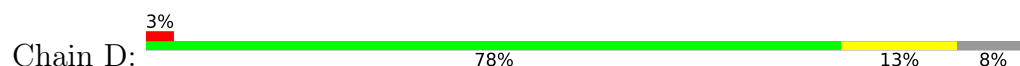
- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic

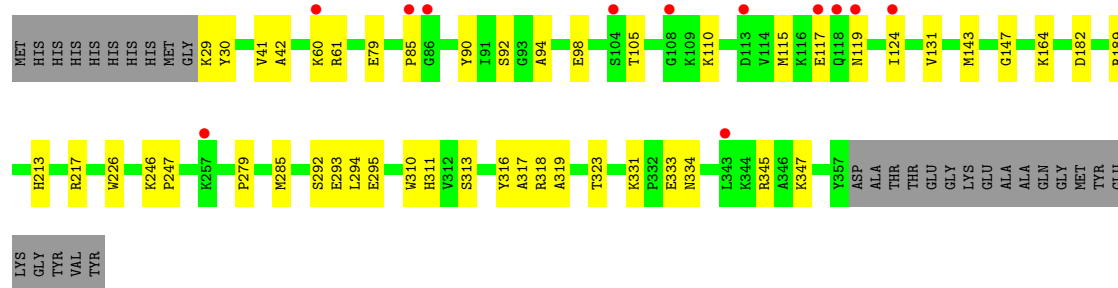


- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic

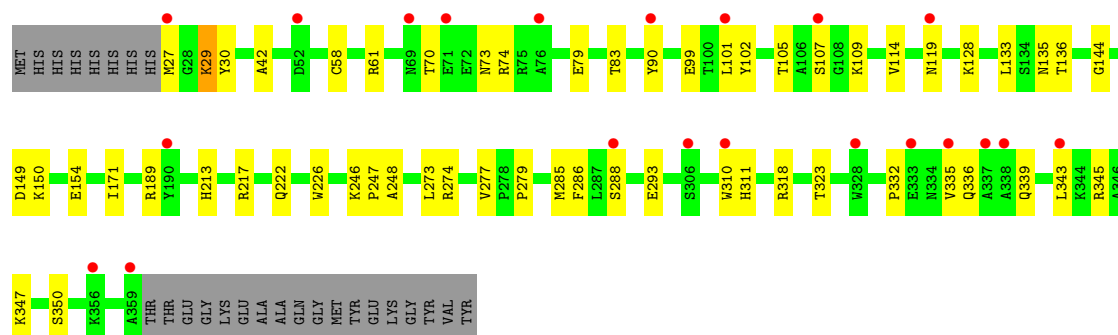
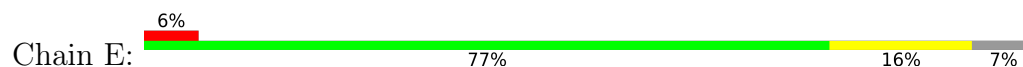


- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic

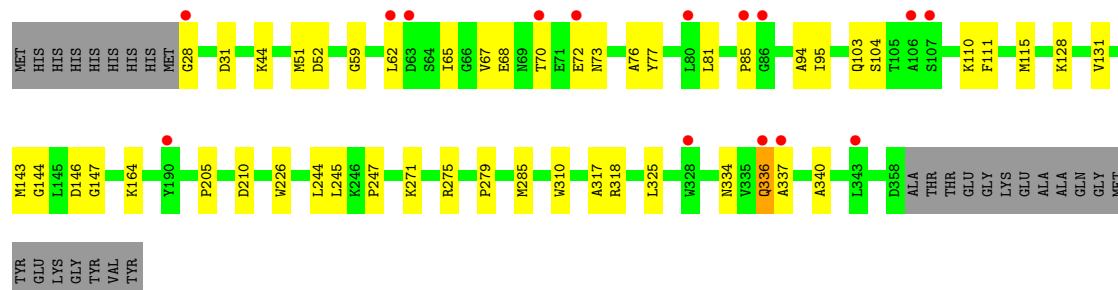
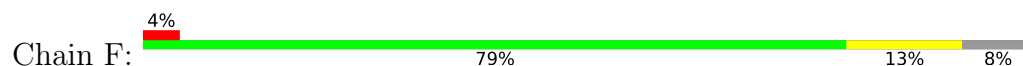




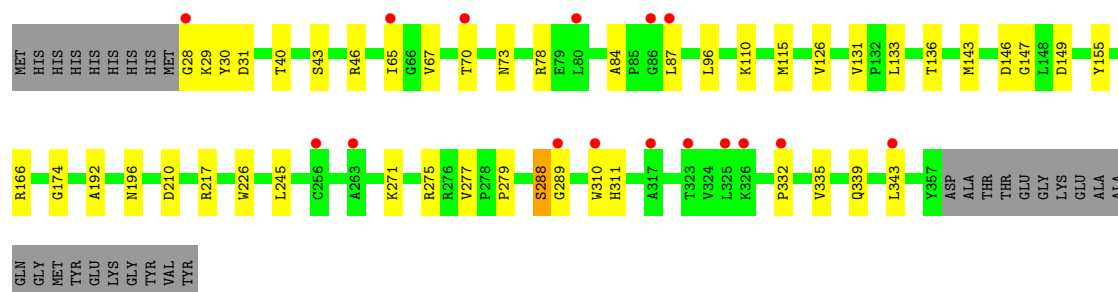
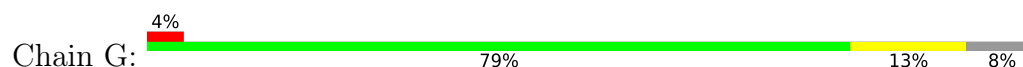
- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic



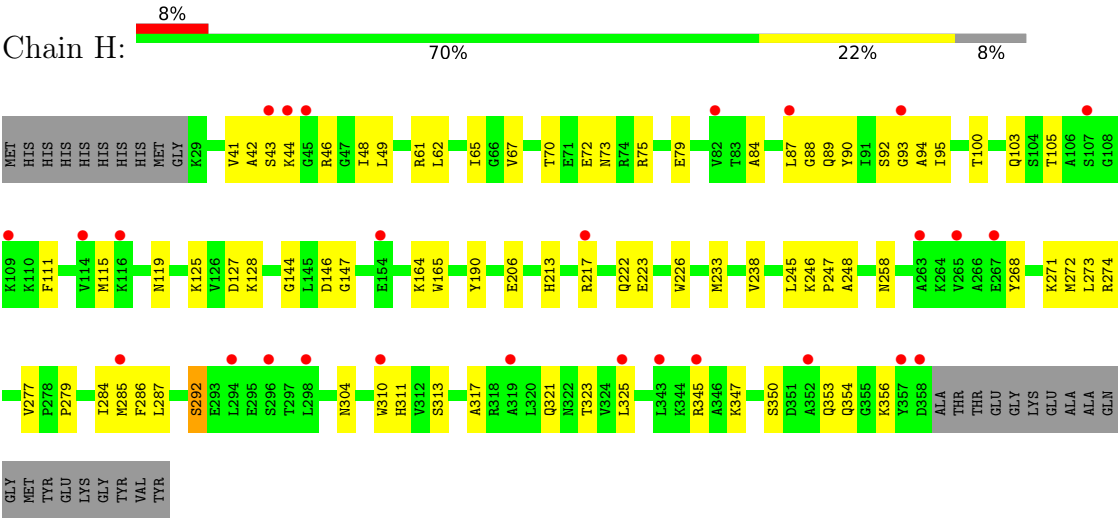
- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic



- Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic



● Molecule 1: Fructose-bisphosphate aldolase 1, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.49Å 251.07Å 126.41Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	46.67 – 2.36 46.67 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.67-2.36) 99.4 (46.67-2.36)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.252 0.203 , 0.250	Depositor DCC
R_{free} test set	1984 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21458	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4

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	0.18	0/2613	0.36	0/3534
1	B	0.30	0/2595	0.44	1/3509 (0.0%)
1	C	0.22	0/2607	0.39	0/3524
1	D	0.16	0/2567	0.36	0/3472
1	E	0.23	0/2592	0.41	0/3505
1	F	0.17	0/2579	0.37	0/3488
1	G	0.25	1/2571 (0.0%)	0.39	0/3477
1	H	0.18	0/2575	0.39	0/3483
All	All	0.21	1/20699 (0.0%)	0.39	1/27992 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	288	SER	C-O	-6.81	1.15	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	GLU	CB-CG-CD	5.37	121.73	112.60

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	2566	0	2572	28	0
1	B	2548	0	2559	18	0
1	C	2560	0	2568	30	0
1	D	2520	0	2535	37	0
1	E	2545	0	2556	47	0
1	F	2532	0	2542	34	0
1	G	2524	0	2538	35	0
1	H	2528	0	2539	56	0
2	A	20	0	0	1	0
2	B	25	0	0	2	0
2	C	25	0	0	1	0
2	D	20	0	0	3	0
2	E	10	0	0	0	0
2	F	25	0	0	4	0
2	G	15	0	0	1	0
2	H	5	0	0	0	0
3	B	1	0	0	0	0
4	A	140	0	0	2	0
4	B	170	0	0	2	0
4	C	152	0	0	5	0
4	D	114	0	0	7	0
4	E	86	0	0	4	0
4	F	138	0	0	1	0
4	G	87	0	0	2	0
4	H	102	0	0	2	0
All	All	21458	0	20409	267	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 7.

All (267) 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:G:279:PRO:HA	1:G:310:TRP:HE1	1.29	0.96
1:C:27:MET:CE	1:E:135:ASN:HD21	1.84	0.91
1:C:27:MET:HE1	1:E:135:ASN:HD21	1.39	0.87
1:D:60:LYS:HE3	1:D:61:ARG:HH12	1.38	0.86
1:B:128:LYS:HD3	1:B:144:GLY:HA2	1.63	0.81
1:H:279:PRO:HA	1:H:310:TRP:HE1	1.44	0.81
1:D:311:HIS:HD2	4:D:592:HOH:O	1.65	0.80
1:E:70:THR:HG23	1:E:73:ASN:H	1.46	0.80
1:E:83:THR:HG22	1:E:114:VAL:HG11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:PRO:HA	1:G:310:TRP:NE1	1.99	0.77
1:B:44:LYS:HE2	2:B:401:SO4:O3	1.87	0.75
1:H:61:ARG:HB3	1:H:325:LEU:HD21	1.69	0.74
1:H:84:ALA:HB3	1:H:87:LEU:HG	1.69	0.73
1:E:339:GLN:O	1:E:343:LEU:HD12	1.89	0.71
1:E:27:MET:HG3	1:E:27:MET:O	1.91	0.70
1:A:256:CYS:SG	4:A:588:HOH:O	2.51	0.69
1:D:131:VAL:HG21	1:D:143:MET:HE3	1.73	0.69
1:H:304:ASN:ND2	1:H:353:GLN:O	2.25	0.69
1:F:164:LYS:NZ	4:F:502:HOH:O	2.26	0.68
1:H:285:MET:SD	1:H:313:SER:HB3	2.34	0.68
1:C:246:LYS:NZ	4:C:502:HOH:O	2.22	0.68
1:E:29:LYS:NZ	4:E:501:HOH:O	2.27	0.67
1:G:28:GLY:HA3	1:G:31:ASP:OD2	1.94	0.67
1:A:86:GLY:H	1:A:343:LEU:HD11	1.60	0.67
1:H:279:PRO:HA	1:H:310:TRP:NE1	2.10	0.66
1:C:128:LYS:HG3	1:C:144:GLY:HA2	1.77	0.66
1:H:42:ALA:O	1:H:311:HIS:ND1	2.25	0.66
1:E:42:ALA:O	1:E:311:HIS:ND1	2.29	0.65
1:F:336:GLN:HG3	1:F:337:ALA:H	1.62	0.65
1:G:131:VAL:HG21	1:G:143:MET:HE3	1.78	0.65
1:A:131:VAL:HG21	1:A:143:MET:HE3	1.79	0.63
1:F:70:THR:HG23	1:F:73:ASN:H	1.62	0.63
1:E:279:PRO:HA	1:E:310:TRP:HE1	1.61	0.63
1:H:222:GLN:NE2	1:H:248:ALA:O	2.30	0.62
1:E:189:ARG:NH1	4:E:503:HOH:O	2.32	0.62
1:G:84:ALA:HB1	1:G:343:LEU:HD21	1.80	0.62
1:E:279:PRO:HA	1:E:310:TRP:NE1	2.14	0.62
1:A:54:SER:HB3	1:A:57:THR:H	1.64	0.62
1:E:277:VAL:O	1:E:310:TRP:HZ2	1.83	0.62
1:E:293:GLU:HG3	1:E:345:ARG:CZ	2.30	0.61
1:D:117:GLU:C	1:D:119:ASN:H	2.08	0.61
1:E:273:LEU:HD11	1:E:286:PHE:HZ	1.65	0.61
1:C:27:MET:HE3	1:E:135:ASN:HD21	1.63	0.61
1:A:317:ALA:HB3	1:A:318:ARG:NH2	2.15	0.61
1:A:49:LEU:HG	1:A:51:MET:HG3	1.83	0.60
1:A:96:LEU:HD21	1:A:115:MET:HE1	1.83	0.60
1:F:128:LYS:HD3	1:F:144:GLY:HA2	1.83	0.59
1:H:323:THR:HB	1:H:345:ARG:NH2	2.17	0.59
1:A:318:ARG:O	1:A:322:ASN:HB2	2.03	0.59
1:G:84:ALA:HB3	1:G:87:LEU:HG	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:70:THR:HG23	1:H:73:ASN:H	1.68	0.58
1:D:42:ALA:O	1:D:311:HIS:ND1	2.37	0.58
1:F:226:TRP:HZ2	1:F:247:PRO:HB3	1.69	0.58
1:G:96:LEU:HD11	1:G:115:MET:HE1	1.86	0.58
1:B:52:ASP:OD2	1:B:125:LYS:HE2	2.03	0.58
1:C:113:ASP:O	1:C:117:GLU:HG3	2.03	0.58
1:D:292:SER:HB3	1:D:295:GLU:HB2	1.84	0.58
1:H:128:LYS:HE3	1:H:144:GLY:HA2	1.86	0.58
1:H:46:ARG:NH2	1:H:119:ASN:O	2.37	0.57
1:F:334:ASN:HA	1:F:336:GLN:HG2	1.86	0.57
1:C:116:LYS:NZ	4:C:507:HOH:O	2.36	0.57
1:A:98:GLU:HA	1:A:124:ILE:HD11	1.85	0.57
1:E:310:TRP:CZ2	1:G:279:PRO:HG2	2.40	0.57
1:F:337:ALA:HA	1:F:340:ALA:HB3	1.86	0.57
1:D:292:SER:OG	1:D:293:GLU:N	2.38	0.57
1:G:40:THR:O	1:G:43:SER:OG	2.22	0.56
1:E:226:TRP:HZ2	1:E:247:PRO:HB3	1.70	0.56
1:H:273:LEU:HD22	1:H:284:ILE:HD13	1.86	0.56
1:D:323:THR:HB	1:D:345:ARG:CZ	2.35	0.56
1:B:126:VAL:O	1:B:151:ARG:NH2	2.39	0.56
1:D:94:ALA:HB3	1:D:115:MET:HE3	1.87	0.56
1:A:90:TYR:CZ	1:A:347:LYS:HG3	2.42	0.55
1:D:98:GLU:HA	1:D:124:ILE:HD11	1.88	0.55
1:H:206:GLU:HG3	1:H:287:LEU:HD21	1.89	0.54
1:G:332:PRO:HA	1:G:335:VAL:HG23	1.88	0.54
1:F:226:TRP:CZ2	1:F:247:PRO:HB3	2.42	0.54
1:E:90:TYR:CZ	1:E:347:LYS:HG3	2.43	0.54
1:F:244:LEU:HD22	1:F:285:MET:HE1	1.88	0.54
1:E:274:ARG:HA	1:E:310:TRP:HH2	1.73	0.54
1:H:62:LEU:HB3	1:H:67:VAL:HB	1.88	0.54
1:H:273:LEU:HD11	1:H:286:PHE:HZ	1.72	0.54
1:E:61:ARG:NH2	1:E:318:ARG:HE	2.05	0.53
1:E:226:TRP:CZ2	1:E:247:PRO:HB3	2.43	0.53
1:H:323:THR:HB	1:H:345:ARG:HH21	1.73	0.53
1:F:77:TYR:CZ	1:F:81:LEU:HD11	2.44	0.53
1:F:318:ARG:NH1	2:F:405:SO4:O3	2.42	0.53
1:B:273:LEU:HD11	1:B:286:PHE:HZ	1.75	0.52
1:D:316:TYR:HB3	1:D:319:ALA:HB3	1.91	0.52
1:D:164:LYS:NZ	4:D:513:HOH:O	2.42	0.52
1:G:166:ARG:NH1	4:G:508:HOH:O	2.40	0.52
1:H:89:GLN:HG2	1:H:90:TYR:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:VAL:O	1:E:310:TRP:CZ2	2.63	0.52
1:H:100:THR:HG23	1:H:103:GLN:HE21	1.75	0.52
1:F:65:ILE:HG13	1:F:67:VAL:HG23	1.91	0.51
1:F:318:ARG:NH1	2:F:405:SO4:S	2.83	0.51
1:E:293:GLU:HG3	1:E:345:ARG:NH1	2.25	0.51
1:F:51:MET:HG2	1:F:95:ILE:O	2.11	0.51
1:H:111:PHE:O	1:H:115:MET:HG3	2.10	0.51
1:C:297:THR:OG1	1:C:345:ARG:NH2	2.44	0.50
1:D:317:ALA:HB3	2:D:404:SO4:O3	2.11	0.50
1:F:226:TRP:CH2	1:F:245:LEU:HG	2.47	0.50
1:B:143:MET:HE2	1:H:146:ASP:HA	1.93	0.50
1:E:29:LYS:HG3	1:E:30:TYR:H	1.76	0.50
1:B:143:MET:HE1	1:H:147:GLY:H	1.75	0.50
1:B:271:LYS:HD2	1:B:275:ARG:NH2	2.27	0.50
1:D:79:GLU:HG3	1:D:105:THR:HG22	1.92	0.50
1:G:339:GLN:O	1:G:343:LEU:HG	2.12	0.50
1:H:292:SER:N	4:H:512:HOH:O	2.45	0.50
1:A:226:TRP:HZ2	1:A:247:PRO:HB3	1.77	0.50
1:C:164:LYS:NZ	4:C:510:HOH:O	2.45	0.50
1:F:44:LYS:HG2	2:F:403:SO4:O3	2.11	0.50
1:H:44:LYS:HE2	1:H:311:HIS:CD2	2.46	0.49
1:G:133:LEU:O	1:G:136:THR:OG1	2.29	0.49
1:H:213:HIS:HA	1:H:217:ARG:HH21	1.76	0.49
1:F:317:ALA:HB3	2:F:405:SO4:O3	2.12	0.49
1:C:277:VAL:O	1:F:279:PRO:HD3	2.12	0.49
1:G:226:TRP:CH2	1:G:245:LEU:HG	2.48	0.49
1:D:279:PRO:HG3	1:H:279:PRO:HG3	1.95	0.49
1:F:103:GLN:HE21	1:F:111:PHE:HE2	1.60	0.49
1:D:164:LYS:HD2	4:D:508:HOH:O	2.11	0.49
1:E:90:TYR:HB3	1:E:350:SER:HB2	1.95	0.49
1:A:226:TRP:CZ2	1:A:247:PRO:HB3	2.48	0.49
1:F:52:ASP:HB3	1:F:95:ILE:HG22	1.94	0.49
1:E:74:ARG:NH1	1:E:99:GLU:OE2	2.46	0.49
1:G:43:SER:HB2	1:G:46:ARG:HD3	1.95	0.49
1:D:292:SER:OG	1:D:294:LEU:N	2.46	0.48
1:C:128:LYS:HB2	1:C:143:MET:HG3	1.95	0.48
1:E:336:GLN:HG2	4:E:544:HOH:O	2.12	0.48
1:E:246:LYS:HA	1:E:285:MET:O	2.13	0.48
1:F:111:PHE:O	1:F:115:MET:HG3	2.13	0.48
1:D:246:LYS:NZ	4:D:508:HOH:O	2.36	0.48
1:E:279:PRO:HG3	1:G:279:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:THR:HA	1:H:103:GLN:HG2	1.96	0.48
1:A:147:GLY:H	1:D:143:MET:HE1	1.78	0.48
1:B:68:GLU:HG2	1:B:70:THR:HG23	1.95	0.48
1:B:354:GLN:HB2	1:B:356:LYS:HG2	1.95	0.48
1:H:246:LYS:HA	1:H:285:MET:O	2.14	0.48
1:B:69:ASN:N	4:B:515:HOH:O	2.47	0.48
1:C:171:ILE:HD12	1:C:213:HIS:CE1	2.48	0.48
1:E:222:GLN:NE2	1:E:248:ALA:O	2.45	0.47
1:H:87:LEU:C	1:H:89:GLN:H	2.21	0.47
1:C:226:TRP:CZ2	1:C:247:PRO:HB3	2.49	0.47
1:B:237:LYS:HE2	4:B:628:HOH:O	2.14	0.47
1:C:44:LYS:NZ	4:C:512:HOH:O	2.47	0.47
1:A:219:LEU:HD12	1:A:272:MET:HB2	1.95	0.47
1:A:169:VAL:HB	1:A:175:PRO:HG3	1.96	0.47
1:B:131:VAL:HG21	1:B:143:MET:HE3	1.97	0.47
1:H:94:ALA:HB3	1:H:115:MET:HE1	1.95	0.47
1:H:222:GLN:HB3	1:H:272:MET:SD	2.54	0.47
1:C:46:ARG:NH2	1:C:119:ASN:O	2.40	0.47
1:C:288:SER:O	1:C:291:GLN:HG2	2.15	0.47
1:F:70:THR:CG2	1:F:73:ASN:H	2.25	0.47
1:D:117:GLU:C	1:D:119:ASN:N	2.73	0.47
1:G:29:LYS:HD3	1:G:30:TYR:CE2	2.50	0.47
1:G:271:LYS:HD2	1:G:275:ARG:NH2	2.30	0.46
1:A:317:ALA:HB3	1:A:318:ARG:HH22	1.81	0.46
1:H:43:SER:OG	1:H:46:ARG:HD3	2.15	0.46
1:A:143:MET:HE1	1:D:147:GLY:H	1.80	0.46
1:E:107:SER:HB2	1:E:109:LYS:HD3	1.98	0.46
1:F:271:LYS:HD2	1:F:275:ARG:NH2	2.30	0.46
1:B:63:ASP:O	1:B:66:GLY:N	2.39	0.46
1:B:46:ARG:NH2	1:B:119:ASN:O	2.48	0.46
1:H:90:TYR:HB3	1:H:350:SER:HB2	1.96	0.46
1:C:226:TRP:HZ2	1:C:247:PRO:HB3	1.79	0.46
1:D:311:HIS:CD2	4:D:592:HOH:O	2.52	0.46
1:E:133:LEU:HD23	1:E:136:THR:HG21	1.98	0.46
1:H:90:TYR:CE1	1:H:347:LYS:HE2	2.50	0.46
1:C:226:TRP:CH2	1:C:245:LEU:HG	2.51	0.46
1:D:285:MET:SD	1:D:313:SER:HB3	2.56	0.45
1:E:171:ILE:HD12	1:E:213:HIS:CE1	2.51	0.45
1:H:65:ILE:HG13	1:H:67:VAL:HG23	1.99	0.45
1:F:131:VAL:HG21	1:F:143:MET:HE3	1.99	0.45
1:G:70:THR:HG23	1:G:73:ASN:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:LYS:HE2	1:E:144:GLY:HA2	1.99	0.45
1:G:279:PRO:CA	1:G:310:TRP:HE1	2.15	0.45
1:B:247:PRO:HG2	1:B:286:PHE:CE1	2.52	0.45
1:D:189:ARG:NH1	4:D:505:HOH:O	2.33	0.45
1:E:323:THR:HG21	1:E:345:ARG:HG3	1.98	0.45
1:A:247:PRO:HG2	1:A:286:PHE:CE1	2.52	0.45
1:A:102:TYR:OH	1:A:154[A]:GLU:OE2	2.30	0.45
1:E:149:ASP:OD1	1:E:150:LYS:N	2.50	0.45
1:G:65:ILE:HG13	1:G:67:VAL:HG23	1.98	0.45
1:C:288:SER:OG	2:C:404:SO4:O2	2.35	0.44
1:F:51:MET:SD	1:F:94:ALA:HB1	2.57	0.44
1:E:279:PRO:HD3	1:G:277:VAL:O	2.17	0.44
1:H:165:TRP:HB3	1:H:190:TYR:CE2	2.53	0.44
1:D:334:ASN:HA	4:D:511:HOH:O	2.18	0.44
1:D:110:LYS:HB3	1:D:110:LYS:HE2	1.74	0.44
1:G:78:ARG:NH1	4:G:515:HOH:O	2.47	0.44
1:A:226:TRP:CH2	1:A:245:LEU:HG	2.53	0.44
1:G:210:ASP:OD1	1:G:210:ASP:N	2.51	0.44
1:A:29:LYS:N	4:A:524:HOH:O	2.51	0.44
1:D:90:TYR:CZ	1:D:347:LYS:HG3	2.52	0.44
1:F:143:MET:HE1	1:G:147:GLY:H	1.82	0.44
1:H:226:TRP:HZ2	1:H:247:PRO:HB3	1.83	0.44
1:A:211:GLY:HA3	2:A:402:SO4:O3	2.18	0.44
1:H:226:TRP:CZ2	1:H:247:PRO:HB3	2.53	0.43
1:C:27:MET:HE1	1:E:135:ASN:ND2	2.21	0.43
1:C:210:ASP:OD1	1:C:210:ASP:N	2.51	0.43
1:E:90:TYR:CE1	1:E:347:LYS:HG3	2.54	0.43
1:H:258:ASN:OD1	1:H:258:ASN:N	2.51	0.43
1:F:147:GLY:H	1:G:143:MET:HE1	1.82	0.43
1:F:146:ASP:HB2	1:G:146:ASP:OD2	2.17	0.43
1:H:279:PRO:CA	1:H:310:TRP:HE1	2.24	0.43
1:H:354:GLN:HB3	1:H:356:LYS:HG2	2.00	0.43
1:D:226:TRP:CZ2	1:D:247:PRO:HB3	2.53	0.43
1:G:174:GLY:O	1:G:217:ARG:NH2	2.52	0.43
1:H:79:GLU:HG3	1:H:105:THR:HG22	2.00	0.43
1:C:267:GLU:OE2	1:C:267:GLU:HA	2.19	0.43
1:E:154:GLU:HG3	4:E:504:HOH:O	2.19	0.42
1:E:101:LEU:HD23	1:E:102:TYR:CE1	2.54	0.42
1:F:325:LEU:HD23	1:F:325:LEU:HA	1.77	0.42
1:A:189:ARG:NH1	1:D:182:ASP:OD1	2.52	0.42
1:H:223:GLU:HG3	1:H:272:MET:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LYS:HZ2	1:A:315:SER:CB	2.32	0.42
1:D:318:ARG:NH2	2:D:404:SO4:S	2.92	0.42
1:F:28:GLY:HA3	1:F:31:ASP:OD2	2.20	0.42
1:H:268:TYR:HA	1:H:271:LYS:HD3	2.00	0.42
1:E:79:GLU:HG3	1:E:105:THR:HG22	2.01	0.42
1:G:110:LYS:HB2	1:G:110:LYS:HE2	1.92	0.42
1:H:49:LEU:O	1:H:94:ALA:HA	2.19	0.42
1:H:226:TRP:CH2	1:H:245:LEU:HG	2.54	0.42
1:C:43:SER:OG	1:C:46:ARG:HD3	2.20	0.42
1:C:259:LYS:HE3	1:C:259:LYS:HB3	1.85	0.42
1:D:41:VAL:HA	1:D:92:SER:HB2	2.02	0.42
1:E:119:ASN:C	1:E:119:ASN:HD22	2.28	0.42
1:C:27:MET:HE3	1:E:135:ASN:ND2	2.34	0.42
1:G:126:VAL:HG12	1:G:155:TYR:CE2	2.55	0.42
1:G:277:VAL:O	1:G:310:TRP:HZ2	2.02	0.42
1:H:274:ARG:NH2	4:H:517:HOH:O	2.53	0.42
1:F:104:SER:OG	1:F:110:LYS:HA	2.20	0.41
1:B:215:ILE:HG21	1:B:264:LYS:HE2	2.02	0.41
1:A:50:ALA:HB3	1:A:317:ALA:HB2	2.01	0.41
1:D:90:TYR:CE1	1:D:347:LYS:HG3	2.56	0.41
1:H:48:ILE:HG23	1:H:93:GLY:C	2.45	0.41
1:A:187:LEU:HD22	1:A:203:VAL:HG13	2.02	0.41
1:H:233:MET:HE2	1:H:238:VAL:HG11	2.01	0.41
1:C:125:LYS:HD2	4:C:510:HOH:O	2.20	0.41
1:H:72:GLU:OE2	1:H:72:GLU:HA	2.19	0.41
1:B:317:ALA:HB3	2:B:404:SO4:O2	2.20	0.41
1:F:59:GLY:HA2	1:F:62:LEU:HD12	2.02	0.41
1:H:277:VAL:HB	1:H:310:TRP:CH2	2.56	0.41
1:D:226:TRP:HZ2	1:D:247:PRO:HB3	1.85	0.41
1:E:58:CYS:SG	1:E:74:ARG:HG2	2.61	0.41
1:C:209:LEU:HD23	1:C:209:LEU:HA	1.89	0.41
1:D:29:LYS:HE2	1:D:30:TYR:CE2	2.56	0.41
1:D:318:ARG:NH2	2:D:404:SO4:O3	2.54	0.41
1:F:72:GLU:O	1:F:76:ALA:N	2.47	0.41
1:H:41:VAL:HA	1:H:92:SER:HB2	2.03	0.41
1:H:125:LYS:NZ	1:H:127:ASP:OD2	2.51	0.41
1:H:317:ALA:O	1:H:321:GLN:HB2	2.21	0.41
1:E:273:LEU:HD11	1:E:286:PHE:CZ	2.52	0.41
1:G:311:HIS:HA	2:G:401:SO4:O3	2.21	0.41
1:H:95:ILE:HD13	1:H:164:LYS:HD3	2.03	0.41
1:C:41:VAL:HA	1:C:92:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:O	1:C:151[B]:ARG:NH2	2.54	0.40
1:C:133:LEU:HD23	1:C:136:THR:HG21	2.04	0.40
1:F:210:ASP:OD1	1:F:210:ASP:N	2.54	0.40
1:A:286:PHE:HE2	1:A:312:VAL:HG13	1.86	0.40
1:E:332:PRO:HA	1:E:335:VAL:HG23	2.03	0.40
1:G:192:ALA:O	1:G:196:ASN:ND2	2.39	0.40
1:G:149:ASP:OD1	1:G:149:ASP:N	2.55	0.40
1:G:277:VAL:HB	1:G:310:TRP:CZ2	2.56	0.40
1:H:75:ARG:NH1	1:H:79:GLU:OE1	2.49	0.40
1:A:293:GLU:H	1:A:293:GLU:CD	2.30	0.40
1:D:213:HIS:HA	1:D:217:ARG:HH21	1.87	0.40
1:D:331:LYS:HD2	1:D:333:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/359 (93%)	322 (97%)	11 (3%)	0	100	100
1	B	331/359 (92%)	321 (97%)	10 (3%)	0	100	100
1	C	332/359 (92%)	321 (97%)	10 (3%)	1 (0%)	36	43
1	D	327/359 (91%)	314 (96%)	12 (4%)	1 (0%)	36	43
1	E	331/359 (92%)	318 (96%)	12 (4%)	1 (0%)	36	43
1	F	329/359 (92%)	314 (95%)	11 (3%)	4 (1%)	10	9
1	G	328/359 (91%)	317 (97%)	10 (3%)	1 (0%)	36	43
1	H	328/359 (91%)	314 (96%)	12 (4%)	2 (1%)	21	24
All	All	2639/2872 (92%)	2541 (96%)	88 (3%)	10 (0%)	30	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	29	LYS
1	F	336	GLN
1	G	289	GLY
1	F	68	GLU
1	H	292	SER
1	C	205	PRO
1	D	85	PRO
1	H	88	GLY
1	F	85	PRO
1	F	205	PRO

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	268/286 (94%)	263 (98%)	5 (2%)	50	65
1	B	265/286 (93%)	263 (99%)	2 (1%)	73	84
1	C	267/286 (93%)	262 (98%)	5 (2%)	50	65
1	D	263/286 (92%)	262 (100%)	1 (0%)	84	91
1	E	265/286 (93%)	263 (99%)	2 (1%)	73	84
1	F	264/286 (92%)	263 (100%)	1 (0%)	84	91
1	G	263/286 (92%)	262 (100%)	1 (0%)	84	91
1	H	264/286 (92%)	264 (100%)	0	100	100
All	All	2119/2288 (93%)	2102 (99%)	17 (1%)	76	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154[A]	GLU
1	A	154[B]	GLU
1	A	170[A]	SER
1	A	170[B]	SER
1	A	310	TRP
1	B	190	TYR

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Mol	Chain	Res	Type
1	B	310	TRP
1	C	27	MET
1	C	154[A]	GLU
1	C	154[B]	GLU
1	C	190	TYR
1	C	310	TRP
1	D	310	TRP
1	E	217	ARG
1	E	288	SER
1	F	310	TRP
1	G	288	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	137	ASN
1	A	308	ASN
1	A	311	HIS
1	B	196	ASN
1	B	258	ASN
1	C	55	ASN
1	C	196	ASN
1	C	258	ASN
1	C	354	GLN
1	D	103	GLN
1	D	118	GLN
1	D	305	GLN
1	D	329	GLN
1	E	89	GLN
1	E	103	GLN
1	E	119	ASN
1	E	135	ASN
1	E	304	ASN
1	E	321	GLN
1	F	118	GLN
1	F	336	GLN
1	F	354	GLN
1	G	89	GLN
1	G	258	ASN
1	G	291	GLN
1	G	304	ASN

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Mol	Chain	Res	Type
1	G	321	GLN
1	H	103	GLN
1	H	308	ASN
1	H	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 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	$\# Z > 2$
2	SO4	B	403	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	H	401	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	F	404	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	F	405	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	F	403	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	E	401	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	G	403	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	E	402	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	C	404	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	C	403	-	4,4,4	0.23	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	F	402	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	C	405	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	G	401	-	4,4,4	0.21	0	6,6,6	0.46	0
2	SO4	D	403	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	B	404	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	B	405	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	G	402	-	4,4,4	0.27	0	6,6,6	0.08	0
2	SO4	A	403	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	B	402	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	402	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	F	401	-	4,4,4	0.27	0	6,6,6	0.07	0
2	SO4	A	404	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	402	-	4,4,4	0.22	0	6,6,6	0.12	0
2	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.05	0
2	SO4	D	402	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	D	404	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SO4	A	401	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	B	401	-	4,4,4	0.26	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	405	SO4	3	0
2	F	403	SO4	1	0
2	C	404	SO4	1	0
2	G	401	SO4	1	0
2	B	404	SO4	1	0
2	A	402	SO4	1	0
2	D	404	SO4	3	0
2	B	401	SO4	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, 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	332/359 (92%)	0.23	10 (3%)	52	59	15, 40, 59, 72	3 (0%)
1	B	332/359 (92%)	-0.15	3 (0%)	81	84	13, 32, 55, 72	1 (0%)
1	C	332/359 (92%)	0.02	6 (1%)	67	72	16, 39, 60, 77	2 (0%)
1	D	329/359 (91%)	0.40	12 (3%)	46	52	26, 49, 68, 77	0
1	E	333/359 (92%)	0.59	21 (6%)	26	29	29, 52, 79, 89	0
1	F	331/359 (92%)	0.36	15 (4%)	38	44	28, 43, 77, 91	0
1	G	330/359 (91%)	0.67	16 (4%)	35	41	33, 52, 70, 81	0
1	H	330/359 (91%)	0.78	27 (8%)	17	20	30, 54, 74, 86	0
All	All	2649/2872 (92%)	0.36	110 (4%)	40	46	13, 45, 71, 91	6 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	ALA	5.8
1	E	359	ALA	4.9
1	B	28	GLY	4.5
1	C	27	MET	4.3
1	G	310	TRP	4.1
1	E	27	MET	3.9
1	H	294	LEU	3.9
1	H	310	TRP	3.9
1	A	319	ALA	3.8
1	D	108	GLY	3.6
1	E	338	ALA	3.4
1	H	285	MET	3.3
1	F	106	ALA	3.3
1	F	337	ALA	3.3
1	A	256	CYS	3.3
1	E	310	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	318	ARG	3.1
1	G	65	ILE	3.0
1	G	80	LEU	3.0
1	H	343	LEU	3.0
1	H	357	TYR	3.0
1	A	289	GLY	2.9
1	F	86	GLY	2.9
1	H	82	VAL	2.9
1	F	107	SER	2.9
1	H	267	GLU	2.9
1	E	343	LEU	2.8
1	E	333	GLU	2.8
1	E	69	ASN	2.8
1	C	293	GLU	2.8
1	H	358	ASP	2.8
1	H	109	LYS	2.7
1	G	323	THR	2.7
1	D	117	GLU	2.7
1	H	217	ARG	2.7
1	H	87	LEU	2.7
1	F	72	GLU	2.7
1	H	263	ALA	2.6
1	E	71	GLU	2.6
1	F	62	LEU	2.6
1	G	70	THR	2.6
1	A	86	GLY	2.6
1	D	86	GLY	2.6
1	H	298	LEU	2.6
1	E	328	TRP	2.6
1	G	289	GLY	2.6
1	E	90	TYR	2.6
1	F	190	TYR	2.6
1	D	118	GLN	2.5
1	E	52	ASP	2.5
1	H	352	ALA	2.5
1	H	93	GLY	2.5
1	A	288	SER	2.5
1	D	119	ASN	2.5
1	E	190	TYR	2.5
1	D	113	ASP	2.5
1	G	317	ALA	2.5
1	F	343	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	358	ASP	2.4
1	B	358	ASP	2.4
1	C	258	ASN	2.4
1	D	60	LYS	2.4
1	A	290	GLY	2.3
1	G	326	LYS	2.3
1	A	343	LEU	2.3
1	F	80	LEU	2.3
1	F	63	ASP	2.3
1	F	70	THR	2.3
1	H	43	SER	2.3
1	H	116	LYS	2.3
1	H	265	VAL	2.3
1	F	28	GLY	2.3
1	H	319	ALA	2.3
1	H	345	ARG	2.3
1	C	257	LYS	2.3
1	H	44	LYS	2.3
1	G	325	LEU	2.2
1	F	85	PRO	2.2
1	G	332	PRO	2.2
1	E	76	ALA	2.2
1	E	337	ALA	2.2
1	E	335	VAL	2.2
1	H	45	GLY	2.2
1	D	257	LYS	2.2
1	E	288	SER	2.2
1	H	325	LEU	2.2
1	F	328	TRP	2.2
1	E	306	SER	2.2
1	D	124	ILE	2.1
1	E	101	LEU	2.1
1	F	336	GLN	2.1
1	G	28	GLY	2.1
1	H	296	SER	2.1
1	G	343	LEU	2.1
1	C	63	ASP	2.1
1	A	321	GLN	2.1
1	A	254	ALA	2.1
1	D	104	SER	2.1
1	D	343	LEU	2.1
1	H	154	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	86	GLY	2.1
1	G	256	CYS	2.1
1	E	119	ASN	2.1
1	D	85	PRO	2.1
1	E	107	SER	2.0
1	H	107	SER	2.0
1	G	263	ALA	2.0
1	H	114	VAL	2.0
1	G	87	LEU	2.0
1	E	356	LYS	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(Å ²)	Q<0.9
2	SO4	D	401	5/5	0.46	0.17	69,86,92,99	0
2	SO4	A	404	5/5	0.67	0.15	75,77,81,96	0
2	SO4	A	401	5/5	0.67	0.14	58,74,94,101	0
2	SO4	E	401	5/5	0.71	0.12	74,78,86,99	0
2	SO4	G	401	5/5	0.72	0.15	80,80,88,94	0
2	SO4	F	405	5/5	0.73	0.20	59,61,74,92	0
2	SO4	C	405	5/5	0.75	0.13	72,78,87,99	0
2	SO4	C	401	5/5	0.76	0.12	67,78,89,90	0
2	SO4	C	404	5/5	0.82	0.15	62,63,74,87	0
2	SO4	A	403	5/5	0.84	0.13	67,72,75,86	0
2	SO4	D	403	5/5	0.85	0.21	57,57,68,87	0
2	SO4	B	405	5/5	0.85	0.14	53,57,61,91	0
2	SO4	G	402	5/5	0.87	0.17	62,67,80,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	404	5/5	0.88	0.16	45,49,73,75	0
2	SO4	C	402	5/5	0.88	0.12	58,59,63,64	0
2	SO4	B	402	5/5	0.89	0.10	67,70,75,78	0
2	SO4	D	404	5/5	0.89	0.18	67,68,81,85	0
2	SO4	F	401	5/5	0.90	0.15	51,61,74,91	0
2	SO4	F	403	5/5	0.91	0.18	60,60,68,68	0
2	SO4	C	403	5/5	0.91	0.16	56,63,75,84	0
2	SO4	B	401	5/5	0.92	0.11	44,50,69,72	0
2	SO4	A	402	5/5	0.92	0.10	51,53,71,75	0
2	SO4	F	404	5/5	0.93	0.18	59,61,72,83	0
2	SO4	G	403	5/5	0.94	0.12	58,60,63,68	0
2	SO4	H	401	5/5	0.94	0.09	49,58,68,69	0
2	SO4	E	402	5/5	0.97	0.08	43,50,53,58	0
2	SO4	F	402	5/5	0.98	0.09	47,48,50,51	0
2	SO4	D	402	5/5	0.98	0.06	47,47,52,61	0
3	CL	B	406	1/1	0.98	0.06	50,50,50,50	0
2	SO4	B	403	5/5	0.99	0.05	37,38,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.