



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:26 pm BST

PDB ID : 3R90
Title : Crystal structure of Malignant T cell-amplified sequence 1 protein
Authors : Hong, B.; Dimov, S.; Tempel, W.; Tong, Y.; Wernimont, A.K.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2011-03-24
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

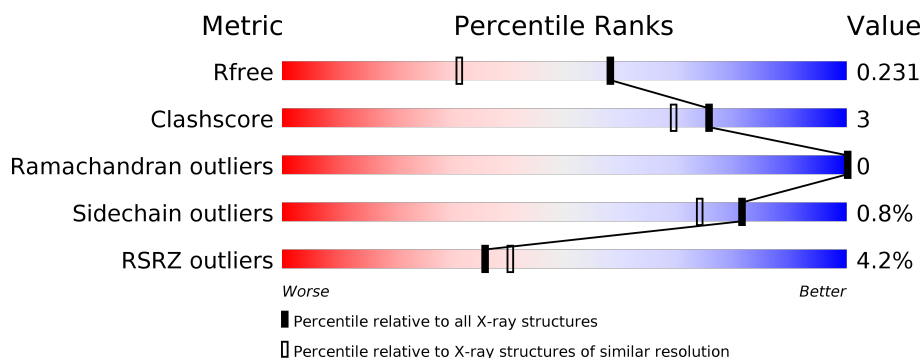
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 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 $\leq 5\%$. 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	188	<div> <div>5%</div> <div>90%</div> <div>8%</div> </div>
1	B	188	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>
1	C	188	<div> <div>8%</div> <div>96%</div> <div>• •</div> </div>
1	D	188	<div> <div>4%</div> <div>92%</div> <div>• •</div> </div>
1	E	188	<div> <div>6%</div> <div>86%</div> <div>10% • •</div> </div>
1	F	188	<div> <div>%</div> <div>92%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	188	
1	H	188	
1	I	188	
1	J	188	
1	K	188	
1	L	188	

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	SO4	K	190	-	-	X	-
3	UNX	I	8972	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19275 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 Malignant T cell-amplified sequence 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	11	0
			1486	976	243	256	11			
1	B	185	Total	C	N	O	S	0	6	0
			1458	950	242	255	11			
1	C	185	Total	C	N	O	S	0	4	0
			1447	939	247	250	11			
1	D	180	Total	C	N	O	S	0	6	0
			1419	932	230	246	11			
1	E	181	Total	C	N	O	S	0	11	0
			1444	948	239	246	11			
1	F	181	Total	C	N	O	S	0	11	0
			1454	954	235	254	11			
1	G	181	Total	C	N	O	S	0	11	0
			1458	958	240	249	11			
1	H	180	Total	C	N	O	S	0	12	0
			1467	964	247	245	11			
1	I	187	Total	C	N	O	S	0	12	0
			1520	994	258	256	12			
1	J	188	Total	C	N	O	S	0	6	0
			1507	981	260	255	11			
1	K	188	Total	C	N	O	S	0	9	0
			1524	996	260	257	11			
1	L	180	Total	C	N	O	S	0	6	0
			1412	924	230	247	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
A	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
A	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
A	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
A	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
A	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
A	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
A	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
A	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
B	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
B	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
B	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
B	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
B	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
B	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
B	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
B	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
B	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
B	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
C	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
C	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
C	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
C	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
C	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
C	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
C	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
C	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
C	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
C	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
D	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
D	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
D	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
D	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
D	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
D	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
D	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
D	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
D	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
D	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
E	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
E	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
E	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
E	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
E	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
E	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
E	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
E	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
E	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
F	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
F	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
F	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
F	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
F	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
F	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
F	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
F	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
F	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
F	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
G	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
G	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
G	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
G	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
G	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
G	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
G	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
G	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
G	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
G	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
H	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
H	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
H	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
H	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
H	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
H	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
H	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
H	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
H	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
H	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
I	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
I	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
I	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
I	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
I	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
I	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
I	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
I	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
I	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
J	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
J	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
J	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
J	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
J	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
J	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
J	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
J	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
J	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
J	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
K	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
K	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
K	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
K	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
K	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
K	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
K	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
K	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
K	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
K	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4
L	137	ALA	GLU	ENGINEERED MUTATION	UNP Q9ULC4
L	139	ALA	LYS	ENGINEERED MUTATION	UNP Q9ULC4
L	140	ALA	GLN	ENGINEERED MUTATION	UNP Q9ULC4
L	182	ALA	-	EXPRESSION TAG	UNP Q9ULC4
L	183	HIS	-	EXPRESSION TAG	UNP Q9ULC4
L	184	HIS	-	EXPRESSION TAG	UNP Q9ULC4
L	185	HIS	-	EXPRESSION TAG	UNP Q9ULC4
L	186	HIS	-	EXPRESSION TAG	UNP Q9ULC4
L	187	HIS	-	EXPRESSION TAG	UNP Q9ULC4
L	188	HIS	-	EXPRESSION TAG	UNP Q9ULC4

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

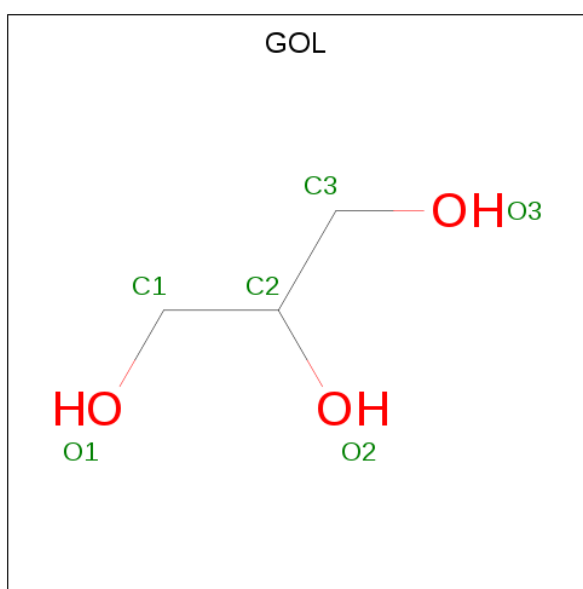
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	13	Total	X	0	0
			13	13		
3	J	14	Total	X	0	0
			14	14		
3	D	8	Total	X	0	0
			8	8		
3	K	16	Total	X	0	0
			16	16		
3	E	11	Total	X	0	0
			11	11		
3	H	20	Total	X	0	0
			20	20		
3	B	9	Total	X	0	0
			9	9		
3	I	23	Total	X	0	0
			23	23		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	14	Total	X	0	0
			14	14		
3	A	17	Total	X	0	0
			17	17		
3	L	12	Total	X	0	0
			12	12		
3	F	17	Total	X	0	0
			17	17		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	111	Total	O	0	0
			111	111		
5	C	63	Total	O	0	0
			63	63		
5	D	88	Total	O	0	0
			88	88		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	87	Total 87	O 87	0	0
5	F	154	Total 154	O 154	0	0
5	G	135	Total 135	O 135	0	0
5	H	140	Total 140	O 140	0	0
5	I	121	Total 121	O 121	0	0
5	J	105	Total 105	O 105	0	0
5	K	144	Total 144	O 144	0	0
5	L	111	Total 111	O 111	0	0

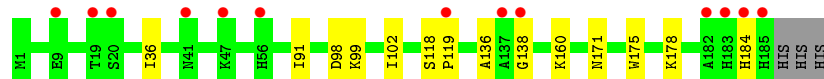
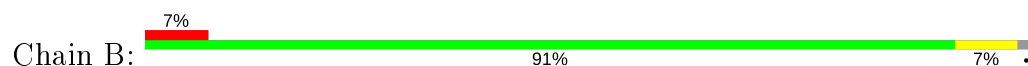
3 Residue-property plots [i](#)

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

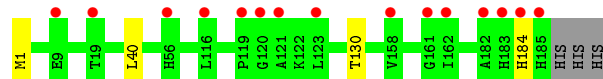
- Molecule 1: Malignant T cell-amplified sequence 1



- Molecule 1: Malignant T cell-amplified sequence 1



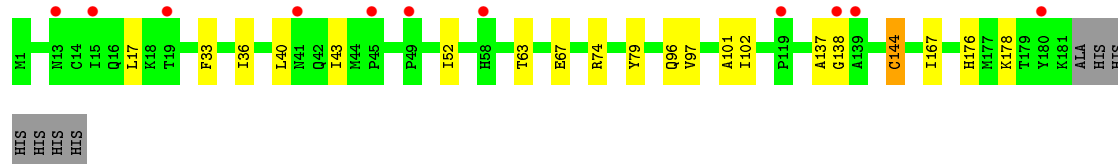
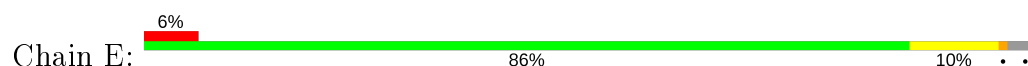
- Molecule 1: Malignant T cell-amplified sequence 1



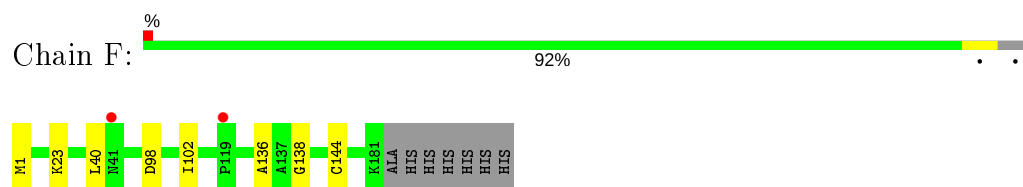
- Molecule 1: Malignant T cell-amplified sequence 1



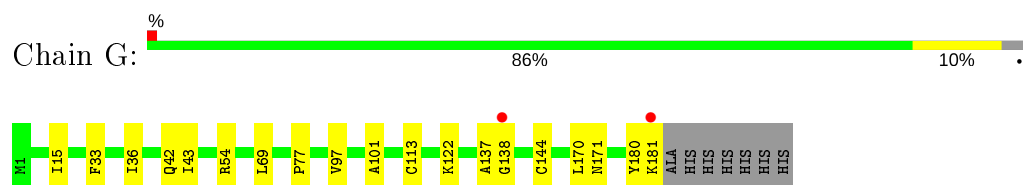
- Molecule 1: Malignant T cell-amplified sequence 1



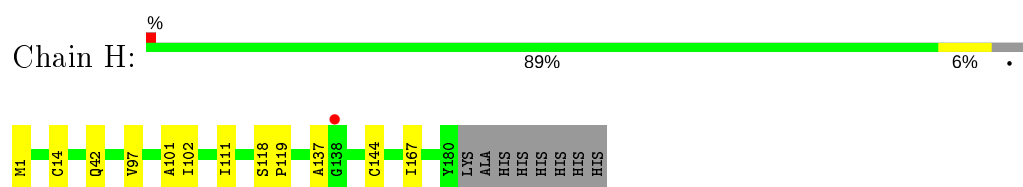
- Molecule 1: Malignant T cell-amplified sequence 1



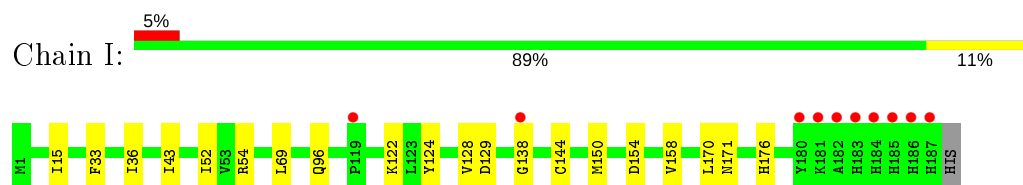
- Molecule 1: Malignant T cell-amplified sequence 1



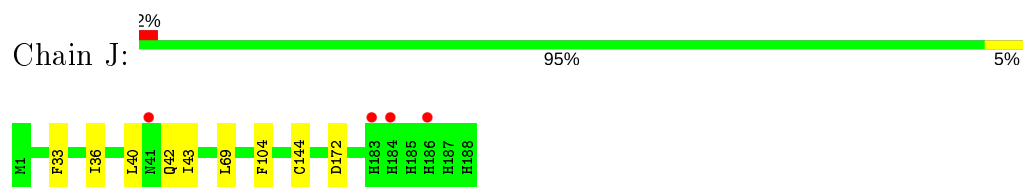
- Molecule 1: Malignant T cell-amplified sequence 1



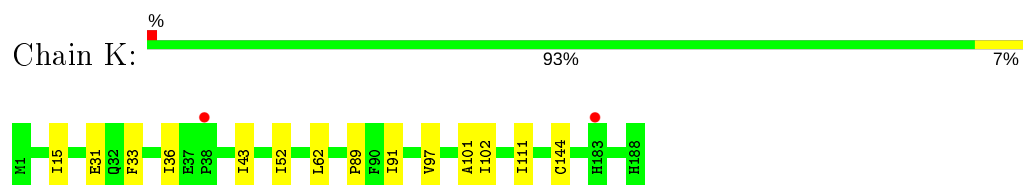
- Molecule 1: Malignant T cell-amplified sequence 1



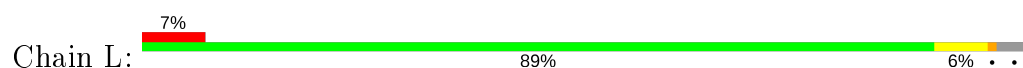
- Molecule 1: Malignant T cell-amplified sequence 1

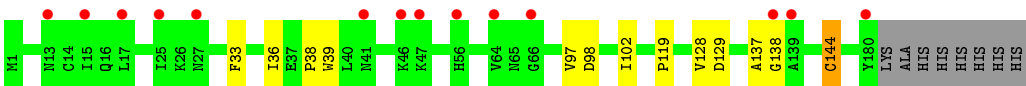


- Molecule 1: Malignant T cell-amplified sequence 1



- Molecule 1: Malignant T cell-amplified sequence 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	115.59Å 115.59Å 157.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.42 – 1.70 28.42 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.42-1.70) 99.9 (28.42-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.202 , 0.235 0.200 , 0.231	Depositor DCC
R_{free} test set	5105 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l 0.023 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19275	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UNX, 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	0.61	0/1557	0.59	0/2112
1	B	0.58	0/1506	0.59	0/2043
1	C	0.55	0/1497	0.57	0/2033
1	D	0.58	0/1473	0.58	0/2001
1	E	0.55	1/1505 (0.1%)	0.59	0/2046
1	F	0.64	0/1522	0.62	0/2065
1	G	0.65	1/1521 (0.1%)	0.62	0/2061
1	H	0.68	1/1533 (0.1%)	0.64	0/2074
1	I	0.63	0/1586	0.60	0/2148
1	J	0.64	1/1566 (0.1%)	0.59	1/2119 (0.0%)
1	K	0.61	0/1593	0.60	0/2158
1	L	0.63	1/1464 (0.1%)	0.64	0/1987
All	All	0.62	5/18323 (0.0%)	0.60	1/24847 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	113	CYS	CB-SG	-5.76	1.72	1.81
1	L	144	CYS	CB-SG	-5.63	1.72	1.81
1	E	144	CYS	CB-SG	-5.50	1.72	1.81
1	J	144	CYS	CB-SG	-5.30	1.73	1.81
1	H	14	CYS	CB-SG	-5.06	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	J	172	ASP	CB-CG-OD1	5.16	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1486	0	1507	9	0
1	B	1458	0	1460	15	0
1	C	1447	0	1429	4	0
1	D	1419	0	1424	4	0
1	E	1444	0	1449	17	0
1	F	1454	0	1481	7	0
1	G	1458	0	1490	14	0
1	H	1467	0	1532	11	0
1	I	1520	0	1542	26	0
1	J	1507	0	1532	6	0
1	K	1524	0	1551	12	0
1	L	1412	0	1422	11	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	15	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	0	0
2	K	15	0	0	2	0
2	L	10	0	0	0	0
3	A	17	0	0	0	0
3	B	9	0	0	0	0
3	C	14	0	0	0	0
3	D	8	0	0	0	0
3	E	11	0	0	0	0
3	F	17	0	0	0	0
3	G	13	0	0	0	0
3	H	20	0	0	0	0
3	I	23	0	0	0	0
3	J	14	0	0	0	0
3	K	16	0	0	0	0
3	L	12	0	0	0	0
4	L	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	115	0	0	0	0
5	B	111	0	0	0	0
5	C	63	0	0	0	0
5	D	88	0	0	0	0
5	E	87	0	0	1	0
5	F	154	0	0	2	0
5	G	135	0	0	0	0
5	H	140	0	0	0	0
5	I	121	0	0	6	0
5	J	105	0	0	0	0
5	K	144	0	0	0	0
5	L	111	0	0	1	0
All	All	19275	0	17827	112	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 (112) 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:I:176[A]:HIS:HD2	5:I:1372:HOH:O	0.85	1.19
1:L:98[B]:ASP:OD2	5:L:1226:HOH:O	1.60	1.17
1:F:98[B]:ASP:OD2	5:F:1057:HOH:O	1.67	1.10
1:I:176[A]:HIS:CD2	5:I:1372:HOH:O	1.65	1.04
1:I:15[A]:ILE:HD11	5:I:1405:HOH:O	1.80	0.82
1:B:102:ILE:HD11	1:B:136:ALA:HB2	1.63	0.81
1:B:160:LYS:HZ3	1:C:130:THR:HG23	1.46	0.81
1:H:1:MET:HE3	1:H:167[A]:ILE:HG23	1.64	0.79
1:I:150[A]:MET:HE3	1:I:158:VAL:HG11	1.64	0.79
1:B:160:LYS:NZ	1:C:130:THR:HG23	1.98	0.79
1:E:74[A]:ARG:O	5:E:1020:HOH:O	2.01	0.78
1:F:138:GLY:HA3	1:H:137[A]:ALA:O	1.87	0.74
1:B:99[B]:LYS:NZ	1:L:137:ALA:O	2.22	0.71
1:B:102:ILE:CD1	1:B:136:ALA:HB2	2.24	0.67
1:A:1:MET:HE3	1:A:167[A]:ILE:HG23	1.77	0.66
1:I:150[A]:MET:CE	1:I:158:VAL:HG11	2.25	0.66
1:G:15:ILE:HD11	1:G:54:ARG:NE	2.12	0.65
1:B:138:GLY:HA3	1:L:138:GLY:H	1.61	0.65
1:A:138:GLY:HA3	1:G:137[A]:ALA:O	1.97	0.64
1:G:97[B]:VAL:HG12	1:G:101:ALA:HB3	1.80	0.63
1:B:36:ILE:HD13	1:B:91:ILE:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97[B]:VAL:HG22	1:H:101:ALA:HB3	1.83	0.60
1:J:40:LEU:HD23	1:J:43[B]:ILE:HD11	1.84	0.60
1:G:97[B]:VAL:CG1	1:G:101:ALA:HB3	2.31	0.59
1:E:79:TYR:CD1	1:E:167[B]:ILE:HD11	2.38	0.59
1:E:178:LYS:NZ	1:J:42:GLN:OE1	2.35	0.58
1:I:176[A]:HIS:ND1	5:I:1265:HOH:O	2.32	0.58
1:D:97[A]:VAL:CG2	1:D:102:ILE:HD13	2.34	0.57
1:K:97[A]:VAL:HG23	1:K:102:ILE:HD11	1.86	0.57
1:H:97[B]:VAL:CG2	1:H:101:ALA:HB3	2.34	0.56
1:F:23[A]:LYS:HG3	5:F:1038:HOH:O	2.04	0.56
1:L:33:PHE:O	1:L:36:ILE:HG22	2.05	0.56
1:K:36:ILE:HD11	1:K:43:ILE:CD1	2.36	0.55
1:E:176[A]:HIS:HE1	1:I:176[A]:HIS:HE1	1.55	0.55
1:K:15[A]:ILE:HD11	2:K:190:SO4:O3	2.06	0.55
1:K:97[A]:VAL:HG23	1:K:102:ILE:CD1	2.36	0.55
1:B:102:ILE:HD11	1:B:136:ALA:CB	2.36	0.54
1:J:33:PHE:O	1:J:36:ILE:HG22	2.07	0.54
1:I:33:PHE:O	1:I:36:ILE:HG22	2.09	0.53
1:K:36:ILE:HD13	1:K:91:ILE:HG21	1.91	0.52
1:I:154:ASP:O	1:I:158:VAL:HG12	2.10	0.52
1:E:63[B]:THR:HG23	1:E:67:GLU:O	2.07	0.52
1:A:99:LYS:HB3	1:G:138[A]:GLY:HA2	1.92	0.51
1:I:43[B]:ILE:HG22	1:I:69:LEU:HD13	1.92	0.51
1:H:118:SER:HB2	1:H:119:PRO:HD2	1.93	0.51
1:L:97:VAL:HG23	1:L:102:ILE:CD1	2.41	0.50
1:G:122:LYS:HE2	1:L:119:PRO:HG2	1.95	0.49
1:D:97[B]:VAL:CG1	1:D:101:ALA:HB3	2.43	0.49
1:K:52:ILE:HD11	1:K:62[A]:LEU:HD13	1.95	0.48
1:E:138:GLY:H	1:I:138:GLY:HA3	1.78	0.48
1:L:97:VAL:HG23	1:L:102:ILE:HD11	1.94	0.48
1:F:138:GLY:CA	1:H:137[A]:ALA:O	2.59	0.48
1:E:33:PHE:O	1:E:36:ILE:HG22	2.14	0.48
1:I:52:ILE:HG22	1:I:54:ARG:HD2	1.95	0.48
1:F:102:ILE:CD1	1:F:136:ALA:HB2	2.44	0.47
1:I:150[A]:MET:CE	1:I:158:VAL:CG1	2.90	0.47
1:A:97[B]:VAL:HG23	1:A:134:ILE:HG23	1.96	0.47
1:I:170:LEU:O	1:I:171[A]:ASN:HB2	2.14	0.47
1:E:79:TYR:CD1	1:E:167[B]:ILE:CD1	2.97	0.47
1:G:170:LEU:O	1:G:171:ASN:HB2	2.13	0.47
1:B:138:GLY:H	1:L:138:GLY:HA3	1.80	0.47
1:K:15[A]:ILE:CD1	2:K:190:SO4:O4	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97[B]:VAL:CG1	1:K:101:ALA:HB3	2.44	0.47
1:K:31[A]:GLU:HA	1:K:31[A]:GLU:OE1	2.15	0.46
1:G:180:TYR:O	1:G:181:LYS:C	2.53	0.46
1:E:96:GLN:NE2	1:E:137:ALA:HB2	2.30	0.46
1:E:97[B]:VAL:CG1	1:E:101:ALA:HB3	2.46	0.46
1:I:128:VAL:O	1:I:129:ASP:HB2	2.15	0.46
1:I:150[A]:MET:HE1	1:I:158:VAL:CG1	2.46	0.46
1:D:97[A]:VAL:CG2	1:D:102:ILE:CD1	2.95	0.45
1:I:43[B]:ILE:HG23	1:I:69:LEU:HD22	1.98	0.45
1:E:97[B]:VAL:HG12	1:E:101:ALA:HB3	1.98	0.45
1:B:138:GLY:HA3	1:L:138:GLY:N	2.29	0.45
1:G:36:ILE:HD11	1:G:43[B]:ILE:CD1	2.46	0.45
1:J:104:PHE:CZ	1:K:89:PRO:HD2	2.52	0.45
1:E:138:GLY:H	1:I:138:GLY:CA	2.30	0.45
1:A:178:LYS:NZ	1:H:42[A]:GLN:OE1	2.41	0.44
1:I:171[A]:ASN:O	1:I:176[A]:HIS:CE1	2.71	0.44
1:C:1:MET:HE2	1:C:1:MET:HB2	1.87	0.44
1:E:40:LEU:HD23	1:E:43:ILE:HD11	2.00	0.44
1:D:36:ILE:CD1	1:D:70:PHE:HZ	2.31	0.43
1:B:178:LYS:NZ	1:G:42[B]:GLN:CD	2.71	0.43
1:A:99:LYS:HA	1:G:138[A]:GLY:O	2.18	0.43
1:H:119:PRO:HD3	1:I:124:TYR:OH	2.19	0.43
1:B:98[A]:ASP:OD2	1:B:99[A]:LYS:N	2.48	0.43
1:K:111:ILE:HD12	1:K:111:ILE:N	2.34	0.43
1:L:38:PRO:HG2	1:L:39:TRP:CD1	2.54	0.43
1:H:97[B]:VAL:HG13	1:H:102:ILE:HD11	1.99	0.43
1:B:178:LYS:HZ1	1:G:42[B]:GLN:CD	2.22	0.43
1:F:1:MET:HE3	1:F:1:MET:HB2	1.85	0.43
1:H:97[B]:VAL:CG2	1:H:101:ALA:CB	2.96	0.43
1:E:176[A]:HIS:CE1	1:I:176[A]:HIS:HE1	2.34	0.42
1:B:118:SER:HB2	1:B:119:PRO:HD2	2.00	0.42
1:F:40:LEU:HD23	1:F:40:LEU:HA	1.93	0.42
1:G:43[B]:ILE:HG23	1:G:69:LEU:HD22	2.01	0.42
1:L:128:VAL:O	1:L:129:ASP:HB2	2.19	0.42
1:J:43[A]:ILE:HG22	1:J:69:LEU:HD13	2.01	0.42
1:E:17:LEU:HD11	1:E:52:ILE:HG13	2.00	0.42
1:I:150[B]:MET:HE1	5:I:1262:HOH:O	2.19	0.42
1:C:40:LEU:HA	1:C:40:LEU:HD23	1.92	0.41
1:E:176[A]:HIS:HE1	1:I:176[A]:HIS:CE1	2.35	0.41
1:H:111:ILE:HD12	1:H:111:ILE:N	2.35	0.41
1:I:176[B]:HIS:ND1	5:I:1372:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HB2	1:A:63:THR:HG23	2.02	0.41
1:E:102:ILE:HG13	1:I:138:GLY:O	2.20	0.41
1:A:171:ASN:HA	1:A:175:TRP:CD1	2.55	0.41
1:B:171:ASN:HA	1:B:175:TRP:CD1	2.55	0.41
1:A:118:SER:HB2	1:A:119:PRO:CD	2.50	0.41
1:I:96:GLN:HB3	1:I:122:LYS:HB2	2.03	0.41
1:J:36:ILE:HD11	1:J:43[A]:ILE:CD1	2.51	0.41
1:G:33:PHE:O	1:G:36:ILE:HG22	2.20	0.41
1:K:33:PHE:O	1:K:36:ILE:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	194/188 (103%)	187 (96%)	7 (4%)	0	100	100
1	B	189/188 (100%)	184 (97%)	5 (3%)	0	100	100
1	C	187/188 (100%)	182 (97%)	5 (3%)	0	100	100
1	D	184/188 (98%)	181 (98%)	3 (2%)	0	100	100
1	E	190/188 (101%)	183 (96%)	7 (4%)	0	100	100
1	F	190/188 (101%)	188 (99%)	2 (1%)	0	100	100
1	G	190/188 (101%)	187 (98%)	3 (2%)	0	100	100
1	H	190/188 (101%)	188 (99%)	2 (1%)	0	100	100
1	I	197/188 (105%)	193 (98%)	4 (2%)	0	100	100
1	J	192/188 (102%)	188 (98%)	4 (2%)	0	100	100
1	K	195/188 (104%)	193 (99%)	2 (1%)	0	100	100
1	L	184/188 (98%)	177 (96%)	7 (4%)	0	100	100
All	All	2282/2256 (101%)	2231 (98%)	51 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	158/162 (98%)	155 (98%)	3 (2%)	57	41
1	B	153/162 (94%)	152 (99%)	1 (1%)	84	77
1	C	150/162 (93%)	149 (99%)	1 (1%)	84	77
1	D	149/162 (92%)	147 (99%)	2 (1%)	69	56
1	E	151/162 (93%)	150 (99%)	1 (1%)	84	77
1	F	157/162 (97%)	156 (99%)	1 (1%)	86	80
1	G	154/162 (95%)	152 (99%)	2 (1%)	69	56
1	H	159/162 (98%)	158 (99%)	1 (1%)	86	80
1	I	160/162 (99%)	159 (99%)	1 (1%)	86	80
1	J	162/162 (100%)	162 (100%)	0	100	100
1	K	164/162 (101%)	163 (99%)	1 (1%)	86	80
1	L	149/162 (92%)	148 (99%)	1 (1%)	84	77
All	All	1866/1944 (96%)	1851 (99%)	15 (1%)	81	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56[A]	HIS
1	A	56[B]	HIS
1	A	144	CYS
1	B	184	HIS
1	C	184	HIS
1	D	124	TYR
1	D	144	CYS
1	E	144	CYS
1	F	144	CYS
1	G	77	PRO
1	G	144	CYS

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Mol	Chain	Res	Type
1	H	144	CYS
1	I	144	CYS
1	K	144	CYS
1	L	144	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 200 ligands modelled in this entry, 174 are unknown - leaving 26 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	SO4	I	189	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	F	191	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	C	189	-	4,4,4	0.13	0	6,6,6	0.26	0
2	SO4	L	190	-	4,4,4	0.20	0	6,6,6	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	H	189	-	4,4,4	0.20	0	6,6,6	0.21	0
2	SO4	C	190	-	4,4,4	0.16	0	6,6,6	0.37	0
2	SO4	K	189	-	4,4,4	0.23	0	6,6,6	0.41	0
2	SO4	L	189	-	4,4,4	0.23	0	6,6,6	0.17	0
2	SO4	J	189	-	4,4,4	0.18	0	6,6,6	0.19	0
2	SO4	K	190	-	4,4,4	0.09	0	6,6,6	0.29	0
2	SO4	A	189	-	4,4,4	0.14	0	6,6,6	0.28	0
2	SO4	D	190	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	A	190	-	4,4,4	0.14	0	6,6,6	0.40	0
2	SO4	D	189	-	4,4,4	0.19	0	6,6,6	0.26	0
2	SO4	A	191	-	4,4,4	0.19	0	6,6,6	0.71	0
2	SO4	H	190	-	4,4,4	0.18	0	6,6,6	0.51	0
2	SO4	E	190	-	4,4,4	0.23	0	6,6,6	0.50	0
2	SO4	K	191	-	4,4,4	0.14	0	6,6,6	0.15	0
4	GOL	L	191	-	5,5,5	0.31	0	5,5,5	0.52	0
2	SO4	E	189	-	4,4,4	0.17	0	6,6,6	0.27	0
2	SO4	F	189	-	4,4,4	0.18	0	6,6,6	0.38	0
2	SO4	F	190	-	4,4,4	0.20	0	6,6,6	0.29	0
2	SO4	B	189	-	4,4,4	0.13	0	6,6,6	0.58	0
2	SO4	G	189	-	4,4,4	0.18	0	6,6,6	0.33	0
2	SO4	B	190	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	J	190	-	4,4,4	0.18	0	6,6,6	0.24	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
4	GOL	L	191	-	-	0/4/4/4	-

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	190	SO4	2	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, 95th 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	185/188 (98%)	0.06	10 (5%) 25 28	10, 19, 34, 50	0
1	B	185/188 (98%)	0.27	13 (7%) 16 18	13, 22, 40, 59	0
1	C	185/188 (98%)	0.45	15 (8%) 12 14	14, 26, 39, 59	0
1	D	180/188 (95%)	0.18	8 (4%) 34 38	15, 23, 36, 43	0
1	E	181/188 (96%)	0.22	11 (6%) 21 23	14, 23, 38, 44	0
1	F	181/188 (96%)	-0.09	2 (1%) 80 83	10, 17, 27, 33	0
1	G	181/188 (96%)	0.03	2 (1%) 80 83	9, 18, 33, 42	0
1	H	180/188 (95%)	-0.18	1 (0%) 89 91	8, 15, 27, 35	0
1	I	187/188 (99%)	0.17	10 (5%) 26 29	9, 19, 34, 54	0
1	J	188/188 (100%)	0.13	4 (2%) 63 67	13, 21, 33, 43	0
1	K	188/188 (100%)	-0.04	2 (1%) 80 83	11, 17, 28, 33	0
1	L	180/188 (95%)	0.46	14 (7%) 13 15	9, 20, 40, 48	0
All	All	2201/2256 (97%)	0.14	92 (4%) 36 40	8, 20, 37, 59	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	ALA	6.0
1	L	180	TYR	5.6
1	C	121	ALA	5.3
1	L	138	GLY	5.2
1	C	183	HIS	5.1
1	B	183	HIS	5.0
1	I	182	ALA	4.9
1	I	183	HIS	4.3
1	I	187	HIS	4.2
1	I	185	HIS	4.0
1	I	184	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	15	ILE	4.0
1	B	185	HIS	3.9
1	C	119	PRO	3.9
1	H	138[A]	GLY	3.8
1	G	138[A]	GLY	3.8
1	D	90[A]	PHE	3.7
1	E	138	GLY	3.6
1	L	15[A]	ILE	3.6
1	C	184	HIS	3.6
1	I	186	HIS	3.4
1	D	180	TYR	3.3
1	E	139	ALA	3.3
1	B	184	HIS	3.3
1	C	162	ILE	3.2
1	C	182	ALA	3.2
1	E	41	ASN	3.1
1	C	123	LEU	3.1
1	B	19	THR	3.1
1	D	14	CYS	3.0
1	L	25	ILE	3.0
1	L	64	VAL	3.0
1	L	139	ALA	2.9
1	C	185	HIS	2.9
1	B	119	PRO	2.9
1	J	183	HIS	2.9
1	L	41	ASN	2.9
1	A	46	LYS	2.8
1	L	17	LEU	2.8
1	B	41	ASN	2.8
1	J	186	HIS	2.8
1	A	182	ALA	2.8
1	E	58	HIS	2.8
1	B	9	GLU	2.8
1	D	119	PRO	2.7
1	I	180	TYR	2.7
1	A	185	HIS	2.7
1	A	14	CYS	2.7
1	C	9	GLU	2.6
1	B	56	HIS	2.6
1	D	19	THR	2.5
1	L	66	GLY	2.5
1	L	46	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	181	LYS	2.5
1	F	119	PRO	2.5
1	L	13	ASN	2.5
1	A	184	HIS	2.4
1	D	65	ASN	2.4
1	L	47	LYS	2.4
1	L	56	HIS	2.4
1	K	38	PRO	2.4
1	B	47	LYS	2.4
1	I	181	LYS	2.3
1	J	41	ASN	2.3
1	B	137	ALA	2.3
1	A	12[A]	SER	2.3
1	C	161	GLY	2.3
1	C	158	VAL	2.3
1	D	8	LYS	2.2
1	F	41	ASN	2.2
1	E	19	THR	2.2
1	C	56[A]	HIS	2.2
1	D	47	LYS	2.2
1	A	41	ASN	2.2
1	E	15	ILE	2.2
1	E	49	PRO	2.2
1	B	20	SER	2.2
1	E	119	PRO	2.2
1	C	120	GLY	2.2
1	E	180	TYR	2.1
1	J	184	HIS	2.1
1	C	116	LEU	2.1
1	A	74	ARG	2.1
1	E	45	PRO	2.1
1	I	138	GLY	2.1
1	C	19	THR	2.1
1	E	13	ASN	2.1
1	A	9	GLU	2.1
1	B	138	GLY	2.0
1	L	27	ASN	2.0
1	K	183	HIS	2.0
1	I	119	PRO	2.0

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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(\AA^2)	Q<0.9
3	UNX	C	9267	1/1	0.45	0.20	49,49,49,49	0
3	UNX	H	8907	1/1	0.53	0.39	42,42,42,42	0
3	UNX	A	9251	1/1	0.63	0.19	43,43,43,43	0
3	UNX	H	9276	1/1	0.63	0.26	38,38,38,38	0
3	UNX	E	8939	1/1	0.66	0.22	38,38,38,38	0
3	UNX	A	9277	1/1	0.66	0.34	38,38,38,38	0
3	UNX	C	9270	1/1	0.70	0.23	43,43,43,43	0
3	UNX	F	8955	1/1	0.71	0.12	37,37,37,37	0
3	UNX	F	9290	1/1	0.72	0.34	38,38,38,38	0
3	UNX	I	8974	1/1	0.72	0.31	24,24,24,24	0
3	UNX	H	9260	1/1	0.73	0.12	37,37,37,37	0
3	UNX	J	8990	1/1	0.74	0.31	36,36,36,36	0
3	UNX	F	8956	1/1	0.74	0.27	22,22,22,22	0
3	UNX	F	9281	1/1	0.75	0.11	40,40,40,40	0
3	UNX	B	9285	1/1	0.75	0.16	37,37,37,37	0
3	UNX	I	9292	1/1	0.76	0.29	39,39,39,39	0
3	UNX	H	9000	1/1	0.77	0.09	42,42,42,42	0
3	UNX	C	9287	1/1	0.77	0.27	34,34,34,34	0
3	UNX	F	8944	1/1	0.78	0.12	33,33,33,33	0
3	UNX	H	8968	1/1	0.78	0.19	26,26,26,26	0
3	UNX	C	9266	1/1	0.80	0.13	37,37,37,37	0
3	UNX	I	8972	1/1	0.80	0.41	36,36,36,36	0
3	UNX	K	8994	1/1	0.80	0.26	34,34,34,34	0
3	UNX	F	8943	1/1	0.81	0.32	32,32,32,32	0
3	UNX	F	9289	1/1	0.81	0.14	33,33,33,33	0
3	UNX	H	8999	1/1	0.82	0.10	46,46,46,46	0
3	UNX	G	9264	1/1	0.82	0.28	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	A	8910	1/1	0.82	0.44	30,30,30,30	0
3	UNX	I	8976	1/1	0.83	0.18	42,42,42,42	0
3	UNX	J	8988	1/1	0.83	0.31	29,29,29,29	0
3	UNX	D	8929	1/1	0.83	0.18	35,35,35,35	0
3	UNX	L	9006	1/1	0.83	0.24	26,26,26,26	0
3	UNX	H	9274	1/1	0.84	0.25	36,36,36,36	0
3	UNX	C	9284	1/1	0.84	0.34	31,31,31,31	0
3	UNX	K	8995	1/1	0.84	0.36	30,30,30,30	0
3	UNX	K	8996	1/1	0.85	0.15	38,38,38,38	0
3	UNX	B	9269	1/1	0.85	0.10	36,36,36,36	0
3	UNX	C	9286	1/1	0.85	0.47	40,40,40,40	0
3	UNX	I	8975	1/1	0.86	0.31	36,36,36,36	0
3	UNX	F	9273	1/1	0.86	0.40	34,34,34,34	0
3	UNX	B	8918	1/1	0.86	0.35	27,27,27,27	0
3	UNX	I	9262	1/1	0.86	0.58	43,43,43,43	0
3	UNX	A	8905	1/1	0.87	0.10	33,33,33,33	0
3	UNX	A	9009	1/1	0.87	0.15	42,42,42,42	0
3	UNX	L	8954	1/1	0.87	0.33	21,21,21,21	0
3	UNX	I	8977	1/1	0.87	0.09	36,36,36,36	0
3	UNX	I	8978	1/1	0.87	0.07	37,37,37,37	0
2	SO4	L	189	5/5	0.87	0.20	61,62,62,63	0
3	UNX	C	9001	1/1	0.87	0.57	34,34,34,34	0
3	UNX	G	8949	1/1	0.87	0.29	31,31,31,31	0
3	UNX	L	9280	1/1	0.88	0.26	37,37,37,37	0
2	SO4	C	189	5/5	0.88	0.17	37,43,46,47	0
3	UNX	F	9263	1/1	0.88	0.54	37,37,37,37	0
3	UNX	A	8906	1/1	0.88	0.56	35,35,35,35	0
3	UNX	A	9229	1/1	0.89	0.34	33,33,33,33	0
3	UNX	I	8982	1/1	0.89	0.11	22,22,22,22	0
3	UNX	K	9322	1/1	0.89	0.16	34,34,34,34	0
3	UNX	E	9288	1/1	0.89	0.17	33,33,33,33	0
3	UNX	B	9248	1/1	0.89	0.41	35,35,35,35	0
3	UNX	C	9271	1/1	0.89	0.11	34,34,34,34	0
3	UNX	J	9268	1/1	0.89	0.16	26,26,26,26	0
3	UNX	B	9265	1/1	0.90	0.51	33,33,33,33	0
3	UNX	G	9278	1/1	0.90	0.28	32,32,32,32	0
3	UNX	E	8935	1/1	0.90	0.09	38,38,38,38	0
3	UNX	K	8928	1/1	0.90	0.34	35,35,35,35	0
3	UNX	H	8959	1/1	0.90	0.26	28,28,28,28	0
3	UNX	K	9005	1/1	0.90	0.21	19,19,19,19	0
3	UNX	D	8938	1/1	0.90	0.32	29,29,29,29	0
3	UNX	I	8979	1/1	0.90	0.13	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	C	8922	1/1	0.90	0.30	26,26,26,26	0
3	UNX	E	8940	1/1	0.90	0.10	41,41,41,41	0
3	UNX	L	8953	1/1	0.90	0.15	32,32,32,32	0
3	UNX	D	9241	1/1	0.90	0.23	22,22,22,22	0
3	UNX	H	9240	1/1	0.91	0.12	28,28,28,28	0
3	UNX	H	9275	1/1	0.91	0.30	28,28,28,28	0
2	SO4	B	189	5/5	0.91	0.12	36,40,43,46	0
3	UNX	L	8992	1/1	0.91	0.21	23,23,23,23	0
3	UNX	I	8924	1/1	0.91	0.26	31,31,31,31	0
3	UNX	E	8931	1/1	0.91	0.39	18,18,18,18	0
3	UNX	G	8965	1/1	0.91	0.33	19,19,19,19	0
3	UNX	I	9359	1/1	0.91	0.10	28,28,28,28	0
3	UNX	E	8930	1/1	0.91	0.14	28,28,28,28	0
3	UNX	L	9245	1/1	0.91	0.28	29,29,29,29	0
2	SO4	K	190	5/5	0.92	0.14	40,41,45,46	0
3	UNX	G	8964	1/1	0.92	0.40	29,29,29,29	0
3	UNX	E	8942	1/1	0.92	0.08	34,34,34,34	0
3	UNX	A	9323	1/1	0.92	0.16	39,39,39,39	0
3	UNX	I	8981	1/1	0.92	0.36	17,17,17,17	0
3	UNX	J	8936	1/1	0.92	0.41	33,33,33,33	0
3	UNX	J	8984	1/1	0.92	0.21	23,23,23,23	0
3	UNX	J	8989	1/1	0.92	0.37	30,30,30,30	0
3	UNX	A	9246	1/1	0.93	0.29	38,38,38,38	0
3	UNX	A	8911	1/1	0.93	0.28	25,25,25,25	0
3	UNX	F	8948	1/1	0.93	0.27	30,30,30,30	0
3	UNX	K	9004	1/1	0.93	0.09	31,31,31,31	0
3	UNX	K	9279	1/1	0.93	0.28	35,35,35,35	0
3	UNX	K	9243	1/1	0.93	0.12	31,31,31,31	0
3	UNX	G	8963	1/1	0.93	0.15	26,26,26,26	0
3	UNX	B	8913	1/1	0.93	0.17	29,29,29,29	0
3	UNX	A	9238	1/1	0.93	0.19	30,30,30,30	0
2	SO4	I	189	5/5	0.93	0.17	33,38,43,43	0
3	UNX	B	8917	1/1	0.93	0.47	32,32,32,32	0
3	UNX	K	8993	1/1	0.93	0.15	26,26,26,26	0
3	UNX	D	8926	1/1	0.93	0.20	34,34,34,34	0
3	UNX	L	8952	1/1	0.93	0.14	28,28,28,28	0
2	SO4	J	190	5/5	0.93	0.11	48,49,52,52	0
2	SO4	J	189	5/5	0.94	0.24	48,50,52,53	0
3	UNX	I	8980	1/1	0.94	0.28	31,31,31,31	0
3	UNX	K	9247	1/1	0.94	0.11	35,35,35,35	0
3	UNX	I	8971	1/1	0.94	0.20	26,26,26,26	0
2	SO4	A	189	5/5	0.94	0.21	32,40,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	D	190	5/5	0.94	0.17	37,41,43,43	0
2	SO4	A	190	5/5	0.94	0.15	33,39,41,43	0
3	UNX	A	8914	1/1	0.94	0.14	28,28,28,28	0
3	UNX	K	8991	1/1	0.94	0.28	13,13,13,13	0
2	SO4	C	190	5/5	0.94	0.12	40,40,45,45	0
3	UNX	J	9250	1/1	0.94	0.14	32,32,32,32	0
3	UNX	C	9002	1/1	0.94	0.41	28,28,28,28	0
3	UNX	H	9324	1/1	0.94	0.17	32,32,32,32	0
3	UNX	C	9283	1/1	0.94	0.28	27,27,27,27	0
3	UNX	K	8998	1/1	0.95	0.17	39,39,39,39	0
3	UNX	L	8951	1/1	0.95	0.20	23,23,23,23	0
3	UNX	I	9242	1/1	0.95	0.41	31,31,31,31	0
2	SO4	B	190	5/5	0.95	0.22	46,47,49,50	0
3	UNX	K	9253	1/1	0.95	0.13	28,28,28,28	0
3	UNX	J	8985	1/1	0.95	0.12	25,25,25,25	0
3	UNX	C	8920	1/1	0.95	0.39	26,26,26,26	0
3	UNX	I	9252	1/1	0.95	0.11	32,32,32,32	0
2	SO4	K	191	5/5	0.95	0.13	51,54,56,56	0
3	UNX	E	8941	1/1	0.95	0.16	31,31,31,31	0
3	UNX	G	8961	1/1	0.95	0.23	19,19,19,19	0
3	UNX	H	9239	1/1	0.95	0.10	18,18,18,18	0
3	UNX	C	8921	1/1	0.96	0.19	26,26,26,26	0
2	SO4	E	190	5/5	0.96	0.11	30,32,36,37	0
3	UNX	I	9258	1/1	0.96	0.29	17,17,17,17	0
3	UNX	A	9259	1/1	0.96	0.21	21,21,21,21	0
3	UNX	D	8927	1/1	0.96	0.48	36,36,36,36	0
2	SO4	K	189	5/5	0.96	0.12	21,25,28,29	0
3	UNX	J	9232	1/1	0.96	0.32	13,13,13,13	0
3	UNX	I	9228	1/1	0.96	0.19	20,20,20,20	0
3	UNX	A	8912	1/1	0.96	0.36	17,17,17,17	0
3	UNX	F	9010	1/1	0.96	0.06	29,29,29,29	0
3	UNX	G	8960	1/1	0.96	0.18	19,19,19,19	0
3	UNX	C	8919	1/1	0.96	0.14	13,13,13,13	0
3	UNX	J	8986	1/1	0.96	0.22	28,28,28,28	0
3	UNX	F	8950	1/1	0.96	0.27	29,29,29,29	0
2	SO4	F	191	5/5	0.96	0.09	37,38,41,45	0
2	SO4	L	190	5/5	0.96	0.13	22,33,35,36	0
3	UNX	I	8973	1/1	0.96	0.11	20,20,20,20	0
3	UNX	J	9282	1/1	0.97	0.18	14,14,14,14	0
2	SO4	F	190	5/5	0.97	0.08	21,28,32,34	0
2	SO4	A	191	5/5	0.97	0.08	25,33,34,36	0
3	UNX	D	9257	1/1	0.97	0.16	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	E	8932	1/1	0.97	0.32	9,9,9,9	0
3	UNX	D	8937	1/1	0.97	0.27	16,16,16,16	0
3	UNX	G	9261	1/1	0.97	0.13	22,22,22,22	0
3	UNX	E	9249	1/1	0.97	0.30	18,18,18,18	0
2	SO4	H	189	5/5	0.97	0.15	21,31,34,35	0
4	GOL	L	191	6/6	0.97	0.06	18,19,20,21	0
2	SO4	E	189	5/5	0.97	0.15	32,37,38,39	0
3	UNX	F	8957	1/1	0.97	0.29	18,18,18,18	0
3	UNX	H	8997	1/1	0.97	0.24	22,22,22,22	0
3	UNX	H	8970	1/1	0.97	0.32	11,11,11,11	0
2	SO4	F	189	5/5	0.97	0.08	32,33,38,40	0
3	UNX	H	9291	1/1	0.97	0.21	18,18,18,18	0
3	UNX	B	9011	1/1	0.97	0.28	34,34,34,34	0
3	UNX	H	8908	1/1	0.98	0.24	8,8,8,8	0
2	SO4	G	189	5/5	0.98	0.12	21,27,30,31	0
2	SO4	H	190	5/5	0.98	0.10	28,31,35,35	0
3	UNX	A	9237	1/1	0.98	0.15	16,16,16,16	0
3	UNX	E	9254	1/1	0.98	0.26	11,11,11,11	0
3	UNX	I	8934	1/1	0.98	0.28	15,15,15,15	0
3	UNX	I	8983	1/1	0.98	0.28	11,11,11,11	0
3	UNX	A	8909	1/1	0.98	0.27	5,5,5,5	0
3	UNX	J	9233	1/1	0.98	0.28	12,12,12,12	0
3	UNX	J	9234	1/1	0.98	0.28	16,16,16,16	0
3	UNX	K	9293	1/1	0.98	0.18	16,16,16,16	0
3	UNX	G	8962	1/1	0.98	0.24	16,16,16,16	0
3	UNX	G	9244	1/1	0.98	0.09	25,25,25,25	0
3	UNX	J	8987	1/1	0.98	0.19	22,22,22,22	0
3	UNX	L	9007	1/1	0.98	0.20	19,19,19,19	0
3	UNX	F	8945	1/1	0.98	0.27	11,11,11,11	0
3	UNX	H	9008	1/1	0.98	0.14	32,32,32,32	0
2	SO4	D	189	5/5	0.99	0.08	32,34,38,39	0
3	UNX	H	8967	1/1	0.99	0.30	2,2,2,2	0
3	UNX	K	9256	1/1	0.99	0.19	12,12,12,12	0
3	UNX	L	8946	1/1	0.99	0.23	11,11,11,11	0
3	UNX	H	8915	1/1	0.99	0.34	7,7,7,7	0
3	UNX	D	8925	1/1	0.99	0.12	20,20,20,20	0
3	UNX	A	9236	1/1	0.99	0.17	15,15,15,15	0
3	UNX	F	9255	1/1	0.99	0.07	20,20,20,20	0
3	UNX	G	8966	1/1	0.99	0.31	6,6,6,6	0
3	UNX	F	8933	1/1	0.99	0.30	6,6,6,6	0
3	UNX	L	8947	1/1	0.99	0.33	3,3,3,3	0
3	UNX	G	9230	1/1	0.99	0.25	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	L	9231	1/1	0.99	0.21	12,12,12,12	0
3	UNX	I	8923	1/1	0.99	0.34	4,4,4,4	0
3	UNX	B	8916	1/1	1.00	0.29	7,7,7,7	0
3	UNX	F	9272	1/1	1.00	0.29	14,14,14,14	0
3	UNX	H	8969	1/1	1.00	0.21	6,6,6,6	0

6.5 Other polymers [i](#)

There are no such residues in this entry.