Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 11:07 pm GMT

PDB ID	:	7QXF
Title	:	Fructose-6-phosphate aldolase (FSA) mutant R134V, S166G, with covalently bound active site ligand
Authors	:	Dobritzsch, D.; Widersten, M.; Engel, S.
Deposited on	:	2022-01-26
Resolution	:	2.62 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:

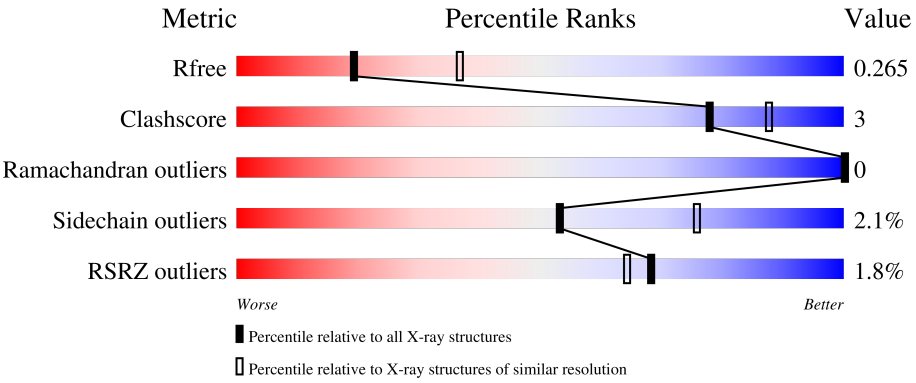
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 <=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	227	88% 8%
1	B	227	5% 89% 7%
1	C	227	2% 91% 6%
1	D	227	87% 8%
1	E	227	89% 7%

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Mol	Chain	Length	Quality of chain
1	F	227	87% 9%
1	G	227	89% 7%
1	H	227	4% 90% 7%
1	I	227	90% 6%
1	J	227	88% 9%
1	K	227	5% 89% 7%
1	L	227	89% 8%
1	M	227	88% 9%
1	N	227	89% 8%
1	O	227	7% 90% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 24511 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-6-phosphate aldolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1615	1033	269	304	9			
1	B	221	Total	C	N	O	S	0	1	0
			1628	1041	271	307	9			
1	C	220	Total	C	N	O	S	0	0	0
			1615	1033	269	304	9			
1	D	219	Total	C	N	O	S	0	3	0
			1627	1041	272	305	9			
1	E	221	Total	C	N	O	S	0	1	0
			1629	1042	272	306	9			
1	F	221	Total	C	N	O	S	0	1	0
			1629	1042	272	306	9			
1	G	221	Total	C	N	O	S	0	1	0
			1629	1042	272	306	9			
1	H	221	Total	C	N	O	S	0	0	0
			1622	1037	270	306	9			
1	I	220	Total	C	N	O	S	0	0	0
			1615	1033	269	304	9			
1	J	220	Total	C	N	O	S	0	0	0
			1615	1033	269	304	9			
1	K	220	Total	C	N	O	S	0	0	0
			1615	1033	269	304	9			
1	L	220	Total	C	N	O	S	0	1	0
			1622	1038	271	304	9			
1	M	221	Total	C	N	O	S	0	0	0
			1622	1037	270	306	9			
1	N	221	Total	C	N	O	S	0	1	0
			1629	1042	272	306	9			
1	O	221	Total	C	N	O	S	0	0	0
			1622	1037	270	306	9			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	VAL	ARG	engineered mutation	UNP P78055
A	166	GLY	SER	engineered mutation	UNP P78055
A	221	THR	-	expression tag	UNP P78055
A	222	SER	-	expression tag	UNP P78055
A	223	HIS	-	expression tag	UNP P78055
A	224	HIS	-	expression tag	UNP P78055
A	225	HIS	-	expression tag	UNP P78055
A	226	HIS	-	expression tag	UNP P78055
A	227	HIS	-	expression tag	UNP P78055
B	134	VAL	ARG	engineered mutation	UNP P78055
B	166	GLY	SER	engineered mutation	UNP P78055
B	221	THR	-	expression tag	UNP P78055
B	222	SER	-	expression tag	UNP P78055
B	223	HIS	-	expression tag	UNP P78055
B	224	HIS	-	expression tag	UNP P78055
B	225	HIS	-	expression tag	UNP P78055
B	226	HIS	-	expression tag	UNP P78055
B	227	HIS	-	expression tag	UNP P78055
C	134	VAL	ARG	engineered mutation	UNP P78055
C	166	GLY	SER	engineered mutation	UNP P78055
C	221	THR	-	expression tag	UNP P78055
C	222	SER	-	expression tag	UNP P78055
C	223	HIS	-	expression tag	UNP P78055
C	224	HIS	-	expression tag	UNP P78055
C	225	HIS	-	expression tag	UNP P78055
C	226	HIS	-	expression tag	UNP P78055
C	227	HIS	-	expression tag	UNP P78055
D	134	VAL	ARG	engineered mutation	UNP P78055
D	166	GLY	SER	engineered mutation	UNP P78055
D	221	THR	-	expression tag	UNP P78055
D	222	SER	-	expression tag	UNP P78055
D	223	HIS	-	expression tag	UNP P78055
D	224	HIS	-	expression tag	UNP P78055
D	225	HIS	-	expression tag	UNP P78055
D	226	HIS	-	expression tag	UNP P78055
D	227	HIS	-	expression tag	UNP P78055
E	134	VAL	ARG	engineered mutation	UNP P78055
E	166	GLY	SER	engineered mutation	UNP P78055
E	221	THR	-	expression tag	UNP P78055
E	222	SER	-	expression tag	UNP P78055
E	223	HIS	-	expression tag	UNP P78055
E	224	HIS	-	expression tag	UNP P78055
E	225	HIS	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
E	226	HIS	-	expression tag	UNP P78055
E	227	HIS	-	expression tag	UNP P78055
F	134	VAL	ARG	engineered mutation	UNP P78055
F	166	GLY	SER	engineered mutation	UNP P78055
F	221	THR	-	expression tag	UNP P78055
F	222	SER	-	expression tag	UNP P78055
F	223	HIS	-	expression tag	UNP P78055
F	224	HIS	-	expression tag	UNP P78055
F	225	HIS	-	expression tag	UNP P78055
F	226	HIS	-	expression tag	UNP P78055
F	227	HIS	-	expression tag	UNP P78055
G	134	VAL	ARG	engineered mutation	UNP P78055
G	166	GLY	SER	engineered mutation	UNP P78055
G	221	THR	-	expression tag	UNP P78055
G	222	SER	-	expression tag	UNP P78055
G	223	HIS	-	expression tag	UNP P78055
G	224	HIS	-	expression tag	UNP P78055
G	225	HIS	-	expression tag	UNP P78055
G	226	HIS	-	expression tag	UNP P78055
G	227	HIS	-	expression tag	UNP P78055
H	134	VAL	ARG	engineered mutation	UNP P78055
H	166	GLY	SER	engineered mutation	UNP P78055
H	221	THR	-	expression tag	UNP P78055
H	222	SER	-	expression tag	UNP P78055
H	223	HIS	-	expression tag	UNP P78055
H	224	HIS	-	expression tag	UNP P78055
H	225	HIS	-	expression tag	UNP P78055
H	226	HIS	-	expression tag	UNP P78055
H	227	HIS	-	expression tag	UNP P78055
I	134	VAL	ARG	engineered mutation	UNP P78055
I	166	GLY	SER	engineered mutation	UNP P78055
I	221	THR	-	expression tag	UNP P78055
I	222	SER	-	expression tag	UNP P78055
I	223	HIS	-	expression tag	UNP P78055
I	224	HIS	-	expression tag	UNP P78055
I	225	HIS	-	expression tag	UNP P78055
I	226	HIS	-	expression tag	UNP P78055
I	227	HIS	-	expression tag	UNP P78055
J	134	VAL	ARG	engineered mutation	UNP P78055
J	166	GLY	SER	engineered mutation	UNP P78055
J	221	THR	-	expression tag	UNP P78055
J	222	SER	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
J	223	HIS	-	expression tag	UNP P78055
J	224	HIS	-	expression tag	UNP P78055
J	225	HIS	-	expression tag	UNP P78055
J	226	HIS	-	expression tag	UNP P78055
J	227	HIS	-	expression tag	UNP P78055
K	134	VAL	ARG	engineered mutation	UNP P78055
K	166	GLY	SER	engineered mutation	UNP P78055
K	221	THR	-	expression tag	UNP P78055
K	222	SER	-	expression tag	UNP P78055
K	223	HIS	-	expression tag	UNP P78055
K	224	HIS	-	expression tag	UNP P78055
K	225	HIS	-	expression tag	UNP P78055
K	226	HIS	-	expression tag	UNP P78055
K	227	HIS	-	expression tag	UNP P78055
L	134	VAL	ARG	engineered mutation	UNP P78055
L	166	GLY	SER	engineered mutation	UNP P78055
L	221	THR	-	expression tag	UNP P78055
L	222	SER	-	expression tag	UNP P78055
L	223	HIS	-	expression tag	UNP P78055
L	224	HIS	-	expression tag	UNP P78055
L	225	HIS	-	expression tag	UNP P78055
L	226	HIS	-	expression tag	UNP P78055
L	227	HIS	-	expression tag	UNP P78055
M	134	VAL	ARG	engineered mutation	UNP P78055
M	166	GLY	SER	engineered mutation	UNP P78055
M	221	THR	-	expression tag	UNP P78055
M	222	SER	-	expression tag	UNP P78055
M	223	HIS	-	expression tag	UNP P78055
M	224	HIS	-	expression tag	UNP P78055
M	225	HIS	-	expression tag	UNP P78055
M	226	HIS	-	expression tag	UNP P78055
M	227	HIS	-	expression tag	UNP P78055
N	134	VAL	ARG	engineered mutation	UNP P78055
N	166	GLY	SER	engineered mutation	UNP P78055
N	221	THR	-	expression tag	UNP P78055
N	222	SER	-	expression tag	UNP P78055
N	223	HIS	-	expression tag	UNP P78055
N	224	HIS	-	expression tag	UNP P78055
N	225	HIS	-	expression tag	UNP P78055
N	226	HIS	-	expression tag	UNP P78055
N	227	HIS	-	expression tag	UNP P78055
O	134	VAL	ARG	engineered mutation	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
O	166	GLY	SER	engineered mutation	UNP P78055
O	221	THR	-	expression tag	UNP P78055
O	222	SER	-	expression tag	UNP P78055
O	223	HIS	-	expression tag	UNP P78055
O	224	HIS	-	expression tag	UNP P78055
O	225	HIS	-	expression tag	UNP P78055
O	226	HIS	-	expression tag	UNP P78055
O	227	HIS	-	expression tag	UNP P78055

- Molecule 2 is water.

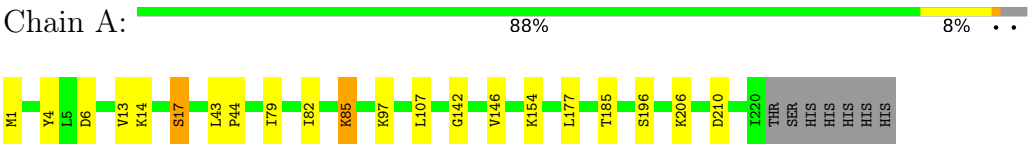
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	9	Total O 9 9	0	0
2	C	4	Total O 4 4	0	0
2	D	15	Total O 15 15	0	0
2	E	18	Total O 18 18	0	0
2	F	29	Total O 29 29	0	0
2	G	16	Total O 16 16	0	0
2	H	8	Total O 8 8	0	0
2	I	3	Total O 3 3	0	0
2	J	9	Total O 9 9	0	0
2	K	7	Total O 7 7	0	0
2	L	8	Total O 8 8	0	0
2	M	16	Total O 16 16	0	0
2	N	12	Total O 12 12	0	0
2	O	10	Total O 10 10	0	0

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.

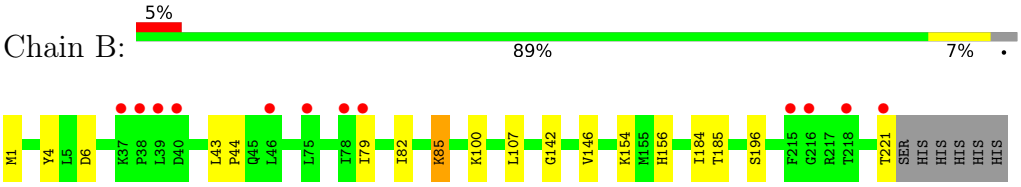
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain A:



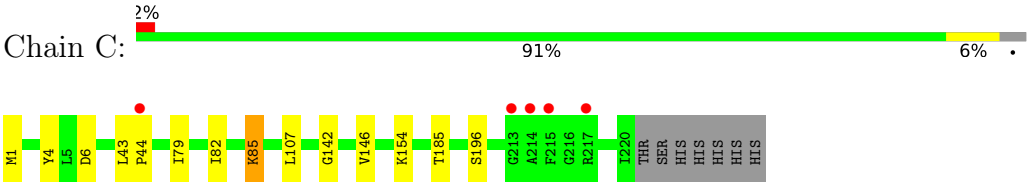
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain B:



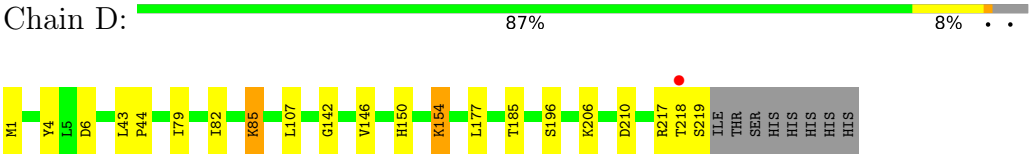
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain C:



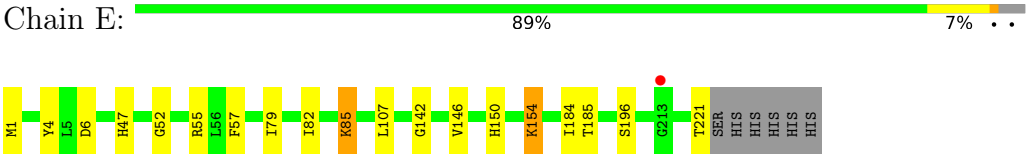
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain D:



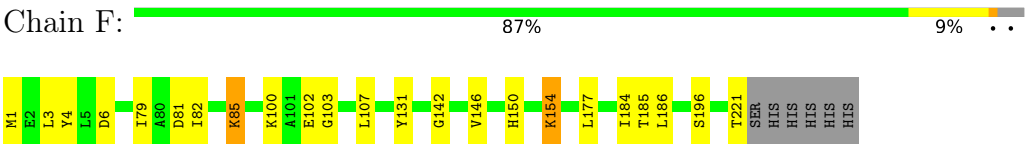
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain E:



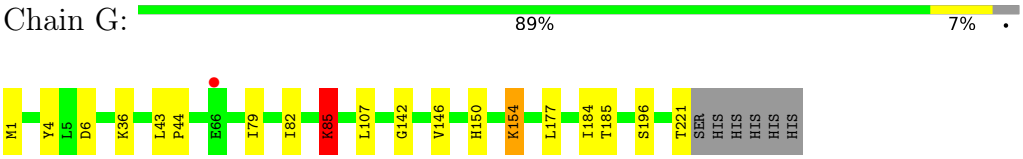
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain F:



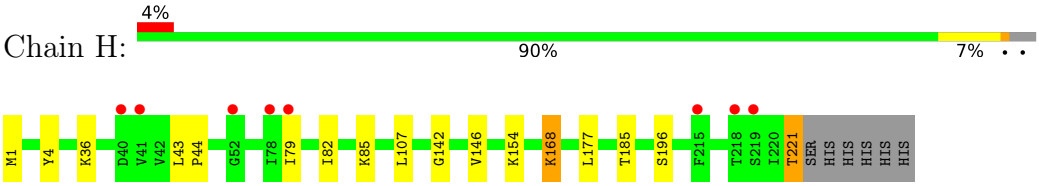
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain G:



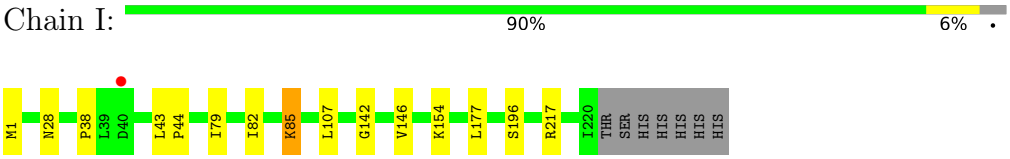
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain H:



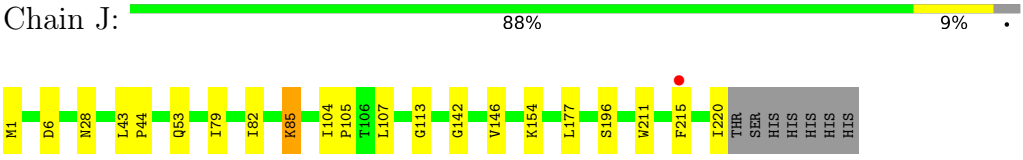
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain I:



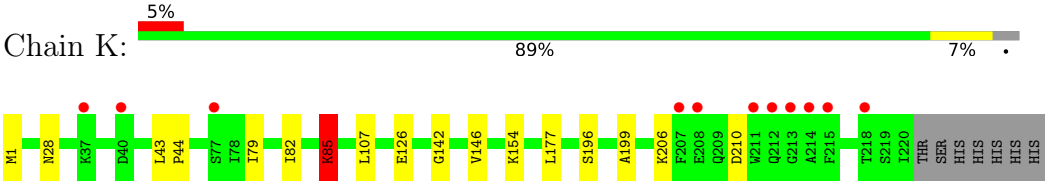
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain J:



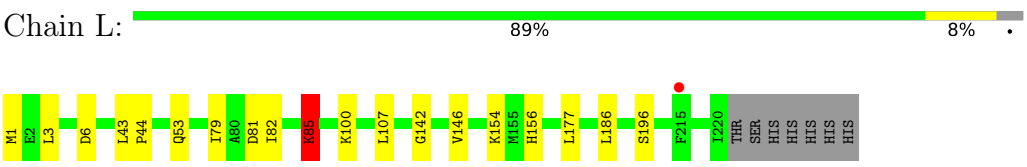
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain K:



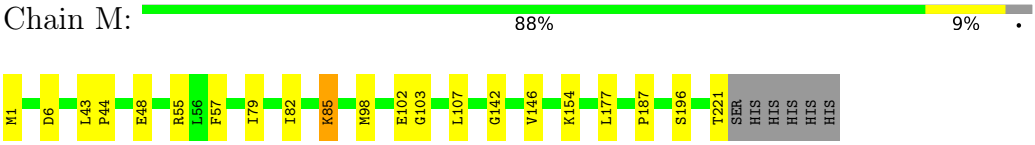
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain L:



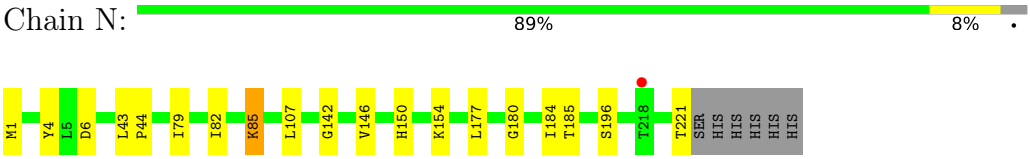
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain M:



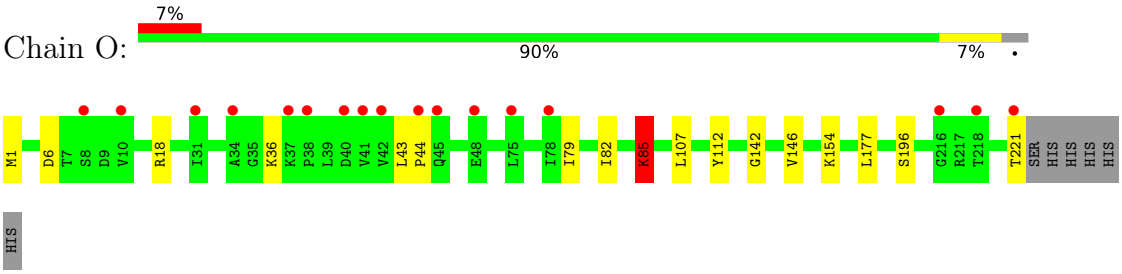
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain N:



• Molecule 1: Fructose-6-phosphate aldolase 1

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.20Å 176.87Å 120.09Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	49.71 – 2.62 49.67 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.71-2.62) 99.0 (49.67-2.62)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.220 , 0.262 0.224 , 0.265	Depositor DCC
R_{free} test set	5735 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 23.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24511	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I2F

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	0.70	0/1621	0.82	0/2206
1	B	0.70	0/1637	0.80	0/2228
1	C	0.71	0/1621	0.81	0/2206
1	D	0.72	0/1644	0.83	0/2237
1	E	0.72	0/1639	0.83	0/2231
1	F	0.73	0/1639	0.83	0/2231
1	G	0.71	0/1639	0.82	0/2231
1	H	0.70	0/1628	0.85	2/2216 (0.1%)
1	I	0.71	0/1621	0.82	0/2206
1	J	0.70	0/1621	0.82	0/2206
1	K	0.71	0/1621	0.81	0/2206
1	L	0.72	0/1632	0.83	0/2221
1	M	0.73	1/1628 (0.1%)	0.83	0/2216
1	N	0.71	0/1639	0.82	0/2231
1	O	0.70	0/1628	0.82	0/2216
All	All	0.71	1/24458 (0.0%)	0.82	2/33288 (0.0%)

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	G	0	1
1	K	0	1
1	L	0	1
1	O	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	48	GLU	CD-OE2	5.37	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	221	THR	CA-C-O	10.83	142.84	120.10
1	H	168	LYS	CA-CB-CG	5.61	125.75	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	85	I2F	Mainchain
1	K	85	I2F	Mainchain
1	L	85	I2F	Mainchain
1	O	85	I2F	Mainchain

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	1615	0	1657	9	0
1	B	1628	0	1671	8	0
1	C	1615	0	1657	9	0
1	D	1627	0	1665	12	0
1	E	1629	0	1671	13	0
1	F	1629	0	1671	14	0
1	G	1629	0	1671	10	0
1	H	1622	0	1664	6	0
1	I	1615	0	1657	7	0
1	J	1615	0	1657	14	0
1	K	1615	0	1656	8	0
1	L	1622	0	1663	12	0
1	M	1622	0	1664	12	0
1	N	1629	0	1671	9	0
1	O	1622	0	1664	8	0
2	A	13	0	0	0	0
2	B	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	4	0	0	0	0
2	D	15	0	0	0	0
2	E	18	0	0	2	0
2	F	29	0	0	2	0
2	G	16	0	0	0	0
2	H	8	0	0	0	0
2	I	3	0	0	0	0
2	J	9	0	0	0	0
2	K	7	0	0	0	0
2	L	8	0	0	0	0
2	M	16	0	0	1	0
2	N	12	0	0	1	0
2	O	10	0	0	0	0
All	All	24511	0	24959	142	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 3.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:O	1:A:17:SER:OG	1.95	0.84
1:F:103:GLY:HA3	1:L:53:GLN:HE22	1.60	0.67
1:F:102:GLU:O	1:L:53:GLN:NE2	2.29	0.66
1:L:6:ASP:OD1	1:L:85:I2F:O4	2.16	0.63
1:F:6:ASP:OD1	1:F:85:I2F:O4	2.17	0.63
1:E:1:MET:HE1	1:E:184:ILE:HG22	1.82	0.61
1:G:6:ASP:OD1	1:G:85:I2F:O4	2.20	0.59
1:D:150[A]:HIS:CE1	1:D:154:LYS:HD3	2.38	0.59
1:E:150[B]:HIS:CE1	1:E:154:LYS:HD3	2.38	0.58
1:G:150[B]:HIS:CE1	1:G:154:LYS:HD3	2.40	0.56
1:F:150[B]:HIS:CE1	1:F:154:LYS:HD3	2.40	0.56
1:I:38:PRO:HA	1:J:215:PHE:HE2	1.71	0.55
1:I:1:MET:HE1	1:I:177:LEU:HD21	1.90	0.54
1:J:53:GLN:NE2	1:M:102:GLU:O	2.40	0.54
1:J:6:ASP:OD1	1:J:85:I2F:O4	2.26	0.54
1:M:6:ASP:OD1	1:M:85:I2F:O4	2.25	0.53
1:E:150[A]:HIS:HD2	2:E:303:HOH:O	1.92	0.53
1:C:6:ASP:OD1	1:C:85:I2F:O4	2.26	0.53
1:F:1:MET:HE1	1:F:177:LEU:HD21	1.89	0.53
1:D:6:ASP:OD2	1:D:85:I2F:O6	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:55:ARG:HD2	1:M:57:PHE:CZ	2.44	0.52
1:G:6:ASP:OD2	1:G:85:I2F:O6	2.27	0.52
1:H:1:MET:HE1	1:H:177:LEU:HD21	1.92	0.52
1:C:6:ASP:OD2	1:C:85:I2F:O6	2.28	0.52
1:E:142:GLY:O	1:E:146:VAL:HG23	2.11	0.51
1:D:217:ARG:HG2	1:D:218:THR:H	1.75	0.51
1:L:1:MET:HE1	1:L:177:LEU:HD21	1.93	0.51
1:E:6:ASP:OD1	1:E:85:I2F:O4	2.29	0.51
1:K:206:LYS:HE2	1:K:210:ASP:OD1	2.11	0.51
1:M:142:GLY:O	1:M:146:VAL:HG23	2.11	0.50
1:A:4:TYR:O	1:A:185:THR:HA	2.12	0.50
1:A:206:LYS:HE2	1:A:210:ASP:OD1	2.10	0.50
1:F:142:GLY:O	1:F:146:VAL:HG23	2.11	0.50
1:C:142:GLY:O	1:C:146:VAL:HG23	2.12	0.50
1:K:142:GLY:O	1:K:146:VAL:HG23	2.12	0.50
1:G:4:TYR:O	1:G:185:THR:HA	2.11	0.50
1:B:142:GLY:O	1:B:146:VAL:HG23	2.12	0.50
1:G:142:GLY:O	1:G:146:VAL:HG23	2.12	0.50
1:D:206:LYS:HE2	1:D:210:ASP:OD1	2.12	0.49
1:N:6:ASP:OD1	1:N:85:I2F:O4	2.28	0.49
1:M:1:MET:HE1	1:M:177:LEU:HD21	1.95	0.49
1:D:6:ASP:OD1	1:D:85:I2F:O4	2.30	0.49
1:D:142:GLY:O	1:D:146:VAL:HG23	2.12	0.49
1:E:150[A]:HIS:CD2	2:E:303:HOH:O	2.64	0.49
1:L:3:LEU:HD11	1:L:186:LEU:CD1	2.42	0.49
1:J:142:GLY:O	1:J:146:VAL:HG23	2.12	0.49
1:N:1:MET:HE1	1:N:184:ILE:HG22	1.94	0.49
1:O:142:GLY:O	1:O:146:VAL:HG23	2.12	0.49
1:A:142:GLY:O	1:A:146:VAL:HG23	2.12	0.49
1:J:6:ASP:OD2	1:J:85:I2F:O6	2.30	0.49
1:N:142:GLY:O	1:N:146:VAL:HG23	2.13	0.49
1:J:211:TRP:CZ2	1:J:220:ILE:CD1	2.96	0.49
1:J:1:MET:HE1	1:J:177:LEU:HD21	1.95	0.48
1:L:142:GLY:O	1:L:146:VAL:HG23	2.12	0.48
1:I:142:GLY:O	1:I:146:VAL:HG23	2.12	0.48
1:K:1:MET:HE1	1:K:177:LEU:HD21	1.95	0.48
1:H:142:GLY:O	1:H:146:VAL:HG23	2.12	0.48
1:N:150[B]:HIS:CE1	1:N:180:GLY:O	2.67	0.48
1:H:4:TYR:O	1:H:185:THR:HA	2.14	0.47
1:I:107:LEU:C	1:I:107:LEU:HD23	2.34	0.47
1:K:107:LEU:C	1:K:107:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:ARG:HG2	1:E:57:PHE:CE1	2.49	0.47
1:E:107:LEU:C	1:E:107:LEU:HD23	2.35	0.47
1:M:107:LEU:C	1:M:107:LEU:HD23	2.35	0.47
1:L:107:LEU:C	1:L:107:LEU:HD23	2.35	0.47
1:D:107:LEU:C	1:D:107:LEU:HD23	2.35	0.47
1:H:107:LEU:C	1:H:107:LEU:HD23	2.35	0.47
1:A:107:LEU:C	1:A:107:LEU:HD23	2.35	0.47
1:B:107:LEU:C	1:B:107:LEU:HD23	2.35	0.47
1:N:107:LEU:HD23	1:N:107:LEU:C	2.35	0.47
1:F:107:LEU:C	1:F:107:LEU:HD23	2.35	0.46
1:C:107:LEU:C	1:C:107:LEU:HD23	2.35	0.46
1:G:107:LEU:C	1:G:107:LEU:HD23	2.35	0.46
1:J:107:LEU:C	1:J:107:LEU:HD23	2.34	0.46
1:O:107:LEU:C	1:O:107:LEU:HD23	2.36	0.46
1:G:1:MET:HE1	1:G:177:LEU:HD21	1.98	0.46
1:D:1:MET:HE1	1:D:177:LEU:HD21	1.99	0.45
1:F:1:MET:HE1	1:F:184:ILE:HG22	1.98	0.45
1:A:1:MET:HE1	1:A:177:LEU:HD21	1.97	0.45
1:J:79:ILE:HB	1:J:82:ILE:HB	1.99	0.45
1:K:28:ASN:HD22	1:K:85:I2F:C5	2.30	0.45
1:N:79:ILE:HB	1:N:82:ILE:HB	1.99	0.45
1:O:1:MET:HE1	1:O:177:LEU:HD21	1.98	0.45
1:D:79:ILE:HB	1:D:82:ILE:HB	1.99	0.45
1:L:3:LEU:HD11	1:L:186:LEU:HD12	1.99	0.45
1:L:79:ILE:HB	1:L:82:ILE:HB	1.99	0.45
1:M:187:PRO:HD3	2:M:307:HOH:O	2.15	0.45
1:B:1:MET:HE1	1:B:184:ILE:HG22	1.99	0.45
1:K:79:ILE:HB	1:K:82:ILE:HB	1.99	0.44
1:N:4:TYR:O	1:N:185:THR:HA	2.16	0.44
1:B:6:ASP:OD1	1:B:85:I2F:O4	2.36	0.44
1:C:79:ILE:HB	1:C:82:ILE:HB	2.00	0.44
1:G:1:MET:HE1	1:G:184:ILE:HG22	2.00	0.44
1:I:79:ILE:HB	1:I:82:ILE:HB	1.99	0.44
1:M:79:ILE:HB	1:M:82:ILE:HB	2.00	0.44
1:G:79:ILE:HB	1:G:82:ILE:HB	2.00	0.44
1:B:4:TYR:O	1:B:185:THR:HA	2.18	0.43
1:E:47:HIS:CD2	1:E:52:GLY:HA2	2.53	0.43
1:H:79:ILE:HB	1:H:82:ILE:HB	2.00	0.43
1:O:79:ILE:HB	1:O:82:ILE:HB	2.00	0.43
1:B:79:ILE:HB	1:B:82:ILE:HB	1.99	0.43
1:D:4:TYR:O	1:D:185:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HB	1:A:82:ILE:HB	2.00	0.43
1:B:43:LEU:HB2	1:B:44:PRO:HD3	2.01	0.43
1:E:79:ILE:HB	1:E:82:ILE:HB	2.00	0.43
1:M:98:MET:HE3	2:N:301:HOH:O	2.19	0.43
1:C:1:MET:HA	1:C:1:MET:HE2	2.01	0.43
1:G:43:LEU:HB2	1:G:44:PRO:HD3	2.01	0.43
1:D:43:LEU:HB2	1:D:44:PRO:HD3	2.01	0.42
1:J:43:LEU:HB2	1:J:44:PRO:HD3	2.01	0.42
1:J:53:GLN:HE22	1:M:103:GLY:HA3	1.84	0.42
1:C:43:LEU:HB2	1:C:44:PRO:HD3	2.02	0.42
1:L:43:LEU:HB2	1:L:44:PRO:HD3	2.01	0.42
1:F:79:ILE:HB	1:F:82:ILE:HB	2.01	0.42
1:A:43:LEU:HB2	1:A:44:PRO:HD3	2.01	0.42
1:N:43:LEU:HB2	1:N:44:PRO:HD3	2.01	0.42
1:F:4:TYR:O	1:F:185:THR:HA	2.20	0.42
1:F:1:MET:CE	1:F:184:ILE:HG22	2.49	0.42
1:F:131:TYR:OH	2:F:301:HOH:O	2.21	0.42
1:H:43:LEU:HB2	1:H:44:PRO:HD3	2.02	0.42
1:I:43:LEU:HB2	1:I:44:PRO:HD3	2.02	0.42
1:J:104:ILE:HA	1:J:105:PRO:HD2	1.94	0.42
1:O:6:ASP:OD1	1:O:85:I2F:O4	2.38	0.42
1:E:55:ARG:HD2	1:E:57:PHE:CZ	2.55	0.41
2:F:308:HOH:O	1:J:113:GLY:HA3	2.20	0.41
1:F:81:ASP:HB3	1:L:81:ASP:HB3	2.02	0.41
1:O:43:LEU:HB2	1:O:44:PRO:HD3	2.02	0.41
1:B:156:HIS:HB3	1:C:1:MET:HB2	2.02	0.41
1:E:4:TYR:O	1:E:185:THR:HA	2.21	0.41
1:E:55:ARG:CD	1:E:57:PHE:CZ	3.04	0.41
1:C:4:TYR:O	1:C:185:THR:HA	2.21	0.41
1:O:6:ASP:OD2	1:O:85:I2F:O6	2.39	0.41
1:J:28:ASN:HD22	1:J:85:I2F:C5	2.32	0.41
1:N:1:MET:HE1	1:N:177:LEU:HD21	2.02	0.41
1:K:43:LEU:HB2	1:K:44:PRO:HD3	2.02	0.41
1:F:3:LEU:HD11	1:F:186:LEU:HD12	2.02	0.40
1:L:156[A]:HIS:HE1	1:M:177:LEU:O	2.04	0.40
1:A:6:ASP:OD1	1:A:85:I2F:O4	2.39	0.40
1:D:185:THR:HG23	1:D:185:THR:O	2.22	0.40
1:I:28:ASN:HD22	1:I:85:I2F:C5	2.35	0.40
1:K:199:ALA:HB1	1:O:112:TYR:CE2	2.57	0.40
1:M:43:LEU:HB2	1:M:44:PRO:HD3	2.02	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	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
1	B	219/227 (96%)	212 (97%)	7 (3%)	0	100	100
1	C	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
1	D	219/227 (96%)	211 (96%)	8 (4%)	0	100	100
1	E	219/227 (96%)	211 (96%)	8 (4%)	0	100	100
1	F	219/227 (96%)	211 (96%)	8 (4%)	0	100	100
1	G	219/227 (96%)	211 (96%)	8 (4%)	0	100	100
1	H	218/227 (96%)	211 (97%)	7 (3%)	0	100	100
1	I	217/227 (96%)	209 (96%)	8 (4%)	0	100	100
1	J	217/227 (96%)	210 (97%)	7 (3%)	0	100	100
1	K	217/227 (96%)	209 (96%)	8 (4%)	0	100	100
1	L	218/227 (96%)	211 (97%)	7 (3%)	0	100	100
1	M	218/227 (96%)	210 (96%)	8 (4%)	0	100	100
1	N	219/227 (96%)	212 (97%)	7 (3%)	0	100	100
1	O	218/227 (96%)	210 (96%)	8 (4%)	0	100	100
All	All	3271/3405 (96%)	3158 (96%)	113 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	165/172 (96%)	160 (97%)	5 (3%)	41	66
1	B	167/172 (97%)	163 (98%)	4 (2%)	49	72
1	C	165/172 (96%)	163 (99%)	2 (1%)	71	86
1	D	167/172 (97%)	164 (98%)	3 (2%)	59	79
1	E	167/172 (97%)	164 (98%)	3 (2%)	59	79
1	F	167/172 (97%)	163 (98%)	4 (2%)	49	72
1	G	167/172 (97%)	163 (98%)	4 (2%)	49	72
1	H	166/172 (96%)	161 (97%)	5 (3%)	41	66
1	I	165/172 (96%)	162 (98%)	3 (2%)	59	79
1	J	165/172 (96%)	163 (99%)	2 (1%)	71	86
1	K	165/172 (96%)	162 (98%)	3 (2%)	59	79
1	L	166/172 (96%)	163 (98%)	3 (2%)	59	79
1	M	166/172 (96%)	163 (98%)	3 (2%)	59	79
1	N	167/172 (97%)	164 (98%)	3 (2%)	59	79
1	O	166/172 (96%)	161 (97%)	5 (3%)	41	66
All	All	2491/2580 (97%)	2439 (98%)	52 (2%)	53	76

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	17	SER
1	A	97	LYS
1	A	154	LYS
1	A	196	SER
1	B	100	LYS
1	B	154	LYS
1	B	196	SER
1	B	221	THR
1	C	154	LYS
1	C	196	SER
1	D	154	LYS
1	D	196	SER
1	D	219	SER
1	E	154	LYS
1	E	196	SER
1	E	221	THR
1	F	100	LYS

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Mol	Chain	Res	Type
1	F	154	LYS
1	F	196	SER
1	F	221	THR
1	G	36	LYS
1	G	154	LYS
1	G	196	SER
1	G	221	THR
1	H	36	LYS
1	H	154	LYS
1	H	168	LYS
1	H	196	SER
1	H	221	THR
1	I	154	LYS
1	I	196	SER
1	I	217	ARG
1	J	154	LYS
1	J	196	SER
1	K	126	GLU
1	K	154	LYS
1	K	196	SER
1	L	100	LYS
1	L	154	LYS
1	L	196	SER
1	M	154	LYS
1	M	196	SER
1	M	221	THR
1	N	154	LYS
1	N	196	SER
1	N	221	THR
1	O	18	ARG
1	O	36	LYS
1	O	154	LYS
1	O	196	SER
1	O	221	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	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)

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	I2F	J	85	1	16,17,18	1.10	1 (6%)	14,20,22	1.15	1 (7%)
1	I2F	M	85	1	16,17,18	1.41	2 (12%)	14,20,22	1.37	2 (14%)
1	I2F	H	85	1	16,17,18	1.53	3 (18%)	14,20,22	1.48	3 (21%)
1	I2F	F	85	1	16,17,18	1.49	3 (18%)	14,20,22	1.71	3 (21%)
1	I2F	B	85	1	16,17,18	1.46	2 (12%)	14,20,22	1.48	4 (28%)
1	I2F	I	85	1	16,17,18	1.14	1 (6%)	14,20,22	1.42	3 (21%)
1	I2F	K	85	1	16,17,18	1.27	1 (6%)	14,20,22	1.39	3 (21%)
1	I2F	O	85	1	16,17,18	1.17	1 (6%)	14,20,22	1.74	4 (28%)
1	I2F	C	85	1	16,17,18	1.37	1 (6%)	14,20,22	1.37	2 (14%)
1	I2F	E	85	1	16,17,18	1.35	2 (12%)	14,20,22	1.15	1 (7%)
1	I2F	L	85	1	16,17,18	1.29	1 (6%)	14,20,22	1.13	2 (14%)
1	I2F	G	85	1	16,17,18	1.13	1 (6%)	14,20,22	1.74	3 (21%)
1	I2F	N	85	1	16,17,18	1.43	3 (18%)	14,20,22	1.65	3 (21%)
1	I2F	D	85	1	16,17,18	1.65	3 (18%)	14,20,22	1.77	3 (21%)
1	I2F	A	85	1	16,17,18	0.93	1 (6%)	14,20,22	0.96	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
1	I2F	J	85	1	-	1/18/20/22	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	I2F	M	85	1	-	7/18/20/22	-
1	I2F	H	85	1	-	5/18/20/22	-
1	I2F	F	85	1	-	6/18/20/22	-
1	I2F	B	85	1	-	1/18/20/22	-
1	I2F	I	85	1	-	3/18/20/22	-
1	I2F	K	85	1	-	4/18/20/22	-
1	I2F	O	85	1	-	5/18/20/22	-
1	I2F	C	85	1	-	5/18/20/22	-
1	I2F	E	85	1	-	3/18/20/22	-
1	I2F	L	85	1	-	5/18/20/22	-
1	I2F	G	85	1	-	1/18/20/22	-
1	I2F	N	85	1	-	3/18/20/22	-
1	I2F	D	85	1	-	5/18/20/22	-
1	I2F	A	85	1	-	7/18/20/22	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	85	I2F	O-C	-4.47	1.23	1.42
1	K	85	I2F	O-C	-3.92	1.25	1.42
1	C	85	I2F	O-C	-3.92	1.25	1.42
1	O	85	I2F	O-C	-3.79	1.26	1.42
1	B	85	I2F	O-C	-3.69	1.26	1.42
1	J	85	I2F	O-C	-3.64	1.27	1.42
1	L	85	I2F	O-C	-3.64	1.27	1.42
1	G	85	I2F	O-C	-3.60	1.27	1.42
1	H	85	I2F	O-C	-3.58	1.27	1.42
1	I	85	I2F	O-C	-3.55	1.27	1.42
1	E	85	I2F	O-C	-3.47	1.27	1.42
1	N	85	I2F	O-C	-3.45	1.27	1.42
1	M	85	I2F	O-C	-3.39	1.28	1.42
1	F	85	I2F	O-C	-3.34	1.28	1.42
1	A	85	I2F	O-C	-3.22	1.28	1.42
1	D	85	I2F	C3-C2	3.04	1.58	1.53
1	N	85	I2F	CB-CA	2.53	1.56	1.53
1	F	85	I2F	C3-C2	2.45	1.57	1.53
1	E	85	I2F	C3-C5	2.42	1.58	1.52
1	F	85	I2F	C3-C5	2.40	1.58	1.52
1	H	85	I2F	C3-C5	2.38	1.58	1.52
1	B	85	I2F	C3-C5	2.36	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	85	I2F	C3-C5	2.34	1.58	1.52
1	D	85	I2F	C3-C5	2.32	1.58	1.52
1	H	85	I2F	CB-CA	2.26	1.56	1.53
1	N	85	I2F	C3-C5	2.01	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	85	I2F	CB-CA-C	-4.10	106.64	112.25
1	F	85	I2F	O4-C2-C3	3.86	118.61	108.69
1	D	85	I2F	C3-C2-CH	3.60	118.90	112.33
1	G	85	I2F	CD-CE-NZ	-3.42	104.43	110.66
1	I	85	I2F	O4-C2-C3	3.42	117.48	108.69
1	D	85	I2F	CB-CA-C	-3.40	107.60	112.25
1	F	85	I2F	CE-NZ-CH	3.23	131.57	122.43
1	H	85	I2F	C3-C2-CH	3.08	117.96	112.33
1	N	85	I2F	C3-C2-CH	3.05	117.89	112.33
1	C	85	I2F	CE-NZ-CH	2.83	130.44	122.43
1	G	85	I2F	O4-C2-C3	2.80	115.89	108.69
1	B	85	I2F	O4-C2-C3	2.68	115.57	108.69
1	C	85	I2F	O4-C2-C3	2.67	115.55	108.69
1	O	85	I2F	CB-CA-N	2.62	116.65	109.03
1	H	85	I2F	O4-C2-C3	2.57	115.30	108.69
1	K	85	I2F	O6-C5-C3	2.56	114.99	109.18
1	B	85	I2F	O-C-CA	2.54	121.54	111.52
1	I	85	I2F	CB-CA-C	-2.44	108.91	112.25
1	O	85	I2F	C3-C2-CH	2.41	116.73	112.33
1	F	85	I2F	CB-CA-N	2.29	115.68	109.03
1	G	85	I2F	O-C-CA	2.29	120.56	111.52
1	N	85	I2F	CB-CA-N	2.25	115.57	109.03
1	E	85	I2F	C3-C2-CH	2.24	116.43	112.33
1	I	85	I2F	CE-NZ-CH	2.24	128.75	122.43
1	K	85	I2F	C3-C2-CH	2.22	116.39	112.33
1	M	85	I2F	CB-CA-C	-2.18	109.27	112.25
1	B	85	I2F	C3-C2-CH	2.16	116.28	112.33
1	O	85	I2F	C1-CH-NZ	-2.14	116.65	124.00
1	H	85	I2F	O1-C6-C5	2.13	120.42	110.20
1	K	85	I2F	CB-CA-C	-2.12	109.35	112.25
1	D	85	I2F	O1-C6-C5	2.07	120.13	110.20
1	J	85	I2F	CE-NZ-CH	2.06	128.26	122.43
1	L	85	I2F	CD-CG-CB	-2.06	106.34	113.62
1	L	85	I2F	CB-CA-C	-2.04	109.47	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	85	I2F	O1-C6-C5	2.03	119.95	110.20
1	M	85	I2F	O4-C2-C3	2.02	113.87	108.69
1	N	85	I2F	O-C-CA	2.00	119.44	111.52

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	85	I2F	O4-C2-C3-C5
1	A	85	I2F	C3-C5-C6-O1
1	B	85	I2F	CD-CE-NZ-CH
1	D	85	I2F	C3-C2-CH-C1
1	D	85	I2F	C3-C5-C6-O1
1	E	85	I2F	C2-C3-C5-C6
1	E	85	I2F	C2-C3-C5-O6
1	F	85	I2F	C3-C5-C6-O1
1	H	85	I2F	O4-C2-C3-C5
1	H	85	I2F	C2-C3-C5-C6
1	H	85	I2F	C2-C3-C5-O6
1	I	85	I2F	CD-CE-NZ-CH
1	L	85	I2F	C3-C2-CH-C1
1	L	85	I2F	C3-C5-C6-O1
1	M	85	I2F	C2-C3-C5-C6
1	M	85	I2F	C3-C5-C6-O1
1	O	85	I2F	O4-C2-CH-C1
1	O	85	I2F	C3-C2-CH-C1
1	I	85	I2F	CE-CD-CG-CB
1	F	85	I2F	C2-C3-C5-C6
1	K	85	I2F	C2-C3-C5-O6
1	M	85	I2F	C2-C3-C5-O6
1	C	85	I2F	CE-CD-CG-CB
1	C	85	I2F	C3-C5-C6-O1
1	D	85	I2F	CE-CD-CG-CB
1	C	85	I2F	O6-C5-C6-O1
1	D	85	I2F	O6-C5-C6-O1
1	L	85	I2F	CE-CD-CG-CB
1	O	85	I2F	CE-CD-CG-CB
1	D	85	I2F	O4-C2-CH-C1
1	F	85	I2F	O4-C2-CH-C1
1	L	85	I2F	O4-C2-CH-C1
1	A	85	I2F	C3-C2-CH-C1
1	F	85	I2F	C3-C2-CH-C1

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Mol	Chain	Res	Type	Atoms
1	C	85	I2F	CD-CE-NZ-CH
1	H	85	I2F	CD-CE-NZ-CH
1	F	85	I2F	CE-CD-CG-CB
1	M	85	I2F	CE-CD-CG-CB
1	A	85	I2F	O6-C5-C6-O1
1	F	85	I2F	O6-C5-C6-O1
1	M	85	I2F	O6-C5-C6-O1
1	C	85	I2F	O-C-CA-CB
1	K	85	I2F	O-C-CA-CB
1	E	85	I2F	O6-C5-C6-O1
1	L	85	I2F	O6-C5-C6-O1
1	M	85	I2F	C3-C2-CH-C1
1	N	85	I2F	C3-C2-CH-C1
1	O	85	I2F	O-C-CA-N
1	O	85	I2F	C2-C3-C5-C6
1	G	85	I2F	N-CA-CB-CG
1	H	85	I2F	CE-CD-CG-CB
1	K	85	I2F	CE-CD-CG-CB
1	J	85	I2F	O4-C2-C3-C5
1	A	85	I2F	CH-C2-C3-C5
1	A	85	I2F	O4-C2-CH-C1
1	M	85	I2F	O4-C2-CH-C1
1	N	85	I2F	O4-C2-CH-C1
1	K	85	I2F	O-C-CA-N
1	N	85	I2F	O4-C2-C3-C5
1	A	85	I2F	N-CA-CB-CG
1	I	85	I2F	N-CA-CB-CG

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	85	I2F	3	0
1	M	85	I2F	1	0
1	F	85	I2F	1	0
1	B	85	I2F	1	0
1	I	85	I2F	1	0
1	K	85	I2F	1	0
1	O	85	I2F	2	0
1	C	85	I2F	2	0
1	E	85	I2F	1	0
1	L	85	I2F	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	85	I2F	2	0
1	N	85	I2F	1	0
1	D	85	I2F	2	0
1	A	85	I2F	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	219/227 (96%)	-0.17	0 100 100	41, 60, 90, 106	0
1	B	220/227 (96%)	0.13	12 (5%) 25 20	47, 68, 99, 143	0
1	C	219/227 (96%)	0.11	5 (2%) 60 55	44, 75, 103, 120	0
1	D	218/227 (96%)	-0.21	1 (0%) 91 89	37, 53, 100, 131	0
1	E	220/227 (96%)	-0.28	1 (0%) 91 89	36, 51, 75, 94	0
1	F	220/227 (96%)	-0.29	0 100 100	36, 49, 75, 132	0
1	G	220/227 (96%)	-0.21	1 (0%) 91 89	41, 56, 86, 119	0
1	H	220/227 (96%)	-0.00	8 (3%) 42 36	41, 65, 94, 119	0
1	I	219/227 (96%)	-0.04	1 (0%) 91 89	40, 66, 95, 113	0
1	J	219/227 (96%)	-0.19	1 (0%) 91 89	34, 52, 91, 112	0
1	K	219/227 (96%)	0.09	11 (5%) 28 23	43, 74, 112, 129	0
1	L	219/227 (96%)	-0.28	1 (0%) 91 89	38, 53, 93, 123	0
1	M	220/227 (96%)	-0.32	0 100 100	36, 53, 76, 106	0
1	N	220/227 (96%)	-0.22	1 (0%) 91 89	41, 61, 91, 114	0
1	O	220/227 (96%)	0.16	17 (7%) 13 10	46, 72, 104, 135	0
All	All	3292/3405 (96%)	-0.11	60 (1%) 68 64	34, 60, 97, 143	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	213	GLY	4.2
1	K	215	PHE	4.2
1	N	218	THR	4.1
1	B	218	THR	3.9
1	H	218	THR	3.8
1	K	214	ALA	3.8
1	O	37	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	215	PHE	3.5
1	K	211	TRP	3.4
1	B	78	ILE	3.4
1	C	215	PHE	3.4
1	O	40	ASP	3.2
1	O	78	ILE	3.1
1	O	42	VAL	3.0
1	O	216	GLY	3.0
1	C	214	ALA	2.9
1	O	34	ALA	2.9
1	K	218	THR	2.8
1	B	79	ILE	2.8
1	B	40	ASP	2.7
1	H	215	PHE	2.7
1	O	218	THR	2.6
1	H	41	VAL	2.6
1	L	215	PHE	2.5
1	D	218	THR	2.5
1	O	41	VAL	2.5
1	H	219	SER	2.5
1	G	66	GLU	2.5
1	C	213	GLY	2.5
1	B	39	LEU	2.5
1	B	46	LEU	2.5
1	O	221	THR	2.4
1	O	31	ILE	2.4
1	C	217	ARG	2.4
1	K	212	GLN	2.4
1	E	213	GLY	2.4
1	H	79	ILE	2.4
1	O	44	PRO	2.3
1	B	75	LEU	2.3
1	H	40	ASP	2.3
1	I	40	ASP	2.3
1	J	215	PHE	2.3
1	K	40	ASP	2.2
1	O	38	PRO	2.2
1	B	216	GLY	2.2
1	O	8	SER	2.2
1	H	78	ILE	2.1
1	K	37	LYS	2.1
1	B	221	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	10	VAL	2.1
1	C	44	PRO	2.1
1	K	208	GLU	2.1
1	H	52	GLY	2.1
1	B	37	LYS	2.0
1	O	75	LEU	2.0
1	K	77	SER	2.0
1	O	45	GLN	2.0
1	B	38	PRO	2.0
1	O	48	GLU	2.0
1	K	207	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	I2F	N	85	18/19	0.88	0.24	58,67,85,92	0
1	I2F	C	85	18/19	0.89	0.19	62,72,84,84	0
1	I2F	H	85	18/19	0.90	0.23	60,69,78,83	0
1	I2F	B	85	18/19	0.91	0.17	56,65,74,76	0
1	I2F	K	85	18/19	0.92	0.24	48,71,91,93	0
1	I2F	A	85	18/19	0.93	0.17	55,62,74,78	0
1	I2F	L	85	18/19	0.93	0.16	43,56,78,78	0
1	I2F	I	85	18/19	0.93	0.19	45,72,87,91	0
1	I2F	E	85	18/19	0.94	0.18	34,56,78,79	0
1	I2F	M	85	18/19	0.94	0.17	36,48,72,73	0
1	I2F	D	85	18/19	0.94	0.18	41,54,69,73	0
1	I2F	F	85	18/19	0.95	0.16	35,50,69,72	0
1	I2F	G	85	18/19	0.95	0.17	49,62,75,80	0
1	I2F	O	85	18/19	0.95	0.16	63,74,83,84	0
1	I2F	J	85	18/19	0.96	0.16	38,51,75,76	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.