Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:54 AM GMT

PDB ID	:	3K2W
Title	:	CRYSTAL STRUCTURE OF betaine-aldehyde dehydrogenase FROM Pseudoalteromonas atlantica T6c
Authors	:	Patskovsky, Y.; Toro, R.; Rutter, M.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2009-09-30
Resolution	:	1.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

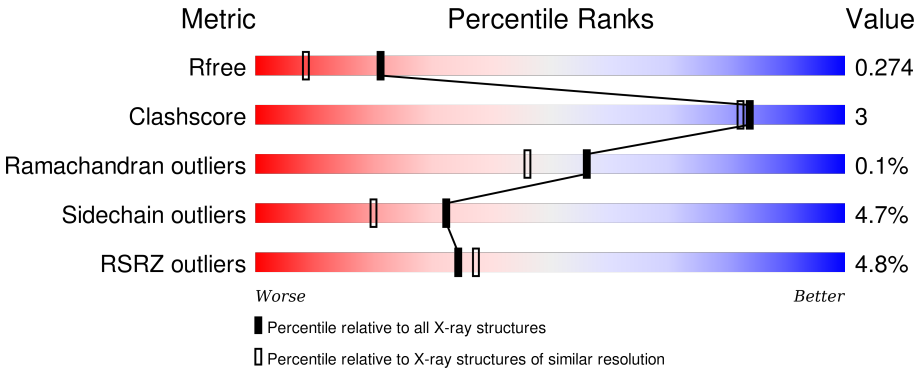
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	497	13% 85% 10%
1	B	497	8% 84% 13%
1	C	497	% 88% 8%
1	D	497	2% 84% 13%
1	E	497	% 90% 8%

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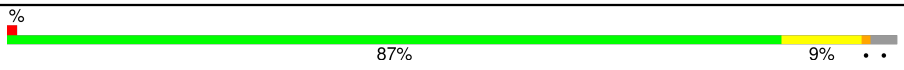
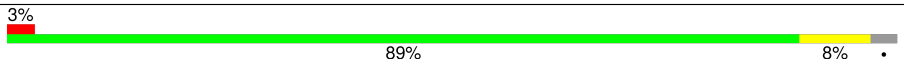
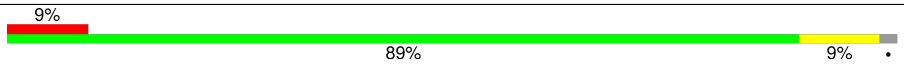
Mol	Chain	Length	Quality of chain
1	F	497	
1	G	497	
1	H	497	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	499	-	-	-	X
2	GOL	E	497	-	-	-	X
2	GOL	F	497	-	-	-	X
2	GOL	G	496	-	-	-	X
4	ACT	D	500	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31410 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 Betaine-aldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	7	0
			3659	2311	617	707	24			
1	B	488	Total	C	N	O	S	0	2	0
			3720	2346	622	728	24			
1	C	484	Total	C	N	O	S	0	5	0
			3708	2341	622	721	24			
1	D	483	Total	C	N	O	S	0	8	0
			3712	2346	622	719	25			
1	E	486	Total	C	N	O	S	0	5	0
			3718	2347	620	726	25			
1	F	483	Total	C	N	O	S	0	9	0
			3720	2354	618	723	25			
1	G	484	Total	C	N	O	S	0	6	0
			3708	2343	619	722	24			
1	H	486	Total	C	N	O	S	0	5	0
			3719	2347	624	723	25			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q15SR9
A	0	SER	-	expression tag	UNP Q15SR9
A	1	LEU	-	expression tag	UNP Q15SR9
A	488	GLU	-	expression tag	UNP Q15SR9
A	489	GLY	-	expression tag	UNP Q15SR9
A	490	HIS	-	expression tag	UNP Q15SR9
A	491	HIS	-	expression tag	UNP Q15SR9
A	492	HIS	-	expression tag	UNP Q15SR9
A	493	HIS	-	expression tag	UNP Q15SR9
A	494	HIS	-	expression tag	UNP Q15SR9
A	495	HIS	-	expression tag	UNP Q15SR9
B	-1	MET	-	expression tag	UNP Q15SR9
B	0	SER	-	expression tag	UNP Q15SR9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	LEU	-	expression tag	UNP Q15SR9
B	488	GLU	-	expression tag	UNP Q15SR9
B	489	GLY	-	expression tag	UNP Q15SR9
B	490	HIS	-	expression tag	UNP Q15SR9
B	491	HIS	-	expression tag	UNP Q15SR9
B	492	HIS	-	expression tag	UNP Q15SR9
B	493	HIS	-	expression tag	UNP Q15SR9
B	494	HIS	-	expression tag	UNP Q15SR9
B	495	HIS	-	expression tag	UNP Q15SR9
C	-1	MET	-	expression tag	UNP Q15SR9
C	0	SER	-	expression tag	UNP Q15SR9
C	1	LEU	-	expression tag	UNP Q15SR9
C	488	GLU	-	expression tag	UNP Q15SR9
C	489	GLY	-	expression tag	UNP Q15SR9
C	490	HIS	-	expression tag	UNP Q15SR9
C	491	HIS	-	expression tag	UNP Q15SR9
C	492	HIS	-	expression tag	UNP Q15SR9
C	493	HIS	-	expression tag	UNP Q15SR9
C	494	HIS	-	expression tag	UNP Q15SR9
C	495	HIS	-	expression tag	UNP Q15SR9
D	-1	MET	-	expression tag	UNP Q15SR9
D	0	SER	-	expression tag	UNP Q15SR9
D	1	LEU	-	expression tag	UNP Q15SR9
D	488	GLU	-	expression tag	UNP Q15SR9
D	489	GLY	-	expression tag	UNP Q15SR9
D	490	HIS	-	expression tag	UNP Q15SR9
D	491	HIS	-	expression tag	UNP Q15SR9
D	492	HIS	-	expression tag	UNP Q15SR9
D	493	HIS	-	expression tag	UNP Q15SR9
D	494	HIS	-	expression tag	UNP Q15SR9
D	495	HIS	-	expression tag	UNP Q15SR9
E	-1	MET	-	expression tag	UNP Q15SR9
E	0	SER	-	expression tag	UNP Q15SR9
E	1	LEU	-	expression tag	UNP Q15SR9
E	488	GLU	-	expression tag	UNP Q15SR9
E	489	GLY	-	expression tag	UNP Q15SR9
E	490	HIS	-	expression tag	UNP Q15SR9
E	491	HIS	-	expression tag	UNP Q15SR9
E	492	HIS	-	expression tag	UNP Q15SR9
E	493	HIS	-	expression tag	UNP Q15SR9
E	494	HIS	-	expression tag	UNP Q15SR9
E	495	HIS	-	expression tag	UNP Q15SR9

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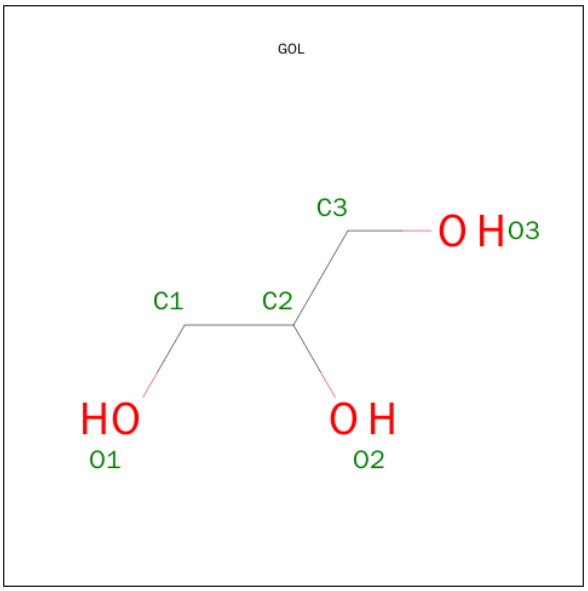
Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	MET	-	expression tag	UNP Q15SR9
F	0	SER	-	expression tag	UNP Q15SR9
F	1	LEU	-	expression tag	UNP Q15SR9
F	488	GLU	-	expression tag	UNP Q15SR9
F	489	GLY	-	expression tag	UNP Q15SR9
F	490	HIS	-	expression tag	UNP Q15SR9
F	491	HIS	-	expression tag	UNP Q15SR9
F	492	HIS	-	expression tag	UNP Q15SR9
F	493	HIS	-	expression tag	UNP Q15SR9
F	494	HIS	-	expression tag	UNP Q15SR9
F	495	HIS	-	expression tag	UNP Q15SR9
G	-1	MET	-	expression tag	UNP Q15SR9
G	0	SER	-	expression tag	UNP Q15SR9
G	1	LEU	-	expression tag	UNP Q15SR9
G	488	GLU	-	expression tag	UNP Q15SR9
G	489	GLY	-	expression tag	UNP Q15SR9
G	490	HIS	-	expression tag	UNP Q15SR9
G	491	HIS	-	expression tag	UNP Q15SR9
G	492	HIS	-	expression tag	UNP Q15SR9
G	493	HIS	-	expression tag	UNP Q15SR9
G	494	HIS	-	expression tag	UNP Q15SR9
G	495	HIS	-	expression tag	UNP Q15SR9
H	-1	MET	-	expression tag	UNP Q15SR9
H	0	SER	-	expression tag	UNP Q15SR9
H	1	LEU	-	expression tag	UNP Q15SR9
H	488	GLU	-	expression tag	UNP Q15SR9
H	489	GLY	-	expression tag	UNP Q15SR9
H	490	HIS	-	expression tag	UNP Q15SR9
H	491	HIS	-	expression tag	UNP Q15SR9
H	492	HIS	-	expression tag	UNP Q15SR9
H	493	HIS	-	expression tag	UNP Q15SR9
H	494	HIS	-	expression tag	UNP Q15SR9
H	495	HIS	-	expression tag	UNP Q15SR9

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

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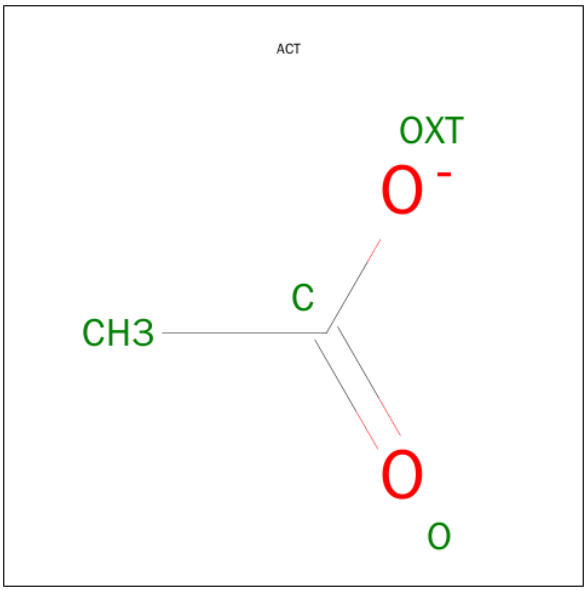
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	154	Total O 154 154	0	0
5	B	170	Total O 170 170	0	0
5	C	224	Total O 224 224	0	0
5	D	218	Total O 218 218	0	0
5	E	227	Total O 227 227	0	0
5	F	220	Total O 220 220	0	0

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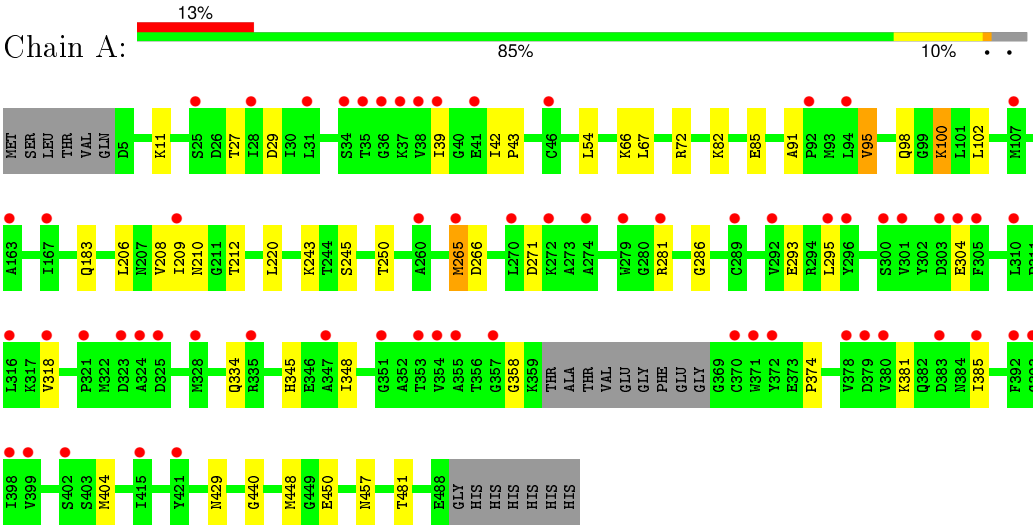
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	220	Total O 220 220	0	0
5	H	179	Total O 179 179	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

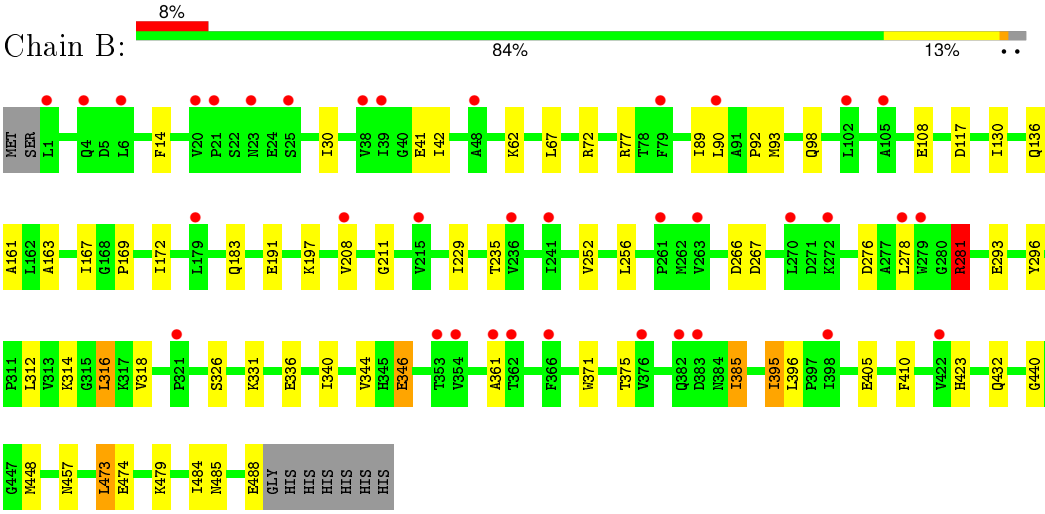
- Molecule 1: Betaine-aldehyde dehydrogenase

Chain A:



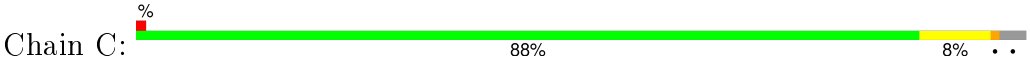
- Molecule 1: Betaine-aldehyde dehydrogenase

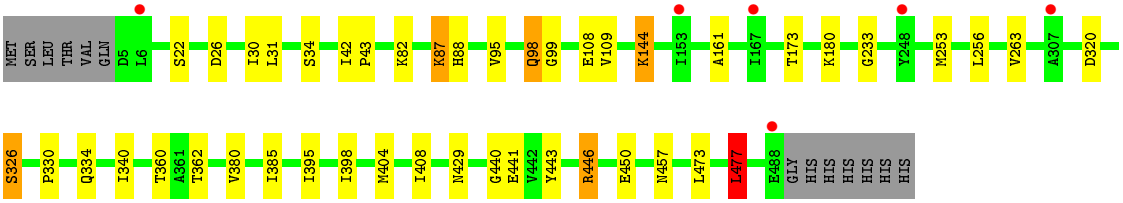
Chain B:



- Molecule 1: Betaine-aldehyde dehydrogenase

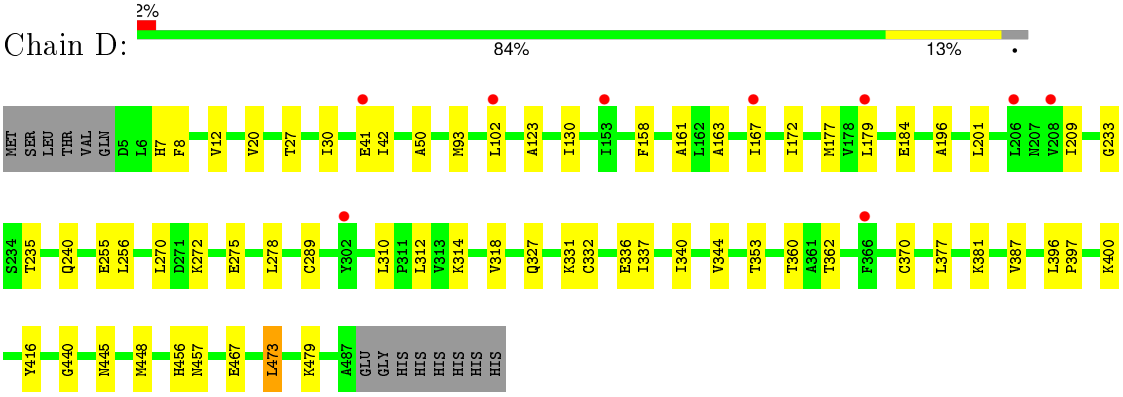
Chain C:





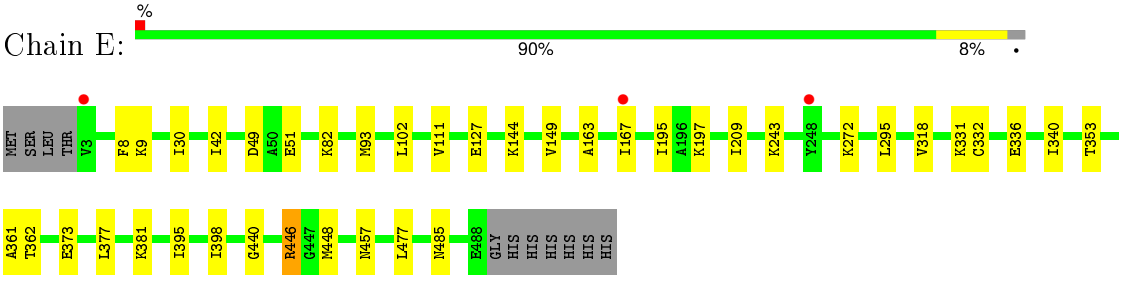
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain D:



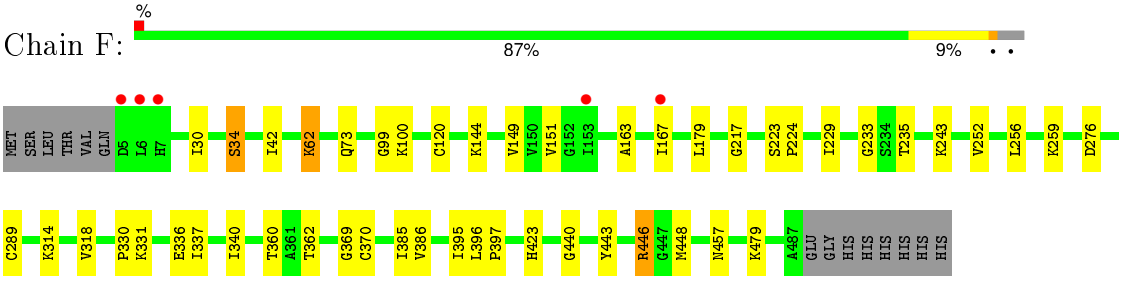
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain E:



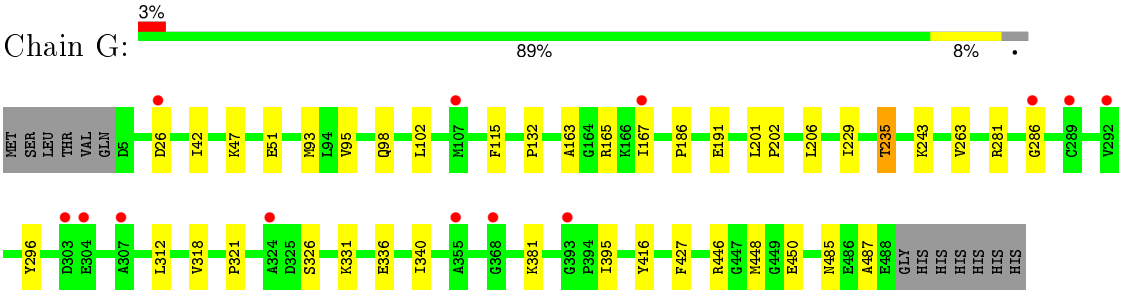
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain F:



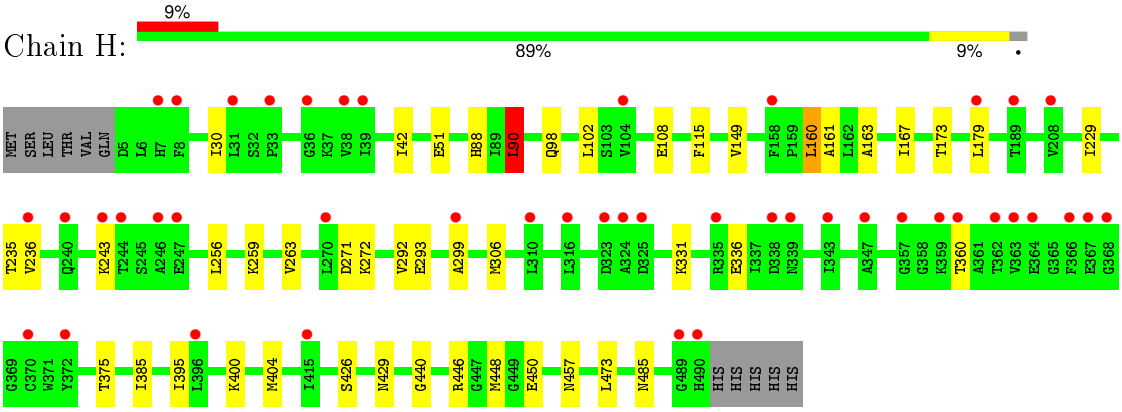
• Molecule 1: Betaine-aldehyde dehydrogenase

Chain G:



• Molecule 1: Betaine-aldehyde dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.78Å 163.72Å 142.07Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 29.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (20.00-1.90) 97.6 (29.97-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.210 , 0.274 0.211 , 0.274	Depositor DCC
R_{free} test set	9231 reflections (3.14%)	DCC
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.4	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 303118 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	31410	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, CL, ACT

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	0.55	2/3745 (0.1%)	0.65	0/5073
1	B	0.56	0/3793	0.67	1/5143 (0.0%)
1	C	0.55	0/3791	0.68	1/5139 (0.0%)
1	D	0.54	0/3804	0.68	1/5154 (0.0%)
1	E	0.56	0/3800	0.67	1/5151 (0.0%)
1	F	0.57	0/3814	0.66	0/5168
1	G	0.54	0/3793	0.66	0/5140
1	H	0.53	0/3802	0.65	1/5151 (0.0%)
All	All	0.55	2/30342 (0.0%)	0.67	5/41119 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLU	CD-OE2	-5.36	1.19	1.25
1	A	127	GLU	CD-OE1	-5.15	1.20	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	446	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	477	LEU	CA-CB-CG	5.58	128.13	115.30
1	D	473	LEU	CA-CB-CG	5.41	127.75	115.30
1	B	281	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	H	90	LEU	CA-CB-CG	5.18	127.22	115.30

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	3659	0	3659	21	0
1	B	3720	0	3693	33	0
1	C	3708	0	3689	26	0
1	D	3712	0	3708	25	0
1	E	3718	0	3697	16	0
1	F	3720	0	3720	23	0
1	G	3708	0	3700	17	0
1	H	3719	0	3700	16	0
2	A	6	0	8	0	0
2	B	18	0	24	3	0
2	C	6	0	8	2	0
2	D	18	0	24	1	0
2	E	12	0	16	0	0
2	F	18	0	24	1	0
2	G	18	0	24	2	0
2	H	6	0	8	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	B	4	0	3	0	0
4	C	8	0	6	0	0
4	D	4	0	3	1	0
4	E	4	0	3	0	0
4	F	4	0	3	0	0
5	A	154	0	0	0	0
5	B	170	0	0	1	0
5	C	224	0	0	2	0
5	D	218	0	0	1	0
5	E	227	0	0	3	0
5	F	220	0	0	1	0
5	G	220	0	0	2	0
5	H	179	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31410	0	29720	176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (176) 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:E:332:CYS:HB3	5:E:1434:HOH:O	1.73	0.87
1:B:163:ALA:O	1:B:167:ILE:HG12	1.77	0.84
1:G:340:ILE:HB	1:G:395:ILE:HD11	1.62	0.80
1:C:95:VAL:O	1:C:99:GLY:HA2	1.84	0.76
1:A:404:MET:HG2	1:A:429[A]:ASN:HB2	1.68	0.76
1:E:336:GLU:HG3	5:E:1434:HOH:O	1.91	0.70
1:B:484:ILE:HG21	2:B:499:GOL:H11	1.74	0.68
1:H:404:MET:HE2	1:H:429:ASN:HB3	1.77	0.67
1:C:404:MET:CE	1:C:429:ASN:HB3	2.25	0.66
1:G:235:THR:HG21	1:G:416:TYR:HE2	1.62	0.65
1:F:163:ALA:O	1:F:167:ILE:HG12	1.96	0.65
1:C:173:THR:HB	1:C:477:LEU:HD13	1.80	0.64
1:A:265:MET:HE2	1:A:266:ASP:HB2	1.80	0.63
1:B:281:ARG:HG2	1:B:396:LEU:HB2	1.81	0.63
1:D:163:ALA:O	1:D:167[A]:ILE:HG12	2.00	0.61
1:B:281:ARG:HD3	1:B:281:ARG:O	2.01	0.61
1:H:235:THR:HA	1:H:256:LEU:HD13	1.82	0.60
1:D:331:LYS:HE3	1:D:336:GLU:HB3	1.84	0.60
1:C:404:MET:HE3	1:C:429:ASN:HB3	1.84	0.60
1:H:331:LYS:HE3	1:H:336:GLU:HB3	1.84	0.60
1:H:404:MET:CE	1:H:429:ASN:HB3	2.33	0.59
1:B:485:ASN:ND2	5:B:878:HOH:O	2.36	0.58
1:C:380:VAL:H	2:C:497:GOL:H12	1.68	0.58
1:B:405:GLU:HG3	1:B:432:GLN:HE22	1.68	0.58
1:D:445:ASN:HB3	4:D:500:ACT:H2	1.85	0.58
1:A:265:MET:CE	1:A:266:ASP:HB2	2.35	0.57
1:C:95:VAL:O	1:C:99:GLY:CA	2.50	0.56
1:D:167[A]:ILE:HD11	1:D:179:LEU:HD22	1.87	0.56
1:F:331:LYS:HE3	1:F:336:GLU:HB3	1.88	0.56
1:G:163:ALA:O	1:G:167[A]:ILE:HG12	2.05	0.56
1:F:276:ASP:OD2	1:F:423:HIS:NE2	2.33	0.54
1:G:93:MET:SD	1:G:191:GLU:HG3	2.47	0.53
1:F:99:GLY:O	1:F:330:PRO:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ILE:HD11	1:C:42:ILE:HG12	1.91	0.53
1:H:485:ASN:ND2	5:H:1732:HOH:O	2.41	0.53
1:B:30:ILE:HD11	1:B:42:ILE:HG12	1.91	0.53
1:G:132:PRO:HD3	2:G:497:GOL:H11	1.91	0.53
1:G:95:VAL:HG13	1:G:321:PRO:HB2	1.90	0.52
1:F:443:TYR:HD1	1:F:446:ARG:HD2	1.73	0.52
1:B:235:THR:HA	1:B:256:LEU:HD13	1.91	0.52
1:E:340:ILE:HB	1:E:395:ILE:HD13	1.92	0.52
1:H:163:ALA:O	1:H:167:ILE:HG12	2.10	0.52
1:A:82:LYS:HA	1:A:85:GLU:HG2	1.91	0.52
1:F:337:ILE:HG13	1:F:370:CYS:HB3	1.90	0.52
1:F:217:GLY:HA3	2:F:498:GOL:H12	1.92	0.52
1:H:173:THR:HA	2:H:496:GOL:H2	1.91	0.52
1:C:404:MET:HE2	1:C:429:ASN:HB3	1.90	0.51
1:H:30:ILE:HD11	1:H:42:ILE:HG12	1.93	0.51
1:B:375:THR:HB	1:B:395:ILE:HG13	1.92	0.51
1:B:281:ARG:HH22	1:B:293:GLU:CD	2.14	0.51
1:C:144:LYS:HB3	1:C:477:LEU:HG	1.91	0.50
1:F:30[B]:ILE:HD11	1:F:42:ILE:HG12	1.94	0.50
1:E:127:GLU:O	1:E:144:LYS:HE2	2.11	0.50
1:A:281:ARG:NH2	1:A:293:GLU:HA	2.26	0.50
1:A:209[B]:ILE:HD11	1:A:220:LEU:HD21	1.93	0.50
1:G:47[A]:LYS:HE3	1:G:51[A]:GLU:HG3	1.93	0.50
1:C:398:ILE:O	2:C:497:GOL:H11	2.12	0.50
1:G:485:ASN:ND2	5:G:637:HOH:O	2.46	0.49
1:E:30:ILE:HD11	1:E:42:ILE:HG12	1.94	0.49
1:B:281:ARG:C	1:B:281:ARG:HD3	2.33	0.49
1:D:167[A]:ILE:HD13	1:D:177:MET:SD	2.52	0.49
1:C:98:GLN:C	1:C:98:GLN:CD	2.72	0.48
1:B:484:ILE:HD12	2:B:499:GOL:H32	1.94	0.48
1:H:440:GLY:HA3	1:H:457:ASN:O	2.14	0.48
1:F:229[A]:ILE:HB	1:F:252:VAL:HG12	1.95	0.48
1:D:27:THR:HB	1:D:41:GLU:HG2	1.95	0.47
1:H:90:LEU:HG	1:H:160:LEU:HD11	1.95	0.47
1:E:485:ASN:ND2	5:E:1707:HOH:O	2.46	0.47
1:A:100:LYS:HE3	1:A:100:LYS:HB3	1.74	0.47
1:F:62:LYS:H	1:F:62:LYS:HZ3	1.63	0.47
1:A:91:ALA:O	1:A:95:VAL:HG12	2.15	0.47
1:F:235:THR:HA	1:F:256:LEU:HD13	1.96	0.47
1:B:229:ILE:HB	1:B:252:VAL:HG12	1.97	0.47
1:D:8:PHE:CE1	1:D:93:MET:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:GLY:HA3	1:A:457:ASN:O	2.15	0.47
1:F:233:GLY:O	1:F:256:LEU:HA	2.15	0.46
1:H:375:THR:HB	1:H:395:ILE:HG13	1.97	0.46
1:B:144:LYS:HE3	1:B:474:GLU:OE2	2.15	0.46
1:A:11:LYS:HE2	1:A:27:THR:HG21	1.97	0.46
1:G:42:ILE:HG21	1:G:186:PRO:HG2	1.98	0.46
1:E:82:LYS:HB3	1:E:195:ILE:HG23	1.96	0.46
1:F:289:CYS:HB2	5:F:548:HOH:O	2.15	0.46
1:G:485:ASN:ND2	1:G:487:ALA:H	2.14	0.46
1:C:253:MET:HG2	5:C:706:HOH:O	2.15	0.46
1:E:361:ALA:HB2	1:E:373:GLU:HG3	1.98	0.46
1:B:296:TYR:CE2	1:B:410:PHE:HB3	2.51	0.46
1:G:331:LYS:HE3	1:G:336:GLU:HB3	1.98	0.46
1:F:34:SER:O	1:F:369:GLY:HA3	2.16	0.46
1:B:169:PRO:HB3	1:B:473:LEU:HG	1.98	0.45
1:A:98[A]:GLN:HG3	1:A:156:TRP:O	2.16	0.45
1:C:404:MET:O	1:C:408:ILE:HG12	2.16	0.45
1:C:173:THR:HB	1:C:477:LEU:CD1	2.46	0.45
1:C:98:GLN:O	1:C:98:GLN:CD	2.54	0.45
1:D:440:GLY:HA3	1:D:457:ASN:O	2.17	0.45
1:H:331:LYS:NZ	1:H:336:GLU:OE1	2.38	0.45
1:G:281:ARG:O	1:G:286:GLY:HA2	2.15	0.45
1:B:93:MET:SD	1:B:191:GLU:HG3	2.56	0.45
1:B:346:GLU:HB3	1:B:385:ILE:HG21	1.98	0.45
1:H:299:ALA:HA	1:H:400:LYS:HD2	1.99	0.45
1:E:8:PHE:CE1	1:E:93:MET:HG2	2.52	0.45
1:B:281:ARG:NH2	1:B:293:GLU:HA	2.32	0.44
1:B:130:ILE:O	2:B:497:GOL:H31	2.17	0.44
1:C:320:ASP:O	1:C:326:SER:OG	2.32	0.44
1:B:108:GLU:HG3	1:B:161:ALA:HB2	1.99	0.44
1:F:167:ILE:HD11	1:F:179:LEU:HD22	1.99	0.44
1:F:151:VAL:HB	1:F:229[A]:ILE:HD13	2.00	0.44
1:D:233:GLY:O	1:D:256:LEU:HA	2.18	0.44
1:A:345:HIS:HA	1:A:348:ILE:HD12	1.99	0.44
1:A:11:LYS:HA	1:A:43:PRO:HD3	1.99	0.44
1:C:440:GLY:HA3	1:C:457:ASN:O	2.18	0.44
1:H:259[B]:LYS:NZ	1:H:293:GLU:HB3	2.33	0.43
1:D:289:CYS:HB2	5:D:1393:HOH:O	2.18	0.43
1:B:340:ILE:O	1:B:344:VAL:HG23	2.18	0.43
1:B:331:LYS:HE3	1:B:336:GLU:HB3	2.01	0.43
1:H:167:ILE:HD11	1:H:179:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:ALA:HB2	1:D:172:ILE:HD11	1.99	0.43
1:B:278:LEU:HD11	1:B:316:LEU:HD11	1.99	0.43
1:G:263:VAL:HG12	1:G:296:TYR:HB2	2.01	0.43
1:B:67:LEU:O	1:B:72:ARG:NH1	2.51	0.43
1:B:440:GLY:HA3	1:B:457:ASN:O	2.19	0.43
1:F:259:LYS:NZ	1:F:386:VAL:O	2.51	0.43
1:A:67:LEU:O	1:A:72:ARG:NH1	2.52	0.42
1:G:427:PHE:HE2	2:G:496:GOL:H11	1.83	0.42
1:C:22:SER:HB2	1:C:43:PRO:HB3	2.01	0.42
1:D:387:VAL:HG12	1:D:387:VAL:O	2.19	0.42
1:D:30:ILE:HD11	1:D:42:ILE:HG12	2.00	0.42
1:E:440:GLY:HA3	1:E:457:ASN:O	2.20	0.42
1:C:87:LYS:HB2	1:C:109:VAL:HG11	2.01	0.42
1:A:42:ILE:HD12	1:A:210:ASN:HB3	2.01	0.42
1:H:108:GLU:HG3	1:H:161:ALA:HB2	2.00	0.42
1:F:100:LYS:HB3	1:F:100:LYS:HE3	1.88	0.42
1:E:144:LYS:HD2	1:E:477:LEU:HD13	2.01	0.42
1:C:340:ILE:HB	1:C:395:ILE:HD13	2.01	0.42
1:E:331:LYS:HE3	1:E:336:GLU:HB3	2.01	0.42
1:C:99:GLY:O	1:C:330:PRO:HD2	2.20	0.42
1:D:235:THR:HA	1:D:256:LEU:HD13	2.02	0.42
1:D:235:THR:HG21	1:D:416:TYR:HE2	1.84	0.42
1:B:89:ILE:O	1:B:92:PRO:HD2	2.19	0.42
1:D:310:LEU:HG	1:D:314:LYS:HE2	2.01	0.42
1:C:233:GLY:O	1:C:256:LEU:HA	2.20	0.41
1:B:77:ARG:NH1	1:B:117[B]:ASP:HB2	2.34	0.41
1:B:14:PHE:HB3	1:B:208:VAL:HG12	2.02	0.41
1:D:337:ILE:HG13	1:D:370:CYS:HB3	2.02	0.41
1:C:88[A]:HIS:ND1	5:C:1653:HOH:O	2.36	0.41
1:A:281:ARG:HH22	1:A:293:GLU:CD	2.24	0.41
1:A:481:THR:O	1:C:441:GLU:HA	2.21	0.41
1:C:443:TYR:HD1	1:C:446:ARG:HD2	1.85	0.41
1:B:172:ILE:HA	1:B:172:ILE:HD12	1.95	0.41
1:B:183:GLN:HB3	1:B:211:GLY:O	2.20	0.41
1:D:50:ALA:HA	1:D:209:ILE:HD13	2.02	0.41
1:D:130:ILE:O	2:D:497:GOL:H31	2.20	0.41
1:G:191:GLU:HG2	5:G:535:HOH:O	2.19	0.41
1:B:361:ALA:HB3	1:B:371:TRP:HB3	2.02	0.41
1:D:158:PHE:HB3	1:D:161:ALA:HB3	2.03	0.41
1:G:201:LEU:HA	1:G:202:PRO:HD3	1.90	0.41
1:F:440:GLY:HA3	1:F:457:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD11	1:A:220:LEU:HA	2.02	0.41
1:B:276:ASP:OD2	1:B:423:HIS:NE2	2.39	0.41
1:C:108:GLU:HG3	1:C:161:ALA:HB2	2.03	0.41
1:F:73:GLN:HG3	1:F:120:CYS:HB3	2.03	0.41
1:F:340:ILE:HB	1:F:395:ILE:HD13	2.03	0.41
1:E:49:ASP:HB3	1:E:209:ILE:HD11	2.03	0.41
1:D:278:LEU:HD13	1:D:312:LEU:HB3	2.02	0.41
1:D:340:ILE:O	1:D:344:VAL:HG23	2.21	0.40
1:F:223:SER:HA	1:F:224:PRO:HD3	2.00	0.40
1:F:396:LEU:HA	1:F:397:PRO:HD2	1.90	0.40
1:A:245:SER:HB2	1:A:250:THR:HB	2.03	0.40
1:D:196:ALA:HB1	1:D:201:LEU:HD22	2.04	0.40
1:E:295:LEU:HD23	1:E:398:ILE:HD13	2.03	0.40
1:E:163:ALA:O	1:E:167[A]:ILE:HG12	2.21	0.40
1:D:396:LEU:HA	1:D:397:PRO:HD2	1.96	0.40
1:G:115:PHE:CE2	1:G:165:ARG:HG3	2.57	0.40
1:A:281:ARG:O	1:A:286:GLY:HA2	2.22	0.40
1:A:183:GLN:HE22	1:A:212:THR:HG22	1.86	0.40
1:D:456:HIS:N	1:D:467:GLU:O	2.54	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	478/497 (96%)	456 (95%)	20 (4%)	2 (0%)	39	27
1	B	488/497 (98%)	468 (96%)	20 (4%)	0	100	100
1	C	487/497 (98%)	474 (97%)	13 (3%)	0	100	100
1	D	489/497 (98%)	472 (96%)	17 (4%)	0	100	100
1	E	489/497 (98%)	475 (97%)	14 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	490/497 (99%)	481 (98%)	9 (2%)	0	100	100
1	G	488/497 (98%)	474 (97%)	14 (3%)	0	100	100
1	H	489/497 (98%)	474 (97%)	14 (3%)	1 (0%)	52	42
All	All	3898/3976 (98%)	3774 (97%)	121 (3%)	3 (0%)	56	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	H	292	VAL
1	A	358	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	396/407 (97%)	375 (95%)	21 (5%)	28	16
1	B	401/407 (98%)	377 (94%)	24 (6%)	24	12
1	C	400/407 (98%)	382 (96%)	18 (4%)	34	21
1	D	402/407 (99%)	379 (94%)	23 (6%)	25	13
1	E	402/407 (99%)	388 (96%)	14 (4%)	43	31
1	F	403/407 (99%)	390 (97%)	13 (3%)	46	35
1	G	401/407 (98%)	387 (96%)	14 (4%)	43	31
1	H	401/407 (98%)	379 (94%)	22 (6%)	27	14
All	All	3206/3256 (98%)	3057 (95%)	149 (5%)	32	21

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	39	ILE
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	95	VAL
1	A	100	LYS
1	A	102	LEU
1	A	206	LEU
1	A	208	VAL
1	A	243	LYS
1	A	265	MET
1	A	271	ASP
1	A	295	LEU
1	A	304	GLU
1	A	314	LYS
1	A	318	VAL
1	A	334	GLN
1	A	381	LYS
1	A	385	ILE
1	A	396	LEU
1	A	448	MET
1	A	450	GLU
1	B	41	GLU
1	B	62	LYS
1	B	90	LEU
1	B	98	GLN
1	B	136	GLN
1	B	137	ASP
1	B	144	LYS
1	B	197	LYS
1	B	266	ASP
1	B	267	ASP
1	B	281	ARG
1	B	312	LEU
1	B	314	LYS
1	B	316	LEU
1	B	318	VAL
1	B	326	SER
1	B	346	GLU
1	B	385	ILE
1	B	395	ILE
1	B	446	ARG
1	B	448	MET
1	B	473	LEU
1	B	479	LYS
1	B	488	GLU

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Mol	Chain	Res	Type
1	C	26	ASP
1	C	31	LEU
1	C	34	SER
1	C	82	LYS
1	C	87	LYS
1	C	98	GLN
1	C	144	LYS
1	C	180	LYS
1	C	263	VAL
1	C	326	SER
1	C	334	GLN
1	C	360	THR
1	C	362	THR
1	C	385	ILE
1	C	446	ARG
1	C	450	GLU
1	C	473	LEU
1	C	477	LEU
1	D	7	HIS
1	D	12	VAL
1	D	20	VAL
1	D	102	LEU
1	D	184	GLU
1	D	240	GLN
1	D	255[A]	GLU
1	D	255[B]	GLU
1	D	270	LEU
1	D	272	LYS
1	D	275	GLU
1	D	318	VAL
1	D	327	GLN
1	D	332	CYS
1	D	353	THR
1	D	360	THR
1	D	362	THR
1	D	377	LEU
1	D	381	LYS
1	D	400	LYS
1	D	448	MET
1	D	473	LEU
1	D	479	LYS
1	E	9	LYS

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Mol	Chain	Res	Type
1	E	51	GLU
1	E	102	LEU
1	E	149	VAL
1	E	197	LYS
1	E	243	LYS
1	E	272	LYS
1	E	318	VAL
1	E	353	THR
1	E	362	THR
1	E	377	LEU
1	E	381	LYS
1	E	446	ARG
1	E	448	MET
1	F	34	SER
1	F	62	LYS
1	F	144	LYS
1	F	149	VAL
1	F	243	LYS
1	F	314	LYS
1	F	318	VAL
1	F	360	THR
1	F	362	THR
1	F	385	ILE
1	F	446	ARG
1	F	448	MET
1	F	479	LYS
1	G	26	ASP
1	G	98	GLN
1	G	102	LEU
1	G	206	LEU
1	G	229	ILE
1	G	235	THR
1	G	243	LYS
1	G	312	LEU
1	G	318	VAL
1	G	326	SER
1	G	381	LYS
1	G	446	ARG
1	G	448	MET
1	G	450	GLU
1	H	51	GLU
1	H	88	HIS

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Mol	Chain	Res	Type
1	H	90	LEU
1	H	98	GLN
1	H	102	LEU
1	H	115	PHE
1	H	149	VAL
1	H	160	LEU
1	H	229	ILE
1	H	236	VAL
1	H	243	LYS
1	H	263	VAL
1	H	271	ASP
1	H	272	LYS
1	H	306	MET
1	H	360	THR
1	H	385	ILE
1	H	426	SER
1	H	446	ARG
1	H	448	MET
1	H	450	GLU
1	H	473	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	183	GLN
1	A	218	GLN
1	A	485	ASN
1	B	327	GLN
1	B	432	GLN
1	B	485	ASN
1	C	23	ASN
1	C	74	ASN
1	C	135	ASN
1	D	327	GLN
1	E	218	GLN
1	E	485	ASN
1	F	334	GLN
1	G	485	ASN
1	H	240	GLN
1	H	485	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GOL	A	496	-	5,5,5	0.44	0	5,5,5	0.09	0
2	GOL	B	496	-	5,5,5	0.35	0	5,5,5	1.00	0
2	GOL	B	497	-	5,5,5	0.53	0	5,5,5	0.60	0
4	ACT	B	498	-	1,3,3	1.49	0	0,3,3	0.00	-
2	GOL	B	499	-	5,5,5	0.37	0	5,5,5	0.80	0
2	GOL	C	497	-	5,5,5	0.39	0	5,5,5	0.38	0
4	ACT	C	498	-	1,3,3	0.68	0	0,3,3	0.00	-
4	ACT	C	499	-	1,3,3	1.03	0	0,3,3	0.00	-
2	GOL	D	496	-	5,5,5	0.46	0	5,5,5	0.41	0
2	GOL	D	497	-	5,5,5	0.37	0	5,5,5	0.62	0
2	GOL	D	498	-	5,5,5	0.36	0	5,5,5	0.43	0
4	ACT	D	500	-	1,3,3	1.02	0	0,3,3	0.00	-
2	GOL	E	496	-	5,5,5	0.54	0	5,5,5	0.39	0
2	GOL	E	497	-	5,5,5	0.55	0	5,5,5	0.75	0
4	ACT	E	499	-	1,3,3	0.37	0	0,3,3	0.00	-
2	GOL	F	496	-	5,5,5	0.48	0	5,5,5	0.81	0
2	GOL	F	497	-	5,5,5	0.31	0	5,5,5	0.36	0
2	GOL	F	498	-	5,5,5	0.33	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	F	500	-	1,3,3	0.31	0	0,3,3	0.00	-
2	GOL	G	496	-	5,5,5	0.46	0	5,5,5	0.42	0
2	GOL	G	497	-	5,5,5	0.39	0	5,5,5	0.70	0
2	GOL	G	498	-	5,5,5	0.30	0	5,5,5	0.41	0
2	GOL	H	496	-	5,5,5	0.40	0	5,5,5	0.53	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	496	-	-	0/4/4/4	0/0/0/0
2	GOL	B	496	-	-	0/4/4/4	0/0/0/0
2	GOL	B	497	-	-	0/4/4/4	0/0/0/0
4	ACT	B	498	-	-	0/0/0/0	0/0/0/0
2	GOL	B	499	-	-	0/4/4/4	0/0/0/0
2	GOL	C	497	-	-	0/4/4/4	0/0/0/0
4	ACT	C	498	-	-	0/0/0/0	0/0/0/0
4	ACT	C	499	-	-	0/0/0/0	0/0/0/0
2	GOL	D	496	-	-	0/4/4/4	0/0/0/0
2	GOL	D	497	-	-	0/4/4/4	0/0/0/0
2	GOL	D	498	-	-	0/4/4/4	0/0/0/0
4	ACT	D	500	-	-	0/0/0/0	0/0/0/0
2	GOL	E	496	-	-	0/4/4/4	0/0/0/0
2	GOL	E	497	-	-	0/4/4/4	0/0/0/0
4	ACT	E	499	-	-	0/0/0/0	0/0/0/0
2	GOL	F	496	-	-	0/4/4/4	0/0/0/0
2	GOL	F	497	-	-	0/4/4/4	0/0/0/0
2	GOL	F	498	-	-	0/4/4/4	0/0/0/0
4	ACT	F	500	-	-	0/0/0/0	0/0/0/0
2	GOL	G	496	-	-	0/4/4/4	0/0/0/0
2	GOL	G	497	-	-	0/4/4/4	0/0/0/0
2	GOL	G	498	-	-	0/4/4/4	0/0/0/0
2	GOL	H	496	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	497	GOL	1	0
2	B	499	GOL	2	0
2	C	497	GOL	2	0
2	D	497	GOL	1	0
4	D	500	ACT	1	0
2	F	498	GOL	1	0
2	G	496	GOL	1	0
2	G	497	GOL	1	0
2	H	496	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	475/497 (95%)	0.74	66 (13%) 4 4	21, 48, 75, 92	0
1	B	488/497 (98%)	0.59	39 (7%) 15 17	20, 42, 62, 72	0
1	C	484/497 (97%)	0.06	6 (1%) 81 83	20, 34, 50, 93	0
1	D	483/497 (97%)	0.19	9 (1%) 70 73	21, 36, 54, 76	0
1	E	486/497 (97%)	0.00	3 (0%) 90 91	21, 35, 52, 78	0
1	F	483/497 (97%)	0.03	5 (1%) 84 86	22, 34, 49, 81	0
1	G	484/497 (97%)	0.21	13 (2%) 58 61	20, 39, 60, 79	0
1	H	486/497 (97%)	0.63	45 (9%) 11 12	20, 45, 70, 93	0
All	All	3869/3976 (97%)	0.31	186 (4%) 34 37	20, 38, 63, 93	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	343	ILE	5.2
1	A	396	LEU	4.9
1	A	39	ILE	4.8
1	H	490	HIS	4.7
1	H	363	VAL	4.7
1	B	20	VAL	4.6
1	H	316	LEU	4.4
1	A	34	SER	4.4
1	A	312	LEU	4.2
1	A	295	LEU	4.2
1	H	489	GLY	4.0
1	A	370	CYS	3.9
1	H	179	LEU	3.9
1	A	371	TRP	3.8
1	H	246	ALA	3.7
1	A	281	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	366	PHE	3.7
1	A	292	VAL	3.7
1	A	321	PRO	3.6
1	A	335	ARG	3.6
1	H	33	PRO	3.6
1	C	488	GLU	3.6
1	B	1	LEU	3.6
1	H	270	LEU	3.6
1	H	415	ILE	3.6
1	A	300	SER	3.5
1	A	385	ILE	3.4
1	B	353	THR	3.4
1	A	310	LEU	3.4
1	B	299	ALA	3.3
1	G	307	ALA	3.3
1	H	335	ARG	3.3
1	B	105	ALA	3.3
1	E	3	VAL	3.3
1	D	366	PHE	3.3
1	B	270	LEU	3.2
1	A	272	LYS	3.2
1	A	398	ILE	3.2
1	H	366	PHE	3.2
1	A	37	LYS	3.2
1	C	248	TYR	3.2
1	A	274	ALA	3.1
1	G	324	ALA	3.1
1	B	25	SER	3.1
1	A	325	ASP	3.1
1	H	31	LEU	3.0
1	H	368	GLY	3.0
1	H	325	ASP	3.0
1	B	310	LEU	3.0
1	A	347	ALA	3.0
1	A	351	GLY	3.0
1	H	338	ASP	3.0
1	H	310	LEU	2.9
1	B	236	VAL	2.9
1	H	362	THR	2.9
1	A	31	LEU	2.9
1	A	304	GLU	2.9
1	H	323	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	2.8
1	H	7	HIS	2.8
1	A	279	TRP	2.8
1	A	355	ALA	2.8
1	B	102	LEU	2.8
1	H	189	THR	2.8
1	G	393	GLY	2.7
1	B	23	ASN	2.7
1	B	48	ALA	2.7
1	B	38	VAL	2.7
1	H	364	GLU	2.7
1	C	307	ALA	2.7
1	H	8	PHE	2.6
1	A	316	LEU	2.6
1	B	362	THR	2.6
1	H	370	CYS	2.6
1	D	167[A]	ILE	2.6
1	B	382	GLN	2.6
1	A	260	ALA	2.6
1	B	208	VAL	2.6
1	A	303	ASP	2.6
1	F	7	HIS	2.6
1	A	354	VAL	2.5
1	G	26	ASP	2.5
1	A	395	ILE	2.5
1	B	422	VAL	2.5
1	A	107	MET	2.5
1	A	379	ASP	2.5
1	A	383	ASP	2.5
1	D	208	VAL	2.5
1	B	39	ILE	2.5
1	H	39	ILE	2.5
1	H	372	TYR	2.5
1	G	304	GLU	2.5
1	G	303	ASP	2.5
1	A	301	VAL	2.5
1	C	153	ILE	2.5
1	G	368	GLY	2.5
1	A	353	THR	2.5
1	H	367	GLU	2.4
1	H	240	GLN	2.4
1	A	92	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	339	ASN	2.4
1	B	90	LEU	2.4
1	H	243	LYS	2.4
1	A	41	GLU	2.4
1	B	398	ILE	2.4
1	F	167	ILE	2.4
1	B	321	PRO	2.4
1	A	318	VAL	2.4
1	A	46	CYS	2.4
1	F	5	ASP	2.4
1	A	296	TYR	2.4
1	D	179	LEU	2.4
1	H	347	ALA	2.4
1	G	107	MET	2.4
1	B	4	GLN	2.3
1	D	41	GLU	2.3
1	G	289	CYS	2.3
1	H	359	LYS	2.3
1	B	21	PRO	2.3
1	B	261	PRO	2.3
1	A	289	CYS	2.3
1	E	248	TYR	2.3
1	A	94	LEU	2.3
1	A	35	THR	2.3
1	A	167	ILE	2.3
1	A	372	TYR	2.3
1	D	206	LEU	2.3
1	G	355	ALA	2.3
1	A	28	ILE	2.3
1	G	167[A]	ILE	2.3
1	A	305	PHE	2.3
1	B	79	PHE	2.3
1	H	244	THR	2.3
1	H	360	THR	2.3
1	H	396	LEU	2.2
1	A	323	ASP	2.2
1	A	38	VAL	2.2
1	C	167	ILE	2.2
1	D	302	TYR	2.2
1	B	215	VAL	2.2
1	B	442	VAL	2.2
1	H	104	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	324	ALA	2.2
1	H	324	ALA	2.2
1	H	247	GLU	2.2
1	H	36	GLY	2.2
1	B	354	VAL	2.2
1	B	279	TRP	2.2
1	A	25	SER	2.2
1	E	167[A]	ILE	2.2
1	C	6	LEU	2.2
1	A	378	VAL	2.2
1	B	263	VAL	2.2
1	B	376	VAL	2.2
1	B	272	LYS	2.2
1	A	392	PHE	2.2
1	D	102	LEU	2.2
1	F	6	LEU	2.2
1	B	179	LEU	2.1
1	A	328	MET	2.1
1	G	292	VAL	2.1
1	H	38	VAL	2.1
1	H	158	PHE	2.1
1	D	153	ILE	2.1
1	F	153	ILE	2.1
1	B	383	ASP	2.1
1	A	421	TYR	2.1
1	A	163	ALA	2.1
1	B	361	ALA	2.1
1	H	236	VAL	2.1
1	A	357	GLY	2.1
1	B	241	ILE	2.1
1	G	286	GLY	2.1
1	H	208	VAL	2.1
1	A	209[A]	ILE	2.1
1	A	380	VAL	2.1
1	A	399	VAL	2.1
1	A	265	MET	2.1
1	H	299	ALA	2.0
1	B	6	LEU	2.0
1	A	402	SER	2.0
1	A	393	GLY	2.0
1	B	278	LEU	2.0
1	A	36	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	357	GLY	2.0
1	A	415	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	G	496	6/6	0.92	0.22	4.40	39,44,55,59	0
2	GOL	F	497	6/6	0.85	0.20	3.91	35,59,67,72	0
2	GOL	E	497	6/6	0.94	0.17	3.38	26,30,50,65	0
2	GOL	B	499	6/6	0.88	0.16	3.31	31,43,50,58	0
4	ACT	D	500	4/4	0.95	0.23	2.69	34,38,44,54	0
4	ACT	C	499	4/4	0.86	0.15	1.95	40,47,47,57	0
2	GOL	D	496	6/6	0.97	0.13	1.75	28,33,39,41	0
4	ACT	E	499	4/4	0.94	0.14	1.44	32,34,42,47	0
2	GOL	C	497	6/6	0.87	0.17	1.17	39,43,58,59	0
2	GOL	B	496	6/6	0.94	0.11	0.94	21,29,39,50	0
2	GOL	G	498	6/6	0.96	0.13	0.86	19,27,32,35	0
4	ACT	B	498	4/4	0.73	0.18	0.50	44,48,52,56	0
4	ACT	F	500	4/4	0.94	0.17	0.42	38,41,46,51	0
2	GOL	H	496	6/6	0.95	0.11	0.38	40,41,46,54	0
2	GOL	D	498	6/6	0.94	0.12	0.37	27,45,50,56	0
2	GOL	D	497	6/6	0.98	0.10	0.16	24,38,41,45	0
2	GOL	F	498	6/6	0.91	0.12	0.08	46,57,58,70	0
2	GOL	A	496	6/6	0.94	0.12	0.02	25,45,47,49	0
2	GOL	E	496	6/6	0.96	0.11	-0.01	21,34,37,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	B	497	6/6	0.97	0.10	-0.48	19,28,44,51	0
2	GOL	F	496	6/6	0.98	0.09	-0.85	22,28,32,35	0
3	CL	B	500	1/1	0.88	0.10	-1.15	47,47,47,47	0
2	GOL	G	497	6/6	0.96	0.08	-1.26	23,33,34,40	0
4	ACT	C	498	4/4	0.98	0.08	-1.27	47,53,54,56	0
3	CL	A	497	1/1	0.93	0.07	-1.55	51,51,51,51	0
3	CL	D	499	1/1	0.99	0.04	-1.90	37,37,37,37	0
3	CL	E	498	1/1	0.99	0.05	-2.02	34,34,34,34	0
3	CL	F	499	1/1	0.98	0.04	-2.03	31,31,31,31	0
3	CL	C	496	1/1	0.98	0.06	-2.13	38,38,38,38	0
3	CL	G	499	1/1	0.97	0.06	-2.33	49,49,49,49	0
3	CL	H	497	1/1	0.98	0.04	-3.03	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.