



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2020 – 08:10 PM BST

PDB ID : 3V5V  
Title : UNLIGANDED E.CLOACAE C115D MURA  
Authors : Zhu, J.-Y.; Yang, Y.; Schonbrunn, E.  
Deposited on : 2011-12-16  
Resolution : 2.70 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.

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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 : 2.13.1  
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

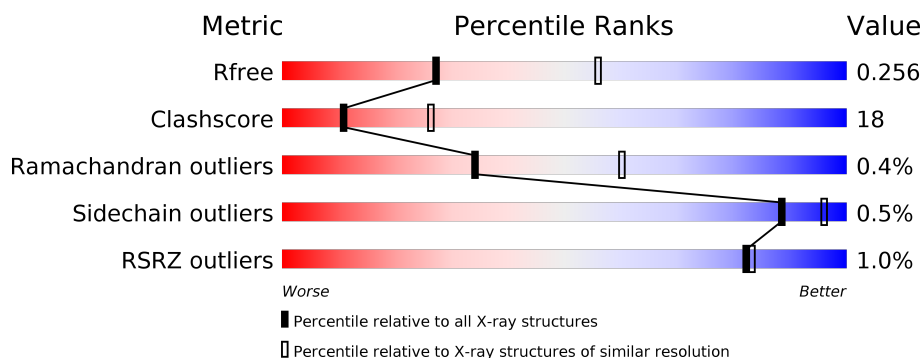
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	419	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>33%</div> </div> </div>
1	B	419	<div> <div>72%</div> <div>27%</div> </div>
1	C	419	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>24%</div> </div> </div>
1	D	419	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>28%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	A	501	-	-	X	-
2	PEG	C	501	-	-	X	-
3	EDO	A	509	-	-	X	-
3	EDO	B	507	-	-	X	-
3	EDO	B	508	-	-	X	-
3	EDO	D	507	-	-	X	-
3	EDO	D	509	-	-	-	X
4	ACT	C	510	-	-	X	-
5	PGE	B	501	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13230 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	B	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	C	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			
1	D	419	Total	C	N	O	S	0	0	0
			3144	1977	554	600	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	SEE REMARK 999	UNP P33038
A	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
B	67	IAS	ASN	SEE REMARK 999	UNP P33038
B	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
C	67	IAS	ASN	SEE REMARK 999	UNP P33038
C	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038
D	67	IAS	ASN	SEE REMARK 999	UNP P33038
D	115	ASP	CYS	ENGINEERED MUTATION	UNP P33038

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	D	1	Total	C	O	0	0
			7	4	3		

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



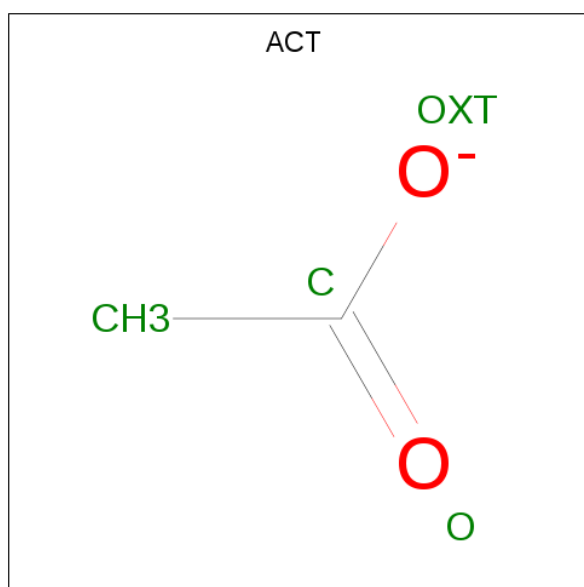
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0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

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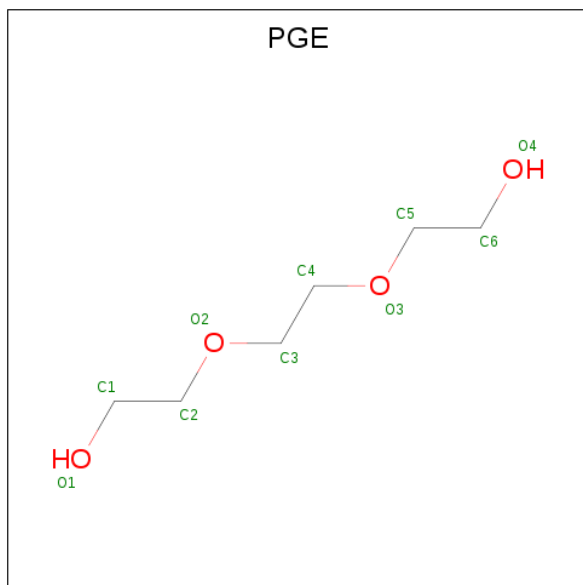
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is water.

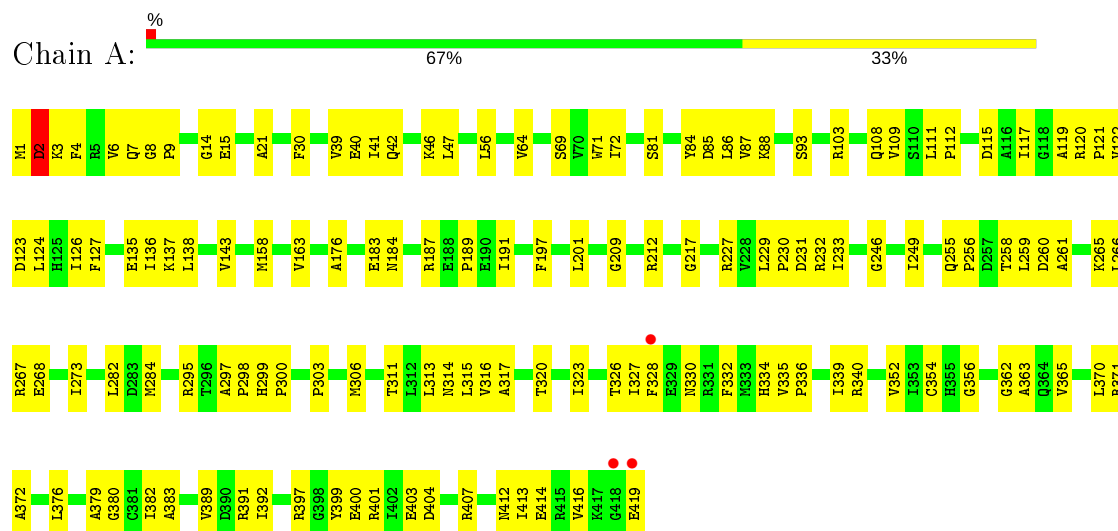
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	122	Total	O	0	0
			122	122		
6	B	131	Total	O	0	0
			131	131		
6	C	111	Total	O	0	0
			111	111		
6	D	112	Total	O	0	0
			112	112		



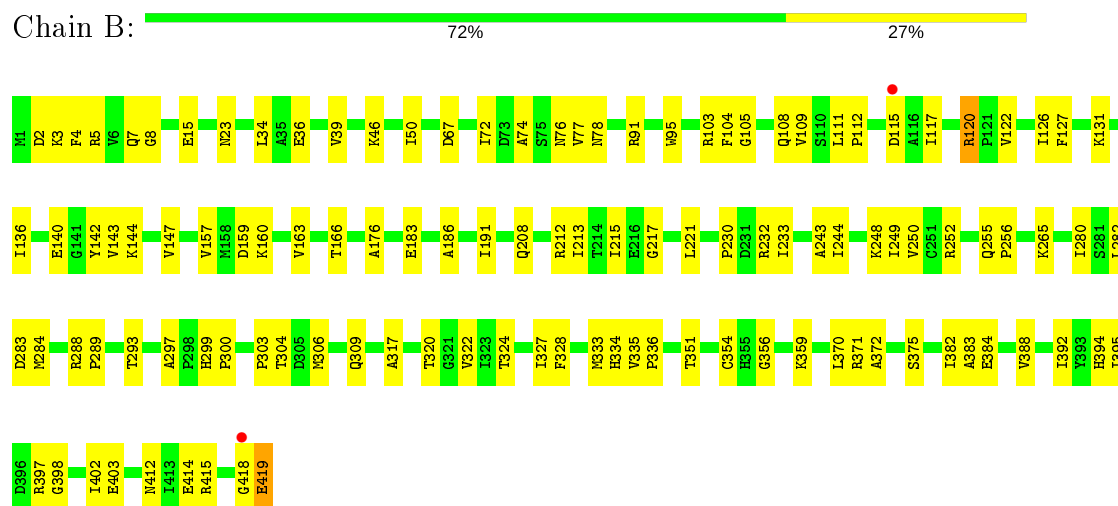
### 3 Residue-property plots

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.

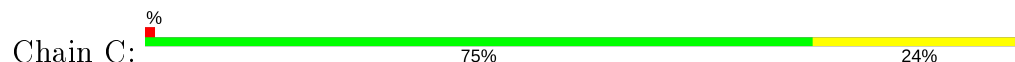
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

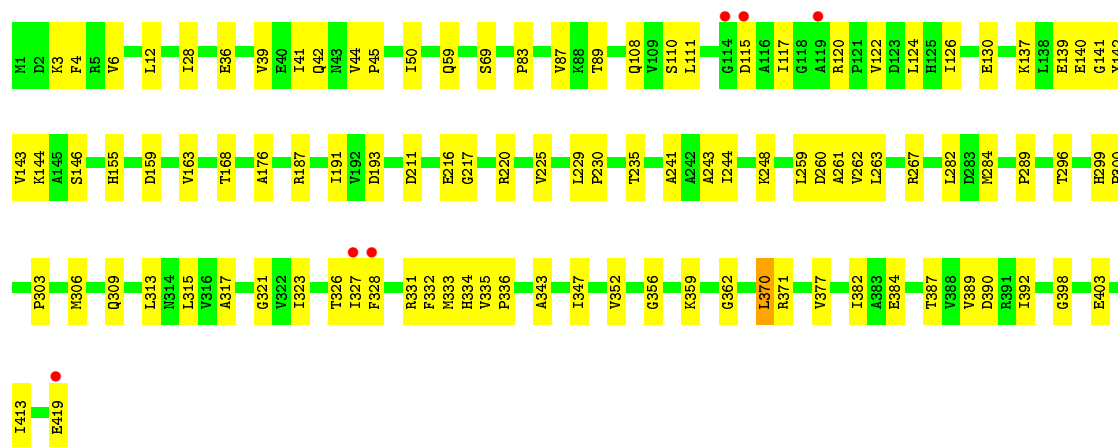


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

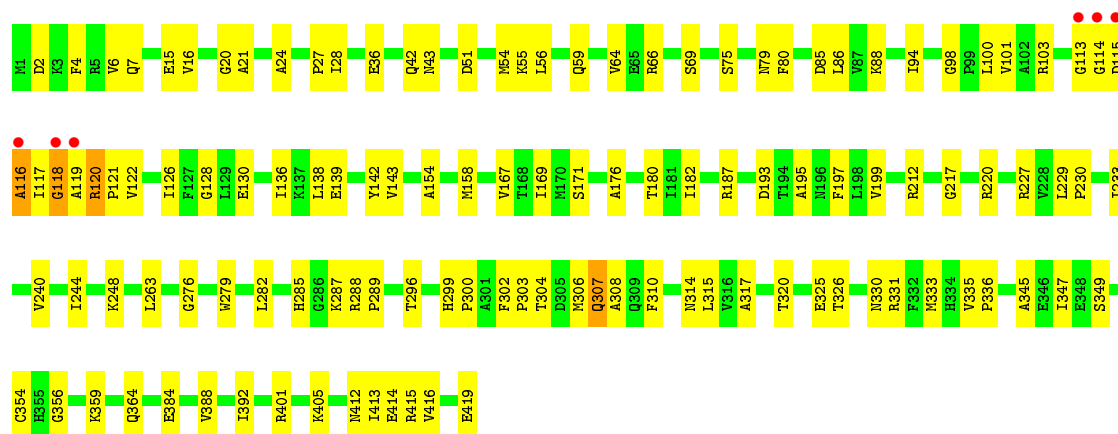


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.14Å 101.69Å 213.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.70 19.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (19.89-2.70) 99.5 (19.89-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.18 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.191 , 0.264 0.182 , 0.256	Depositor DCC
$R_{free}$ test set	1223 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE, EDO, IAS, ACT

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	0.43	0/3180	0.89	0/4308
1	B	0.44	0/3180	0.90	0/4308
1	C	0.44	0/3180	0.90	0/4308
1	D	0.48	0/3180	0.91	2/4308 (0.0%)
All	All	0.45	0/12720	0.90	2/17232 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	GLY	N-CA-C	-6.39	97.11	113.10
1	D	419	GLU	N-CA-C	5.59	126.10	111.00

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	3144	0	3215	140	0
1	B	3144	0	3215	125	0
1	C	3144	0	3215	122	0
1	D	3144	0	3215	104	0
2	A	14	0	19	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	7	0	10	12	0
2	D	7	0	9	0	0
3	A	32	0	48	8	0
3	B	28	0	42	15	0
3	C	32	0	48	5	0
3	D	40	0	60	15	0
4	A	4	0	3	0	0
4	C	4	0	3	4	0
5	B	10	0	14	10	0
6	A	122	0	0	5	0
6	B	131	0	0	4	0
6	C	111	0	0	4	0
6	D	112	0	0	1	0
All	All	13230	0	13116	470	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 18.

The worst 5 of 470 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:C:327:ILE:HG22	1:C:328:PHE:CD1	1.65	1.30
1:C:193:ASP:HB2	1:C:229:LEU:HD23	1.24	1.16
1:B:163:VAL:HG11	5:B:501:PGE:H62	1.10	1.10
1:A:230:PRO:HB2	3:A:509:EDO:H11	1.37	1.06
1:B:230:PRO:HB2	3:B:508:EDO:H12	1.39	1.01

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	A	415/419 (99%)	383 (92%)	30 (7%)	2 (0%)	29	54
1	B	415/419 (99%)	400 (96%)	14 (3%)	1 (0%)	47	73
1	C	415/419 (99%)	392 (94%)	22 (5%)	1 (0%)	47	73
1	D	415/419 (99%)	391 (94%)	22 (5%)	2 (0%)	29	54
All	All	1660/1676 (99%)	1566 (94%)	88 (5%)	6 (0%)	34	60

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	ASP
1	C	333	MET
1	D	120	ARG
1	A	2	ASP
1	A	115	ASP

### 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	329/329 (100%)	328 (100%)	1 (0%)	92	98
1	B	329/329 (100%)	326 (99%)	3 (1%)	78	92
1	C	329/329 (100%)	327 (99%)	2 (1%)	86	95
1	D	329/329 (100%)	328 (100%)	1 (0%)	92	98
All	All	1316/1316 (100%)	1309 (100%)	7 (0%)	88	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	419	GLU
1	D	307	GLN
1	C	115	ASP
1	B	78	ASN
1	C	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	GLN
1	C	42	GLN
1	D	59	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	IAS	A	67	1	4,7,8	0.81	0	2,8,10	1.13	0
1	IAS	D	67	1	4,7,8	0.59	0	2,8,10	1.16	0
1	IAS	B	67	1	4,7,8	0.68	0	2,8,10	1.19	0
1	IAS	C	67	1	4,7,8	0.75	0	2,8,10	1.17	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
1	IAS	A	67	1	-	0/3/7/8	-
1	IAS	D	67	1	-	0/3/7/8	-
1	IAS	B	67	1	-	0/3/7/8	-
1	IAS	C	67	1	-	0/3/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	67	IAS	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

40 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	$\# Z  > 2$
4	ACT	C	510	-	1,3,3	1.52	0	0,3,3	0.00	-
3	EDO	B	506	-	3,3,3	0.63	0	2,2,2	0.26	0
3	EDO	C	508	-	3,3,3	0.60	0	2,2,2	0.27	0
2	PEG	C	501	-	6,6,6	0.35	0	5,5,5	0.87	0
3	EDO	C	505	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	B	507	-	3,3,3	0.49	0	2,2,2	0.38	0
3	EDO	C	504	-	3,3,3	0.51	0	2,2,2	0.30	0
3	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	D	510	-	3,3,3	0.60	0	2,2,2	0.27	0
3	EDO	B	508	-	3,3,3	0.52	0	2,2,2	0.25	0
4	ACT	A	511	-	1,3,3	1.37	0	0,3,3	0.00	-
3	EDO	A	510	-	3,3,3	0.65	0	2,2,2	0.19	0
3	EDO	A	506	-	3,3,3	0.32	0	2,2,2	0.26	0
3	EDO	C	509	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	D	502	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	D	509	-	3,3,3	0.50	0	2,2,2	0.25	0
3	EDO	D	503	-	3,3,3	0.51	0	2,2,2	0.29	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	D	511	-	3,3,3	0.55	0	2,2,2	0.21	0
3	EDO	A	504	-	3,3,3	0.55	0	2,2,2	0.30	0
3	EDO	B	505	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	D	505	-	3,3,3	0.52	0	2,2,2	0.31	0
3	EDO	D	508	-	3,3,3	0.55	0	2,2,2	0.24	0
3	EDO	A	508	-	3,3,3	0.54	0	2,2,2	0.28	0
3	EDO	C	502	-	3,3,3	0.35	0	2,2,2	0.40	0
3	EDO	D	507	-	3,3,3	0.53	0	2,2,2	0.30	0
3	EDO	B	503	-	3,3,3	0.54	0	2,2,2	0.27	0
3	EDO	A	505	-	3,3,3	0.29	0	2,2,2	0.38	0
2	PEG	A	501	-	6,6,6	0.28	0	5,5,5	1.35	1 (20%)
3	EDO	D	504	-	3,3,3	0.68	0	2,2,2	0.14	0
2	PEG	D	501	-	6,6,6	1.59	1 (16%)	5,5,5	0.21	0
3	EDO	A	509	-	3,3,3	0.49	0	2,2,2	0.26	0
2	PEG	A	502	-	6,6,6	1.56	1 (16%)	5,5,5	0.23	0
3	EDO	A	507	-	3,3,3	0.49	0	2,2,2	0.31	0
3	EDO	B	502	-	3,3,3	0.55	0	2,2,2	0.28	0
3	EDO	D	506	-	3,3,3	0.51	0	2,2,2	0.28	0
3	EDO	C	506	-	3,3,3	0.29	0	2,2,2	0.24	0
3	EDO	B	504	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	C	503	-	3,3,3	0.54	0	2,2,2	0.26	0
5	PGE	B	501	-	9,9,9	0.44	0	8,8,8	0.29	0
3	EDO	C	507	-	3,3,3	0.52	0	2,2,2	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	506	-	-	1/1/1/1	-
3	EDO	C	508	-	-	0/1/1/1	-
2	PEG	C	501	-	-	3/4/4/4	-
3	EDO	C	505	-	-	1/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	D	510	-	-	1/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	A	506	-	-	1/1/1/1	-
3	EDO	C	509	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	502	-	-	1/1/1/1	-
3	EDO	D	509	-	-	1/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	D	511	-	-	1/1/1/1	-
3	EDO	A	504	-	-	1/1/1/1	-
3	EDO	B	505	-	-	1/1/1/1	-
3	EDO	D	505	-	-	0/1/1/1	-
3	EDO	D	508	-	-	1/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	C	502	-	-	1/1/1/1	-
3	EDO	D	507	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	A	505	-	-	1/1/1/1	-
2	PEG	A	501	-	-	2/4/4/4	-
3	EDO	D	504	-	-	1/1/1/1	-
2	PEG	D	501	-	-	2/4/4/4	-
2	PEG	A	502	-	-	3/4/4/4	-
3	EDO	A	507	-	-	1/1/1/1	-
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	D	506	-	-	1/1/1/1	-
3	EDO	C	506	-	-	1/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	C	503	-	-	0/1/1/1	-
5	PGE	B	501	-	-	6/7/7/7	-
3	EDO	C	507	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	PEG	O1-C1	-3.63	1.23	1.42
2	A	502	PEG	O1-C1	-3.48	1.24	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	PEG	C3-O2-C2	2.33	123.36	113.29

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	501	PGE	C4-C3-O2-C2
2	A	501	PEG	O2-C3-C4-O4
2	A	502	PEG	O2-C3-C4-O4
5	B	501	PGE	O1-C1-C2-O2
2	D	501	PEG	O1-C1-C2-O2

There are no ring outliers.

23 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	510	ACT	4	0
2	C	501	PEG	12	0
3	B	507	EDO	9	0
3	A	503	EDO	2	0
3	B	508	EDO	4	0
3	A	510	EDO	1	0
3	D	502	EDO	1	0
3	D	509	EDO	1	0
3	D	503	EDO	2	0
3	D	511	EDO	1	0
3	D	505	EDO	2	0
3	D	508	EDO	3	0
3	C	502	EDO	2	0
3	D	507	EDO	4	0
3	B	503	EDO	2	0
2	A	501	PEG	12	0
3	D	504	EDO	1	0
3	A	509	EDO	4	0
3	A	507	EDO	1	0
3	C	506	EDO	1	0
3	C	503	EDO	1	0
5	B	501	PGE	10	0
3	C	507	EDO	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	67:IAS	C	68:GLY	N	4.51
1	A	67:IAS	C	68:GLY	N	4.42
1	D	67:IAS	C	68:GLY	N	4.42
1	C	67:IAS	C	68:GLY	N	4.35

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	418/419 (99%)	-0.51	3 (0%) 87 89	6, 21, 44, 80	0
1	B	418/419 (99%)	-0.59	2 (0%) 91 92	6, 19, 38, 65	0
1	C	418/419 (99%)	-0.48	6 (1%) 75 77	6, 21, 49, 70	0
1	D	418/419 (99%)	-0.51	6 (1%) 75 77	5, 21, 42, 82	0
All	All	1672/1676 (99%)	-0.52	17 (1%) 82 83	5, 20, 43, 82	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	ASP	4.9
1	D	116	ALA	4.7
1	A	419	GLU	4.2
1	D	115	ASP	4.0
1	A	418	GLY	3.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
1	IAS	C	67	8/9	0.94	0.16	22,24,25,25	0
1	IAS	B	67	8/9	0.95	0.16	34,34,35,36	0
1	IAS	A	67	8/9	0.95	0.11	16,17,18,18	0
1	IAS	D	67	8/9	0.96	0.18	24,26,27,27	0

## 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(Å <sup>2</sup> )	Q<0.9
3	EDO	D	509	4/4	0.73	0.41	57,58,58,59	0
3	EDO	A	510	4/4	0.79	0.31	35,36,36,37	0
3	EDO	B	503	4/4	0.80	0.20	43,43,43,43	0
3	EDO	A	505	4/4	0.81	0.29	42,45,46,47	0
2	PEG	D	501	7/7	0.82	0.36	57,59,60,60	0
2	PEG	A	502	7/7	0.82	0.38	49,53,54,55	0
5	PGE	B	501	10/10	0.82	0.33	37,45,47,48	0
3	EDO	A	504	4/4	0.83	0.41	47,48,48,49	0
3	EDO	C	502	4/4	0.84	0.26	42,45,47,48	0
3	EDO	A	508	4/4	0.84	0.31	46,46,47,48	0
3	EDO	B	506	4/4	0.84	0.33	30,31,31,34	0
3	EDO	C	506	4/4	0.85	0.22	38,41,41,43	0
3	EDO	C	508	4/4	0.85	0.28	33,36,36,36	0
2	PEG	A	501	7/7	0.86	0.28	43,47,48,48	0
3	EDO	D	504	4/4	0.86	0.37	31,32,34,34	0
4	ACT	A	511	4/4	0.86	0.33	71,71,71,72	0
3	EDO	D	510	4/4	0.87	0.19	39,40,41,42	0
3	EDO	B	502	4/4	0.87	0.34	42,43,43,43	0
3	EDO	A	506	4/4	0.88	0.27	57,58,58,59	0
2	PEG	C	501	7/7	0.88	0.31	71,75,76,76	0
3	EDO	C	503	4/4	0.90	0.26	46,46,47,48	0
3	EDO	B	507	4/4	0.91	0.28	32,36,36,37	0
3	EDO	D	508	4/4	0.91	0.30	50,50,51,51	0
3	EDO	C	507	4/4	0.91	0.21	34,36,37,37	0
3	EDO	D	503	4/4	0.92	0.43	46,48,49,49	0
3	EDO	C	509	4/4	0.92	0.28	35,37,37,38	0
3	EDO	B	505	4/4	0.92	0.22	41,41,41,41	0
3	EDO	D	507	4/4	0.92	0.24	43,44,44,44	0
3	EDO	D	505	4/4	0.92	0.23	35,36,37,38	0
3	EDO	A	503	4/4	0.93	0.22	37,37,37,37	0
3	EDO	C	505	4/4	0.93	0.15	40,41,41,41	0
3	EDO	A	509	4/4	0.93	0.23	51,52,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	D	511	4/4	0.94	0.25	47,47,48,49	0
3	EDO	D	502	4/4	0.94	0.21	40,41,42,44	0
4	ACT	C	510	4/4	0.94	0.17	40,41,42,43	0
3	EDO	C	504	4/4	0.94	0.27	34,34,35,35	0
3	EDO	D	506	4/4	0.95	0.33	33,35,36,36	0
3	EDO	A	507	4/4	0.96	0.14	25,28,28,30	0
3	EDO	B	504	4/4	0.97	0.31	25,26,27,27	0
3	EDO	B	508	4/4	0.97	0.13	32,34,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.