Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2024 – 04:29 PM JST

PDB ID	:	9JER
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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.

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

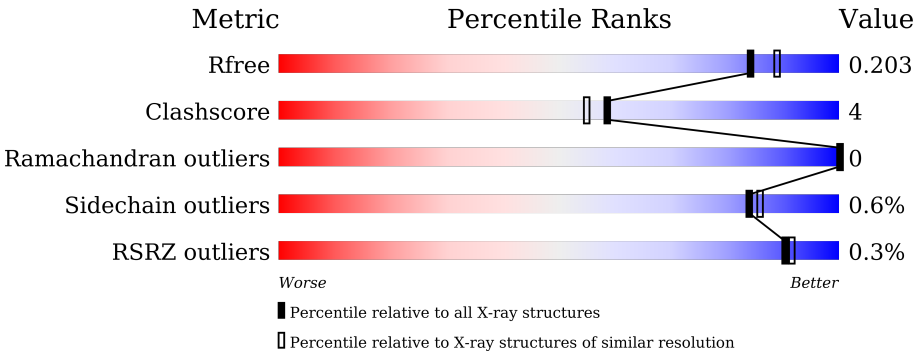
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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 >=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 <=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	76% 6% 18%
1	B	462	74% 9% 18%
1	C	462	77% 5% 18%
1	D	462	77% 5% 18%
2	E	42	93% 5% .
2	F	42	95% . .

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Mol	Chain	Length	Quality of chain
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
1	A	381	Total	C	N	O	S	0	9	0
			3029	1926	515	576	12			
1	B	381	Total	C	N	O	S	0	11	0
			3043	1935	517	579	12			
1	C	381	Total	C	N	O	S	0	5	0
			3004	1909	508	576	11			
1	D	381	Total	C	N	O	S	0	7	0
			3017	1917	510	579	11			

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

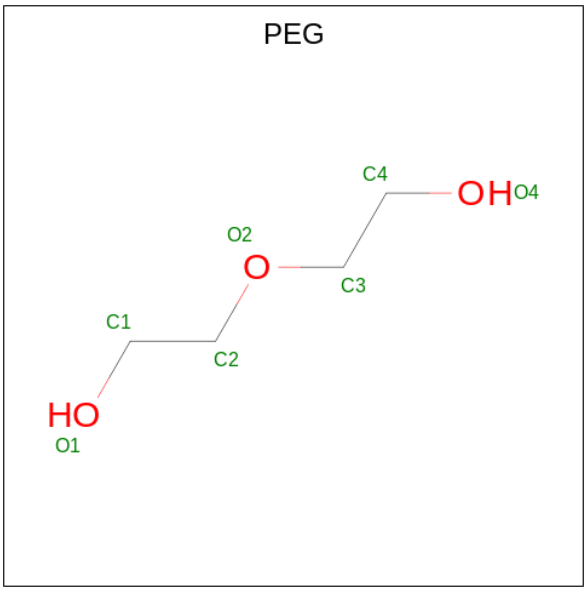
- Molecule 2 is a protein called L-tryptophan decarboxylase PsiD-like domain-containing protein.

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:

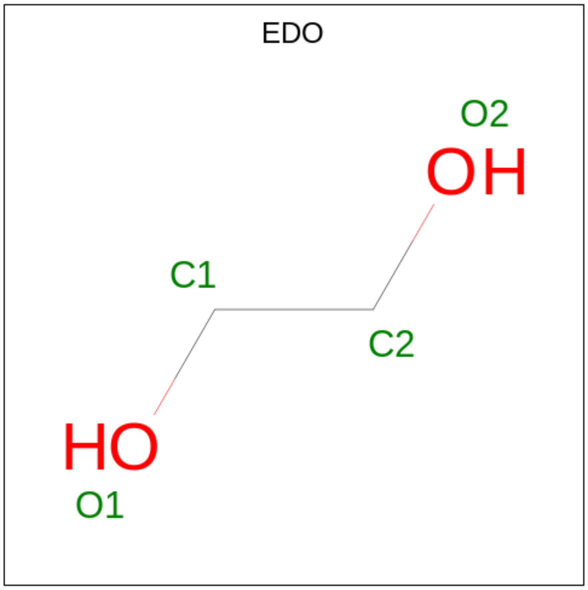
Chain	Residue	Modelled	Actual	Comment	Reference
E	501	PYR	-	modified residue	UNP Q2UAM5
F	501	PYR	-	modified residue	UNP Q2UAM5
G	501	PYR	-	modified residue	UNP Q2UAM5
H	501	PYR	-	modified residue	UNP Q2UAM5

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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	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 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	1
4	B	1	Total C O 4 2 2	0	1
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	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 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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

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

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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.

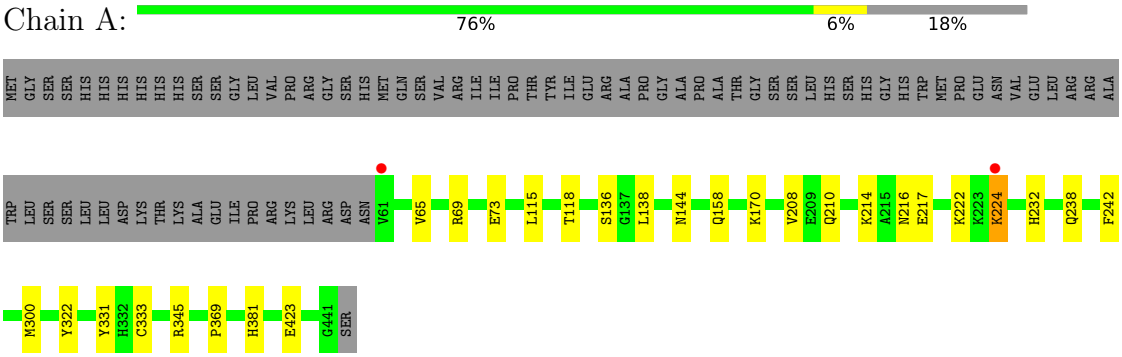
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	417	Total O 418 418	0	1
5	E	42	Total O 42 42	0	0
5	B	374	Total O 376 376	0	2
5	F	32	Total O 32 32	0	0
5	C	365	Total O 366 366	0	1
5	G	34	Total O 35 35	0	1
5	D	407	Total O 407 407	0	0
5	H	37	Total O 37 37	0	0

3 Residue-property plots (i)

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.

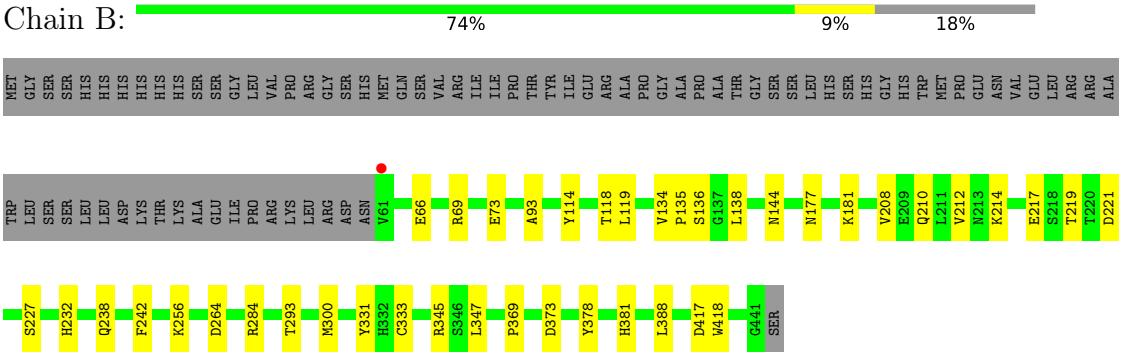
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain A:



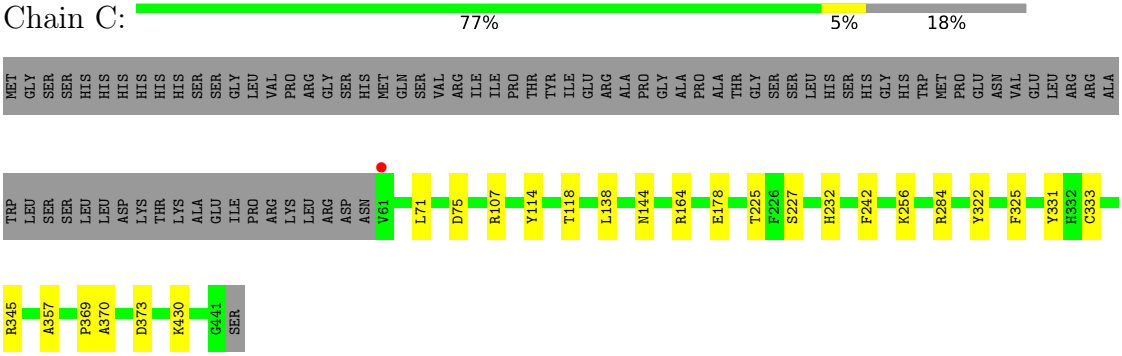
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain B:



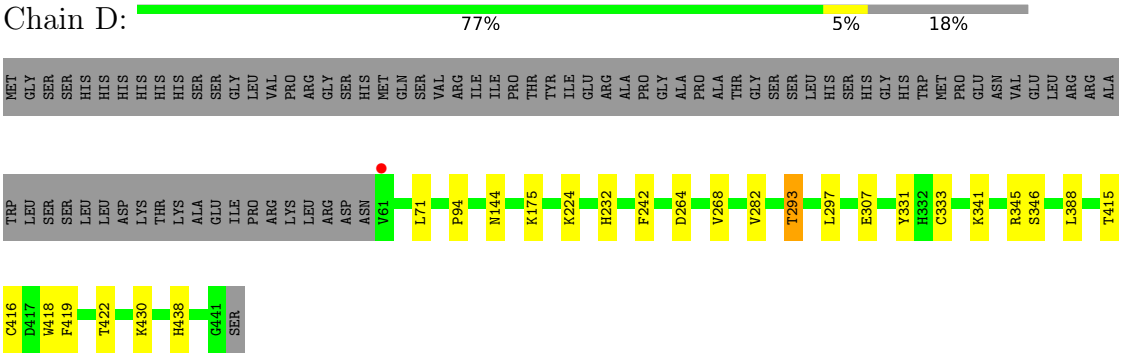
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain C:



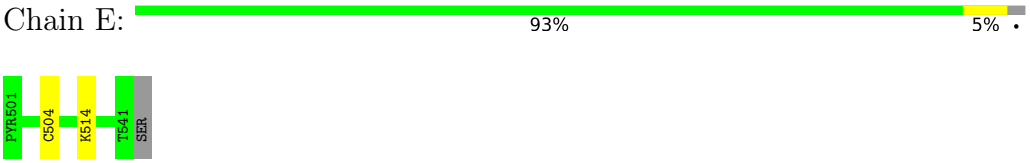
• Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain D:



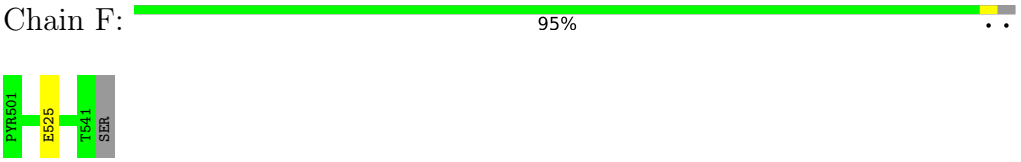
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain E:



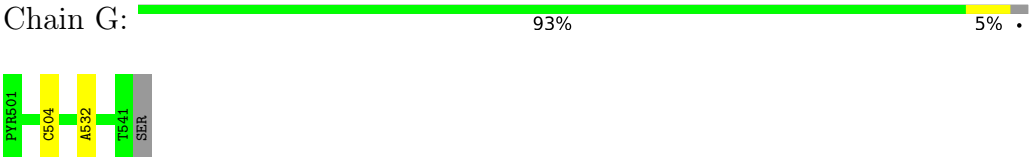
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain F:



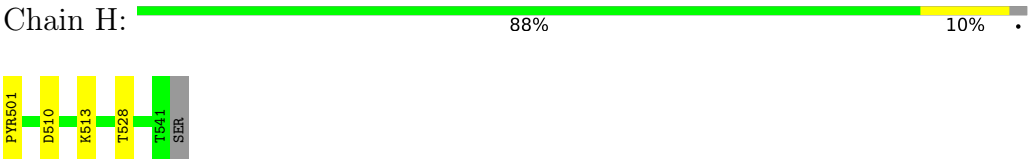
• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain G:



• Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.24 (at 1.90Å)	Xtriage
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	10159 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15694	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, EDO, PYR

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	0.37	0/3134	0.57	0/4257
1	B	0.37	0/3154	0.57	0/4283
1	C	0.36	0/3097	0.56	0/4209
1	D	0.36	0/3113	0.57	0/4232
2	E	0.36	0/331	0.57	0/448
2	F	0.35	0/331	0.56	0/448
2	G	0.32	0/322	0.56	0/436
2	H	0.36	0/331	0.55	0/448
All	All	0.36	0/13813	0.57	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 (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	3029	0	2930	25	0
1	B	3043	0	2945	36	0
1	C	3004	0	2884	23	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	5	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	121	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 (121) 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
1:C:430:LYS:HE2	4:C:527:EDO:H21	1.73	0.69
1:C:75:ASP:HA	4:C:523:EDO:H22	1.78	0.65
1:C:357:ALA:H	4:C:505:EDO:H11	1.62	0.64
1:B:369:PRO:HG3	4:B:537:EDO:H11	1.83	0.60
1:D:416:CYS:HB2	4:D:523:EDO:H12	1.83	0.60
1:B:300[B]:MET:HG3	1:B:381:HIS:CD2	2.37	0.60
1:B:219[B]:THR:HG22	1:B:221:ASP:H	1.66	0.59
1:B:345:ARG:HE	3:B:504:PEG:H21	1.65	0.59
1:B:93:ALA:O	4:B:517:EDO:H12	2.03	0.59
1:D:341:LYS:NZ	5:D:602:HOH:O	2.28	0.59
1:D:71:LEU:HD13	4:D:525:EDO:H22	1.86	0.58
1:B:284[B]:ARG:NH2	4:B:531:EDO:O1	2.36	0.57
1:B:134:VAL:HA	3:B:503:PEG:H41	1.86	0.57
1:C:114:TYR:O	1:C:118:THR:HG23	2.05	0.56
1:A:331:TYR:CZ	1:A:333:CYS:HB2	2.40	0.56
1:A:300[B]:MET:HG3	1:A:381:HIS:CD2	2.40	0.56
3:D:501:PEG:H11	5:D:768:HOH:O	2.04	0.56
1:A:115:LEU:O	1:A:118[B]:THR:HG22	2.06	0.56
1:C:370:ALA:O	3:C:501[A]:PEG:H31	2.05	0.55
1:D:331:TYR:CZ	1:D:333:CYS:HB2	2.41	0.55
1:A:65:VAL:HG12	4:A:520:EDO:H21	1.87	0.55
1:B:177:ASN:OD1	1:B:181:LYS:HE3	2.07	0.55
1:C:325:PHE:CZ	3:C:502[B]:PEG:H11	2.39	0.54
1:D:264:ASP:HA	4:D:519:EDO:H11	1.89	0.54
1:A:158:GLN:NE2	4:A:531:EDO:O1	2.22	0.54
1:B:227:SER:O	1:B:256:LYS:HD2	2.08	0.53
1:C:331:TYR:CZ	1:C:333:CYS:HB2	2.43	0.53
1:D:232:HIS:NE2	4:D:524:EDO:H22	2.24	0.53
1:A:69[B]:ARG:NH1	1:A:73:GLU:OE1	2.42	0.52
1:A:423:GLU:HG2	5:A:981:HOH:O	2.10	0.52
4:C:531:EDO:H12	4:C:533:EDO:H21	1.91	0.52
4:A:530:EDO:H21	1:C:164:ARG:NH2	2.25	0.52
1:B:331:TYR:CZ	1:B:333:CYS:HB2	2.45	0.52
3:B:501:PEG:H21	4:B:510:EDO:O2	2.10	0.52
2:G:532:ALA:H	4:G:603:EDO:C1	2.22	0.51
1:B:210[A]:GLN:NE2	4:B:521:EDO:O1	2.42	0.51
1:B:284[A]:ARG:H	4:B:531:EDO:HO2	1.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284[B]:ARG:H	4:B:531:EDO:HO2	1.55	0.51
1:A:345:ARG:HE	3:A:502:PEG:C3	2.24	0.51
1:A:210:GLN:HG3	4:A:525:EDO:H11	1.93	0.51
1:D:293[B]:THR:HG23	4:D:510:EDO:O1	2.11	0.50
1:C:357:ALA:H	4:C:505:EDO:C1	2.24	0.50
2:G:532:ALA:H	4:G:603:EDO:H11	1.77	0.49
4:A:530:EDO:H21	1:C:164:ARG:HH21	1.78	0.49
1:D:345:ARG:HH11	1:D:422[B]:THR:HG23	1.77	0.49
1:B:135:PRO:HD3	3:B:503:PEG:H41	1.94	0.48
1:B:66[B]:GLU:OE2	5:B:601:HOH:O	2.20	0.48
1:B:119:LEU:HD21	3:B:501:PEG:H31	1.96	0.48
1:C:225:THR:HB	4:C:525:EDO:H12	1.96	0.48
1:B:284[A]:ARG:HH22	4:B:509:EDO:H12	1.79	0.48
1:D:293[A]:THR:HG22	4:D:510:EDO:O1	2.13	0.48
1:A:136:SER:O	4:A:524:EDO:H12	2.14	0.47
2:H:528:THR:HG22	4:H:601:EDO:H12	1.96	0.47
4:A:524:EDO:H22	5:A:737:HOH:O	2.14	0.47
1:B:69[A]:ARG:NH1	1:B:73:GLU:OE1	2.47	0.47
1:A:345:ARG:HE	3:A:502:PEG:H32	1.80	0.47
1:B:135:PRO:HB3	4:B:537:EDO:H12	1.96	0.47
1:B:417:ASP:OD1	5:B:602:HOH:O	2.20	0.47
1:A:224:LYS:HD2	1:A:224:LYS:N	2.21	0.47
2:E:514:LYS:NZ	5:E:702:HOH:O	2.46	0.47
1:C:227:SER:O	1:C:256:LYS:HD2	2.15	0.46
1:D:415:THR:HB	1:D:438:HIS:HB2	1.97	0.46
3:C:502[B]:PEG:H12	5:C:661:HOH:O	2.16	0.46
1:D:388:LEU:HB2	1:D:418:TRP:CH2	2.50	0.46
1:A:118[A]:THR:HG21	4:A:526:EDO:H22	1.97	0.46
5:A:652:HOH:O	4:H:601:EDO:H22	2.16	0.46
1:B:214:LYS:O	1:B:217:GLU:HG2	2.17	0.45
1:C:284:ARG:NH1	4:C:506:EDO:O2	2.40	0.45
1:B:232:HIS:CG	1:B:242:PHE:HB3	2.51	0.45
1:D:419:PHE:O	1:D:422[B]:THR:HG22	2.16	0.45
1:A:216:ASN:HB3	1:A:222:LYS:HG2	1.98	0.44
1:D:293[A]:THR:HG21	5:D:873:HOH:O	2.16	0.44
1:B:66[A]:GLU:OE2	1:B:69[A]:ARG:NH2	2.31	0.44
1:C:369:PRO:HG3	4:C:532:EDO:H12	1.99	0.44
1:A:115:LEU:HD22	4:A:526:EDO:H11	1.99	0.44
1:B:114:TYR:O	1:B:118:THR:HG23	2.18	0.44
1:B:212:VAL:HG21	3:B:502:PEG:H22	1.99	0.44
1:A:208:VAL:HG21	1:A:238:GLN:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LYS:HD2	4:A:518:EDO:C1	2.47	0.43
1:A:369:PRO:HG3	4:A:517:EDO:H21	2.00	0.43
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.84	0.43
1:D:94:PRO:HD3	4:D:522:EDO:H21	2.00	0.43
1:B:208:VAL:HG21	1:B:238:GLN:HG3	2.00	0.43
1:D:345:ARG:HD3	1:D:422[B]:THR:HG23	2.00	0.43
1:B:136:SER:HB2	4:B:521:EDO:H12	2.00	0.43
1:A:214:LYS:O	1:A:217:GLU:HG2	2.19	0.43
3:B:504:PEG:H41	3:B:504:PEG:H22	1.79	0.43
1:C:232:HIS:CG	1:C:242:PHE:HB3	2.54	0.43
2:F:525[B]:GLU:CD	1:C:107[B]:ARG:H	2.22	0.42
4:A:528:EDO:O1	4:B:530:EDO:H11	2.19	0.42
1:C:373:ASP:HB2	3:C:501[A]:PEG:H21	2.02	0.42
1:B:369:PRO:CG	4:B:537:EDO:H11	2.47	0.42
1:D:232:HIS:CG	1:D:242:PHE:HB3	2.54	0.42
1:A:322:TYR:O	2:E:504:CYS:HA	2.21	0.41
1:C:71:LEU:HD13	4:C:516:EDO:H21	2.02	0.41
2:H:510:ASP:HA	2:H:513:LYS:HD3	2.02	0.41
1:D:346:SER:HA	3:D:501:PEG:H31	2.02	0.41
1:B:347:LEU:HD11	4:B:533:EDO:H11	2.02	0.41
1:B:373:ASP:HB2	4:B:511:EDO:H12	2.02	0.41
1:A:170:LYS:HD2	4:A:518:EDO:H11	2.02	0.41
1:D:293[B]:THR:HG21	5:D:873:HOH:O	2.21	0.41
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.86	0.41
1:D:268:VAL:HG13	1:D:430:LYS:HD2	2.03	0.41
1:A:232:HIS:CG	1:A:242:PHE:HB3	2.56	0.41
1:C:178[B]:GLU:HG2	4:C:511:EDO:H12	2.02	0.41
1:D:175:LYS:HB2	1:D:175:LYS:HE2	1.91	0.41
1:C:373:ASP:OD1	4:C:510:EDO:H12	2.20	0.41
5:A:666:HOH:O	4:C:528:EDO:H21	2.21	0.40
1:B:388:LEU:HB2	1:B:418:TRP:CH2	2.56	0.40
1:B:293:THR:HG21	1:B:378:TYR:N	2.36	0.40
1:B:135:PRO:N	3:B:503:PEG:H11	2.36	0.40
1:B:227:SER:O	4:B:526:EDO:O1	2.40	0.40
1:A:210:GLN:O	4:A:525:EDO:H22	2.21	0.40
1:C:322:TYR:O	2:G:504:CYS:HA	2.21	0.40
1:D:282:VAL:HG23	1:D:297:LEU:HD11	2.03	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	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%)	326 (99%)	2 (1%)	84	86
1	B	330/389 (85%)	329 (100%)	1 (0%)	91	92
1	C	324/389 (83%)	322 (99%)	2 (1%)	84	86
1	D	326/389 (84%)	321 (98%)	5 (2%)	60	59
2	E	36/36 (100%)	36 (100%)	0	100	100
2	F	36/36 (100%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	1441 (99%)	10 (1%)	84 83

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	224	LYS
1	B	144	ASN
1	C	138	LEU
1	C	144	ASN
1	D	144	ASN
1	D	224	LYS
1	D	293[A]	THR
1	D	293[B]	THR
1	D	307	GLU

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 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	A	507	-	3,3,3	0.24	0	2,2,2	0.33	0
4	EDO	D	503	-	3,3,3	0.25	0	2,2,2	0.25	0
4	EDO	B	506	-	3,3,3	0.25	0	2,2,2	0.53	0
4	EDO	C	523	-	3,3,3	0.29	0	2,2,2	0.06	0
4	EDO	A	532	-	3,3,3	0.20	0	2,2,2	0.78	0
4	EDO	A	525	-	3,3,3	0.29	0	2,2,2	0.32	0
4	EDO	B	528	-	3,3,3	0.27	0	2,2,2	0.35	0
4	EDO	H	601	-	3,3,3	0.27	0	2,2,2	0.14	0
4	EDO	D	506	-	3,3,3	0.29	0	2,2,2	0.17	0
4	EDO	C	529	-	3,3,3	0.36	0	2,2,2	0.25	0
4	EDO	C	531	-	3,3,3	0.36	0	2,2,2	0.51	0
4	EDO	C	503	-	3,3,3	0.26	0	2,2,2	0.25	0
4	EDO	C	533	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	B	536	-	3,3,3	0.33	0	2,2,2	0.35	0
4	EDO	C	511	-	3,3,3	0.27	0	2,2,2	0.24	0
4	EDO	D	514	-	3,3,3	0.26	0	2,2,2	0.45	0
3	PEG	C	501[A]	-	6,6,6	0.20	0	5,5,5	0.25	0
4	EDO	E	602	-	3,3,3	0.27	0	2,2,2	0.50	0
4	EDO	B	534	-	3,3,3	0.24	0	2,2,2	0.22	0
4	EDO	B	523	-	3,3,3	0.26	0	2,2,2	0.27	0
3	PEG	A	501	-	6,6,6	0.33	0	5,5,5	0.46	0
4	EDO	A	514	-	3,3,3	0.32	0	2,2,2	0.29	0
4	EDO	B	510	-	3,3,3	0.27	0	2,2,2	0.18	0
4	EDO	D	520	-	3,3,3	0.27	0	2,2,2	0.19	0
4	EDO	D	518	-	3,3,3	0.28	0	2,2,2	0.27	0
4	EDO	D	524	-	3,3,3	0.26	0	2,2,2	0.22	0
4	EDO	C	532	-	3,3,3	0.43	0	2,2,2	0.40	0
4	EDO	A	524	-	3,3,3	0.21	0	2,2,2	0.28	0
4	EDO	C	512	-	3,3,3	0.23	0	2,2,2	0.54	0
4	EDO	C	534	-	3,3,3	0.28	0	2,2,2	0.19	0
4	EDO	B	513	-	3,3,3	0.31	0	2,2,2	0.19	0
4	EDO	C	507	-	3,3,3	0.32	0	2,2,2	0.17	0
3	PEG	C	502[B]	-	6,6,6	0.24	0	5,5,5	0.58	0
4	EDO	A	505	-	3,3,3	0.20	0	2,2,2	0.46	0
4	EDO	C	515	-	3,3,3	0.29	0	2,2,2	0.19	0
4	EDO	A	516	-	3,3,3	0.31	0	2,2,2	0.11	0
3	PEG	B	503	-	6,6,6	0.24	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	B	531	-	3,3,3	0.32	0	2,2,2	0.30	0
4	EDO	A	520	-	3,3,3	0.28	0	2,2,2	0.26	0
4	EDO	C	521	-	3,3,3	0.30	0	2,2,2	0.13	0
4	EDO	D	515	-	3,3,3	0.26	0	2,2,2	0.25	0
4	EDO	A	522	-	3,3,3	0.28	0	2,2,2	0.11	0
3	PEG	B	501	-	6,6,6	0.24	0	5,5,5	0.47	0
3	PEG	B	504	-	6,6,6	0.26	0	5,5,5	0.43	0
4	EDO	B	511	-	3,3,3	0.26	0	2,2,2	0.35	0
4	EDO	C	527	-	3,3,3	0.28	0	2,2,2	0.14	0
4	EDO	A	529	-	3,3,3	0.24	0	2,2,2	0.35	0
4	EDO	A	533	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	B	530	-	3,3,3	0.28	0	2,2,2	0.26	0
4	EDO	B	537	-	3,3,3	0.27	0	2,2,2	0.35	0
4	EDO	C	524	-	3,3,3	0.29	0	2,2,2	0.10	0
4	EDO	A	531	-	3,3,3	0.20	0	2,2,2	0.43	0
4	EDO	C	514	-	3,3,3	0.28	0	2,2,2	0.16	0
4	EDO	A	513	-	3,3,3	0.36	0	2,2,2	0.32	0
4	EDO	C	505	-	3,3,3	0.33	0	2,2,2	0.59	0
4	EDO	C	509	-	3,3,3	0.27	0	2,2,2	0.38	0
4	EDO	D	505	-	3,3,3	0.31	0	2,2,2	0.08	0
4	EDO	D	525	-	3,3,3	0.25	0	2,2,2	0.17	0
4	EDO	B	524	-	3,3,3	0.26	0	2,2,2	0.49	0
4	EDO	B	526	-	3,3,3	0.28	0	2,2,2	0.22	0
4	EDO	A	508	-	3,3,3	0.27	0	2,2,2	0.21	0
4	EDO	B	512	-	3,3,3	0.33	0	2,2,2	0.02	0
4	EDO	A	530	-	3,3,3	0.32	0	2,2,2	0.50	0
4	EDO	B	505	-	3,3,3	0.18	0	2,2,2	0.62	0
4	EDO	D	511	-	3,3,3	0.28	0	2,2,2	0.36	0
4	EDO	A	504	-	3,3,3	0.27	0	2,2,2	0.34	0
4	EDO	B	525	-	3,3,3	0.24	0	2,2,2	0.33	0
4	EDO	D	512	-	3,3,3	0.30	0	2,2,2	0.19	0
4	EDO	B	522	-	3,3,3	0.29	0	2,2,2	0.19	0
4	EDO	A	518	-	3,3,3	0.28	0	2,2,2	0.07	0
4	EDO	B	529	-	3,3,3	0.25	0	2,2,2	0.37	0
4	EDO	B	521	-	3,3,3	0.30	0	2,2,2	0.27	0
4	EDO	B	533	-	3,3,3	0.33	0	2,2,2	0.18	0
4	EDO	B	516	-	3,3,3	0.28	0	2,2,2	0.31	0
4	EDO	A	506	-	3,3,3	0.23	0	2,2,2	0.51	0
4	EDO	A	512	-	3,3,3	0.23	0	2,2,2	0.31	0
3	PEG	D	502	-	6,6,6	0.25	0	5,5,5	0.52	0
4	EDO	C	504	-	3,3,3	0.26	0	2,2,2	0.33	0
4	EDO	B	538	-	3,3,3	0.27	0	2,2,2	0.26	0
4	EDO	B	509	-	3,3,3	0.28	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	521	-	3,3,3	0.26	0	2,2,2	0.25	0
4	EDO	D	510	-	3,3,3	0.27	0	2,2,2	0.26	0
4	EDO	A	519	-	3,3,3	0.27	0	2,2,2	0.21	0
4	EDO	D	508	-	3,3,3	0.27	0	2,2,2	0.21	0
4	EDO	A	511	-	3,3,3	0.30	0	2,2,2	0.34	0
4	EDO	E	601	-	3,3,3	0.27	0	2,2,2	0.09	0
4	EDO	B	532	-	3,3,3	0.28	0	2,2,2	0.23	0
4	EDO	D	507	-	3,3,3	0.19	0	2,2,2	0.92	0
4	EDO	C	508	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	G	601	-	3,3,3	0.33	0	2,2,2	0.19	0
4	EDO	A	503	-	3,3,3	0.35	0	2,2,2	0.09	0
4	EDO	A	510	-	3,3,3	0.27	0	2,2,2	0.14	0
4	EDO	A	526	-	3,3,3	0.25	0	2,2,2	0.39	0
4	EDO	B	508	-	3,3,3	0.23	0	2,2,2	0.30	0
4	EDO	D	523	-	3,3,3	0.32	0	2,2,2	0.51	0
4	EDO	C	519	-	3,3,3	0.27	0	2,2,2	0.14	0
4	EDO	D	519	-	3,3,3	0.28	0	2,2,2	0.31	0
4	EDO	A	515	-	3,3,3	0.27	0	2,2,2	0.34	0
3	PEG	D	501	-	6,6,6	0.21	0	5,5,5	0.48	0
4	EDO	B	517	-	3,3,3	0.26	0	2,2,2	0.29	0
4	EDO	B	515	-	3,3,3	0.28	0	2,2,2	0.38	0
4	EDO	C	510	-	3,3,3	0.26	0	2,2,2	0.25	0
4	EDO	C	518	-	3,3,3	0.32	0	2,2,2	0.14	0
4	EDO	C	522	-	3,3,3	0.27	0	2,2,2	0.29	0
4	EDO	C	525	-	3,3,3	0.29	0	2,2,2	0.11	0
4	EDO	B	507	-	3,3,3	0.27	0	2,2,2	0.21	0
4	EDO	D	504	-	3,3,3	0.18	0	2,2,2	1.03	0
4	EDO	D	513	-	3,3,3	0.26	0	2,2,2	0.29	0
4	EDO	E	603	-	3,3,3	0.30	0	2,2,2	0.21	0
4	EDO	A	527	-	3,3,3	0.28	0	2,2,2	0.18	0
4	EDO	C	530	-	3,3,3	0.27	0	2,2,2	0.18	0
4	EDO	C	506	-	3,3,3	0.29	0	2,2,2	0.30	0
4	EDO	C	513	-	3,3,3	0.35	0	2,2,2	0.02	0
4	EDO	A	517	-	3,3,3	0.40	0	2,2,2	0.38	0
4	EDO	C	528	-	3,3,3	0.25	0	2,2,2	0.46	0
4	EDO	B	520[B]	-	3,3,3	0.25	0	2,2,2	0.42	0
4	EDO	G	602	-	3,3,3	0.29	0	2,2,2	0.36	0
4	EDO	B	535	-	3,3,3	0.27	0	2,2,2	0.20	0
4	EDO	B	514	-	3,3,3	0.28	0	2,2,2	0.21	0
4	EDO	C	526	-	3,3,3	0.25	0	2,2,2	0.26	0
4	EDO	A	528	-	3,3,3	0.22	0	2,2,2	0.26	0
4	EDO	D	522	-	3,3,3	0.29	0	2,2,2	0.15	0
4	EDO	D	521	-	3,3,3	0.26	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	C	520	-	3,3,3	0.26	0	2,2,2	0.42	0
4	EDO	A	509	-	3,3,3	0.26	0	2,2,2	0.41	0
4	EDO	A	523	-	3,3,3	0.27	0	2,2,2	0.19	0
4	EDO	C	517	-	3,3,3	0.29	0	2,2,2	0.25	0
3	PEG	A	502	-	6,6,6	0.24	0	5,5,5	0.62	0
4	EDO	D	517	-	3,3,3	0.26	0	2,2,2	0.31	0
4	EDO	B	519[A]	-	3,3,3	0.27	0	2,2,2	0.31	0
4	EDO	B	518	-	3,3,3	0.26	0	2,2,2	0.42	0
4	EDO	G	603	-	3,3,3	0.27	0	2,2,2	0.37	0
4	EDO	B	527	-	3,3,3	0.29	0	2,2,2	0.18	0
4	EDO	F	601	-	3,3,3	0.31	0	2,2,2	0.32	0
4	EDO	D	509	-	3,3,3	0.18	0	2,2,2	0.55	0
3	PEG	B	502	-	6,6,6	0.28	0	5,5,5	0.24	0
4	EDO	C	516	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	D	516	-	3,3,3	0.35	0	2,2,2	0.10	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
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	C	523	-	-	1/1/1/1	-
4	EDO	A	532	-	-	1/1/1/1	-
4	EDO	A	525	-	-	0/1/1/1	-
4	EDO	B	528	-	-	0/1/1/1	-
4	EDO	H	601	-	-	0/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	C	529	-	-	0/1/1/1	-
4	EDO	C	531	-	-	1/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	C	533	-	-	0/1/1/1	-
4	EDO	B	536	-	-	1/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-
4	EDO	D	514	-	-	1/1/1/1	-
3	PEG	C	501[A]	-	-	4/4/4/4	-
4	EDO	E	602	-	-	0/1/1/1	-
4	EDO	B	534	-	-	0/1/1/1	-
4	EDO	B	523	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	501	-	-	3/4/4/4	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	D	524	-	-	0/1/1/1	-
4	EDO	C	532	-	-	1/1/1/1	-
4	EDO	A	524	-	-	0/1/1/1	-
4	EDO	C	512	-	-	1/1/1/1	-
4	EDO	C	534	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
3	PEG	C	502[B]	-	-	2/4/4/4	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	A	516	-	-	1/1/1/1	-
3	PEG	B	503	-	-	4/4/4/4	-
4	EDO	B	531	-	-	0/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
4	EDO	C	521	-	-	0/1/1/1	-
4	EDO	D	515	-	-	0/1/1/1	-
4	EDO	A	522	-	-	0/1/1/1	-
3	PEG	B	501	-	-	2/4/4/4	-
3	PEG	B	504	-	-	2/4/4/4	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	C	527	-	-	1/1/1/1	-
4	EDO	A	529	-	-	0/1/1/1	-
4	EDO	A	533	-	-	1/1/1/1	-
4	EDO	B	530	-	-	1/1/1/1	-
4	EDO	B	537	-	-	1/1/1/1	-
4	EDO	C	524	-	-	1/1/1/1	-
4	EDO	A	531	-	-	1/1/1/1	-
4	EDO	C	514	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	C	505	-	-	1/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	D	525	-	-	1/1/1/1	-
4	EDO	B	524	-	-	0/1/1/1	-
4	EDO	B	526	-	-	0/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	512	-	-	0/1/1/1	-
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	B	525	-	-	0/1/1/1	-
4	EDO	D	512	-	-	0/1/1/1	-
4	EDO	B	522	-	-	0/1/1/1	-
4	EDO	A	518	-	-	1/1/1/1	-
4	EDO	B	529	-	-	1/1/1/1	-
4	EDO	B	521	-	-	1/1/1/1	-
4	EDO	B	533	-	-	0/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
3	PEG	D	502	-	-	1/4/4/4	-
4	EDO	C	504	-	-	0/1/1/1	-
4	EDO	B	538	-	-	1/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
4	EDO	A	521	-	-	0/1/1/1	-
4	EDO	D	510	-	-	0/1/1/1	-
4	EDO	A	519	-	-	1/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	E	601	-	-	1/1/1/1	-
4	EDO	B	532	-	-	0/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	G	601	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	A	526	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	D	523	-	-	1/1/1/1	-
4	EDO	C	519	-	-	1/1/1/1	-
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	A	515	-	-	0/1/1/1	-
3	PEG	D	501	-	-	1/4/4/4	-
4	EDO	B	517	-	-	1/1/1/1	-
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	522	-	-	1/1/1/1	-
4	EDO	C	525	-	-	0/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	D	504	-	-	1/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	E	603	-	-	1/1/1/1	-
4	EDO	A	527	-	-	1/1/1/1	-
4	EDO	C	530	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	A	517	-	-	1/1/1/1	-
4	EDO	C	528	-	-	0/1/1/1	-
4	EDO	B	520[B]	-	-	0/1/1/1	-
4	EDO	G	602	-	-	1/1/1/1	-
4	EDO	B	535	-	-	1/1/1/1	-
4	EDO	B	514	-	-	1/1/1/1	-
4	EDO	C	526	-	-	1/1/1/1	-
4	EDO	A	528	-	-	0/1/1/1	-
4	EDO	D	522	-	-	0/1/1/1	-
4	EDO	D	521	-	-	0/1/1/1	-
4	EDO	C	520	-	-	0/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	523	-	-	0/1/1/1	-
4	EDO	C	517	-	-	0/1/1/1	-
3	PEG	A	502	-	-	3/4/4/4	-
4	EDO	D	517	-	-	1/1/1/1	-
4	EDO	B	519[A]	-	-	1/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
4	EDO	G	603	-	-	1/1/1/1	-
4	EDO	B	527	-	-	1/1/1/1	-
4	EDO	F	601	-	-	0/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
3	PEG	B	502	-	-	2/4/4/4	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (81) 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	504	EDO	O1-C1-C2-O2
4	A	516	EDO	O1-C1-C2-O2
4	A	517	EDO	O1-C1-C2-O2
4	A	530	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
4	B	514	EDO	O1-C1-C2-O2
4	B	517	EDO	O1-C1-C2-O2
4	B	523	EDO	O1-C1-C2-O2
4	B	530	EDO	O1-C1-C2-O2
4	B	537	EDO	O1-C1-C2-O2
4	C	514	EDO	O1-C1-C2-O2
4	C	523	EDO	O1-C1-C2-O2
4	C	527	EDO	O1-C1-C2-O2
4	C	532	EDO	O1-C1-C2-O2
4	G	603	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
4	D	520	EDO	O1-C1-C2-O2
4	D	525	EDO	O1-C1-C2-O2
3	A	501	PEG	O2-C3-C4-O4
3	A	502	PEG	O2-C3-C4-O4
3	B	503	PEG	O2-C3-C4-O4
3	C	501[A]	PEG	O1-C1-C2-O2
4	A	519	EDO	O1-C1-C2-O2
4	E	603	EDO	O1-C1-C2-O2
4	C	518	EDO	O1-C1-C2-O2
4	C	519	EDO	O1-C1-C2-O2
4	G	602	EDO	O1-C1-C2-O2
4	B	509	EDO	O1-C1-C2-O2
4	B	529	EDO	O1-C1-C2-O2
4	B	538	EDO	O1-C1-C2-O2
4	C	522	EDO	O1-C1-C2-O2
4	C	524	EDO	O1-C1-C2-O2
3	B	502	PEG	O1-C1-C2-O2
3	C	502[B]	PEG	O2-C3-C4-O4
3	C	501[A]	PEG	C1-C2-O2-C3
3	C	501[A]	PEG	C4-C3-O2-C2
3	B	501	PEG	C1-C2-O2-C3
3	B	502	PEG	C1-C2-O2-C3
3	A	501	PEG	O1-C1-C2-O2
3	B	503	PEG	O1-C1-C2-O2
4	A	532	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	533	EDO	O1-C1-C2-O2
4	B	535	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2
4	A	531	EDO	O1-C1-C2-O2
4	B	521	EDO	O1-C1-C2-O2
4	B	536	EDO	O1-C1-C2-O2
4	C	508	EDO	O1-C1-C2-O2
4	C	511	EDO	O1-C1-C2-O2
4	C	531	EDO	O1-C1-C2-O2
4	D	513	EDO	O1-C1-C2-O2
3	C	502[B]	PEG	C4-C3-O2-C2
3	B	501	PEG	C4-C3-O2-C2
3	D	502	PEG	C1-C2-O2-C3
4	A	527	EDO	O1-C1-C2-O2
4	D	504	EDO	O1-C1-C2-O2
3	A	501	PEG	C1-C2-O2-C3
3	B	503	PEG	C1-C2-O2-C3
3	D	501	PEG	C4-C3-O2-C2
4	B	505	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	B	527	EDO	O1-C1-C2-O2
4	C	526	EDO	O1-C1-C2-O2
4	G	601	EDO	O1-C1-C2-O2
4	A	518	EDO	O1-C1-C2-O2
4	E	601	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	B	519[A]	EDO	O1-C1-C2-O2
4	C	505	EDO	O1-C1-C2-O2
4	C	512	EDO	O1-C1-C2-O2
4	C	534	EDO	O1-C1-C2-O2
4	D	514	EDO	O1-C1-C2-O2
4	D	517	EDO	O1-C1-C2-O2
4	D	523	EDO	O1-C1-C2-O2
3	A	502	PEG	O1-C1-C2-O2
3	A	502	PEG	C4-C3-O2-C2
3	B	503	PEG	C4-C3-O2-C2
3	B	504	PEG	C1-C2-O2-C3

There are no ring outliers.

50 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	523	EDO	1	0
4	A	525	EDO	2	0
4	B	528	EDO	1	0
4	H	601	EDO	2	0
4	C	529	EDO	1	0
4	C	531	EDO	1	0
4	C	533	EDO	1	0
4	C	511	EDO	1	0
3	C	501[A]	PEG	2	0
4	B	510	EDO	1	0
4	D	524	EDO	1	0
4	C	532	EDO	1	0
4	A	524	EDO	2	0
3	C	502[B]	PEG	3	0
4	C	515	EDO	1	0
3	B	503	PEG	3	0
4	B	531	EDO	3	0
4	A	520	EDO	1	0
3	B	501	PEG	2	0
3	B	504	PEG	2	0
4	B	511	EDO	1	0
4	C	527	EDO	1	0
4	B	530	EDO	1	0
4	B	537	EDO	3	0
4	A	531	EDO	1	0
4	C	505	EDO	2	0
4	D	525	EDO	1	0
4	B	526	EDO	1	0
4	A	530	EDO	2	0
4	A	518	EDO	2	0
4	B	521	EDO	2	0
4	B	533	EDO	1	0
4	B	509	EDO	1	0
4	D	510	EDO	2	0
4	A	526	EDO	2	0
4	D	523	EDO	1	0
4	D	519	EDO	1	0
3	D	501	PEG	2	0
4	B	517	EDO	1	0
4	C	510	EDO	1	0
4	C	525	EDO	1	0
4	C	506	EDO	1	0
4	A	517	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	528	EDO	1	0
4	A	528	EDO	1	0
4	D	522	EDO	1	0
3	A	502	PEG	2	0
4	G	603	EDO	2	0
3	B	502	PEG	1	0
4	C	516	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	A	381/462 (82%)	-0.56	2 (0%)	87	88	12, 24, 34, 63	9 (2%)
1	B	381/462 (82%)	-0.46	1 (0%)	90	91	12, 25, 38, 66	11 (2%)
1	C	381/462 (82%)	-0.18	1 (0%)	90	91	12, 28, 42, 55	5 (1%)
1	D	381/462 (82%)	-0.34	1 (0%)	90	91	13, 27, 38, 56	7 (1%)
2	E	40/42 (95%)	-0.40	0	100	100	12, 26, 43, 48	1 (2%)
2	F	40/42 (95%)	-0.34	0	100	100	16, 27, 41, 48	1 (2%)
2	G	40/42 (95%)	-0.07	0	100	100	24, 28, 48, 51	0
2	H	40/42 (95%)	-0.23	0	100	100	15, 27, 43, 44	1 (2%)
All	All	1684/2016 (83%)	-0.37	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	5.3
1	B	61	VAL	4.4
1	D	61	VAL	3.2
1	A	224	LYS	2.4
1	C	61	VAL	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 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^{th} 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^2)	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(Å^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(Å^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^2)	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.