



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 06:53 PM JST

PDB ID : 7D5V  
Title : Structure of the C646A mutant of peptidylarginine deiminase type III (PAD3)  
Authors : Akimoto, M.; Mashimo, R.; Unno, M.  
Deposited on : 2020-09-28  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

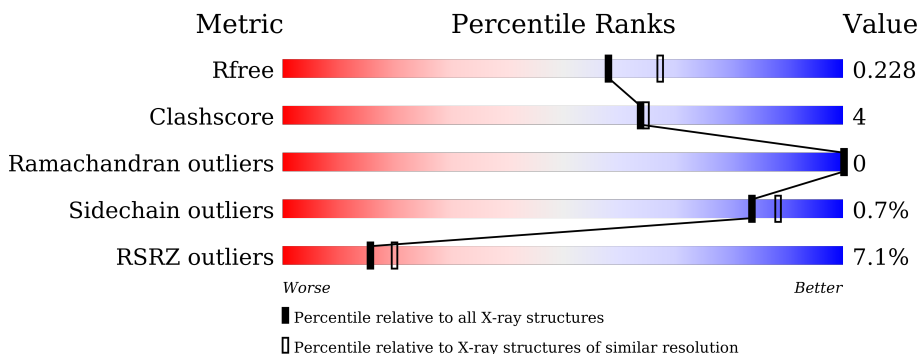
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of 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	664	
1	B	664	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10302 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.

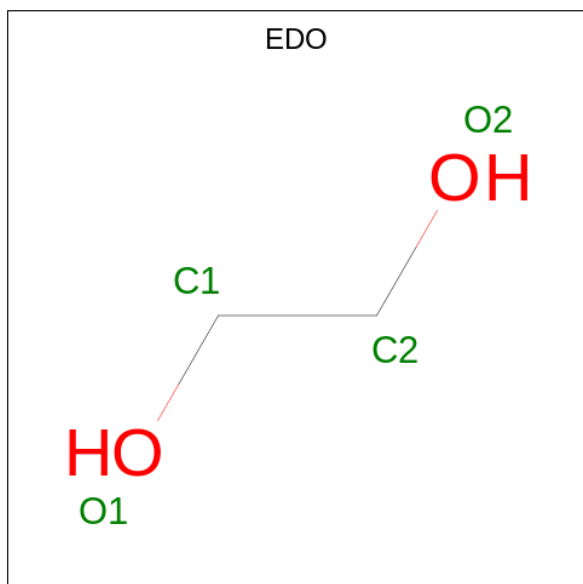
- Molecule 1 is a protein called Protein-arginine deiminase type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	620	4837	3093	823	891	30	0	7	0
1	B	620	4830	3092	818	890	30	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	646	ALA	CYS	engineered mutation	UNP Q9ULW8
B	646	ALA	CYS	engineered mutation	UNP Q9ULW8

- Molecule 2 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
			Total	C	O		
2	A	1	4	2	2	0	0

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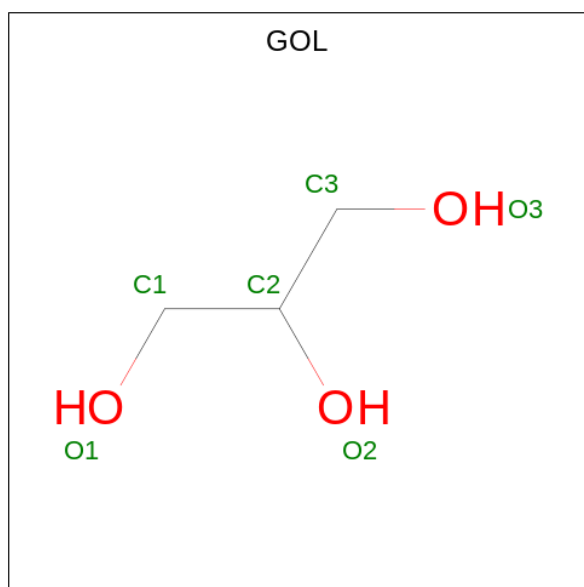
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total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

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

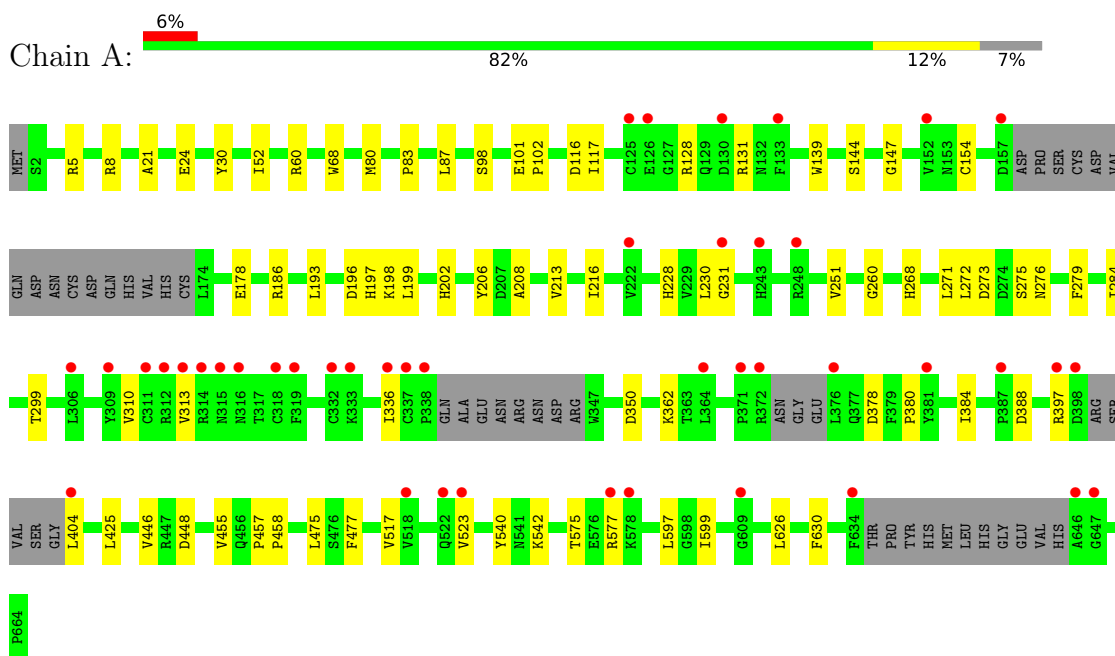
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total 246	O 246	0	0
4	B	241	Total 241	O 241	0	0

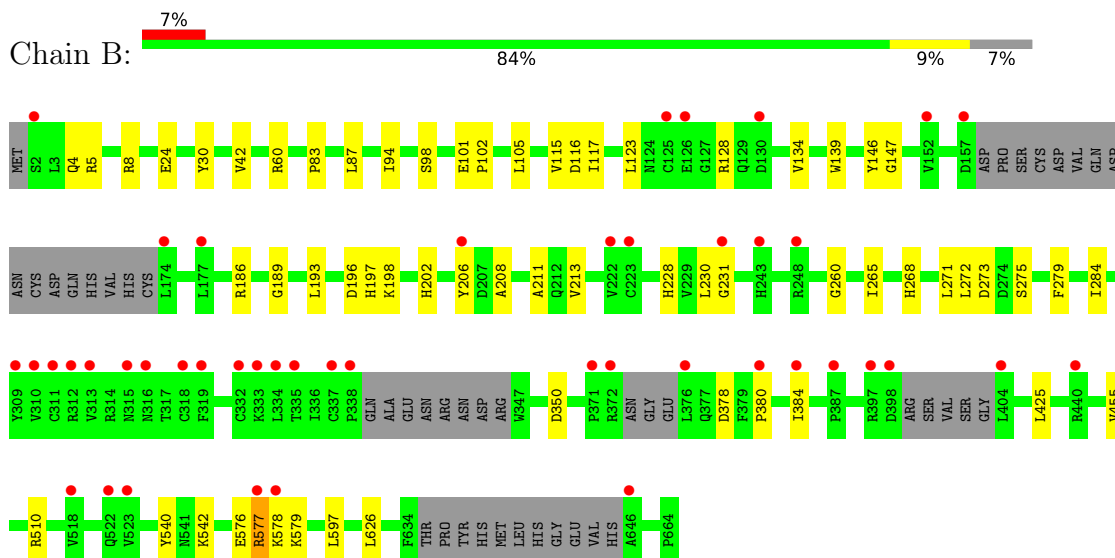
### 3 Residue-property plots

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: Protein-arginine deiminase type-3



- Molecule 1: Protein-arginine deiminase type-3



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.48Å 115.48Å 330.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.52 – 2.10 29.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.52-2.10) 99.8 (29.52-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.60 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.212 , 0.228 0.212 , 0.228	Depositor DCC
$R_{free}$ test set	4810 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.473	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.488 for -h-k,k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: EDO, GOL

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	0.25	0/4974	0.45	0/6765
1	B	0.25	0/4970	0.45	0/6759
All	All	0.25	0/9944	0.45	0/13524

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	576	GLU	Peptide

### 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	4837	0	4711	48	0
1	B	4830	0	4702	38	0
2	A	56	0	84	4	0
2	B	44	0	66	3	0
3	A	24	0	32	2	0
3	B	24	0	32	0	0
4	A	246	0	0	1	0
4	B	241	0	0	1	0
All	All	10302	0	9627	82	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.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:H	2:A:704:EDO:H11	1.48	0.78
1:A:102:PRO:HA	2:A:711:EDO:H11	1.66	0.78
1:B:102:PRO:HA	2:B:709:EDO:H22	1.73	0.71
1:A:128:ARG:HB3	1:A:144:SER:HA	1.73	0.70
1:A:213:VAL:HB	1:A:230:LEU:HB2	1.78	0.65
1:A:196[A]:ASP:HB3	1:A:275:SER:HB3	1.86	0.58
1:A:178:GLU:OE1	1:A:362:LYS:NZ	2.38	0.56
1:A:196[B]:ASP:HB2	1:A:275:SER:HB3	1.87	0.56
1:B:213:VAL:HB	1:B:230:LEU:HB2	1.87	0.56
1:B:577:ARG:HH21	1:B:577:ARG:H	1.55	0.55
1:A:388:ASP:HA	3:A:716:GOL:H31	1.89	0.54
1:B:196[B]:ASP:OD1	1:B:197:HIS:ND1	2.37	0.53
1:A:196[B]:ASP:OD1	1:A:197:HIS:ND1	2.40	0.53
1:B:577:ARG:H	1:B:577:ARG:NH2	2.05	0.53
1:B:206:TYR:OH	1:B:260:GLY:O	2.27	0.52
1:A:117:ILE:HA	1:A:186:ARG:O	2.10	0.52
1:A:213:VAL:HG22	1:A:251:VAL:HG22	1.92	0.51
1:B:42:VAL:HG12	1:B:94:ILE:HG12	1.93	0.51
1:B:24:GLU:OE2	1:B:60:ARG:NH1	2.44	0.51
1:A:83:PRO:HG3	1:A:116:ASP:HB2	1.92	0.51
1:A:597:LEU:HD11	1:A:626:LEU:HD13	1.92	0.51
1:B:273:ASP:HB2	1:B:284[A]:ILE:HD11	1.93	0.51
1:B:597:LEU:HD11	1:B:626:LEU:HD13	1.93	0.51
1:B:228:HIS:CE1	1:B:231:GLY:HA3	2.46	0.50
1:B:83:PRO:HG3	1:B:116:ASP:HB2	1.92	0.50
1:B:380:PRO:HG2	1:B:384:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:OE2	1:A:60:ARG:NH1	2.44	0.49
1:B:123:LEU:HD13	1:B:134:VAL:HG11	1.95	0.49
1:A:206:TYR:OH	1:A:260:GLY:O	2.25	0.49
1:A:380:PRO:HG2	1:A:384:ILE:HD13	1.95	0.48
1:B:134:VAL:HG13	1:B:146:TYR:CE1	2.48	0.48
1:A:228:HIS:CE1	1:A:231:GLY:HA3	2.49	0.48
1:A:404:LEU:HD23	1:A:446:VAL:HG21	1.95	0.48
1:A:208:ALA:HB1	1:A:231:GLY:O	2.14	0.48
1:A:276:ASN:HB3	1:A:279:PHE:CD2	2.49	0.48
1:B:8:ARG:HB2	1:B:30:TYR:CZ	2.49	0.48
1:A:397:ARG:NH2	1:A:448:ASP:OD2	2.47	0.47
1:B:208:ALA:HB1	1:B:231:GLY:O	2.14	0.47
1:A:273:ASP:HB2	1:A:284[A]:ILE:HD11	1.96	0.47
1:B:5:ARG:CZ	1:B:284[A]:ILE:HG23	2.44	0.47
1:B:378:ASP:N	1:B:378:ASP:OD1	2.48	0.47
1:B:211:ALA:HB2	1:B:265:ILE:HD13	1.97	0.47
1:A:378:ASP:N	1:A:378:ASP:OD1	2.48	0.47
1:A:139:TRP:CD1	1:A:147:GLY:HA3	2.50	0.46
1:A:5:ARG:CZ	1:A:284[A]:ILE:HG23	2.46	0.46
1:A:8:ARG:HB2	1:A:30:TYR:CZ	2.50	0.46
1:A:542:LYS:HB3	1:B:30:TYR:CZ	2.52	0.45
1:B:87:LEU:HD21	1:B:193:LEU:HB2	1.96	0.45
1:A:117:ILE:HD12	1:A:271:LEU:HD22	1.97	0.45
1:A:517:VAL:HG11	1:A:523:VAL:HG11	1.98	0.45
1:B:117:ILE:HD12	1:B:271:LEU:HD22	1.98	0.44
1:A:98:SER:O	2:A:711:EDO:H22	2.17	0.44
1:A:30:TYR:CZ	1:B:542:LYS:HB3	2.52	0.44
1:A:154:CYS:HB3	3:A:717:GOL:H32	1.98	0.44
1:A:457:PRO:HA	1:A:458:PRO:HD3	1.79	0.44
1:A:279:PHE:CE1	1:B:540:TYR:HD1	2.36	0.43
1:A:475:LEU:HD21	1:A:477:PHE:CE2	2.53	0.43
1:B:578:LYS:O	1:B:579:LYS:HD3	2.18	0.43
1:A:101:GLU:HB2	4:A:942:HOH:O	2.18	0.43
1:B:139:TRP:CD1	1:B:147:GLY:HA3	2.54	0.43
1:B:101:GLU:O	2:B:709:EDO:O1	2.24	0.43
1:B:425:LEU:HD12	1:B:455:VAL:HB	2.01	0.43
1:B:115:VAL:HG12	1:B:189:GLY:HA3	2.01	0.43
1:B:202:HIS:CE1	1:B:268:HIS:HB2	2.54	0.43
1:A:202:HIS:CE1	1:A:268:HIS:HB2	2.54	0.43
1:B:198:LYS:HE3	1:B:272:LEU:HD12	2.01	0.42
1:A:117:ILE:HD13	1:A:199:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196[A]:ASP:HB3	1:B:275:SER:HB3	2.00	0.42
1:A:21:ALA:HA	1:A:80:MET:O	2.20	0.42
1:A:52:ILE:HD11	1:A:68:TRP:CH2	2.54	0.42
1:B:98:SER:HB3	1:B:105:LEU:HD11	2.01	0.41
1:B:117:ILE:HA	1:B:186:ARG:O	2.19	0.41
1:A:599:ILE:O	1:A:630:PHE:HA	2.21	0.41
1:B:510:ARG:HG2	2:B:701:EDO:H22	2.03	0.41
1:A:310:VAL:O	1:A:336:ILE:HA	2.21	0.40
1:A:575:THR:HG22	2:A:710:EDO:O1	2.21	0.40
1:A:87:LEU:HD21	1:A:193:LEU:HB2	2.02	0.40
1:A:198:LYS:HE3	1:A:272:LEU:HD12	2.04	0.40
1:B:4:GLN:OE1	4:B:801:HOH:O	2.22	0.40
1:A:425:LEU:HD12	1:A:455:VAL:HB	2.03	0.40
1:A:540:TYR:HD1	1:B:279:PHE:CE1	2.40	0.40

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	615/664 (93%)	601 (98%)	14 (2%)	0	100	100
1	B	616/664 (93%)	599 (97%)	17 (3%)	0	100	100
All	All	1231/1328 (93%)	1200 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	529/587 (90%)	525 (99%)	4 (1%)	81	86
1	B	527/587 (90%)	524 (99%)	3 (1%)	86	90
All	All	1056/1174 (90%)	1049 (99%)	7 (1%)	84	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	ARG
1	A	313	VAL
1	A	350	ASP
1	A	577	ARG
1	B	128	ARG
1	B	350	ASP
1	B	577	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

33 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
3	GOL	A	716	-	5,5,5	0.90	0	5,5,5	0.99	0
2	EDO	B	701	-	3,3,3	0.44	0	2,2,2	0.35	0
2	EDO	B	708	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	706	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	A	712	-	3,3,3	0.46	0	2,2,2	0.32	0
3	GOL	B	714	-	5,5,5	0.90	0	5,5,5	0.97	0
2	EDO	B	711	-	3,3,3	0.46	0	2,2,2	0.32	0
3	GOL	A	715	-	5,5,5	0.87	0	5,5,5	1.04	0
3	GOL	B	713	-	5,5,5	0.91	0	5,5,5	1.02	0
3	GOL	A	718	-	5,5,5	0.91	0	5,5,5	0.97	0
2	EDO	A	701	-	3,3,3	0.44	0	2,2,2	0.39	0
2	EDO	A	708	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	A	711	-	3,3,3	0.45	0	2,2,2	0.24	0
2	EDO	A	706	-	3,3,3	0.45	0	2,2,2	0.36	0
2	EDO	B	704	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	B	707	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	B	710	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	A	714	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	A	704	-	3,3,3	0.45	0	2,2,2	0.32	0
3	GOL	A	717	-	5,5,5	0.90	0	5,5,5	1.00	0
2	EDO	A	702	-	3,3,3	0.47	0	2,2,2	0.32	0
3	GOL	B	712	-	5,5,5	0.87	0	5,5,5	1.04	0
2	EDO	A	713	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	709	-	3,3,3	0.46	0	2,2,2	0.25	0
2	EDO	A	709	-	3,3,3	0.46	0	2,2,2	0.30	0
2	EDO	A	707	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	B	703	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	A	703	-	3,3,3	0.46	0	2,2,2	0.33	0
3	GOL	B	715	-	5,5,5	0.89	0	5,5,5	1.01	0
2	EDO	A	710	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	B	705	-	3,3,3	0.45	0	2,2,2	0.35	0
2	EDO	A	705	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	702	-	3,3,3	0.47	0	2,2,2	0.30	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	716	-	-	2/4/4/4	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	B	708	-	-	0/1/1/1	-
2	EDO	B	706	-	-	0/1/1/1	-
2	EDO	A	712	-	-	0/1/1/1	-
3	GOL	B	714	-	-	3/4/4/4	-
2	EDO	B	711	-	-	0/1/1/1	-
3	GOL	A	715	-	-	0/4/4/4	-
3	GOL	B	713	-	-	0/4/4/4	-
3	GOL	A	718	-	-	0/4/4/4	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	A	708	-	-	0/1/1/1	-
2	EDO	A	711	-	-	0/1/1/1	-
2	EDO	A	706	-	-	0/1/1/1	-
2	EDO	B	704	-	-	0/1/1/1	-
2	EDO	B	707	-	-	0/1/1/1	-
2	EDO	B	710	-	-	0/1/1/1	-
2	EDO	A	714	-	-	0/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
3	GOL	A	717	-	-	0/4/4/4	-
2	EDO	A	702	-	-	0/1/1/1	-
3	GOL	B	712	-	-	2/4/4/4	-
2	EDO	A	713	-	-	0/1/1/1	-
2	EDO	B	709	-	-	0/1/1/1	-
2	EDO	A	709	-	-	0/1/1/1	-
2	EDO	A	707	-	-	0/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
3	GOL	B	715	-	-	0/4/4/4	-
2	EDO	A	710	-	-	0/1/1/1	-
2	EDO	B	705	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	714	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	712	GOL	O1-C1-C2-O2
3	A	716	GOL	O1-C1-C2-C3
3	B	712	GOL	O1-C1-C2-C3
3	B	714	GOL	O2-C2-C3-O3
3	B	714	GOL	O1-C1-C2-C3
3	A	716	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	716	GOL	1	0
2	B	701	EDO	1	0
2	A	711	EDO	2	0
2	A	704	EDO	1	0
3	A	717	GOL	1	0
2	B	709	EDO	2	0
2	A	710	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 [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	620/664 (93%)	0.39	43 (6%) 16 21	25, 47, 111, 144	0
1	B	620/664 (93%)	0.38	45 (7%) 15 19	25, 47, 109, 138	0
All	All	1240/1328 (93%)	0.38	88 (7%) 16 20	25, 47, 111, 144	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	CYS	9.6
1	A	337	CYS	9.1
1	B	522	GLN	6.4
1	B	311	CYS	5.8
1	B	319	PHE	5.3
1	A	646	ALA	5.1
1	A	518	VAL	5.1
1	A	319	PHE	5.0
1	B	398	ASP	5.0
1	A	315	ASN	4.8
1	B	338	PRO	4.7
1	B	523	VAL	4.7
1	A	577	ARG	4.6
1	A	133	PHE	4.5
1	A	311	CYS	4.5
1	A	522	GLN	4.5
1	B	313	VAL	4.4
1	A	125	CYS	4.4
1	A	376	LEU	4.2
1	B	376	LEU	4.2
1	B	125	CYS	4.2
1	A	313	VAL	4.1
1	B	518	VAL	4.1
1	B	2	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	523	VAL	4.0
1	B	577	ARG	3.7
1	B	130	ASP	3.7
1	A	130	ASP	3.7
1	A	312	ARG	3.6
1	B	222	VAL	3.6
1	B	646	ALA	3.4
1	B	309	TYR	3.4
1	B	332	CYS	3.4
1	A	314	ARG	3.3
1	B	380	PRO	3.3
1	A	338	PRO	3.3
1	A	157	ASP	3.2
1	B	177	LEU	3.2
1	A	371	PRO	3.1
1	B	316	ASN	3.1
1	A	126	GLU	3.1
1	A	316	ASN	3.0
1	A	372	ARG	3.0
1	A	309	TYR	3.0
1	B	333	LYS	2.9
1	B	318	CYS	2.9
1	A	364	LEU	2.9
1	B	126	GLU	2.9
1	B	243	HIS	2.8
1	B	372	ARG	2.8
1	B	371	PRO	2.8
1	A	398	ASP	2.8
1	B	157	ASP	2.8
1	A	318	CYS	2.8
1	A	634	PHE	2.8
1	B	223	CYS	2.7
1	B	384	ILE	2.7
1	B	174	LEU	2.7
1	A	222	VAL	2.7
1	B	312	ARG	2.6
1	A	152	VAL	2.5
1	B	248[A]	ARG	2.5
1	A	332	CYS	2.5
1	B	397	ARG	2.5
1	B	404	LEU	2.5
1	A	609	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	387	PRO	2.4
1	A	248[A]	ARG	2.4
1	A	387	PRO	2.4
1	B	231	GLY	2.3
1	B	310	VAL	2.3
1	B	315	ASN	2.3
1	B	335	THR	2.3
1	B	206	TYR	2.2
1	B	334	LEU	2.2
1	A	381	TYR	2.2
1	A	336	ILE	2.2
1	A	647	GLY	2.2
1	B	152	VAL	2.2
1	A	306	LEU	2.1
1	A	397	ARG	2.1
1	B	578	LYS	2.1
1	A	243	HIS	2.1
1	A	231	GLY	2.1
1	B	440	ARG	2.1
1	A	404	LEU	2.0
1	A	578	LYS	2.0
1	A	333	LYS	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [\(i\)](#)

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( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	716	6/6	0.59	0.17	101,102,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	713	6/6	0.62	0.19	103,104,106,106	0
3	GOL	B	714	6/6	0.66	0.15	88,90,93,95	0
2	EDO	A	711	4/4	0.71	0.21	62,63,63,65	0
2	EDO	B	709	4/4	0.75	0.19	56,58,60,61	0
3	GOL	A	718	6/6	0.76	0.20	81,83,84,85	0
3	GOL	B	712	6/6	0.79	0.17	62,64,65,67	0
3	GOL	A	715	6/6	0.80	0.18	76,78,78,78	0
3	GOL	A	717	6/6	0.80	0.13	77,79,82,84	0
2	EDO	B	711	4/4	0.83	0.18	70,71,72,73	0
2	EDO	A	709	4/4	0.83	0.14	58,58,58,58	0
2	EDO	A	704	4/4	0.84	0.19	75,76,76,76	0
2	EDO	A	713	4/4	0.84	0.16	65,67,69,69	0
2	EDO	B	704	4/4	0.84	0.17	56,56,57,58	0
3	GOL	B	715	6/6	0.84	0.15	59,61,61,62	0
2	EDO	A	708	4/4	0.85	0.24	56,58,59,60	0
2	EDO	B	707	4/4	0.85	0.19	69,70,72,74	0
2	EDO	A	712	4/4	0.85	0.21	91,92,92,93	0
2	EDO	A	705	4/4	0.85	0.15	58,61,63,65	0
2	EDO	A	701	4/4	0.86	0.19	46,46,46,48	0
2	EDO	A	707	4/4	0.87	0.23	60,61,61,62	0
2	EDO	A	714	4/4	0.87	0.14	65,65,66,66	0
2	EDO	B	702	4/4	0.87	0.16	53,56,58,60	0
2	EDO	B	705	4/4	0.88	0.26	45,45,46,46	0
2	EDO	B	708	4/4	0.88	0.16	74,74,74,74	0
2	EDO	A	703	4/4	0.89	0.17	78,79,79,79	0
2	EDO	B	703	4/4	0.89	0.14	49,54,58,60	0
2	EDO	B	706	4/4	0.89	0.17	47,47,47,47	0
2	EDO	A	702	4/4	0.92	0.11	47,51,54,55	0
2	EDO	A	710	4/4	0.92	0.23	67,68,69,70	0
2	EDO	B	710	4/4	0.92	0.17	85,85,85,85	0
2	EDO	A	706	4/4	0.92	0.17	42,43,44,44	0
2	EDO	B	701	4/4	0.98	0.15	45,47,48,50	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.