Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 11:29 AM JST

PDB ID	:	7CJ8
Title	:	Crystal structure of N-terminal His-tagged D-allulose 3-epimerase from Methylomonas sp. in complex with D-allulose
Authors	:	Yoshida, H.; Yoshihara, A.; Kamitori, S.
Deposited on	:	2020-07-09
Resolution	:	2.05 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:

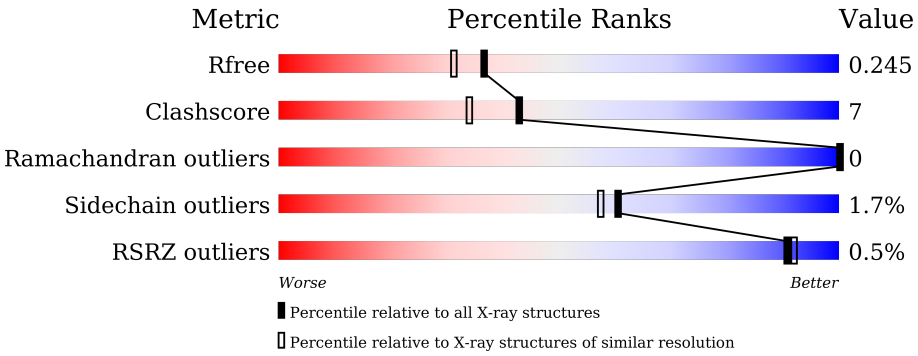
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	307	81% 12% • 7%
1	B	307	84% 9% 7%
1	C	307	% 78% 15% • 7%
1	D	307	85% 8% 6%
1	E	307	% 83% 9% • 7%
1	F	307	82% 11% 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14395 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 Epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2213	1401	382	422	8			
1	B	287	Total	C	N	O	S	0	0	0
			2213	1401	382	422	8			
1	C	287	Total	C	N	O	S	0	0	0
			2213	1401	382	422	8			
1	D	288	Total	C	N	O	S	0	0	0
			2223	1407	385	423	8			
1	E	287	Total	C	N	O	S	0	0	0
			2213	1401	382	422	8			
1	F	287	Total	C	N	O	S	0	0	0
			2213	1401	382	422	8			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A172U6X0
A	-19	GLY	-	expression tag	UNP A0A172U6X0
A	-18	SER	-	expression tag	UNP A0A172U6X0
A	-17	SER	-	expression tag	UNP A0A172U6X0
A	-16	HIS	-	expression tag	UNP A0A172U6X0
A	-15	HIS	-	expression tag	UNP A0A172U6X0
A	-14	HIS	-	expression tag	UNP A0A172U6X0
A	-13	HIS	-	expression tag	UNP A0A172U6X0
A	-12	HIS	-	expression tag	UNP A0A172U6X0
A	-11	HIS	-	expression tag	UNP A0A172U6X0
A	-10	SER	-	expression tag	UNP A0A172U6X0
A	-9	SER	-	expression tag	UNP A0A172U6X0
A	-8	GLY	-	expression tag	UNP A0A172U6X0
A	-7	LEU	-	expression tag	UNP A0A172U6X0
A	-6	VAL	-	expression tag	UNP A0A172U6X0
A	-5	PRO	-	expression tag	UNP A0A172U6X0
A	-4	ARG	-	expression tag	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP A0A172U6X0
A	-2	SER	-	expression tag	UNP A0A172U6X0
A	-1	HIS	-	expression tag	UNP A0A172U6X0
A	0	SER	-	expression tag	UNP A0A172U6X0
B	-20	MET	-	initiating methionine	UNP A0A172U6X0
B	-19	GLY	-	expression tag	UNP A0A172U6X0
B	-18	SER	-	expression tag	UNP A0A172U6X0
B	-17	SER	-	expression tag	UNP A0A172U6X0
B	-16	HIS	-	expression tag	UNP A0A172U6X0
B	-15	HIS	-	expression tag	UNP A0A172U6X0
B	-14	HIS	-	expression tag	UNP A0A172U6X0
B	-13	HIS	-	expression tag	UNP A0A172U6X0
B	-12	HIS	-	expression tag	UNP A0A172U6X0
B	-11	HIS	-	expression tag	UNP A0A172U6X0
B	-10	SER	-	expression tag	UNP A0A172U6X0
B	-9	SER	-	expression tag	UNP A0A172U6X0
B	-8	GLY	-	expression tag	UNP A0A172U6X0
B	-7	LEU	-	expression tag	UNP A0A172U6X0
B	-6	VAL	-	expression tag	UNP A0A172U6X0
B	-5	PRO	-	expression tag	UNP A0A172U6X0
B	-4	ARG	-	expression tag	UNP A0A172U6X0
B	-3	GLY	-	expression tag	UNP A0A172U6X0
B	-2	SER	-	expression tag	UNP A0A172U6X0
B	-1	HIS	-	expression tag	UNP A0A172U6X0
B	0	SER	-	expression tag	UNP A0A172U6X0
C	-20	MET	-	initiating methionine	UNP A0A172U6X0
C	-19	GLY	-	expression tag	UNP A0A172U6X0
C	-18	SER	-	expression tag	UNP A0A172U6X0
C	-17	SER	-	expression tag	UNP A0A172U6X0
C	-16	HIS	-	expression tag	UNP A0A172U6X0
C	-15	HIS	-	expression tag	UNP A0A172U6X0
C	-14	HIS	-	expression tag	UNP A0A172U6X0
C	-13	HIS	-	expression tag	UNP A0A172U6X0
C	-12	HIS	-	expression tag	UNP A0A172U6X0
C	-11	HIS	-	expression tag	UNP A0A172U6X0
C	-10	SER	-	expression tag	UNP A0A172U6X0
C	-9	SER	-	expression tag	UNP A0A172U6X0
C	-8	GLY	-	expression tag	UNP A0A172U6X0
C	-7	LEU	-	expression tag	UNP A0A172U6X0
C	-6	VAL	-	expression tag	UNP A0A172U6X0
C	-5	PRO	-	expression tag	UNP A0A172U6X0
C	-4	ARG	-	expression tag	UNP A0A172U6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP A0A172U6X0
C	-2	SER	-	expression tag	UNP A0A172U6X0
C	-1	HIS	-	expression tag	UNP A0A172U6X0
C	0	SER	-	expression tag	UNP A0A172U6X0
D	-20	MET	-	initiating methionine	UNP A0A172U6X0
D	-19	GLY	-	expression tag	UNP A0A172U6X0
D	-18	SER	-	expression tag	UNP A0A172U6X0
D	-17	SER	-	expression tag	UNP A0A172U6X0
D	-16	HIS	-	expression tag	UNP A0A172U6X0
D	-15	HIS	-	expression tag	UNP A0A172U6X0
D	-14	HIS	-	expression tag	UNP A0A172U6X0
D	-13	HIS	-	expression tag	UNP A0A172U6X0
D	-12	HIS	-	expression tag	UNP A0A172U6X0
D	-11	HIS	-	expression tag	UNP A0A172U6X0
D	-10	SER	-	expression tag	UNP A0A172U6X0
D	-9	SER	-	expression tag	UNP A0A172U6X0
D	-8	GLY	-	expression tag	UNP A0A172U6X0
D	-7	LEU	-	expression tag	UNP A0A172U6X0
D	-6	VAL	-	expression tag	UNP A0A172U6X0
D	-5	PRO	-	expression tag	UNP A0A172U6X0
D	-4	ARG	-	expression tag	UNP A0A172U6X0
D	-3	GLY	-	expression tag	UNP A0A172U6X0
D	-2	SER	-	expression tag	UNP A0A172U6X0
D	-1	HIS	-	expression tag	UNP A0A172U6X0
D	0	SER	-	expression tag	UNP A0A172U6X0
E	-20	MET	-	initiating methionine	UNP A0A172U6X0
E	-19	GLY	-	expression tag	UNP A0A172U6X0
E	-18	SER	-	expression tag	UNP A0A172U6X0
E	-17	SER	-	expression tag	UNP A0A172U6X0
E	-16	HIS	-	expression tag	UNP A0A172U6X0
E	-15	HIS	-	expression tag	UNP A0A172U6X0
E	-14	HIS	-	expression tag	UNP A0A172U6X0
E	-13	HIS	-	expression tag	UNP A0A172U6X0
E	-12	HIS	-	expression tag	UNP A0A172U6X0
E	-11	HIS	-	expression tag	UNP A0A172U6X0
E	-10	SER	-	expression tag	UNP A0A172U6X0
E	-9	SER	-	expression tag	UNP A0A172U6X0
E	-8	GLY	-	expression tag	UNP A0A172U6X0
E	-7	LEU	-	expression tag	UNP A0A172U6X0
E	-6	VAL	-	expression tag	UNP A0A172U6X0
E	-5	PRO	-	expression tag	UNP A0A172U6X0
E	-4	ARG	-	expression tag	UNP A0A172U6X0

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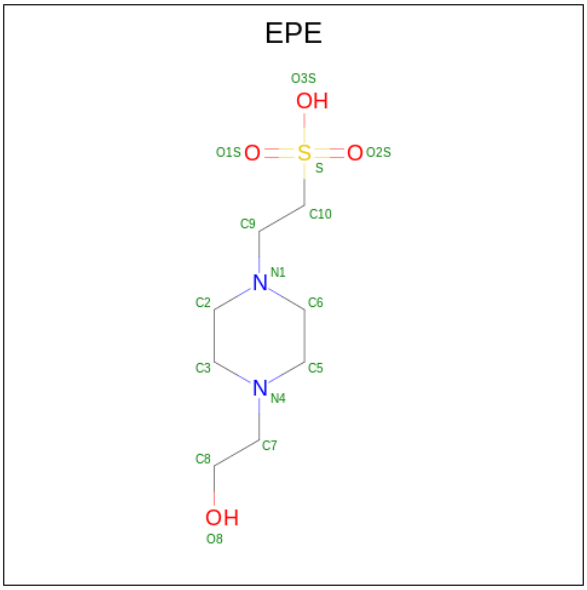
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP A0A172U6X0
E	-2	SER	-	expression tag	UNP A0A172U6X0
E	-1	HIS	-	expression tag	UNP A0A172U6X0
E	0	SER	-	expression tag	UNP A0A172U6X0
F	-20	MET	-	initiating methionine	UNP A0A172U6X0
F	-19	GLY	-	expression tag	UNP A0A172U6X0
F	-18	SER	-	expression tag	UNP A0A172U6X0
F	-17	SER	-	expression tag	UNP A0A172U6X0
F	-16	HIS	-	expression tag	UNP A0A172U6X0
F	-15	HIS	-	expression tag	UNP A0A172U6X0
F	-14	HIS	-	expression tag	UNP A0A172U6X0
F	-13	HIS	-	expression tag	UNP A0A172U6X0
F	-12	HIS	-	expression tag	UNP A0A172U6X0
F	-11	HIS	-	expression tag	UNP A0A172U6X0
F	-10	SER	-	expression tag	UNP A0A172U6X0
F	-9	SER	-	expression tag	UNP A0A172U6X0
F	-8	GLY	-	expression tag	UNP A0A172U6X0
F	-7	LEU	-	expression tag	UNP A0A172U6X0
F	-6	VAL	-	expression tag	UNP A0A172U6X0
F	-5	PRO	-	expression tag	UNP A0A172U6X0
F	-4	ARG	-	expression tag	UNP A0A172U6X0
F	-3	GLY	-	expression tag	UNP A0A172U6X0
F	-2	SER	-	expression tag	UNP A0A172U6X0
F	-1	HIS	-	expression tag	UNP A0A172U6X0
F	0	SER	-	expression tag	UNP A0A172U6X0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

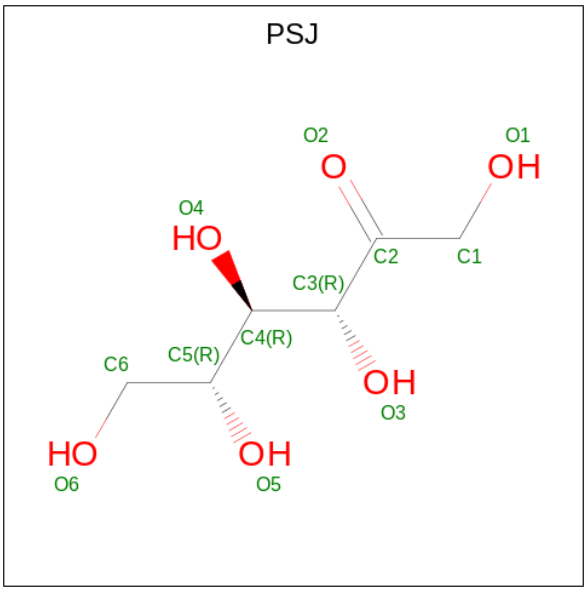
- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is D-psicose (three-letter code: PSJ) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	0
4	B	1	Total C O 12 6 6	0	0
4	C	1	Total C O 12 6 6	0	0
4	D	1	Total C O 12 6 6	0	0
4	E	1	Total C O 12 6 6	0	0
4	F	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

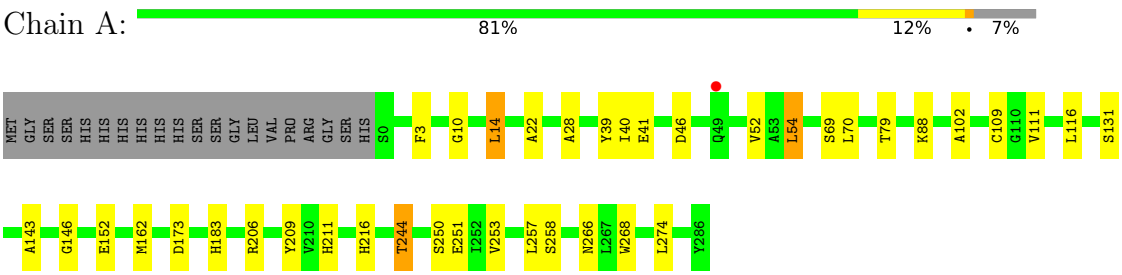
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	163	Total O 163 163	0	0
5	B	153	Total O 153 153	0	0
5	C	141	Total O 141 141	0	0
5	D	173	Total O 173 173	0	0
5	E	133	Total O 133 133	0	0
5	F	176	Total O 176 176	0	0

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.

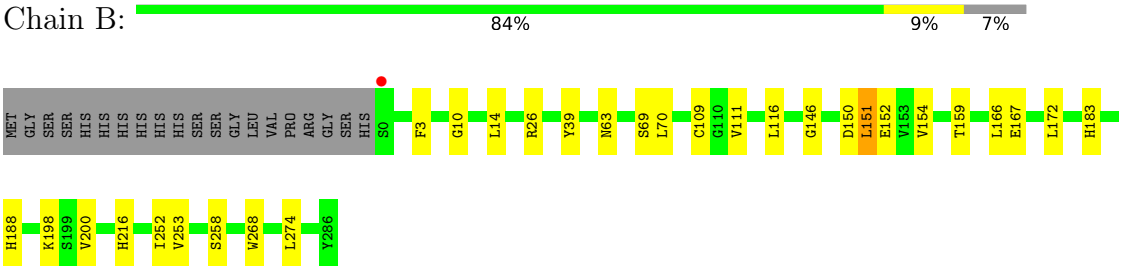
• Molecule 1: Epimerase

Chain A:



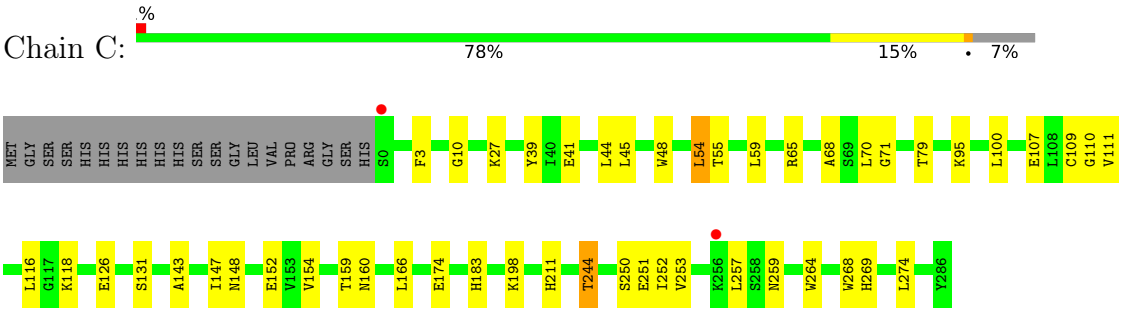
• Molecule 1: Epimerase

Chain B:



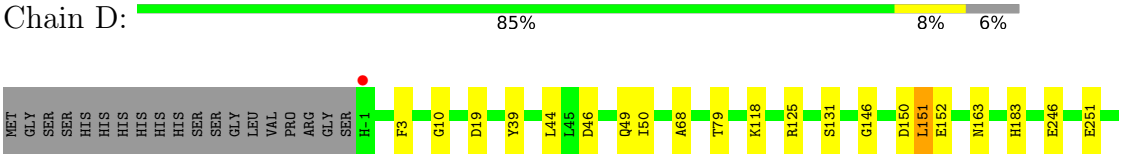
• Molecule 1: Epimerase

Chain C:



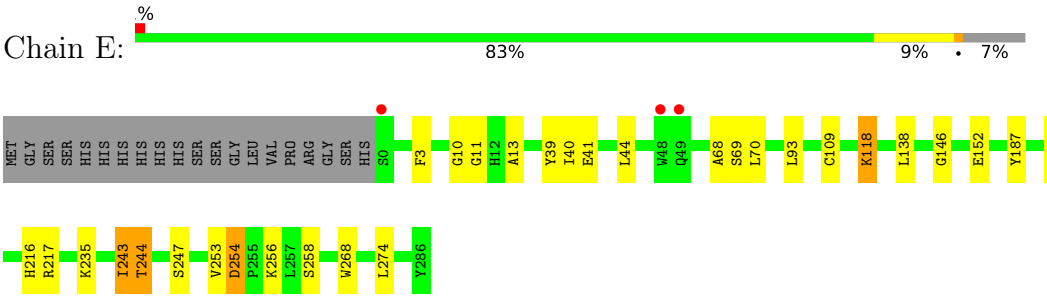
• Molecule 1: Epimerase

Chain D:



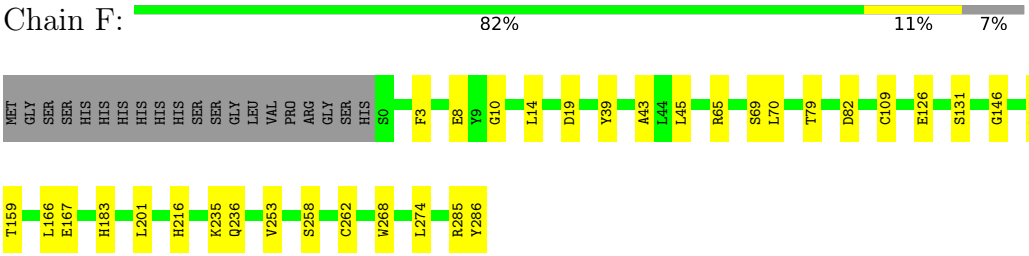
• Molecule 1: Epimerase

Chain E:



• Molecule 1: Epimerase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.02Å 81.05Å 106.13Å 99.30° 101.50° 87.24°	Depositor
Resolution (Å)	48.84 – 2.05 48.84 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.84-2.05) 97.7 (48.84-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.162 , 0.241 0.169 , 0.245	Depositor DCC
R_{free} test set	5031 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14395	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8395e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: EPE, MN, PSJ

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	0.64	0/2260	0.67	0/3066
1	B	0.64	0/2260	0.66	0/3066
1	C	0.64	0/2260	0.66	0/3066
1	D	0.64	0/2271	0.66	0/3081
1	E	0.65	0/2260	0.68	0/3066
1	F	0.65	0/2260	0.67	0/3066
All	All	0.64	0/13571	0.67	0/18411

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2213	0	2158	31	0
1	B	2213	0	2158	27	0
1	C	2213	0	2158	42	0
1	D	2223	0	2165	25	0
1	E	2213	0	2158	30	0
1	F	2213	0	2158	26	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	15	0	18	0	0
3	B	15	0	18	5	0
3	C	15	0	18	3	0
3	D	15	0	18	0	0
3	E	15	0	18	0	0
3	F	15	0	18	3	0
4	A	12	0	11	1	0
4	B	12	0	12	2	0
4	C	12	0	11	1	0
4	D	12	0	11	3	0
4	E	12	0	11	1	0
4	F	12	0	12	2	0
5	A	163	0	0	2	0
5	B	153	0	0	5	0
5	C	141	0	0	3	0
5	D	173	0	0	1	0
5	E	133	0	0	0	0
5	F	176	0	0	1	0
All	All	14395	0	13131	181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (181) 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:41:GLU:OE1	1:A:244:THR:HG21	1.62	0.98
1:D:152:GLU:OE1	4:D:303:PSJ:H3	1.67	0.94
1:C:41:GLU:OE1	1:C:244:THR:HG21	1.66	0.94
1:E:41:GLU:OE1	1:E:244:THR:HG21	1.67	0.94
1:A:152:GLU:OE1	4:A:303:PSJ:H3	1.76	0.85
1:C:166:LEU:HD11	1:C:198:LYS:HE2	1.59	0.85
1:F:152:GLU:OE1	4:F:303:PSJ:H3	1.78	0.83
1:E:212:ILE:HG12	1:E:243:ILE:HD12	1.64	0.80
1:A:79:THR:HG22	1:A:131:SER:HB2	1.71	0.70
1:C:166:LEU:HD11	1:C:198:LYS:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASN:O	1:D:118:LYS:NZ	2.25	0.69
3:C:302:EPE:H21	5:C:525:HOH:O	1.92	0.69
1:B:198:LYS:NZ	1:F:82:ASP:OD2	2.21	0.69
1:B:151:LEU:HD22	1:B:151:LEU:N	2.07	0.68
1:B:167:GLU:CD	3:B:302:EPE:H32	2.14	0.68
1:D:151:LEU:N	1:D:151:LEU:HD22	2.09	0.68
1:A:250:SER:O	1:A:253:VAL:HG23	1.94	0.67
1:B:151:LEU:HD23	1:B:172:LEU:HD21	1.77	0.66
1:D:79:THR:HG22	1:D:131:SER:HB2	1.77	0.66
1:C:268:TRP:CD2	1:C:274:LEU:HD22	2.32	0.65
1:B:268:TRP:CD2	1:B:274:LEU:HD22	2.32	0.64
1:A:14:LEU:HD12	1:A:257:LEU:HD23	1.78	0.64
1:B:167:GLU:OE2	3:B:302:EPE:H32	1.98	0.63
1:E:212:ILE:CG1	1:E:243:ILE:HD12	2.28	0.63
1:F:79:THR:HG22	1:F:131:SER:HB2	1.81	0.63
1:E:243:ILE:O	1:E:243:ILE:HG13	1.98	0.63
1:E:70:LEU:HD12	1:E:70:LEU:C	2.19	0.62
1:E:39:TYR:OH	1:E:244:THR:HG22	2.00	0.61
1:B:152:GLU:OE1	4:B:303:PSJ:H3	2.00	0.60
1:F:253:VAL:HG23	1:F:258:SER:HB3	1.84	0.59
1:F:253:VAL:CG2	1:F:258:SER:HB3	2.32	0.59
4:F:303:PSJ:O3	4:F:303:PSJ:O5	2.19	0.58
1:F:151:LEU:N	1:F:151:LEU:HD23	2.17	0.58
1:F:235:LYS:NZ	1:F:285:ARG:O	2.31	0.58
1:C:152:GLU:OE1	4:C:303:PSJ:H3	2.04	0.58
1:D:44:LEU:HD12	1:D:68:ALA:HB1	1.86	0.57
1:B:198:LYS:HG3	1:F:82:ASP:HB2	1.86	0.57
1:F:268:TRP:CD2	1:F:274:LEU:HD22	2.40	0.57
1:A:251:GLU:OE1	1:A:266:ASN:ND2	2.36	0.56
1:E:212:ILE:CG1	1:E:243:ILE:CD1	2.82	0.56
1:C:39:TYR:OH	1:C:244:THR:HG22	2.06	0.56
1:E:10:GLY:O	1:E:244:THR:HA	2.06	0.55
1:C:252:ILE:HD12	1:C:268:TRP:CZ3	2.42	0.55
1:E:268:TRP:CD2	1:E:274:LEU:HD22	2.42	0.55
1:A:211:HIS:CD2	1:A:244:THR:HG23	2.42	0.55
1:B:188:HIS:HB3	5:B:504:HOH:O	2.05	0.55
1:D:151:LEU:N	1:D:151:LEU:CD2	2.71	0.54
1:A:10:GLY:HA3	1:A:39:TYR:CE1	2.42	0.54
1:F:152:GLU:HA	1:F:183:HIS:HB3	1.90	0.54
1:C:211:HIS:CD2	1:C:244:THR:HG23	2.43	0.53
1:A:52:VAL:HG11	1:A:102:ALA:HB1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:ALA:HA	1:E:40:ILE:HD11	1.90	0.53
1:D:152:GLU:HA	1:D:183:HIS:HB3	1.90	0.52
1:B:10:GLY:HA3	1:B:39:TYR:CZ	2.44	0.52
1:E:152:GLU:OE1	4:E:303:PSJ:H3	2.09	0.52
1:D:125:ARG:NE	5:D:404:HOH:O	2.38	0.52
1:D:251:GLU:HG2	1:D:269:HIS:HA	1.91	0.52
1:A:173:ASP:OD1	1:A:206:ARG:NH2	2.43	0.52
1:E:212:ILE:HG13	1:E:243:ILE:CD1	2.40	0.52
1:F:167:GLU:CD	3:F:302:EPE:H32	2.30	0.52
1:C:268:TRP:CE2	1:C:274:LEU:HD22	2.45	0.52
1:F:167:GLU:OE2	3:F:302:EPE:H32	2.09	0.52
1:B:151:LEU:N	1:B:151:LEU:CD2	2.73	0.51
1:C:3:PHE:HE2	1:C:143:ALA:HA	1.74	0.51
1:C:48:TRP:CD1	1:C:95:LYS:HE2	2.45	0.51
1:D:44:LEU:CD2	1:D:50:ILE:HG13	2.41	0.51
1:F:70:LEU:C	1:F:70:LEU:HD12	2.32	0.51
4:B:303:PSJ:O5	4:B:303:PSJ:O3	2.28	0.51
1:D:10:GLY:HA3	1:D:39:TYR:CZ	2.46	0.50
1:A:152:GLU:HA	1:A:183:HIS:HB3	1.92	0.50
1:C:250:SER:O	1:C:253:VAL:HG23	2.10	0.50
3:B:302:EPE:H92	5:B:539:HOH:O	2.11	0.50
1:D:268:TRP:CD2	1:D:274:LEU:HD22	2.47	0.50
1:B:252:ILE:HD12	1:B:268:TRP:CH2	2.47	0.50
1:C:71:GLY:HA2	1:C:111:VAL:O	2.12	0.50
1:D:268:TRP:CE2	1:D:274:LEU:HD22	2.47	0.49
1:A:69:SER:HA	1:A:109:CYS:O	2.11	0.49
1:E:11:GLY:O	1:E:40:ILE:HD12	2.12	0.49
1:A:28:ALA:HB1	1:A:40:ILE:HD11	1.95	0.49
1:A:14:LEU:CD1	1:A:257:LEU:HD23	2.42	0.48
1:B:69:SER:HA	1:B:109:CYS:O	2.13	0.48
1:C:118:LYS:HD2	1:D:262:CYS:SG	2.54	0.48
1:A:88:LYS:HE2	5:A:500:HOH:O	2.12	0.48
1:F:268:TRP:CE2	1:F:274:LEU:HD22	2.48	0.48
1:D:10:GLY:HA3	1:D:39:TYR:CE1	2.49	0.47
1:E:254:ASP:OD2	1:E:254:ASP:C	2.53	0.47
1:E:10:GLY:HA3	1:E:39:TYR:CZ	2.50	0.47
1:B:111:VAL:HG21	1:B:116:LEU:HD13	1.97	0.47
1:C:54:LEU:O	1:C:54:LEU:HD22	2.15	0.47
1:F:43:ALA:HB1	1:F:45:LEU:HD13	1.97	0.47
1:C:10:GLY:HA3	1:C:39:TYR:CE1	2.49	0.47
1:E:217:ARG:O	1:E:247:SER:OG	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:HA3	1:A:39:TYR:CZ	2.50	0.47
1:B:10:GLY:HA3	1:B:39:TYR:CE1	2.50	0.47
1:B:253:VAL:CG2	1:B:258:SER:HB3	2.45	0.47
1:A:268:TRP:CD2	1:A:274:LEU:HD22	2.51	0.46
1:B:200:VAL:HG23	5:B:443:HOH:O	2.14	0.46
1:F:3:PHE:CE1	1:F:146:GLY:HA2	2.50	0.46
1:B:151:LEU:HD22	1:B:151:LEU:H	1.76	0.46
1:A:253:VAL:HG13	1:A:258:SER:CB	2.46	0.46
1:A:22:ALA:HA	1:A:54:LEU:HD11	1.98	0.46
1:B:63:ASN:HA	5:B:479:HOH:O	2.15	0.46
1:C:10:GLY:O	1:C:244:THR:HA	2.16	0.46
1:A:46:ASP:HA	5:A:446:HOH:O	2.15	0.46
1:C:27:LYS:HE2	5:C:533:HOH:O	2.16	0.46
1:C:44:LEU:HD12	1:C:68:ALA:HB1	1.96	0.46
1:E:3:PHE:CE1	1:E:146:GLY:HA2	2.50	0.46
3:F:302:EPE:H21	5:F:557:HOH:O	2.16	0.46
3:B:302:EPE:H82	3:B:302:EPE:H31	1.57	0.45
3:C:302:EPE:H32	3:C:302:EPE:H82	1.76	0.45
1:C:10:GLY:HA3	1:C:39:TYR:CZ	2.51	0.45
1:E:187:TYR:CD1	1:E:217:ARG:HG2	2.51	0.45
1:E:211:HIS:CD2	1:E:244:THR:HG23	2.51	0.45
1:C:251:GLU:HG2	1:C:269:HIS:HA	1.98	0.45
1:E:44:LEU:HD12	1:E:68:ALA:HB1	1.98	0.45
1:B:268:TRP:CE2	1:B:274:LEU:HD22	2.52	0.45
1:C:126:GLU:HB2	5:C:510:HOH:O	2.16	0.45
1:C:55:THR:O	1:C:59:LEU:HG	2.16	0.45
1:B:151:LEU:CD2	1:B:151:LEU:H	2.29	0.45
1:C:79:THR:HG22	1:C:131:SER:HB2	1.98	0.45
1:B:70:LEU:HD12	1:B:70:LEU:C	2.38	0.45
1:C:268:TRP:CG	1:C:274:LEU:HD22	2.50	0.45
1:A:70:LEU:C	1:A:70:LEU:HD12	2.37	0.44
1:F:201:LEU:CD2	1:F:236:GLN:HG2	2.46	0.44
1:F:235:LYS:HG2	1:F:286:TYR:CE1	2.53	0.44
1:D:19:ASP:OD2	1:D:19:ASP:C	2.56	0.44
1:D:151:LEU:CD2	1:D:151:LEU:H	2.31	0.44
1:E:211:HIS:HD2	1:E:244:THR:HG23	1.83	0.44
1:B:154:VAL:HG23	1:B:159:THR:HG22	1.99	0.43
1:C:110:GLY:HA2	1:C:152:GLU:OE1	2.18	0.43
1:C:211:HIS:HD2	1:C:244:THR:HG23	1.83	0.43
1:E:69:SER:HA	1:E:109:CYS:O	2.19	0.43
1:E:118:LYS:HE2	1:F:262:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:GLY:HA2	1:F:39:TYR:O	2.18	0.43
1:C:252:ILE:HD12	1:C:268:TRP:HZ3	1.84	0.43
1:E:209:TYR:HE1	1:E:244:THR:CG2	2.31	0.43
1:C:118:LYS:CD	1:D:262:CYS:SG	3.07	0.43
1:C:154:VAL:HG23	1:C:159:THR:HG22	2.00	0.43
1:D:46:ASP:CG	1:D:49:GLN:HG2	2.39	0.43
1:A:162:MET:O	1:A:162:MET:HG3	2.19	0.43
1:A:253:VAL:HG13	1:A:258:SER:HB2	2.00	0.42
1:C:160:ASN:HA	1:D:264:TRP:CD1	2.53	0.42
1:C:264:TRP:HD1	1:D:163:ASN:HD21	1.65	0.42
1:C:111:VAL:HG21	1:C:116:LEU:HD13	2.00	0.42
1:D:246:GLU:OE2	4:D:303:PSJ:O3	2.37	0.42
1:A:39:TYR:OH	1:A:244:THR:HG22	2.20	0.42
1:F:8:GLU:CD	1:F:65:ARG:HH11	2.23	0.42
1:D:44:LEU:HD12	1:D:68:ALA:CB	2.49	0.42
1:A:3:PHE:CE1	1:A:146:GLY:HA2	2.55	0.42
1:A:88:LYS:HD3	1:A:88:LYS:HA	1.86	0.42
1:C:39:TYR:HA	1:C:65:ARG:O	2.20	0.42
1:C:45:LEU:HD21	1:C:257:LEU:HD13	2.01	0.42
1:E:253:VAL:CG2	1:E:258:SER:HB3	2.50	0.42
1:B:109:CYS:HB2	1:B:183:HIS:HD1	1.85	0.42
1:F:235:LYS:HG2	1:F:286:TYR:HE1	1.85	0.42
1:C:100:LEU:HD23	1:C:147:ILE:HD13	2.02	0.42
1:C:107:GLU:OE1	1:C:148:ASN:HB2	2.20	0.42
1:E:3:PHE:CD1	1:E:146:GLY:HA2	2.55	0.42
1:A:268:TRP:CE2	1:A:274:LEU:HD22	2.54	0.41
1:A:3:PHE:HE2	1:A:143:ALA:HA	1.85	0.41
1:B:3:PHE:CE1	1:B:146:GLY:HA2	2.55	0.41
1:B:109:CYS:HB2	1:B:183:HIS:ND1	2.35	0.41
1:F:154:VAL:HG23	1:F:159:THR:HG22	2.02	0.41
3:B:302:EPE:H21	5:B:539:HOH:O	2.20	0.41
1:D:3:PHE:CD1	1:D:146:GLY:HA2	2.55	0.41
1:E:93:LEU:HD13	1:E:138:LEU:HD22	2.03	0.41
1:A:10:GLY:O	1:A:244:THR:HA	2.20	0.41
1:C:109:CYS:HB2	1:C:183:HIS:ND1	2.36	0.41
1:E:10:GLY:HA3	1:E:39:TYR:CE1	2.56	0.41
1:F:19:ASP:OD1	1:F:19:ASP:C	2.59	0.41
1:B:26:ARG:HD3	1:C:174:GLU:O	2.21	0.41
3:C:302:EPE:H21	3:C:302:EPE:H101	1.74	0.41
1:C:268:TRP:CE2	1:C:274:LEU:CD2	3.05	0.40
1:D:246:GLU:OE2	4:D:303:PSJ:O5	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:HE1	1:A:244:THR:CG2	2.34	0.40
1:E:268:TRP:CE2	1:E:274:LEU:HD22	2.56	0.40
1:A:111:VAL:HG21	1:A:116:LEU:HD13	2.03	0.40
1:E:254:ASP:OD2	1:E:256:LYS:N	2.46	0.40
1:C:70:LEU:HD12	1:C:70:LEU:C	2.42	0.40
1:F:10:GLY:HA3	1:F:39:TYR:CE1	2.57	0.40
1:F:69:SER:HA	1:F:109:CYS:O	2.22	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	285/307 (93%)	278 (98%)	7 (2%)	0	100	100
1	B	285/307 (93%)	281 (99%)	4 (1%)	0	100	100
1	C	285/307 (93%)	278 (98%)	7 (2%)	0	100	100
1	D	286/307 (93%)	279 (98%)	7 (2%)	0	100	100
1	E	285/307 (93%)	278 (98%)	7 (2%)	0	100	100
1	F	285/307 (93%)	281 (99%)	4 (1%)	0	100	100
All	All	1711/1842 (93%)	1675 (98%)	36 (2%)	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	224/241 (93%)	220 (98%)	4 (2%)	59	55
1	B	224/241 (93%)	219 (98%)	5 (2%)	52	46
1	C	224/241 (93%)	222 (99%)	2 (1%)	78	79
1	D	225/241 (93%)	223 (99%)	2 (1%)	78	79
1	E	224/241 (93%)	218 (97%)	6 (3%)	44	38
1	F	224/241 (93%)	220 (98%)	4 (2%)	59	55
All	All	1345/1446 (93%)	1322 (98%)	23 (2%)	60	57

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	54	LEU
1	A	216	HIS
1	A	244	THR
1	B	14	LEU
1	B	150	ASP
1	B	151	LEU
1	B	166	LEU
1	B	216	HIS
1	C	54	LEU
1	C	244	THR
1	D	150	ASP
1	D	151	LEU
1	E	118	LYS
1	E	216	HIS
1	E	235	LYS
1	E	243	ILE
1	E	244	THR
1	E	254	ASP
1	F	14	LEU
1	F	126	GLU
1	F	166	LEU
1	F	216	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	60	GLN
1	D	163	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PSJ	A	303	2	10,11,11	0.47	0	9,14,14	1.08	0
3	EPE	F	302	-	15,15,15	1.74	1 (6%)	18,20,20	1.43	2 (11%)
4	PSJ	E	303	2	10,11,11	0.44	0	9,14,14	0.83	0
4	PSJ	F	303	2	10,11,11	0.56	0	9,14,14	0.99	0
4	PSJ	C	303	2	10,11,11	0.42	0	9,14,14	1.21	1 (11%)
3	EPE	B	302	-	15,15,15	1.86	1 (6%)	18,20,20	1.30	2 (11%)
3	EPE	E	302	-	15,15,15	1.88	1 (6%)	18,20,20	1.27	2 (11%)
4	PSJ	B	303	2	10,11,11	0.51	0	9,14,14	0.64	0
3	EPE	D	302	-	15,15,15	2.08	1 (6%)	18,20,20	1.21	2 (11%)
4	PSJ	D	303	2	10,11,11	0.55	0	9,14,14	1.04	0
3	EPE	A	302	-	15,15,15	1.81	1 (6%)	18,20,20	1.67	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EPE	C	302	-	15,15,15	1.97	1 (6%)	18,20,20	1.10	3 (16%)

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
4	PSJ	A	303	2	-	10/16/16/16	-
3	EPE	F	302	-	-	7/9/19/19	0/1/1/1
4	PSJ	E	303	2	-	6/16/16/16	-
4	PSJ	F	303	2	-	14/16/16/16	-
4	PSJ	C	303	2	-	9/16/16/16	-
3	EPE	B	302	-	-	3/9/19/19	0/1/1/1
3	EPE	E	302	-	-	2/9/19/19	0/1/1/1
4	PSJ	B	303	2	-	6/16/16/16	-
3	EPE	D	302	-	-	4/9/19/19	0/1/1/1
4	PSJ	D	303	2	-	8/16/16/16	-
3	EPE	A	302	-	-	5/9/19/19	0/1/1/1
3	EPE	C	302	-	-	4/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	EPE	C10-S	-7.81	1.66	1.77
3	C	302	EPE	C10-S	-7.32	1.67	1.77
3	E	302	EPE	C10-S	-7.01	1.67	1.77
3	B	302	EPE	C10-S	-6.92	1.67	1.77
3	A	302	EPE	C10-S	-6.62	1.68	1.77
3	F	302	EPE	C10-S	-6.32	1.68	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	EPE	O3S-S-C10	4.18	112.52	105.77
3	F	302	EPE	O2S-S-C10	3.82	111.51	106.92
3	E	302	EPE	O1S-S-C10	3.33	110.93	106.92
3	B	302	EPE	O3S-S-C10	3.00	110.62	105.77
3	A	302	EPE	C9-N1-C6	2.78	118.33	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	302	EPE	O2S-S-C10	2.67	110.13	106.92
4	C	303	PSJ	O6-C6-C5	-2.63	105.34	111.07
3	C	302	EPE	O1S-S-C10	2.45	109.86	106.92
3	C	302	EPE	O2S-S-C10	2.40	109.80	106.92
3	E	302	EPE	O3S-S-C10	2.36	109.59	105.77
3	D	302	EPE	O1S-S-C10	2.32	109.71	106.92
3	D	302	EPE	O2S-S-C10	2.26	109.64	106.92
3	A	302	EPE	C3-C2-N1	-2.26	106.01	110.64
3	F	302	EPE	O3S-S-C10	2.24	109.39	105.77
3	C	302	EPE	O3S-S-C10	2.07	109.11	105.77

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	EPE	C10-C9-N1-C6
3	A	302	EPE	C9-C10-S-O1S
3	A	302	EPE	C9-C10-S-O2S
3	A	302	EPE	C9-C10-S-O3S
3	B	302	EPE	C8-C7-N4-C3
3	B	302	EPE	N4-C7-C8-O8
3	C	302	EPE	C10-C9-N1-C2
3	C	302	EPE	C8-C7-N4-C3
3	D	302	EPE	C10-C9-N1-C2
3	D	302	EPE	C10-C9-N1-C6
3	F	302	EPE	C10-C9-N1-C6
3	F	302	EPE	C8-C7-N4-C3
4	A	303	PSJ	C1-C2-C3-C4
4	A	303	PSJ	O2-C2-C3-C4
4	A	303	PSJ	C2-C3-C4-O4
4	A	303	PSJ	C2-C3-C4-C5
4	A	303	PSJ	O3-C3-C4-O4
4	A	303	PSJ	O3-C3-C4-C5
4	A	303	PSJ	O5-C5-C6-O6
4	B	303	PSJ	C1-C2-C3-C4
4	B	303	PSJ	O2-C2-C3-C4
4	C	303	PSJ	C1-C2-C3-O3
4	C	303	PSJ	C1-C2-C3-C4
4	C	303	PSJ	O2-C2-C3-C4
4	C	303	PSJ	O3-C3-C4-C5
4	C	303	PSJ	C4-C5-C6-O6
4	C	303	PSJ	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	303	PSJ	C1-C2-C3-C4
4	D	303	PSJ	O2-C2-C3-C4
4	D	303	PSJ	C2-C3-C4-O4
4	D	303	PSJ	C2-C3-C4-C5
4	D	303	PSJ	O3-C3-C4-O4
4	D	303	PSJ	O3-C3-C4-C5
4	E	303	PSJ	C1-C2-C3-C4
4	E	303	PSJ	O2-C2-C3-C4
4	F	303	PSJ	C1-C2-C3-O3
4	F	303	PSJ	C1-C2-C3-C4
4	F	303	PSJ	O2-C2-C3-O3
4	F	303	PSJ	O2-C2-C3-C4
4	F	303	PSJ	O3-C3-C4-O4
4	F	303	PSJ	O3-C3-C4-C5
3	C	302	EPE	N4-C7-C8-O8
3	F	302	EPE	N4-C7-C8-O8
4	E	303	PSJ	O5-C5-C6-O6
4	A	303	PSJ	C4-C5-C6-O6
4	E	303	PSJ	C4-C5-C6-O6
4	F	303	PSJ	O4-C4-C5-C6
4	C	303	PSJ	O3-C3-C4-O4
3	F	302	EPE	C9-C10-S-O3S
4	F	303	PSJ	C4-C5-C6-O6
4	F	303	PSJ	O5-C5-C6-O6
4	F	303	PSJ	C3-C4-C5-O5
3	F	302	EPE	C8-C7-N4-C5
4	F	303	PSJ	C2-C3-C4-O4
4	F	303	PSJ	C2-C3-C4-C5
4	F	303	PSJ	O4-C4-C5-O5
3	C	302	EPE	C8-C7-N4-C5
4	F	303	PSJ	C3-C4-C5-C6
4	B	303	PSJ	O5-C5-C6-O6
3	D	302	EPE	C9-C10-S-O1S
3	F	302	EPE	C9-C10-S-O1S
3	F	302	EPE	C9-C10-S-O2S
4	A	303	PSJ	O2-C2-C3-O3
4	B	303	PSJ	O2-C2-C3-O3
4	C	303	PSJ	O2-C2-C3-O3
4	D	303	PSJ	O2-C2-C3-O3
4	E	303	PSJ	O2-C2-C3-O3
4	A	303	PSJ	C1-C2-C3-O3
4	B	303	PSJ	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	303	PSJ	C1-C2-C3-O3
4	E	303	PSJ	C1-C2-C3-O3
3	B	302	EPE	C8-C7-N4-C5
3	D	302	EPE	C9-C10-S-O3S
3	A	302	EPE	C10-C9-N1-C2
3	E	302	EPE	C10-C9-N1-C2
3	E	302	EPE	C10-C9-N1-C6
4	C	303	PSJ	C2-C3-C4-O4
4	B	303	PSJ	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	303	PSJ	1	0
3	F	302	EPE	3	0
4	E	303	PSJ	1	0
4	F	303	PSJ	2	0
4	C	303	PSJ	1	0
3	B	302	EPE	5	0
4	B	303	PSJ	2	0
4	D	303	PSJ	3	0
3	C	302	EPE	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	287/307 (93%)	-0.35	1 (0%)	94	94	17, 27, 41, 58	0
1	B	287/307 (93%)	-0.42	1 (0%)	94	94	20, 28, 40, 64	0
1	C	287/307 (93%)	-0.40	2 (0%)	87	89	17, 28, 42, 66	0
1	D	288/307 (93%)	-0.41	1 (0%)	94	94	16, 25, 39, 48	0
1	E	287/307 (93%)	-0.21	3 (1%)	82	84	19, 30, 46, 72	0
1	F	287/307 (93%)	-0.37	0	100	100	17, 25, 38, 52	0
All	All	1723/1842 (93%)	-0.36	8 (0%)	91	92	16, 27, 42, 72	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	0	SER	4.8
1	E	0	SER	3.7
1	C	256	LYS	3.5
1	E	49	GLN	3.3
1	E	48	TRP	2.7
1	B	0	SER	2.5
1	A	49	GLN	2.4
1	D	-1	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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
4	PSJ	C	303	12/12	0.88	0.16	23,35,39,41	0
3	EPE	C	302	15/15	0.89	0.21	33,50,81,81	0
4	PSJ	E	303	12/12	0.89	0.16	23,41,44,51	0
4	PSJ	B	303	12/12	0.92	0.16	22,40,52,59	0
4	PSJ	A	303	12/12	0.93	0.12	26,36,41,44	0
3	EPE	F	302	15/15	0.93	0.11	25,32,53,54	0
3	EPE	E	302	15/15	0.94	0.11	28,38,59,60	0
3	EPE	B	302	15/15	0.94	0.13	24,31,53,56	0
4	PSJ	D	303	12/12	0.94	0.13	24,33,43,46	0
3	EPE	D	302	15/15	0.94	0.12	24,34,57,60	0
4	PSJ	F	303	12/12	0.94	0.11	27,36,42,45	0
3	EPE	A	302	15/15	0.95	0.12	24,26,41,48	0
2	MN	A	301	1/1	0.99	0.02	33,33,33,33	0
2	MN	D	301	1/1	0.99	0.03	36,36,36,36	0
2	MN	C	301	1/1	1.00	0.02	38,38,38,38	0
2	MN	B	301	1/1	1.00	0.03	34,34,34,34	0
2	MN	E	301	1/1	1.00	0.02	34,34,34,34	0
2	MN	F	301	1/1	1.00	0.04	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.