



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:09 am BST

PDB ID : 5L2O  
Title : Crystal Structure of ALDH1A1 in complex with BUC22  
Authors : Buchman, C.D.; Hurley, T.D.  
Deposited on : 2016-08-02  
Resolution : 2.05 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](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.

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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 : 1.8.5 (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

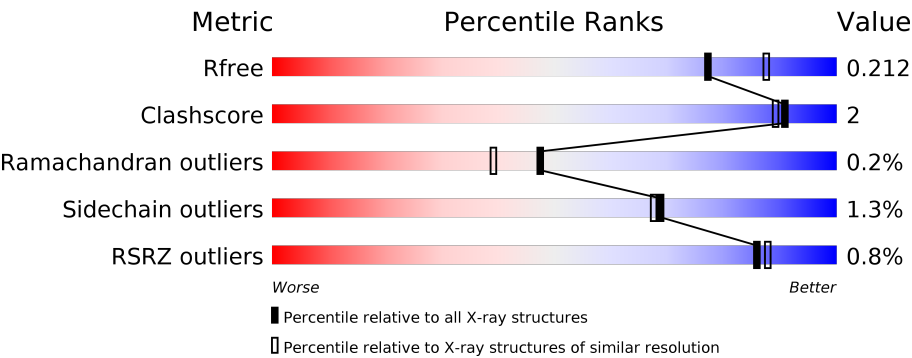
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	501	<div><div></div><div>95%</div><div></div><div></div><div></div></div>
1	B	501	<div><div>%</div><div>94%</div><div>5%</div><div></div><div></div></div>
1	C	501	<div><div></div><div>95%</div><div></div><div></div><div></div></div>
1	D	501	<div><div>%</div><div>93%</div><div>5%</div><div></div><div></div></div>
1	E	501	<div><div></div><div>94%</div><div></div><div></div><div></div></div>
1	F	501	<div><div>2%</div><div>93%</div><div>5%</div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	501	<div><div>%</div><div><div></div><div>93%</div><div>5% •</div></div></div>
1	H	501	<div><div></div><div>93%</div><div>5% •</div></div>

## 2 Entry composition

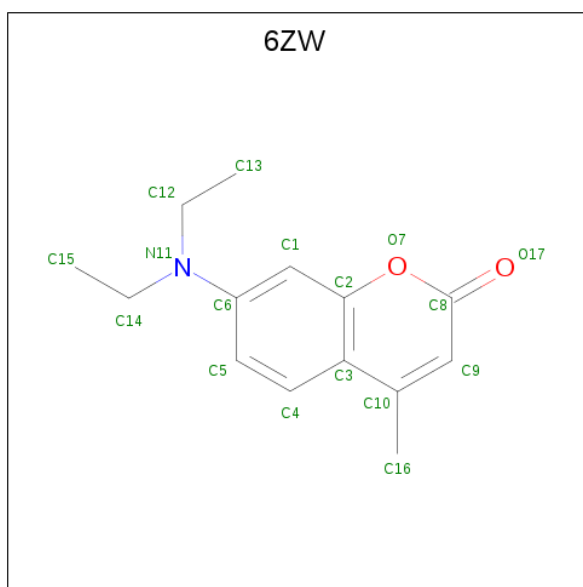
There are 5 unique types of molecules in this entry. The entry contains 33056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinal dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3828	2445	644	719	20			
1	B	494	Total	C	N	O	S	0	2	0
			3828	2445	644	719	20			
1	C	493	Total	C	N	O	S	0	2	0
			3820	2441	643	716	20			
1	D	493	Total	C	N	O	S	0	3	0
			3823	2443	643	716	21			
1	E	493	Total	C	N	O	S	0	3	0
			3823	2443	643	716	21			
1	F	493	Total	C	N	O	S	0	2	0
			3820	2441	643	716	20			
1	G	494	Total	C	N	O	S	0	2	0
			3822	2439	644	718	21			
1	H	493	Total	C	N	O	S	0	2	0
			3814	2435	643	715	21			

- Molecule 2 is 7-(diethylamino)-4-methyl-2H-1-benzopyran-2-one (three-letter code: 6ZW) (formula: C<sub>14</sub>H<sub>17</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	14	1	2		
2	B	1	Total	C	N	O	0	0
			17	14	1	2		
2	C	1	Total	C	N	O	0	0
			17	14	1	2		
2	D	1	Total	C	N	O	0	0
			17	14	1	2		
2	E	1	Total	C	N	O	0	0
			17	14	1	2		
2	F	1	Total	C	N	O	0	0
			17	14	1	2		
2	G	1	Total	C	N	O	0	0
			17	14	1	2		
2	H	1	Total	C	N	O	0	0
			17	14	1	2		

- Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Yb	0	0
			1	1		
3	D	1	Total	Yb	0	0
			1	1		
3	E	2	Total	Yb	0	0
			2	2		
3	H	1	Total	Yb	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Yb 1	0	0
3	A	1	Total 1	Yb 1	0	0
3	F	1	Total 1	Yb 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	303	Total 303	O 303	0	0
5	B	287	Total 287	O 287	0	0
5	C	312	Total 312	O 312	0	0
5	D	325	Total 325	O 325	0	0
5	E	292	Total 292	O 292	0	0
5	F	236	Total 236	O 236	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	287	Total 287	O 287	0	0
5	H	284	Total 284	O 284	0	0

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

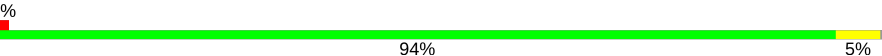
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Retinal dehydrogenase 1

Chain A:  95% ..



- Molecule 1: Retinal dehydrogenase 1

Chain B:  94% 5% .

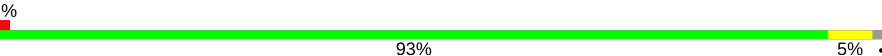


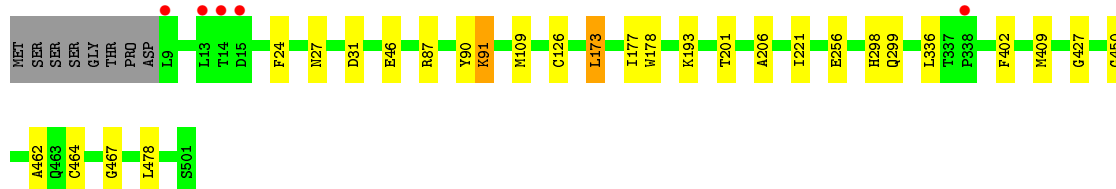
- Molecule 1: Retinal dehydrogenase 1

Chain C:  95% ..



- Molecule 1: Retinal dehydrogenase 1

Chain D:  93% 5% .



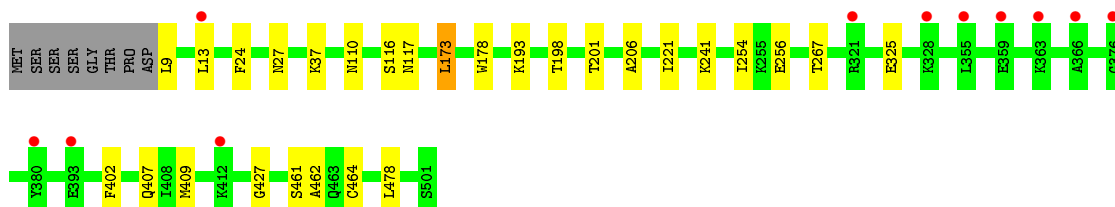
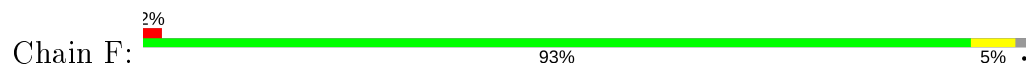
- Molecule 1: Retinal dehydrogenase 1

Chain E:  94% . . .

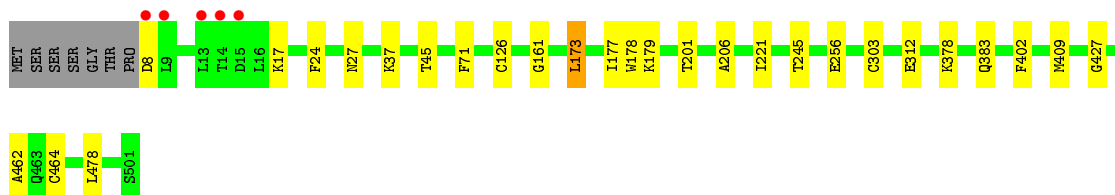




- Molecule 1: Retinal dehydrogenase 1



- Molecule 1: Retinal dehydrogenase 1



- Molecule 1: Retinal dehydrogenase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.98 Å 98.29 Å 127.32 Å 80.55° 86.23° 64.36°	Depositor
Resolution (Å)	50.00 – 2.05 49.72 – 2.05	Depositor EDS
% Data completeness (in resolution range)	90.5 (50.00-2.05) 90.6 (49.72-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.05 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.174 , 0.204 0.183 , 0.212	Depositor DCC
$R_{free}$ test set	11177 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	33056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YB, 6ZW, 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	A	0.59	0/3917	0.71	0/5301
1	B	0.59	0/3917	0.70	2/5301 (0.0%)
1	C	0.67	4/3909 (0.1%)	0.71	2/5290 (0.0%)
1	D	0.69	2/3915 (0.1%)	0.74	3/5298 (0.1%)
1	E	0.61	1/3915 (0.0%)	0.74	3/5298 (0.1%)
1	F	0.61	3/3909 (0.1%)	0.73	6/5290 (0.1%)
1	G	0.60	0/3910	0.71	1/5291 (0.0%)
1	H	0.59	1/3902 (0.0%)	0.73	2/5280 (0.0%)
All	All	0.62	11/31294 (0.0%)	0.72	19/42349 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	GLU	CD-OE2	14.54	1.41	1.25
1	C	349	GLU	CD-OE2	13.72	1.40	1.25
1	F	325	GLU	CD-OE2	10.07	1.36	1.25
1	D	46	GLU	CG-CD	9.68	1.66	1.51
1	E	359	GLU	CG-CD	9.59	1.66	1.51
1	F	325	GLU	CG-CD	9.41	1.66	1.51
1	C	349	GLU	CB-CG	7.42	1.66	1.52
1	C	349	GLU	CG-CD	7.41	1.63	1.51
1	F	325	GLU	CB-CG	6.71	1.64	1.52
1	C	464	CYS	CB-SG	-5.83	1.72	1.81
1	H	9	LEU	N-CA	5.32	1.56	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	359	GLU	OE1-CD-OE2	-15.01	105.29	123.30
1	H	285	ASP	CB-CG-OD2	10.29	127.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	285	ASP	CB-CG-OD1	-9.71	109.56	118.30
1	D	31	ASP	CB-CG-OD2	9.32	126.69	118.30
1	F	325	GLU	CA-CB-CG	8.78	132.71	113.40
1	F	325	GLU	CG-CD-OE2	7.10	132.50	118.30
1	C	349	GLU	CG-CD-OE2	6.83	131.96	118.30
1	F	13	LEU	CA-CB-CG	6.46	130.17	115.30
1	E	359	GLU	CA-CB-CG	6.38	127.44	113.40
1	D	91	LYS	CB-CG-CD	6.27	127.90	111.60
1	E	359	GLU	CG-CD-OE1	6.11	130.52	118.30
1	C	349	GLU	CG-CD-OE1	-5.90	106.50	118.30
1	D	87	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	87	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	325	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	G	37	LYS	CD-CE-NZ	-5.57	98.89	111.70
1	F	254	ILE	CA-CB-CG1	-5.28	100.97	111.00
1	B	87	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	F	254	ILE	CB-CG1-CD1	5.02	127.95	113.90

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	A	3828	0	3827	12	0
1	B	3828	0	3827	13	0
1	C	3820	0	3823	10	0
1	D	3823	0	3828	17	0
1	E	3823	0	3829	15	0
1	F	3820	0	3824	15	0
1	G	3822	0	3824	15	0
1	H	3814	0	3820	16	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	17	0	0	0	0
2	F	17	0	0	0	0
2	G	17	0	0	0	0
2	H	17	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	303	0	0	0	0
5	B	287	0	0	2	0
5	C	312	0	0	1	0
5	D	325	0	0	2	0
5	E	292	0	0	1	0
5	F	236	0	0	2	0
5	G	287	0	0	4	0
5	H	284	0	0	3	0
All	All	33056	0	30602	104	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 2.

All (104) 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:B:462:ALA:HA	1:B:478:LEU:HD23	1.68	0.75
1:F:117:ASN:ND2	5:F:701:HOH:O	2.23	0.70
1:E:126[B]:CYS:SG	1:E:177:ILE:HG13	2.33	0.68
1:D:126[B]:CYS:SG	1:D:177:ILE:HG13	2.35	0.67
1:G:45:THR:O	1:G:378:LYS:HE2	1.95	0.67
1:H:312:GLU:HG3	5:H:929:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:MET:HG2	1:D:336:LEU:HD11	1.79	0.64
1:A:8:ASP:OD1	1:A:9:LEU:HG	1.98	0.64
1:D:109:MET:CG	1:D:336:LEU:HD11	2.28	0.64
1:F:9:LEU:HD11	1:F:116:SER:HB3	1.79	0.64
1:H:126[B]:CYS:SG	1:H:177:ILE:HG13	2.40	0.62
1:F:462:ALA:HA	1:F:478:LEU:HD13	1.83	0.60
1:D:462:ALA:HA	1:D:478:LEU:HD13	1.83	0.60
1:E:147:ILE:HG13	1:F:461:SER:OG	2.02	0.59
1:G:126[B]:CYS:SG	1:G:177:ILE:HG13	2.42	0.58
1:F:241:LYS:NZ	1:F:267:THR:OG1	2.37	0.58
1:H:462:ALA:HA	1:H:478:LEU:HD13	1.86	0.57
1:G:462:ALA:HA	1:G:478:LEU:HD13	1.86	0.57
1:C:462:ALA:HA	1:C:478:LEU:HD13	1.86	0.57
1:E:126[B]:CYS:SG	1:E:177:ILE:CG1	2.93	0.56
1:A:90[B]:TYR:CE1	1:C:90[B]:TYR:CZ	2.92	0.56
1:B:90[B]:TYR:CZ	1:D:90[B]:TYR:CE1	2.93	0.56
1:E:462:ALA:HA	1:E:478:LEU:HD13	1.88	0.55
1:A:462:ALA:HA	1:A:478:LEU:HD13	1.88	0.54
1:F:9:LEU:HD11	1:F:116:SER:CB	2.38	0.54
1:B:178:TRP:CE3	1:B:478:LEU:HD13	2.43	0.53
1:H:178:TRP:CZ2	1:H:478:LEU:HD12	2.44	0.53
1:B:90[B]:TYR:CE1	1:D:90[B]:TYR:CZ	2.97	0.53
1:G:312:GLU:HG3	5:G:915:HOH:O	2.09	0.52
1:C:178:TRP:CZ2	1:C:478:LEU:HD12	2.44	0.52
1:A:393:GLU:OE1	1:A:393:GLU:N	2.44	0.51
1:A:90[B]:TYR:CZ	1:C:90[B]:TYR:CE1	2.98	0.51
1:D:178:TRP:CZ2	1:D:478:LEU:HD12	2.46	0.50
1:A:178:TRP:CZ2	1:A:478:LEU:HD12	2.46	0.50
1:C:256:GLU:HG3	1:D:256:GLU:HG3	1.93	0.50
1:F:178:TRP:CZ2	1:F:478:LEU:HD12	2.46	0.50
1:G:178:TRP:CZ2	1:G:478:LEU:HD12	2.47	0.49
1:G:179:LYS:HD3	5:G:778:HOH:O	2.12	0.49
1:E:178:TRP:CZ2	1:E:478:LEU:HD12	2.47	0.49
1:G:383:GLN:NE2	5:G:706:HOH:O	2.46	0.49
1:D:126[B]:CYS:SG	1:D:177:ILE:CG1	2.99	0.48
1:H:377:ASN:N	1:H:377:ASN:OD1	2.46	0.48
1:D:178:TRP:CE2	1:D:478:LEU:HD12	2.49	0.48
1:A:17:LYS:HE3	1:A:17:LYS:HA	1.95	0.48
1:E:193:LYS:HG2	1:E:222:VAL:O	2.14	0.48
1:A:295:VAL:HG23	1:A:306:ALA:O	2.14	0.47
1:H:178:TRP:CE2	1:H:478:LEU:HD12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HB2	1:A:221:ILE:HD12	1.96	0.47
1:D:298:HIS:HD2	5:D:738:HOH:O	1.96	0.47
1:H:87:ARG:HG2	5:H:827:HOH:O	2.13	0.47
1:E:178:TRP:CE2	1:E:478:LEU:HD12	2.50	0.47
1:A:256:GLU:HG3	1:B:256:GLU:HG3	1.96	0.46
1:B:337:THR:OG1	5:B:701:HOH:O	2.20	0.46
1:F:178:TRP:CE2	1:F:478:LEU:HD12	2.50	0.46
1:F:206:ALA:HB2	1:F:221:ILE:HD12	1.98	0.46
1:C:206:ALA:HB2	1:C:221:ILE:HD12	1.98	0.46
1:B:295:VAL:HG23	1:B:306:ALA:O	2.15	0.46
1:H:14:THR:HG22	5:H:957:HOH:O	2.15	0.46
1:B:299:GLN:HA	5:B:728:HOH:O	2.16	0.46
1:C:178:TRP:CE2	1:C:478:LEU:HD12	2.52	0.46
1:H:206:ALA:HB2	1:H:221:ILE:HD12	1.98	0.46
1:A:178:TRP:CE2	1:A:478:LEU:HD12	2.51	0.45
1:D:206:ALA:HB2	1:D:221:ILE:HD12	1.98	0.45
1:G:303[A]:CYS:SG	5:G:828:HOH:O	2.57	0.45
1:H:126[B]:CYS:SG	1:H:177:ILE:CG1	3.04	0.45
1:E:24:PHE:CZ	1:E:27:ASN:HA	2.52	0.45
1:E:299:GLN:HA	5:E:824:HOH:O	2.16	0.45
1:G:178:TRP:CE2	1:G:478:LEU:HD12	2.52	0.45
1:G:206:ALA:HB2	1:G:221:ILE:HD12	1.97	0.44
1:A:179:LYS:NZ	1:A:245:THR:OG1	2.49	0.44
1:F:37:LYS:HD2	5:F:708:HOH:O	2.16	0.44
1:F:407:GLN:OE1	1:F:407:GLN:N	2.50	0.44
1:C:24:PHE:CZ	1:C:27:ASN:HA	2.53	0.44
1:H:24:PHE:CZ	1:H:27:ASN:HA	2.53	0.44
1:D:24:PHE:CZ	1:D:27:ASN:HA	2.53	0.44
1:C:57:LYS:HE3	5:C:847:HOH:O	2.19	0.43
1:E:206:ALA:HB2	1:E:221:ILE:HD12	1.99	0.43
1:B:206:ALA:HB2	1:B:221:ILE:HD12	1.99	0.43
1:G:24:PHE:CZ	1:G:27:ASN:HA	2.54	0.43
1:D:299:GLN:HA	5:D:892:HOH:O	2.18	0.43
1:E:173:LEU:HD13	1:E:201:THR:HB	2.01	0.42
1:F:173:LEU:HD13	1:F:201:THR:HB	2.02	0.42
1:H:179:LYS:NZ	1:H:245:THR:OG1	2.49	0.42
1:H:173:LEU:HD13	1:H:201:THR:HB	2.01	0.42
1:B:24:PHE:CZ	1:B:27:ASN:HA	2.55	0.42
1:C:179:LYS:NZ	1:C:245:THR:OG1	2.49	0.42
1:E:147:ILE:HG21	1:E:147:ILE:HD13	1.76	0.42
1:E:179:LYS:NZ	1:E:245:THR:OG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:GLU:HG3	1:H:256:GLU:HG3	2.03	0.41
1:D:450:GLY:HA3	1:D:467:GLY:O	2.21	0.41
1:E:256:GLU:HG3	1:F:256:GLU:HG3	2.02	0.41
1:F:24:PHE:CZ	1:F:27:ASN:HA	2.56	0.41
1:B:179:LYS:NZ	1:B:245:THR:OG1	2.50	0.41
1:B:71:PHE:CZ	1:B:161:GLY:HA2	2.56	0.41
1:D:173:LEU:HD13	1:D:201:THR:HB	2.03	0.41
1:D:178:TRP:CE2	1:D:478:LEU:CD1	3.04	0.41
1:B:14:THR:HG22	1:B:15:ASP:N	2.36	0.41
1:H:178:TRP:CE2	1:H:478:LEU:CD1	3.03	0.41
1:G:173:LEU:HD13	1:G:201:THR:HB	2.03	0.40
1:G:71:PHE:CZ	1:G:161:GLY:HA2	2.57	0.40
1:H:193:LYS:HE3	1:H:194:PRO:O	2.21	0.40
1:G:179:LYS:NZ	1:G:245:THR:OG1	2.50	0.40
1:E:178:TRP:CE2	1:E:478:LEU:CD1	3.05	0.40
1:F:110:ASN:HD21	1:F:198:THR:HA	1.87	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	494/501 (99%)	481 (97%)	12 (2%)	1 (0%)	47	39
1	B	494/501 (99%)	481 (97%)	12 (2%)	1 (0%)	47	39
1	C	493/501 (98%)	478 (97%)	14 (3%)	1 (0%)	47	39
1	D	494/501 (99%)	479 (97%)	14 (3%)	1 (0%)	47	39
1	E	494/501 (99%)	480 (97%)	13 (3%)	1 (0%)	47	39
1	F	493/501 (98%)	479 (97%)	13 (3%)	1 (0%)	47	39
1	G	494/501 (99%)	478 (97%)	15 (3%)	1 (0%)	47	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	493/501 (98%)	477 (97%)	15 (3%)	1 (0%)	47	39
All	All	3949/4008 (98%)	3833 (97%)	108 (3%)	8 (0%)	47	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	427	GLY
1	D	427	GLY
1	E	427	GLY
1	F	427	GLY
1	H	427	GLY
1	A	427	GLY
1	B	427	GLY
1	G	427	GLY

### 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	411/415 (99%)	406 (99%)	5 (1%)	71	70
1	B	411/415 (99%)	407 (99%)	4 (1%)	76	75
1	C	410/415 (99%)	404 (98%)	6 (2%)	65	63
1	D	411/415 (99%)	405 (98%)	6 (2%)	65	63
1	E	411/415 (99%)	404 (98%)	7 (2%)	60	57
1	F	410/415 (99%)	405 (99%)	5 (1%)	71	70
1	G	411/415 (99%)	405 (98%)	6 (2%)	65	63
1	H	410/415 (99%)	405 (99%)	5 (1%)	71	70
All	All	3285/3320 (99%)	3241 (99%)	44 (1%)	69	67

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	193	LYS
1	A	402	PHE
1	A	409	MET
1	A	464	CYS
1	B	193	LYS
1	B	402	PHE
1	B	409	MET
1	B	464	CYS
1	C	90[A]	TYR
1	C	90[B]	TYR
1	C	193	LYS
1	C	402	PHE
1	C	409	MET
1	C	464	CYS
1	D	91	LYS
1	D	173	LEU
1	D	193	LYS
1	D	402	PHE
1	D	409	MET
1	D	464	CYS
1	E	173	LEU
1	E	179	LYS
1	E	193	LYS
1	E	313	GLU
1	E	402	PHE
1	E	409	MET
1	E	464	CYS
1	F	173	LEU
1	F	193	LYS
1	F	402	PHE
1	F	409	MET
1	F	464	CYS
1	G	8	ASP
1	G	17	LYS
1	G	173	LEU
1	G	402	PHE
1	G	409	MET
1	G	464	CYS
1	H	173	LEU
1	H	193	LYS
1	H	402	PHE
1	H	409	MET

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Mol	Chain	Res	Type
1	H	464	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	B	299	GLN
1	D	298	HIS
1	D	299	GLN
1	G	383	GLN
1	H	383	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 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	6ZW	C	601	-	16,18,18	1.51	3 (18%)	21,25,25	1.24	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	6ZW	F	601	-	16,18,18	1.56	2 (12%)	21,25,25	1.35	3 (14%)
2	6ZW	G	601	-	16,18,18	1.55	2 (12%)	21,25,25	1.44	5 (23%)
2	6ZW	D	601	-	16,18,18	1.46	3 (18%)	21,25,25	1.55	4 (19%)
2	6ZW	H	601	-	16,18,18	1.73	4 (25%)	21,25,25	1.19	3 (14%)
2	6ZW	A	601	-	16,18,18	1.42	2 (12%)	21,25,25	1.32	4 (19%)
2	6ZW	E	601	-	16,18,18	1.66	2 (12%)	21,25,25	1.32	3 (14%)
2	6ZW	B	601	-	16,18,18	1.84	2 (12%)	21,25,25	1.76	6 (28%)

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	6ZW	C	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	F	601	-	-	4/8/8/8	0/2/2/2
2	6ZW	G	601	-	-	3/8/8/8	0/2/2/2
2	6ZW	D	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	H	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	A	601	-	-	1/8/8/8	0/2/2/2
2	6ZW	E	601	-	-	0/8/8/8	0/2/2/2
2	6ZW	B	601	-	-	4/8/8/8	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6ZW	C3-C2	5.84	1.49	1.41
2	F	601	6ZW	C3-C2	5.09	1.48	1.41
2	H	601	6ZW	C3-C2	4.74	1.47	1.41
2	E	601	6ZW	C3-C2	4.31	1.47	1.41
2	G	601	6ZW	C3-C2	4.26	1.47	1.41
2	C	601	6ZW	C3-C2	4.26	1.47	1.41
2	A	601	6ZW	C3-C2	3.84	1.46	1.41
2	E	601	6ZW	C10-C3	3.49	1.50	1.42
2	D	601	6ZW	C10-C3	3.39	1.49	1.42
2	G	601	6ZW	C10-C3	3.08	1.49	1.42
2	A	601	6ZW	C10-C3	2.94	1.48	1.42
2	H	601	6ZW	C10-C3	2.85	1.48	1.42
2	D	601	6ZW	C3-C2	2.78	1.45	1.41
2	B	601	6ZW	C10-C3	2.76	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	6ZW	C10-C3	2.53	1.48	1.42
2	C	601	6ZW	C4-C3	-2.50	1.37	1.42
2	F	601	6ZW	C10-C3	2.45	1.47	1.42
2	D	601	6ZW	C6-N11	2.21	1.44	1.38
2	H	601	6ZW	C9-C8	2.14	1.41	1.37
2	H	601	6ZW	C4-C3	-2.08	1.38	1.42

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	6ZW	O7-C2-C1	4.08	120.87	116.03
2	D	601	6ZW	O7-C2-C1	3.87	120.62	116.03
2	G	601	6ZW	O7-C2-C1	3.43	120.09	116.03
2	D	601	6ZW	O7-C2-C3	-3.36	117.96	121.20
2	E	601	6ZW	O7-C2-C1	3.30	119.94	116.03
2	B	601	6ZW	O7-C8-C9	3.20	123.35	119.27
2	C	601	6ZW	O7-C2-C1	2.96	119.54	116.03
2	F	601	6ZW	O7-C2-C1	2.91	119.48	116.03
2	F	601	6ZW	O7-C8-C9	2.87	122.93	119.27
2	C	601	6ZW	O7-C8-C9	2.82	122.87	119.27
2	A	601	6ZW	C1-C2-C3	-2.80	119.94	123.05
2	B	601	6ZW	C5-C6-N11	-2.75	117.58	121.38
2	B	601	6ZW	C1-C2-C3	-2.48	120.31	123.05
2	B	601	6ZW	O7-C2-C3	-2.47	118.82	121.20
2	H	601	6ZW	C1-C2-C3	-2.47	120.32	123.05
2	G	601	6ZW	O7-C8-C9	2.42	122.35	119.27
2	A	601	6ZW	O7-C8-C9	2.41	122.34	119.27
2	H	601	6ZW	O7-C8-C9	2.36	122.28	119.27
2	H	601	6ZW	O7-C2-C1	2.35	118.82	116.03
2	B	601	6ZW	C10-C3-C2	2.28	119.41	118.05
2	A	601	6ZW	O7-C2-C1	2.28	118.74	116.03
2	E	601	6ZW	O7-C8-C9	2.21	122.09	119.27
2	G	601	6ZW	C1-C2-C3	-2.17	120.65	123.05
2	E	601	6ZW	C1-C2-C3	-2.14	120.68	123.05
2	D	601	6ZW	C16-C10-C9	-2.07	117.72	120.74
2	A	601	6ZW	C1-C6-N11	-2.06	119.50	121.99
2	D	601	6ZW	C6-C1-C2	2.03	121.39	119.46
2	G	601	6ZW	C12-N11-C6	2.03	124.39	121.39
2	F	601	6ZW	C1-C6-N11	-2.02	119.54	121.99
2	G	601	6ZW	O7-C2-C3	-2.02	119.25	121.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	601	6ZW	C13-C12-N11-C6
2	B	601	6ZW	C5-C6-N11-C12
2	G	601	6ZW	C13-C12-N11-C14
2	B	601	6ZW	C1-C6-N11-C14
2	B	601	6ZW	C1-C6-N11-C12
2	B	601	6ZW	C5-C6-N11-C14
2	F	601	6ZW	C5-C6-N11-C12
2	F	601	6ZW	C1-C6-N11-C12
2	F	601	6ZW	C5-C6-N11-C14
2	F	601	6ZW	C1-C6-N11-C14
2	G	601	6ZW	C5-C6-N11-C14
2	A	601	6ZW	C15-C14-N11-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 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	494/501 (98%)	-0.32	2 (0%) 92 93	9, 17, 33, 51	0
1	B	494/501 (98%)	-0.40	4 (0%) 86 88	9, 18, 34, 60	0
1	C	493/501 (98%)	-0.39	2 (0%) 92 93	7, 15, 31, 52	0
1	D	493/501 (98%)	-0.50	5 (1%) 82 84	7, 15, 30, 62	0
1	E	493/501 (98%)	-0.40	0 100 100	9, 18, 31, 48	0
1	F	493/501 (98%)	-0.12	11 (2%) 62 66	9, 21, 46, 63	0
1	G	494/501 (98%)	-0.39	5 (1%) 82 84	9, 16, 31, 63	0
1	H	493/501 (98%)	-0.34	1 (0%) 95 95	10, 18, 31, 44	0
All	All	3947/4008 (98%)	-0.36	30 (0%) 86 88	7, 17, 35, 63	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	LEU	5.0
1	C	14	THR	4.1
1	G	13	LEU	3.7
1	B	13	LEU	3.6
1	D	338	PRO	3.4
1	G	8	ASP	2.8
1	F	13	LEU	2.8
1	G	9	LEU	2.8
1	F	363	LYS	2.6
1	B	8	ASP	2.5
1	F	376	GLY	2.5
1	D	15	ASP	2.4
1	F	393	GLU	2.4
1	F	412	LYS	2.4
1	F	366	ALA	2.4
1	H	375	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	321	ARG	2.4
1	C	13	LEU	2.3
1	B	14	THR	2.3
1	G	14	THR	2.3
1	F	380	TYR	2.2
1	A	17	LYS	2.2
1	G	15	ASP	2.2
1	F	328	LYS	2.2
1	B	15	ASP	2.2
1	D	14	THR	2.1
1	A	14	THR	2.1
1	D	9	LEU	2.1
1	F	359	GLU	2.0
1	F	355	LEU	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, 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(Å <sup>2</sup> )	Q<0.9
2	6ZW	E	601	17/17	0.89	0.14	26,32,40,45	0
2	6ZW	B	601	17/17	0.90	0.15	23,26,43,44	0
2	6ZW	C	601	17/17	0.90	0.13	20,23,29,31	0
2	6ZW	D	601	17/17	0.92	0.12	17,19,34,37	0
2	6ZW	A	601	17/17	0.93	0.12	22,26,36,37	0
2	6ZW	F	601	17/17	0.93	0.12	25,27,36,36	0
2	6ZW	H	601	17/17	0.93	0.17	24,30,43,44	0
2	6ZW	G	601	17/17	0.94	0.13	21,23,33,34	0
3	YB	E	603	1/1	0.98	0.04	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	YB	F	602	1/1	0.99	0.06	49,49,49,49	0
4	CL	G	603	1/1	0.99	0.13	16,16,16,16	0
3	YB	B	602	1/1	0.99	0.03	27,27,27,27	0
4	CL	D	603	1/1	0.99	0.09	16,16,16,16	0
4	CL	C	602	1/1	0.99	0.08	17,17,17,17	0
3	YB	H	602	1/1	0.99	0.03	25,25,25,25	0
3	YB	E	602	1/1	0.99	0.02	32,32,32,32	0
4	CL	B	603	1/1	0.99	0.13	18,18,18,18	0
4	CL	F	603	1/1	0.99	0.16	19,19,19,19	0
4	CL	A	603	1/1	0.99	0.14	18,18,18,18	0
3	YB	D	602	1/1	0.99	0.02	35,35,35,35	0
3	YB	A	602	1/1	0.99	0.02	29,29,29,29	0
4	CL	E	604	1/1	1.00	0.12	17,17,17,17	0
4	CL	H	603	1/1	1.00	0.14	16,16,16,16	0
3	YB	G	602	1/1	1.00	0.03	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.