



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2020 – 09:19 AM BST

PDB ID : 1ZO8  
Title : X-ray Structure of the haloalcohol dehalogenase HheC of Agrobacterium radiobacter AD1 in complex with (S)-para-nitrostyrene oxide, with a water molecule in the halide-binding site  
Authors : de Jong, R.M.; Tiesinga, J.J.W.; Tang, L.; Villa, A.; Janssen, D.B.; Dijkstra, B.W.  
Deposited on : 2005-05-12  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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	:	2.13
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)	:	2.13

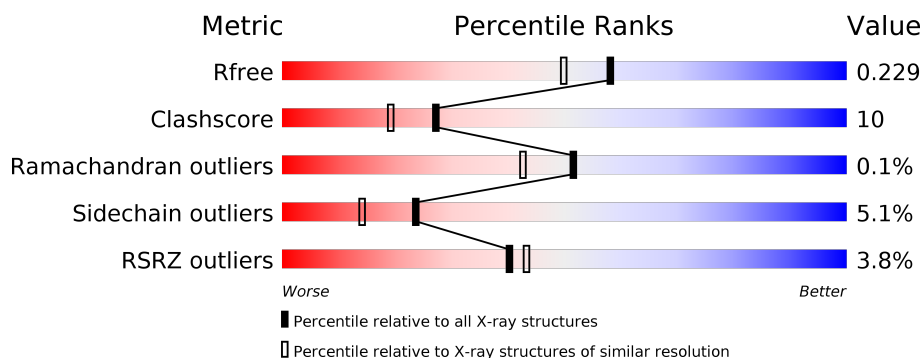
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	254	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	254	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	C	254	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	D	254	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div> </div>
1	E	254	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	F	254	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>..</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	254	
1	H	254	
1	I	254	
1	J	254	
1	K	254	
1	L	254	
1	M	254	
1	N	254	
1	O	254	
1	P	254	

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	SNO	C	5003	-	-	X	-
2	SNO	H	5008	-	-	-	X
2	SNO	J	5009	-	-	X	-
2	SNO	M	5014	-	-	-	X

## 2 Entry composition

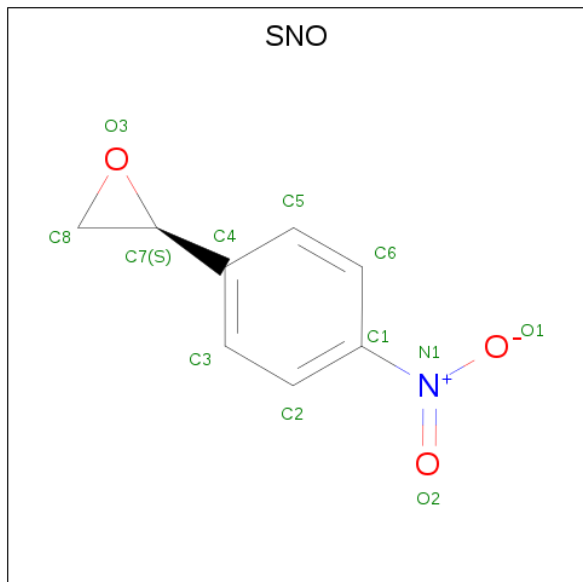
There are 3 unique types of molecules in this entry. The entry contains 32814 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 halohydrin dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1915	1233	319	355	8			
1	B	252	Total	C	N	O	S	0	0	0
			1919	1234	318	359	8			
1	C	252	Total	C	N	O	S	0	0	0
			1915	1232	318	357	8			
1	D	252	Total	C	N	O	S	0	0	0
			1919	1236	320	355	8			
1	E	252	Total	C	N	O	S	0	0	0
			1915	1233	319	355	8			
1	F	252	Total	C	N	O	S	0	0	0
			1919	1234	318	359	8			
1	G	252	Total	C	N	O	S	0	0	0
			1915	1232	318	357	8			
1	H	252	Total	C	N	O	S	0	0	0
			1919	1236	320	355	8			
1	I	252	Total	C	N	O	S	0	0	0
			1915	1233	319	355	8			
1	J	252	Total	C	N	O	S	0	0	0
			1919	1234	318	359	8			
1	K	252	Total	C	N	O	S	0	0	0
			1915	1232	318	357	8			
1	L	252	Total	C	N	O	S	0	0	0
			1919	1236	320	355	8			
1	M	252	Total	C	N	O	S	0	0	0
			1915	1233	319	355	8			
1	N	252	Total	C	N	O	S	0	0	0
			1919	1234	318	359	8			
1	O	252	Total	C	N	O	S	0	0	0
			1915	1233	319	355	8			
1	P	252	Total	C	N	O	S	0	0	0
			1915	1233	319	355	8			

- Molecule 2 is (S)-PARA-NITROSTYRENE OXIDE (three-letter code: SNO) (formula:  $C_8H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	8	1	3		
2	B	1	Total	C	N	O	0	0
			12	8	1	3		
2	C	1	Total	C	N	O	0	0
			12	8	1	3		
2	D	1	Total	C	N	O	0	0
			12	8	1	3		
2	E	1	Total	C	N	O	0	0
			12	8	1	3		
2	F	1	Total	C	N	O	0	0
			12	8	1	3		
2	G	1	Total	C	N	O	0	0
			12	8	1	3		
2	H	1	Total	C	N	O	0	0
			12	8	1	3		
2	I	1	Total	C	N	O	0	0
			12	8	1	3		
2	J	1	Total	C	N	O	0	0
			12	8	1	3		
2	K	1	Total	C	N	O	0	0
			12	8	1	3		
2	L	1	Total	C	N	O	0	0
			12	8	1	3		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	N	O	0	0
			12	8	1	3		
2	N	1	Total	C	N	O	0	0
			12	8	1	3		
2	O	1	Total	C	N	O	0	0
			12	8	1	3		
2	P	1	Total	C	N	O	0	0
			12	8	1	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total	O	0	0
			127	127		
3	B	120	Total	O	0	0
			120	120		
3	C	111	Total	O	0	0
			111	111		
3	D	106	Total	O	0	0
			106	106		
3	E	132	Total	O	0	0
			132	132		
3	F	129	Total	O	0	0
			129	129		
3	G	165	Total	O	0	0
			165	165		
3	H	148	Total	O	0	0
			148	148		
3	I	147	Total	O	0	0
			147	147		
3	J	112	Total	O	0	0
			112	112		
3	K	132	Total	O	0	0
			132	132		
3	L	125	Total	O	0	0
			125	125		
3	M	98	Total	O	0	0
			98	98		
3	N	102	Total	O	0	0
			102	102		
3	O	88	Total	O	0	0
			88	88		

*Continued on next page...*

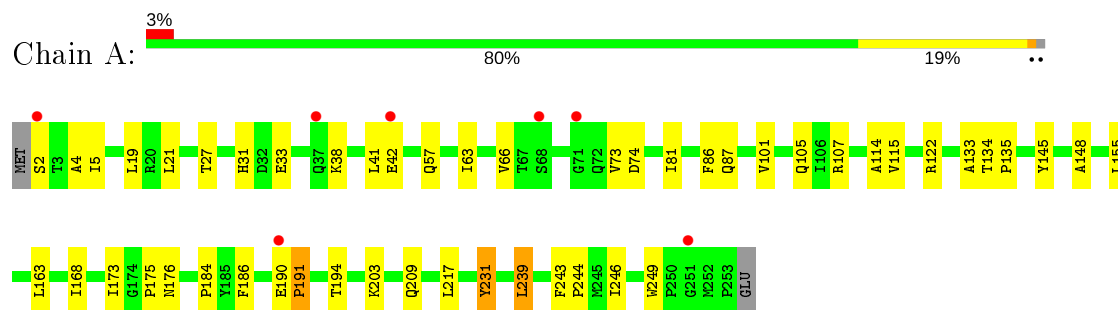
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	112	Total	O	0	0
			112	112		

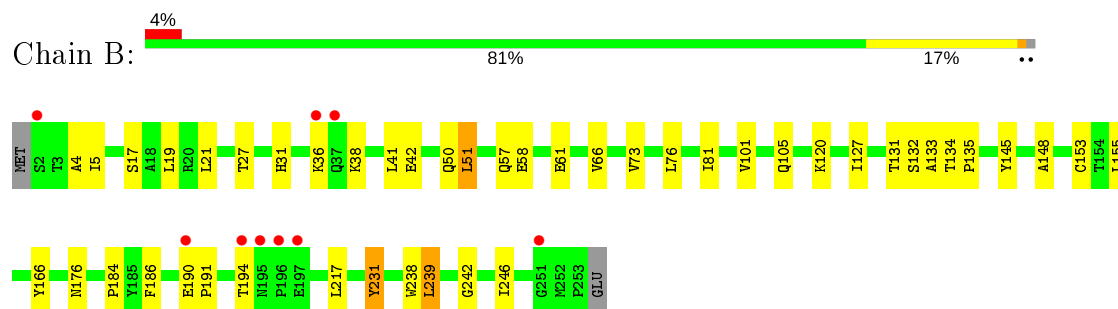
### 3 Residue-property plots [i](#)

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.

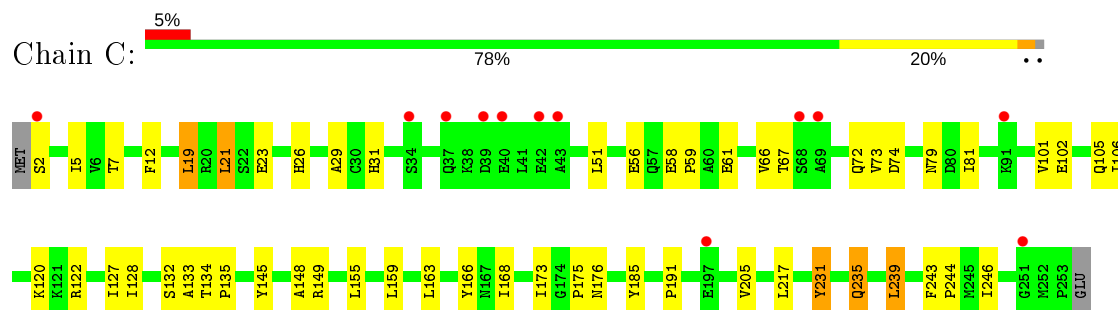
- Molecule 1: halohydrin dehalogenase



- Molecule 1: halohydrin dehalogenase



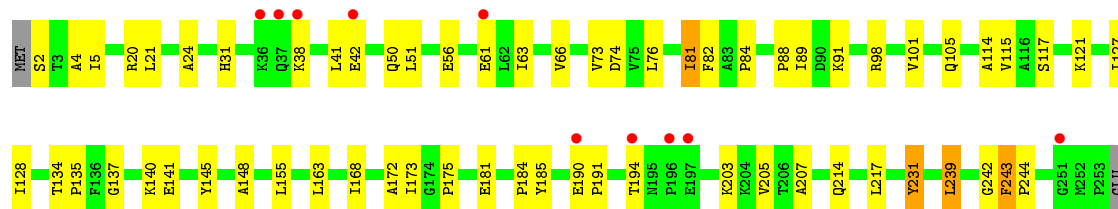
- Molecule 1: halohydrin dehalogenase



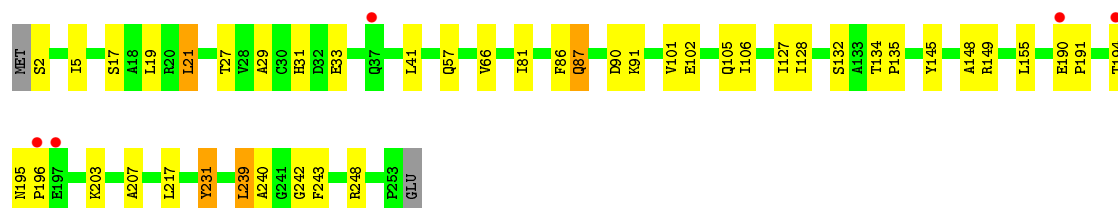
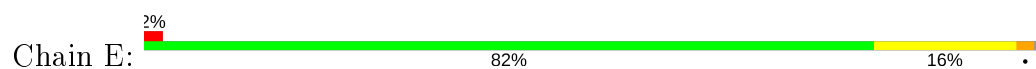
- Molecule 1: halohydrin dehalogenase



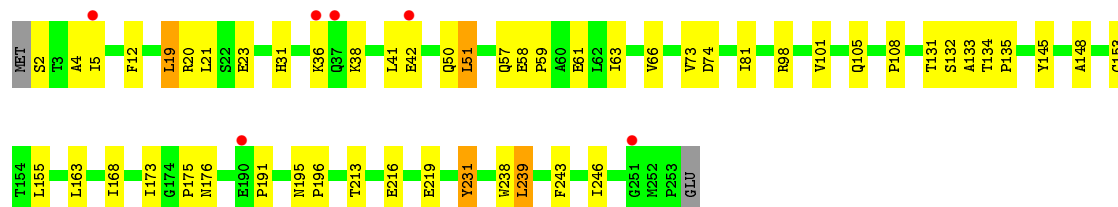
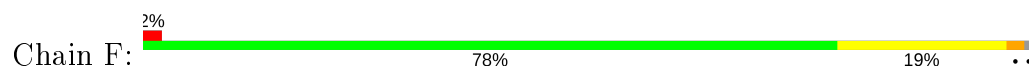




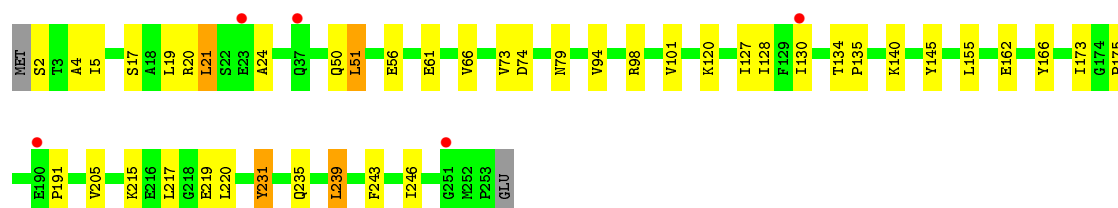
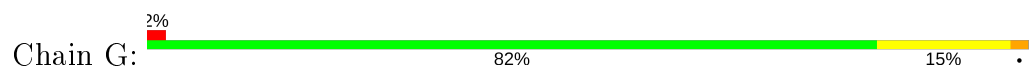
- Molecule 1: halohydrin dehalogenase



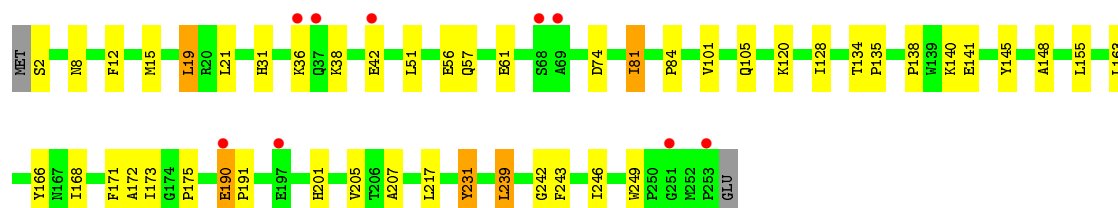
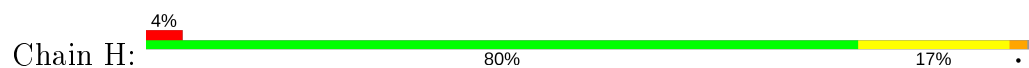
- Molecule 1: halohydrin dehalogenase



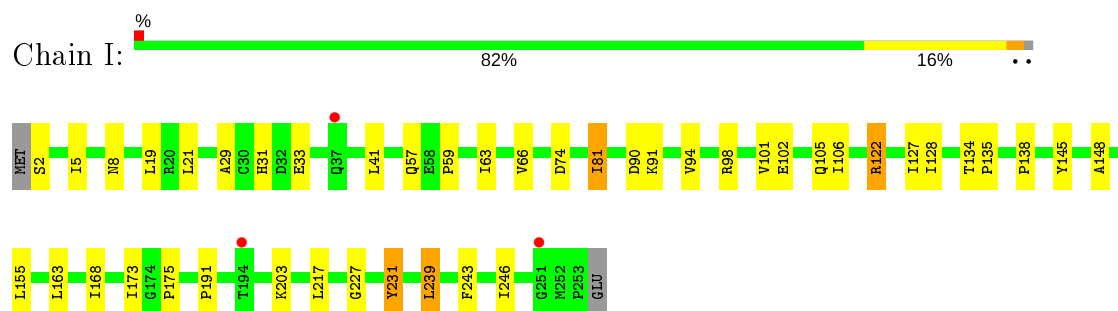
- Molecule 1: halohydrin dehalogenase



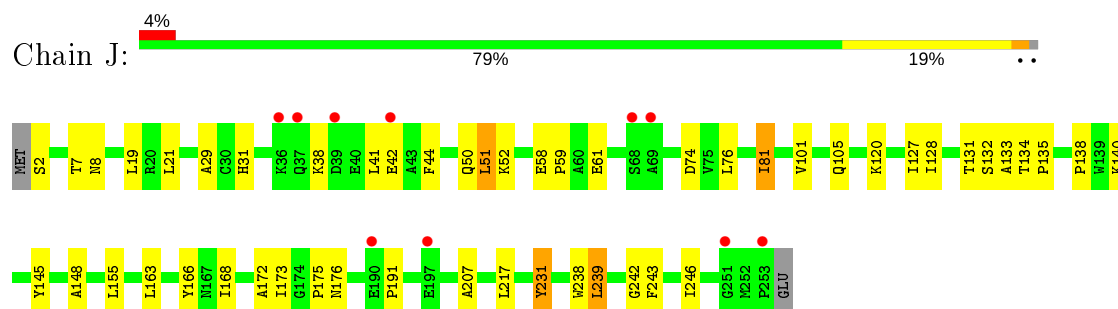
- Molecule 1: halohydrin dehalogenase



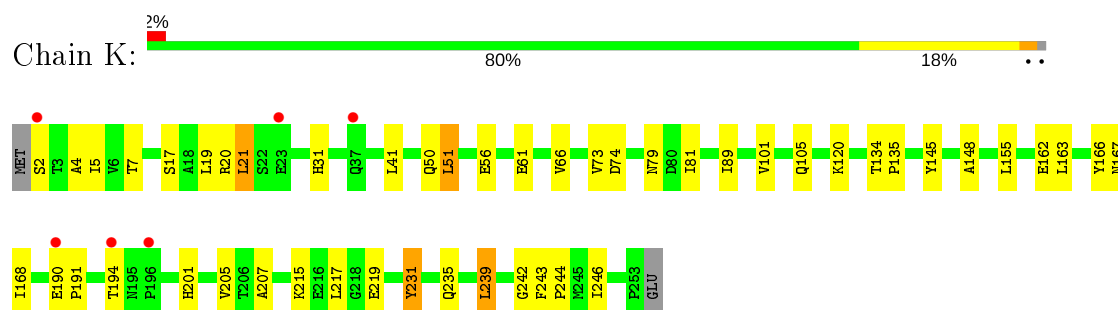
- Molecule 1: halohydrin dehalogenase



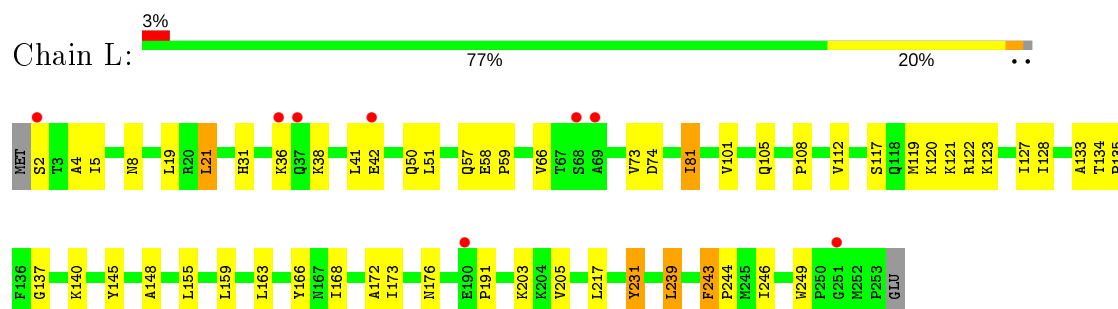
- Molecule 1: halohydrin dehalogenase



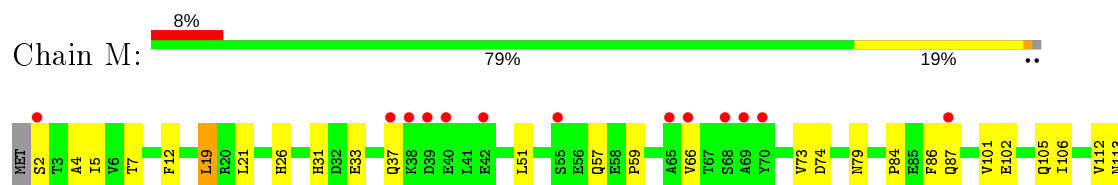
- Molecule 1: halohydrin dehalogenase



- Molecule 1: halohydrin dehalogenase

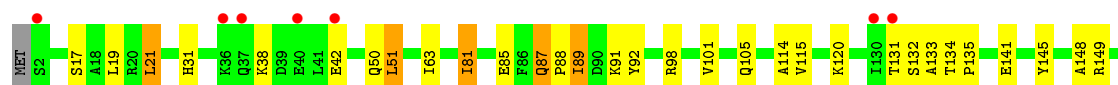
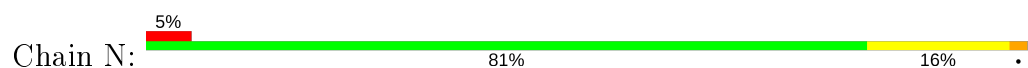


- Molecule 1: halohydrin dehalogenase

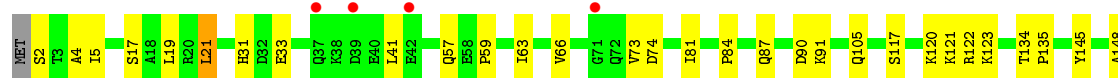
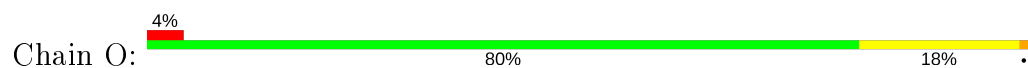




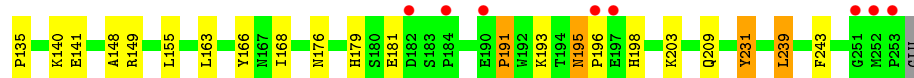
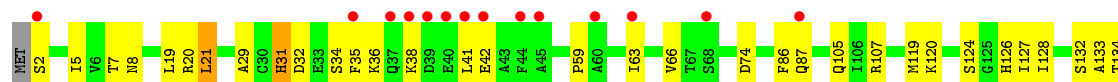
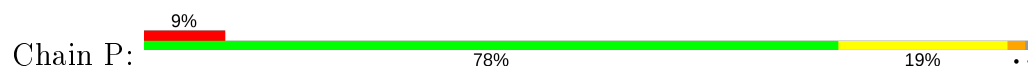
- Molecule 1: halohydrin dehalogenase



- Molecule 1: halohydrin dehalogenase



- Molecule 1: halohydrin dehalogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.75Å 292.82Å 146.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 1.90 29.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.94-1.90) 98.3 (29.93-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1, CNX	Depositor
R, $R_{free}$	0.208 , 0.235 0.203 , 0.229	Depositor DCC
$R_{free}$ test set	20038 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32814	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3292e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SNO

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	0.34	0/1969	0.63	1/2686 (0.0%)
1	B	0.33	0/1973	0.64	1/2692 (0.0%)
1	C	0.32	0/1969	0.62	0/2687
1	D	0.33	0/1973	0.63	0/2690
1	E	0.34	0/1969	0.64	1/2686 (0.0%)
1	F	0.33	0/1973	0.65	0/2692
1	G	0.34	0/1969	0.64	0/2687
1	H	0.34	0/1973	0.63	0/2690
1	I	0.34	0/1969	0.63	0/2686
1	J	0.32	0/1973	0.63	0/2692
1	K	0.34	0/1969	0.64	0/2687
1	L	0.34	0/1973	0.64	0/2690
1	M	0.33	0/1969	0.61	0/2686
1	N	0.32	0/1973	0.62	0/2692
1	O	0.32	0/1969	0.62	0/2686
1	P	0.32	0/1969	0.60	0/2686
All	All	0.33	0/31532	0.63	3/43015 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	27	THR	N-CA-C	-5.13	97.14	111.00
1	A	27	THR	N-CA-C	-5.07	97.32	111.00
1	B	27	THR	N-CA-C	-5.04	97.41	111.00

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	1915	0	1846	43	0
1	B	1919	0	1843	36	0
1	C	1915	0	1839	45	0
1	D	1919	0	1857	56	0
1	E	1915	0	1846	37	0
1	F	1919	0	1843	42	0
1	G	1915	0	1839	39	0
1	H	1919	0	1857	43	0
1	I	1915	0	1846	39	0
1	J	1919	0	1843	51	0
1	K	1915	0	1839	43	0
1	L	1919	0	1857	63	0
1	M	1915	0	1846	40	0
1	N	1919	0	1843	38	0
1	O	1915	0	1846	32	0
1	P	1915	0	1846	47	0
2	A	12	0	6	1	0
2	B	12	0	6	1	0
2	C	12	0	6	4	0
2	D	12	0	6	1	0
2	E	12	0	6	2	0
2	F	12	0	6	3	0
2	G	12	0	6	2	0
2	H	12	0	6	2	0
2	I	12	0	6	1	0
2	J	12	0	6	5	0
2	K	12	0	6	2	0
2	L	12	0	6	2	0
2	M	12	0	6	2	0
2	N	12	0	6	1	0
2	O	12	0	6	0	0
2	P	12	0	6	0	0
3	A	127	0	0	3	0
3	B	120	0	0	1	0
3	C	111	0	0	1	0
3	D	106	0	0	0	0
3	E	132	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	129	0	0	1	0
3	G	165	0	0	1	0
3	H	148	0	0	1	0
3	I	147	0	0	2	0
3	J	112	0	0	0	0
3	K	132	0	0	0	0
3	L	125	0	0	4	0
3	M	98	0	0	1	1
3	N	102	0	0	0	0
3	O	88	0	0	0	0
3	P	112	0	0	1	0
All	All	32814	0	29632	613	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 613 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:101:VAL:HG11	1:B:101:VAL:HG11	1.23	1.18
1:E:101:VAL:HG11	1:F:101:VAL:HG11	1.15	1.14
1:G:101:VAL:HG11	1:H:101:VAL:HG11	1.17	1.14
1:C:5:ILE:HD11	1:C:66:VAL:HG21	1.17	1.10
1:C:101:VAL:HG11	1:D:101:VAL:HG11	1.22	1.09

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:5082:HOH:O	3:M:5082:HOH:O[2_755]	2.06	0.14

## 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	250/254 (98%)	240 (96%)	10 (4%)	0	100	100
1	B	250/254 (98%)	238 (95%)	12 (5%)	0	100	100
1	C	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
1	D	250/254 (98%)	238 (95%)	12 (5%)	0	100	100
1	E	250/254 (98%)	241 (96%)	9 (4%)	0	100	100
1	F	250/254 (98%)	238 (95%)	12 (5%)	0	100	100
1	G	250/254 (98%)	237 (95%)	13 (5%)	0	100	100
1	H	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
1	I	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
1	J	250/254 (98%)	236 (94%)	14 (6%)	0	100	100
1	K	250/254 (98%)	240 (96%)	10 (4%)	0	100	100
1	L	250/254 (98%)	238 (95%)	12 (5%)	0	100	100
1	M	250/254 (98%)	239 (96%)	10 (4%)	1 (0%)	34	24
1	N	250/254 (98%)	239 (96%)	11 (4%)	0	100	100
1	O	250/254 (98%)	235 (94%)	15 (6%)	0	100	100
1	P	250/254 (98%)	233 (93%)	16 (6%)	1 (0%)	34	24
All	All	4000/4064 (98%)	3809 (95%)	189 (5%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	35	PHE
1	M	59	PRO

### 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	196/208 (94%)	188 (96%)	8 (4%)	30	21

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	197/208 (95%)	190 (96%)	7 (4%)	35	26
1	C	196/208 (94%)	185 (94%)	11 (6%)	21	11
1	D	197/208 (95%)	189 (96%)	8 (4%)	30	21
1	E	196/208 (94%)	187 (95%)	9 (5%)	27	17
1	F	197/208 (95%)	187 (95%)	10 (5%)	24	14
1	G	196/208 (94%)	188 (96%)	8 (4%)	30	21
1	H	197/208 (95%)	184 (93%)	13 (7%)	16	8
1	I	196/208 (94%)	185 (94%)	11 (6%)	21	11
1	J	197/208 (95%)	187 (95%)	10 (5%)	24	14
1	K	196/208 (94%)	186 (95%)	10 (5%)	24	14
1	L	197/208 (95%)	188 (95%)	9 (5%)	27	17
1	M	196/208 (94%)	184 (94%)	12 (6%)	18	9
1	N	197/208 (95%)	184 (93%)	13 (7%)	16	8
1	O	196/208 (94%)	186 (95%)	10 (5%)	24	14
1	P	196/208 (94%)	186 (95%)	10 (5%)	24	14
All	All	3143/3328 (94%)	2984 (95%)	159 (5%)	24	14

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	231	TYR
1	J	81	ILE
1	O	231	TYR
1	I	19	LEU
1	I	191	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	105	GLN
1	J	105	GLN
1	P	57	GLN
1	H	195	ASN
1	I	87	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 ⓘ

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SNO	I	5010	-	12,13,13	1.13	0	16,18,18	0.51	0
2	SNO	D	5004	-	12,13,13	1.16	0	16,18,18	0.51	0
2	SNO	L	5012	-	12,13,13	1.14	1 (8%)	16,18,18	0.46	0
2	SNO	B	5001	-	12,13,13	1.13	0	16,18,18	0.55	0
2	SNO	J	5009	-	12,13,13	1.14	0	16,18,18	0.61	0
2	SNO	M	5014	-	12,13,13	1.15	1 (8%)	16,18,18	0.52	0
2	SNO	N	5013	-	12,13,13	1.17	0	16,18,18	0.55	0
2	SNO	E	5006	-	12,13,13	1.22	1 (8%)	16,18,18	0.49	0
2	SNO	O	5016	-	12,13,13	1.20	0	16,18,18	0.57	0
2	SNO	H	5008	-	12,13,13	1.13	1 (8%)	16,18,18	0.54	0
2	SNO	A	5002	-	12,13,13	1.13	1 (8%)	16,18,18	0.46	0
2	SNO	F	5005	-	12,13,13	1.07	0	16,18,18	0.52	0
2	SNO	K	5011	-	12,13,13	1.13	0	16,18,18	0.54	0
2	SNO	G	5007	-	12,13,13	1.11	0	16,18,18	0.56	0
2	SNO	C	5003	-	12,13,13	1.19	1 (8%)	16,18,18	0.51	0
2	SNO	P	5015	-	12,13,13	1.17	1 (8%)	16,18,18	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SNO	I	5010	-	-	2/6/10/10	0/2/2/2
2	SNO	D	5004	-	-	2/6/10/10	0/2/2/2
2	SNO	L	5012	-	-	2/6/10/10	0/2/2/2
2	SNO	B	5001	-	-	2/6/10/10	0/2/2/2
2	SNO	J	5009	-	-	2/6/10/10	0/2/2/2
2	SNO	M	5014	-	-	2/6/10/10	0/2/2/2
2	SNO	N	5013	-	-	2/6/10/10	0/2/2/2
2	SNO	E	5006	-	-	2/6/10/10	0/2/2/2
2	SNO	O	5016	-	-	2/6/10/10	0/2/2/2
2	SNO	H	5008	-	-	2/6/10/10	0/2/2/2
2	SNO	A	5002	-	-	2/6/10/10	0/2/2/2
2	SNO	F	5005	-	-	2/6/10/10	0/2/2/2
2	SNO	K	5011	-	-	2/6/10/10	0/2/2/2
2	SNO	G	5007	-	-	2/6/10/10	0/2/2/2
2	SNO	C	5003	-	-	2/6/10/10	0/2/2/2
2	SNO	P	5015	-	-	2/6/10/10	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	5012	SNO	C1-N1	2.23	1.50	1.45
2	E	5006	SNO	C1-N1	2.22	1.50	1.45
2	C	5003	SNO	C1-N1	2.22	1.50	1.45
2	H	5008	SNO	C1-N1	2.15	1.50	1.45
2	M	5014	SNO	C1-N1	2.12	1.50	1.45

There are no bond angle outliers.

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	5007	SNO	C3-C4-C7-O3
2	G	5007	SNO	C5-C4-C7-O3
2	J	5009	SNO	C3-C4-C7-O3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	J	5009	SNO	C5-C4-C7-O3
2	O	5016	SNO	C3-C4-C7-O3

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	5010	SNO	1	0
2	D	5004	SNO	1	0
2	L	5012	SNO	2	0
2	B	5001	SNO	1	0
2	J	5009	SNO	5	0
2	M	5014	SNO	2	0
2	N	5013	SNO	1	0
2	E	5006	SNO	2	0
2	H	5008	SNO	2	0
2	A	5002	SNO	1	0
2	F	5005	SNO	3	0
2	K	5011	SNO	2	0
2	G	5007	SNO	2	0
2	C	5003	SNO	4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	252/254 (99%)	0.09	7 (2%) 53 56	14, 22, 32, 42	0
1	B	252/254 (99%)	0.16	9 (3%) 42 45	13, 22, 35, 40	0
1	C	252/254 (99%)	0.17	12 (4%) 30 33	14, 23, 34, 42	0
1	D	252/254 (99%)	0.27	10 (3%) 38 41	13, 23, 35, 41	0
1	E	252/254 (99%)	0.03	5 (1%) 65 68	12, 20, 32, 38	0
1	F	252/254 (99%)	-0.06	6 (2%) 59 62	12, 20, 32, 41	0
1	G	252/254 (99%)	-0.06	5 (1%) 65 68	12, 19, 31, 41	0
1	H	252/254 (99%)	0.01	9 (3%) 42 45	12, 20, 32, 40	0
1	I	252/254 (99%)	0.01	3 (1%) 79 81	12, 20, 32, 41	0
1	J	252/254 (99%)	0.04	10 (3%) 38 41	13, 22, 33, 41	0
1	K	252/254 (99%)	0.02	6 (2%) 59 62	14, 21, 33, 39	0
1	L	252/254 (99%)	0.04	8 (3%) 47 50	13, 21, 34, 42	0
1	M	252/254 (99%)	0.44	20 (7%) 12 14	14, 26, 37, 43	0
1	N	252/254 (99%)	0.25	12 (4%) 30 33	14, 24, 38, 42	0
1	O	252/254 (99%)	0.26	11 (4%) 34 37	13, 25, 39, 44	0
1	P	252/254 (99%)	0.52	22 (8%) 10 11	15, 26, 40, 46	0
All	All	4032/4064 (99%)	0.14	155 (3%) 40 43	12, 22, 35, 46	0

The worst 5 of 155 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	37	GLN	6.7
1	O	196	PRO	6.6
1	M	37	GLN	4.9
1	M	251	GLY	4.8
1	O	194	THR	4.6

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	SNO	O	5016	12/12	0.56	0.36	41,45,50,51	0
2	SNO	I	5010	12/12	0.58	0.38	42,44,48,50	0
2	SNO	J	5009	12/12	0.61	0.38	43,45,50,52	0
2	SNO	P	5015	12/12	0.61	0.38	44,46,51,51	0
2	SNO	C	5003	12/12	0.62	0.37	44,47,51,52	0
2	SNO	H	5008	12/12	0.64	0.41	43,45,47,48	0
2	SNO	B	5001	12/12	0.65	0.32	43,44,46,47	0
2	SNO	N	5013	12/12	0.66	0.39	41,46,51,52	0
2	SNO	K	5011	12/12	0.68	0.35	42,44,47,48	0
2	SNO	M	5014	12/12	0.70	0.42	45,46,50,52	0
2	SNO	L	5012	12/12	0.70	0.38	44,46,50,52	0
2	SNO	G	5007	12/12	0.73	0.33	41,43,47,48	0
2	SNO	E	5006	12/12	0.74	0.29	42,45,47,49	0
2	SNO	D	5004	12/12	0.76	0.29	44,45,49,49	0
2	SNO	F	5005	12/12	0.76	0.38	43,44,49,51	0
2	SNO	A	5002	12/12	0.77	0.32	43,46,48,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.