



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:22 AM UTC

PDB ID : 9JER / pdb\_00009jer  
Title : Arginine decarboxylase in *Aspergillus oryzae*, ligand-free form  
Authors : Mikami, B.; Yasukawa, K.; Fujiwara, S.; Takita, T.; Mizutani, K.; Odagaki, Y.; Murakami, Y.  
Deposited on : 2024-09-03  
Resolution : 1.90 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

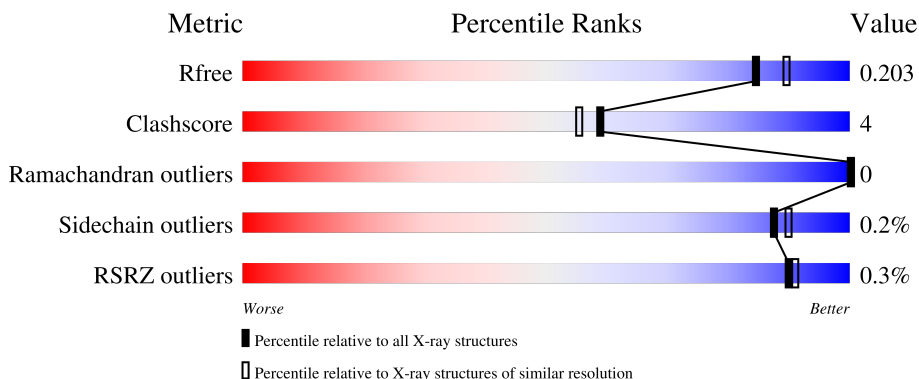
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



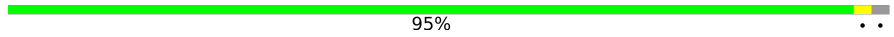
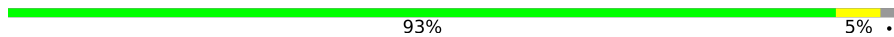

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	462	
1	B	462	
1	C	462	
1	D	462	
2	E	42	

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Mol	Chain	Length	Quality of chain
2	F	42	 95% ..
2	G	42	 93% 5% •
2	H	42	 88% 10% •

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15694 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 L-tryptophan decarboxylase PsiD-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	381	3029	1926	515	576	12	0	9	0
1	B	381	3043	1935	517	579	12	0	11	0
1	C	381	3004	1909	508	576	11	0	5	0
1	D	381	3017	1917	510	579	11	0	7	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q2UAM5
A	-18	GLY	-	expression tag	UNP Q2UAM5
A	-17	SER	-	expression tag	UNP Q2UAM5
A	-16	SER	-	expression tag	UNP Q2UAM5
A	-15	HIS	-	expression tag	UNP Q2UAM5
A	-14	HIS	-	expression tag	UNP Q2UAM5
A	-13	HIS	-	expression tag	UNP Q2UAM5
A	-12	HIS	-	expression tag	UNP Q2UAM5
A	-11	HIS	-	expression tag	UNP Q2UAM5
A	-10	HIS	-	expression tag	UNP Q2UAM5
A	-9	SER	-	expression tag	UNP Q2UAM5
A	-8	SER	-	expression tag	UNP Q2UAM5
A	-7	GLY	-	expression tag	UNP Q2UAM5
A	-6	LEU	-	expression tag	UNP Q2UAM5
A	-5	VAL	-	expression tag	UNP Q2UAM5
A	-4	PRO	-	expression tag	UNP Q2UAM5
A	-3	ARG	-	expression tag	UNP Q2UAM5
A	-2	GLY	-	expression tag	UNP Q2UAM5
A	-1	SER	-	expression tag	UNP Q2UAM5
A	0	HIS	-	expression tag	UNP Q2UAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q2UAM5
B	-18	GLY	-	expression tag	UNP Q2UAM5
B	-17	SER	-	expression tag	UNP Q2UAM5
B	-16	SER	-	expression tag	UNP Q2UAM5
B	-15	HIS	-	expression tag	UNP Q2UAM5
B	-14	HIS	-	expression tag	UNP Q2UAM5
B	-13	HIS	-	expression tag	UNP Q2UAM5
B	-12	HIS	-	expression tag	UNP Q2UAM5
B	-11	HIS	-	expression tag	UNP Q2UAM5
B	-10	HIS	-	expression tag	UNP Q2UAM5
B	-9	SER	-	expression tag	UNP Q2UAM5
B	-8	SER	-	expression tag	UNP Q2UAM5
B	-7	GLY	-	expression tag	UNP Q2UAM5
B	-6	LEU	-	expression tag	UNP Q2UAM5
B	-5	VAL	-	expression tag	UNP Q2UAM5
B	-4	PRO	-	expression tag	UNP Q2UAM5
B	-3	ARG	-	expression tag	UNP Q2UAM5
B	-2	GLY	-	expression tag	UNP Q2UAM5
B	-1	SER	-	expression tag	UNP Q2UAM5
B	0	HIS	-	expression tag	UNP Q2UAM5
C	-19	MET	-	initiating methionine	UNP Q2UAM5
C	-18	GLY	-	expression tag	UNP Q2UAM5
C	-17	SER	-	expression tag	UNP Q2UAM5
C	-16	SER	-	expression tag	UNP Q2UAM5
C	-15	HIS	-	expression tag	UNP Q2UAM5
C	-14	HIS	-	expression tag	UNP Q2UAM5
C	-13	HIS	-	expression tag	UNP Q2UAM5
C	-12	HIS	-	expression tag	UNP Q2UAM5
C	-11	HIS	-	expression tag	UNP Q2UAM5
C	-10	HIS	-	expression tag	UNP Q2UAM5
C	-9	SER	-	expression tag	UNP Q2UAM5
C	-8	SER	-	expression tag	UNP Q2UAM5
C	-7	GLY	-	expression tag	UNP Q2UAM5
C	-6	LEU	-	expression tag	UNP Q2UAM5
C	-5	VAL	-	expression tag	UNP Q2UAM5
C	-4	PRO	-	expression tag	UNP Q2UAM5
C	-3	ARG	-	expression tag	UNP Q2UAM5
C	-2	GLY	-	expression tag	UNP Q2UAM5
C	-1	SER	-	expression tag	UNP Q2UAM5
C	0	HIS	-	expression tag	UNP Q2UAM5
D	-19	MET	-	initiating methionine	UNP Q2UAM5
D	-18	GLY	-	expression tag	UNP Q2UAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q2UAM5
D	-16	SER	-	expression tag	UNP Q2UAM5
D	-15	HIS	-	expression tag	UNP Q2UAM5
D	-14	HIS	-	expression tag	UNP Q2UAM5
D	-13	HIS	-	expression tag	UNP Q2UAM5
D	-12	HIS	-	expression tag	UNP Q2UAM5
D	-11	HIS	-	expression tag	UNP Q2UAM5
D	-10	HIS	-	expression tag	UNP Q2UAM5
D	-9	SER	-	expression tag	UNP Q2UAM5
D	-8	SER	-	expression tag	UNP Q2UAM5
D	-7	GLY	-	expression tag	UNP Q2UAM5
D	-6	LEU	-	expression tag	UNP Q2UAM5
D	-5	VAL	-	expression tag	UNP Q2UAM5
D	-4	PRO	-	expression tag	UNP Q2UAM5
D	-3	ARG	-	expression tag	UNP Q2UAM5
D	-2	GLY	-	expression tag	UNP Q2UAM5
D	-1	SER	-	expression tag	UNP Q2UAM5
D	0	HIS	-	expression tag	UNP Q2UAM5

- Molecule 2 is a protein called L-tryptophan decarboxylase PsiD-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	41	Total	C	N	O	S	0	1	0
			328	212	54	61	1			
2	F	41	Total	C	N	O	S	0	1	0
			328	212	54	61	1			
2	G	41	Total	C	N	O	S	0	0	0
			322	208	54	59	1			
2	H	41	Total	C	N	O	S	0	1	0
			328	212	54	61	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	501	PYR	-	modified residue	UNP Q2UAM5
F	501	PYR	-	modified residue	UNP Q2UAM5
G	501	PYR	-	modified residue	UNP Q2UAM5
H	501	PYR	-	modified residue	UNP Q2UAM5

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	417	Total O 418 418	0	1
5	E	42	Total O 42 42	0	0
5	B	374	Total O 376 376	0	2
5	F	32	Total O 32 32	0	0
5	C	365	Total O 366 366	0	1
5	G	34	Total O 35 35	0	1
5	D	407	Total O 407 407	0	0
5	H	37	Total O 37 37	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.69Å 196.48Å 196.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.77 – 1.90 43.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.77-1.90) 99.9 (43.77-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.169 , 0.202 0.170 , 0.203	Depositor DCC
$R_{free}$ test set	10160 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtrriage
Anisotropy	0.458	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	15694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: EDO, PYR, PEG

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	0.28	0/3134	0.47	0/4257
1	B	0.27	0/3154	0.46	0/4283
1	C	0.27	0/3097	0.45	0/4209
1	D	0.27	0/3113	0.46	0/4232
2	E	0.24	0/331	0.46	0/448
2	F	0.25	0/331	0.47	0/448
2	G	0.22	0/322	0.45	0/436
2	H	0.24	0/331	0.44	0/448
All	All	0.27	0/13813	0.46	0/18761

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
2	H	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
2	H	501	PYR	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3029	0	2930	26	0
1	B	3043	0	2945	36	0
1	C	3004	0	2884	24	0
1	D	3017	0	2901	22	0
2	E	328	0	340	2	0
2	F	328	0	340	1	0
2	G	322	0	334	3	0
2	H	328	0	340	2	0
3	A	14	0	20	2	0
3	B	28	0	40	8	0
3	C	14	0	20	6	0
3	D	14	0	20	2	0
4	A	124	0	186	14	0
4	B	136	0	204	16	0
4	C	128	0	192	14	0
4	D	92	0	138	7	0
4	E	12	0	18	0	0
4	F	4	0	6	0	0
4	G	12	0	18	2	0
4	H	4	0	6	2	0
5	A	418	0	0	4	0
5	B	376	0	0	2	0
5	C	366	0	0	1	0
5	D	407	0	0	5	0
5	E	42	0	0	1	0
5	F	32	0	0	0	0
5	G	35	0	0	0	0
5	H	37	0	0	0	0
All	All	15694	0	13882	123	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 123 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:224:LYS:HD2	1:A:224:LYS:H	1.41	0.86
1:C:345:ARG:HH21	4:C:515:EDO:H12	1.44	0.80
1:B:264:ASP:HA	4:B:528:EDO:H22	1.66	0.78
1:D:293[B]:THR:HG22	5:D:641:HOH:O	1.90	0.71
1:C:325:PHE:HZ	3:C:502[B]:PEG:H11	1.55	0.71

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	388/462 (84%)	379 (98%)	9 (2%)	0	100	100
1	B	390/462 (84%)	385 (99%)	5 (1%)	0	100	100
1	C	384/462 (83%)	373 (97%)	11 (3%)	0	100	100
1	D	386/462 (84%)	375 (97%)	11 (3%)	0	100	100
2	E	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
2	F	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
2	G	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
2	H	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
All	All	1707/2016 (85%)	1667 (98%)	40 (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	328/389 (84%)	328 (100%)	0	100	100
1	B	330/389 (85%)	329 (100%)	1 (0%)	86	88
1	C	324/389 (83%)	323 (100%)	1 (0%)	86	88
1	D	326/389 (84%)	324 (99%)	2 (1%)	78	81
2	E	36/36 (100%)	36 (100%)	0	100	100
2	F	36/36 (100%)	36 (100%)	0	100	100
2	G	35/36 (97%)	35 (100%)	0	100	100
2	H	36/36 (100%)	36 (100%)	0	100	100
All	All	1451/1700 (85%)	1447 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	VAL
1	C	138	LEU
1	D	293[A]	THR
1	D	293[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	194	ASN
1	C	332	HIS
2	H	530	ASN
1	D	194	ASN
2	H	516	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

138 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	EDO	D	514	-	3,3,3	0.24	0	2,2,2	0.48	0
4	EDO	B	518	-	3,3,3	0.24	0	2,2,2	0.45	0
4	EDO	C	506	-	3,3,3	0.26	0	2,2,2	0.34	0
4	EDO	C	525	-	3,3,3	0.26	0	2,2,2	0.16	0
4	EDO	B	526	-	3,3,3	0.25	0	2,2,2	0.27	0
4	EDO	B	532	-	3,3,3	0.26	0	2,2,2	0.28	0
4	EDO	H	601	-	3,3,3	0.25	0	2,2,2	0.08	0
4	EDO	A	522	-	3,3,3	0.25	0	2,2,2	0.15	0
4	EDO	A	518	-	3,3,3	0.26	0	2,2,2	0.08	0
4	EDO	B	522	-	3,3,3	0.27	0	2,2,2	0.24	0
4	EDO	B	509	-	3,3,3	0.25	0	2,2,2	0.38	0
3	PEG	A	502	-	6,6,6	0.25	0	5,5,5	0.61	0
4	EDO	B	535	-	3,3,3	0.24	0	2,2,2	0.25	0
4	EDO	G	601	-	3,3,3	0.31	0	2,2,2	0.12	0
4	EDO	C	521	-	3,3,3	0.27	0	2,2,2	0.19	0
4	EDO	D	522	-	3,3,3	0.26	0	2,2,2	0.20	0
4	EDO	B	530	-	3,3,3	0.26	0	2,2,2	0.28	0
4	EDO	B	533	-	3,3,3	0.31	0	2,2,2	0.19	0
4	EDO	D	519	-	3,3,3	0.26	0	2,2,2	0.35	0
4	EDO	C	515	-	3,3,3	0.26	0	2,2,2	0.23	0
4	EDO	B	515	-	3,3,3	0.25	0	2,2,2	0.42	0
4	EDO	A	527	-	3,3,3	0.25	0	2,2,2	0.19	0
4	EDO	A	524	-	3,3,3	0.19	0	2,2,2	0.30	0
4	EDO	B	537	-	3,3,3	0.24	0	2,2,2	0.33	0
3	PEG	D	502	-	6,6,6	0.26	0	5,5,5	0.51	0
4	EDO	B	529	-	3,3,3	0.23	0	2,2,2	0.41	0
4	EDO	B	513	-	3,3,3	0.28	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	529	-	3,3,3	0.33	0	2,2,2	0.19	0
4	EDO	B	506	-	3,3,3	0.23	0	2,2,2	0.57	0
4	EDO	C	509	-	3,3,3	0.26	0	2,2,2	0.42	0
4	EDO	A	528	-	3,3,3	0.21	0	2,2,2	0.31	0
4	EDO	B	536	-	3,3,3	0.30	0	2,2,2	0.28	0
4	EDO	C	520	-	3,3,3	0.24	0	2,2,2	0.46	0
4	EDO	C	533	-	3,3,3	0.21	0	2,2,2	0.41	0
4	EDO	A	525	-	3,3,3	0.26	0	2,2,2	0.35	0
4	EDO	C	503	-	3,3,3	0.24	0	2,2,2	0.30	0
3	PEG	B	502	-	6,6,6	0.29	0	5,5,5	0.24	0
4	EDO	C	531	-	3,3,3	0.34	0	2,2,2	0.42	0
4	EDO	B	538	-	3,3,3	0.24	0	2,2,2	0.31	0
4	EDO	C	528	-	3,3,3	0.23	0	2,2,2	0.49	0
4	EDO	C	526	-	3,3,3	0.23	0	2,2,2	0.30	0
3	PEG	B	501	-	6,6,6	0.25	0	5,5,5	0.46	0
4	EDO	E	603	-	3,3,3	0.28	0	2,2,2	0.19	0
4	EDO	A	505	-	3,3,3	0.19	0	2,2,2	0.50	0
4	EDO	C	514	-	3,3,3	0.26	0	2,2,2	0.19	0
3	PEG	B	504	-	6,6,6	0.27	0	5,5,5	0.42	0
4	EDO	G	603	-	3,3,3	0.24	0	2,2,2	0.36	0
4	EDO	B	534	-	3,3,3	0.22	0	2,2,2	0.26	0
4	EDO	C	532	-	3,3,3	0.40	0	2,2,2	0.32	0
4	EDO	D	505	-	3,3,3	0.28	0	2,2,2	0.11	0
4	EDO	B	527	-	3,3,3	0.26	0	2,2,2	0.23	0
4	EDO	A	521	-	3,3,3	0.24	0	2,2,2	0.30	0
4	EDO	A	533	-	3,3,3	0.22	0	2,2,2	0.37	0
4	EDO	C	517	-	3,3,3	0.26	0	2,2,2	0.29	0
4	EDO	C	534	-	3,3,3	0.26	0	2,2,2	0.24	0
4	EDO	A	515	-	3,3,3	0.25	0	2,2,2	0.39	0
4	EDO	D	520	-	3,3,3	0.24	0	2,2,2	0.24	0
4	EDO	B	523	-	3,3,3	0.24	0	2,2,2	0.31	0
4	EDO	C	523	-	3,3,3	0.26	0	2,2,2	0.11	0
4	EDO	C	516	-	3,3,3	0.23	0	2,2,2	0.38	0
4	EDO	A	517	-	3,3,3	0.37	0	2,2,2	0.31	0
4	EDO	D	523	-	3,3,3	0.30	0	2,2,2	0.53	0
4	EDO	C	513	-	3,3,3	0.31	0	2,2,2	0.06	0
4	EDO	D	521	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	A	520	-	3,3,3	0.26	0	2,2,2	0.30	0
4	EDO	C	507	-	3,3,3	0.29	0	2,2,2	0.23	0
4	EDO	B	528	-	3,3,3	0.25	0	2,2,2	0.38	0
4	EDO	C	504	-	3,3,3	0.24	0	2,2,2	0.37	0
4	EDO	D	516	-	3,3,3	0.32	0	2,2,2	0.12	0
4	EDO	C	530	-	3,3,3	0.25	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	503	-	3,3,3	0.32	0	2,2,2	0.14	0
4	EDO	A	526	-	3,3,3	0.23	0	2,2,2	0.43	0
4	EDO	C	511	-	3,3,3	0.25	0	2,2,2	0.29	0
4	EDO	B	512	-	3,3,3	0.30	0	2,2,2	0.08	0
4	EDO	D	510	-	3,3,3	0.24	0	2,2,2	0.31	0
4	EDO	A	516	-	3,3,3	0.28	0	2,2,2	0.17	0
4	EDO	C	512	-	3,3,3	0.21	0	2,2,2	0.58	0
4	EDO	A	531	-	3,3,3	0.19	0	2,2,2	0.47	0
4	EDO	E	602	-	3,3,3	0.25	0	2,2,2	0.54	0
4	EDO	A	532	-	3,3,3	0.19	0	2,2,2	0.80	0
4	EDO	D	503	-	3,3,3	0.23	0	2,2,2	0.30	0
4	EDO	C	519	-	3,3,3	0.24	0	2,2,2	0.20	0
4	EDO	E	601	-	3,3,3	0.25	0	2,2,2	0.09	0
4	EDO	D	515	-	3,3,3	0.24	0	2,2,2	0.30	0
4	EDO	D	513	-	3,3,3	0.24	0	2,2,2	0.33	0
4	EDO	G	602	-	3,3,3	0.26	0	2,2,2	0.40	0
4	EDO	D	507	-	3,3,3	0.19	0	2,2,2	0.93	0
4	EDO	D	518	-	3,3,3	0.25	0	2,2,2	0.32	0
4	EDO	C	510	-	3,3,3	0.24	0	2,2,2	0.30	0
4	EDO	A	513	-	3,3,3	0.33	0	2,2,2	0.25	0
4	EDO	A	523	-	3,3,3	0.25	0	2,2,2	0.25	0
4	EDO	B	510	-	3,3,3	0.25	0	2,2,2	0.15	0
4	EDO	B	517	-	3,3,3	0.24	0	2,2,2	0.32	0
4	EDO	D	512	-	3,3,3	0.27	0	2,2,2	0.24	0
4	EDO	B	521	-	3,3,3	0.28	0	2,2,2	0.32	0
4	EDO	B	508	-	3,3,3	0.21	0	2,2,2	0.34	0
4	EDO	B	511	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	D	517	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	A	507	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	B	516	-	3,3,3	0.26	0	2,2,2	0.36	0
4	EDO	C	527	-	3,3,3	0.25	0	2,2,2	0.19	0
4	EDO	D	508	-	3,3,3	0.25	0	2,2,2	0.22	0
4	EDO	D	511	-	3,3,3	0.26	0	2,2,2	0.41	0
4	EDO	D	525	-	3,3,3	0.23	0	2,2,2	0.22	0
4	EDO	A	504	-	3,3,3	0.25	0	2,2,2	0.38	0
4	EDO	B	519[A]	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	A	530	-	3,3,3	0.30	0	2,2,2	0.41	0
4	EDO	A	508	-	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	D	509	-	3,3,3	0.17	0	2,2,2	0.58	0
3	PEG	A	501	-	6,6,6	0.34	0	5,5,5	0.45	0
3	PEG	C	501[A]	-	6,6,6	0.21	0	5,5,5	0.25	0
4	EDO	A	529	-	3,3,3	0.22	0	2,2,2	0.40	0
4	EDO	D	504	-	3,3,3	0.17	0	2,2,2	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PEG	D	501	-	6,6,6	0.22	0	5,5,5	0.47	0
4	EDO	A	511	-	3,3,3	0.27	0	2,2,2	0.39	0
4	EDO	C	508	-	3,3,3	0.23	0	2,2,2	0.39	0
4	EDO	B	525	-	3,3,3	0.22	0	2,2,2	0.38	0
4	EDO	A	512	-	3,3,3	0.21	0	2,2,2	0.35	0
4	EDO	B	524	-	3,3,3	0.24	0	2,2,2	0.51	0
4	EDO	C	522	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	A	509	-	3,3,3	0.23	0	2,2,2	0.45	0
4	EDO	C	505	-	3,3,3	0.32	0	2,2,2	0.62	0
4	EDO	C	518	-	3,3,3	0.29	0	2,2,2	0.20	0
4	EDO	A	519	-	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	B	505	-	3,3,3	0.18	0	2,2,2	0.65	0
3	PEG	C	502[B]	-	6,6,6	0.25	0	5,5,5	0.57	0
4	EDO	B	507	-	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	D	524	-	3,3,3	0.24	0	2,2,2	0.26	0
4	EDO	A	514	-	3,3,3	0.29	0	2,2,2	0.33	0
4	EDO	A	510	-	3,3,3	0.24	0	2,2,2	0.19	0
4	EDO	B	531	-	3,3,3	0.30	0	2,2,2	0.35	0
4	EDO	B	520[B]	-	3,3,3	0.23	0	2,2,2	0.46	0
4	EDO	D	506	-	3,3,3	0.27	0	2,2,2	0.22	0
3	PEG	B	503	-	6,6,6	0.25	0	5,5,5	0.19	0
4	EDO	B	514	-	3,3,3	0.26	0	2,2,2	0.27	0
4	EDO	A	506	-	3,3,3	0.21	0	2,2,2	0.55	0
4	EDO	C	524	-	3,3,3	0.26	0	2,2,2	0.15	0
4	EDO	F	601	-	3,3,3	0.28	0	2,2,2	0.37	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
4	EDO	D	514	-	-	1/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
4	EDO	C	525	-	-	0/1/1/1	-
4	EDO	B	526	-	-	0/1/1/1	-
4	EDO	B	532	-	-	0/1/1/1	-
4	EDO	H	601	-	-	0/1/1/1	-
4	EDO	A	522	-	-	0/1/1/1	-
4	EDO	A	518	-	-	1/1/1/1	-
4	EDO	B	522	-	-	0/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	502	-	-	3/4/4/4	-
4	EDO	B	535	-	-	1/1/1/1	-
4	EDO	G	601	-	-	1/1/1/1	-
4	EDO	C	521	-	-	0/1/1/1	-
4	EDO	D	522	-	-	0/1/1/1	-
4	EDO	B	530	-	-	1/1/1/1	-
4	EDO	B	533	-	-	0/1/1/1	-
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	A	527	-	-	1/1/1/1	-
4	EDO	A	524	-	-	0/1/1/1	-
4	EDO	B	537	-	-	1/1/1/1	-
3	PEG	D	502	-	-	1/4/4/4	-
4	EDO	B	529	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	C	529	-	-	0/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	A	528	-	-	0/1/1/1	-
4	EDO	B	536	-	-	1/1/1/1	-
4	EDO	C	520	-	-	0/1/1/1	-
4	EDO	C	533	-	-	0/1/1/1	-
4	EDO	A	525	-	-	0/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
3	PEG	B	502	-	-	2/4/4/4	-
4	EDO	C	531	-	-	1/1/1/1	-
4	EDO	B	538	-	-	1/1/1/1	-
4	EDO	C	528	-	-	0/1/1/1	-
4	EDO	C	526	-	-	1/1/1/1	-
3	PEG	B	501	-	-	2/4/4/4	-
4	EDO	E	603	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	C	514	-	-	1/1/1/1	-
3	PEG	B	504	-	-	2/4/4/4	-
4	EDO	G	603	-	-	1/1/1/1	-
4	EDO	B	534	-	-	1/1/1/1	-
4	EDO	C	532	-	-	1/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	B	527	-	-	1/1/1/1	-
4	EDO	A	521	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	533	-	-	1/1/1/1	-
4	EDO	C	517	-	-	0/1/1/1	-
4	EDO	C	534	-	-	1/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	B	523	-	-	1/1/1/1	-
4	EDO	C	523	-	-	1/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	D	523	-	-	1/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	D	521	-	-	0/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
4	EDO	B	528	-	-	0/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-
4	EDO	C	530	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	A	526	-	-	0/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-
4	EDO	B	512	-	-	0/1/1/1	-
4	EDO	D	510	-	-	0/1/1/1	-
4	EDO	A	516	-	-	1/1/1/1	-
4	EDO	C	512	-	-	1/1/1/1	-
4	EDO	A	531	-	-	1/1/1/1	-
4	EDO	E	602	-	-	0/1/1/1	-
4	EDO	A	532	-	-	1/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	C	519	-	-	1/1/1/1	-
4	EDO	E	601	-	-	1/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	G	602	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	A	523	-	-	0/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	B	517	-	-	1/1/1/1	-
4	EDO	D	512	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	521	-	-	1/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	D	517	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	C	527	-	-	1/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	D	525	-	-	1/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	B	519[A]	-	-	1/1/1/1	-
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
3	PEG	A	501	-	-	3/4/4/4	-
3	PEG	C	501[A]	-	-	4/4/4/4	-
4	EDO	A	529	-	-	0/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-
3	PEG	D	501	-	-	1/4/4/4	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	B	525	-	-	0/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	B	524	-	-	0/1/1/1	-
4	EDO	C	522	-	-	1/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
4	EDO	A	519	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
3	PEG	C	502[B]	-	-	2/4/4/4	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	D	524	-	-	0/1/1/1	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	B	531	-	-	0/1/1/1	-
4	EDO	B	520[B]	-	-	0/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
3	PEG	B	503	-	-	4/4/4/4	-
4	EDO	B	514	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	C	524	-	-	1/1/1/1	-
4	EDO	F	601	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504	PEG	C4-C3-O2-C2
3	C	501[A]	PEG	O2-C3-C4-O4
4	A	517	EDO	O1-C1-C2-O2
4	A	530	EDO	O1-C1-C2-O2
4	B	517	EDO	O1-C1-C2-O2

There are no ring outliers.

50 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	506	EDO	1	0
4	C	525	EDO	1	0
4	B	526	EDO	1	0
4	H	601	EDO	2	0
4	A	518	EDO	2	0
4	B	509	EDO	1	0
3	A	502	PEG	2	0
4	D	522	EDO	1	0
4	B	530	EDO	1	0
4	B	533	EDO	1	0
4	D	519	EDO	1	0
4	C	515	EDO	1	0
4	A	524	EDO	2	0
4	B	537	EDO	3	0
4	C	529	EDO	1	0
4	A	528	EDO	1	0
4	C	533	EDO	1	0
4	A	525	EDO	2	0
3	B	502	PEG	1	0
4	C	531	EDO	1	0
4	C	528	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	PEG	2	0
3	B	504	PEG	2	0
4	G	603	EDO	2	0
4	C	532	EDO	1	0
4	C	523	EDO	1	0
4	C	516	EDO	1	0
4	A	517	EDO	1	0
4	D	523	EDO	1	0
4	A	520	EDO	1	0
4	B	528	EDO	1	0
4	A	526	EDO	2	0
4	C	511	EDO	1	0
4	D	510	EDO	2	0
4	A	531	EDO	1	0
4	C	510	EDO	1	0
4	B	510	EDO	1	0
4	B	517	EDO	1	0
4	B	521	EDO	2	0
4	B	511	EDO	1	0
4	C	527	EDO	1	0
4	D	525	EDO	1	0
4	A	530	EDO	2	0
3	C	501[A]	PEG	3	0
3	D	501	PEG	2	0
4	C	505	EDO	2	0
3	C	502[B]	PEG	3	0
4	D	524	EDO	1	0
4	B	531	EDO	3	0
3	B	503	PEG	3	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	381/462 (82%)	-0.47	2 (0%) 87 89	12, 24, 34, 63	9 (2%)
1	B	381/462 (82%)	-0.37	1 (0%) 90 91	12, 25, 38, 66	11 (2%)
1	C	381/462 (82%)	-0.08	1 (0%) 90 91	12, 28, 42, 55	5 (1%)
1	D	381/462 (82%)	-0.24	1 (0%) 90 91	13, 27, 38, 56	7 (1%)
2	E	40/42 (95%)	-0.30	0 100 100	12, 26, 43, 48	1 (2%)
2	F	40/42 (95%)	-0.24	0 100 100	16, 27, 41, 48	1 (2%)
2	G	40/42 (95%)	0.03	0 100 100	24, 28, 48, 51	0
2	H	40/42 (95%)	-0.13	0 100 100	15, 27, 43, 44	1 (2%)
All	All	1684/2016 (83%)	-0.28	5 (0%) 90 91	12, 26, 40, 66	35 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	VAL	5.5
1	B	61	VAL	4.6
1	D	61	VAL	3.4
1	A	224	LYS	2.5
1	C	61	VAL	2.2

### 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 oligosaccharides 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
4	EDO	A	530	4/4	0.59	0.29	36,42,45,48	0
4	EDO	C	531	4/4	0.72	0.22	32,35,38,39	0
4	EDO	C	521	4/4	0.73	0.23	51,51,52,58	0
3	PEG	D	502	7/7	0.74	0.20	35,43,54,57	0
3	PEG	B	501	7/7	0.74	0.22	37,44,51,56	0
4	EDO	D	515	4/4	0.75	0.28	43,48,53,58	0
4	EDO	B	514	4/4	0.76	0.23	41,44,45,53	0
4	EDO	B	527	4/4	0.76	0.16	54,57,62,62	0
3	PEG	A	501	7/7	0.76	0.19	27,36,46,50	0
3	PEG	C	501[A]	7/7	0.76	0.24	24,27,30,37	7
4	EDO	A	533	4/4	0.76	0.19	40,44,46,48	0
3	PEG	C	502[B]	7/7	0.77	0.26	24,28,30,33	7
4	EDO	C	526	4/4	0.77	0.14	44,54,55,59	0
4	EDO	A	524	4/4	0.78	0.20	37,41,42,52	0
4	EDO	A	525	4/4	0.78	0.23	36,41,45,48	0
4	EDO	A	513	4/4	0.78	0.20	36,38,41,43	0
4	EDO	C	510	4/4	0.78	0.20	44,46,51,62	0
4	EDO	E	603	4/4	0.79	0.24	28,40,43,46	0
3	PEG	B	503	7/7	0.79	0.14	42,45,56,62	0
4	EDO	B	524	4/4	0.79	0.23	38,42,45,47	0
4	EDO	A	526	4/4	0.79	0.19	43,46,47,56	0
4	EDO	B	538	4/4	0.79	0.15	52,56,58,58	0
4	EDO	D	518	4/4	0.79	0.16	47,48,53,56	0
4	EDO	A	517	4/4	0.80	0.24	27,28,42,43	0
4	EDO	D	519	4/4	0.80	0.17	41,44,45,52	0
4	EDO	C	518	4/4	0.81	0.29	38,41,46,46	0
4	EDO	C	532	4/4	0.81	0.24	34,40,41,44	0
4	EDO	D	509	4/4	0.81	0.19	33,40,42,45	0
4	EDO	B	525	4/4	0.81	0.17	44,47,51,57	0
4	EDO	C	515	4/4	0.81	0.16	38,40,43,44	0
4	EDO	C	530	4/4	0.81	0.23	43,48,49,53	0
4	EDO	A	521	4/4	0.82	0.18	39,43,52,54	0
4	EDO	D	517	4/4	0.82	0.19	43,46,47,55	0
4	EDO	B	537	4/4	0.82	0.25	35,35,46,48	0
4	EDO	A	519	4/4	0.82	0.21	35,44,44,49	0
4	EDO	D	520	4/4	0.82	0.20	41,45,49,53	0
4	EDO	B	534	4/4	0.83	0.22	35,46,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	C	527	4/4	0.83	0.18	46,50,52,56	0
4	EDO	B	535	4/4	0.83	0.20	47,49,49,53	0
4	EDO	B	522	4/4	0.83	0.15	44,45,53,54	0
4	EDO	B	511	4/4	0.83	0.19	30,38,38,41	0
4	EDO	G	603	4/4	0.83	0.19	33,34,45,45	0
4	EDO	D	523	4/4	0.83	0.22	28,31,34,40	0
4	EDO	H	601	4/4	0.83	0.26	39,42,44,46	0
4	EDO	B	523	4/4	0.84	0.19	42,44,45,61	0
4	EDO	D	514	4/4	0.84	0.17	42,45,53,56	0
4	EDO	D	504	4/4	0.84	0.17	36,37,39,44	0
4	EDO	B	536	4/4	0.85	0.18	30,32,37,40	0
3	PEG	B	502	7/7	0.85	0.14	38,43,51,55	0
4	EDO	B	528	4/4	0.85	0.19	38,44,45,53	0
4	EDO	C	508	4/4	0.85	0.15	34,39,46,51	0
4	EDO	D	522	4/4	0.85	0.20	44,47,54,54	0
4	EDO	B	517	4/4	0.85	0.14	31,45,46,55	0
3	PEG	D	501	7/7	0.85	0.14	31,38,48,49	0
4	EDO	C	520	4/4	0.86	0.17	44,45,50,53	0
4	EDO	B	509	4/4	0.86	0.14	29,38,49,49	0
4	EDO	C	533	4/4	0.86	0.15	36,36,37,40	0
4	EDO	C	524	4/4	0.86	0.12	51,51,54,60	0
4	EDO	E	601	4/4	0.86	0.22	34,34,34,39	0
4	EDO	D	508	4/4	0.86	0.19	40,42,43,54	0
4	EDO	B	520[B]	4/4	0.86	0.13	31,34,39,43	4
4	EDO	C	519	4/4	0.86	0.15	42,49,50,54	0
4	EDO	C	516	4/4	0.87	0.28	42,46,46,49	0
4	EDO	B	529	4/4	0.87	0.21	38,38,45,47	0
4	EDO	B	530	4/4	0.87	0.15	37,44,51,52	0
4	EDO	B	533	4/4	0.87	0.24	34,37,44,47	0
4	EDO	A	507	4/4	0.87	0.20	39,40,42,43	0
4	EDO	A	531	4/4	0.87	0.16	35,37,39,52	0
4	EDO	A	520	4/4	0.87	0.14	39,43,45,58	0
4	EDO	A	511	4/4	0.87	0.13	38,39,42,62	0
4	EDO	C	529	4/4	0.87	0.20	40,41,41,41	0
3	PEG	A	502	7/7	0.87	0.13	31,35,44,47	0
4	EDO	A	516	4/4	0.87	0.18	39,41,47,50	0
4	EDO	A	504	4/4	0.87	0.21	33,44,46,53	0
4	EDO	D	524	4/4	0.87	0.18	46,47,50,53	0
4	EDO	A	528	4/4	0.87	0.27	33,39,45,53	0
4	EDO	A	527	4/4	0.88	0.17	30,40,42,42	0
4	EDO	C	525	4/4	0.88	0.14	40,40,43,52	0
4	EDO	D	510	4/4	0.88	0.14	32,35,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	515	4/4	0.88	0.13	45,46,52,56	0
4	EDO	C	511	4/4	0.88	0.15	29,34,45,51	0
4	EDO	A	512	4/4	0.88	0.19	40,42,44,52	0
4	EDO	A	514	4/4	0.88	0.14	33,37,46,46	0
4	EDO	B	531	4/4	0.88	0.17	32,42,42,48	0
4	EDO	B	532	4/4	0.88	0.17	44,46,47,57	0
4	EDO	C	505	4/4	0.88	0.14	31,33,37,42	0
4	EDO	C	506	4/4	0.88	0.17	37,43,49,50	0
4	EDO	C	522	4/4	0.88	0.11	41,49,49,54	0
4	EDO	D	525	4/4	0.88	0.22	41,43,44,50	0
4	EDO	D	506	4/4	0.88	0.16	35,43,44,49	0
4	EDO	A	523	4/4	0.89	0.14	45,46,49,50	0
4	EDO	B	512	4/4	0.89	0.15	36,36,36,39	0
4	EDO	B	508	4/4	0.89	0.15	35,37,38,45	0
4	EDO	C	534	4/4	0.89	0.20	35,36,37,42	0
4	EDO	A	522	4/4	0.89	0.14	43,47,54,54	0
4	EDO	B	518	4/4	0.89	0.15	33,39,40,49	0
4	EDO	B	526	4/4	0.89	0.17	36,39,46,48	0
4	EDO	C	513	4/4	0.90	0.15	28,41,43,47	0
4	EDO	D	521	4/4	0.90	0.13	36,39,46,48	0
4	EDO	C	514	4/4	0.90	0.20	30,33,39,47	0
4	EDO	A	509	4/4	0.90	0.13	42,46,47,52	0
4	EDO	B	521	4/4	0.90	0.13	37,40,42,54	0
4	EDO	A	505	4/4	0.90	0.13	34,35,44,46	0
3	PEG	B	504	7/7	0.90	0.11	35,38,47,48	0
4	EDO	A	518	4/4	0.91	0.19	31,33,34,45	0
4	EDO	G	601	4/4	0.91	0.23	36,36,39,40	0
4	EDO	F	601	4/4	0.91	0.13	29,33,36,39	0
4	EDO	B	506	4/4	0.91	0.12	35,36,38,39	0
4	EDO	D	505	4/4	0.91	0.12	40,40,40,43	0
4	EDO	A	529	4/4	0.91	0.12	30,32,33,43	0
4	EDO	C	528	4/4	0.91	0.19	34,36,41,52	0
4	EDO	C	523	4/4	0.92	0.15	26,40,41,45	0
4	EDO	B	516	4/4	0.92	0.10	36,38,43,46	0
4	EDO	B	519[A]	4/4	0.92	0.11	32,32,34,42	4
4	EDO	E	602	4/4	0.92	0.11	28,28,34,41	0
4	EDO	D	512	4/4	0.92	0.09	45,49,49,50	0
4	EDO	D	513	4/4	0.92	0.11	31,31,34,48	0
4	EDO	A	506	4/4	0.93	0.15	35,38,39,40	0
4	EDO	D	511	4/4	0.93	0.10	27,28,37,41	0
4	EDO	C	512	4/4	0.93	0.12	33,37,39,42	0
4	EDO	C	504	4/4	0.93	0.10	32,33,38,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	C	503	4/4	0.94	0.08	30,31,31,42	0
4	EDO	A	510	4/4	0.94	0.10	31,32,33,34	0
4	EDO	B	505	4/4	0.94	0.11	29,33,37,37	0
4	EDO	C	517	4/4	0.94	0.12	35,36,37,43	0
4	EDO	A	532	4/4	0.95	0.09	31,32,35,40	0
4	EDO	G	602	4/4	0.95	0.10	29,30,37,44	0
4	EDO	D	507	4/4	0.95	0.10	32,34,35,38	0
4	EDO	B	510	4/4	0.96	0.07	22,26,30,31	0
4	EDO	D	503	4/4	0.96	0.09	25,29,30,33	0
4	EDO	B	515	4/4	0.96	0.07	29,30,30,43	0
4	EDO	A	503	4/4	0.97	0.07	21,22,24,26	0
4	EDO	D	516	4/4	0.97	0.06	21,21,23,25	0
4	EDO	C	509	4/4	0.97	0.07	27,29,32,34	0
4	EDO	B	513	4/4	0.97	0.08	28,32,33,33	0
4	EDO	A	508	4/4	0.98	0.06	25,26,26,31	0
4	EDO	B	507	4/4	0.98	0.04	21,24,25,25	0
4	EDO	C	507	4/4	0.98	0.04	21,22,23,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.