Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2024 – 04:49 AM EDT

PDB ID	:	3WWP
Title	:	S-selective hydroxynitrile lyase from Baliospermum montanum (apo2)
Authors	:	Nakano, S.; Dadashipour, M.; Asano, Y.
Deposited on	:	2014-06-23
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
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:

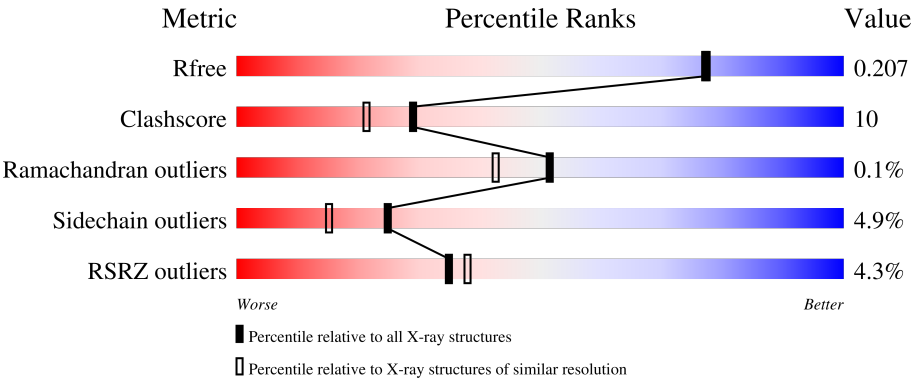
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	288	79% 11% 8%
1	B	288	81% 8% 9%
1	G	288	75% 14% 9%
1	L	288	78% 9% 11%
1	M	288	16% 71% 16% 10%

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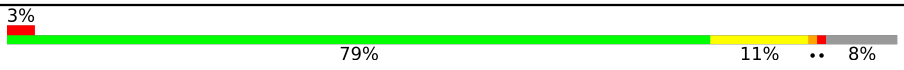
Mol	Chain	Length	Quality of chain
1	R	288	

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	CIT	G	301	-	X	-	-
3	EDO	A	304	-	-	X	-
3	EDO	L	302	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14563 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 (S)-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2104	1356	341	403	4			
1	B	261	Total	C	N	O	S	0	0	0
			2075	1337	337	397	4			
1	G	262	Total	C	N	O	S	0	0	0
			2084	1342	338	400	4			
1	L	257	Total	C	N	O	S	0	0	0
			2048	1321	333	390	4			
1	M	258	Total	C	N	O	S	0	0	0
			2053	1324	334	391	4			
1	R	265	Total	C	N	O	S	0	0	0
			2100	1354	341	401	4			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP D1MX73
A	-23	ASN	-	expression tag	UNP D1MX73
A	-22	HIS	-	expression tag	UNP D1MX73
A	-21	LYS	-	expression tag	UNP D1MX73
A	-20	VAL	-	expression tag	UNP D1MX73
A	-19	HIS	-	expression tag	UNP D1MX73
A	-18	HIS	-	expression tag	UNP D1MX73
A	-17	HIS	-	expression tag	UNP D1MX73
A	-16	HIS	-	expression tag	UNP D1MX73
A	-15	HIS	-	expression tag	UNP D1MX73
A	-14	HIS	-	expression tag	UNP D1MX73
A	-13	ILE	-	expression tag	UNP D1MX73
A	-12	GLU	-	expression tag	UNP D1MX73
A	-11	GLY	-	expression tag	UNP D1MX73
A	-10	ARG	-	expression tag	UNP D1MX73
A	-9	HIS	-	expression tag	UNP D1MX73
A	-8	MET	-	expression tag	UNP D1MX73

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLU	-	expression tag	UNP D1MX73
A	-6	LEU	-	expression tag	UNP D1MX73
A	-5	GLY	-	expression tag	UNP D1MX73
A	-4	THR	-	expression tag	UNP D1MX73
A	-3	LEU	-	expression tag	UNP D1MX73
A	-2	GLU	-	expression tag	UNP D1MX73
A	-1	GLY	-	expression tag	UNP D1MX73
A	0	PHE	-	expression tag	UNP D1MX73
B	-24	MET	-	expression tag	UNP D1MX73
B	-23	ASN	-	expression tag	UNP D1MX73
B	-22	HIS	-	expression tag	UNP D1MX73
B	-21	LYS	-	expression tag	UNP D1MX73
B	-20	VAL	-	expression tag	UNP D1MX73
B	-19	HIS	-	expression tag	UNP D1MX73
B	-18	HIS	-	expression tag	UNP D1MX73
B	-17	HIS	-	expression tag	UNP D1MX73
B	-16	HIS	-	expression tag	UNP D1MX73
B	-15	HIS	-	expression tag	UNP D1MX73
B	-14	HIS	-	expression tag	UNP D1MX73
B	-13	ILE	-	expression tag	UNP D1MX73
B	-12	GLU	-	expression tag	UNP D1MX73
B	-11	GLY	-	expression tag	UNP D1MX73
B	-10	ARG	-	expression tag	UNP D1MX73
B	-9	HIS	-	expression tag	UNP D1MX73
B	-8	MET	-	expression tag	UNP D1MX73
B	-7	GLU	-	expression tag	UNP D1MX73
B	-6	LEU	-	expression tag	UNP D1MX73
B	-5	GLY	-	expression tag	UNP D1MX73
B	-4	THR	-	expression tag	UNP D1MX73
B	-3	LEU	-	expression tag	UNP D1MX73
B	-2	GLU	-	expression tag	UNP D1MX73
B	-1	GLY	-	expression tag	UNP D1MX73
B	0	PHE	-	expression tag	UNP D1MX73
G	-24	MET	-	expression tag	UNP D1MX73
G	-23	ASN	-	expression tag	UNP D1MX73
G	-22	HIS	-	expression tag	UNP D1MX73
G	-21	LYS	-	expression tag	UNP D1MX73
G	-20	VAL	-	expression tag	UNP D1MX73
G	-19	HIS	-	expression tag	UNP D1MX73
G	-18	HIS	-	expression tag	UNP D1MX73
G	-17	HIS	-	expression tag	UNP D1MX73
G	-16	HIS	-	expression tag	UNP D1MX73

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-15	HIS	-	expression tag	UNP D1MX73
G	-14	HIS	-	expression tag	UNP D1MX73
G	-13	ILE	-	expression tag	UNP D1MX73
G	-12	GLU	-	expression tag	UNP D1MX73
G	-11	GLY	-	expression tag	UNP D1MX73
G	-10	ARG	-	expression tag	UNP D1MX73
G	-9	HIS	-	expression tag	UNP D1MX73
G	-8	MET	-	expression tag	UNP D1MX73
G	-7	GLU	-	expression tag	UNP D1MX73
G	-6	LEU	-	expression tag	UNP D1MX73
G	-5	GLY	-	expression tag	UNP D1MX73
G	-4	THR	-	expression tag	UNP D1MX73
G	-3	LEU	-	expression tag	UNP D1MX73
G	-2	GLU	-	expression tag	UNP D1MX73
G	-1	GLY	-	expression tag	UNP D1MX73
G	0	PHE	-	expression tag	UNP D1MX73
L	-24	MET	-	expression tag	UNP D1MX73
L	-23	ASN	-	expression tag	UNP D1MX73
L	-22	HIS	-	expression tag	UNP D1MX73
L	-21	LYS	-	expression tag	UNP D1MX73
L	-20	VAL	-	expression tag	UNP D1MX73
L	-19	HIS	-	expression tag	UNP D1MX73
L	-18	HIS	-	expression tag	UNP D1MX73
L	-17	HIS	-	expression tag	UNP D1MX73
L	-16	HIS	-	expression tag	UNP D1MX73
L	-15	HIS	-	expression tag	UNP D1MX73
L	-14	HIS	-	expression tag	UNP D1MX73
L	-13	ILE	-	expression tag	UNP D1MX73
L	-12	GLU	-	expression tag	UNP D1MX73
L	-11	GLY	-	expression tag	UNP D1MX73
L	-10	ARG	-	expression tag	UNP D1MX73
L	-9	HIS	-	expression tag	UNP D1MX73
L	-8	MET	-	expression tag	UNP D1MX73
L	-7	GLU	-	expression tag	UNP D1MX73
L	-6	LEU	-	expression tag	UNP D1MX73
L	-5	GLY	-	expression tag	UNP D1MX73
L	-4	THR	-	expression tag	UNP D1MX73
L	-3	LEU	-	expression tag	UNP D1MX73
L	-2	GLU	-	expression tag	UNP D1MX73
L	-1	GLY	-	expression tag	UNP D1MX73
L	0	PHE	-	expression tag	UNP D1MX73
M	-24	MET	-	expression tag	UNP D1MX73

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-23	ASN	-	expression tag	UNP D1MX73
M	-22	HIS	-	expression tag	UNP D1MX73
M	-21	LYS	-	expression tag	UNP D1MX73
M	-20	VAL	-	expression tag	UNP D1MX73
M	-19	HIS	-	expression tag	UNP D1MX73
M	-18	HIS	-	expression tag	UNP D1MX73
M	-17	HIS	-	expression tag	UNP D1MX73
M	-16	HIS	-	expression tag	UNP D1MX73
M	-15	HIS	-	expression tag	UNP D1MX73
M	-14	HIS	-	expression tag	UNP D1MX73
M	-13	ILE	-	expression tag	UNP D1MX73
M	-12	GLU	-	expression tag	UNP D1MX73
M	-11	GLY	-	expression tag	UNP D1MX73
M	-10	ARG	-	expression tag	UNP D1MX73
M	-9	HIS	-	expression tag	UNP D1MX73
M	-8	MET	-	expression tag	UNP D1MX73
M	-7	GLU	-	expression tag	UNP D1MX73
M	-6	LEU	-	expression tag	UNP D1MX73
M	-5	GLY	-	expression tag	UNP D1MX73
M	-4	THR	-	expression tag	UNP D1MX73
M	-3	LEU	-	expression tag	UNP D1MX73
M	-2	GLU	-	expression tag	UNP D1MX73
M	-1	GLY	-	expression tag	UNP D1MX73
M	0	PHE	-	expression tag	UNP D1MX73
R	-24	MET	-	expression tag	UNP D1MX73
R	-23	ASN	-	expression tag	UNP D1MX73
R	-22	HIS	-	expression tag	UNP D1MX73
R	-21	LYS	-	expression tag	UNP D1MX73
R	-20	VAL	-	expression tag	UNP D1MX73
R	-19	HIS	-	expression tag	UNP D1MX73
R	-18	HIS	-	expression tag	UNP D1MX73
R	-17	HIS	-	expression tag	UNP D1MX73
R	-16	HIS	-	expression tag	UNP D1MX73
R	-15	HIS	-	expression tag	UNP D1MX73
R	-14	HIS	-	expression tag	UNP D1MX73
R	-13	ILE	-	expression tag	UNP D1MX73
R	-12	GLU	-	expression tag	UNP D1MX73
R	-11	GLY	-	expression tag	UNP D1MX73
R	-10	ARG	-	expression tag	UNP D1MX73
R	-9	HIS	-	expression tag	UNP D1MX73
R	-8	MET	-	expression tag	UNP D1MX73
R	-7	GLU	-	expression tag	UNP D1MX73

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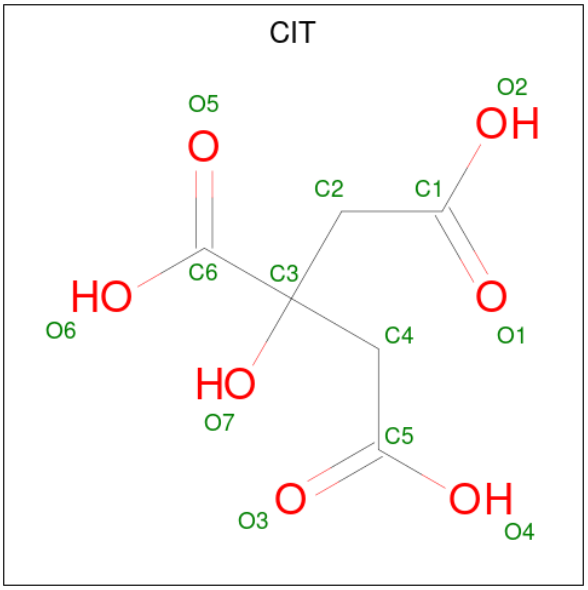
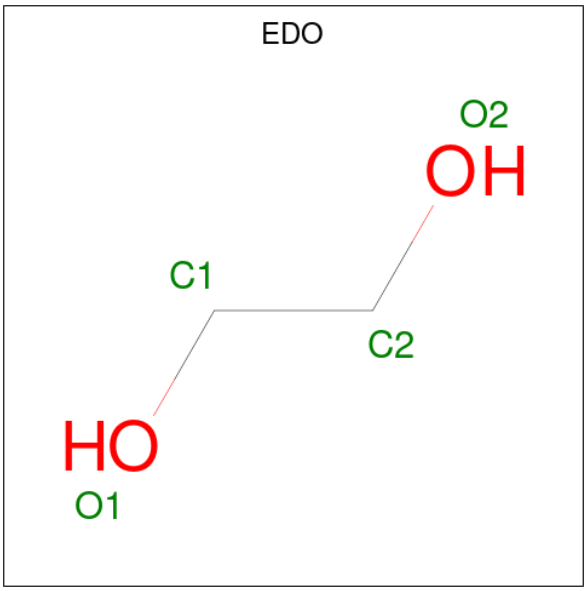
Chain	Residue	Modelled	Actual	Comment	Reference
R	-6	LEU	-	expression tag	UNP D1MX73
R	-5	GLY	-	expression tag	UNP D1MX73
R	-4	THR	-	expression tag	UNP D1MX73
R	-3	LEU	-	expression tag	UNP D1MX73
R	-2	GLU	-	expression tag	UNP D1MX73
R	-1	GLY	-	expression tag	UNP D1MX73
R	0	PHE	-	expression tag	UNP D1MX73

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	L	1	Total C O 13 6 7	0	0
2	M	1	Total C O 13 6 7	0	0
2	R	1	Total C O 13 6 7	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		
3	L	1	Total	C	O	0	0
			4	2	2		

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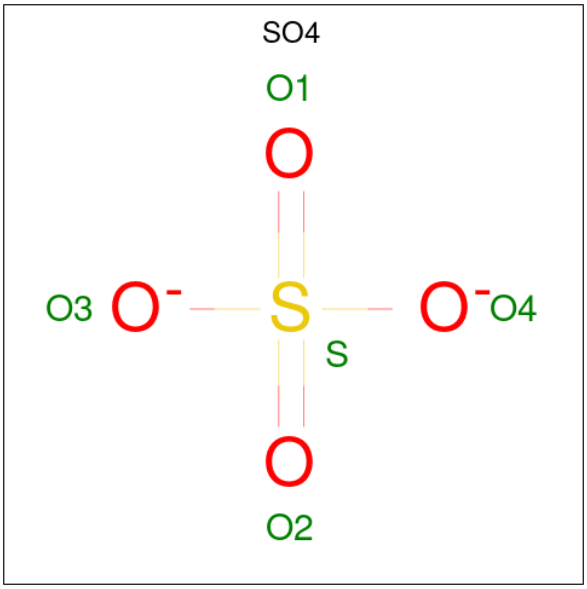
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	R	1	Total C O 4 2 2	0	0
3	R	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0
5	M	1	Total Cl 1 1	0	0
5	R	1	Total Cl 1 1	0	0

- Molecule 6 is water.

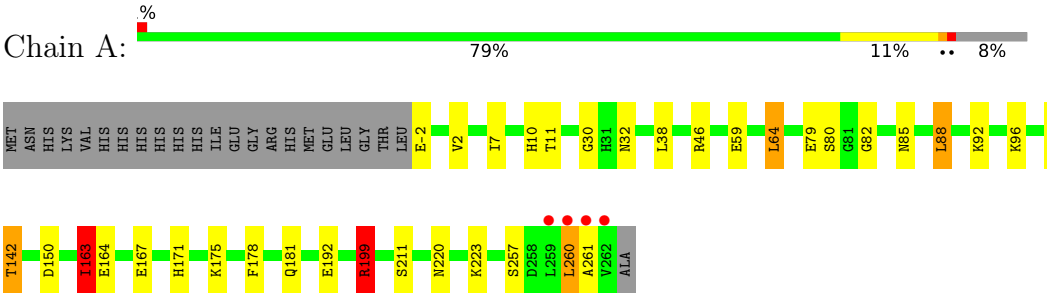
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	419	Total O 419 419	0	0
6	B	391	Total O 391 391	0	0
6	G	249	Total O 249 249	0	0
6	L	342	Total O 342 342	0	0
6	M	144	Total O 144 144	0	0
6	R	304	Total O 304 304	0	0

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.

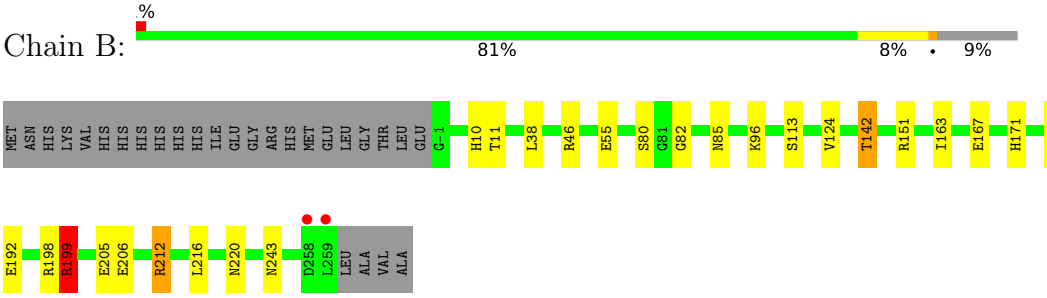
• Molecule 1: (S)-hydroxynitrile lyase

Chain A:



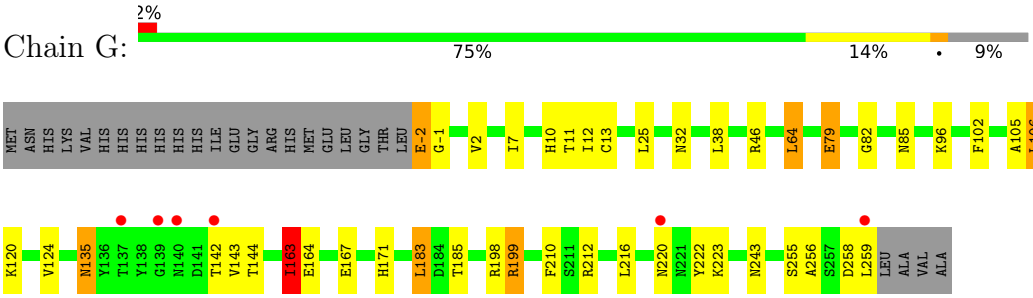
• Molecule 1: (S)-hydroxynitrile lyase

Chain B:



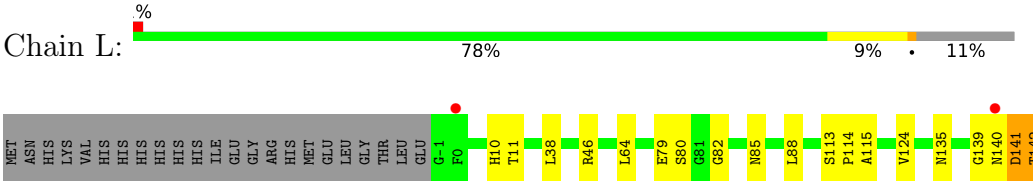
• Molecule 1: (S)-hydroxynitrile lyase

Chain G:



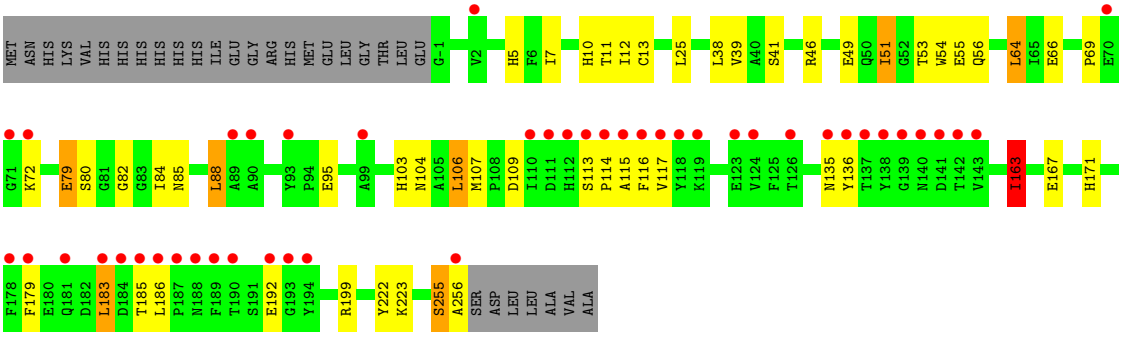
• Molecule 1: (S)-hydroxynitrile lyase

Chain L:



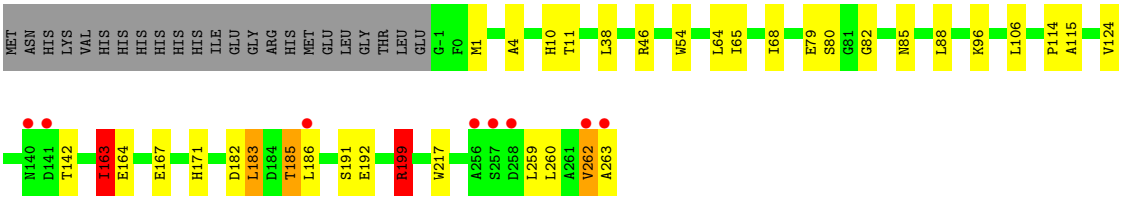
• Molecule 1: (S)-hydroxynitrile lyase

Chain M:



• Molecule 1: (S)-hydroxynitrile lyase

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	191.96Å 261.58Å 91.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.99 – 1.90 45.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.99-1.90) 99.8 (45.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.160 , 0.199 0.171 , 0.207	Depositor DCC
R_{free} test set	9074 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14563	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: CIT, CL, EDO, 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	0.62	0/2157	0.78	6/2934 (0.2%)
1	B	0.58	0/2128	0.76	3/2894 (0.1%)
1	G	0.47	0/2137	0.64	2/2906 (0.1%)
1	L	0.60	0/2101	0.75	2/2857 (0.1%)
1	M	0.42	0/2106	0.59	1/2864 (0.0%)
1	R	0.54	0/2153	0.72	2/2929 (0.1%)
All	All	0.54	0/12782	0.71	16/17384 (0.1%)

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	A	0	1
1	B	0	1
1	G	0	1
1	L	0	3
1	R	0	2
All	All	0	8

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	ARG	NE-CZ-NH2	-12.83	113.89	120.30
1	A	199	ARG	NE-CZ-NH2	-12.02	114.29	120.30
1	R	199	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	L	199	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	B	212	ARG	NE-CZ-NH1	7.07	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	88	LEU	CB-CG-CD1	6.69	122.37	111.00
1	B	212	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	163	ILE	CB-CA-C	-5.97	99.66	111.60
1	L	199	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	163	ILE	CG1-CB-CG2	5.72	123.99	111.40
1	M	163	ILE	CB-CA-C	-5.61	100.38	111.60
1	G	163	ILE	CB-CA-C	-5.54	100.52	111.60
1	A	150	ASP	CB-CG-OD1	5.24	123.02	118.30
1	G	199	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	R	163	ILE	CB-CA-C	-5.11	101.38	111.60
1	A	199	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ARG	Sidechain
1	B	199	ARG	Sidechain
1	G	135	ASN	Mainchain
1	L	135	ASN	Mainchain
1	L	141	ASP	Peptide
1	L	199	ARG	Sidechain
1	R	199	ARG	Sidechain
1	R	262	VAL	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	2104	0	2049	40	0
1	B	2075	0	2018	33	0
1	G	2084	0	2024	38	0
1	L	2048	0	1993	33	0
1	M	2053	0	1998	39	0
1	R	2100	0	2048	37	0
2	A	13	0	5	0	0
2	B	13	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	13	0	5	2	0
2	L	13	0	5	0	0
2	M	13	0	5	0	0
2	R	13	0	5	0	0
3	A	16	0	24	7	0
3	B	16	0	24	4	0
3	G	8	0	12	0	0
3	L	16	0	24	7	0
3	M	12	0	18	2	0
3	R	8	0	12	2	0
4	A	15	0	0	1	0
4	B	25	0	0	1	0
4	G	15	0	0	0	0
4	L	15	0	0	1	0
4	R	20	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	G	1	0	0	0	0
5	L	1	0	0	1	0
5	M	1	0	0	0	0
5	R	1	0	0	0	0
6	A	419	0	0	37	1
6	B	391	0	0	26	1
6	G	249	0	0	14	0
6	L	342	0	0	29	1
6	M	144	0	0	15	1
6	R	304	0	0	18	0
All	All	14563	0	12274	240	3

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 10.

All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ASN:HB3	6:A:792:HOH:O	1.13	1.31
1:B:206:GLU:HG3	6:B:790:HOH:O	1.30	1.31
6:A:807:HOH:O	1:R:260:LEU:HD11	1.37	1.22
1:B:163:ILE:HB	6:B:783:HOH:O	1.04	1.20
1:B:55:GLU:HG2	6:B:748:HOH:O	1.42	1.16
1:B:205:GLU:O	1:B:212:ARG:NH2	1.87	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:GLU:HB3	6:L:722:HOH:O	1.62	0.97
1:R:263:ALA:HB3	6:R:638:HOH:O	1.64	0.97
1:G:32:ASN:HB2	6:G:546:HOH:O	1.64	0.96
1:A:178:PHE:CD1	6:A:806:HOH:O	2.17	0.95
1:L:199:ARG:HD2	6:L:735:HOH:O	1.64	0.95
1:R:185:THR:CG2	6:R:689:HOH:O	2.20	0.90
1:A:59:GLU:HG3	6:A:763:HOH:O	1.71	0.90
1:B:220:ASN:HB2	6:B:594:HOH:O	1.71	0.90
1:L:199:ARG:CD	6:L:735:HOH:O	2.19	0.89
1:B:181:GLN:HG3	6:B:611:HOH:O	1.72	0.88
6:A:807:HOH:O	1:R:260:LEU:HD21	1.75	0.87
1:A:10:HIS:HE1	1:A:38:LEU:H	1.16	0.86
1:L:10:HIS:HE1	1:L:38:LEU:H	1.24	0.86
1:R:217:TRP:NE1	4:R:307:SO4:O2	2.08	0.85
3:L:303:EDO:H21	6:L:738:HOH:O	1.75	0.85
1:A:92:LYS:HD2	6:A:711:HOH:O	1.77	0.85
3:B:302:EDO:O2	6:B:786:HOH:O	1.95	0.85
1:A:261:ALA:HB1	6:A:643:HOH:O	1.77	0.84
3:A:302:EDO:H22	6:A:793:HOH:O	1.76	0.84
1:G:-2:GLU:HB2	6:G:639:HOH:O	1.76	0.84
1:A:96:LYS:HE2	6:A:641:HOH:O	1.77	0.84
1:L:140:ASN:C	6:L:601:HOH:O	2.17	0.83
1:G:220:ASN:HB3	6:G:524:HOH:O	1.77	0.83
1:R:164:GLU:CG	6:R:564:HOH:O	2.27	0.82
1:B:10:HIS:HE1	1:B:38:LEU:H	1.25	0.82
1:R:199:ARG:HD3	6:R:443:HOH:O	1.80	0.81
1:L:170:LYS:NZ	6:L:628:HOH:O	2.13	0.81
3:B:302:EDO:C1	6:B:613:HOH:O	2.28	0.81
1:G:243:ASN:ND2	2:G:301:CIT:O1	2.14	0.81
1:R:10:HIS:HE1	1:R:38:LEU:H	1.29	0.80
1:G:10:HIS:HE1	1:G:38:LEU:H	1.29	0.79
1:G:115:ALA:HA	1:G:183:LEU:HD13	1.65	0.78
1:A:181:GLN:HB3	6:A:681:HOH:O	1.84	0.78
3:B:302:EDO:H12	6:B:613:HOH:O	1.84	0.78
3:L:303:EDO:C2	6:L:738:HOH:O	2.31	0.77
1:M:10:HIS:HE1	1:M:38:LEU:H	1.32	0.77
1:A:167:GLU:OE2	1:A:171:HIS:HE1	1.70	0.75
1:M:55:GLU:O	6:M:505:HOH:O	2.05	0.74
1:A:199:ARG:CD	6:A:429:HOH:O	2.36	0.73
6:G:413:HOH:O	1:L:171:HIS:HD2	1.71	0.72
1:A:199:ARG:HD2	6:A:429:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:167:GLU:OE2	1:M:171:HIS:HE1	1.73	0.72
4:R:306:SO4:O3	6:R:607:HOH:O	2.07	0.72
3:A:304:EDO:C1	6:A:680:HOH:O	2.39	0.71
1:B:142:THR:HG22	6:B:678:HOH:O	1.89	0.70
1:G:199:ARG:HD3	6:G:429:HOH:O	1.90	0.70
1:L:170:LYS:CD	6:L:628:HOH:O	2.40	0.69
1:L:82:GLY:HA2	1:L:85:ASN:HD22	1.58	0.69
3:A:302:EDO:C2	6:A:793:HOH:O	2.36	0.69
1:B:199:ARG:CD	6:B:433:HOH:O	2.41	0.69
1:M:10:HIS:HD2	1:M:11:THR:O	1.77	0.68
1:A:-2:GLU:HG2	1:R:4:ALA:HA	1.75	0.68
1:M:115:ALA:HA	1:M:183:LEU:HD13	1.76	0.68
1:A:10:HIS:CE1	1:A:38:LEU:H	2.07	0.67
1:B:10:HIS:HD2	1:B:11:THR:O	1.77	0.67
1:B:205:GLU:C	1:B:212:ARG:HH22	1.97	0.66
1:R:82:GLY:HA2	1:R:85:ASN:HD22	1.60	0.66
4:L:307:SO4:O3	6:L:734:HOH:O	2.13	0.66
3:R:302:EDO:C1	6:R:698:HOH:O	2.43	0.65
1:R:10:HIS:HD2	1:R:11:THR:O	1.80	0.65
1:A:175:LYS:CE	6:A:663:HOH:O	2.45	0.65
1:L:115:ALA:HA	1:L:183:LEU:HD13	1.79	0.65
3:A:304:EDO:C2	6:A:810:HOH:O	2.46	0.64
1:B:167:GLU:OE2	1:B:171:HIS:HE1	1.80	0.64
1:R:10:HIS:CE1	1:R:38:LEU:H	2.15	0.64
1:L:142:THR:HG23	6:L:688:HOH:O	1.98	0.64
1:L:186:LEU:O	6:L:639:HOH:O	2.15	0.64
1:B:199:ARG:HD3	6:B:433:HOH:O	1.97	0.64
1:L:139:GLY:O	6:L:685:HOH:O	2.15	0.63
1:L:10:HIS:HD2	1:L:11:THR:O	1.81	0.63
1:L:206:GLU:CG	6:L:722:HOH:O	2.45	0.63
1:G:10:HIS:CE1	1:G:38:LEU:H	2.15	0.63
1:A:10:HIS:HD2	1:A:11:THR:O	1.83	0.62
1:L:140:ASN:HB3	6:L:601:HOH:O	2.00	0.62
1:B:82:GLY:HA2	1:B:85:ASN:HD22	1.63	0.62
1:M:199:ARG:NH2	1:M:222:TYR:O	2.32	0.62
1:M:179:PHE:CB	6:M:536:HOH:O	2.47	0.62
1:B:192:GLU:HG2	6:B:614:HOH:O	1.98	0.62
1:L:140:ASN:CB	6:L:601:HOH:O	2.47	0.62
1:G:171:HIS:HD2	6:L:483:HOH:O	1.82	0.62
1:A:135:ASN:CB	6:A:792:HOH:O	1.95	0.61
1:A:82:GLY:HA2	1:A:85:ASN:HD22	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:302:EDO:C1	6:M:539:HOH:O	2.48	0.61
1:M:179:PHE:HB2	6:M:536:HOH:O	2.00	0.61
1:L:226:LYS:HE2	6:L:668:HOH:O	2.00	0.61
6:M:424:HOH:O	1:R:171:HIS:HD2	1.82	0.61
1:A:192:GLU:HG2	6:A:644:HOH:O	2.00	0.60
1:L:206:GLU:CB	6:L:722:HOH:O	2.32	0.60
1:M:106:LEU:HG	1:M:117:VAL:HG12	1.84	0.60
6:A:807:HOH:O	1:R:260:LEU:CG	2.47	0.60
1:L:167:GLU:OE2	1:L:171:HIS:HE1	1.84	0.60
3:A:304:EDO:H21	6:A:810:HOH:O	2.02	0.60
1:G:10:HIS:HD2	1:G:11:THR:O	1.84	0.59
4:A:308:SO4:O4	6:A:787:HOH:O	2.16	0.59
3:R:302:EDO:O1	6:R:698:HOH:O	2.17	0.59
1:G:167:GLU:OE2	1:G:171:HIS:HE1	1.84	0.59
1:G:243:ASN:HD22	2:G:301:CIT:C1	2.14	0.59
1:L:199:ARG:HD3	6:L:735:HOH:O	1.94	0.59
3:L:302:EDO:H11	5:L:309:CL:CL	2.40	0.59
1:M:171:HIS:HD2	6:R:448:HOH:O	1.85	0.59
3:L:303:EDO:O2	6:L:738:HOH:O	2.17	0.58
1:M:12:ILE:O	1:M:13:CYS:HB2	2.03	0.58
1:L:10:HIS:CE1	1:L:38:LEU:H	2.12	0.58
1:M:10:HIS:CE1	1:M:38:LEU:H	2.18	0.58
1:G:32:ASN:CB	6:G:546:HOH:O	2.34	0.57
1:M:82:GLY:HA2	1:M:85:ASN:HD22	1.69	0.57
1:M:39:VAL:HG11	1:M:51:ILE:HD13	1.85	0.57
1:G:82:GLY:HA2	1:G:85:ASN:HD22	1.70	0.57
1:B:199:ARG:HD2	6:B:433:HOH:O	2.02	0.57
1:G:220:ASN:CB	6:G:524:HOH:O	2.47	0.56
1:G:212:ARG:HG3	6:G:582:HOH:O	2.05	0.56
1:R:167:GLU:OE2	1:R:171:HIS:HE1	1.89	0.56
1:R:192:GLU:HG2	6:R:562:HOH:O	2.05	0.56
1:A:171:HIS:HD2	6:B:468:HOH:O	1.89	0.55
1:L:164:GLU:HG3	6:L:541:HOH:O	2.05	0.55
1:A:199:ARG:HD3	6:A:429:HOH:O	2.06	0.55
3:A:304:EDO:H12	6:A:810:HOH:O	2.05	0.55
1:L:141:ASP:N	6:L:601:HOH:O	2.34	0.55
1:R:163:ILE:HD12	1:R:164:GLU:OE2	2.07	0.55
1:R:164:GLU:HG3	6:R:564:HOH:O	2.01	0.55
1:B:10:HIS:CE1	1:B:38:LEU:H	2.16	0.55
1:B:189:PHE:CE1	3:B:304:EDO:H22	2.42	0.54
1:R:114:PRO:HB2	1:R:183:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:GLU:HG3	6:G:632:HOH:O	2.07	0.54
3:L:302:EDO:C2	6:L:583:HOH:O	2.55	0.54
1:L:170:LYS:HD3	6:L:628:HOH:O	2.04	0.54
1:M:255:SER:OG	1:M:256:ALA:N	2.40	0.54
1:M:255:SER:O	1:M:256:ALA:C	2.47	0.53
1:A:178:PHE:HD1	6:A:806:HOH:O	1.74	0.53
1:R:185:THR:HG22	6:R:689:HOH:O	1.99	0.53
1:M:167:GLU:OE2	1:M:171:HIS:CE1	2.60	0.53
1:M:69:PRO:HB2	1:M:72:LYS:HG3	1.90	0.53
1:B:243:ASN:ND2	2:B:301:CIT:O3	2.41	0.52
1:A:220:ASN:O	1:A:223:LYS:HE2	2.08	0.52
6:A:807:HOH:O	1:R:260:LEU:CD2	2.40	0.52
3:M:302:EDO:H12	6:M:539:HOH:O	2.08	0.52
6:A:497:HOH:O	1:B:171:HIS:HD2	1.90	0.52
1:A:135:ASN:ND2	6:A:792:HOH:O	2.24	0.52
1:A:2:VAL:HB	1:A:257:SER:HB2	1.91	0.52
1:A:92:LYS:HG3	6:A:646:HOH:O	2.10	0.52
1:M:11:THR:HB	1:M:80:SER:HB3	1.92	0.51
1:G:96:LYS:HE2	6:G:598:HOH:O	2.10	0.51
1:M:107:MET:O	1:M:117:VAL:HG21	2.11	0.51
1:B:163:ILE:CG2	6:B:783:HOH:O	2.46	0.50
1:G:106:LEU:HD13	1:G:210:PHE:CZ	2.47	0.50
1:L:229:CYS:SG	6:L:733:HOH:O	2.60	0.50
1:R:54:TRP:NE1	1:R:183:LEU:HG	2.26	0.50
1:R:259:LEU:CD1	6:R:701:HOH:O	2.60	0.50
1:M:5:HIS:HE1	6:M:476:HOH:O	1.95	0.50
1:L:80:SER:OG	3:L:302:EDO:H21	2.12	0.50
1:G:11:THR:HG22	1:G:79:GLU:OE2	2.12	0.49
1:M:199:ARG:HD3	6:M:537:HOH:O	2.10	0.49
1:G:115:ALA:CA	1:G:183:LEU:HD13	2.41	0.49
1:A:175:LYS:NZ	6:A:663:HOH:O	2.41	0.49
1:L:142:THR:CG2	6:L:688:HOH:O	2.59	0.49
1:G:-2:GLU:CG	1:G:-1:GLY:H	2.25	0.49
1:B:198:ARG:HD3	6:B:610:HOH:O	2.12	0.49
1:M:114:PRO:HB2	1:M:183:LEU:HD22	1.94	0.48
3:A:304:EDO:C1	6:A:810:HOH:O	2.60	0.48
1:R:199:ARG:CD	6:R:443:HOH:O	2.48	0.47
1:G:114:PRO:HB2	1:G:183:LEU:HD22	1.95	0.47
1:G:163:ILE:HD11	6:G:541:HOH:O	2.13	0.47
1:L:114:PRO:HB2	1:L:183:LEU:HD22	1.96	0.47
1:A:7:ILE:HD13	1:A:64:LEU:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ASN:CB	1:G:143:VAL:O	2.62	0.47
1:G:199:ARG:NH2	1:G:222:TYR:O	2.48	0.47
1:M:12:ILE:O	1:M:13:CYS:CB	2.64	0.46
1:M:113:SER:HB3	6:M:540:HOH:O	2.15	0.46
1:L:163:ILE:HD11	6:L:560:HOH:O	2.16	0.46
1:R:182:ASP:O	1:R:185:THR:HG22	2.15	0.46
1:M:5:HIS:CE1	6:M:476:HOH:O	2.68	0.46
1:A:11:THR:HB	1:A:80:SER:HB3	1.97	0.46
1:G:-2:GLU:HG2	6:G:621:HOH:O	2.16	0.46
1:M:163:ILE:HG13	6:M:423:HOH:O	2.15	0.46
1:R:163:ILE:HG13	6:R:433:HOH:O	2.16	0.46
1:M:53:THR:HA	6:M:536:HOH:O	2.15	0.46
1:M:54:TRP:CD1	6:M:536:HOH:O	2.56	0.46
1:B:96:LYS:HE2	6:B:540:HOH:O	2.15	0.46
4:B:306:SO4:O1	6:B:588:HOH:O	2.21	0.46
1:M:115:ALA:O	1:M:116:PHE:C	2.54	0.46
1:G:102:PHE:HB3	1:G:105:ALA:HB3	1.98	0.45
1:B:220:ASN:CB	6:B:594:HOH:O	2.45	0.45
1:A:167:GLU:OE2	1:A:171:HIS:CE1	2.60	0.45
1:B:198:ARG:NH2	6:B:605:HOH:O	2.41	0.45
1:R:11:THR:HB	1:R:80:SER:HB3	1.98	0.45
1:R:262:VAL:HG13	6:R:565:HOH:O	2.15	0.45
1:A:260:LEU:HD12	6:A:633:HOH:O	2.16	0.45
1:A:142:THR:HB	6:A:624:HOH:O	2.16	0.44
1:G:7:ILE:HD13	1:G:64:LEU:HD13	1.99	0.44
1:L:141:ASP:HA	6:L:601:HOH:O	2.17	0.44
1:B:11:THR:HB	1:B:80:SER:HB3	1.99	0.44
1:G:96:LYS:HA	1:G:96:LYS:HD2	1.87	0.44
1:R:68:ILE:HB	1:R:96:LYS:HE3	1.99	0.44
1:A:163:ILE:H	1:A:163:ILE:HG13	1.65	0.44
6:B:574:HOH:O	1:R:260:LEU:HD22	2.18	0.44
1:B:142:THR:HG21	6:B:745:HOH:O	2.17	0.44
1:B:216:LEU:CD2	6:B:787:HOH:O	2.66	0.44
1:M:84:ILE:HG22	1:M:88:LEU:HD22	2.00	0.44
1:M:7:ILE:HD13	1:M:64:LEU:HD13	1.99	0.44
1:A:30:GLY:HA3	1:R:1:MET:HE3	2.00	0.43
1:A:163:ILE:HG13	6:A:446:HOH:O	2.18	0.43
1:R:259:LEU:HG	6:R:701:HOH:O	2.18	0.43
1:A:175:LYS:HE3	6:A:663:HOH:O	2.13	0.43
1:L:178:PHE:HZ	3:L:302:EDO:H22	1.83	0.43
1:M:115:ALA:CA	1:M:183:LEU:HD13	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLU:C	1:B:212:ARG:NH2	2.63	0.43
1:M:49:GLU:HA	1:M:136:TYR:CE2	2.54	0.43
1:M:11:THR:HG22	1:M:79:GLU:OE2	2.18	0.43
1:B:55:GLU:CG	6:B:748:HOH:O	2.26	0.43
1:R:164:GLU:HG2	6:R:564:HOH:O	2.08	0.43
1:M:109:ASP:HB2	6:M:510:HOH:O	2.19	0.42
1:A:261:ALA:CB	6:A:643:HOH:O	2.48	0.42
1:A:163:ILE:HD11	6:A:559:HOH:O	2.19	0.42
1:A:92:LYS:HB3	1:A:92:LYS:HE3	1.75	0.42
1:B:163:ILE:CD1	1:R:260:LEU:HD23	2.50	0.42
1:G:12:ILE:O	1:G:13:CYS:HB2	2.20	0.41
1:G:198:ARG:NH1	1:G:255:SER:OG	2.53	0.41
1:R:115:ALA:HA	1:R:183:LEU:HD13	2.01	0.41
1:A:192:GLU:CG	6:A:644:HOH:O	2.63	0.41
1:M:41:SER:HA	6:M:449:HOH:O	2.20	0.41
1:B:216:LEU:HD21	6:B:787:HOH:O	2.20	0.41
1:G:256:ALA:HA	6:G:647:HOH:O	2.20	0.41
1:R:164:GLU:CD	6:R:564:HOH:O	2.54	0.41
1:L:164:GLU:CG	6:L:721:HOH:O	2.69	0.41
1:M:103:HIS:O	1:M:104:ASN:C	2.59	0.41
1:B:151:ARG:CD	6:B:612:HOH:O	2.69	0.41
1:G:163:ILE:HD12	1:G:164:GLU:OE1	2.20	0.41
1:M:51:ILE:CG1	1:M:56:GLN:HB3	2.51	0.41
1:G:135:ASN:HB3	1:G:144:THR:HA	2.03	0.41
1:G:120:LYS:O	1:G:124:VAL:HB	2.22	0.40
1:G:-2:GLU:CG	1:G:-1:GLY:N	2.85	0.40
1:A:163:ILE:HD12	1:A:164:GLU:N	2.36	0.40
1:G:216:LEU:HD21	6:G:640:HOH:O	2.22	0.40
1:R:65:ILE:HA	1:R:68:ILE:HD12	2.02	0.40

All (3) 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)
6:M:492:HOH:O	6:M:492:HOH:O[6_445]	1.93	0.27
6:A:761:HOH:O	6:B:539:HOH:O[4_554]	2.05	0.15
6:L:563:HOH:O	6:L:642:HOH:O[6_445]	2.17	0.03

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	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	34 24
1	B	259/288 (90%)	245 (95%)	14 (5%)	0	100 100
1	G	260/288 (90%)	247 (95%)	13 (5%)	0	100 100
1	L	255/288 (88%)	243 (95%)	12 (5%)	0	100 100
1	M	256/288 (89%)	240 (94%)	16 (6%)	0	100 100
1	R	263/288 (91%)	250 (95%)	13 (5%)	0	100 100
All	All	1556/1728 (90%)	1475 (95%)	80 (5%)	1 (0%)	51 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	229/249 (92%)	219 (96%)	10 (4%)	28 19
1	B	226/249 (91%)	222 (98%)	4 (2%)	59 55
1	G	227/249 (91%)	213 (94%)	14 (6%)	18 9
1	L	223/249 (90%)	214 (96%)	9 (4%)	31 22
1	M	223/249 (90%)	206 (92%)	17 (8%)	13 5
1	R	228/249 (92%)	216 (95%)	12 (5%)	22 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1356/1494 (91%)	1290 (95%)	66 (5%)	25 15

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	46	ARG
1	A	64	LEU
1	A	79	GLU
1	A	88	LEU
1	A	113	SER
1	A	142	THR
1	A	163	ILE
1	A	199	ARG
1	A	260	LEU
1	B	46	ARG
1	B	113	SER
1	B	124	VAL
1	B	142	THR
1	G	-2	GLU
1	G	2	VAL
1	G	25	LEU
1	G	46	ARG
1	G	64	LEU
1	G	79	GLU
1	G	106	LEU
1	G	142	THR
1	G	163	ILE
1	G	183	LEU
1	G	185	THR
1	G	223	LYS
1	G	258	ASP
1	G	259	LEU
1	L	46	ARG
1	L	64	LEU
1	L	79	GLU
1	L	88	LEU
1	L	113	SER
1	L	124	VAL
1	L	142	THR
1	L	163	ILE
1	L	183	LEU

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Mol	Chain	Res	Type
1	M	25	LEU
1	M	46	ARG
1	M	51	ILE
1	M	64	LEU
1	M	66	GLU
1	M	79	GLU
1	M	88	LEU
1	M	95	GLU
1	M	106	LEU
1	M	135	ASN
1	M	163	ILE
1	M	183	LEU
1	M	185	THR
1	M	186	LEU
1	M	192	GLU
1	M	223	LYS
1	M	255	SER
1	R	46	ARG
1	R	64	LEU
1	R	79	GLU
1	R	88	LEU
1	R	106	LEU
1	R	124	VAL
1	R	142	THR
1	R	163	ILE
1	R	183	LEU
1	R	185	THR
1	R	186	LEU
1	R	191	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	47	GLN
1	A	85	ASN
1	A	171	HIS
1	A	220	ASN
1	A	250	GLN
1	A	254	ASN
1	B	10	HIS
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	140	ASN
1	B	171	HIS
1	G	10	HIS
1	G	47	GLN
1	G	85	ASN
1	G	171	HIS
1	G	181	GLN
1	G	220	ASN
1	G	243	ASN
1	G	247	GLN
1	L	10	HIS
1	L	47	GLN
1	L	85	ASN
1	L	140	ASN
1	L	171	HIS
1	M	10	HIS
1	M	47	GLN
1	M	85	ASN
1	M	171	HIS
1	M	181	GLN
1	M	220	ASN
1	R	10	HIS
1	R	47	GLN
1	R	85	ASN
1	R	171	HIS
1	R	181	GLN
1	R	250	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 49 ligands modelled in this entry, 6 are monoatomic - leaving 43 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	310	-	4,4,4	0.40	0	6,6,6	0.14	0
3	EDO	B	303	-	3,3,3	0.21	0	2,2,2	0.92	0
3	EDO	R	302	-	3,3,3	0.47	0	2,2,2	0.71	0
4	SO4	L	307	-	4,4,4	0.44	0	6,6,6	0.26	0
4	SO4	L	308	-	4,4,4	0.37	0	6,6,6	0.22	0
4	SO4	B	308	-	4,4,4	0.39	0	6,6,6	0.30	0
3	EDO	L	303	-	3,3,3	0.36	0	2,2,2	0.60	0
2	CIT	A	301	-	12,12,12	1.26	0	17,17,17	1.77	4 (23%)
4	SO4	B	307	-	4,4,4	0.34	0	6,6,6	0.50	0
4	SO4	R	305	-	4,4,4	0.39	0	6,6,6	0.45	0
3	EDO	A	304	-	3,3,3	0.38	0	2,2,2	0.44	0
4	SO4	A	308	-	4,4,4	0.41	0	6,6,6	0.25	0
4	SO4	G	304	-	4,4,4	0.34	0	6,6,6	0.35	0
3	EDO	A	305	-	3,3,3	0.56	0	2,2,2	0.17	0
2	CIT	M	301	-	12,12,12	1.01	0	17,17,17	1.54	3 (17%)
4	SO4	B	306	-	4,4,4	0.24	0	6,6,6	0.32	0
4	SO4	A	306	-	4,4,4	0.23	0	6,6,6	0.53	0
3	EDO	B	305	-	3,3,3	0.57	0	2,2,2	0.14	0
3	EDO	G	303	-	3,3,3	0.43	0	2,2,2	0.20	0
3	EDO	L	305	-	3,3,3	0.52	0	2,2,2	0.13	0
3	EDO	L	302	-	3,3,3	0.56	0	2,2,2	0.45	0
3	EDO	R	303	-	3,3,3	0.50	0	2,2,2	0.05	0
2	CIT	G	301	-	12,12,12	1.43	3 (25%)	17,17,17	2.37	8 (47%)
3	EDO	B	304	-	3,3,3	0.38	0	2,2,2	0.70	0
2	CIT	L	301	-	12,12,12	1.98	2 (16%)	17,17,17	3.99	6 (35%)
4	SO4	B	309	-	4,4,4	0.44	0	6,6,6	0.32	0
4	SO4	L	306	-	4,4,4	0.22	0	6,6,6	0.37	0
3	EDO	G	302	-	3,3,3	0.41	0	2,2,2	0.89	0
2	CIT	B	301	-	12,12,12	1.15	1 (8%)	17,17,17	2.14	8 (47%)
4	SO4	R	306	-	4,4,4	0.26	0	6,6,6	0.39	0
4	SO4	G	305	-	4,4,4	0.29	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	R	307	-	4,4,4	0.37	0	6,6,6	0.28	0
3	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.33	0
4	SO4	R	304	-	4,4,4	0.31	0	6,6,6	0.27	0
3	EDO	M	302	-	3,3,3	0.37	0	2,2,2	0.64	0
3	EDO	A	302	-	3,3,3	0.56	0	2,2,2	0.17	0
4	SO4	G	306	-	4,4,4	0.43	0	6,6,6	0.25	0
3	EDO	M	303	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	M	304	-	3,3,3	0.48	0	2,2,2	0.19	0
4	SO4	A	307	-	4,4,4	0.37	0	6,6,6	0.30	0
3	EDO	B	302	-	3,3,3	0.50	0	2,2,2	0.03	0
2	CIT	R	301	-	12,12,12	0.96	0	17,17,17	2.04	3 (17%)
3	EDO	L	304	-	3,3,3	0.54	0	2,2,2	0.13	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	EDO	B	303	-	-	1/1/1/1	-
3	EDO	R	302	-	-	1/1/1/1	-
3	EDO	L	303	-	-	0/1/1/1	-
2	CIT	A	301	-	-	2/16/16/16	-
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	A	305	-	-	1/1/1/1	-
2	CIT	M	301	-	-	3/16/16/16	-
3	EDO	B	305	-	-	1/1/1/1	-
3	EDO	G	303	-	-	1/1/1/1	-
3	EDO	L	305	-	-	1/1/1/1	-
3	EDO	L	302	-	-	1/1/1/1	-
3	EDO	R	303	-	-	1/1/1/1	-
2	CIT	G	301	-	-	8/16/16/16	-
3	EDO	B	304	-	-	1/1/1/1	-
2	CIT	L	301	-	-	2/16/16/16	-
3	EDO	G	302	-	-	1/1/1/1	-
2	CIT	B	301	-	-	3/16/16/16	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	M	302	-	-	1/1/1/1	-
3	EDO	A	302	-	-	0/1/1/1	-
3	EDO	M	303	-	-	0/1/1/1	-
3	EDO	M	304	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	302	-	-	1/1/1/1	-
2	CIT	R	301	-	-	6/16/16/16	-
3	EDO	L	304	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	301	CIT	C3-C6	-5.44	1.47	1.53
2	G	301	CIT	C2-C3	-2.32	1.50	1.53
2	G	301	CIT	C4-C3	-2.26	1.51	1.53
2	G	301	CIT	C3-C6	-2.24	1.51	1.53
2	L	301	CIT	O5-C6	2.08	1.28	1.22
2	B	301	CIT	C3-C6	-2.01	1.51	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	301	CIT	O7-C3-C6	-12.83	90.86	108.86
2	L	301	CIT	O5-C6-C3	-6.55	112.97	122.25
2	R	301	CIT	O7-C3-C6	-4.75	102.19	108.86
2	G	301	CIT	C4-C3-C6	-4.68	100.06	110.11
2	G	301	CIT	C4-C3-C2	4.33	120.47	109.16
2	L	301	CIT	C4-C3-C2	4.18	120.07	109.16
2	R	301	CIT	O6-C6-C3	4.15	120.25	113.05
2	A	301	CIT	C4-C3-C6	-3.99	101.52	110.11
2	L	301	CIT	C2-C3-C6	-3.85	101.84	110.11
2	G	301	CIT	O5-C6-C3	-3.59	117.16	122.25
2	B	301	CIT	O7-C3-C4	-3.35	101.56	109.40
2	B	301	CIT	C2-C3-C6	-3.30	103.01	110.11
2	L	301	CIT	O7-C3-C4	3.30	117.13	109.40
2	A	301	CIT	O6-C6-C3	3.25	118.69	113.05
2	B	301	CIT	O7-C3-C2	3.09	116.64	109.40
2	M	301	CIT	O6-C6-C3	3.04	118.33	113.05
2	M	301	CIT	O5-C6-C3	-2.77	118.33	122.25
2	B	301	CIT	O1-C1-C2	-2.76	114.88	122.94
2	B	301	CIT	O5-C6-C3	-2.75	118.35	122.25
2	G	301	CIT	O6-C6-C3	2.68	117.71	113.05
2	M	301	CIT	C2-C3-C6	-2.60	104.53	110.11
2	G	301	CIT	O3-C5-C4	-2.57	115.44	122.94
2	G	301	CIT	O7-C3-C6	-2.56	105.27	108.86
2	R	301	CIT	O1-C1-C2	-2.49	115.66	122.94
2	G	301	CIT	O7-C3-C4	2.48	115.21	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	301	CIT	O6-C6-O5	2.38	131.40	123.82
2	A	301	CIT	C4-C3-C2	2.35	115.29	109.16
2	B	301	CIT	C4-C3-C2	2.35	115.29	109.16
2	G	301	CIT	C3-C2-C1	-2.31	108.22	113.81
2	B	301	CIT	O6-C6-C3	2.08	116.67	113.05
2	A	301	CIT	C3-C4-C5	-2.04	108.88	113.81
2	B	301	CIT	C3-C4-C5	-2.01	108.95	113.81

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	301	CIT	O7-C3-C6-O6
2	M	301	CIT	C1-C2-C3-C4
2	M	301	CIT	C1-C2-C3-C6
3	R	302	EDO	O1-C1-C2-O2
2	B	301	CIT	C1-C2-C3-C6
3	A	305	EDO	O1-C1-C2-O2
3	B	305	EDO	O1-C1-C2-O2
3	L	302	EDO	O1-C1-C2-O2
2	L	301	CIT	C1-C2-C3-O7
2	M	301	CIT	C1-C2-C3-O7
2	A	301	CIT	C2-C3-C4-C5
2	R	301	CIT	O7-C3-C4-C5
3	L	304	EDO	O1-C1-C2-O2
3	L	305	EDO	O1-C1-C2-O2
2	G	301	CIT	O7-C3-C6-O5
2	G	301	CIT	C2-C3-C6-O5
2	G	301	CIT	C2-C3-C6-O6
2	R	301	CIT	C2-C3-C6-O5
2	R	301	CIT	C4-C3-C6-O5
2	R	301	CIT	C4-C3-C6-O6
2	A	301	CIT	C6-C3-C4-C5
3	G	303	EDO	O1-C1-C2-O2
2	B	301	CIT	C1-C2-C3-C4
2	G	301	CIT	C4-C3-C6-O5
2	R	301	CIT	C2-C3-C6-O6
3	G	302	EDO	O1-C1-C2-O2
3	M	304	EDO	O1-C1-C2-O2
2	G	301	CIT	C2-C3-C4-C5
2	G	301	CIT	C4-C3-C6-O6
2	L	301	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
3	M	302	EDO	O1-C1-C2-O2
3	R	303	EDO	O1-C1-C2-O2
2	G	301	CIT	C1-C2-C3-O7
3	B	302	EDO	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2
3	B	304	EDO	O1-C1-C2-O2
2	B	301	CIT	C1-C2-C3-O7
2	R	301	CIT	C1-C2-C3-O7

There are no ring outliers.

15 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	302	EDO	2	0
4	L	307	SO4	1	0
3	L	303	EDO	3	0
3	A	304	EDO	5	0
4	A	308	SO4	1	0
4	B	306	SO4	1	0
3	L	302	EDO	4	0
2	G	301	CIT	2	0
3	B	304	EDO	1	0
2	B	301	CIT	1	0
4	R	306	SO4	1	0
4	R	307	SO4	1	0
3	M	302	EDO	2	0
3	A	302	EDO	2	0
3	B	302	EDO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	265/288 (92%)	-0.25	4 (1%) 73 76	11, 17, 32, 64	0
1	B	261/288 (90%)	-0.15	2 (0%) 86 87	11, 19, 34, 81	0
1	G	262/288 (90%)	0.05	6 (2%) 60 63	17, 29, 50, 77	0
1	L	257/288 (89%)	-0.40	2 (0%) 86 87	14, 21, 39, 68	0
1	M	258/288 (89%)	0.80	45 (17%) 1 1	18, 42, 67, 94	0
1	R	265/288 (92%)	-0.02	8 (3%) 50 53	15, 25, 45, 77	0
All	All	1568/1728 (90%)	0.00	67 (4%) 35 38	11, 24, 54, 94	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	256	ALA	6.9
1	M	189	PHE	5.5
1	R	140	ASN	4.9
1	M	186	LEU	4.8
1	M	181	GLN	4.8
1	M	110	ILE	4.5
1	B	259	LEU	4.4
1	M	140	ASN	4.4
1	M	190	THR	4.3
1	M	139	GLY	4.3
1	M	142	THR	4.2
1	M	184	ASP	4.2
1	M	137	THR	4.1
1	M	185	THR	4.0
1	G	140	ASN	4.0
1	M	143	VAL	3.9
1	A	262	VAL	3.8
1	G	259	LEU	3.7
1	R	256	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	M	123	GLU	3.6
1	M	187	PRO	3.6
1	M	183	LEU	3.5
1	M	141	ASP	3.5
1	M	178	PHE	3.4
1	B	258	ASP	3.4
1	M	193	GLY	3.3
1	M	138	TYR	3.3
1	M	194	TYR	3.2
1	M	116	PHE	3.1
1	M	113	SER	3.1
1	M	70	GLU	3.1
1	M	114	PRO	3.0
1	M	119	LYS	3.0
1	G	139	GLY	3.0
1	M	117	VAL	2.8
1	M	188	ASN	2.8
1	M	72	LYS	2.7
1	M	2	VAL	2.7
1	A	261	ALA	2.7
1	M	118	TYR	2.7
1	M	93	TYR	2.6
1	M	124	VAL	2.6
1	R	257	SER	2.6
1	M	89	ALA	2.5
1	M	192	GLU	2.5
1	R	186	LEU	2.5
1	M	90	ALA	2.5
1	L	0	PHE	2.4
1	G	220	ASN	2.4
1	R	141	ASP	2.4
1	A	259	LEU	2.3
1	A	260	LEU	2.3
1	R	263	ALA	2.2
1	M	112	HIS	2.1
1	M	136	TYR	2.1
1	L	140	ASN	2.1
1	G	137	THR	2.1
1	M	179	PHE	2.1
1	G	142	THR	2.1
1	M	111	ASP	2.1
1	R	258	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	126	THR	2.0
1	R	262	VAL	2.0
1	M	99	ALA	2.0
1	M	115	ALA	2.0
1	M	71	GLY	2.0
1	M	135	ASN	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	EDO	L	304	4/4	0.67	0.39	430,478,500,500	0
4	SO4	R	307	5/5	0.78	0.27	59,76,96,118	0
3	EDO	R	302	4/4	0.83	0.17	44,48,50,52	0
2	CIT	M	301	13/13	0.83	0.24	42,54,74,89	0
2	CIT	B	301	13/13	0.85	0.20	26,45,67,68	0
3	EDO	A	303	4/4	0.85	0.18	37,37,39,42	0
3	EDO	L	302	4/4	0.85	0.19	30,47,50,51	0
3	EDO	G	302	4/4	0.86	0.22	50,52,58,60	0
3	EDO	A	302	4/4	0.87	0.18	37,47,47,49	0
3	EDO	M	303	4/4	0.88	0.18	32,35,39,47	0
3	EDO	A	304	4/4	0.88	0.13	29,40,42,57	0
2	CIT	L	301	13/13	0.88	0.26	24,39,70,70	0
3	EDO	B	305	4/4	0.89	0.14	41,43,46,47	0
2	CIT	G	301	13/13	0.89	0.21	34,39,60,61	0
3	EDO	B	304	4/4	0.89	0.23	39,39,43,47	0
3	EDO	L	303	4/4	0.89	0.17	26,28,30,39	0
3	EDO	B	303	4/4	0.90	0.24	24,27,34,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	302	4/4	0.91	0.15	35,46,48,54	0
4	SO4	B	310	5/5	0.91	0.23	50,65,75,89	0
4	SO4	L	308	5/5	0.91	0.25	61,68,75,92	0
4	SO4	R	306	5/5	0.91	0.20	36,38,42,43	5
3	EDO	G	303	4/4	0.91	0.26	51,59,59,63	0
4	SO4	L	307	5/5	0.92	0.22	52,56,68,75	0
2	CIT	R	301	13/13	0.92	0.14	22,32,55,71	0
3	EDO	L	305	4/4	0.93	0.16	39,49,52,52	0
3	EDO	A	305	4/4	0.93	0.18	38,44,45,48	0
3	EDO	M	304	4/4	0.93	0.25	54,56,64,64	0
2	CIT	A	301	13/13	0.94	0.14	18,25,47,49	0
3	EDO	R	303	4/4	0.94	0.24	55,57,57,61	0
4	SO4	A	308	5/5	0.94	0.31	53,54,68,80	0
3	EDO	M	302	4/4	0.94	0.10	47,53,55,57	0
4	SO4	G	304	5/5	0.95	0.17	53,61,64,70	0
4	SO4	G	306	5/5	0.95	0.09	54,57,60,68	0
4	SO4	B	308	5/5	0.95	0.17	55,68,73,83	0
4	SO4	G	305	5/5	0.96	0.18	49,53,62,73	0
4	SO4	R	305	5/5	0.96	0.12	38,53,62,71	0
4	SO4	A	307	5/5	0.96	0.16	39,40,43,49	0
4	SO4	B	309	5/5	0.96	0.18	34,46,50,55	0
4	SO4	R	304	5/5	0.97	0.19	55,56,59,62	0
4	SO4	B	306	5/5	0.97	0.11	47,47,53,63	0
5	CL	R	308	1/1	0.97	0.09	26,26,26,26	0
4	SO4	B	307	5/5	0.98	0.15	38,39,42,51	0
4	SO4	L	306	5/5	0.98	0.12	44,44,47,64	0
5	CL	L	309	1/1	0.98	0.06	20,20,20,20	0
4	SO4	A	306	5/5	0.98	0.11	33,34,41,60	0
5	CL	G	307	1/1	0.99	0.07	30,30,30,30	0
5	CL	A	309	1/1	0.99	0.09	20,20,20,20	0
5	CL	M	305	1/1	0.99	0.06	36,36,36,36	0
5	CL	B	311	1/1	0.99	0.11	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.