Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2024 – 08:42 AM JST

PDB ID	:	5ZOL
Title	:	Crystal structure of a three sites mutantion of FSAA complexed with HA and product
Authors	:	Wu, L.; Yang, X.H.; Yu, H.W.; Zhou, J.H.
Deposited on	:	2018-04-13
Resolution	:	2.17 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:

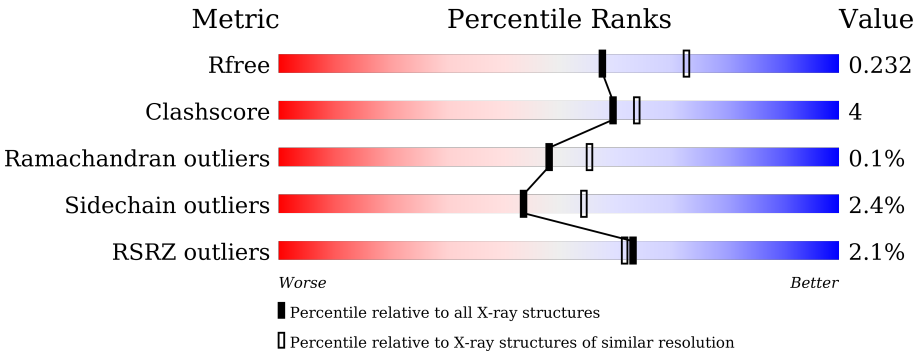
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.17 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}	164625	8336 (2.20-2.16)
Clashscore	180529	9404 (2.20-2.16)
Ramachandran outliers	177936	9297 (2.20-2.16)
Sidechain outliers	177891	9297 (2.20-2.16)
RSRZ outliers	164620	8337 (2.20-2.16)

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	255	% 78% 9% 13%
1	B	255	2% 80% 5% • 13%
1	C	255	2% 79% 7% • 13%
1	D	255	77% 9% 13%
1	E	255	% 75% 11% • 13%
1	F	255	4% 76% 9% • 13%

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Mol	Chain	Length	Quality of chain
1	G	255	2% 79% 7% 13%
1	H	255	% 77% 10% 13%
1	I	255	4% 73% 13% 13%
1	J	255	3% 77% 9% 13%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17350 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	222	Total	C	N	O	S	3	1	0
			1631	1036	277	308	10			
1	B	221	Total	C	N	O	S	0	2	0
			1626	1034	273	309	10			
1	C	221	Total	C	N	O	S	0	0	0
			1617	1028	273	307	9			
1	D	221	Total	C	N	O	S	0	1	0
			1623	1032	273	309	9			
1	E	221	Total	C	N	O	S	0	0	0
			1617	1028	273	307	9			
1	F	221	Total	C	N	O	S	0	2	0
			1626	1034	273	309	10			
1	G	222	Total	C	N	O	S	0	1	0
			1637	1042	277	309	9			
1	H	221	Total	C	N	O	S	0	0	0
			1617	1028	273	307	9			
1	I	221	Total	C	N	O	S	0	0	0
			1617	1028	273	307	9			
1	J	221	Total	C	N	O	S	0	1	0
			1622	1032	273	308	9			

There are 380 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	HIS	-	expression tag	UNP P78055
A	-33	HIS	-	expression tag	UNP P78055
A	-32	HIS	-	expression tag	UNP P78055
A	-31	HIS	-	expression tag	UNP P78055
A	-30	HIS	-	expression tag	UNP P78055
A	-29	HIS	-	expression tag	UNP P78055
A	-28	SER	-	expression tag	UNP P78055
A	-27	SER	-	expression tag	UNP P78055
A	-26	GLY	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	LEU	-	expression tag	UNP P78055
A	-24	VAL	-	expression tag	UNP P78055
A	-23	PRO	-	expression tag	UNP P78055
A	-22	ARG	-	expression tag	UNP P78055
A	-21	GLY	-	expression tag	UNP P78055
A	-20	SER	-	expression tag	UNP P78055
A	-19	GLY	-	expression tag	UNP P78055
A	-18	MET	-	expression tag	UNP P78055
A	-17	LYS	-	expression tag	UNP P78055
A	-16	GLU	-	expression tag	UNP P78055
A	-15	THR	-	expression tag	UNP P78055
A	-14	ALA	-	expression tag	UNP P78055
A	-13	ALA	-	expression tag	UNP P78055
A	-12	ALA	-	expression tag	UNP P78055
A	-11	LYS	-	expression tag	UNP P78055
A	-10	PHE	-	expression tag	UNP P78055
A	-9	GLU	-	expression tag	UNP P78055
A	-8	ARG	-	expression tag	UNP P78055
A	-7	GLN	-	expression tag	UNP P78055
A	-6	HIS	-	expression tag	UNP P78055
A	-5	MET	-	expression tag	UNP P78055
A	-4	ASP	-	expression tag	UNP P78055
A	-3	SER	-	expression tag	UNP P78055
A	-2	PRO	-	expression tag	UNP P78055
A	-1	ARG	-	expression tag	UNP P78055
A	0	SER	-	expression tag	UNP P78055
A	31	THR	ILE	engineered mutation	UNP P78055
A	59	THR	GLN	engineered mutation	UNP P78055
A	195	GLN	ILE	engineered mutation	UNP P78055
B	-34	HIS	-	expression tag	UNP P78055
B	-33	HIS	-	expression tag	UNP P78055
B	-32	HIS	-	expression tag	UNP P78055
B	-31	HIS	-	expression tag	UNP P78055
B	-30	HIS	-	expression tag	UNP P78055
B	-29	HIS	-	expression tag	UNP P78055
B	-28	SER	-	expression tag	UNP P78055
B	-27	SER	-	expression tag	UNP P78055
B	-26	GLY	-	expression tag	UNP P78055
B	-25	LEU	-	expression tag	UNP P78055
B	-24	VAL	-	expression tag	UNP P78055
B	-23	PRO	-	expression tag	UNP P78055
B	-22	ARG	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	GLY	-	expression tag	UNP P78055
B	-20	SER	-	expression tag	UNP P78055
B	-19	GLY	-	expression tag	UNP P78055
B	-18	MET	-	expression tag	UNP P78055
B	-17	LYS	-	expression tag	UNP P78055
B	-16	GLU	-	expression tag	UNP P78055
B	-15	THR	-	expression tag	UNP P78055
B	-14	ALA	-	expression tag	UNP P78055
B	-13	ALA	-	expression tag	UNP P78055
B	-12	ALA	-	expression tag	UNP P78055
B	-11	LYS	-	expression tag	UNP P78055
B	-10	PHE	-	expression tag	UNP P78055
B	-9	GLU	-	expression tag	UNP P78055
B	-8	ARG	-	expression tag	UNP P78055
B	-7	GLN	-	expression tag	UNP P78055
B	-6	HIS	-	expression tag	UNP P78055
B	-5	MET	-	expression tag	UNP P78055
B	-4	ASP	-	expression tag	UNP P78055
B	-3	SER	-	expression tag	UNP P78055
B	-2	PRO	-	expression tag	UNP P78055
B	-1	ARG	-	expression tag	UNP P78055
B	0	SER	-	expression tag	UNP P78055
B	31	THR	ILE	engineered mutation	UNP P78055
B	59	THR	GLN	engineered mutation	UNP P78055
B	195	GLN	ILE	engineered mutation	UNP P78055
C	-34	HIS	-	expression tag	UNP P78055
C	-33	HIS	-	expression tag	UNP P78055
C	-32	HIS	-	expression tag	UNP P78055
C	-31	HIS	-	expression tag	UNP P78055
C	-30	HIS	-	expression tag	UNP P78055
C	-29	HIS	-	expression tag	UNP P78055
C	-28	SER	-	expression tag	UNP P78055
C	-27	SER	-	expression tag	UNP P78055
C	-26	GLY	-	expression tag	UNP P78055
C	-25	LEU	-	expression tag	UNP P78055
C	-24	VAL	-	expression tag	UNP P78055
C	-23	PRO	-	expression tag	UNP P78055
C	-22	ARG	-	expression tag	UNP P78055
C	-21	GLY	-	expression tag	UNP P78055
C	-20	SER	-	expression tag	UNP P78055
C	-19	GLY	-	expression tag	UNP P78055
C	-18	MET	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	LYS	-	expression tag	UNP P78055
C	-16	GLU	-	expression tag	UNP P78055
C	-15	THR	-	expression tag	UNP P78055
C	-14	ALA	-	expression tag	UNP P78055
C	-13	ALA	-	expression tag	UNP P78055
C	-12	ALA	-	expression tag	UNP P78055
C	-11	LYS	-	expression tag	UNP P78055
C	-10	PHE	-	expression tag	UNP P78055
C	-9	GLU	-	expression tag	UNP P78055
C	-8	ARG	-	expression tag	UNP P78055
C	-7	GLN	-	expression tag	UNP P78055
C	-6	HIS	-	expression tag	UNP P78055
C	-5	MET	-	expression tag	UNP P78055
C	-4	ASP	-	expression tag	UNP P78055
C	-3	SER	-	expression tag	UNP P78055
C	-2	PRO	-	expression tag	UNP P78055
C	-1	ARG	-	expression tag	UNP P78055
C	0	SER	-	expression tag	UNP P78055
C	31	THR	ILE	engineered mutation	UNP P78055
C	59	THR	GLN	engineered mutation	UNP P78055
C	195	GLN	ILE	engineered mutation	UNP P78055
D	-34	HIS	-	expression tag	UNP P78055
D	-33	HIS	-	expression tag	UNP P78055
D	-32	HIS	-	expression tag	UNP P78055
D	-31	HIS	-	expression tag	UNP P78055
D	-30	HIS	-	expression tag	UNP P78055
D	-29	HIS	-	expression tag	UNP P78055
D	-28	SER	-	expression tag	UNP P78055
D	-27	SER	-	expression tag	UNP P78055
D	-26	GLY	-	expression tag	UNP P78055
D	-25	LEU	-	expression tag	UNP P78055
D	-24	VAL	-	expression tag	UNP P78055
D	-23	PRO	-	expression tag	UNP P78055
D	-22	ARG	-	expression tag	UNP P78055
D	-21	GLY	-	expression tag	UNP P78055
D	-20	SER	-	expression tag	UNP P78055
D	-19	GLY	-	expression tag	UNP P78055
D	-18	MET	-	expression tag	UNP P78055
D	-17	LYS	-	expression tag	UNP P78055
D	-16	GLU	-	expression tag	UNP P78055
D	-15	THR	-	expression tag	UNP P78055
D	-14	ALA	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	ALA	-	expression tag	UNP P78055
D	-12	ALA	-	expression tag	UNP P78055
D	-11	LYS	-	expression tag	UNP P78055
D	-10	PHE	-	expression tag	UNP P78055
D	-9	GLU	-	expression tag	UNP P78055
D	-8	ARG	-	expression tag	UNP P78055
D	-7	GLN	-	expression tag	UNP P78055
D	-6	HIS	-	expression tag	UNP P78055
D	-5	MET	-	expression tag	UNP P78055
D	-4	ASP	-	expression tag	UNP P78055
D	-3	SER	-	expression tag	UNP P78055
D	-2	PRO	-	expression tag	UNP P78055
D	-1	ARG	-	expression tag	UNP P78055
D	0	SER	-	expression tag	UNP P78055
D	31	THR	ILE	engineered mutation	UNP P78055
D	59	THR	GLN	engineered mutation	UNP P78055
D	195	GLN	ILE	engineered mutation	UNP P78055
E	-34	HIS	-	expression tag	UNP P78055
E	-33	HIS	-	expression tag	UNP P78055
E	-32	HIS	-	expression tag	UNP P78055
E	-31	HIS	-	expression tag	UNP P78055
E	-30	HIS	-	expression tag	UNP P78055
E	-29	HIS	-	expression tag	UNP P78055
E	-28	SER	-	expression tag	UNP P78055
E	-27	SER	-	expression tag	UNP P78055
E	-26	GLY	-	expression tag	UNP P78055
E	-25	LEU	-	expression tag	UNP P78055
E	-24	VAL	-	expression tag	UNP P78055
E	-23	PRO	-	expression tag	UNP P78055
E	-22	ARG	-	expression tag	UNP P78055
E	-21	GLY	-	expression tag	UNP P78055
E	-20	SER	-	expression tag	UNP P78055
E	-19	GLY	-	expression tag	UNP P78055
E	-18	MET	-	expression tag	UNP P78055
E	-17	LYS	-	expression tag	UNP P78055
E	-16	GLU	-	expression tag	UNP P78055
E	-15	THR	-	expression tag	UNP P78055
E	-14	ALA	-	expression tag	UNP P78055
E	-13	ALA	-	expression tag	UNP P78055
E	-12	ALA	-	expression tag	UNP P78055
E	-11	LYS	-	expression tag	UNP P78055
E	-10	PHE	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	GLU	-	expression tag	UNP P78055
E	-8	ARG	-	expression tag	UNP P78055
E	-7	GLN	-	expression tag	UNP P78055
E	-6	HIS	-	expression tag	UNP P78055
E	-5	MET	-	expression tag	UNP P78055
E	-4	ASP	-	expression tag	UNP P78055
E	-3	SER	-	expression tag	UNP P78055
E	-2	PRO	-	expression tag	UNP P78055
E	-1	ARG	-	expression tag	UNP P78055
E	0	SER	-	expression tag	UNP P78055
E	31	THR	ILE	engineered mutation	UNP P78055
E	59	THR	GLN	engineered mutation	UNP P78055
E	195	GLN	ILE	engineered mutation	UNP P78055
F	-34	HIS	-	expression tag	UNP P78055
F	-33	HIS	-	expression tag	UNP P78055
F	-32	HIS	-	expression tag	UNP P78055
F	-31	HIS	-	expression tag	UNP P78055
F	-30	HIS	-	expression tag	UNP P78055
F	-29	HIS	-	expression tag	UNP P78055
F	-28	SER	-	expression tag	UNP P78055
F	-27	SER	-	expression tag	UNP P78055
F	-26	GLY	-	expression tag	UNP P78055
F	-25	LEU	-	expression tag	UNP P78055
F	-24	VAL	-	expression tag	UNP P78055
F	-23	PRO	-	expression tag	UNP P78055
F	-22	ARG	-	expression tag	UNP P78055
F	-21	GLY	-	expression tag	UNP P78055
F	-20	SER	-	expression tag	UNP P78055
F	-19	GLY	-	expression tag	UNP P78055
F	-18	MET	-	expression tag	UNP P78055
F	-17	LYS	-	expression tag	UNP P78055
F	-16	GLU	-	expression tag	UNP P78055
F	-15	THR	-	expression tag	UNP P78055
F	-14	ALA	-	expression tag	UNP P78055
F	-13	ALA	-	expression tag	UNP P78055
F	-12	ALA	-	expression tag	UNP P78055
F	-11	LYS	-	expression tag	UNP P78055
F	-10	PHE	-	expression tag	UNP P78055
F	-9	GLU	-	expression tag	UNP P78055
F	-8	ARG	-	expression tag	UNP P78055
F	-7	GLN	-	expression tag	UNP P78055
F	-6	HIS	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	MET	-	expression tag	UNP P78055
F	-4	ASP	-	expression tag	UNP P78055
F	-3	SER	-	expression tag	UNP P78055
F	-2	PRO	-	expression tag	UNP P78055
F	-1	ARG	-	expression tag	UNP P78055
F	0	SER	-	expression tag	UNP P78055
F	31	THR	ILE	engineered mutation	UNP P78055
F	59	THR	GLN	engineered mutation	UNP P78055
F	195	GLN	ILE	engineered mutation	UNP P78055
G	-34	HIS	-	expression tag	UNP P78055
G	-33	HIS	-	expression tag	UNP P78055
G	-32	HIS	-	expression tag	UNP P78055
G	-31	HIS	-	expression tag	UNP P78055
G	-30	HIS	-	expression tag	UNP P78055
G	-29	HIS	-	expression tag	UNP P78055
G	-28	SER	-	expression tag	UNP P78055
G	-27	SER	-	expression tag	UNP P78055
G	-26	GLY	-	expression tag	UNP P78055
G	-25	LEU	-	expression tag	UNP P78055
G	-24	VAL	-	expression tag	UNP P78055
G	-23	PRO	-	expression tag	UNP P78055
G	-22	ARG	-	expression tag	UNP P78055
G	-21	GLY	-	expression tag	UNP P78055
G	-20	SER	-	expression tag	UNP P78055
G	-19	GLY	-	expression tag	UNP P78055
G	-18	MET	-	expression tag	UNP P78055
G	-17	LYS	-	expression tag	UNP P78055
G	-16	GLU	-	expression tag	UNP P78055
G	-15	THR	-	expression tag	UNP P78055
G	-14	ALA	-	expression tag	UNP P78055
G	-13	ALA	-	expression tag	UNP P78055
G	-12	ALA	-	expression tag	UNP P78055
G	-11	LYS	-	expression tag	UNP P78055
G	-10	PHE	-	expression tag	UNP P78055
G	-9	GLU	-	expression tag	UNP P78055
G	-8	ARG	-	expression tag	UNP P78055
G	-7	GLN	-	expression tag	UNP P78055
G	-6	HIS	-	expression tag	UNP P78055
G	-5	MET	-	expression tag	UNP P78055
G	-4	ASP	-	expression tag	UNP P78055
G	-3	SER	-	expression tag	UNP P78055
G	-2	PRO	-	expression tag	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	ARG	-	expression tag	UNP P78055
G	0	SER	-	expression tag	UNP P78055
G	31	THR	ILE	engineered mutation	UNP P78055
G	59	THR	GLN	engineered mutation	UNP P78055
G	195	GLN	ILE	engineered mutation	UNP P78055
H	-34	HIS	-	expression tag	UNP P78055
H	-33	HIS	-	expression tag	UNP P78055
H	-32	HIS	-	expression tag	UNP P78055
H	-31	HIS	-	expression tag	UNP P78055
H	-30	HIS	-	expression tag	UNP P78055
H	-29	HIS	-	expression tag	UNP P78055
H	-28	SER	-	expression tag	UNP P78055
H	-27	SER	-	expression tag	UNP P78055
H	-26	GLY	-	expression tag	UNP P78055
H	-25	LEU	-	expression tag	UNP P78055
H	-24	VAL	-	expression tag	UNP P78055
H	-23	PRO	-	expression tag	UNP P78055
H	-22	ARG	-	expression tag	UNP P78055
H	-21	GLY	-	expression tag	UNP P78055
H	-20	SER	-	expression tag	UNP P78055
H	-19	GLY	-	expression tag	UNP P78055
H	-18	MET	-	expression tag	UNP P78055
H	-17	LYS	-	expression tag	UNP P78055
H	-16	GLU	-	expression tag	UNP P78055
H	-15	THR	-	expression tag	UNP P78055
H	-14	ALA	-	expression tag	UNP P78055
H	-13	ALA	-	expression tag	UNP P78055
H	-12	ALA	-	expression tag	UNP P78055
H	-11	LYS	-	expression tag	UNP P78055
H	-10	PHE	-	expression tag	UNP P78055
H	-9	GLU	-	expression tag	UNP P78055
H	-8	ARG	-	expression tag	UNP P78055
H	-7	GLN	-	expression tag	UNP P78055
H	-6	HIS	-	expression tag	UNP P78055
H	-5	MET	-	expression tag	UNP P78055
H	-4	ASP	-	expression tag	UNP P78055
H	-3	SER	-	expression tag	UNP P78055
H	-2	PRO	-	expression tag	UNP P78055
H	-1	ARG	-	expression tag	UNP P78055
H	0	SER	-	expression tag	UNP P78055
H	31	THR	ILE	engineered mutation	UNP P78055
H	59	THR	GLN	engineered mutation	UNP P78055

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Chain	Residue	Modelled	Actual	Comment	Reference
H	195	GLN	ILE	engineered mutation	UNP P78055
I	-34	HIS	-	expression tag	UNP P78055
I	-33	HIS	-	expression tag	UNP P78055
I	-32	HIS	-	expression tag	UNP P78055
I	-31	HIS	-	expression tag	UNP P78055
I	-30	HIS	-	expression tag	UNP P78055
I	-29	HIS	-	expression tag	UNP P78055
I	-28	SER	-	expression tag	UNP P78055
I	-27	SER	-	expression tag	UNP P78055
I	-26	GLY	-	expression tag	UNP P78055
I	-25	LEU	-	expression tag	UNP P78055
I	-24	VAL	-	expression tag	UNP P78055
I	-23	PRO	-	expression tag	UNP P78055
I	-22	ARG	-	expression tag	UNP P78055
I	-21	GLY	-	expression tag	UNP P78055
I	-20	SER	-	expression tag	UNP P78055
I	-19	GLY	-	expression tag	UNP P78055
I	-18	MET	-	expression tag	UNP P78055
I	-17	LYS	-	expression tag	UNP P78055
I	-16	GLU	-	expression tag	UNP P78055
I	-15	THR	-	expression tag	UNP P78055
I	-14	ALA	-	expression tag	UNP P78055
I	-13	ALA	-	expression tag	UNP P78055
I	-12	ALA	-	expression tag	UNP P78055
I	-11	LYS	-	expression tag	UNP P78055
I	-10	PHE	-	expression tag	UNP P78055
I	-9	GLU	-	expression tag	UNP P78055
I	-8	ARG	-	expression tag	UNP P78055
I	-7	GLN	-	expression tag	UNP P78055
I	-6	HIS	-	expression tag	UNP P78055
I	-5	MET	-	expression tag	UNP P78055
I	-4	ASP	-	expression tag	UNP P78055
I	-3	SER	-	expression tag	UNP P78055
I	-2	PRO	-	expression tag	UNP P78055
I	-1	ARG	-	expression tag	UNP P78055
I	0	SER	-	expression tag	UNP P78055
I	31	THR	ILE	engineered mutation	UNP P78055
I	59	THR	GLN	engineered mutation	UNP P78055
I	195	GLN	ILE	engineered mutation	UNP P78055
J	-34	HIS	-	expression tag	UNP P78055
J	-33	HIS	-	expression tag	UNP P78055
J	-32	HIS	-	expression tag	UNP P78055

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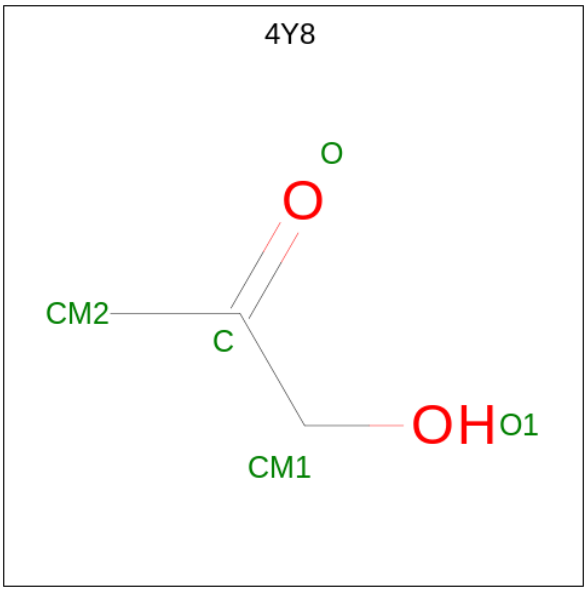
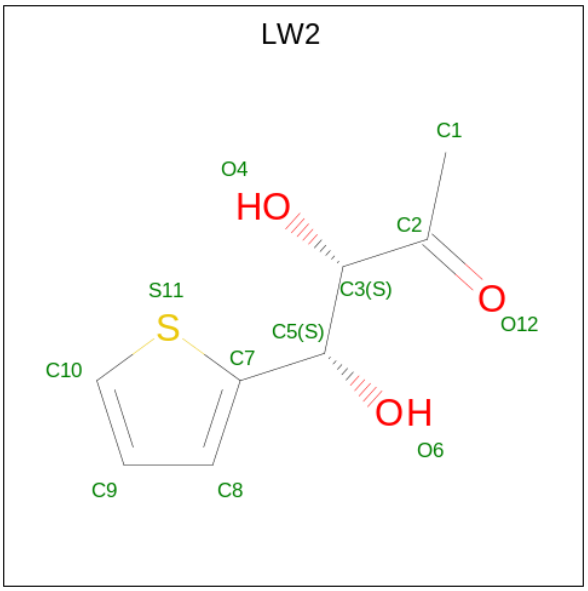
Chain	Residue	Modelled	Actual	Comment	Reference
J	-31	HIS	-	expression tag	UNP P78055
J	-30	HIS	-	expression tag	UNP P78055
J	-29	HIS	-	expression tag	UNP P78055
J	-28	SER	-	expression tag	UNP P78055
J	-27	SER	-	expression tag	UNP P78055
J	-26	GLY	-	expression tag	UNP P78055
J	-25	LEU	-	expression tag	UNP P78055
J	-24	VAL	-	expression tag	UNP P78055
J	-23	PRO	-	expression tag	UNP P78055
J	-22	ARG	-	expression tag	UNP P78055
J	-21	GLY	-	expression tag	UNP P78055
J	-20	SER	-	expression tag	UNP P78055
J	-19	GLY	-	expression tag	UNP P78055
J	-18	MET	-	expression tag	UNP P78055
J	-17	LYS	-	expression tag	UNP P78055
J	-16	GLU	-	expression tag	UNP P78055
J	-15	THR	-	expression tag	UNP P78055
J	-14	ALA	-	expression tag	UNP P78055
J	-13	ALA	-	expression tag	UNP P78055
J	-12	ALA	-	expression tag	UNP P78055
J	-11	LYS	-	expression tag	UNP P78055
J	-10	PHE	-	expression tag	UNP P78055
J	-9	GLU	-	expression tag	UNP P78055
J	-8	ARG	-	expression tag	UNP P78055
J	-7	GLN	-	expression tag	UNP P78055
J	-6	HIS	-	expression tag	UNP P78055
J	-5	MET	-	expression tag	UNP P78055
J	-4	ASP	-	expression tag	UNP P78055
J	-3	SER	-	expression tag	UNP P78055
J	-2	PRO	-	expression tag	UNP P78055
J	-1	ARG	-	expression tag	UNP P78055
J	0	SER	-	expression tag	UNP P78055
J	31	THR	ILE	engineered mutation	UNP P78055
J	59	THR	GLN	engineered mutation	UNP P78055
J	195	GLN	ILE	engineered mutation	UNP P78055

- Molecule 2 is 1-hydroxypropan-2-one (three-letter code: 4Y8) (formula: $C_3H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		
2	B	1	Total	C	O	0	0
			4	3	1		
2	C	1	Total	C	O	0	0
			4	3	1		
2	D	1	Total	C	O	0	0
			4	3	1		
2	E	1	Total	C	O	0	0
			4	3	1		
2	F	1	Total	C	O	0	0
			4	3	1		
2	G	1	Total	C	O	0	0
			4	3	1		
2	H	1	Total	C	O	0	0
			4	3	1		
2	I	1	Total	C	O	0	0
			4	3	1		
2	J	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is (3S,4S)-3,4-dihydroxy-4-(thiophen-2-yl)butan-2-one (three-letter code: LW2) (formula: $C_8H_{10}O_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 12 8 3 1	0	0
3	B	1	Total C O S 12 8 3 1	0	0
3	C	1	Total C O S 12 8 3 1	0	0
3	D	1	Total C O S 12 8 3 1	0	0
3	E	1	Total C O S 12 8 3 1	0	0
3	F	1	Total C O S 12 8 3 1	0	0
3	H	1	Total C O S 12 8 3 1	0	0
3	I	1	Total C O S 12 8 3 1	0	0
3	J	1	Total C O S 12 8 3 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0

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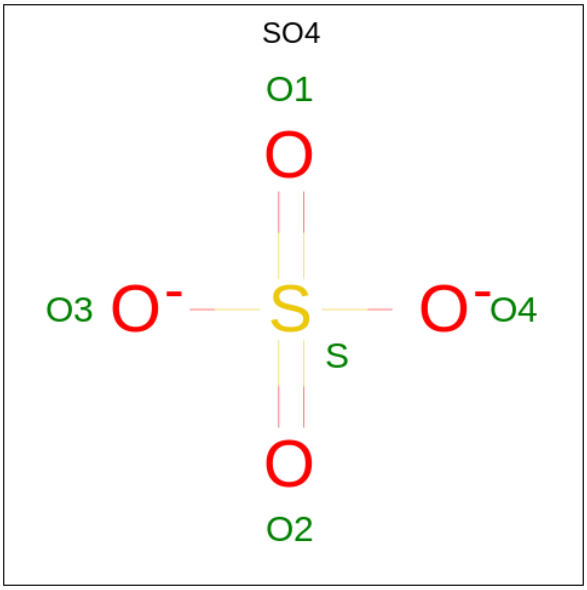
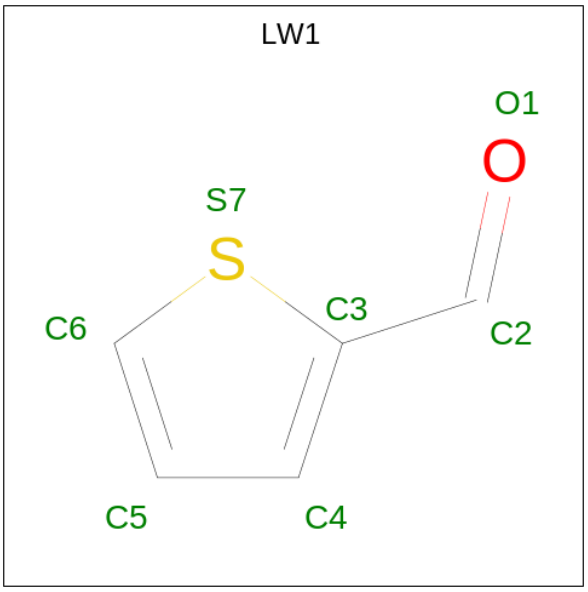
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total Cl 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	J	1	Total O S 5 4 1	0	0

- Molecule 6 is thiophene-2-carbaldehyde (three-letter code: LW1) (formula: C_5H_4OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total C O S 7 5 1 1	0	0

- Molecule 7 is water.

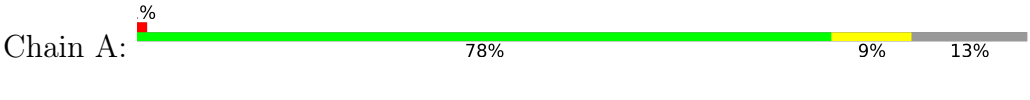
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	72	Total O 72 72	0	0
7	B	86	Total O 86 86	0	0
7	C	104	Total O 104 104	0	0
7	D	95	Total O 95 95	0	0
7	E	110	Total O 110 110	0	0
7	F	85	Total O 85 85	0	0
7	G	133	Total O 133 133	0	0
7	H	91	Total O 91 91	0	0
7	I	64	Total O 64 64	0	0
7	J	73	Total O 73 73	0	0

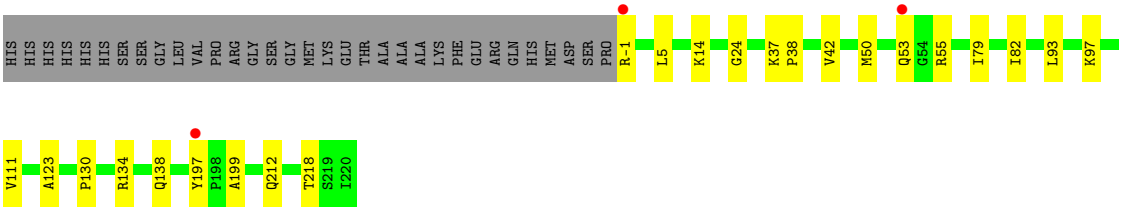
3 Residue-property plots (i)

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

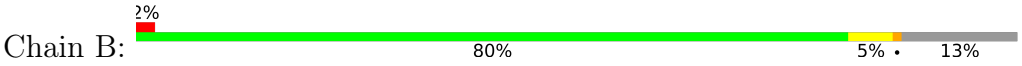
Chain A:

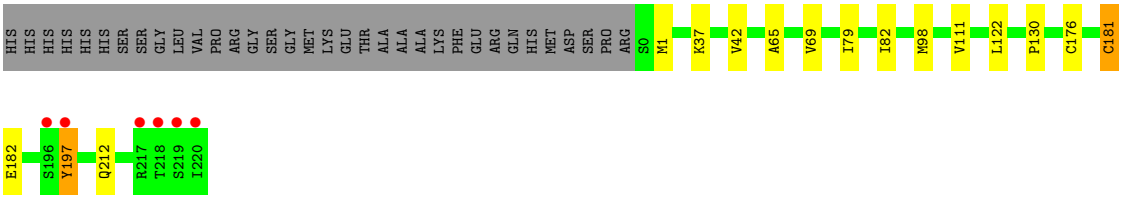




• Molecule 1: Fructose-6-phosphate aldolase 1

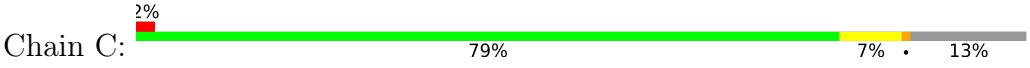
Chain B:

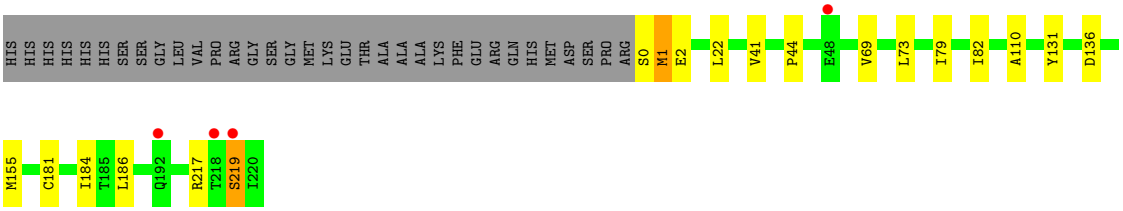




• Molecule 1: Fructose-6-phosphate aldolase 1

Chain C:



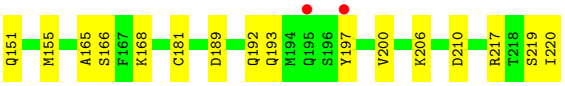


• Molecule 1: Fructose-6-phosphate aldolase 1

Chain D:

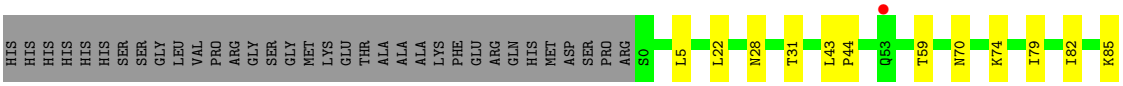
• Molecule 1: Fructose-6-phosphate aldolase 1

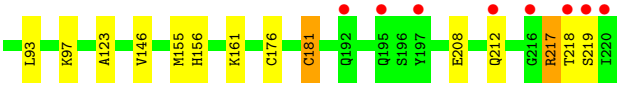
Chain E:



• Molecule 1: Fructose-6-phosphate aldolase 1

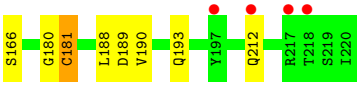
Chain F:





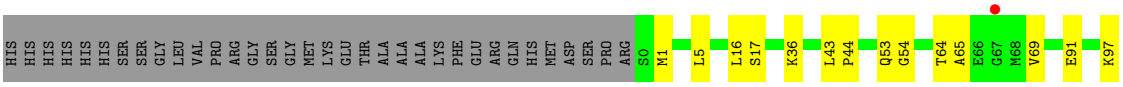
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain G:



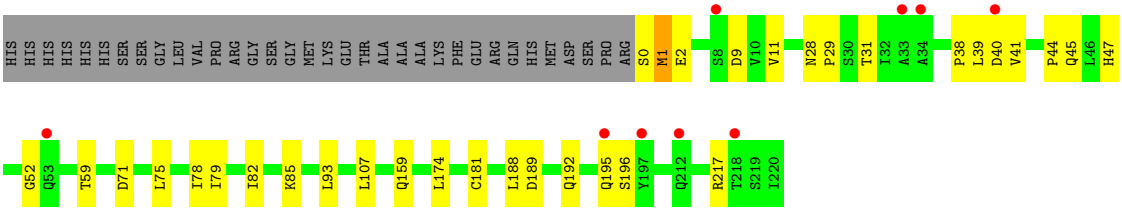
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain H:

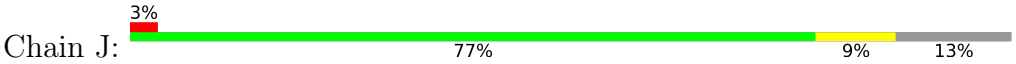


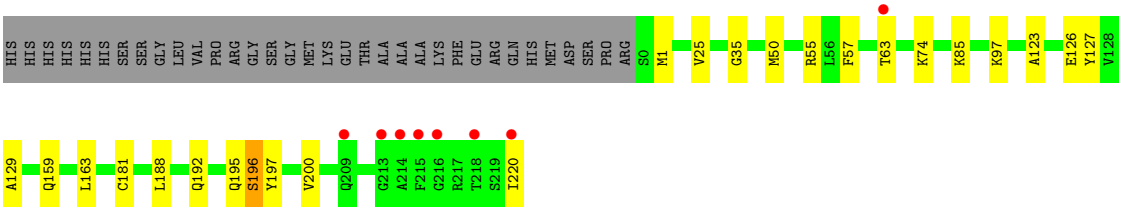
• Molecule 1: Fructose-6-phosphate aldolase 1

Chain I:



• Molecule 1: Fructose-6-phosphate aldolase 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.08Å 103.08Å 492.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	22.70 – 2.17 22.70 – 2.17	Depositor EDS
% Data completeness (in resolution range)	96.8 (22.70-2.17) 96.7 (22.70-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.191 , 0.232 0.192 , 0.232	Depositor DCC
R_{free} test set	8055 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17350	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: 4Y8, LW1, LW2, 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	0.37	0/1659	0.54	0/2255
1	B	0.42	0/1657	0.59	0/2253
1	C	0.46	1/1642 (0.1%)	0.61	0/2233
1	D	0.46	1/1651 (0.1%)	0.58	0/2245
1	E	0.45	1/1642 (0.1%)	0.59	0/2233
1	F	0.43	2/1657 (0.1%)	0.59	0/2253
1	G	0.48	1/1666 (0.1%)	0.60	0/2266
1	H	0.42	1/1642 (0.1%)	0.57	0/2233
1	I	0.41	1/1642 (0.1%)	0.54	0/2233
1	J	0.42	1/1650 (0.1%)	0.57	0/2245
All	All	0.43	9/16508 (0.1%)	0.58	0/22449

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	181	CYS	CB-SG	-8.65	1.67	1.82
1	D	181	CYS	CB-SG	-7.34	1.69	1.82
1	C	181	CYS	CB-SG	-6.93	1.70	1.82
1	G	181	CYS	CB-SG	-6.71	1.70	1.82
1	J	181	CYS	CB-SG	-6.27	1.71	1.82
1	H	181	CYS	CB-SG	-5.57	1.72	1.81
1	I	181	CYS	CB-SG	-5.51	1.72	1.81
1	F	181[A]	CYS	CB-SG	-5.33	1.73	1.81
1	F	181[B]	CYS	CB-SG	-5.33	1.73	1.81

There are no bond angle outliers.

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	1631	0	1689	12	0
1	B	1626	0	1682	8	0
1	C	1617	0	1671	10	0
1	D	1623	0	1677	11	0
1	E	1617	0	1671	19	0
1	F	1626	0	1683	19	0
1	G	1637	0	1693	15	0
1	H	1617	0	1671	20	0
1	I	1617	0	1670	28	0
1	J	1622	0	1677	13	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	0	0
2	H	4	0	3	0	0
2	I	4	0	3	1	0
2	J	4	0	3	0	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
3	C	12	0	0	0	0
3	D	12	0	0	0	0
3	E	12	0	0	1	0
3	F	12	0	0	0	0
3	H	12	0	0	1	0
3	I	12	0	0	0	0
3	J	12	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	5	0	0	0	0
5	G	5	0	0	0	0
5	H	5	0	0	0	0
5	I	5	0	0	0	0
5	J	5	0	0	1	0
6	G	7	0	0	1	0
7	A	72	0	0	2	0
7	B	86	0	0	0	0
7	C	104	0	0	2	0
7	D	95	0	0	1	0
7	E	110	0	0	4	0
7	F	85	0	0	2	0
7	G	133	0	0	1	0
7	H	91	0	0	0	0
7	I	64	0	0	0	0
7	J	73	0	0	1	0
All	All	17350	0	16814	140	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 4.

All (140) 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:69:VAL:O	1:C:73:LEU:HD12	1.66	0.96
1:A:37:LYS:HB2	1:A:42:VAL:HG13	1.70	0.73
1:H:156:HIS:HB3	1:I:1:MET:CE	2.20	0.72
1:E:136:ASP:OD2	7:E:401:HOH:O	2.11	0.69
1:F:161:LYS:NZ	7:F:401:HOH:O	2.27	0.67
1:G:43:LEU:HB3	1:G:79:ILE:HD11	1.80	0.64
1:H:102:GLU:HB3	1:H:104:ILE:HD12	1.81	0.62
1:H:156:HIS:HB3	1:I:1:MET:HE3	1.82	0.61
1:A:79:ILE:HB	1:A:82:ILE:HB	1.81	0.61
1:H:156:HIS:HB3	1:I:1:MET:HE2	1.83	0.60
1:F:5:LEU:HD13	1:F:22:LEU:CD2	2.32	0.60
1:G:138:GLN:NE2	7:G:402:HOH:O	2.23	0.60
1:F:5:LEU:HD13	1:F:22:LEU:HD22	1.84	0.59
1:I:188:LEU:O	1:I:192:GLN:HG3	2.03	0.59
1:J:197:TYR:HB2	1:J:200:VAL:HG23	1.85	0.56
1:C:184:ILE:HD12	1:C:186:LEU:HD21	1.88	0.56
1:F:28:ASN:H	1:F:31:THR:HG22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ALA:HB1	1:E:138:GLN:HE22	1.72	0.55
1:E:97:LYS:NZ	7:E:403:HOH:O	2.41	0.55
1:G:122:LEU:HD21	1:H:1:MET:HG2	1.88	0.55
1:C:136:ASP:OD2	7:C:401:HOH:O	2.18	0.54
1:I:41:VAL:O	1:I:45:GLN:HG3	2.08	0.54
1:I:39:LEU:HD12	1:J:220:ILE:HG23	1.91	0.53
1:I:29:PRO:HD3	1:I:59:THR:HB	1.91	0.53
1:J:97:LYS:HG2	1:J:123:ALA:HB1	1.91	0.53
1:B:65:ALA:O	1:B:69:VAL:HG23	2.10	0.52
1:F:5:LEU:HD22	1:F:22:LEU:HD11	1.91	0.52
1:H:118:LEU:HD21	1:I:1:MET:CE	2.40	0.52
1:D:24:GLY:HA2	1:D:50:MET:SD	2.50	0.52
1:F:31:THR:HG21	7:F:403:HOH:O	2.10	0.52
1:H:5:LEU:HD21	1:H:16:LEU:HD12	1.92	0.52
1:G:166:SER:HA	6:G:302:LW1:C4	2.41	0.51
1:G:43:LEU:HB3	1:G:79:ILE:CD1	2.40	0.51
1:H:118:LEU:HD21	1:I:1:MET:HE2	1.93	0.50
1:H:65:ALA:N	1:H:91:GLU:HG3	2.26	0.50
1:I:41:VAL:O	1:I:44:PRO:HD2	2.11	0.50
1:E:60:VAL:HG21	1:E:68:MET:HG2	1.94	0.50
1:E:151:GLN:O	1:E:155:MET:HG2	2.11	0.50
1:F:156:HIS:HB3	1:G:1:MET:HB3	1.95	0.49
1:C:1:MET:HG2	1:C:2:GLU:N	2.26	0.49
1:D:70:ASN:O	1:D:74:LYS:HG3	2.13	0.48
1:I:59:THR:HA	1:I:85:LYS:HB2	1.96	0.48
1:I:9:ASP:OD1	1:I:11:VAL:HG22	2.13	0.48
1:H:53:GLN:HG2	1:H:54:GLY:H	1.79	0.48
1:F:79:ILE:HB	1:F:82:ILE:HB	1.95	0.47
1:I:28:ASN:HD22	2:I:301:4Y8:CM2	2.26	0.47
1:D:79:ILE:HB	1:D:82:ILE:HB	1.97	0.47
1:I:159:GLN:H	1:I:159:GLN:CD	2.17	0.47
1:A:199:ALA:CB	1:E:138:GLN:HE22	2.26	0.47
1:E:189:ASP:O	1:E:193:GLN:HG3	2.14	0.47
1:I:85:LYS:HG2	1:I:107:LEU:HD22	1.96	0.47
1:J:159:GLN:H	1:J:159:GLN:CD	2.17	0.47
1:D:29:PRO:HD3	1:D:59:THR:HB	1.97	0.47
1:H:65:ALA:O	1:H:69:VAL:HG23	2.15	0.47
1:J:129:ALA:HA	1:J:163:LEU:O	2.15	0.47
1:E:134:ARG:HG2	7:E:435:HOH:O	2.15	0.47
1:H:53:GLN:HG2	1:H:54:GLY:N	2.30	0.46
1:I:195:GLN:HA	1:I:195:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:GLN:HG2	7:E:507:HOH:O	2.16	0.46
1:H:43:LEU:HB2	1:H:44:PRO:HD3	1.98	0.46
1:E:219:SER:O	1:E:220:ILE:HG22	2.16	0.46
1:I:1:MET:HG2	1:I:2:GLU:N	2.31	0.46
1:B:65:ALA:HB1	1:B:98:MET:CE	2.46	0.46
1:E:79:ILE:HB	1:E:82:ILE:HB	1.98	0.46
1:F:43:LEU:HB2	1:F:44:PRO:HD3	1.98	0.46
1:H:152:LEU:HD11	1:I:174:LEU:HD11	1.98	0.45
1:D:40:ASP:HA	1:D:78:ILE:HD13	1.98	0.45
1:E:168:LYS:HD3	1:E:168:LYS:HA	1.78	0.45
1:I:1:MET:HE3	1:I:1:MET:HB3	1.55	0.45
3:H:302:LW2:S11	3:H:302:LW2:O4	2.75	0.45
1:F:5:LEU:HD22	1:F:22:LEU:CD1	2.47	0.45
1:B:37:LYS:HB2	1:B:42:VAL:HB	1.99	0.45
1:H:156:HIS:HB3	1:I:1:MET:HB2	1.99	0.44
1:H:64:THR:HA	1:H:91:GLU:HG2	1.99	0.44
1:I:39:LEU:HD13	1:I:75:LEU:HD21	1.98	0.44
1:A:111:VAL:O	1:A:130:PRO:HA	2.17	0.44
1:E:165:ALA:O	1:E:166:SER:HB3	2.17	0.44
1:E:197:TYR:HB2	1:E:200:VAL:HG23	1.99	0.44
1:E:111:VAL:O	1:E:130:PRO:HA	2.18	0.44
1:F:176:CYS:O	1:F:181[B]:CYS:HB2	2.17	0.44
1:F:208:GLU:O	1:F:212:GLN:HG3	2.17	0.44
1:I:189:ASP:N	1:I:189:ASP:OD1	2.50	0.44
1:D:14:LYS:HG2	1:D:49:ALA:HB1	2.00	0.44
1:J:126:GLU:HG2	1:J:127:TYR:CD1	2.53	0.44
1:G:189:ASP:O	1:G:193:GLN:HG3	2.18	0.43
1:A:134:ARG:O	1:A:138:GLN:HG2	2.17	0.43
1:B:111:VAL:O	1:B:130:PRO:HA	2.18	0.43
1:F:97:LYS:HG2	1:F:123:ALA:HB1	2.00	0.43
1:D:39:LEU:HD22	1:D:43:LEU:HD11	2.00	0.43
1:I:47:HIS:CE1	1:I:52:GLY:HA2	2.54	0.43
1:A:24:GLY:HA2	1:A:50:MET:SD	2.59	0.43
1:H:156:HIS:CB	1:I:1:MET:HE2	2.47	0.43
1:C:79:ILE:HB	1:C:82:ILE:HB	1.99	0.43
1:C:41:VAL:O	1:C:44:PRO:HD2	2.18	0.43
1:D:201:ASP:OD2	7:D:401:HOH:O	2.20	0.43
1:B:79:ILE:HB	1:B:82:ILE:HB	2.00	0.43
1:D:176:CYS:O	1:D:181:CYS:HB3	2.18	0.43
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.86	0.43
1:G:188:LEU:HD23	1:G:188:LEU:HA	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:CYS:O	1:B:181[A]:CYS:HB2	2.19	0.43
1:G:189:ASP:OD1	1:G:190:VAL:N	2.51	0.43
1:I:79:ILE:HB	1:I:82:ILE:HB	1.99	0.43
1:A:38:PRO:O	1:A:42:VAL:HG22	2.19	0.42
1:E:134:ARG:NE	3:E:302:LW2:O4	2.52	0.42
1:J:63:THR:HG22	5:J:303:SO4:O4	2.18	0.42
1:C:22:LEU:HB2	7:C:474:HOH:O	2.18	0.42
1:F:212:GLN:HG2	1:F:217:ARG:O	2.19	0.42
1:F:218:THR:O	1:F:219:SER:HB3	2.18	0.42
1:A:14:LYS:HB2	1:A:14:LYS:HE2	1.86	0.42
1:G:126:GLU:HG2	1:G:127:TYR:CD2	2.54	0.42
1:D:85:LYS:HG2	1:D:107:LEU:HD22	2.01	0.42
1:I:40:ASP:HA	1:I:78:ILE:HD13	2.02	0.42
1:J:57:PHE:HB3	1:J:85:LYS:HD2	2.01	0.42
1:A:53:GLN:HB3	7:A:437:HOH:O	2.19	0.42
1:F:59:THR:HA	1:F:85:LYS:HB2	2.02	0.42
1:J:25:VAL:HG23	1:J:50:MET:SD	2.60	0.42
7:A:401:HOH:O	1:E:97:LYS:HG3	2.20	0.42
1:C:110:ALA:HA	1:C:131:TYR:CE2	2.54	0.41
1:I:71:ASP:HB3	1:J:220:ILE:HD12	2.02	0.41
1:B:65:ALA:HB1	1:B:98:MET:HE1	2.02	0.41
1:D:74:LYS:O	1:D:77:SER:OG	2.29	0.41
1:A:97:LYS:HG2	1:A:123:ALA:HB1	2.01	0.41
1:F:155:MET:SD	1:G:180:GLY:HA2	2.60	0.41
1:E:206:LYS:HE3	1:E:210:ASP:OD1	2.21	0.41
1:G:131:TYR:HB3	1:G:134:ARG:HG3	2.03	0.41
1:E:1:MET:HG2	1:E:2:GLU:N	2.35	0.41
1:H:36:LYS:HA	1:H:36:LYS:HD3	1.95	0.41
1:I:38:PRO:HG2	1:I:41:VAL:HG23	2.01	0.41
1:A:5:LEU:HD12	1:A:5:LEU:HA	1.94	0.41
1:H:97:LYS:HG2	1:H:123:ALA:HB1	2.02	0.41
1:G:24:GLY:HA2	1:G:50:MET:SD	2.60	0.41
1:F:70:ASN:O	1:F:74:LYS:HG2	2.21	0.41
1:F:146:VAL:HG13	1:F:181[B]:CYS:SG	2.61	0.41
1:H:189:ASP:O	1:H:193:GLN:HG3	2.20	0.41
1:J:188:LEU:O	1:J:192:GLN:HG2	2.21	0.41
1:J:192:GLN:O	1:J:195:GLN:HG2	2.20	0.41
1:B:122:LEU:HD11	1:C:1:MET:SD	2.60	0.41
1:G:79:ILE:HB	1:G:82:ILE:HB	2.03	0.40
1:J:35:GLY:HA3	7:J:438:HOH:O	2.21	0.40
1:C:217:ARG:HG2	1:C:219:SER:H	1.86	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	221/255 (87%)	213 (96%)	8 (4%)	0	100	100
1	B	221/255 (87%)	210 (95%)	9 (4%)	2 (1%)	14	13
1	C	219/255 (86%)	214 (98%)	5 (2%)	0	100	100
1	D	220/255 (86%)	216 (98%)	4 (2%)	0	100	100
1	E	219/255 (86%)	214 (98%)	5 (2%)	0	100	100
1	F	221/255 (87%)	211 (96%)	10 (4%)	0	100	100
1	G	221/255 (87%)	211 (96%)	10 (4%)	0	100	100
1	H	219/255 (86%)	213 (97%)	6 (3%)	0	100	100
1	I	219/255 (86%)	213 (97%)	6 (3%)	0	100	100
1	J	220/255 (86%)	212 (96%)	7 (3%)	1 (0%)	25	26
All	All	2200/2550 (86%)	2127 (97%)	70 (3%)	3 (0%)	48	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	TYR
1	B	1	MET
1	J	196	SER

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	170/196 (87%)	164 (96%)	6 (4%)	31	38
1	B	170/196 (87%)	164 (96%)	6 (4%)	31	38
1	C	168/196 (86%)	164 (98%)	4 (2%)	44	54
1	D	169/196 (86%)	164 (97%)	5 (3%)	36	45
1	E	168/196 (86%)	164 (98%)	4 (2%)	44	54
1	F	170/196 (87%)	168 (99%)	2 (1%)	67	78
1	G	170/196 (87%)	167 (98%)	3 (2%)	54	66
1	H	168/196 (86%)	165 (98%)	3 (2%)	54	66
1	I	168/196 (86%)	162 (96%)	6 (4%)	30	37
1	J	169/196 (86%)	165 (98%)	4 (2%)	44	54
All	All	1690/1960 (86%)	1647 (98%)	43 (2%)	44	53

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	55	ARG
1	A	93	LEU
1	A	197	TYR
1	A	212	GLN
1	A	218	THR
1	B	181[A]	CYS
1	B	181[B]	CYS
1	B	182[A]	GLU
1	B	182[B]	GLU
1	B	197	TYR
1	B	212	GLN
1	C	0	SER
1	C	1	MET
1	C	155	MET
1	C	219	SER
1	D	17	SER
1	D	93	LEU
1	D	100	LYS
1	D	102	GLU
1	D	181	CYS
1	E	1	MET
1	E	134	ARG
1	E	192	GLN

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Mol	Chain	Res	Type
1	E	217	ARG
1	F	93	LEU
1	F	217	ARG
1	G	134	ARG
1	G	181	CYS
1	G	212	GLN
1	H	17	SER
1	H	126	GLU
1	H	197	TYR
1	I	0	SER
1	I	1	MET
1	I	31	THR
1	I	93	LEU
1	I	196	SER
1	I	217	ARG
1	J	1	MET
1	J	55	ARG
1	J	74	LYS
1	J	196	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	70	ASN
1	E	138	GLN
1	G	195	GLN
1	I	45	GLN
1	J	195	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 33 ligands modelled in this entry, 4 are 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	$\#\|Z\| > 2$
5	SO4	I	304	-	4,4,4	0.12	0	6,6,6	0.20	0
2	4Y8	D	301	1	3,3,4	0.51	0	2,2,4	0.64	0
2	4Y8	A	301	1	3,3,4	0.44	0	2,2,4	0.65	0
2	4Y8	H	301	1	3,3,4	0.35	0	2,2,4	0.71	0
3	LW2	I	302	-	11,12,12	3.96	4 (36%)	9,16,16	5.04	7 (77%)
5	SO4	G	303	-	4,4,4	0.18	0	6,6,6	0.18	0
5	SO4	J	303	-	4,4,4	0.18	0	6,6,6	0.33	0
3	LW2	D	302	-	11,12,12	4.30	4 (36%)	9,16,16	4.93	5 (55%)
6	LW1	G	302	-	7,7,7	1.78	1 (14%)	3,8,8	0.93	0
5	SO4	B	303	-	4,4,4	0.17	0	6,6,6	0.22	0
3	LW2	F	302	-	11,12,12	1.77	3 (27%)	9,16,16	4.50	4 (44%)
3	LW2	H	302	-	11,12,12	3.45	4 (36%)	9,16,16	4.23	5 (55%)
5	SO4	E	303	-	4,4,4	0.16	0	6,6,6	0.24	0
2	4Y8	G	301	1	3,3,4	0.34	0	2,2,4	0.59	0
2	4Y8	J	301	1	3,3,4	0.35	0	2,2,4	0.63	0
5	SO4	D	303	-	4,4,4	0.17	0	6,6,6	0.25	0
3	LW2	J	302	-	11,12,12	4.53	4 (36%)	9,16,16	4.66	4 (44%)
5	SO4	H	303	-	4,4,4	0.13	0	6,6,6	0.17	0
2	4Y8	B	301	1	3,3,4	0.22	0	2,2,4	0.70	0
5	SO4	F	304	-	4,4,4	0.14	0	6,6,6	0.16	0
3	LW2	C	302	-	11,12,12	2.23	3 (27%)	9,16,16	4.11	5 (55%)
2	4Y8	E	301	1	3,3,4	0.33	0	2,2,4	0.59	0
2	4Y8	C	301	1	3,3,4	0.40	0	2,2,4	0.62	0
2	4Y8	F	301	1	3,3,4	0.32	0	2,2,4	0.65	0
3	LW2	A	302	-	11,12,12	3.19	4 (36%)	9,16,16	3.83	4 (44%)
5	SO4	A	304	-	4,4,4	0.15	0	6,6,6	0.17	0
3	LW2	B	302	-	11,12,12	2.42	4 (36%)	9,16,16	4.08	3 (33%)
2	4Y8	I	301	1	3,3,4	0.36	0	2,2,4	0.63	0
3	LW2	E	302	-	11,12,12	3.54	4 (36%)	9,16,16	4.36	5 (55%)

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	4Y8	D	301	1	-	0/1/1/2	-
2	4Y8	A	301	1	-	0/1/1/2	-
2	4Y8	H	301	1	-	0/1/1/2	-
3	LW2	I	302	-	-	2/8/12/12	0/1/1/1
3	LW2	D	302	-	-	4/8/12/12	0/1/1/1
6	LW1	G	302	-	-	0/0/2/2	0/1/1/1
3	LW2	F	302	-	-	8/8/12/12	0/1/1/1
3	LW2	H	302	-	-	2/8/12/12	0/1/1/1
2	4Y8	G	301	1	-	0/1/1/2	-
2	4Y8	J	301	1	-	0/1/1/2	-
3	LW2	J	302	-	-	6/8/12/12	0/1/1/1
2	4Y8	B	301	1	-	0/1/1/2	-
3	LW2	C	302	-	-	4/8/12/12	0/1/1/1
2	4Y8	E	301	1	-	0/1/1/2	-
2	4Y8	C	301	1	-	0/1/1/2	-
2	4Y8	F	301	1	-	1/1/1/2	-
3	LW2	A	302	-	-	4/8/12/12	0/1/1/1
3	LW2	B	302	-	-	3/8/12/12	0/1/1/1
2	4Y8	I	301	1	-	0/1/1/2	-
3	LW2	E	302	-	-	6/8/12/12	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	302	LW2	C3-C2	13.41	1.63	1.52
3	D	302	LW2	C3-C2	12.91	1.63	1.52
3	I	302	LW2	C3-C2	9.93	1.60	1.52
3	E	302	LW2	C3-C2	9.81	1.60	1.52
3	H	302	LW2	C3-C2	9.73	1.60	1.52
3	A	302	LW2	C3-C2	9.36	1.60	1.52
3	I	302	LW2	C7-C5	7.30	1.59	1.51
3	B	302	LW2	C3-C2	5.86	1.57	1.52
3	C	302	LW2	C3-C2	5.75	1.57	1.52
3	J	302	LW2	C7-C5	5.01	1.56	1.51
3	E	302	LW2	C7-C5	4.47	1.56	1.51
3	D	302	LW2	C7-C5	3.93	1.55	1.51
3	H	302	LW2	C7-C5	3.92	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	302	LW1	C3-C2	3.73	1.52	1.48
3	F	302	LW2	C3-C2	3.64	1.55	1.52
3	E	302	LW2	C9-C8	3.60	1.51	1.39
3	B	302	LW2	C9-C8	3.51	1.51	1.39
3	C	302	LW2	C9-C8	3.42	1.50	1.39
3	J	302	LW2	C9-C8	3.38	1.50	1.39
3	F	302	LW2	C9-C8	3.38	1.50	1.39
3	H	302	LW2	C9-C8	3.35	1.50	1.39
3	I	302	LW2	C9-C8	3.33	1.50	1.39
3	D	302	LW2	C9-C8	3.22	1.50	1.39
3	A	302	LW2	C9-C8	3.03	1.49	1.39
3	B	302	LW2	C7-C5	2.93	1.54	1.51
3	A	302	LW2	C7-C5	2.62	1.54	1.51
3	C	302	LW2	C9-C10	2.20	1.41	1.34
3	F	302	LW2	C9-C10	2.19	1.41	1.34
3	D	302	LW2	C9-C10	2.17	1.41	1.34
3	B	302	LW2	C9-C10	2.16	1.41	1.34
3	J	302	LW2	C9-C10	2.13	1.40	1.34
3	E	302	LW2	C9-C10	2.13	1.40	1.34
3	I	302	LW2	C9-C10	2.11	1.40	1.34
3	H	302	LW2	C9-C10	2.09	1.40	1.34
3	A	302	LW2	C9-C10	2.08	1.40	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	302	LW2	C1-C2-C3	12.96	127.26	118.39
3	I	302	LW2	C1-C2-C3	12.95	127.25	118.39
3	J	302	LW2	C1-C2-C3	12.18	126.73	118.39
3	H	302	LW2	C1-C2-C3	10.82	125.80	118.39
3	F	302	LW2	C1-C2-C3	10.76	125.76	118.39
3	E	302	LW2	C1-C2-C3	10.60	125.64	118.39
3	C	302	LW2	C1-C2-C3	10.40	125.51	118.39
3	B	302	LW2	C1-C2-C3	10.04	125.26	118.39
3	A	302	LW2	C1-C2-C3	9.78	125.08	118.39
3	F	302	LW2	O4-C3-C2	-5.96	101.47	111.04
3	E	302	LW2	O4-C3-C2	-4.84	103.26	111.04
3	B	302	LW2	O4-C3-C2	-4.67	103.54	111.04
3	I	302	LW2	C9-C10-S11	-4.38	109.42	112.98
3	E	302	LW2	C9-C10-S11	-4.33	109.47	112.98
3	D	302	LW2	C9-C10-S11	-4.32	109.48	112.98
3	C	302	LW2	O4-C3-C2	-4.17	104.34	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	302	LW2	C9-C10-S11	-4.12	109.64	112.98
3	I	302	LW2	O4-C3-C2	-4.00	104.62	111.04
3	A	302	LW2	C9-C10-S11	-3.88	109.83	112.98
3	F	302	LW2	C9-C10-S11	-3.87	109.84	112.98
3	B	302	LW2	C9-C10-S11	-3.86	109.85	112.98
3	H	302	LW2	C9-C10-S11	-3.74	109.95	112.98
3	H	302	LW2	O4-C3-C2	-3.26	105.79	111.04
3	J	302	LW2	O4-C3-C2	-3.18	105.92	111.04
3	C	302	LW2	C9-C10-S11	-3.15	110.42	112.98
3	A	302	LW2	O4-C3-C2	-3.13	106.02	111.04
3	D	302	LW2	O4-C3-C2	-2.94	106.32	111.04
3	D	302	LW2	O12-C2-C1	-2.79	116.19	121.15
3	J	302	LW2	O12-C2-C1	-2.73	116.30	121.15
3	E	302	LW2	O12-C2-C1	-2.65	116.44	121.15
3	I	302	LW2	O12-C2-C3	-2.53	116.07	118.98
3	I	302	LW2	O12-C2-C1	-2.52	116.67	121.15
3	F	302	LW2	O12-C2-C3	-2.38	116.24	118.98
3	C	302	LW2	O6-C5-C3	-2.18	101.83	108.97
3	A	302	LW2	O12-C2-C1	-2.18	117.28	121.15
3	I	302	LW2	C8-C7-S11	-2.15	106.34	111.36
3	D	302	LW2	O12-C2-C3	-2.12	116.54	118.98
3	H	302	LW2	C7-C5-C3	-2.11	109.07	113.64
3	H	302	LW2	O12-C2-C1	-2.11	117.40	121.15
3	C	302	LW2	O12-C2-C3	-2.11	116.56	118.98
3	I	302	LW2	C7-C5-C3	2.08	118.14	113.64
3	E	302	LW2	C8-C7-S11	-2.00	106.67	111.36

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	LW2	C1-C2-C3-C5
3	A	302	LW2	O12-C2-C3-C5
3	B	302	LW2	C1-C2-C3-C5
3	B	302	LW2	O12-C2-C3-O4
3	C	302	LW2	C1-C2-C3-C5
3	C	302	LW2	O12-C2-C3-C5
3	D	302	LW2	C1-C2-C3-C5
3	D	302	LW2	O12-C2-C3-C5
3	E	302	LW2	C1-C2-C3-C5
3	E	302	LW2	O12-C2-C3-O4
3	F	302	LW2	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
3	F	302	LW2	C1-C2-C3-O4
3	F	302	LW2	O12-C2-C3-C5
3	F	302	LW2	O12-C2-C3-O4
3	F	302	LW2	C2-C3-C5-C7
3	F	302	LW2	C2-C3-C5-O6
3	F	302	LW2	O4-C3-C5-C7
3	H	302	LW2	O12-C2-C3-O4
3	I	302	LW2	O12-C2-C3-C5
3	J	302	LW2	O12-C2-C3-C5
3	J	302	LW2	C2-C3-C5-C7
3	J	302	LW2	C2-C3-C5-O6
3	J	302	LW2	O4-C3-C5-C7
3	J	302	LW2	O4-C3-C5-O6
3	F	302	LW2	O4-C3-C5-O6
2	F	301	4Y8	CM2-C-CM1-O1
3	A	302	LW2	O12-C2-C3-O4
3	C	302	LW2	O12-C2-C3-O4
3	D	302	LW2	O12-C2-C3-O4
3	I	302	LW2	C1-C2-C3-C5
3	J	302	LW2	C1-C2-C3-C5
3	B	302	LW2	O12-C2-C3-C5
3	E	302	LW2	O12-C2-C3-C5
3	C	302	LW2	C1-C2-C3-O4
3	H	302	LW2	C1-C2-C3-O4
3	E	302	LW2	C2-C3-C5-O6
3	E	302	LW2	O4-C3-C5-C7
3	A	302	LW2	C1-C2-C3-O4
3	D	302	LW2	C1-C2-C3-O4
3	E	302	LW2	C2-C3-C5-C7

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	303	SO4	1	0
6	G	302	LW1	1	0
3	H	302	LW2	1	0
2	I	301	4Y8	1	0
3	E	302	LW2	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, 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	222/255 (87%)	0.00	3 (1%)	73	72	19, 39, 58, 78	1 (0%)
1	B	221/255 (86%)	-0.08	6 (2%)	56	55	14, 31, 74, 103	2 (0%)
1	C	221/255 (86%)	-0.30	4 (1%)	67	66	14, 28, 62, 77	0
1	D	221/255 (86%)	-0.30	0	100	100	13, 31, 54, 64	1 (0%)
1	E	221/255 (86%)	-0.30	2 (0%)	81	80	18, 31, 53, 72	0
1	F	221/255 (86%)	-0.06	9 (4%)	42	41	14, 34, 65, 98	2 (0%)
1	G	222/255 (87%)	-0.41	4 (1%)	67	66	16, 25, 60, 83	1 (0%)
1	H	221/255 (86%)	-0.22	2 (0%)	81	80	16, 33, 55, 72	0
1	I	221/255 (86%)	0.26	9 (4%)	42	41	20, 40, 69, 86	0
1	J	221/255 (86%)	-0.01	8 (3%)	46	45	20, 35, 69, 88	1 (0%)
All	All	2212/2550 (86%)	-0.14	47 (2%)	63	62	13, 33, 63, 103	8 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	218	THR	4.3
1	G	197[A]	TYR	4.2
1	F	218	THR	4.1
1	B	197	TYR	3.5
1	F	197	TYR	3.5
1	C	219	SER	3.4
1	J	213	GLY	3.0
1	J	214	ALA	3.0
1	G	218	THR	3.0
1	J	215	PHE	2.8
1	I	197	TYR	2.8
1	E	195	GLN	2.8
1	F	219	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	48	GLU	2.7
1	F	220	ILE	2.7
1	B	217	ARG	2.6
1	H	218	THR	2.6
1	B	219	SER	2.6
1	C	218	THR	2.5
1	I	218	THR	2.5
1	F	216	GLY	2.5
1	A	197	TYR	2.5
1	F	53	GLN	2.5
1	I	53	GLN	2.5
1	G	217	ARG	2.4
1	F	192	GLN	2.4
1	J	63	THR	2.4
1	B	196	SER	2.4
1	I	8	SER	2.4
1	F	212	GLN	2.4
1	H	67	GLY	2.4
1	B	220	ILE	2.4
1	A	-1	ARG	2.3
1	F	195	GLN	2.3
1	J	216	GLY	2.3
1	J	209	GLN	2.3
1	I	212	GLN	2.2
1	I	34	ALA	2.2
1	A	53	GLN	2.2
1	J	220	ILE	2.1
1	E	197	TYR	2.1
1	C	192	GLN	2.1
1	I	195	GLN	2.1
1	G	212	GLN	2.1
1	B	218	THR	2.1
1	I	33	ALA	2.0
1	I	40	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	LW2	D	302	12/12	0.63	0.20	46,59,77,92	0
3	LW2	H	302	12/12	0.69	0.23	50,71,79,89	0
6	LW1	G	302	7/7	0.70	0.18	53,55,73,95	0
3	LW2	A	302	12/12	0.72	0.22	56,64,75,80	0
3	LW2	B	302	12/12	0.73	0.21	41,53,62,62	12
5	SO4	J	303	5/5	0.74	0.14	59,65,73,80	5
3	LW2	I	302	12/12	0.74	0.22	47,58,65,79	12
3	LW2	F	302	12/12	0.76	0.21	51,61,71,73	12
3	LW2	J	302	12/12	0.77	0.18	47,62,69,88	0
4	CL	F	303	1/1	0.78	0.15	66,66,66,66	0
3	LW2	C	302	12/12	0.78	0.18	37,46,59,72	12
3	LW2	E	302	12/12	0.78	0.18	44,52,58,70	12
5	SO4	I	304	5/5	0.84	0.14	58,60,68,69	5
5	SO4	E	303	5/5	0.87	0.12	46,60,65,71	5
2	4Y8	I	301	4/5	0.87	0.15	35,36,42,48	0
4	CL	A	303	1/1	0.88	0.11	57,57,57,57	0
5	SO4	H	303	5/5	0.90	0.12	57,58,69,73	5
5	SO4	B	303	5/5	0.90	0.17	59,62,81,85	0
5	SO4	A	304	5/5	0.90	0.11	57,58,70,71	5
5	SO4	F	304	5/5	0.90	0.11	54,54,63,69	5
2	4Y8	E	301	4/5	0.91	0.11	26,26,31,33	0
5	SO4	G	303	5/5	0.91	0.10	34,46,56,57	5
5	SO4	D	303	5/5	0.94	0.08	42,44,52,59	5
4	CL	I	303	1/1	0.94	0.11	60,60,60,60	0
2	4Y8	H	301	4/5	0.95	0.07	28,30,31,32	0
2	4Y8	D	301	4/5	0.95	0.07	22,25,28,34	0
2	4Y8	C	301	4/5	0.95	0.08	25,31,33,33	0
2	4Y8	F	301	4/5	0.95	0.07	28,32,34,38	0
2	4Y8	B	301	4/5	0.96	0.07	24,28,29,32	0
2	4Y8	J	301	4/5	0.96	0.08	30,33,33,35	0
2	4Y8	A	301	4/5	0.96	0.09	31,36,38,42	0
2	4Y8	G	301	4/5	0.97	0.05	20,21,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	C	303	1/1	0.98	0.08	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.