



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

PDB ID : 3ZNJ  
Title : Crystal structure of unliganded ClcF from R.opacus 1CP in crystal form 1.  
Authors : Roth, C.; Groening, J.A.D.; Kaschabek, S.R.; Schloemann, M.; Straeter, N.  
Deposited on : 2013-02-14  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

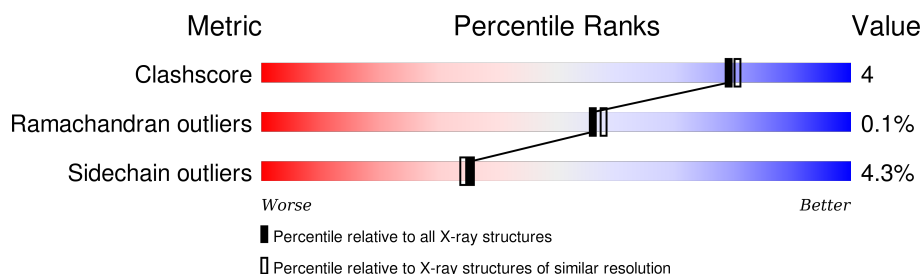
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)









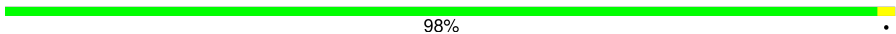
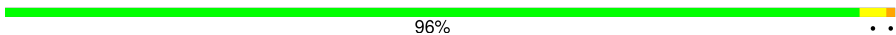



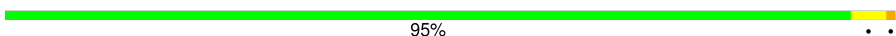

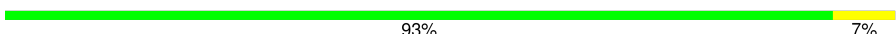


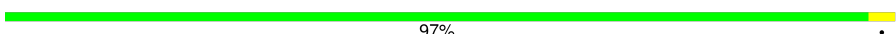






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	94	
1	2	94	
1	3	94	
1	4	94	
1	5	94	
1	6	94	
1	7	94	

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Mol	Chain	Length	Quality of chain
1	8	94	 84% 14% ..
1	9	94	 83% 13% . .
1	A	94	 81% 18% .
1	B	94	 84% 11% 5%
1	C	94	 93% 7%
1	D	94	 82% 18%
1	E	94	 79% 21%
1	F	94	 81% 14% 5%
1	G	94	 98% .
1	H	94	 96% . .
1	I	94	 91% 9%
1	J	94	 93% 7%
1	K	94	 94% 5% .
1	L	94	 95% . .
1	M	94	 91% 9%
1	N	94	 93% 7%
1	O	94	 89% 11%
1	P	94	 85% 13% .
1	R	94	 97% .
1	S	94	 89% 11%
1	T	94	 90% 7% .
1	U	94	 86% 12% .
1	V	94	 81% 16% .
1	W	94	 82% 17% .
1	X	94	 91% 7% .

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Mol	Chain	Length	Quality of chain
1	Y	94	 83%12% . .
1	Z	94	 93%6% .
1	a	94	 95%5%
1	b	94	 94%6%
1	c	94	 97%.
1	d	94	 90%10%
1	e	94	 95% . .
1	f	94	 99% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 66372 atoms, of which 31697 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 5-CHLOROMUCONOLACTONE DEHALOGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	2	93	Total	C	H	N	O	S	0	0	0
			1562	500	779	142	139	2			
1	3	92	Total	C	H	N	O	S	0	0	0
			1544	494	768	141	139	2			
1	4	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	5	92	Total	C	H	N	O	S	0	0	0
			1540	494	766	140	138	2			
1	6	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	7	92	Total	C	H	N	O	S	0	0	0
			1540	494	766	140	138	2			
1	8	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	9	91	Total	C	H	N	O	S	0	0	0
			1523	490	759	136	136	2			
1	A	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	B	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	C	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	D	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	E	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	F	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	G	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	I	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	J	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	K	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	L	94	Total	C	H	N	O	S	0	1	0
			1587	508	789	143	145	2			
1	M	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	N	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	O	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	P	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	R	94	Total	C	H	N	O	S	0	1	0
			1591	509	794	143	143	2			
1	S	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	T	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	U	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	V	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	W	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	X	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	Y	91	Total	C	H	N	O	S	0	1	0
			1545	496	769	139	139	2			
1	Z	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	a	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	b	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	c	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	d	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			
1	e	92	Total	C	H	N	O	S	0	0	0
			1540	494	766	140	138	2			
1	f	94	Total	C	H	N	O	S	0	0	0
			1575	504	783	143	143	2			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Cl	0	0
			1	1		
2	K	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	c	1	Total	Cl	0	0
			1	1		
2	6	1	Total	Cl	0	0
			1	1		
2	W	1	Total	Cl	0	0
			1	1		
2	N	1	Total	Cl	0	0
			1	1		
2	X	1	Total	Cl	0	0
			1	1		
2	2	1	Total	Cl	0	0
			1	1		
2	S	1	Total	Cl	0	0
			1	1		
2	f	1	Total	Cl	0	0
			1	1		
2	J	1	Total	Cl	0	0
			1	1		
2	E	1	Total	Cl	0	0
			1	1		
2	b	1	Total	Cl	0	0
			1	1		
2	V	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	5	1	Total Cl 1 1	0	0
2	R	1	Total Cl 1 1	0	0
2	M	1	Total Cl 1 1	0	0
2	1	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	e	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0
2	Z	1	Total Cl 1 1	0	0
2	a	1	Total Cl 1 1	0	0
2	4	1	Total Cl 1 1	0	0
2	U	1	Total Cl 1 1	0	0
2	9	1	Total Cl 1 1	0	0
2	L	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0
2	d	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	7	1	Total Cl 1 1	0	0
2	T	1	Total Cl 1 1	0	0
2	8	1	Total Cl 1 1	0	0
2	O	1	Total Cl 1 1	0	0

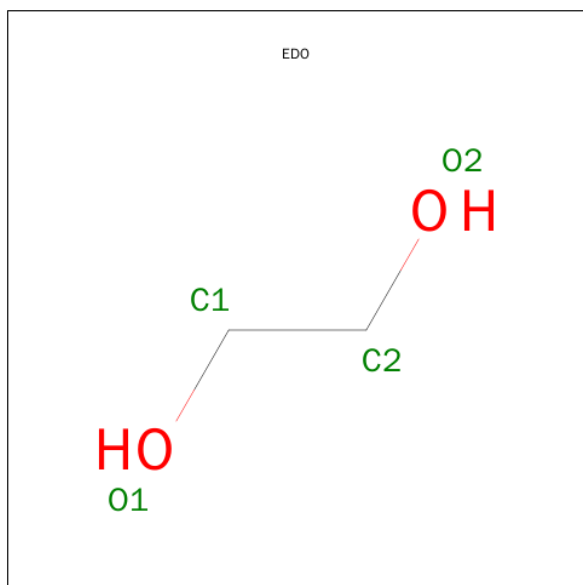
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Y	1	Total	Cl	0	0
			1	1		
2	3	1	Total	Cl	0	0
			1	1		
2	F	1	Total	Cl	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	1	1	Total	C	H	O	0	0
			10	2	6	2		
3	1	1	Total	C	H	O	0	0
			10	2	6	2		
3	2	1	Total	C	H	O	0	0
			10	2	6	2		
3	2	1	Total	C	H	O	0	0
			10	2	6	2		
3	3	1	Total	C	H	O	0	0
			10	2	6	2		
3	3	1	Total	C	H	O	0	0
			10	2	6	2		
3	4	1	Total	C	H	O	0	0
			10	2	6	2		
3	4	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	5	1	Total	C	H	O	0	0
			10	2	6	2		
3	5	1	Total	C	H	O	0	0
			10	2	6	2		
3	6	1	Total	C	H	O	0	0
			10	2	6	2		
3	6	1	Total	C	H	O	0	0
			10	2	6	2		
3	7	1	Total	C	H	O	0	0
			10	2	6	2		
3	7	1	Total	C	H	O	0	0
			10	2	6	2		
3	8	1	Total	C	H	O	0	0
			10	2	6	2		
3	8	1	Total	C	H	O	0	0
			10	2	6	2		
3	9	1	Total	C	H	O	0	0
			10	2	6	2		
3	9	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	E	1	Total	C	H	O	0	0
			10	2	6	2		
3	F	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	G	1	Total	C	H	O	0	0
			10	2	6	2		
3	H	1	Total	C	H	O	0	0
			10	2	6	2		
3	H	1	Total	C	H	O	0	0
			10	2	6	2		
3	I	1	Total	C	H	O	0	0
			10	2	6	2		
3	I	1	Total	C	H	O	0	0
			10	2	6	2		
3	J	1	Total	C	H	O	0	0
			10	2	6	2		
3	J	1	Total	C	H	O	0	0
			10	2	6	2		
3	K	1	Total	C	H	O	0	0
			10	2	6	2		
3	K	1	Total	C	H	O	0	0
			10	2	6	2		
3	L	1	Total	C	H	O	0	0
			10	2	6	2		
3	L	1	Total	C	H	O	0	0
			10	2	6	2		
3	M	1	Total	C	H	O	0	0
			10	2	6	2		
3	M	1	Total	C	H	O	0	0
			10	2	6	2		
3	N	1	Total	C	H	O	0	0
			10	2	6	2		
3	N	1	Total	C	H	O	0	0
			10	2	6	2		
3	O	1	Total	C	H	O	0	0
			10	2	6	2		
3	O	1	Total	C	H	O	0	0
			10	2	6	2		
3	P	1	Total	C	H	O	0	0
			10	2	6	2		
3	P	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	R	1	Total 10	C 2	H 6	O 2	0	0
3	R	1	Total 10	C 2	H 6	O 2	0	0
3	S	1	Total 10	C 2	H 6	O 2	0	0
3	S	1	Total 10	C 2	H 6	O 2	0	0
3	T	1	Total 10	C 2	H 6	O 2	0	0
3	T	1	Total 10	C 2	H 6	O 2	0	0
3	U	1	Total 10	C 2	H 6	O 2	0	0
3	V	1	Total 10	C 2	H 6	O 2	0	0
3	V	1	Total 10	C 2	H 6	O 2	0	0
3	W	1	Total 10	C 2	H 6	O 2	0	0
3	W	1	Total 10	C 2	H 6	O 2	0	0
3	X	1	Total 10	C 2	H 6	O 2	0	0
3	X	1	Total 10	C 2	H 6	O 2	0	0
3	Y	1	Total 10	C 2	H 6	O 2	0	0
3	Y	1	Total 10	C 2	H 6	O 2	0	0
3	Z	1	Total 10	C 2	H 6	O 2	0	0
3	a	1	Total 10	C 2	H 6	O 2	0	0
3	a	1	Total 10	C 2	H 6	O 2	0	0
3	b	1	Total 10	C 2	H 6	O 2	0	0
3	b	1	Total 10	C 2	H 6	O 2	0	0
3	c	1	Total 10	C 2	H 6	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	c	1	Total	C	H	O	0	0
			10	2	6	2		
3	d	1	Total	C	H	O	0	0
			10	2	6	2		
3	d	1	Total	C	H	O	0	0
			10	2	6	2		
3	e	1	Total	C	H	O	0	0
			10	2	6	2		
3	e	1	Total	C	H	O	0	0
			10	2	6	2		
3	f	1	Total	C	H	O	0	0
			10	2	6	2		
3	f	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	57	Total	O	0	0
			57	57		
4	2	59	Total	O	0	0
			59	59		
4	3	68	Total	O	0	0
			68	68		
4	4	38	Total	O	0	0
			38	38		
4	5	47	Total	O	0	0
			47	47		
4	6	46	Total	O	0	0
			46	46		
4	7	41	Total	O	0	0
			41	41		
4	8	56	Total	O	0	0
			56	56		
4	9	50	Total	O	0	0
			50	50		
4	A	155	Total	O	0	0
			155	155		
4	B	143	Total	O	0	0
			143	143		
4	C	169	Total	O	0	0
			169	169		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	147	Total 147	O 147	0	0
4	E	161	Total 161	O 161	0	0
4	F	122	Total 122	O 122	0	0
4	G	138	Total 138	O 138	0	0
4	H	93	Total 93	O 93	0	0
4	I	75	Total 75	O 75	0	0
4	J	90	Total 90	O 90	0	0
4	K	103	Total 103	O 103	0	0
4	L	87	Total 87	O 87	0	0
4	M	84	Total 84	O 84	0	0
4	N	78	Total 78	O 78	0	0
4	O	64	Total 64	O 64	0	0
4	P	67	Total 67	O 67	0	0
4	R	95	Total 95	O 95	0	0
4	S	88	Total 88	O 88	0	0
4	T	82	Total 82	O 82	0	0
4	U	54	Total 54	O 54	0	0
4	V	46	Total 46	O 46	0	0
4	W	37	Total 37	O 37	0	0
4	X	42	Total 42	O 42	0	0
4	Y	29	Total 29	O 29	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Z	44	Total	O	0	0
			44	44		

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.


Note EDS failed to run properly.

#### • Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 1: 




#### • Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 2: 




#### • Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 3: 




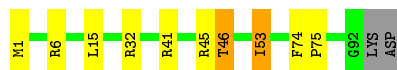
#### • Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 4: 




#### • Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 5: 



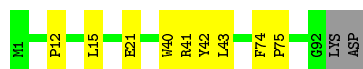
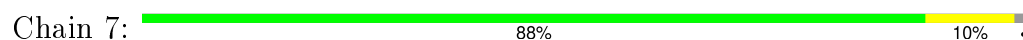
#### • Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain 6: 

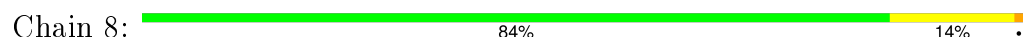




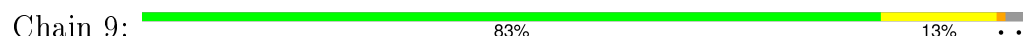
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



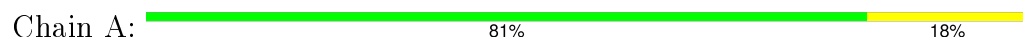
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



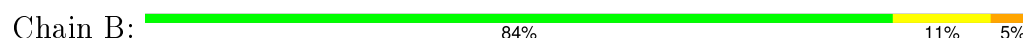
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



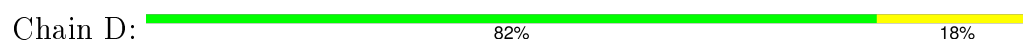
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE




- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE




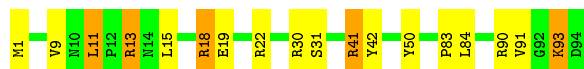
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain E:  79% 21%



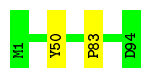
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain F:  81% 14% 5%



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain G:  98% .




- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain H:  96% . .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain I:  91% 9%



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain J:  93% 7%



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain K:  94% 5% .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain L:  95% . .




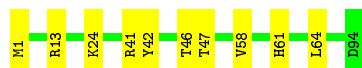
## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain M:  91% 9%


## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain N:  93% 7%

## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain O:  89% 11%


## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain P:  85% 13% .


## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain R:  97% .


## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain S:  89% 11%

## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain T:  90% 7% .

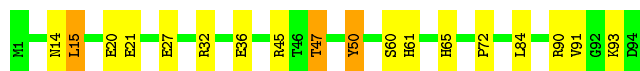
## ● Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain U:  86% 12% .



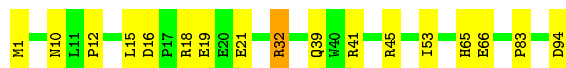
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain V: 81% 16% .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain W: 82% 17% .



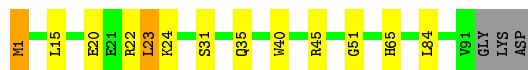
- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain X: 91% 7% .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain Y: 83% 12% . .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain Z: 93% 6% .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain a: 95% 5%




- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain b: 94% 6%



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain c:  97% .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain d:  90% 10%



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain e:  95% . .



- Molecule 1: 5-CHLOROMUCONOLACTONE DEHALOGENASE

Chain f:  99% .



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.14Å 79.43Å 198.97Å 90.00° 93.41° 90.00°	Depositor
Resolution (Å)	19.90 – 2.10	Depositor
% Data completeness (in resolution range)	95.3 (19.90-2.10)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.33 (at 2.09Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1172)	Depositor
R, $R_{free}$	0.164 , 0.224	Depositor
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.187	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 261658 reflections	Xtriage
Total number of atoms	66372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: EDO, CL

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	1	0.23	0/814	0.44	0/1103
1	2	0.23	0/805	0.44	0/1092
1	3	0.23	0/797	0.45	0/1077
1	4	0.24	0/814	0.44	0/1103
1	5	0.23	0/796	0.42	0/1081
1	6	0.23	0/814	0.44	0/1103
1	7	0.23	0/796	0.45	0/1081
1	8	0.24	0/814	0.52	1/1103 (0.1%)
1	9	0.22	0/785	0.44	0/1064
1	A	0.23	0/814	0.44	0/1103
1	B	0.24	0/814	0.43	0/1103
1	C	0.23	0/814	0.43	0/1103
1	D	0.24	0/814	0.45	0/1103
1	E	0.24	0/814	0.44	0/1103
1	F	0.24	0/814	0.45	0/1103
1	G	0.24	0/814	0.43	0/1103
1	H	0.24	0/814	0.47	0/1103
1	I	0.24	0/814	0.44	0/1103
1	J	0.24	0/814	0.45	0/1103
1	K	0.23	0/814	0.45	0/1103
1	L	0.24	0/823	0.45	0/1115
1	M	0.23	0/814	0.44	0/1103
1	N	0.23	0/814	0.45	0/1103
1	O	0.24	0/814	0.45	0/1103
1	P	0.24	0/814	0.45	0/1103
1	R	0.24	0/822	0.44	0/1114
1	S	0.24	0/814	0.44	0/1103
1	T	0.24	0/814	0.45	0/1103
1	U	0.24	0/814	0.47	0/1103
1	V	0.23	0/814	0.44	0/1103
1	W	0.24	0/814	0.47	0/1103
1	X	0.23	0/814	0.44	0/1103

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	Y	0.24	0/801	0.44	0/1088
1	Z	0.24	0/814	0.45	0/1103
1	a	0.23	0/814	0.45	0/1103
1	b	0.23	0/814	0.44	0/1103
1	c	0.23	0/814	0.43	0/1103
1	d	0.24	0/814	0.45	0/1103
1	e	0.24	0/796	0.49	0/1081
1	f	0.25	0/814	0.45	0/1103
All	All	0.24	0/32455	0.45	1/43986 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	8	18	ARG	NE-CZ-NH1	7.32	123.96	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	792	783	779	9	0
1	2	783	779	775	8	0
1	3	776	768	764	5	0
1	4	792	783	779	12	0
1	5	774	766	762	7	0
1	6	792	783	779	9	0
1	7	774	766	762	6	0
1	8	792	783	779	8	0
1	9	764	759	755	6	0
1	A	792	783	779	11	0
1	B	792	783	779	15	0
1	C	792	783	779	6	0
1	D	792	783	779	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	792	783	779	17	0
1	F	792	783	779	18	0
1	G	792	783	779	1	0
1	H	792	783	779	5	0
1	I	792	783	779	6	0
1	J	792	783	779	2	0
1	K	792	783	779	4	0
1	L	798	789	785	2	0
1	M	792	783	779	7	0
1	N	792	783	779	5	0
1	O	792	783	779	6	0
1	P	792	783	779	11	0
1	R	797	794	790	2	0
1	S	792	783	779	9	0
1	T	792	783	779	5	0
1	U	792	783	779	17	0
1	V	792	783	779	15	0
1	W	792	783	779	12	0
1	X	792	783	779	5	0
1	Y	776	769	765	8	0
1	Z	792	783	779	4	0
1	a	792	783	779	0	0
1	b	792	783	779	0	0
1	c	792	783	779	0	0
1	d	792	783	779	0	0
1	e	774	766	762	0	0
1	f	792	783	779	0	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
2	6	1	0	0	0	0
2	7	1	0	0	0	0
2	8	1	0	0	0	0
2	9	1	0	0	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	1	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	X	1	0	0	1	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
2	a	1	0	0	0	0
2	b	1	0	0	0	0
2	c	1	0	0	0	0
2	d	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
3	1	8	12	12	0	0
3	2	8	12	12	0	0
3	3	8	12	12	1	0
3	4	8	12	12	0	0
3	5	8	12	12	0	0
3	6	8	12	12	1	0
3	7	8	12	12	0	0
3	8	8	12	12	0	0
3	9	8	12	12	0	0
3	A	8	12	12	1	0
3	B	8	12	12	0	0
3	C	8	12	12	0	0
3	D	8	12	12	0	0
3	E	8	12	12	0	0
3	F	8	12	12	1	0
3	G	8	12	12	0	0
3	H	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	8	12	12	0	0
3	J	8	12	12	0	0
3	K	8	12	12	0	0
3	L	8	12	12	1	0
3	M	8	12	12	0	0
3	N	8	12	12	0	0
3	O	8	12	12	0	0
3	P	8	12	12	1	0
3	R	8	12	12	0	0
3	S	8	12	12	0	0
3	T	8	12	12	0	0
3	U	4	6	6	0	0
3	V	8	12	12	0	0
3	W	8	12	12	0	0
3	X	8	12	12	0	0
3	Y	8	12	12	1	0
3	Z	4	6	6	0	0
3	a	8	12	12	0	0
3	b	8	12	12	0	0
3	c	8	12	12	0	0
3	d	8	12	12	0	0
3	e	8	12	12	0	0
3	f	8	12	12	0	0
4	1	57	0	0	1	0
4	2	59	0	0	0	0
4	3	68	0	0	0	0
4	4	38	0	0	1	0
4	5	47	0	0	0	0
4	6	46	0	0	0	0
4	7	41	0	0	0	0
4	8	56	0	0	0	0
4	9	50	0	0	0	0
4	A	155	0	0	0	0
4	B	143	0	0	1	0
4	C	169	0	0	0	0
4	D	147	0	0	1	0
4	E	161	0	0	1	0
4	F	122	0	0	1	0
4	G	138	0	0	0	0
4	H	93	0	0	0	0
4	I	75	0	0	0	0
4	J	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	103	0	0	0	0
4	L	87	0	0	1	0
4	M	84	0	0	1	0
4	N	78	0	0	0	0
4	O	64	0	0	0	0
4	P	67	0	0	0	0
4	R	95	0	0	0	0
4	S	88	0	0	0	0
4	T	82	0	0	1	0
4	U	54	0	0	0	0
4	V	46	0	0	1	0
4	W	37	0	0	2	0
4	X	42	0	0	0	0
4	Y	29	0	0	0	0
4	Z	44	0	0	1	0
All	All	34675	31697	31537	222	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 4.

The worst 5 of 222 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:D:41:ARG:NH1	1:D:94:ASP:O	2.83	0.74
1:M:93:LYS:O	1:M:94:ASP:HB2	1.88	0.72
1:V:50:TYR:OH	4:V:2029:HOH:O	2.07	0.71
1:6:41:ARG:NH2	1:6:94:ASP:O	2.24	0.70
1:F:41:ARG:NH2	4:F:2080:HOH:O	2.25	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	17	11
1	2	91/94 (97%)	89 (98%)	2 (2%)	0	100	100
1	3	88/94 (94%)	86 (98%)	2 (2%)	0	100	100
1	4	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	5	90/94 (96%)	88 (98%)	2 (2%)	0	100	100
1	6	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	7	90/94 (96%)	86 (96%)	4 (4%)	0	100	100
1	8	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	9	87/94 (93%)	85 (98%)	2 (2%)	0	100	100
1	A	92/94 (98%)	90 (98%)	1 (1%)	1 (1%)	17	11
1	B	92/94 (98%)	92 (100%)	0	0	100	100
1	C	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	D	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	E	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	F	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	G	92/94 (98%)	92 (100%)	0	0	100	100
1	H	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	I	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	J	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	K	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	L	93/94 (99%)	93 (100%)	0	0	100	100
1	M	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	N	92/94 (98%)	92 (100%)	0	0	100	100
1	O	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	P	92/94 (98%)	92 (100%)	0	0	100	100
1	R	93/94 (99%)	93 (100%)	0	0	100	100
1	S	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	T	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	U	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
1	V	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
1	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
1	X	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
1	Z	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	a	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	b	92/94 (98%)	92 (100%)	0	0	100	100
1	c	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	e	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
1	f	92/94 (98%)	92 (100%)	0	0	100	100
All	All	3664/3760 (97%)	3609 (98%)	53 (1%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	17	PRO
1	A	17	PRO

### 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	1	87/87 (100%)	83 (95%)	4 (5%)	33	31
1	2	86/87 (99%)	79 (92%)	7 (8%)	15	10
1	3	85/87 (98%)	81 (95%)	4 (5%)	32	30
1	4	87/87 (100%)	85 (98%)	2 (2%)	58	62
1	5	85/87 (98%)	80 (94%)	5 (6%)	24	20
1	6	87/87 (100%)	83 (95%)	4 (5%)	33	31
1	7	85/87 (98%)	84 (99%)	1 (1%)	78	84
1	8	87/87 (100%)	81 (93%)	6 (7%)	19	15
1	9	84/87 (97%)	79 (94%)	5 (6%)	24	20
1	A	87/87 (100%)	85 (98%)	2 (2%)	58	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	87/87 (100%)	81 (93%)	6 (7%)	19	15
1	C	87/87 (100%)	86 (99%)	1 (1%)	80	85
1	D	87/87 (100%)	84 (97%)	3 (3%)	44	45
1	E	87/87 (100%)	83 (95%)	4 (5%)	33	31
1	F	87/87 (100%)	78 (90%)	9 (10%)	9	5
1	G	87/87 (100%)	86 (99%)	1 (1%)	80	85
1	H	87/87 (100%)	85 (98%)	2 (2%)	58	62
1	I	87/87 (100%)	87 (100%)	0	100	100
1	J	87/87 (100%)	83 (95%)	4 (5%)	33	31
1	K	87/87 (100%)	86 (99%)	1 (1%)	80	85
1	L	88/87 (101%)	84 (96%)	4 (4%)	34	32
1	M	87/87 (100%)	84 (97%)	3 (3%)	44	45
1	N	87/87 (100%)	85 (98%)	2 (2%)	58	62
1	O	87/87 (100%)	84 (97%)	3 (3%)	44	45
1	P	87/87 (100%)	83 (95%)	4 (5%)	33	31
1	R	88/87 (101%)	87 (99%)	1 (1%)	80	85
1	S	87/87 (100%)	86 (99%)	1 (1%)	80	85
1	T	87/87 (100%)	84 (97%)	3 (3%)	44	45
1	U	87/87 (100%)	82 (94%)	5 (6%)	25	22
1	V	87/87 (100%)	82 (94%)	5 (6%)	25	22
1	W	87/87 (100%)	82 (94%)	5 (6%)	25	22
1	X	87/87 (100%)	81 (93%)	6 (7%)	19	15
1	Y	86/87 (99%)	81 (94%)	5 (6%)	25	21
1	Z	87/87 (100%)	84 (97%)	3 (3%)	44	45
1	a	87/87 (100%)	82 (94%)	5 (6%)	25	22
1	b	87/87 (100%)	81 (93%)	6 (7%)	19	15
1	c	87/87 (100%)	84 (97%)	3 (3%)	44	45
1	d	87/87 (100%)	78 (90%)	9 (10%)	9	5
1	e	85/87 (98%)	82 (96%)	3 (4%)	43	44
1	f	87/87 (100%)	86 (99%)	1 (1%)	80	85
All	All	3469/3480 (100%)	3321 (96%)	148 (4%)	35	34

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	13	ARG
1	O	47	THR
1	d	13	ARG
1	J	23	LEU
1	M	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	61	HIS
1	P	61	HIS
1	V	61	HIS
1	J	61	HIS
1	V	14	ASN

### 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 118 ligands modelled in this entry, 40 are monoatomic - leaving 78 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
3	EDO	1	1096	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	1	1097	-	3,3,3	0.48	0	2,2,2	0.40	0
3	EDO	2	1095	-	3,3,3	0.48	0	2,2,2	0.31	0
3	EDO	2	1096	-	3,3,3	0.47	0	2,2,2	0.41	0
3	EDO	3	1096	-	3,3,3	0.45	0	2,2,2	0.33	0
3	EDO	3	1097	-	3,3,3	0.48	0	2,2,2	0.45	0
3	EDO	4	1096	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	4	1097	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	5	1094	-	3,3,3	0.47	0	2,2,2	0.42	0
3	EDO	5	1095	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	6	1096	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	6	1097	-	3,3,3	0.43	0	2,2,2	0.29	0
3	EDO	7	1094	-	3,3,3	0.46	0	2,2,2	0.47	0
3	EDO	7	1095	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	8	1096	-	3,3,3	0.44	0	2,2,2	0.67	0
3	EDO	8	1097	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	9	1095	-	3,3,3	0.44	0	2,2,2	0.71	0
3	EDO	9	1096	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	A	1096	-	3,3,3	0.44	0	2,2,2	0.43	0
3	EDO	A	1097	-	3,3,3	0.48	0	2,2,2	0.33	0
3	EDO	B	1096	-	3,3,3	0.52	0	2,2,2	0.42	0
3	EDO	B	1097	-	3,3,3	0.45	0	2,2,2	0.42	0
3	EDO	C	1096	-	3,3,3	0.54	0	2,2,2	0.46	0
3	EDO	C	1097	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	D	1096	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	D	1097	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	E	1096	-	3,3,3	0.54	0	2,2,2	0.28	0
3	EDO	E	1097	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	F	1096	-	3,3,3	0.50	0	2,2,2	0.42	0
3	EDO	F	1097	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	G	1096	-	3,3,3	0.45	0	2,2,2	0.40	0
3	EDO	G	1097	-	3,3,3	0.42	0	2,2,2	0.56	0
3	EDO	H	1096	-	3,3,3	0.58	0	2,2,2	0.46	0
3	EDO	H	1097	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	I	1096	-	3,3,3	0.38	0	2,2,2	0.90	0
3	EDO	I	1097	-	3,3,3	0.46	0	2,2,2	0.44	0
3	EDO	J	1096	-	3,3,3	0.44	0	2,2,2	0.40	0
3	EDO	J	1097	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	K	1096	-	3,3,3	0.44	0	2,2,2	0.89	0
3	EDO	K	1097	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	L	1096	-	3,3,3	0.48	0	2,2,2	0.43	0
3	EDO	L	1097	-	3,3,3	0.47	0	2,2,2	0.36	0
3	EDO	M	1096	-	3,3,3	0.49	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	M	1097	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	N	1096	-	3,3,3	0.50	0	2,2,2	0.36	0
3	EDO	N	1097	-	3,3,3	0.47	0	2,2,2	0.41	0
3	EDO	O	1096	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	O	1097	-	3,3,3	0.48	0	2,2,2	0.38	0
3	EDO	P	1096	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	P	1097	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	R	1096	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	R	1097	-	3,3,3	0.47	0	2,2,2	0.44	0
3	EDO	S	1096	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	S	1097	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	T	1096	-	3,3,3	0.46	0	2,2,2	0.41	0
3	EDO	T	1097	-	3,3,3	0.48	0	2,2,2	0.46	0
3	EDO	U	1096	-	3,3,3	0.47	0	2,2,2	0.44	0
3	EDO	V	1096	-	3,3,3	0.43	0	2,2,2	0.43	0
3	EDO	V	1097	-	3,3,3	0.47	0	2,2,2	0.39	0
3	EDO	W	1096	-	3,3,3	0.44	0	2,2,2	0.44	0
3	EDO	W	1097	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	X	1096	-	3,3,3	0.52	0	2,2,2	0.31	0
3	EDO	X	1097	-	3,3,3	0.47	0	2,2,2	0.37	0
3	EDO	Y	1093	-	3,3,3	0.43	0	2,2,2	0.53	0
3	EDO	Y	1094	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	Z	1096	-	3,3,3	0.46	0	2,2,2	0.42	0
3	EDO	a	1096	-	3,3,3	0.51	0	2,2,2	0.49	0
3	EDO	a	1097	-	3,3,3	0.46	0	2,2,2	0.39	0
3	EDO	b	1096	-	3,3,3	0.43	0	2,2,2	0.61	0
3	EDO	b	1097	-	3,3,3	0.48	0	2,2,2	0.35	0
3	EDO	c	1096	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	c	1097	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EDO	d	1096	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	d	1097	-	3,3,3	0.46	0	2,2,2	0.40	0
3	EDO	e	1094	-	3,3,3	0.49	0	2,2,2	0.55	0
3	EDO	e	1095	-	3,3,3	0.47	0	2,2,2	0.35	0
3	EDO	f	1096	-	3,3,3	0.49	0	2,2,2	0.44	0
3	EDO	f	1097	-	3,3,3	0.48	0	2,2,2	0.34	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	1	1096	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	1	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	2	1095	-	-	0/1/1/1	0/0/0/0
3	EDO	2	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	3	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	3	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	4	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	4	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	5	1094	-	-	0/1/1/1	0/0/0/0
3	EDO	5	1095	-	-	0/1/1/1	0/0/0/0
3	EDO	6	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	6	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	7	1094	-	-	0/1/1/1	0/0/0/0
3	EDO	7	1095	-	-	0/1/1/1	0/0/0/0
3	EDO	8	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	8	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	9	1095	-	-	0/1/1/1	0/0/0/0
3	EDO	9	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	E	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	F	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	F	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	G	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	G	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	H	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	H	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	I	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	I	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	J	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	J	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	K	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	K	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	L	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	L	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	M	1096	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	M	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	N	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	N	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	O	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	O	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	P	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	P	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	R	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	R	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	S	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	S	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	T	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	T	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	U	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	V	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	V	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	W	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	W	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	X	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	X	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	Y	1093	-	-	0/1/1/1	0/0/0/0
3	EDO	Y	1094	-	-	0/1/1/1	0/0/0/0
3	EDO	Z	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	a	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	a	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	b	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	b	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	c	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	c	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	d	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	d	1097	-	-	0/1/1/1	0/0/0/0
3	EDO	e	1094	-	-	0/1/1/1	0/0/0/0
3	EDO	e	1095	-	-	0/1/1/1	0/0/0/0
3	EDO	f	1096	-	-	0/1/1/1	0/0/0/0
3	EDO	f	1097	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3	1096	EDO	1	0
3	6	1097	EDO	1	0
3	A	1096	EDO	1	0
3	F	1097	EDO	1	0
3	L	1097	EDO	1	0
3	P	1097	EDO	1	0
3	Y	1094	EDO	1	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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.