Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 09:36 AM EDT

PDB ID	:	3EK1
Title	:	Crystal structure of aldehyde dehydrogenase from brucella melitensis biovar abortus 2308
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2008-09-18
Resolution	:	2.10 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:

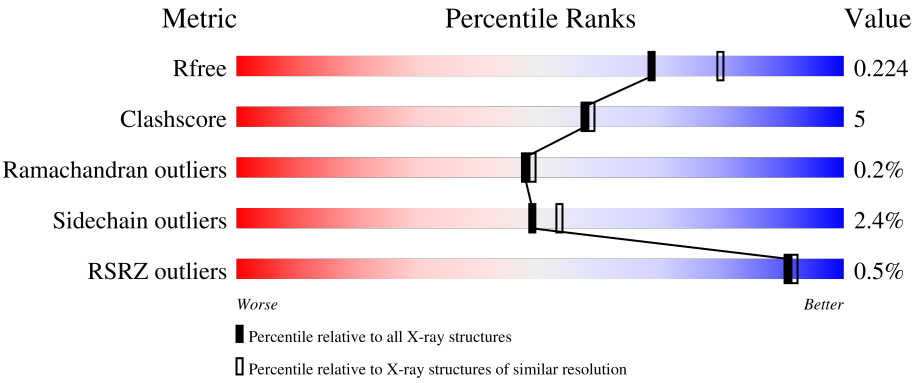
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	504	87% 9% .
1	B	504	87% 8% . .
1	C	504	86% 9% . .
1	D	504	81% 13% . .
1	E	504	% 83% 12% . .

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Mol	Chain	Length	Quality of chain
1	F	504	86% 10%
1	G	504	% 84% 11%
1	H	504	2% 81% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32199 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 Aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	3	0
			3635	2312	615	692	16			
1	B	483	Total	C	N	O	S	0	3	0
			3611	2299	611	686	15			
1	C	483	Total	C	N	O	S	0	3	0
			3614	2300	610	688	16			
1	D	483	Total	C	N	O	S	0	2	0
			3608	2296	610	686	16			
1	E	483	Total	C	N	O	S	0	3	0
			3604	2295	607	686	16			
1	F	483	Total	C	N	O	S	0	3	0
			3617	2301	611	689	16			
1	G	482	Total	C	N	O	S	0	3	0
			3605	2294	610	686	15			
1	H	483	Total	C	N	O	S	0	4	0
			3627	2308	612	691	16			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q2YRI3
A	-19	ALA	-	expression tag	UNP Q2YRI3
A	-18	HIS	-	expression tag	UNP Q2YRI3
A	-17	HIS	-	expression tag	UNP Q2YRI3
A	-16	HIS	-	expression tag	UNP Q2YRI3
A	-15	HIS	-	expression tag	UNP Q2YRI3
A	-14	HIS	-	expression tag	UNP Q2YRI3
A	-13	HIS	-	expression tag	UNP Q2YRI3
A	-12	MET	-	expression tag	UNP Q2YRI3
A	-11	GLY	-	expression tag	UNP Q2YRI3
A	-10	THR	-	expression tag	UNP Q2YRI3
A	-9	LEU	-	expression tag	UNP Q2YRI3
A	-8	GLU	-	expression tag	UNP Q2YRI3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	expression tag	UNP Q2YRI3
A	-6	GLN	-	expression tag	UNP Q2YRI3
A	-5	THR	-	expression tag	UNP Q2YRI3
A	-4	GLN	-	expression tag	UNP Q2YRI3
A	-3	GLY	-	expression tag	UNP Q2YRI3
A	-2	PRO	-	expression tag	UNP Q2YRI3
A	-1	GLY	-	expression tag	UNP Q2YRI3
A	0	SER	-	expression tag	UNP Q2YRI3
B	-20	MET	-	expression tag	UNP Q2YRI3
B	-19	ALA	-	expression tag	UNP Q2YRI3
B	-18	HIS	-	expression tag	UNP Q2YRI3
B	-17	HIS	-	expression tag	UNP Q2YRI3
B	-16	HIS	-	expression tag	UNP Q2YRI3
B	-15	HIS	-	expression tag	UNP Q2YRI3
B	-14	HIS	-	expression tag	UNP Q2YRI3
B	-13	HIS	-	expression tag	UNP Q2YRI3
B	-12	MET	-	expression tag	UNP Q2YRI3
B	-11	GLY	-	expression tag	UNP Q2YRI3
B	-10	THR	-	expression tag	UNP Q2YRI3
B	-9	LEU	-	expression tag	UNP Q2YRI3
B	-8	GLU	-	expression tag	UNP Q2YRI3
B	-7	ALA	-	expression tag	UNP Q2YRI3
B	-6	GLN	-	expression tag	UNP Q2YRI3
B	-5	THR	-	expression tag	UNP Q2YRI3
B	-4	GLN	-	expression tag	UNP Q2YRI3
B	-3	GLY	-	expression tag	UNP Q2YRI3
B	-2	PRO	-	expression tag	UNP Q2YRI3
B	-1	GLY	-	expression tag	UNP Q2YRI3
B	0	SER	-	expression tag	UNP Q2YRI3
C	-20	MET	-	expression tag	UNP Q2YRI3
C	-19	ALA	-	expression tag	UNP Q2YRI3
C	-18	HIS	-	expression tag	UNP Q2YRI3
C	-17	HIS	-	expression tag	UNP Q2YRI3
C	-16	HIS	-	expression tag	UNP Q2YRI3
C	-15	HIS	-	expression tag	UNP Q2YRI3
C	-14	HIS	-	expression tag	UNP Q2YRI3
C	-13	HIS	-	expression tag	UNP Q2YRI3
C	-12	MET	-	expression tag	UNP Q2YRI3
C	-11	GLY	-	expression tag	UNP Q2YRI3
C	-10	THR	-	expression tag	UNP Q2YRI3
C	-9	LEU	-	expression tag	UNP Q2YRI3
C	-8	GLU	-	expression tag	UNP Q2YRI3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	expression tag	UNP Q2YRI3
C	-6	GLN	-	expression tag	UNP Q2YRI3
C	-5	THR	-	expression tag	UNP Q2YRI3
C	-4	GLN	-	expression tag	UNP Q2YRI3
C	-3	GLY	-	expression tag	UNP Q2YRI3
C	-2	PRO	-	expression tag	UNP Q2YRI3
C	-1	GLY	-	expression tag	UNP Q2YRI3
C	0	SER	-	expression tag	UNP Q2YRI3
D	-20	MET	-	expression tag	UNP Q2YRI3
D	-19	ALA	-	expression tag	UNP Q2YRI3
D	-18	HIS	-	expression tag	UNP Q2YRI3
D	-17	HIS	-	expression tag	UNP Q2YRI3
D	-16	HIS	-	expression tag	UNP Q2YRI3
D	-15	HIS	-	expression tag	UNP Q2YRI3
D	-14	HIS	-	expression tag	UNP Q2YRI3
D	-13	HIS	-	expression tag	UNP Q2YRI3
D	-12	MET	-	expression tag	UNP Q2YRI3
D	-11	GLY	-	expression tag	UNP Q2YRI3
D	-10	THR	-	expression tag	UNP Q2YRI3
D	-9	LEU	-	expression tag	UNP Q2YRI3
D	-8	GLU	-	expression tag	UNP Q2YRI3
D	-7	ALA	-	expression tag	UNP Q2YRI3
D	-6	GLN	-	expression tag	UNP Q2YRI3
D	-5	THR	-	expression tag	UNP Q2YRI3
D	-4	GLN	-	expression tag	UNP Q2YRI3
D	-3	GLY	-	expression tag	UNP Q2YRI3
D	-2	PRO	-	expression tag	UNP Q2YRI3
D	-1	GLY	-	expression tag	UNP Q2YRI3
D	0	SER	-	expression tag	UNP Q2YRI3
E	-20	MET	-	expression tag	UNP Q2YRI3
E	-19	ALA	-	expression tag	UNP Q2YRI3
E	-18	HIS	-	expression tag	UNP Q2YRI3
E	-17	HIS	-	expression tag	UNP Q2YRI3
E	-16	HIS	-	expression tag	UNP Q2YRI3
E	-15	HIS	-	expression tag	UNP Q2YRI3
E	-14	HIS	-	expression tag	UNP Q2YRI3
E	-13	HIS	-	expression tag	UNP Q2YRI3
E	-12	MET	-	expression tag	UNP Q2YRI3
E	-11	GLY	-	expression tag	UNP Q2YRI3
E	-10	THR	-	expression tag	UNP Q2YRI3
E	-9	LEU	-	expression tag	UNP Q2YRI3
E	-8	GLU	-	expression tag	UNP Q2YRI3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ALA	-	expression tag	UNP Q2YRI3
E	-6	GLN	-	expression tag	UNP Q2YRI3
E	-5	THR	-	expression tag	UNP Q2YRI3
E	-4	GLN	-	expression tag	UNP Q2YRI3
E	-3	GLY	-	expression tag	UNP Q2YRI3
E	-2	PRO	-	expression tag	UNP Q2YRI3
E	-1	GLY	-	expression tag	UNP Q2YRI3
E	0	SER	-	expression tag	UNP Q2YRI3
F	-20	MET	-	expression tag	UNP Q2YRI3
F	-19	ALA	-	expression tag	UNP Q2YRI3
F	-18	HIS	-	expression tag	UNP Q2YRI3
F	-17	HIS	-	expression tag	UNP Q2YRI3
F	-16	HIS	-	expression tag	UNP Q2YRI3
F	-15	HIS	-	expression tag	UNP Q2YRI3
F	-14	HIS	-	expression tag	UNP Q2YRI3
F	-13	HIS	-	expression tag	UNP Q2YRI3
F	-12	MET	-	expression tag	UNP Q2YRI3
F	-11	GLY	-	expression tag	UNP Q2YRI3
F	-10	THR	-	expression tag	UNP Q2YRI3
F	-9	LEU	-	expression tag	UNP Q2YRI3
F	-8	GLU	-	expression tag	UNP Q2YRI3
F	-7	ALA	-	expression tag	UNP Q2YRI3
F	-6	GLN	-	expression tag	UNP Q2YRI3
F	-5	THR	-	expression tag	UNP Q2YRI3
F	-4	GLN	-	expression tag	UNP Q2YRI3
F	-3	GLY	-	expression tag	UNP Q2YRI3
F	-2	PRO	-	expression tag	UNP Q2YRI3
F	-1	GLY	-	expression tag	UNP Q2YRI3
F	0	SER	-	expression tag	UNP Q2YRI3
G	-20	MET	-	expression tag	UNP Q2YRI3
G	-19	ALA	-	expression tag	UNP Q2YRI3
G	-18	HIS	-	expression tag	UNP Q2YRI3
G	-17	HIS	-	expression tag	UNP Q2YRI3
G	-16	HIS	-	expression tag	UNP Q2YRI3
G	-15	HIS	-	expression tag	UNP Q2YRI3
G	-14	HIS	-	expression tag	UNP Q2YRI3
G	-13	HIS	-	expression tag	UNP Q2YRI3
G	-12	MET	-	expression tag	UNP Q2YRI3
G	-11	GLY	-	expression tag	UNP Q2YRI3
G	-10	THR	-	expression tag	UNP Q2YRI3
G	-9	LEU	-	expression tag	UNP Q2YRI3
G	-8	GLU	-	expression tag	UNP Q2YRI3

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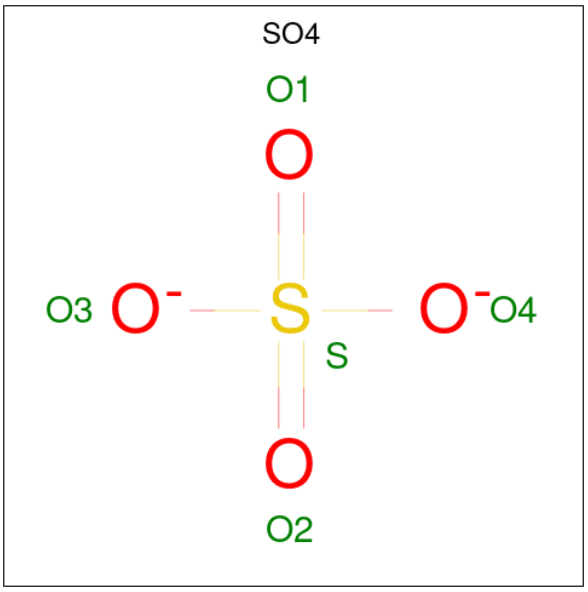
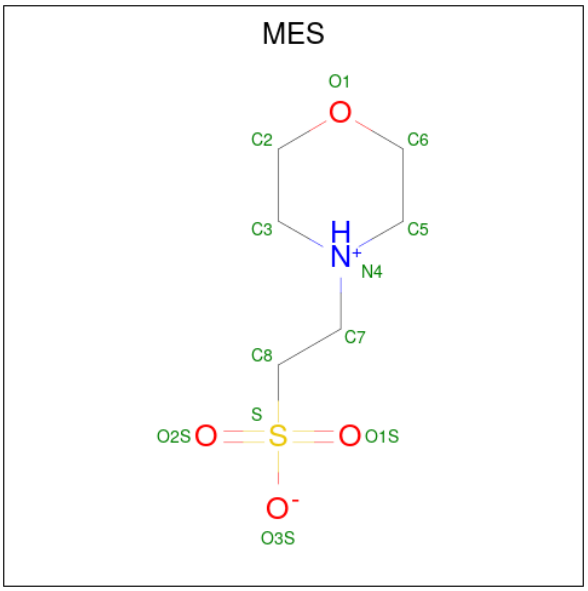
Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ALA	-	expression tag	UNP Q2YRI3
G	-6	GLN	-	expression tag	UNP Q2YRI3
G	-5	THR	-	expression tag	UNP Q2YRI3
G	-4	GLN	-	expression tag	UNP Q2YRI3
G	-3	GLY	-	expression tag	UNP Q2YRI3
G	-2	PRO	-	expression tag	UNP Q2YRI3
G	-1	GLY	-	expression tag	UNP Q2YRI3
G	0	SER	-	expression tag	UNP Q2YRI3
H	-20	MET	-	expression tag	UNP Q2YRI3
H	-19	ALA	-	expression tag	UNP Q2YRI3
H	-18	HIS	-	expression tag	UNP Q2YRI3
H	-17	HIS	-	expression tag	UNP Q2YRI3
H	-16	HIS	-	expression tag	UNP Q2YRI3
H	-15	HIS	-	expression tag	UNP Q2YRI3
H	-14	HIS	-	expression tag	UNP Q2YRI3
H	-13	HIS	-	expression tag	UNP Q2YRI3
H	-12	MET	-	expression tag	UNP Q2YRI3
H	-11	GLY	-	expression tag	UNP Q2YRI3
H	-10	THR	-	expression tag	UNP Q2YRI3
H	-9	LEU	-	expression tag	UNP Q2YRI3
H	-8	GLU	-	expression tag	UNP Q2YRI3
H	-7	ALA	-	expression tag	UNP Q2YRI3
H	-6	GLN	-	expression tag	UNP Q2YRI3
H	-5	THR	-	expression tag	UNP Q2YRI3
H	-4	GLN	-	expression tag	UNP Q2YRI3
H	-3	GLY	-	expression tag	UNP Q2YRI3
H	-2	PRO	-	expression tag	UNP Q2YRI3
H	-1	GLY	-	expression tag	UNP Q2YRI3
H	0	SER	-	expression tag	UNP Q2YRI3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0
3	C	1	Total C N O S 12 6 1 4 1	0	0
3	D	1	Total C N O S 12 6 1 4 1	0	0
3	E	1	Total C N O S 12 6 1 4 1	0	0
3	F	1	Total C N O S 12 6 1 4 1	0	0
3	G	1	Total C N O S 12 6 1 4 1	0	0
3	H	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	553	Total O 553 553	0	0
4	B	470	Total O 470 470	0	0
4	C	406	Total O 406 406	0	0
4	D	359	Total O 359 359	0	0

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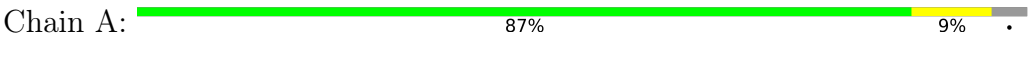
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	282	Total O 282 282	0	0
4	F	446	Total O 446 446	0	0
4	G	346	Total O 346 346	0	0
4	H	280	Total O 280 280	0	0

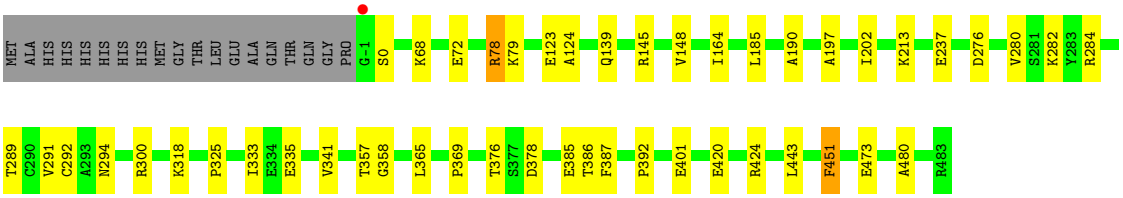
3 Residue-property plots (i)

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: Aldehyde dehydrogenase

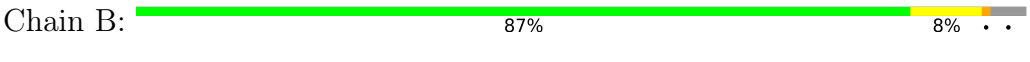
Chain A:

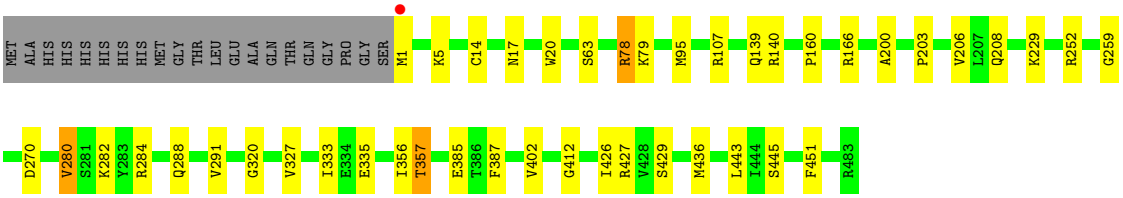




• Molecule 1: Aldehyde dehydrogenase

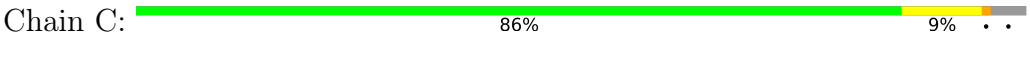
Chain B:

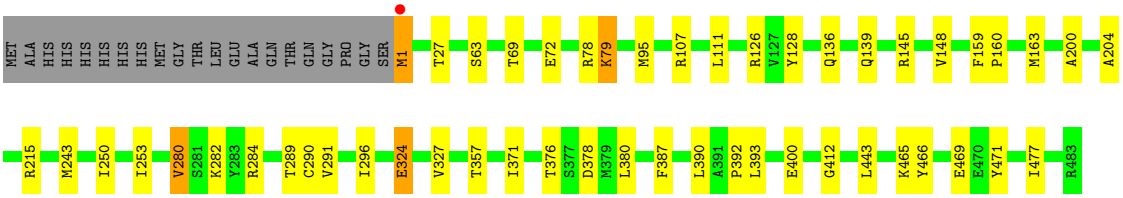




• Molecule 1: Aldehyde dehydrogenase

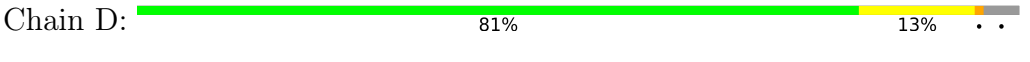
Chain C:

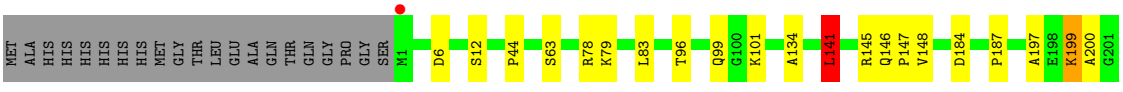


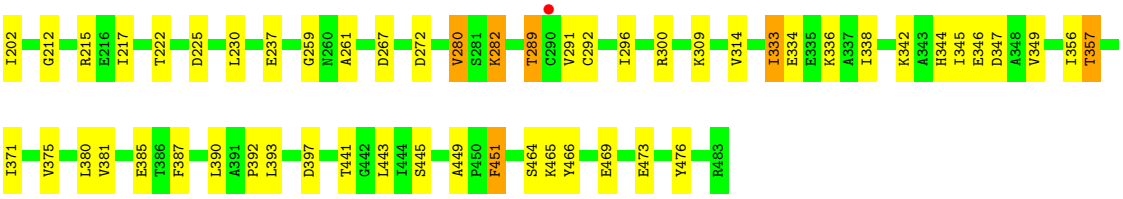


• Molecule 1: Aldehyde dehydrogenase

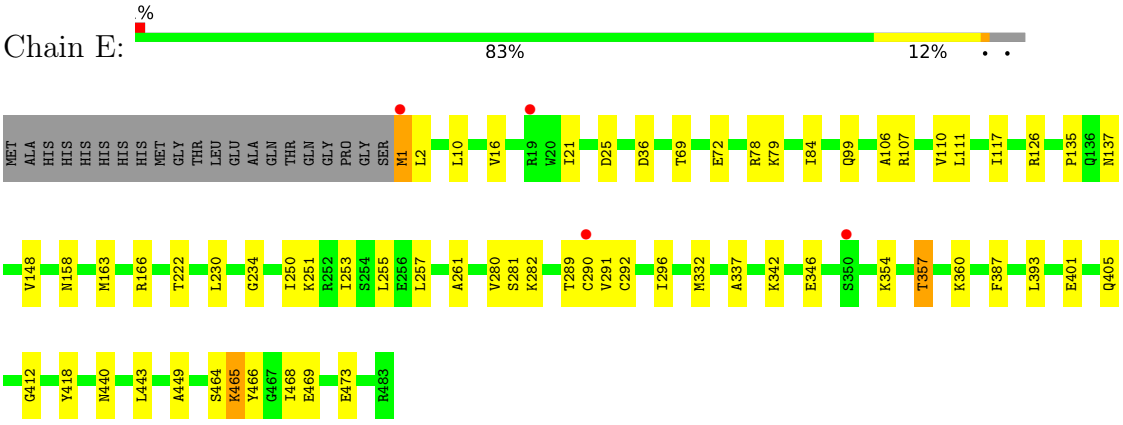
Chain D:



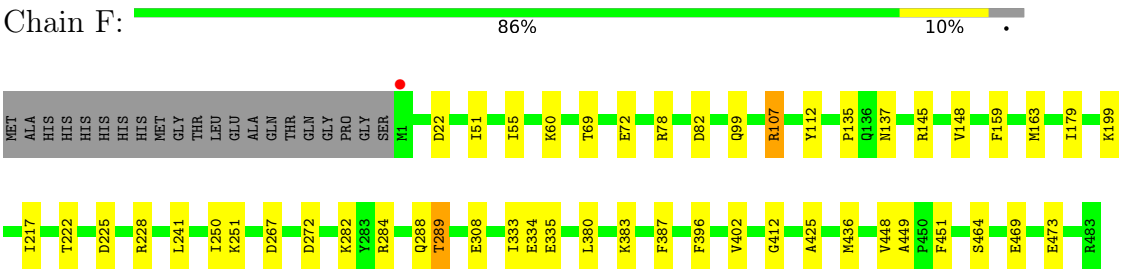




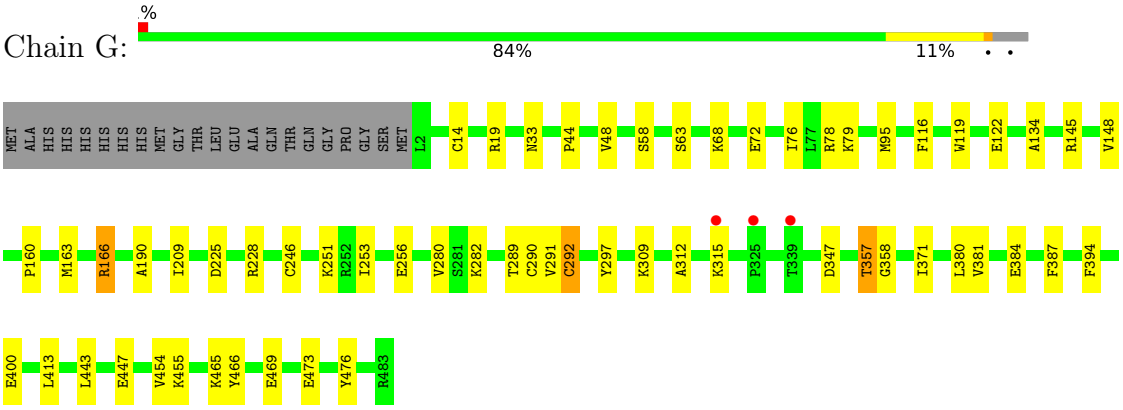
• Molecule 1: Aldehyde dehydrogenase



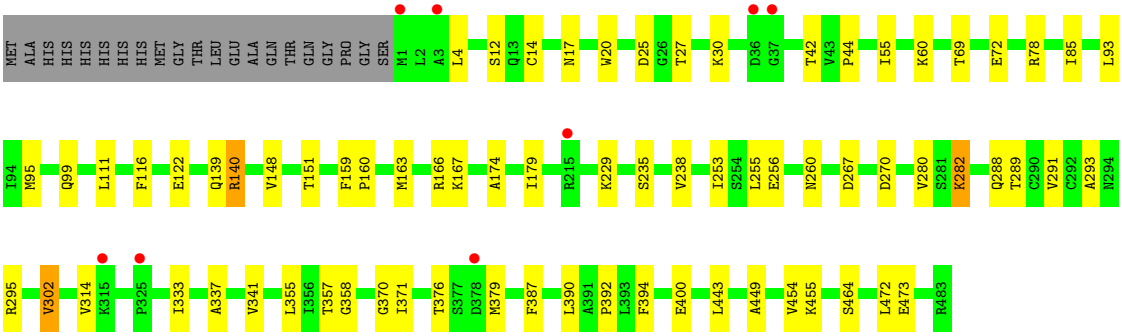
• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase



• Molecule 1: Aldehyde dehydrogenase


MET ALA HIS HIS HIS HIS HIS MET GLY THR LEU GLU ALA GLN THR GLN GLY PRO GLY SER M1 L2 A3 L4 S12 Q13 C14 N17 W20 D25 G26 T27 K30 D36 G37 T42 V43 P44 I55 K60 T69 E72 R78 I85 L93
I94 M95 Q99 L111 F116 E122 Q139 R140 V148 T151 F159 P160 M163 R166 K167 A174 I179 R215 K229 S235 V238 I253 S254 L255 E256 N260 D267 D270 V280 S281 K282 Q288 T289 C290 V291 C292 A293 N294
R296 V302 V314 K315 P325 I333 A337 V341 L355 I356 T357 G368 G370 I371 T376 S377 D378 M379 F387 L390 A391 P392 L393 F394 E400 L443 A449 V454 K455 S464 L472 E473 R483

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.87Å 93.01Å 143.70Å 92.03° 107.58° 109.65°	Depositor
Resolution (Å)	19.78 – 2.10 19.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.78-2.10) 94.2 (19.77-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.161 , 0.225 0.164 , 0.224	Depositor DCC
R_{free} test set	11634 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32199	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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 (i)

5.1 Standard geometry (i)

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

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	0.97	2/3702 (0.1%)	0.84	3/5015 (0.1%)
1	B	0.93	0/3681	0.86	7/4990 (0.1%)
1	C	0.90	2/3684 (0.1%)	0.84	2/4994 (0.0%)
1	D	0.81	0/3669	0.79	2/4974 (0.0%)
1	E	0.79	0/3674	0.78	2/4982 (0.0%)
1	F	0.90	2/3684 (0.1%)	0.87	7/4994 (0.1%)
1	G	0.83	2/3672 (0.1%)	0.79	4/4979 (0.1%)
1	H	0.76	1/3697 (0.0%)	0.76	4/5010 (0.1%)
All	All	0.86	9/29463 (0.0%)	0.82	31/39938 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	GLU	CB-CG	6.16	1.63	1.52
1	A	335	GLU	CG-CD	6.03	1.60	1.51
1	G	400	GLU	CG-CD	5.92	1.60	1.51
1	F	267	ASP	CB-CG	-5.85	1.39	1.51
1	G	292	CYS	CB-SG	5.73	1.92	1.82
1	F	448	VAL	CB-CG2	5.72	1.64	1.52
1	C	204	ALA	CA-CB	5.69	1.64	1.52
1	H	400	GLU	CG-CD	5.40	1.60	1.51
1	C	400	GLU	CG-CD	5.15	1.59	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	267	ASP	CB-CG-OD1	-8.93	110.26	118.30
1	H	78	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	F	107[A]	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	F	107[B]	ARG	NE-CZ-NH2	-6.30	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	78	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	H	140	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	78	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	166	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	F	82	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	78	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	78	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	E	78	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	F	272	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	424	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	G	166	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	276	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	380	LEU	CA-CB-CG	5.39	127.69	115.30
1	G	78	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	E	126	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	141	LEU	CB-CG-CD1	5.24	119.91	111.00
1	B	140	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	280	VAL	CB-CA-C	-5.12	101.67	111.40
1	H	295	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	F	145	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	427	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	G	228	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	126	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	H	295	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	G	78	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	78	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	270	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	3635	0	3717	32	0
1	B	3611	0	3688	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3614	0	3688	28	0
1	D	3608	0	3676	47	0
1	E	3604	0	3673	44	0
1	F	3617	0	3687	31	0
1	G	3605	0	3671	34	0
1	H	3627	0	3704	40	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	12	0	13	2	0
3	B	12	0	12	2	0
3	C	12	0	13	3	0
3	D	12	0	13	2	0
3	E	12	0	13	3	0
3	F	12	0	13	3	0
3	G	12	0	13	3	0
3	H	12	0	13	2	0
4	A	553	0	0	12	0
4	B	470	0	0	7	1
4	C	406	0	0	11	0
4	D	359	0	0	11	0
4	E	282	0	0	10	0
4	F	446	0	0	16	0
4	G	346	0	0	10	1
4	H	280	0	0	2	0
All	All	32199	0	29607	290	1

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 5.

All (290) 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:B:280:VAL:HG11	1:B:443:LEU:HD21	1.41	1.00
1:B:280:VAL:CG1	1:B:443:LEU:HD21	1.93	0.99
1:F:241:LEU:HD22	4:F:872:HOH:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:VAL:HG11	1:B:443:LEU:CD2	2.02	0.88
1:F:107[A]:ARG:HD3	4:F:878:HOH:O	1.77	0.84
1:A:145:ARG:NH1	4:A:683:HOH:O	2.13	0.80
1:B:17:ASN:H	1:B:208:GLN:HE21	1.26	0.80
1:G:280:VAL:HG11	1:G:443:LEU:HG	1.64	0.79
1:E:280:VAL:CG1	1:E:443:LEU:HD21	2.13	0.79
1:H:69:THR:OG1	1:H:72[B]:GLU:HG3	1.82	0.78
1:G:291:VAL:HG22	3:G:485:MES:O3S	1.84	0.77
1:E:137:ASN:ND2	4:E:742:HOH:O	2.12	0.75
1:D:344:HIS:CD2	1:D:380:LEU:HD23	2.21	0.75
1:E:2:LEU:HD12	1:E:10:LEU:HD22	1.70	0.74
1:H:282:LYS:HE2	1:H:293:ALA:O	1.89	0.73
1:C:79:LYS:HE3	1:C:200:ALA:O	1.90	0.71
1:E:280:VAL:HG11	1:E:443:LEU:HD21	1.71	0.71
1:D:289:THR:O	4:D:835:HOH:O	2.08	0.70
1:G:454:VAL:HG23	1:G:455:LYS:HG3	1.73	0.70
1:A:68:LYS:HB3	1:A:72[B]:GLU:HG3	1.74	0.70
1:E:280:VAL:HG11	1:E:443:LEU:CD2	2.22	0.69
1:F:284:ARG:HG2	4:F:847:HOH:O	1.93	0.69
1:C:290[B]:CYS:SG	4:C:836:HOH:O	2.50	0.68
1:B:17:ASN:H	1:B:208:GLN:NE2	1.93	0.67
1:F:335:GLU:HG3	4:F:766:HOH:O	1.94	0.67
1:D:280:VAL:HG11	1:D:443:LEU:HG	1.77	0.67
1:H:291:VAL:HG13	3:H:485:MES:O3S	1.95	0.67
1:D:289:THR:HG23	1:D:292:CYS:SG	2.35	0.66
1:H:256[A]:GLU:OE2	4:H:489:HOH:O	2.13	0.66
1:A:357:THR:HG21	4:A:621:HOH:O	1.94	0.66
1:B:139:GLN:OE1	4:B:927:HOH:O	2.12	0.66
1:D:267:ASP:OD2	4:D:720:HOH:O	2.14	0.66
1:B:17:ASN:N	1:B:208:GLN:HE21	1.94	0.66
1:F:288:GLN:HE22	1:F:333:ILE:H	1.44	0.66
1:D:333:ILE:HG23	1:D:334:GLU:HG2	1.77	0.65
1:H:14:CYS:SG	1:H:44:PRO:HG2	2.36	0.65
1:D:237:GLU:OE2	4:D:840:HOH:O	2.14	0.65
1:E:72[A]:GLU:OE2	4:E:531:HOH:O	2.13	0.65
1:F:22:ASP:OD1	4:F:883:HOH:O	2.14	0.64
1:E:354:LYS:NZ	4:E:741:HOH:O	2.29	0.63
1:G:357:THR:HG22	1:G:371:ILE:H	1.64	0.62
1:B:79:LYS:HE3	1:B:200:ALA:O	2.00	0.62
1:B:280:VAL:CG1	1:B:443:LEU:CD2	2.70	0.62
1:D:451:PHE:HD1	4:D:493:HOH:O	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:VAL:HG11	1:B:443:LEU:CG	2.29	0.62
1:G:357:THR:HG22	1:G:371:ILE:N	2.15	0.62
1:C:1:MET:HG2	4:C:880:HOH:O	2.00	0.61
1:E:280:VAL:HG11	1:E:443:LEU:HG	1.81	0.61
1:A:79:LYS:HE2	4:A:906:HOH:O	2.01	0.61
1:B:291:VAL:HG22	3:B:485:MES:O3S	2.00	0.61
1:A:148:VAL:HG22	1:A:473:GLU:HG2	1.81	0.61
1:C:139:GLN:OE1	4:C:738:HOH:O	2.16	0.60
1:G:145:ARG:NH1	4:G:784:HOH:O	2.34	0.60
1:G:256:GLU:OE2	4:G:824:HOH:O	2.16	0.60
1:A:139:GLN:OE1	4:A:991:HOH:O	2.16	0.59
1:G:148:VAL:HG22	1:G:473:GLU:HG2	1.85	0.59
1:H:355:LEU:HD21	1:H:358:GLY:O	2.03	0.59
1:E:280:VAL:HG11	1:E:443:LEU:CG	2.33	0.58
1:H:148:VAL:HG22	1:H:473:GLU:HG2	1.85	0.58
1:H:314:VAL:HG21	1:H:371:ILE:HD11	1.86	0.58
1:B:1:MET:N	4:B:918:HOH:O	2.36	0.57
1:H:25:ASP:OD1	1:H:27:THR:HG23	2.04	0.57
1:H:357:THR:HG23	1:H:370:GLY:HA2	1.86	0.57
1:D:134:ALA:HA	1:D:141:LEU:HD22	1.86	0.57
1:C:145:ARG:NH1	4:C:828:HOH:O	2.38	0.56
1:E:342:LYS:O	1:E:346:GLU:HG2	2.05	0.56
1:D:145:ARG:NH1	4:D:669:HOH:O	2.37	0.56
1:E:280:VAL:CG1	1:E:443:LEU:CD2	2.80	0.56
1:F:148:VAL:HG22	1:F:473:GLU:HG2	1.87	0.56
1:G:309:LYS:O	4:G:797:HOH:O	2.18	0.56
1:D:314:VAL:HG21	1:D:371:ILE:HD11	1.88	0.55
3:C:485:MES:H32	3:C:485:MES:O3S	2.06	0.55
1:E:163:MET:HE2	1:E:166:ARG:HD3	1.88	0.55
1:E:79:LYS:CE	4:E:723:HOH:O	2.55	0.55
1:B:280:VAL:HG12	1:B:280:VAL:O	2.06	0.55
1:F:289:THR:HG21	4:F:871:HOH:O	2.06	0.55
1:H:357:THR:HG21	1:H:371:ILE:HD12	1.89	0.55
1:H:280:VAL:HG11	1:H:443:LEU:HG	1.89	0.54
1:G:68:LYS:HB3	1:G:72[B]:GLU:HG3	1.89	0.54
1:H:270:ASP:C	1:H:270:ASP:OD1	2.46	0.54
1:C:69:THR:OG1	1:C:72[B]:GLU:HG3	2.07	0.54
1:G:312:ALA:HB3	4:G:797:HOH:O	2.07	0.54
1:B:356:ILE:HG13	1:B:357:THR:HG22	1.90	0.54
1:H:288:GLN:HE22	1:H:333:ILE:H	1.56	0.53
1:A:280:VAL:CG1	1:A:443:LEU:HD21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:CYS:HB2	4:D:835:HOH:O	2.07	0.53
1:C:1:MET:CA	4:C:662:HOH:O	2.55	0.53
1:D:356:ILE:HG13	1:D:357:THR:HG22	1.91	0.53
1:F:469:GLU:HG3	4:F:856:HOH:O	2.08	0.53
1:H:337:ALA:O	1:H:341:VAL:HG23	2.08	0.53
1:D:79:LYS:CE	1:D:200:ALA:O	2.57	0.53
1:B:445:SER:HA	1:B:451:PHE:CZ	2.44	0.52
1:H:30:LYS:HG2	1:H:42:THR:HG22	1.91	0.52
1:A:284:ARG:HD2	3:A:485:MES:H21	1.91	0.52
1:G:14:CYS:SG	1:G:44:PRO:HG2	2.49	0.52
1:A:300:ARG:NH2	4:A:938:HOH:O	2.43	0.52
1:E:69:THR:OG1	1:E:72[B]:GLU:HG2	2.08	0.52
1:B:78:ARG:HD3	4:B:868:HOH:O	2.09	0.52
1:B:436:MET:SD	1:B:451:PHE:CD1	3.03	0.52
1:C:357:THR:HG21	1:C:371:ILE:HD12	1.91	0.52
1:A:289:THR:HG23	1:A:292:CYS:SG	2.50	0.52
1:E:84:ILE:HD12	1:E:117:ILE:HD12	1.92	0.52
1:G:63:SER:HB2	4:G:776:HOH:O	2.09	0.52
1:A:385:GLU:OE2	4:A:1018:HOH:O	2.19	0.51
1:C:128:TYR:CE2	1:D:465:LYS:HD3	2.46	0.51
1:C:250:ILE:HG22	1:C:250:ILE:O	2.11	0.51
1:F:284:ARG:CG	4:F:847:HOH:O	2.54	0.51
1:H:12:SER:O	1:H:44:PRO:HD3	2.11	0.51
1:C:280:VAL:HG11	1:C:443:LEU:HG	1.93	0.51
1:E:332:MET:HE1	1:E:337:ALA:HB1	1.93	0.51
1:D:342:LYS:O	1:D:346:GLU:HG2	2.11	0.51
1:G:72[A]:GLU:OE2	4:G:717:HOH:O	2.19	0.51
1:A:79:LYS:NZ	4:A:1028:HOH:O	2.37	0.50
1:C:390:LEU:O	1:C:392:PRO:HD3	2.10	0.50
1:D:222:THR:HG22	1:D:230:LEU:HD22	1.94	0.50
1:D:466:TYR:O	1:D:469:GLU:HG2	2.12	0.50
1:D:357:THR:HG21	1:D:371:ILE:HD12	1.93	0.49
1:G:291:VAL:CG2	3:G:485:MES:O3S	2.58	0.49
1:E:253:ILE:HD11	1:E:255:LEU:HD21	1.94	0.49
1:F:112:TYR:CE2	3:F:485:MES:H52	2.48	0.49
1:E:230:LEU:HD23	1:E:253:ILE:HD12	1.94	0.49
1:G:466:TYR:O	1:G:469:GLU:HG2	2.13	0.49
1:F:159:PHE:HB2	1:F:163:MET:HG2	1.95	0.49
1:E:25:ASP:OD1	1:E:25:ASP:C	2.51	0.49
1:B:280:VAL:CG1	1:B:280:VAL:O	2.60	0.48
1:D:148:VAL:HG22	1:D:473:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:GLU:OE1	4:A:832:HOH:O	2.19	0.48
1:B:259:GLY:O	1:B:385:GLU:HG3	2.13	0.48
1:G:76:ILE:HA	1:G:79:LYS:HE3	1.95	0.48
1:C:148:VAL:HG23	1:C:471:TYR:C	2.34	0.48
1:E:357:THR:HG22	4:E:729:HOH:O	2.12	0.48
1:B:107[A]:ARG:HD2	4:B:596:HOH:O	2.13	0.48
1:D:63:SER:HB2	4:D:675:HOH:O	2.14	0.48
1:C:78:ARG:HD3	4:C:829:HOH:O	2.13	0.48
1:D:345:ILE:O	1:D:349:VAL:HG23	2.13	0.48
1:G:48:VAL:HG23	4:G:596:HOH:O	2.13	0.48
1:A:185:LEU:HD13	1:A:333:ILE:HG13	1.96	0.48
1:E:250:ILE:HG22	1:E:250:ILE:O	2.14	0.48
1:E:332:MET:CE	1:E:337:ALA:HB1	2.44	0.48
1:E:466:TYR:O	1:E:469:GLU:HG2	2.13	0.48
1:A:318:LYS:NZ	1:A:325:PRO:O	2.46	0.47
1:E:107[A]:ARG:HD3	4:E:725:HOH:O	2.14	0.47
1:C:27:THR:O	4:C:660:HOH:O	2.20	0.47
1:E:158:ASN:CG	4:E:724:HOH:O	2.52	0.47
1:A:451:PHE:HD1	4:A:580:HOH:O	1.96	0.47
1:H:235:SER:OG	1:H:238:VAL:HG23	2.14	0.47
1:A:480:ALA:HB2	1:D:441:THR:HB	1.97	0.47
1:C:296:ILE:HB	1:C:393:LEU:HD23	1.95	0.47
1:D:184:ASP:OD2	4:D:747:HOH:O	2.20	0.47
1:D:300:ARG:NH1	1:D:397:ASP:OD1	2.48	0.47
1:H:14:CYS:O	1:H:20:TRP:HA	2.14	0.47
1:D:272:ASP:OD1	1:D:309:LYS:NZ	2.42	0.47
1:H:174:ALA:HB1	1:H:472:LEU:HD21	1.97	0.47
1:H:267:ASP:HB2	4:H:726:HOH:O	2.13	0.47
1:E:16:VAL:HG21	1:E:21:ILE:HD11	1.96	0.46
1:F:228:ARG:CZ	1:G:455:LYS:HD2	2.45	0.46
1:C:376:THR:OG1	1:C:378:ASP:OD1	2.31	0.46
1:H:357:THR:HG22	1:H:371:ILE:HB	1.96	0.46
1:G:116:PHE:CE1	1:G:166:ARG:HG2	2.50	0.46
1:H:174:ALA:HB1	1:H:472:LEU:CD2	2.44	0.46
1:D:83:LEU:HD13	1:D:199:LYS:HB3	1.98	0.46
1:D:259:GLY:O	1:D:385:GLU:CD	2.53	0.46
1:D:261:ALA:HB3	1:D:292:CYS:O	2.16	0.46
1:D:184:ASP:O	1:D:187:PRO:HD3	2.15	0.46
1:G:246:CYS:HB3	1:G:251:LYS:HB2	1.97	0.46
1:B:203:PRO:HD2	1:B:206:VAL:HG21	1.98	0.46
1:D:338:ILE:HG22	1:D:342:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:ARG:NH1	4:D:725:HOH:O	2.47	0.46
1:D:336:LYS:HB2	4:D:842:HOH:O	2.15	0.46
1:G:119:TRP:HB2	1:G:447:GLU:HG3	1.97	0.46
1:E:401:GLU:HG3	1:E:405:GLN:HE21	1.80	0.45
1:H:163:MET:O	1:H:167:LYS:HD2	2.16	0.45
1:E:449:ALA:C	1:E:464:SER:HB3	2.37	0.45
1:E:1:MET:HE3	1:E:2:LEU:O	2.16	0.45
1:H:4:LEU:HD23	1:H:93:LEU:HD23	1.98	0.45
1:B:445:SER:OG	3:B:485:MES:H32	2.16	0.45
3:C:485:MES:H82	3:C:485:MES:H31	1.06	0.45
1:H:151:THR:HG22	1:H:229:LYS:HB3	1.97	0.45
1:A:78:ARG:HD3	4:A:973:HOH:O	2.16	0.45
3:H:485:MES:H31	3:H:485:MES:H82	1.59	0.45
1:C:136:GLN:NE2	4:C:887:HOH:O	2.50	0.45
1:F:241:LEU:HB3	4:F:872:HOH:O	2.17	0.45
1:A:197:ALA:HB1	1:A:202:ILE:HD12	1.99	0.45
1:H:95:MET:HG3	1:H:160:PRO:HG2	1.99	0.45
1:A:376:THR:OG1	1:A:378:ASP:OD2	2.28	0.45
1:F:51:ILE:HG13	1:F:217:ILE:HG12	1.99	0.45
2:D:484:SO4:O2	4:D:548:HOH:O	2.21	0.44
1:F:289:THR:CG2	4:F:871:HOH:O	2.65	0.44
1:D:291:VAL:HG22	3:D:485:MES:O3S	2.17	0.44
1:D:375:VAL:HG21	1:D:392:PRO:CB	2.48	0.44
1:E:148:VAL:HG22	1:E:473:GLU:HG2	1.99	0.44
1:G:381:VAL:O	1:G:381:VAL:HG22	2.16	0.44
1:C:215:ARG:NH2	4:C:677:HOH:O	2.50	0.44
1:F:425:ALA:HB3	4:F:882:HOH:O	2.17	0.44
1:H:267:ASP:OD1	1:H:302:VAL:HG22	2.17	0.44
1:B:280:VAL:HG11	1:B:443:LEU:HG	1.97	0.44
1:B:429:SER:HB2	1:C:477:ILE:HD13	1.99	0.44
1:G:290[B]:CYS:O	1:G:413:LEU:HD23	2.18	0.44
1:A:68:LYS:HB3	1:A:72[B]:GLU:CG	2.47	0.44
1:A:123:GLU:O	1:A:124:ALA:C	2.55	0.44
1:F:69:THR:OG1	1:F:72[B]:GLU:HG3	2.17	0.44
1:D:96:THR:HG23	1:D:101:LYS:O	2.18	0.44
1:E:84:ILE:HD12	1:E:117:ILE:CD1	2.48	0.44
1:F:333:ILE:HG23	1:F:334:GLU:HG2	2.00	0.44
1:A:213:LYS:NZ	4:A:930:HOH:O	2.50	0.43
1:C:291:VAL:HG22	3:C:485:MES:O3S	2.18	0.43
1:E:234:GLY:O	1:E:257:LEU:HA	2.18	0.43
3:G:485:MES:H31	3:G:485:MES:H82	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:ILE:HA	1:H:179:ILE:HD11	2.00	0.43
1:E:291:VAL:HG22	3:E:485:MES:O3S	2.17	0.43
1:F:383:LYS:HE3	4:F:817:HOH:O	2.18	0.43
1:C:95:MET:HG3	1:C:160:PRO:HG2	1.99	0.43
1:D:212:GLY:HA3	1:D:217:ILE:HD11	1.99	0.43
1:E:296:ILE:HB	1:E:393:LEU:HD23	2.01	0.43
1:H:116:PHE:CE1	1:H:166:ARG:HG2	2.53	0.43
1:D:445:SER:OG	3:D:485:MES:H32	2.18	0.43
1:G:380:LEU:HD11	1:G:384:GLU:OE2	2.17	0.43
1:H:139:GLN:O	1:H:140:ARG:NH1	2.51	0.43
1:B:288:GLN:HE22	1:B:333:ILE:H	1.65	0.43
1:D:12:SER:O	1:D:44:PRO:HD3	2.19	0.43
1:F:396:PHE:CD1	1:F:402:VAL:HB	2.54	0.43
1:G:289:THR:HG23	1:G:292:CYS:SG	2.58	0.43
1:D:197:ALA:HB1	1:D:202:ILE:HD12	2.00	0.43
1:G:19:ARG:CG	4:G:673:HOH:O	2.67	0.43
1:G:190:ALA:O	1:G:209:ILE:HD13	2.19	0.43
1:F:289:THR:OG1	4:F:871:HOH:O	2.15	0.43
1:E:291:VAL:CG2	3:E:485:MES:O3S	2.67	0.43
1:B:284:ARG:NH2	4:B:926:HOH:O	2.49	0.43
1:E:135:PRO:HD2	4:E:573:HOH:O	2.19	0.43
1:G:33:ASN:C	1:G:33:ASN:OD1	2.58	0.42
3:E:485:MES:H82	3:E:485:MES:H31	1.55	0.42
1:G:122:GLU:HG2	1:H:122:GLU:HG2	2.01	0.42
1:D:6:ASP:OD1	1:D:6:ASP:C	2.57	0.42
1:D:381:VAL:HG21	1:D:392:PRO:HG3	2.01	0.42
1:F:250:ILE:O	1:F:250:ILE:HG22	2.20	0.42
1:G:134:ALA:HB3	4:G:706:HOH:O	2.19	0.42
1:B:229:LYS:HA	1:B:252:ARG:O	2.20	0.42
1:A:365:LEU:HD23	1:A:365:LEU:HA	1.88	0.42
1:F:199:LYS:CE	4:F:862:HOH:O	2.67	0.42
1:H:282:LYS:HE3	1:H:390:LEU:O	2.20	0.42
1:H:390:LEU:O	1:H:392:PRO:HD3	2.19	0.42
1:E:79:LYS:HE3	4:E:723:HOH:O	2.17	0.42
3:F:485:MES:H82	3:F:485:MES:H31	1.57	0.42
1:A:291:VAL:HG22	3:A:485:MES:H71	2.02	0.42
1:E:468:ILE:HG22	4:E:582:HOH:O	2.20	0.42
1:H:376:THR:HG23	1:H:379:MET:CE	2.50	0.42
1:F:137:ASN:HD22	1:F:137:ASN:HA	1.76	0.42
1:D:296:ILE:HB	1:D:393:LEU:HD23	2.01	0.41
1:D:282:LYS:HD3	1:D:390:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:THR:CG2	1:D:371:ILE:HD12	2.50	0.41
1:H:85:ILE:HD12	1:H:111:LEU:HD22	2.03	0.41
1:A:79:LYS:HD2	4:A:620:HOH:O	2.20	0.41
1:E:106:ALA:O	1:E:110:VAL:HG23	2.20	0.41
1:H:449:ALA:C	1:H:464:SER:HB3	2.41	0.41
1:G:297:TYR:CD1	1:G:394:PHE:HB2	2.54	0.41
1:H:454:VAL:HG23	1:H:455:LYS:HG3	2.01	0.41
1:A:294:ASN:O	1:A:392:PRO:HG2	2.20	0.41
1:B:14:CYS:O	1:B:20:TRP:HA	2.21	0.41
1:F:284:ARG:NH1	3:F:485:MES:O1	2.53	0.41
1:H:159:PHE:CZ	1:H:289:THR:HG22	2.55	0.41
1:H:253:ILE:HD11	1:H:255:LEU:HD21	2.02	0.41
1:A:237:GLU:CD	1:A:237:GLU:H	2.24	0.41
1:E:332:MET:HB3	1:E:332:MET:HE2	1.93	0.41
1:F:449:ALA:C	1:F:464:SER:HB3	2.40	0.41
1:G:95:MET:HG3	1:G:160:PRO:HG2	2.01	0.41
1:E:222:THR:O	1:E:251:LYS:HE2	2.20	0.41
1:A:341:VAL:HG22	1:A:386:THR:HG22	2.02	0.41
1:A:358:GLY:HA3	1:A:369:PRO:O	2.21	0.41
1:D:146:GLN:HB3	1:D:147:PRO:HD2	2.02	0.41
1:E:465:LYS:HG3	4:F:657:HOH:O	2.21	0.41
1:F:55:ILE:HA	1:F:179:ILE:HD11	2.02	0.41
1:B:426:ILE:HD13	4:B:882:HOH:O	2.20	0.41
1:C:63:SER:CB	4:C:749:HOH:O	2.67	0.41
1:C:324:GLU:HG3	1:C:327:VAL:HG23	2.03	0.41
1:E:418:TYR:CD1	1:E:440:ASN:HA	2.56	0.41
1:F:135:PRO:HD2	4:F:797:HOH:O	2.19	0.41
1:G:19:ARG:HG2	4:G:673:HOH:O	2.21	0.41
1:A:164:ILE:CD1	1:A:190:ALA:HB2	2.51	0.41
1:C:159:PHE:HB2	1:C:163:MET:HG2	2.03	0.41
1:C:243:MET:HA	1:C:253:ILE:CD1	2.51	0.40
1:C:466:TYR:O	1:C:469:GLU:HG2	2.20	0.40
1:D:449:ALA:C	1:D:464:SER:HB3	2.41	0.40
1:F:222:THR:O	1:F:251:LYS:HE2	2.21	0.40
1:B:320:GLY:O	1:B:327:VAL:HG11	2.22	0.40
1:F:436:MET:SD	1:F:451:PHE:CD1	3.15	0.40
1:B:95:MET:HG3	1:B:160:PRO:HG2	2.02	0.40
1:A:280:VAL:HG12	1:A:443:LEU:HD21	2.03	0.40
1:B:357:THR:HG21	4:B:762:HOH:O	2.21	0.40
1:C:107[A]:ARG:NH2	4:C:845:HOH:O	2.54	0.40
1:E:261:ALA:HB3	1:E:292:CYS:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:833:HOH:O	4:G:799:HOH:O[1_455]	2.10	0.10

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	486/504 (96%)	475 (98%)	11 (2%)	0	100	100
1	B	484/504 (96%)	472 (98%)	11 (2%)	1 (0%)	47	49
1	C	484/504 (96%)	474 (98%)	9 (2%)	1 (0%)	47	49
1	D	483/504 (96%)	465 (96%)	18 (4%)	0	100	100
1	E	484/504 (96%)	466 (96%)	16 (3%)	2 (0%)	34	32
1	F	484/504 (96%)	469 (97%)	14 (3%)	1 (0%)	47	49
1	G	483/504 (96%)	467 (97%)	15 (3%)	1 (0%)	47	49
1	H	485/504 (96%)	470 (97%)	13 (3%)	2 (0%)	34	32
All	All	3873/4032 (96%)	3758 (97%)	107 (3%)	8 (0%)	47	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	358	GLY
1	H	17	ASN
1	H	260	ASN
1	E	36	ASP
1	F	412	GLY
1	B	412	GLY
1	C	412	GLY
1	E	412	GLY

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	374/386 (97%)	369 (99%)	5 (1%)	69	75
1	B	370/386 (96%)	363 (98%)	7 (2%)	57	63
1	C	371/386 (96%)	361 (97%)	10 (3%)	44	48
1	D	369/386 (96%)	356 (96%)	13 (4%)	36	38
1	E	369/386 (96%)	357 (97%)	12 (3%)	38	40
1	F	371/386 (96%)	363 (98%)	8 (2%)	52	57
1	G	369/386 (96%)	358 (97%)	11 (3%)	41	44
1	H	373/386 (97%)	367 (98%)	6 (2%)	62	69
All	All	2966/3088 (96%)	2894 (98%)	72 (2%)	49	53

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	282	LYS
1	A	387	PHE
1	A	401	GLU
1	A	451	PHE
1	B	5	LYS
1	B	63	SER
1	B	282	LYS
1	B	335	GLU
1	B	357	THR
1	B	387	PHE
1	B	402	VAL
1	C	1	MET
1	C	79	LYS
1	C	111	LEU
1	C	280	VAL
1	C	282	LYS
1	C	284	ARG
1	C	289	THR

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Mol	Chain	Res	Type
1	C	324	GLU
1	C	387	PHE
1	C	465	LYS
1	D	99	GLN
1	D	141	LEU
1	D	199	LYS
1	D	225	ASP
1	D	280	VAL
1	D	282	LYS
1	D	289	THR
1	D	333	ILE
1	D	347	ASP
1	D	357	THR
1	D	387	PHE
1	D	451	PHE
1	D	476	TYR
1	E	1	MET
1	E	99	GLN
1	E	111	LEU
1	E	281	SER
1	E	282	LYS
1	E	289	THR
1	E	290[A]	CYS
1	E	290[B]	CYS
1	E	357	THR
1	E	360	LYS
1	E	387	PHE
1	E	465	LYS
1	F	60	LYS
1	F	99	GLN
1	F	225	ASP
1	F	282	LYS
1	F	289	THR
1	F	308	GLU
1	F	380	LEU
1	F	387	PHE
1	G	58	SER
1	G	163	MET
1	G	225	ASP
1	G	253	ILE
1	G	282	LYS
1	G	315	LYS

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Mol	Chain	Res	Type
1	G	347	ASP
1	G	357	THR
1	G	387	PHE
1	G	465	LYS
1	G	476	TYR
1	H	60	LYS
1	H	99	GLN
1	H	282	LYS
1	H	302	VAL
1	H	387	PHE
1	H	394	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	136	GLN
1	B	208	GLN
1	E	405	GLN
1	F	136	GLN
1	F	137	ASN
1	F	288	GLN
1	H	288	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands 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	$\#\|Z\| > 2$
3	MES	C	485	-	12,12,12	2.32	1 (8%)	14,16,16	1.62	2 (14%)
3	MES	D	485	-	12,12,12	2.47	1 (8%)	14,16,16	2.92	4 (28%)
2	SO4	G	484	-	4,4,4	0.16	0	6,6,6	0.36	0
2	SO4	H	484	-	4,4,4	0.17	0	6,6,6	0.29	0
3	MES	E	485	-	12,12,12	2.47	1 (8%)	14,16,16	2.03	3 (21%)
2	SO4	C	484	-	4,4,4	0.18	0	6,6,6	0.34	0
3	MES	A	485	-	12,12,12	2.55	1 (8%)	14,16,16	3.06	4 (28%)
3	MES	F	485	-	12,12,12	2.74	1 (8%)	14,16,16	2.59	4 (28%)
2	SO4	F	484	-	4,4,4	0.20	0	6,6,6	0.15	0
3	MES	G	485	-	12,12,12	2.21	1 (8%)	14,16,16	2.54	4 (28%)
2	SO4	A	484	-	4,4,4	0.21	0	6,6,6	0.55	0
2	SO4	E	484	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	D	484	-	4,4,4	0.14	0	6,6,6	0.24	0
3	MES	B	485	-	12,12,12	2.38	1 (8%)	14,16,16	2.15	5 (35%)
2	SO4	B	484	-	4,4,4	0.20	0	6,6,6	0.33	0
3	MES	H	485	-	12,12,12	2.05	1 (8%)	14,16,16	1.78	5 (35%)

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
3	MES	C	485	-	-	3/6/14/14	0/1/1/1
3	MES	D	485	-	-	3/6/14/14	0/1/1/1
3	MES	F	485	-	-	1/6/14/14	0/1/1/1
3	MES	E	485	-	-	2/6/14/14	0/1/1/1
3	MES	A	485	-	-	5/6/14/14	0/1/1/1
3	MES	G	485	-	-	3/6/14/14	0/1/1/1
3	MES	B	485	-	-	6/6/14/14	0/1/1/1
3	MES	H	485	-	-	1/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	485	MES	C8-S	-9.20	1.64	1.77
3	A	485	MES	C8-S	-8.46	1.65	1.77
3	E	485	MES	C8-S	-8.29	1.65	1.77
3	D	485	MES	C8-S	-8.18	1.65	1.77
3	B	485	MES	C8-S	-7.94	1.66	1.77
3	C	485	MES	C8-S	-7.73	1.66	1.77
3	G	485	MES	C8-S	-7.27	1.67	1.77
3	H	485	MES	C8-S	-6.75	1.67	1.77

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	485	MES	O1S-S-C8	9.64	118.53	106.92
3	D	485	MES	O1S-S-C8	7.24	115.63	106.92
3	G	485	MES	O1S-S-C8	6.52	114.77	106.92
3	F	485	MES	O1S-S-C8	6.01	114.16	106.92
3	E	485	MES	O1S-S-C8	5.52	113.57	106.92
3	D	485	MES	O2S-S-C8	-5.32	100.51	106.92
3	F	485	MES	C2-C3-N4	-5.07	102.41	110.10
3	D	485	MES	C5-N4-C3	4.79	119.61	108.83
3	G	485	MES	O2S-S-C8	4.78	112.67	106.92
3	B	485	MES	C5-N4-C3	4.15	118.16	108.83
3	E	485	MES	C2-C3-N4	-3.48	104.83	110.10
3	B	485	MES	O3S-S-C8	3.46	111.36	105.77
3	B	485	MES	O1S-S-C8	3.43	111.04	106.92
3	A	485	MES	C2-C3-N4	-3.39	104.97	110.10
3	H	485	MES	O2S-S-C8	3.32	110.91	106.92
3	F	485	MES	C6-C5-N4	-3.22	105.22	110.10
3	G	485	MES	O3S-S-O1S	-3.21	103.43	111.27
3	H	485	MES	O3S-S-C8	3.09	110.77	105.77
3	C	485	MES	O3S-S-C8	3.06	110.71	105.77
3	D	485	MES	O3S-S-C8	2.99	110.60	105.77
3	C	485	MES	C2-C3-N4	-2.94	105.64	110.10
3	F	485	MES	O1-C6-C5	-2.83	105.57	111.80
3	H	485	MES	O3S-S-O1S	-2.51	105.15	111.27
3	H	485	MES	C6-C5-N4	-2.47	106.36	110.10
3	G	485	MES	C2-C3-N4	-2.32	106.59	110.10
3	A	485	MES	C7-N4-C3	-2.31	105.32	111.23
3	B	485	MES	C2-C3-N4	-2.31	106.60	110.10
3	H	485	MES	O1S-S-C8	2.28	109.66	106.92
3	B	485	MES	O1-C2-C3	-2.21	106.93	111.80
3	A	485	MES	O3S-S-O2S	-2.13	106.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	485	MES	C6-O1-C2	2.02	116.65	109.89

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	485	MES	C8-C7-N4-C5
3	A	485	MES	C7-C8-S-O2S
3	A	485	MES	C7-C8-S-O3S
3	B	485	MES	N4-C7-C8-S
3	B	485	MES	C7-C8-S-O1S
3	C	485	MES	C8-C7-N4-C3
3	C	485	MES	N4-C7-C8-S
3	D	485	MES	C8-C7-N4-C5
3	D	485	MES	N4-C7-C8-S
3	E	485	MES	C8-C7-N4-C3
3	E	485	MES	N4-C7-C8-S
3	F	485	MES	C8-C7-N4-C3
3	G	485	MES	C8-C7-N4-C3
3	G	485	MES	N4-C7-C8-S
3	H	485	MES	C8-C7-N4-C3
3	B	485	MES	C7-C8-S-O3S
3	B	485	MES	C8-C7-N4-C3
3	B	485	MES	C8-C7-N4-C5
3	D	485	MES	C8-C7-N4-C3
3	G	485	MES	C8-C7-N4-C5
3	A	485	MES	C7-C8-S-O1S
3	B	485	MES	C7-C8-S-O2S
3	A	485	MES	C8-C7-N4-C3
3	C	485	MES	C8-C7-N4-C5

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	485	MES	3	0
3	D	485	MES	2	0
3	E	485	MES	3	0
3	A	485	MES	2	0
3	F	485	MES	3	0
3	G	485	MES	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	484	SO4	1	0
3	B	485	MES	2	0
3	H	485	MES	2	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	485/504 (96%)	-0.72	1 (0%)	95	95	10, 18, 29, 39	0
1	B	483/504 (95%)	-0.73	1 (0%)	95	95	11, 20, 30, 40	0
1	C	483/504 (95%)	-0.57	1 (0%)	95	95	13, 23, 34, 56	0
1	D	483/504 (95%)	-0.50	2 (0%)	92	93	13, 26, 41, 60	0
1	E	483/504 (95%)	-0.37	4 (0%)	86	88	17, 30, 42, 64	0
1	F	483/504 (95%)	-0.72	1 (0%)	95	95	13, 20, 30, 54	0
1	G	482/504 (95%)	-0.47	3 (0%)	89	91	14, 26, 45, 54	0
1	H	483/504 (95%)	-0.30	8 (1%)	70	74	18, 31, 43, 63	0
All	All	3865/4032 (95%)	-0.55	21 (0%)	91	92	10, 24, 40, 64	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	6.6
1	D	1	MET	5.1
1	F	1	MET	5.1
1	H	1	MET	5.0
1	C	1	MET	3.9
1	A	-1	GLY	3.7
1	H	3	ALA	2.8
1	E	19	ARG	2.7
1	D	290[A]	CYS	2.6
1	B	1	MET	2.6
1	H	37	GLY	2.5
1	H	325	PRO	2.4
1	G	325	PRO	2.4
1	G	339	THR	2.2
1	E	290[A]	CYS	2.2
1	H	215	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	36	ASP	2.1
1	G	315	LYS	2.1
1	H	315	LYS	2.1
1	H	378	ASP	2.1
1	E	350	SER	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	MES	C	485	12/12	0.87	0.46	19,21,24,25	12
3	MES	F	485	12/12	0.88	0.31	28,30,33,35	12
3	MES	E	485	12/12	0.89	0.25	34,35,36,37	12
2	SO4	H	484	5/5	0.89	0.18	88,88,89,89	0
3	MES	H	485	12/12	0.90	0.23	28,29,31,32	12
2	SO4	C	484	5/5	0.91	0.17	61,62,63,63	0
3	MES	A	485	12/12	0.91	0.28	16,20,21,23	12
3	MES	D	485	12/12	0.92	0.21	27,29,32,32	12
3	MES	G	485	12/12	0.93	0.21	25,27,27,30	12
3	MES	B	485	12/12	0.94	0.24	26,27,29,30	12
2	SO4	E	484	5/5	0.95	0.17	75,75,75,77	0
2	SO4	G	484	5/5	0.97	0.11	45,49,50,53	0
2	SO4	A	484	5/5	0.98	0.15	49,51,54,54	0
2	SO4	F	484	5/5	0.98	0.14	47,48,50,50	0
2	SO4	D	484	5/5	0.98	0.18	49,51,52,54	0
2	SO4	B	484	5/5	0.99	0.11	42,43,44,45	0

6.5 Other polymers (i)

There are no such residues in this entry.