wwPDB X-ray Structure Validation Summary Report (i)

Jun 15, 2024 – 10:24 AM EDT

PDB ID	:	2P0I
Title	:	Crystal structure of L-rhamnonate dehydratase from Gibberella zeae
Authors	:	Patskovsky, Y.; Toro, R.; Sauder, J.M.; Dickey, M.; Logan, C.; Gheyi, T.; Wasserman, S.R.; Smith, D.; Gerlt, J.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2007-02-28
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

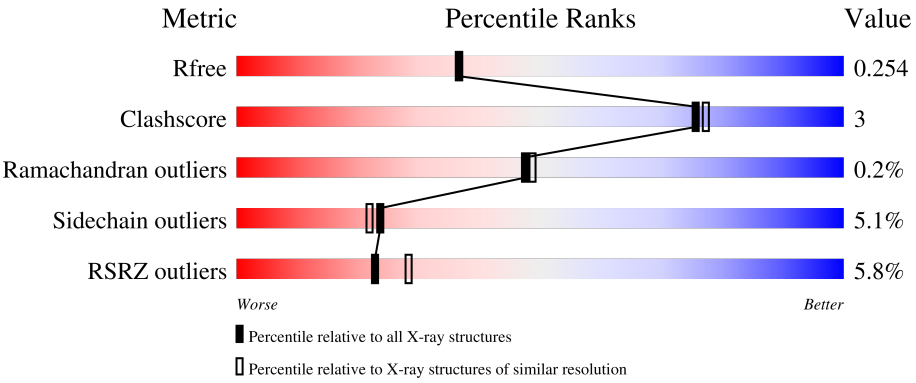
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	456	4% 77% 9% • 14%
1	B	456	3% 76% 9% • 14%
1	C	456	6% 77% 8% • 14%
1	D	456	8% 76% 9% • 14%
1	E	456	6% 77% 9% 14%

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Mol	Chain	Length	Quality of chain
1	F	456	4% 77% 8% • 14%
1	G	456	4% 77% 7% • 14%
1	H	456	4% 80% 6% • 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26261 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 L-rhamnonate dehydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	Se	0	5	0
			3137	2038	522	565	6	6			
1	B	392	Total	C	N	O	S	Se	0	6	0
			3135	2038	523	562	6	6			
1	C	393	Total	C	N	O	S	Se	0	3	0
			3121	2028	516	565	6	6			
1	D	392	Total	C	N	O	S	Se	0	5	0
			3123	2028	515	568	6	6			
1	E	393	Total	C	N	O	S	Se	0	6	0
			3142	2044	520	566	6	6			
1	F	393	Total	C	N	O	S	Se	0	4	0
			3126	2031	517	566	6	6			
1	G	393	Total	C	N	O	S	Se	0	6	0
			3137	2037	518	570	6	6			
1	H	393	Total	C	N	O	S	Se	0	6	0
			3135	2040	517	566	6	6			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP Q4HYS5
A	1	LEU	-	cloning artifact	UNP Q4HYS5
A	115	MSE	MET	modified residue	UNP Q4HYS5
A	120	MSE	MET	modified residue	UNP Q4HYS5
A	178	MSE	MET	modified residue	UNP Q4HYS5
A	219	MSE	MET	modified residue	UNP Q4HYS5
A	224	MSE	MET	modified residue	UNP Q4HYS5
A	299	MSE	MET	modified residue	UNP Q4HYS5
A	448	GLU	-	cloning artifact	UNP Q4HYS5
A	449	GLY	-	cloning artifact	UNP Q4HYS5
A	450	HIS	-	cloning artifact	UNP Q4HYS5
A	451	HIS	-	cloning artifact	UNP Q4HYS5
A	452	HIS	-	cloning artifact	UNP Q4HYS5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	453	HIS	-	cloning artifact	UNP Q4HYS5
A	454	HIS	-	cloning artifact	UNP Q4HYS5
A	455	HIS	-	cloning artifact	UNP Q4HYS5
B	0	SER	-	cloning artifact	UNP Q4HYS5
B	1	LEU	-	cloning artifact	UNP Q4HYS5
B	115	MSE	MET	modified residue	UNP Q4HYS5
B	120	MSE	MET	modified residue	UNP Q4HYS5
B	178	MSE	MET	modified residue	UNP Q4HYS5
B	219	MSE	MET	modified residue	UNP Q4HYS5
B	224	MSE	MET	modified residue	UNP Q4HYS5
B	299	MSE	MET	modified residue	UNP Q4HYS5
B	448	GLU	-	cloning artifact	UNP Q4HYS5
B	449	GLY	-	cloning artifact	UNP Q4HYS5
B	450	HIS	-	cloning artifact	UNP Q4HYS5
B	451	HIS	-	cloning artifact	UNP Q4HYS5
B	452	HIS	-	cloning artifact	UNP Q4HYS5
B	453	HIS	-	cloning artifact	UNP Q4HYS5
B	454	HIS	-	cloning artifact	UNP Q4HYS5
B	455	HIS	-	cloning artifact	UNP Q4HYS5
C	0	SER	-	cloning artifact	UNP Q4HYS5
C	1	LEU	-	cloning artifact	UNP Q4HYS5
C	115	MSE	MET	modified residue	UNP Q4HYS5
C	120	MSE	MET	modified residue	UNP Q4HYS5
C	178	MSE	MET	modified residue	UNP Q4HYS5
C	219	MSE	MET	modified residue	UNP Q4HYS5
C	224	MSE	MET	modified residue	UNP Q4HYS5
C	299	MSE	MET	modified residue	UNP Q4HYS5
C	448	GLU	-	cloning artifact	UNP Q4HYS5
C	449	GLY	-	cloning artifact	UNP Q4HYS5
C	450	HIS	-	cloning artifact	UNP Q4HYS5
C	451	HIS	-	cloning artifact	UNP Q4HYS5
C	452	HIS	-	cloning artifact	UNP Q4HYS5
C	453	HIS	-	cloning artifact	UNP Q4HYS5
C	454	HIS	-	cloning artifact	UNP Q4HYS5
C	455	HIS	-	cloning artifact	UNP Q4HYS5
D	0	SER	-	cloning artifact	UNP Q4HYS5
D	1	LEU	-	cloning artifact	UNP Q4HYS5
D	115	MSE	MET	modified residue	UNP Q4HYS5
D	120	MSE	MET	modified residue	UNP Q4HYS5
D	178	MSE	MET	modified residue	UNP Q4HYS5
D	219	MSE	MET	modified residue	UNP Q4HYS5
D	224	MSE	MET	modified residue	UNP Q4HYS5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	299	MSE	MET	modified residue	UNP Q4HYS5
D	448	GLU	-	cloning artifact	UNP Q4HYS5
D	449	GLY	-	cloning artifact	UNP Q4HYS5
D	450	HIS	-	cloning artifact	UNP Q4HYS5
D	451	HIS	-	cloning artifact	UNP Q4HYS5
D	452	HIS	-	cloning artifact	UNP Q4HYS5
D	453	HIS	-	cloning artifact	UNP Q4HYS5
D	454	HIS	-	cloning artifact	UNP Q4HYS5
D	455	HIS	-	cloning artifact	UNP Q4HYS5
E	0	SER	-	cloning artifact	UNP Q4HYS5
E	1	LEU	-	cloning artifact	UNP Q4HYS5
E	115	MSE	MET	modified residue	UNP Q4HYS5
E	120	MSE	MET	modified residue	UNP Q4HYS5
E	178	MSE	MET	modified residue	UNP Q4HYS5
E	219	MSE	MET	modified residue	UNP Q4HYS5
E	224	MSE	MET	modified residue	UNP Q4HYS5
E	299	MSE	MET	modified residue	UNP Q4HYS5
E	448	GLU	-	cloning artifact	UNP Q4HYS5
E	449	GLY	-	cloning artifact	UNP Q4HYS5
E	450	HIS	-	cloning artifact	UNP Q4HYS5
E	451	HIS	-	cloning artifact	UNP Q4HYS5
E	452	HIS	-	cloning artifact	UNP Q4HYS5
E	453	HIS	-	cloning artifact	UNP Q4HYS5
E	454	HIS	-	cloning artifact	UNP Q4HYS5
E	455	HIS	-	cloning artifact	UNP Q4HYS5
F	0	SER	-	cloning artifact	UNP Q4HYS5
F	1	LEU	-	cloning artifact	UNP Q4HYS5
F	115	MSE	MET	modified residue	UNP Q4HYS5
F	120	MSE	MET	modified residue	UNP Q4HYS5
F	178	MSE	MET	modified residue	UNP Q4HYS5
F	219	MSE	MET	modified residue	UNP Q4HYS5
F	224	MSE	MET	modified residue	UNP Q4HYS5
F	299	MSE	MET	modified residue	UNP Q4HYS5
F	448	GLU	-	cloning artifact	UNP Q4HYS5
F	449	GLY	-	cloning artifact	UNP Q4HYS5
F	450	HIS	-	cloning artifact	UNP Q4HYS5
F	451	HIS	-	cloning artifact	UNP Q4HYS5
F	452	HIS	-	cloning artifact	UNP Q4HYS5
F	453	HIS	-	cloning artifact	UNP Q4HYS5
F	454	HIS	-	cloning artifact	UNP Q4HYS5
F	455	HIS	-	cloning artifact	UNP Q4HYS5
G	0	SER	-	cloning artifact	UNP Q4HYS5

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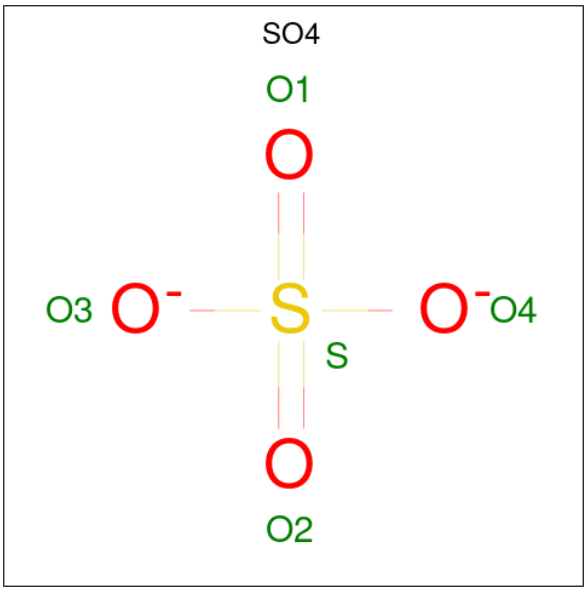
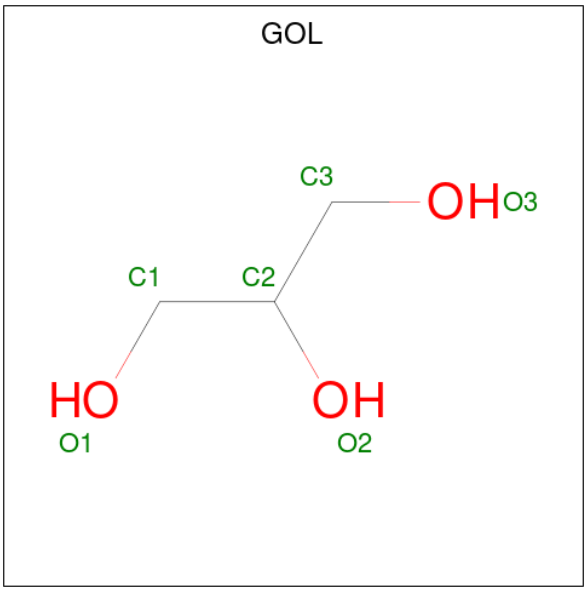
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	LEU	-	cloning artifact	UNP Q4HYS5
G	115	MSE	MET	modified residue	UNP Q4HYS5
G	120	MSE	MET	modified residue	UNP Q4HYS5
G	178	MSE	MET	modified residue	UNP Q4HYS5
G	219	MSE	MET	modified residue	UNP Q4HYS5
G	224	MSE	MET	modified residue	UNP Q4HYS5
G	299	MSE	MET	modified residue	UNP Q4HYS5
G	448	GLU	-	cloning artifact	UNP Q4HYS5
G	449	GLY	-	cloning artifact	UNP Q4HYS5
G	450	HIS	-	cloning artifact	UNP Q4HYS5
G	451	HIS	-	cloning artifact	UNP Q4HYS5
G	452	HIS	-	cloning artifact	UNP Q4HYS5
G	453	HIS	-	cloning artifact	UNP Q4HYS5
G	454	HIS	-	cloning artifact	UNP Q4HYS5
G	455	HIS	-	cloning artifact	UNP Q4HYS5
H	0	SER	-	cloning artifact	UNP Q4HYS5
H	1	LEU	-	cloning artifact	UNP Q4HYS5
H	115	MSE	MET	modified residue	UNP Q4HYS5
H	120	MSE	MET	modified residue	UNP Q4HYS5
H	178	MSE	MET	modified residue	UNP Q4HYS5
H	219	MSE	MET	modified residue	UNP Q4HYS5
H	224	MSE	MET	modified residue	UNP Q4HYS5
H	299	MSE	MET	modified residue	UNP Q4HYS5
H	448	GLU	-	cloning artifact	UNP Q4HYS5
H	449	GLY	-	cloning artifact	UNP Q4HYS5
H	450	HIS	-	cloning artifact	UNP Q4HYS5
H	451	HIS	-	cloning artifact	UNP Q4HYS5
H	452	HIS	-	cloning artifact	UNP Q4HYS5
H	453	HIS	-	cloning artifact	UNP Q4HYS5
H	454	HIS	-	cloning artifact	UNP Q4HYS5
H	455	HIS	-	cloning artifact	UNP Q4HYS5

- 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	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	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	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	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is water.

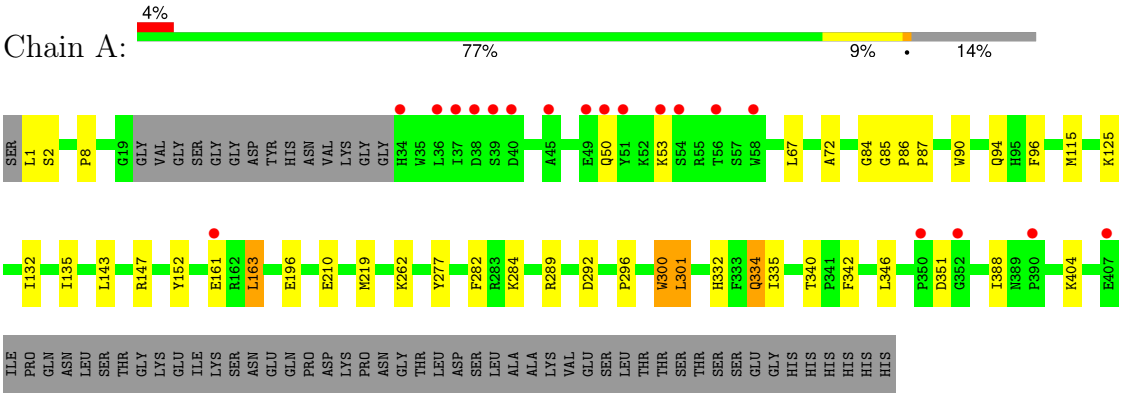
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0
4	B	151	Total O 151 151	0	0
4	C	126	Total O 126 126	0	0
4	D	128	Total O 128 128	0	0
4	E	121	Total O 121 121	0	0
4	F	107	Total O 107 107	0	0
4	G	131	Total O 131 131	0	0
4	H	115	Total O 115 115	0	0

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.

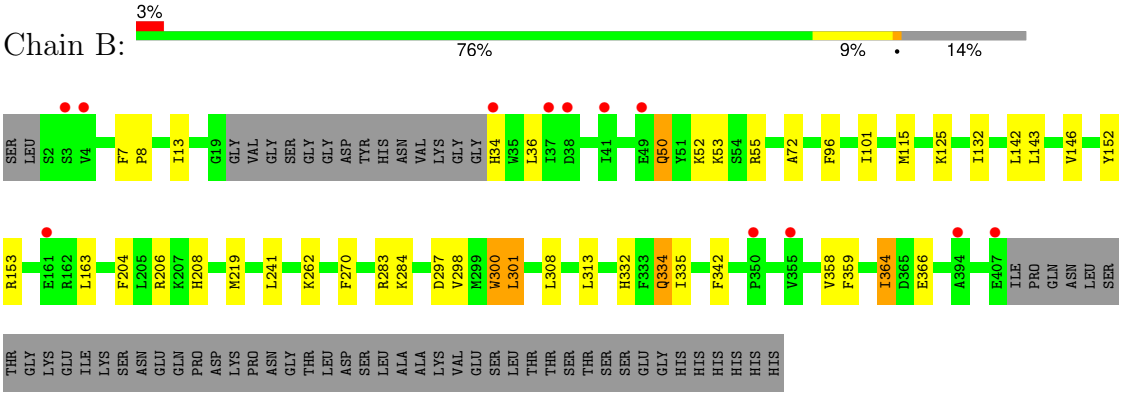
• Molecule 1: L-rhamnonate dehydratase

Chain A:



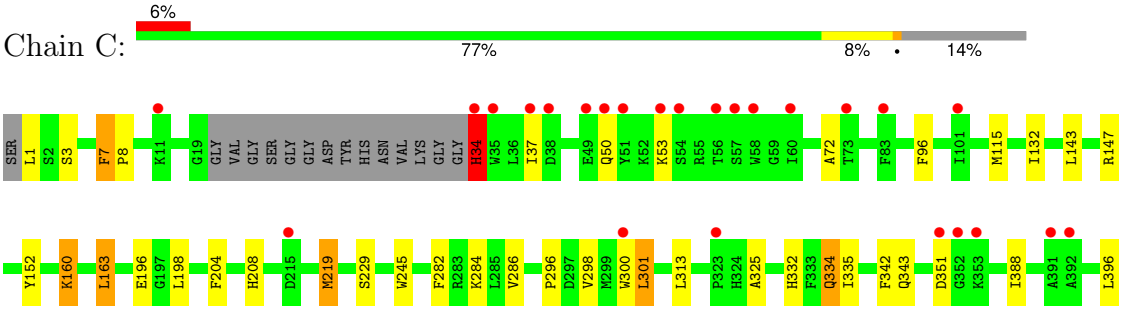
• Molecule 1: L-rhamnonate dehydratase

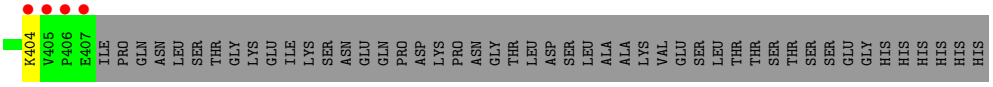
Chain B:



• Molecule 1: L-rhamnonate dehydratase

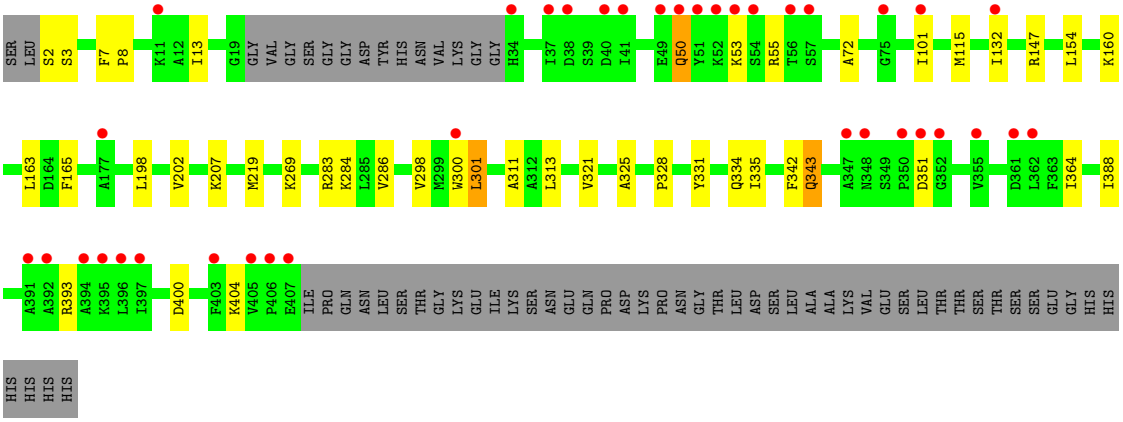
Chain C:





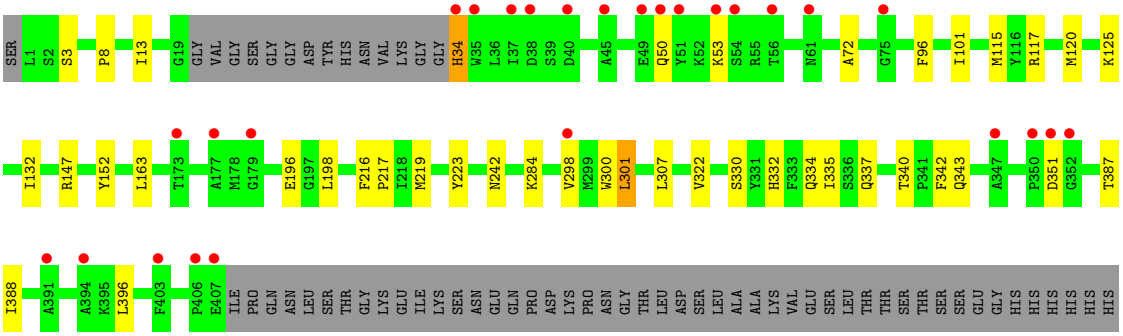
• Molecule 1: L-rhamnonate dehydratase

Chain D:



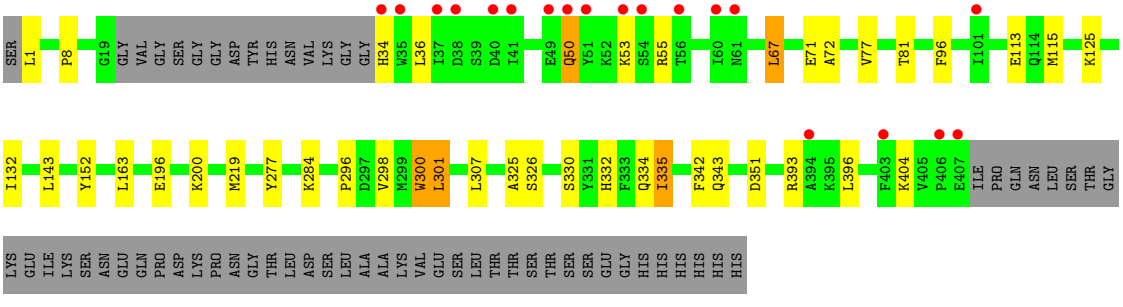
• Molecule 1: L-rhamnonate dehydratase

Chain E:



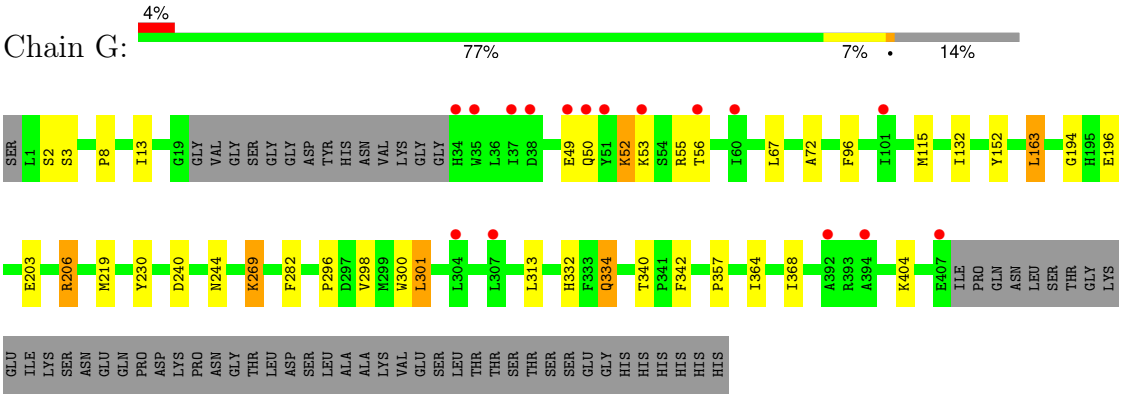
• Molecule 1: L-rhamnonate dehydratase

Chain F:



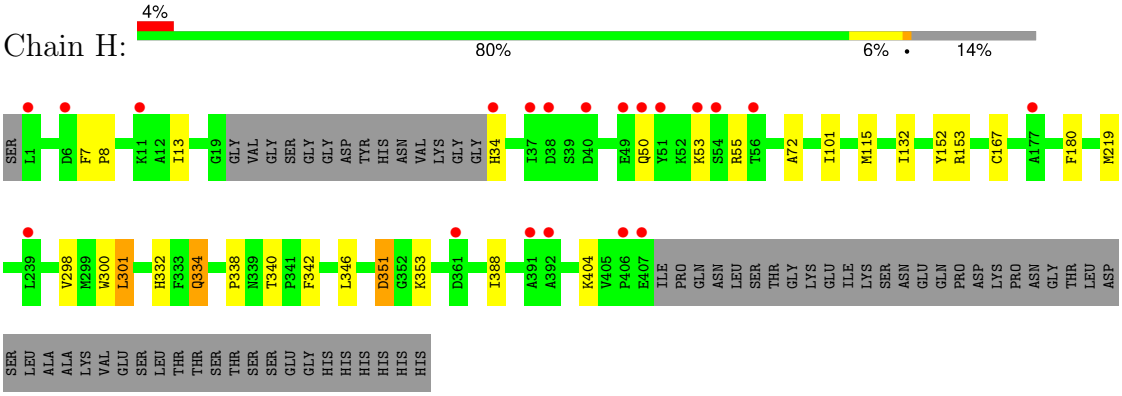
• Molecule 1: L-rhamnonate dehydratase

Chain G:



• Molecule 1: L-rhamnonate dehydratase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	201.40Å 201.13Å 82.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 34.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-2.10) 95.5 (34.02-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.3.0028	Depositor
R, R_{free}	0.190 , 0.256 0.192 , 0.254	Depositor DCC
R_{free} test set	5687 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	36.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.028 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26261	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	0/3233	0.57	0/4387
1	B	0.43	0/3240	0.56	0/4395
1	C	0.44	0/3211	0.56	0/4359
1	D	0.40	0/3219	0.55	0/4370
1	E	0.40	0/3238	0.56	0/4393
1	F	0.41	0/3219	0.56	0/4370
1	G	0.40	0/3233	0.56	0/4390
1	H	0.40	0/3234	0.56	0/4389
All	All	0.41	0/25827	0.56	0/35053

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	34	HIS	Peptide
1	D	2	SER	Peptide

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Mol	Chain	Res	Type	Group
1	E	34	HIS	Peptide

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	3137	0	3109	19	0
1	B	3135	0	3116	28	0
1	C	3121	0	3082	19	0
1	D	3123	0	3076	13	0
1	E	3142	0	3120	24	0
1	F	3126	0	3088	25	0
1	G	3137	0	3096	17	0
1	H	3135	0	3111	11	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	15	0	0	0	0
2	F	5	0	0	0	0
2	H	10	0	0	0	0
3	A	24	0	32	5	0
3	B	6	0	8	2	0
3	D	12	0	16	1	0
3	E	12	0	16	3	0
3	F	24	0	32	0	0
3	G	30	0	40	2	0
3	H	12	0	16	2	0
4	A	146	0	0	0	0
4	B	151	0	0	0	0
4	C	126	0	0	1	0
4	D	128	0	0	0	0
4	E	121	0	0	1	0
4	F	107	0	0	0	0
4	G	131	0	0	0	0
4	H	115	0	0	0	0
All	All	26261	0	24958	155	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.

The worst 5 of 155 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:G:163:LEU:HD23	1:G:334[A]:GLN:OE1	1.76	0.85
1:E:163:LEU:CD1	1:E:335:ILE:HD13	2.07	0.85
1:A:115:MSE:HE2	1:A:132:ILE:HG12	1.58	0.84
1:B:163:LEU:HD11	1:B:335:ILE:HD13	1.61	0.80
1:H:152:TYR:H	1:H:332:HIS:HD2	1.33	0.76

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	394/456 (86%)	379 (96%)	13 (3%)	2 (0%)	29	26
1	B	394/456 (86%)	386 (98%)	8 (2%)	0	100	100
1	C	392/456 (86%)	378 (96%)	13 (3%)	1 (0%)	41	41
1	D	393/456 (86%)	376 (96%)	15 (4%)	2 (0%)	29	26
1	E	395/456 (87%)	379 (96%)	14 (4%)	2 (0%)	29	26
1	F	393/456 (86%)	381 (97%)	11 (3%)	1 (0%)	41	41
1	G	395/456 (87%)	385 (98%)	10 (2%)	0	100	100
1	H	395/456 (87%)	382 (97%)	13 (3%)	0	100	100
All	All	3151/3648 (86%)	3046 (97%)	97 (3%)	8 (0%)	47	41

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	242	ASN

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Mol	Chain	Res	Type
1	A	289[A]	ARG
1	A	289[B]	ARG
1	F	325	ALA
1	C	325	ALA

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	336/378 (89%)	317 (94%)	19 (6%)	20	18
1	B	337/378 (89%)	325 (96%)	12 (4%)	35	36
1	C	334/378 (88%)	311 (93%)	23 (7%)	15	12
1	D	335/378 (89%)	314 (94%)	21 (6%)	18	15
1	E	337/378 (89%)	324 (96%)	13 (4%)	32	33
1	F	335/378 (89%)	318 (95%)	17 (5%)	24	22
1	G	337/378 (89%)	315 (94%)	22 (6%)	17	14
1	H	337/378 (89%)	322 (96%)	15 (4%)	27	27
All	All	2688/3024 (89%)	2546 (95%)	142 (5%)	24	20

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	196	GLU
1	G	269	LYS
1	H	53	LYS
1	C	334[B]	GLN
1	C	334[A]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	343	GLN

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Mol	Chain	Res	Type
1	F	343	GLN
1	F	34	HIS
1	F	244	ASN
1	G	50	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)

32 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	$\#\|Z\| > 2$
2	SO4	C	1209	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	F	1210	-	4,4,4	0.26	0	6,6,6	0.07	0
3	GOL	D	1306	-	5,5,5	0.30	0	5,5,5	0.42	0
2	SO4	D	1207	-	4,4,4	0.24	0	6,6,6	0.06	0
3	GOL	G	1315	-	5,5,5	0.42	0	5,5,5	0.31	0
3	GOL	F	1317	-	5,5,5	0.35	0	5,5,5	0.48	0
3	GOL	D	1310	-	5,5,5	0.81	0	5,5,5	0.59	0
2	SO4	B	1205	-	4,4,4	0.33	0	6,6,6	0.16	0
3	GOL	B	1308	-	5,5,5	0.37	0	5,5,5	0.41	0
2	SO4	H	1211	-	4,4,4	0.24	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	G	1318	-	5,5,5	0.48	0	5,5,5	0.36	0
3	GOL	A	1314	-	5,5,5	0.37	0	5,5,5	0.28	0
3	GOL	G	1307	-	5,5,5	0.34	0	5,5,5	0.52	0
3	GOL	F	1313	-	5,5,5	0.36	0	5,5,5	0.32	0
2	SO4	E	1202	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	E	1201	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	A	1204	-	4,4,4	0.25	0	6,6,6	0.17	0
2	SO4	D	1206	-	4,4,4	0.26	0	6,6,6	0.09	0
3	GOL	A	1316	-	5,5,5	0.40	0	5,5,5	0.49	0
3	GOL	A	1304	-	5,5,5	0.31	0	5,5,5	0.57	0
2	SO4	B	1212	-	4,4,4	0.24	0	6,6,6	0.13	0
3	GOL	E	1305	-	5,5,5	0.41	0	5,5,5	0.51	0
3	GOL	G	1309	-	5,5,5	0.38	0	5,5,5	0.31	0
2	SO4	H	1203	-	4,4,4	0.27	0	6,6,6	0.05	0
3	GOL	H	1302	-	5,5,5	0.44	0	5,5,5	0.59	0
3	GOL	E	1301	-	5,5,5	0.48	0	5,5,5	0.48	0
3	GOL	H	1311	-	5,5,5	0.40	0	5,5,5	0.31	0
3	GOL	G	1320	-	5,5,5	0.38	0	5,5,5	0.54	0
3	GOL	F	1312	-	5,5,5	0.42	0	5,5,5	0.30	0
3	GOL	A	1303	-	5,5,5	0.45	0	5,5,5	0.24	0
3	GOL	F	1319	-	5,5,5	0.34	0	5,5,5	0.33	0
2	SO4	E	1208	-	4,4,4	0.38	0	6,6,6	0.30	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
3	GOL	D	1306	-	-	2/4/4/4	-
3	GOL	G	1315	-	-	1/4/4/4	-
3	GOL	F	1317	-	-	1/4/4/4	-
3	GOL	D	1310	-	-	2/4/4/4	-
3	GOL	B	1308	-	-	2/4/4/4	-
3	GOL	G	1318	-	-	4/4/4/4	-
3	GOL	A	1314	-	-	1/4/4/4	-
3	GOL	G	1307	-	-	3/4/4/4	-
3	GOL	F	1313	-	-	2/4/4/4	-
3	GOL	A	1316	-	-	3/4/4/4	-
3	GOL	A	1304	-	-	0/4/4/4	-
3	GOL	G	1309	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	1305	-	-	2/4/4/4	-
3	GOL	H	1302	-	-	0/4/4/4	-
3	GOL	E	1301	-	-	4/4/4/4	-
3	GOL	H	1311	-	-	2/4/4/4	-
3	GOL	G	1320	-	-	4/4/4/4	-
3	GOL	F	1312	-	-	2/4/4/4	-
3	GOL	A	1303	-	-	2/4/4/4	-
3	GOL	F	1319	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1303	GOL	O1-C1-C2-C3
3	A	1316	GOL	O1-C1-C2-C3
3	B	1308	GOL	O1-C1-C2-C3
3	D	1306	GOL	C1-C2-C3-O3
3	E	1301	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1306	GOL	1	0
3	B	1308	GOL	2	0
3	G	1318	GOL	1	0
3	A	1304	GOL	2	0
3	E	1305	GOL	1	0
3	G	1309	GOL	1	0
3	E	1301	GOL	2	0
3	H	1311	GOL	2	0
3	A	1303	GOL	3	0

5.7 Other polymers

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	387/456 (84%)	-0.04	19 (4%)	29	35	21, 35, 70, 116	0
1	B	386/456 (84%)	-0.09	12 (3%)	49	55	20, 37, 66, 109	0
1	C	387/456 (84%)	0.18	29 (7%)	14	18	21, 42, 77, 122	0
1	D	386/456 (84%)	0.22	37 (9%)	8	10	25, 45, 88, 113	0
1	E	387/456 (84%)	0.08	27 (6%)	16	20	23, 45, 80, 115	0
1	F	387/456 (84%)	0.07	19 (4%)	29	35	21, 44, 75, 113	0
1	G	387/456 (84%)	-0.05	16 (4%)	37	43	20, 41, 72, 105	0
1	H	387/456 (84%)	0.04	20 (5%)	27	32	25, 43, 79, 119	0
All	All	3094/3648 (84%)	0.05	179 (5%)	23	28	20, 42, 77, 122	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ILE	8.1
1	F	37	ILE	7.4
1	A	37	ILE	6.6
1	H	392	ALA	6.5
1	C	37	ILE	6.4

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
3	GOL	G	1309	6/6	0.64	0.25	67,78,84,86	0
3	GOL	G	1318	6/6	0.64	0.24	55,60,65,69	0
2	SO4	B	1205	5/5	0.67	0.27	50,77,85,103	0
3	GOL	F	1312	6/6	0.79	0.18	48,62,69,74	0
3	GOL	A	1316	6/6	0.80	0.28	46,58,63,71	0
2	SO4	F	1210	5/5	0.81	0.23	85,106,111,113	0
3	GOL	G	1320	6/6	0.81	0.15	36,64,73,79	0
3	GOL	F	1313	6/6	0.84	0.38	57,62,72,76	0
3	GOL	F	1319	6/6	0.86	0.19	48,58,65,66	0
2	SO4	A	1204	5/5	0.88	0.23	66,85,93,99	0
2	SO4	B	1212	5/5	0.88	0.16	74,93,107,108	0
2	SO4	D	1207	5/5	0.88	0.24	89,97,98,99	0
2	SO4	E	1208	5/5	0.88	0.13	120,122,123,127	0
3	GOL	B	1308	6/6	0.89	0.17	46,54,61,70	0
3	GOL	D	1310	6/6	0.89	0.13	53,70,78,85	0
2	SO4	C	1209	5/5	0.91	0.15	59,68,85,90	0
3	GOL	G	1315	6/6	0.91	0.14	60,61,63,75	0
3	GOL	F	1317	6/6	0.91	0.12	43,55,68,68	0
2	SO4	H	1211	5/5	0.91	0.16	103,105,110,111	0
3	GOL	H	1311	6/6	0.92	0.13	44,51,57,60	0
2	SO4	D	1206	5/5	0.93	0.22	84,101,106,108	0
3	GOL	A	1303	6/6	0.94	0.15	33,34,45,46	0
3	GOL	H	1302	6/6	0.94	0.17	43,46,51,58	0
3	GOL	D	1306	6/6	0.94	0.15	41,48,53,53	0
2	SO4	E	1202	5/5	0.95	0.15	55,65,86,93	0
3	GOL	E	1305	6/6	0.95	0.14	32,41,44,51	0
3	GOL	A	1314	6/6	0.96	0.25	21,45,53,58	0
2	SO4	H	1203	5/5	0.97	0.20	52,71,87,91	0
3	GOL	G	1307	6/6	0.97	0.10	30,38,46,47	0
3	GOL	E	1301	6/6	0.97	0.13	39,48,50,58	0
3	GOL	A	1304	6/6	0.97	0.11	27,34,45,54	0
2	SO4	E	1201	5/5	0.98	0.27	67,69,79,86	0

6.5 Other polymers (i)

There are no such residues in this entry.