



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 08:43 AM EST

PDB ID : 3W88  
Title : Structure of Trypanosoma cruzi dihydroorotate dehydrogenase in complex with SH-1-200  
Authors : Inaoka, D.K.; Hashimoto, S.; Rocha, J.R.; Iida, M.; Tabuchi, T.; Lee, N.; Matsuoka, S.; Kuranaga, T.; Shiba, T.; Balogun, E.O.; Sakamoto, K.; Suzuki, S.; Montanari, C.A.; Nara, T.; Aoki, T.; Inoue, M.; Honma, T.; Tanaka, A.; Harada, S.; Kita, K.  
Deposited on : unknown  
Resolution : 1.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

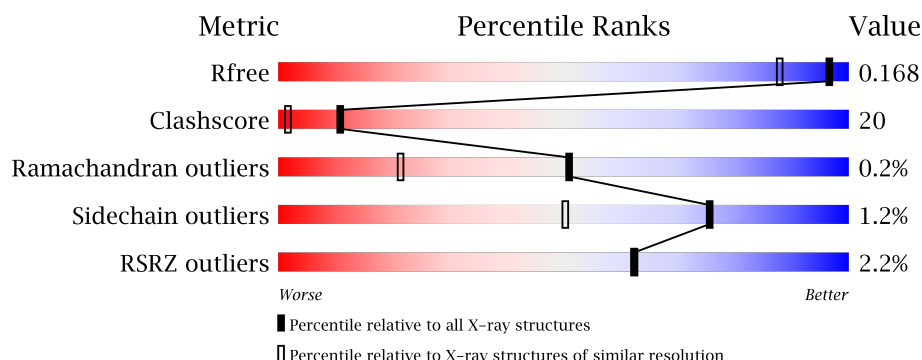
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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))
$R_{free}$	100719	1307 (1.40-1.40)
Clashscore	112137	1411 (1.40-1.40)
Ramachandran outliers	110173	1373 (1.40-1.40)
Sidechain outliers	110143	1372 (1.40-1.40)
RSRZ outliers	101464	1315 (1.40-1.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	314	<div> <div>3%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	B	314	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	406	-	-	-	X
3	GOL	A	407[A]	-	-	-	X
3	GOL	A	409	-	-	-	X
3	GOL	A	410	-	-	-	X
3	GOL	A	412	-	-	-	X
3	GOL	A	414	-	-	-	X
3	GOL	B	402	-	-	-	X
3	GOL	B	403	-	-	-	X
3	GOL	B	404[A]	-	-	-	X
3	GOL	B	406	-	-	-	X
3	GOL	B	407	-	-	-	X
3	GOL	B	408	-	-	-	X
3	GOL	B	409	-	-	-	X
3	GOL	B	410	-	-	-	X
3	GOL	B	412	-	-	X	X
4	CAC	A	415	-	-	-	X
4	CAC	B	413	-	-	-	X
6	EDO	A	418	-	-	-	X
6	EDO	A	422	-	-	-	X
6	EDO	A	423	-	-	X	X
6	EDO	A	424	-	-	-	X
6	EDO	A	432	-	-	-	X
6	EDO	A	433	-	-	X	-
6	EDO	A	434	-	-	X	X
6	EDO	A	435	-	-	X	X
6	EDO	B	416	-	-	X	X
6	EDO	B	418	-	-	X	X
6	EDO	B	421	-	-	-	X
6	EDO	B	422	-	-	-	X
6	EDO	B	424	-	-	X	X
6	EDO	B	425	-	-	-	X
6	EDO	B	426	-	-	-	X
6	EDO	B	427	-	-	-	X
7	PEG	A	436	-	-	-	X
7	PEG	A	437[A]	-	-	X	-
7	PEG	A	437[B]	-	-	X	-
7	PEG	A	438	-	-	X	X
7	PEG	A	439	-	-	X	-
7	PEG	A	440	-	-	X	-
7	PEG	B	432	-	-	X	X
7	PEG	B	433	-	-	X	X
8	NCO	A	441	-	-	-	X
8	NCO	A	442[A]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NCO	A	442[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6466 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.

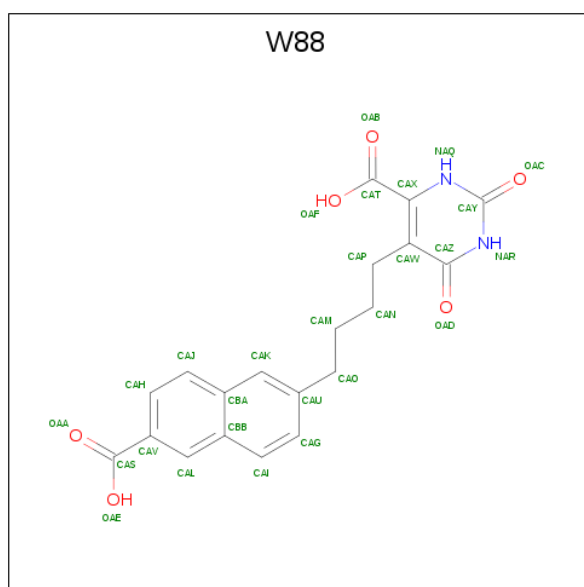
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (fumarate).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	19	0
			2554	1629	427	479	19			
1	B	314	Total	C	N	O	S	0	17	0
			2533	1609	427	478	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q4D3W2
B	-1	SER	-	EXPRESSION TAG	UNP Q4D3W2

- Molecule 2 is 5-[4-(6-carboxynaphthalen-2-yl)butyl]-2,6-dioxo-1,2,3,6-tetrahydropyrimidine-4-carboxylic acid (three-letter code: W88) (formula: C<sub>20</sub>H<sub>18</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	20	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	1
			56	40	4	12		

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



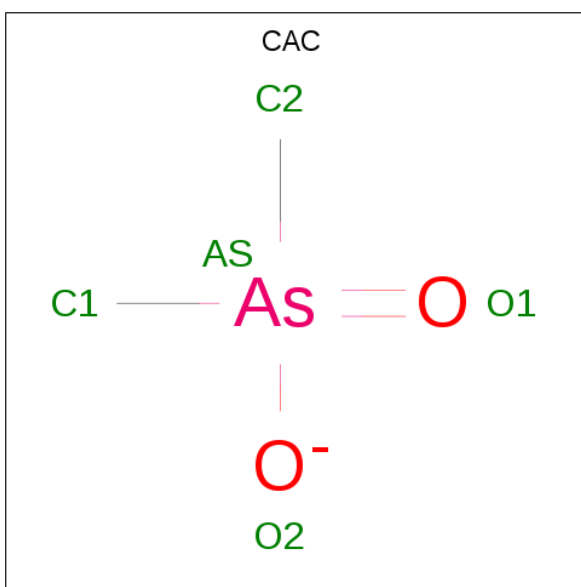
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	1
			12	6	6		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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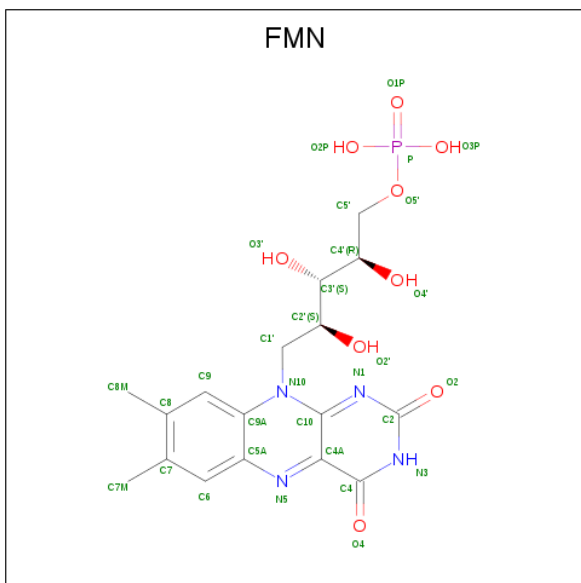
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
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 CACODYLATE ION (three-letter code: CAC) (formula:  $\text{C}_2\text{H}_6\text{AsO}_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	A	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		
4	B	1	Total	As	C	O	0	0
			5	1	2	2		

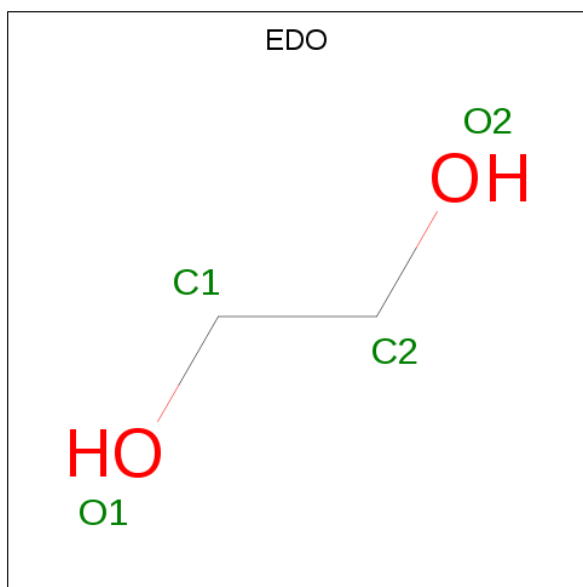
- Molecule 5 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
5	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 6 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
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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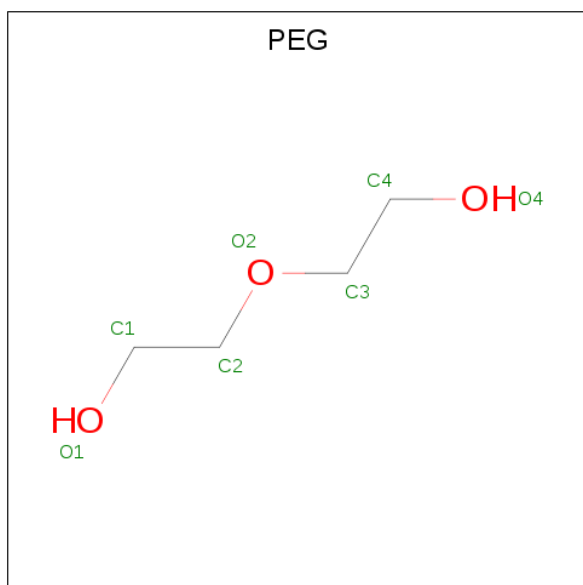
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	A	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0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

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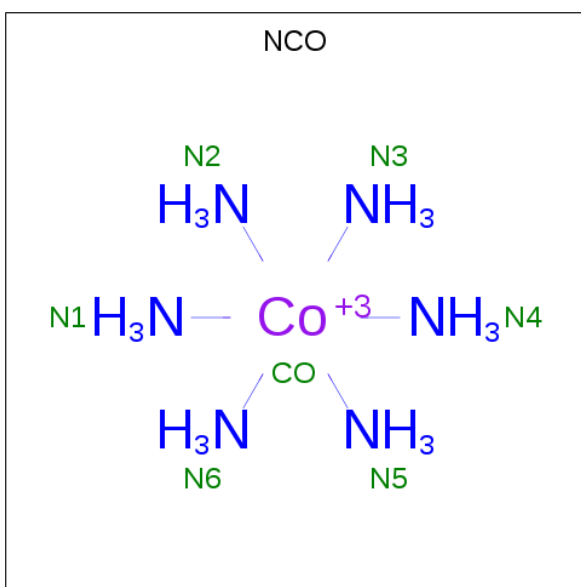
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	1
			14	8	6		
7	A	1	Total	C	O	0	0
			7	4	3		
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	1
			14	8	6		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula:  $CoH_{18}N_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	Co	N	0	0
			7	1	6		
8	A	1	Total	Co	N	0	1
			14	2	12		

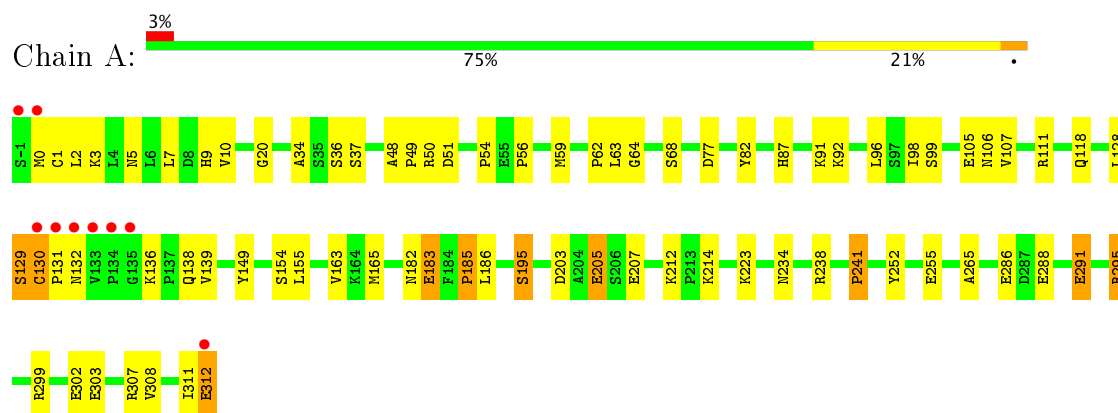
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	371	Total	O	0	10
			381	381		
9	B	440	Total	O	0	7
			447	447		

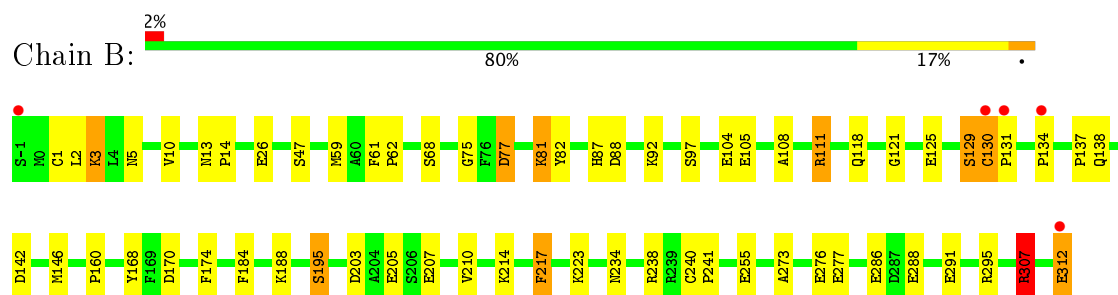
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dihydroorotate dehydrogenase (fumarate)



- Molecule 1: Dihydroorotate dehydrogenase (fumarate)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.97Å 71.52Å 129.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.96 – 1.40 36.96 – 1.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (36.96-1.40) 95.1 (36.96-1.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.139 , 0.166 0.143 , 0.168	Depositor DCC
$R_{free}$ test set	5941 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.3	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6466	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6031e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, W88, EDO, FMN, NCO, CAC, 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	1.62	29/2606 (1.1%)	1.21	6/3524 (0.2%)
1	B	1.52	27/2585 (1.0%)	1.29	26/3496 (0.7%)
All	All	1.57	56/5191 (1.1%)	1.25	32/7020 (0.5%)

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	A	0	2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130[A]	CYS	C-N	18.62	1.69	1.34
1	A	130[B]	CYS	C-N	18.62	1.69	1.34
1	B	205[A]	GLU	CD-OE2	-11.18	1.13	1.25
1	B	205[B]	GLU	CD-OE2	-11.18	1.13	1.25
1	B	105	GLU	CD-OE1	-10.49	1.14	1.25
1	A	303	GLU	CD-OE1	-10.22	1.14	1.25
1	B	255	GLU	CD-OE1	-9.26	1.15	1.25
1	A	255	GLU	CD-OE1	-9.19	1.15	1.25
1	B	207	GLU	CD-OE1	-8.60	1.16	1.25
1	A	288	GLU	CD-OE2	-8.58	1.16	1.25
1	A	207	GLU	CD-OE1	-8.39	1.16	1.25
1	B	291	GLU	CG-CD	8.21	1.64	1.51
1	A	183	GLU	CD-OE2	-7.76	1.17	1.25
1	B	3	LYS	CE-NZ	7.74	1.68	1.49
1	B	195	SER	CB-OG	-7.39	1.32	1.42
1	A	183	GLU	CD-OE1	-7.15	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	N-CD	7.04	1.57	1.47
1	B	1	CYS	CB-SG	-7.04	1.70	1.82
1	A	185	PRO	N-CD	7.03	1.57	1.47
1	A	62	PRO	N-CD	6.99	1.57	1.47
1	A	49	PRO	N-CD	6.97	1.57	1.47
1	A	64	GLY	C-O	-6.91	1.12	1.23
1	B	3	LYS	CD-CE	6.81	1.68	1.51
1	B	288	GLU	CD-OE2	-6.71	1.18	1.25
1	B	288	GLU	CD-OE1	-6.48	1.18	1.25
1	A	241	PRO	N-CD	6.33	1.56	1.47
1	B	286	GLU	CD-OE1	-6.21	1.18	1.25
1	A	288	GLU	CD-OE1	-6.12	1.19	1.25
1	A	99	SER	CB-OG	-6.11	1.34	1.42
1	A	205[A]	GLU	CD-OE1	-6.07	1.19	1.25
1	A	205[B]	GLU	CD-OE1	-6.07	1.19	1.25
1	B	207	GLU	CD-OE2	-6.00	1.19	1.25
1	A	195	SER	CB-OG	-5.88	1.34	1.42
1	A	105	GLU	CD-OE2	-5.82	1.19	1.25
1	B	240	CYS	CB-SG	-5.75	1.72	1.81
1	A	295	ARG	CZ-NH2	-5.70	1.25	1.33
1	B	26	GLU	CD-OE1	-5.63	1.19	1.25
1	B	295	ARG	CZ-NH2	-5.52	1.25	1.33
1	B	307[A]	ARG	CG-CD	-5.46	1.38	1.51
1	B	307[B]	ARG	CG-CD	-5.46	1.38	1.51
1	B	255	GLU	CD-OE2	-5.45	1.19	1.25
1	B	134	PRO	N-CD	5.45	1.55	1.47
1	A	54	PRO	N-CD	5.44	1.55	1.47
1	B	130[A]	CYS	CA-C	5.37	1.67	1.52
1	B	130[B]	CYS	CA-C	5.37	1.67	1.52
1	B	61	PHE	CB-CG	-5.34	1.42	1.51
1	A	59	MET	C-O	-5.29	1.13	1.23
1	A	36	SER	CB-OG	-5.24	1.35	1.42
1	B	26	GLU	CD-OE2	-5.22	1.20	1.25
1	B	137	PRO	N-CD	5.17	1.55	1.47
1	A	265	ALA	C-O	-5.16	1.13	1.23
1	A	136	LYS	N-CA	5.14	1.56	1.46
1	A	48	ALA	C-O	-5.08	1.13	1.23
1	B	75	GLY	C-O	-5.02	1.15	1.23
1	A	96	LEU	CB-CG	-5.02	1.38	1.52
1	A	291	GLU	CG-CD	5.00	1.59	1.51

All (32) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	LYS	CD-CE-NZ	14.44	144.92	111.70
1	A	129	SER	O-C-N	-10.41	106.03	122.70
1	B	129	SER	O-C-N	-9.33	107.77	122.70
1	B	130[A]	CYS	CA-CB-SG	9.05	130.28	114.00
1	B	130[B]	CYS	CA-CB-SG	9.05	130.28	114.00
1	B	1	CYS	N-CA-CB	-8.41	95.47	110.60
1	B	307[A]	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	B	307[B]	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	B	77	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	B	307[A]	ARG	CG-CD-NE	-8.20	94.59	111.80
1	B	307[B]	ARG	CG-CD-NE	-8.20	94.59	111.80
1	B	146	MET	CG-SD-CE	-7.87	87.61	100.20
1	A	77	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	299	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	B	307[A]	ARG	NE-CZ-NH2	6.93	123.76	120.30
1	B	307[B]	ARG	NE-CZ-NH2	6.93	123.76	120.30
1	B	142	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	111[A]	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	B	111[B]	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	51	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	129	SER	CA-C-N	5.62	129.55	117.20
1	A	291	GLU	CB-CG-CD	5.51	129.09	114.20
1	B	111[A]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	111[B]	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	130[A]	CYS	N-CA-CB	-5.29	101.09	110.60
1	B	130[B]	CYS	N-CA-CB	-5.29	101.09	110.60
1	B	81	LYS	CD-CE-NZ	5.25	123.77	111.70
1	B	217	PHE	CB-CG-CD1	5.24	124.47	120.80
1	B	174	PHE	CB-CG-CD1	5.23	124.46	120.80
1	B	184	PHE	CB-CG-CD2	5.17	124.42	120.80
1	B	88	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	302	GLU	OE1-CD-OE2	-5.09	117.19	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	SER	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	2554	0	2540	115	0
1	B	2533	0	2512	62	0
2	A	28	0	16	1	0
2	B	56	0	32	8	0
3	A	90	0	119	6	0
3	B	72	0	95	12	0
4	A	10	0	0	2	0
4	B	10	0	0	0	0
5	A	31	0	19	1	0
5	B	31	0	19	0	0
6	A	72	0	107	34	0
6	B	60	0	88	31	0
7	A	42	0	59	38	0
7	B	28	0	40	18	0
8	A	21	0	0	2	0
9	A	381	0	0	25	0
9	B	447	0	0	28	0
All	All	6466	0	5646	230	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 20.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:NZ	1:B:3:LYS:CE	1.68	1.54
1:A:130[A]:CYS:C	1:A:131:PRO:N	1.69	1.42
1:A:130[B]:CYS:C	1:A:131:PRO:N	1.73	1.39
1:A:1:CYS:HB2	7:A:437[B]:PEG:H22	1.33	1.11
2:B:401[A]:W88:CAI	7:B:433:PEG:H22	1.81	1.10
1:A:2:LEU:HD12	1:A:286:GLU:HG3	1.29	1.09
1:A:130[A]:CYS:SG	1:A:139:VAL:HG23	1.94	1.07
1:A:128:LEU:CD1	1:A:163[B]:VAL:HG21	1.86	1.05
1:A:1:CYS:HB2	7:A:437[A]:PEG:H22	1.32	1.04
2:B:401[A]:W88:H17	7:B:433:PEG:C2	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401[A]:W88:H17	7:B:433:PEG:H22	1.01	1.00
1:A:312[A]:GLU:OE2	1:A:312[A]:GLU:HA	1.57	1.00
1:A:185:PRO:HG2	7:A:440:PEG:H22	1.44	0.96
1:A:5:ASN:HB3	6:A:433:EDO:C2	1.98	0.94
1:A:5:ASN:ND2	1:A:10[A]:VAL:HG22	1.83	0.93
1:B:130[B]:CYS:SG	1:B:131:PRO:HD2	2.09	0.93
1:A:2:LEU:HD12	1:A:286:GLU:CG	2.01	0.90
1:B:195:SER:OG	3:B:402:GOL:H11	1.73	0.89
1:A:128:LEU:HD12	1:A:163[B]:VAL:HG21	1.56	0.88
1:A:312[A]:GLU:CA	1:A:312[A]:GLU:OE2	2.18	0.88
7:A:438:PEG:H31	7:A:440:PEG:C1	2.05	0.86
6:B:429:EDO:H22	9:B:875:HOH:O	1.75	0.86
1:B:111[B]:ARG:NH2	7:B:432:PEG:C2	2.39	0.86
1:B:131:PRO:HD3	2:B:401[B]:W88:CAK	2.07	0.85
1:B:277:GLU:HB2	6:B:418:EDO:H12	1.60	0.84
7:A:438:PEG:H31	7:A:440:PEG:H12	1.57	0.84
1:A:5:ASN:HD21	1:A:10[A]:VAL:HG22	1.42	0.82
1:A:312[A]:GLU:HG3	9:B:744:HOH:O	1.78	0.82
2:B:401[A]:W88:CAI	7:B:433:PEG:C2	2.55	0.81
1:A:131:PRO:HB3	2:A:401:W88:CAI	2.12	0.80
1:A:234:ASN:HD21	1:A:238:ARG:HE	1.30	0.80
1:A:128:LEU:CD1	1:A:163[B]:VAL:CG2	2.60	0.79
1:B:130[B]:CYS:SG	1:B:131:PRO:CD	2.71	0.79
1:A:128:LEU:HD11	1:A:163[B]:VAL:HG21	1.65	0.79
1:A:128:LEU:HG	1:A:163[B]:VAL:HG23	1.63	0.78
1:A:5:ASN:HB3	6:A:433:EDO:O2	1.84	0.77
1:A:185:PRO:HG2	7:A:440:PEG:C2	2.14	0.77
1:A:128:LEU:HG	1:A:163[B]:VAL:CG2	2.15	0.76
1:A:138[B]:GLN:HG2	1:B:170:ASP:OD2	1.86	0.76
1:A:2:LEU:CD1	1:A:286:GLU:HG3	2.12	0.76
7:B:431[B]:PEG:O1	7:B:431[B]:PEG:H32	1.76	0.75
6:B:421:EDO:H11	9:B:584:HOH:O	1.87	0.74
1:B:59:MET:HE3	9:B:601:HOH:O	1.87	0.74
1:A:5:ASN:HB3	6:A:433:EDO:H21	1.71	0.73
1:A:185:PRO:HD2	7:A:439:PEG:H42	1.70	0.72
1:B:59:MET:CE	9:B:601:HOH:O	2.38	0.72
1:B:195:SER:OG	3:B:402:GOL:C1	2.37	0.72
6:B:429:EDO:H12	9:B:555:HOH:O	1.88	0.72
6:A:434:EDO:H12	8:A:442[B]:NCO:N1	2.05	0.72
1:A:91:LYS:O	6:A:423:EDO:H22	1.89	0.71
1:A:154:SER:CB	7:A:438:PEG:H22	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:HD11	6:B:419:EDO:H22	1.74	0.70
1:A:2:LEU:HB2	7:A:437[B]:PEG:H12	1.72	0.70
1:A:154:SER:HB3	7:A:438:PEG:H22	1.73	0.70
1:B:273:ALA:HB1	6:B:418:EDO:H11	1.75	0.69
1:B:111[B]:ARG:NH2	7:B:432:PEG:H21	2.07	0.69
1:B:47[B]:SER:O	6:B:416:EDO:H12	1.92	0.69
1:B:111[B]:ARG:NH2	7:B:432:PEG:H22	2.09	0.67
1:A:138[B]:GLN:CG	1:B:170:ASP:OD2	2.43	0.67
1:B:234:ASN:HD21	1:B:238:ARG:HE	1.40	0.67
1:B:131:PRO:CD	2:B:401[B]:W88:CAK	2.73	0.66
7:A:438:PEG:C3	7:A:440:PEG:C1	2.73	0.66
1:B:81:LYS:HE2	9:B:904:HOH:O	1.94	0.66
6:A:434:EDO:H22	8:A:442[A]:NCO:N6	2.10	0.65
6:B:419:EDO:H21	9:B:863:HOH:O	1.96	0.65
6:B:430:EDO:H12	9:B:940:HOH:O	1.97	0.65
7:A:439:PEG:H32	9:A:870:HOH:O	1.96	0.64
1:A:138[A]:GLN:HG3	9:A:855:HOH:O	1.97	0.64
7:A:438:PEG:H31	7:A:440:PEG:H11	1.79	0.63
1:A:106:ASN:CG	1:A:149[B]:TYR:OH	2.37	0.63
1:B:111[B]:ARG:HH22	7:B:432:PEG:H22	1.63	0.63
1:A:2:LEU:H	7:A:437[A]:PEG:C2	2.12	0.62
7:A:438:PEG:C3	7:A:440:PEG:H12	2.27	0.62
1:A:154:SER:O	7:A:438:PEG:H41	1.99	0.62
1:A:128:LEU:HD12	1:A:163[A]:VAL:CG1	2.28	0.62
1:A:2:LEU:H	7:A:437[B]:PEG:C2	2.12	0.62
1:B:276:GLU:HB2	6:B:418:EDO:H22	1.81	0.62
7:A:439:PEG:C3	9:A:870:HOH:O	2.48	0.62
1:A:68[B]:SER:OG	1:A:214[B]:LYS:NZ	2.33	0.61
1:B:68[B]:SER:OG	1:B:214[B]:LYS:NZ	2.32	0.61
3:B:409:GOL:C3	9:B:693:HOH:O	2.49	0.61
6:A:420:EDO:H21	9:A:534:HOH:O	2.00	0.61
6:A:434:EDO:H11	9:A:734[A]:HOH:O	2.00	0.61
1:A:128:LEU:CG	1:A:163[B]:VAL:CG2	2.79	0.61
6:B:421:EDO:C1	9:B:584:HOH:O	2.46	0.60
6:A:427:EDO:H21	9:A:665:HOH:O	2.01	0.60
1:A:82:TYR:OH	1:A:87:HIS:HD2	1.84	0.60
3:B:412:GOL:C1	9:B:628:HOH:O	2.49	0.60
1:A:3[C]:LYS:HZ3	1:A:3[C]:LYS:C	2.05	0.60
1:B:195:SER:HB3	9:B:675:HOH:O	2.01	0.60
1:A:241:PRO:HB3	3:A:413:GOL:H12	1.84	0.60
1:A:2:LEU:H	7:A:437[B]:PEG:C1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:CD1	1:A:163[A]:VAL:CG1	2.80	0.59
7:A:437[A]:PEG:H11	9:A:653:HOH:O	2.02	0.59
1:A:3[A]:LYS:N	7:A:437[A]:PEG:H21	2.18	0.58
1:B:5[B]:ASN:ND2	1:B:10:VAL:HG22	2.18	0.58
1:A:3[C]:LYS:NZ	1:A:3[C]:LYS:C	2.57	0.58
1:A:183:GLU:HB3	7:A:439:PEG:H12	1.85	0.58
1:A:163[A]:VAL:HG12	1:A:165:MET:SD	2.44	0.58
1:A:98[A]:ILE:O	1:A:98[A]:ILE:HG13	2.04	0.58
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG13	2.35	0.57
1:B:82:TYR:OH	1:B:87:HIS:HD2	1.88	0.57
7:A:437[B]:PEG:H11	9:A:653:HOH:O	2.04	0.57
6:A:435:EDO:C2	9:A:657:HOH:O	2.53	0.57
1:B:92:LYS:HE2	6:B:424:EDO:H12	1.86	0.57
1:B:223[B]:LYS:NZ	3:B:412:GOL:H2	2.20	0.57
4:A:416:CAC:C2	6:A:427:EDO:H11	2.35	0.56
1:A:2:LEU:HB2	7:A:437[A]:PEG:H12	1.88	0.56
1:A:182:ASN:O	6:A:435:EDO:H21	2.05	0.56
1:A:149[A]:TYR:HE1	9:A:689:HOH:O	1.89	0.55
2:B:401[A]:W88:H18	7:B:433:PEG:H12	1.88	0.55
1:A:130[B]:CYS:C	1:A:131:PRO:CD	2.69	0.55
1:A:312[A]:GLU:OE2	1:A:312[A]:GLU:N	2.40	0.55
1:B:241:PRO:HA	3:B:408:GOL:H31	1.89	0.55
1:B:121:GLY:CA	6:B:423:EDO:H22	2.37	0.55
1:A:234:ASN:ND2	1:A:238:ARG:HE	2.02	0.54
1:A:1:CYS:CB	7:A:437[A]:PEG:H22	2.23	0.54
1:A:1:CYS:CB	7:A:437[B]:PEG:H22	2.24	0.54
6:B:416:EDO:H11	9:B:539:HOH:O	2.07	0.54
1:A:130[A]:CYS:SG	1:A:139:VAL:CG2	2.85	0.54
1:A:312[A]:GLU:CG	9:B:744:HOH:O	2.48	0.54
1:B:108:ALA:CB	7:B:432:PEG:H12	2.37	0.54
1:A:128:LEU:HD12	1:A:163[B]:VAL:CG2	2.32	0.53
1:B:234:ASN:ND2	1:B:238:ARG:HE	2.07	0.53
1:B:111[B]:ARG:HH21	7:B:432:PEG:C1	2.21	0.53
1:A:130[A]:CYS:C	1:A:131:PRO:CA	2.70	0.53
7:A:436:PEG:H21	9:B:808:HOH:O	2.08	0.53
1:B:47[B]:SER:O	6:B:416:EDO:C1	2.57	0.53
1:A:128:LEU:HD12	1:A:163[A]:VAL:HG11	1.90	0.53
3:A:411:GOL:H12	9:A:799:HOH:O	2.08	0.53
1:A:5:ASN:CB	6:A:433:EDO:O2	2.55	0.53
1:A:2:LEU:CD1	1:A:286:GLU:CG	2.78	0.52
1:A:154:SER:HB2	7:A:438:PEG:H22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PRO:HB3	6:B:430:EDO:H21	1.91	0.52
1:A:92:LYS:HE2	6:A:423:EDO:H11	1.92	0.51
6:A:435:EDO:C1	9:A:657:HOH:O	2.58	0.51
1:A:87:HIS:HE1	1:A:92:LYS:O	1.92	0.51
1:A:128:LEU:HG	1:A:163[A]:VAL:HG13	1.93	0.51
1:B:62:PRO:HD3	7:B:431[B]:PEG:H21	1.93	0.51
1:A:195:SER:HB3	9:A:798:HOH:O	2.11	0.50
1:B:203:ASP:HB2	3:B:410:GOL:H12	1.94	0.50
1:B:87:HIS:HE1	1:B:92:LYS:O	1.93	0.50
7:A:438:PEG:H21	7:A:440:PEG:O1	2.11	0.50
6:B:422:EDO:H11	9:B:527:HOH:O	2.11	0.50
1:A:128:LEU:CD1	1:A:163[A]:VAL:HG11	2.43	0.49
1:A:308:VAL:O	6:A:418:EDO:H21	2.11	0.49
1:A:205[A]:GLU:HG2	6:B:426:EDO:H12	1.94	0.49
1:B:131:PRO:HD3	2:B:401[B]:W88:H12	1.93	0.49
6:B:429:EDO:C2	9:B:875:HOH:O	2.49	0.49
1:A:130[A]:CYS:C	1:A:131:PRO:CD	2.73	0.48
1:A:203:ASP:HB2	6:A:434:EDO:H21	1.95	0.48
1:A:223[B]:LYS:HG3	1:A:252:TYR:CE1	2.48	0.48
1:B:160:PRO:HB2	6:B:425:EDO:H22	1.95	0.48
6:A:435:EDO:H22	9:A:657:HOH:O	2.12	0.48
1:B:104:GLU:HB3	7:B:432:PEG:H31	1.95	0.48
1:A:138[A]:GLN:CG	9:A:855:HOH:O	2.59	0.48
1:A:9:HIS:HE1	9:A:522:HOH:O	1.97	0.48
4:A:415:CAC:C1	9:A:784:HOH:O	2.62	0.48
3:B:412:GOL:H11	9:B:628:HOH:O	2.14	0.48
1:A:7:LEU:O	1:A:9:HIS:HD2	1.97	0.48
1:A:212:LYS:NZ	1:B:312:GLU:HG2	2.28	0.47
1:B:130[A]:CYS:SG	9:B:832:HOH:O	2.28	0.47
1:A:182:ASN:O	6:A:435:EDO:C2	2.63	0.47
1:A:2:LEU:N	7:A:437[B]:PEG:C2	2.77	0.47
1:A:91:LYS:O	6:A:423:EDO:C2	2.61	0.47
1:B:210:VAL:HA	3:B:410:GOL:H31	1.97	0.47
1:B:77:ASP:H	6:B:416:EDO:H11	1.78	0.47
1:A:37:SER:O	6:A:423:EDO:H11	2.14	0.47
1:A:2:LEU:N	7:A:437[A]:PEG:C2	2.77	0.47
6:A:434:EDO:C1	9:A:734[A]:HOH:O	2.59	0.46
7:A:436:PEG:H41	7:A:436:PEG:H21	1.49	0.46
1:A:2:LEU:H	7:A:437[A]:PEG:C1	2.25	0.46
1:B:129:SER:HA	1:B:138:GLN:NE2	2.31	0.46
6:A:432:EDO:C1	9:A:579:HOH:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223[A]:LYS:HE3	3:B:412:GOL:H2	1.97	0.46
1:A:34:ALA:HB3	3:A:402[A]:GOL:H11	1.97	0.46
1:A:3[C]:LYS:HZ2	1:A:3[C]:LYS:HB3	1.80	0.46
7:A:438:PEG:C3	7:A:440:PEG:H11	2.44	0.46
1:A:186:LEU:HD21	7:A:440:PEG:H31	1.98	0.46
1:A:132:ASN:HB2	9:A:591:HOH:O	2.16	0.45
6:B:424:EDO:C2	9:B:634:HOH:O	2.63	0.45
1:A:106:ASN:ND2	1:A:149[B]:TYR:OH	2.49	0.45
1:A:312[A]:GLU:N	1:A:312[A]:GLU:CD	2.69	0.45
1:B:223[B]:LYS:HZ1	3:B:412:GOL:H2	1.81	0.45
6:B:424:EDO:H21	9:B:634:HOH:O	2.16	0.45
1:A:2:LEU:N	7:A:437[A]:PEG:H21	2.31	0.45
1:A:182:ASN:O	6:A:435:EDO:C1	2.65	0.44
1:B:108:ALA:HB2	7:B:432:PEG:H12	1.98	0.44
1:A:107:VAL:O	1:A:111[A]:ARG:HG3	2.17	0.44
1:A:163[A]:VAL:CG1	1:A:165:MET:SD	3.05	0.44
1:A:130[B]:CYS:SG	1:A:131:PRO:HD2	2.59	0.43
7:B:431[B]:PEG:O1	7:B:431[B]:PEG:C3	2.55	0.43
3:A:406:GOL:O3	6:A:434:EDO:C2	2.66	0.43
6:B:416:EDO:C2	9:B:539:HOH:O	2.66	0.43
6:A:425:EDO:H21	9:A:633:HOH:O	2.18	0.43
1:B:307[B]:ARG:NH2	9:B:825:HOH:O	2.44	0.43
1:A:130[B]:CYS:O	1:A:138[B]:GLN:NE2	2.49	0.43
1:B:130[B]:CYS:SG	1:B:131:PRO:N	2.90	0.43
1:A:155:LEU:HB2	7:A:438:PEG:H11	2.01	0.43
6:B:424:EDO:H11	9:B:512:HOH:O	2.19	0.43
1:A:238:ARG:NH2	6:A:418:EDO:H22	2.34	0.43
1:A:138[B]:GLN:HG3	1:B:170:ASP:OD2	2.19	0.42
1:B:188:LYS:HE3	9:B:909:HOH:O	2.19	0.42
3:A:414:GOL:H32	9:A:739:HOH:O	2.19	0.42
1:A:205[A]:GLU:HA	6:B:426:EDO:H21	2.01	0.42
1:B:2:LEU:HG	6:B:427:EDO:H12	2.00	0.42
6:B:420:EDO:H12	9:B:829:HOH:O	2.19	0.42
1:A:98[A]:ILE:CG1	1:A:98[A]:ILE:O	2.67	0.42
1:B:13:ASN:HB2	1:B:14:PRO:HD2	2.01	0.42
6:A:435:EDO:H12	9:A:657:HOH:O	2.18	0.42
1:B:241:PRO:HA	3:B:408:GOL:C3	2.49	0.42
1:B:97:SER:HA	1:B:125:GLU:O	2.20	0.42
7:B:433:PEG:H12	9:B:938[A]:HOH:O	2.19	0.42
1:A:205[B]:GLU:HA	6:B:426:EDO:H21	2.02	0.42
1:A:20:GLY:HA3	5:A:417:FMN:N5	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:420:EDO:C1	9:A:611:HOH:O	2.68	0.42
1:A:128:LEU:HD11	1:A:163[B]:VAL:CG2	2.43	0.41
1:A:308:VAL:O	6:A:418:EDO:C2	2.68	0.41
1:A:50:ARG:HA	6:A:420:EDO:H12	2.02	0.41
6:A:431:EDO:H22	9:A:689:HOH:O	2.20	0.41
1:B:111[B]:ARG:NH2	7:B:432:PEG:C1	2.81	0.41
1:B:160:PRO:HB3	1:B:188:LYS:HG3	2.03	0.41
1:A:107:VAL:O	1:A:111[B]:ARG:HG3	2.19	0.41
1:B:77:ASP:H	6:B:416:EDO:C1	2.33	0.41
1:A:307:ARG:HH22	6:A:426:EDO:H22	1.86	0.41
7:A:436:PEG:H12	1:B:168:TYR:HA	2.03	0.41
1:B:277:GLU:CB	6:B:418:EDO:H12	2.40	0.41
1:A:295:ARG:HH21	6:A:424:EDO:C1	2.34	0.40
3:A:403:GOL:H31	1:B:217:PHE:CE1	2.56	0.40
1:A:311:ILE:HG22	1:A:312[A]:GLU:HG2	2.02	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	330/314 (105%)	323 (98%)	6 (2%)	1 (0%)	44	18
1	B	329/314 (105%)	318 (97%)	11 (3%)	0	100	100
All	All	659/628 (105%)	641 (97%)	17 (3%)	1 (0%)	51	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	MET



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	278/259 (107%)	274 (99%)	4 (1%)	71	43
1	B	276/259 (107%)	272 (99%)	4 (1%)	71	43
All	All	554/518 (107%)	546 (99%)	8 (1%)	75	43

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	291	GLU
1	A	312[A]	GLU
1	A	312[B]	GLU
1	B	118	GLN
1	B	307[A]	ARG
1	B	307[B]	ARG
1	B	312	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	9	HIS
1	A	87	HIS
1	A	151	GLN
1	A	234	ASN
1	A	275	GLN
1	B	87	HIS
1	B	118	GLN
1	B	138	GLN
1	B	234	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

82 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$
2	W88	A	401	-	22,30,30	2.06	6 (27%)	23,42,42	2.28	1 (4%)
3	GOL	A	402[A]	-	5,5,5	1.13	0	5,5,5	0.72	0
3	GOL	A	402[B]	-	5,5,5	1.19	0	5,5,5	1.26	1 (20%)
3	GOL	A	403	-	5,5,5	0.89	0	5,5,5	1.08	0
3	GOL	A	404	-	5,5,5	0.49	0	5,5,5	0.50	0
3	GOL	A	405	-	5,5,5	1.42	1 (20%)	5,5,5	1.67	1 (20%)
3	GOL	A	406	-	5,5,5	0.81	0	5,5,5	1.39	1 (20%)
3	GOL	A	407[A]	-	5,5,5	0.29	0	5,5,5	0.31	0
3	GOL	A	407[B]	-	5,5,5	0.36	0	5,5,5	0.65	0
3	GOL	A	408	-	5,5,5	0.37	0	5,5,5	0.53	0
3	GOL	A	409	-	5,5,5	0.83	0	5,5,5	1.13	1 (20%)
3	GOL	A	410	-	5,5,5	0.93	0	5,5,5	1.29	1 (20%)
3	GOL	A	411	-	5,5,5	0.83	0	5,5,5	0.78	0
3	GOL	A	412	-	5,5,5	0.78	0	5,5,5	1.35	0
3	GOL	A	413	-	5,5,5	0.77	0	5,5,5	0.92	0
3	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.30	0
4	CAC	A	415	-	0,4,4	0.00	-	0,6,6	0.00	-
4	CAC	A	416	-	0,4,4	0.00	-	0,6,6	0.00	-
5	FMN	A	417	-	31,33,33	1.18	2 (6%)	38,50,50	2.84	9 (23%)
6	EDO	A	418	-	3,3,3	1.13	0	2,2,2	0.65	0
6	EDO	A	419	-	3,3,3	0.54	0	2,2,2	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	A	420	-	3,3,3	0.86	0	2,2,2	1.30	0
6	EDO	A	421	-	3,3,3	0.34	0	2,2,2	1.40	0
6	EDO	A	422	-	3,3,3	1.02	0	2,2,2	0.48	0
6	EDO	A	423	-	3,3,3	0.74	0	2,2,2	1.08	0
6	EDO	A	424	-	3,3,3	0.54	0	2,2,2	0.41	0
6	EDO	A	425	-	3,3,3	0.82	0	2,2,2	0.20	0
6	EDO	A	426	-	3,3,3	0.54	0	2,2,2	0.36	0
6	EDO	A	427	-	3,3,3	0.56	0	2,2,2	0.03	0
6	EDO	A	428	-	3,3,3	0.60	0	2,2,2	0.42	0
6	EDO	A	429	-	3,3,3	0.87	0	2,2,2	0.42	0
6	EDO	A	430	-	3,3,3	0.65	0	2,2,2	0.58	0
6	EDO	A	431	-	3,3,3	0.78	0	2,2,2	0.42	0
6	EDO	A	432	-	3,3,3	0.79	0	2,2,2	0.71	0
6	EDO	A	433	-	3,3,3	1.15	0	2,2,2	1.08	0
6	EDO	A	434	-	3,3,3	0.49	0	2,2,2	0.91	0
6	EDO	A	435	-	3,3,3	0.88	0	2,2,2	0.51	0
7	PEG	A	436	-	6,6,6	1.01	0	5,5,5	1.56	2 (40%)
7	PEG	A	437[A]	-	6,6,6	0.82	0	5,5,5	1.60	1 (20%)
7	PEG	A	437[B]	-	6,6,6	0.68	0	5,5,5	1.48	1 (20%)
7	PEG	A	438	-	6,6,6	0.36	0	5,5,5	1.43	0
7	PEG	A	439	-	6,6,6	0.72	0	5,5,5	1.72	1 (20%)
7	PEG	A	440	-	6,6,6	0.50	0	5,5,5	0.94	0
8	NCO	A	441	-	6,6,6	2.43	5 (83%)	0,15,15	0.00	-
8	NCO	A	442[A]	-	6,6,6	0.77	0	0,15,15	0.00	-
8	NCO	A	442[B]	-	6,6,6	1.02	0	0,15,15	0.00	-
2	W88	B	401[A]	-	22,30,30	2.00	4 (18%)	23,42,42	2.67	5 (21%)
2	W88	B	401[B]	-	22,30,30	2.01	6 (27%)	23,42,42	2.48	4 (17%)
3	GOL	B	402	-	5,5,5	0.59	0	5,5,5	1.02	0
3	GOL	B	403	-	5,5,5	1.30	1 (20%)	5,5,5	1.06	0
3	GOL	B	404[A]	-	5,5,5	0.99	0	5,5,5	0.74	0
3	GOL	B	404[B]	-	5,5,5	0.44	0	5,5,5	1.35	0
3	GOL	B	405	-	5,5,5	0.94	0	5,5,5	1.34	1 (20%)
3	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.35	0
3	GOL	B	407	-	5,5,5	0.63	0	5,5,5	0.75	0
3	GOL	B	408	-	5,5,5	1.14	1 (20%)	5,5,5	0.99	0
3	GOL	B	409	-	5,5,5	0.70	0	5,5,5	0.60	0
3	GOL	B	410	-	5,5,5	0.52	0	5,5,5	1.35	1 (20%)
3	GOL	B	411	-	5,5,5	0.64	0	5,5,5	0.89	0
3	GOL	B	412	-	5,5,5	0.62	0	5,5,5	0.88	0
4	CAC	B	413	-	0,4,4	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CAC	B	414	-	0,4,4	0.00	-	0,6,6	0.00	-
5	FMN	B	415	-	31,33,33	1.40	4 (12%)	38,50,50	2.24	9 (23%)
6	EDO	B	416	-	3,3,3	1.41	0	2,2,2	1.47	0
6	EDO	B	417	-	3,3,3	0.25	0	2,2,2	1.20	0
6	EDO	B	418	-	3,3,3	0.79	0	2,2,2	0.86	0
6	EDO	B	419	-	3,3,3	0.76	0	2,2,2	0.80	0
6	EDO	B	420	-	3,3,3	0.59	0	2,2,2	0.11	0
6	EDO	B	421	-	3,3,3	0.58	0	2,2,2	0.32	0
6	EDO	B	422	-	3,3,3	0.34	0	2,2,2	0.06	0
6	EDO	B	423	-	3,3,3	0.80	0	2,2,2	1.05	0
6	EDO	B	424	-	3,3,3	0.91	0	2,2,2	1.79	1 (50%)
6	EDO	B	425	-	3,3,3	1.00	0	2,2,2	0.83	0
6	EDO	B	426	-	3,3,3	0.50	0	2,2,2	1.15	0
6	EDO	B	427	-	3,3,3	0.69	0	2,2,2	0.67	0
6	EDO	B	428	-	3,3,3	0.59	0	2,2,2	0.15	0
6	EDO	B	429	-	3,3,3	0.56	0	2,2,2	0.29	0
6	EDO	B	430	-	3,3,3	0.84	0	2,2,2	0.45	0
7	PEG	B	431[A]	-	6,6,6	0.58	0	5,5,5	0.37	0
7	PEG	B	431[B]	-	6,6,6	0.54	0	5,5,5	0.78	0
7	PEG	B	432	-	6,6,6	1.29	0	5,5,5	1.63	2 (40%)
7	PEG	B	433	-	6,6,6	0.42	0	5,5,5	0.94	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
2	W88	A	401	-	-	0/7/15/15	0/3/3/3
3	GOL	A	402[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	402[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	403	-	-	0/4/4/4	0/0/0/0
3	GOL	A	404	-	-	0/4/4/4	0/0/0/0
3	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	GOL	A	406	-	-	0/4/4/4	0/0/0/0
3	GOL	A	407[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	407[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	A	408	-	-	0/4/4/4	0/0/0/0
3	GOL	A	409	-	-	0/4/4/4	0/0/0/0
3	GOL	A	410	-	-	0/4/4/4	0/0/0/0
3	GOL	A	411	-	-	0/4/4/4	0/0/0/0
3	GOL	A	412	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	413	-	-	0/4/4/4	0/0/0/0
3	GOL	A	414	-	-	0/4/4/4	0/0/0/0
4	CAC	A	415	-	-	0/0/0/0	0/0/0/0
4	CAC	A	416	-	-	0/0/0/0	0/0/0/0
5	FMN	A	417	-	-	0/16/18/18	0/3/3/3
6	EDO	A	418	-	-	0/1/1/1	0/0/0/0
6	EDO	A	419	-	-	0/1/1/1	0/0/0/0
6	EDO	A	420	-	-	0/1/1/1	0/0/0/0
6	EDO	A	421	-	-	0/1/1/1	0/0/0/0
6	EDO	A	422	-	-	0/1/1/1	0/0/0/0
6	EDO	A	423	-	-	0/1/1/1	0/0/0/0
6	EDO	A	424	-	-	0/1/1/1	0/0/0/0
6	EDO	A	425	-	-	0/1/1/1	0/0/0/0
6	EDO	A	426	-	-	0/1/1/1	0/0/0/0
6	EDO	A	427	-	-	0/1/1/1	0/0/0/0
6	EDO	A	428	-	-	0/1/1/1	0/0/0/0
6	EDO	A	429	-	-	0/1/1/1	0/0/0/0
6	EDO	A	430	-	-	0/1/1/1	0/0/0/0
6	EDO	A	431	-	-	0/1/1/1	0/0/0/0
6	EDO	A	432	-	-	0/1/1/1	0/0/0/0
6	EDO	A	433	-	-	0/1/1/1	0/0/0/0
6	EDO	A	434	-	-	0/1/1/1	0/0/0/0
6	EDO	A	435	-	-	0/1/1/1	0/0/0/0
7	PEG	A	436	-	-	0/4/4/4	0/0/0/0
7	PEG	A	437[A]	-	-	0/4/4/4	0/0/0/0
7	PEG	A	437[B]	-	-	0/4/4/4	0/0/0/0
7	PEG	A	438	-	-	0/4/4/4	0/0/0/0
7	PEG	A	439	-	-	0/4/4/4	0/0/0/0
7	PEG	A	440	-	-	0/4/4/4	0/0/0/0
8	NCO	A	441	-	-	0/0/0/0	0/0/0/0
8	NCO	A	442[A]	-	-	0/0/0/0	0/0/0/0
8	NCO	A	442[B]	-	-	0/0/0/0	0/0/0/0
2	W88	B	401[A]	-	-	0/7/15/15	0/3/3/3
2	W88	B	401[B]	-	-	0/7/15/15	0/3/3/3
3	GOL	B	402	-	-	0/4/4/4	0/0/0/0
3	GOL	B	403	-	-	0/4/4/4	0/0/0/0
3	GOL	B	404[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	404[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	B	405	-	-	0/4/4/4	0/0/0/0
3	GOL	B	406	-	-	0/4/4/4	0/0/0/0
3	GOL	B	407	-	-	0/4/4/4	0/0/0/0
3	GOL	B	408	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	409	-	-	0/4/4/4	0/0/0/0
3	GOL	B	410	-	-	0/4/4/4	0/0/0/0
3	GOL	B	411	-	-	0/4/4/4	0/0/0/0
3	GOL	B	412	-	-	0/4/4/4	0/0/0/0
4	CAC	B	413	-	-	0/0/0/0	0/0/0/0
4	CAC	B	414	-	-	0/0/0/0	0/0/0/0
5	FMN	B	415	-	-	0/16/18/18	0/3/3/3
6	EDO	B	416	-	-	0/1/1/1	0/0/0/0
6	EDO	B	417	-	-	0/1/1/1	0/0/0/0
6	EDO	B	418	-	-	0/1/1/1	0/0/0/0
6	EDO	B	419	-	-	0/1/1/1	0/0/0/0
6	EDO	B	420	-	-	0/1/1/1	0/0/0/0
6	EDO	B	421	-	-	0/1/1/1	0/0/0/0
6	EDO	B	422	-	-	0/1/1/1	0/0/0/0
6	EDO	B	423	-	-	0/1/1/1	0/0/0/0
6	EDO	B	424	-	-	0/1/1/1	0/0/0/0
6	EDO	B	425	-	-	0/1/1/1	0/0/0/0
6	EDO	B	426	-	-	0/1/1/1	0/0/0/0
6	EDO	B	427	-	-	0/1/1/1	0/0/0/0
6	EDO	B	428	-	-	0/1/1/1	0/0/0/0
6	EDO	B	429	-	-	0/1/1/1	0/0/0/0
6	EDO	B	430	-	-	0/1/1/1	0/0/0/0
7	PEG	B	431[A]	-	-	0/4/4/4	0/0/0/0
7	PEG	B	431[B]	-	-	0/4/4/4	0/0/0/0
7	PEG	B	432	-	-	0/4/4/4	0/0/0/0
7	PEG	B	433	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401[B]	W88	CAP-CAW	-4.64	1.43	1.52
2	B	401[A]	W88	CAP-CAW	-4.12	1.44	1.52
5	B	415	FMN	C6-C5A	-3.86	1.36	1.41
2	B	401[B]	W88	CAO-CAU	-3.42	1.41	1.51
2	B	401[A]	W88	CAO-CAU	-3.21	1.42	1.51
2	A	401	W88	CAO-CAU	-2.97	1.43	1.51
5	B	415	FMN	C8M-C8	-2.63	1.45	1.51
5	B	415	FMN	C2-N1	-2.42	1.33	1.38
3	B	403	GOL	O2-C2	-2.39	1.36	1.43
5	A	417	FMN	C1'-N10	-2.29	1.46	1.48
2	B	401[B]	W88	CAX-CAW	-2.04	1.37	1.41
8	A	441	NCO	CO-N2	2.03	2.05	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	408	GOL	C1-C2	2.08	1.60	1.52
8	A	441	NCO	CO-N4	2.15	2.05	1.97
2	B	401[B]	W88	CAJ-CAH	2.27	1.41	1.36
3	A	405	GOL	C3-C2	2.36	1.61	1.52
8	A	441	NCO	CO-N6	2.55	2.07	1.97
2	A	401	W88	CAI-CAG	2.62	1.42	1.36
2	A	401	W88	CAL-CAV	2.70	1.44	1.38
5	A	417	FMN	C4A-C10	2.77	1.45	1.41
2	A	401	W88	CAJ-CAH	2.77	1.42	1.36
8	A	441	NCO	CO-N5	2.79	2.08	1.97
5	B	415	FMN	C9A-N10	2.84	1.42	1.38
8	A	441	NCO	CO-N3	2.99	2.08	1.97
2	B	401[B]	W88	CAZ-NAR	3.75	1.39	1.33
2	B	401[A]	W88	CAZ-NAR	3.77	1.39	1.33
2	A	401	W88	CAX-NAQ	4.60	1.41	1.34
2	A	401	W88	CAZ-NAR	4.89	1.41	1.33
2	B	401[B]	W88	CAX-NAQ	4.92	1.42	1.34
2	B	401[A]	W88	CAX-NAQ	5.09	1.42	1.34

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	417	FMN	C4-C4A-C10	-8.84	112.81	119.96
5	A	417	FMN	C4A-C10-N10	-5.59	116.64	120.52
5	B	415	FMN	C4A-C4-N3	-4.65	116.86	123.48
2	B	401[A]	W88	CAH-CAV-CAS	-4.07	114.98	120.45
7	A	439	PEG	O2-C2-C1	-3.37	94.60	110.15
5	B	415	FMN	C4-C4A-C10	-3.29	117.30	119.96
2	B	401[A]	W88	CAV-CAL-CBB	-2.77	116.99	121.52
5	B	415	FMN	C4A-C10-N10	-2.56	118.74	120.52
6	B	424	EDO	O2-C2-C1	-2.53	93.98	112.08
5	A	417	FMN	C4A-C4-N3	-2.49	119.94	123.48
2	B	401[B]	W88	CAI-CBB-CAL	-2.46	117.67	122.05
2	B	401[B]	W88	CAW-CAX-NAQ	-2.41	119.45	122.75
2	B	401[A]	W88	CAW-CAX-NAQ	-2.38	119.49	122.75
3	A	410	GOL	C3-C2-C1	-2.34	102.20	111.52
2	B	401[B]	W88	CAN-CAM-CAO	-2.32	104.49	113.70
5	B	415	FMN	C6-C7-C8	-2.20	116.02	119.95
7	A	436	PEG	O2-C3-C4	-2.19	100.03	110.15
3	B	410	GOL	O1-C1-C2	-2.06	99.71	110.07
3	A	409	GOL	O3-C3-C2	2.02	120.25	110.07
3	B	405	GOL	O1-C1-C2	2.07	120.50	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	436	PEG	O1-C1-C2	2.08	123.81	111.89
3	A	406	GOL	O2-C2-C1	2.10	118.78	108.84
7	B	432	PEG	O2-C2-C1	2.19	120.27	110.15
5	B	415	FMN	C1'-N10-C10	2.25	120.81	118.50
7	B	432	PEG	O1-C1-C2	2.29	125.01	111.89
5	A	417	FMN	C10-C4A-N5	2.33	123.28	120.59
3	A	402[B]	GOL	C3-C2-C1	2.41	121.08	111.52
5	B	415	FMN	C6-C5A-N5	2.44	121.83	118.97
2	B	401[A]	W88	CAH-CAV-CAL	2.61	122.11	118.19
5	A	417	FMN	C5A-C9A-N10	2.63	119.61	117.66
7	A	437[B]	PEG	C3-O2-C2	2.91	125.91	113.30
3	A	405	GOL	O3-C3-C2	3.20	126.20	110.07
5	B	415	FMN	C7-C6-C5A	3.26	126.13	121.08
5	A	417	FMN	C1'-N10-C9A	3.31	121.38	118.35
5	A	417	FMN	C4A-N5-C5A	3.49	120.44	116.76
7	A	437[A]	PEG	C3-O2-C2	3.50	128.48	113.30
5	B	415	FMN	C4A-N5-C5A	3.61	120.57	116.76
5	A	417	FMN	C4-C4A-N5	4.14	123.22	118.68
2	A	401	W88	CAZ-NAR-CAY	9.40	123.38	115.16
5	B	415	FMN	C4-N3-C2	9.45	123.43	115.16
2	B	401[B]	W88	CAZ-NAR-CAY	10.37	124.23	115.16
2	B	401[A]	W88	CAZ-NAR-CAY	10.41	124.26	115.16
5	A	417	FMN	C4-N3-C2	10.72	124.53	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

53 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	W88	1	0
3	A	402[A]	GOL	1	0
3	A	403	GOL	1	0
3	A	406	GOL	1	0
3	A	411	GOL	1	0
3	A	413	GOL	1	0
3	A	414	GOL	1	0
4	A	415	CAC	1	0
4	A	416	CAC	1	0
5	A	417	FMN	1	0
6	A	418	EDO	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	420	EDO	3	0
6	A	423	EDO	4	0
6	A	424	EDO	1	0
6	A	425	EDO	1	0
6	A	426	EDO	1	0
6	A	427	EDO	2	0
6	A	431	EDO	1	0
6	A	432	EDO	1	0
6	A	433	EDO	4	0
6	A	434	EDO	6	0
6	A	435	EDO	7	0
7	A	436	PEG	3	0
7	A	437[A]	PEG	9	0
7	A	437[B]	PEG	7	0
7	A	438	PEG	12	0
7	A	439	PEG	4	0
7	A	440	PEG	10	0
8	A	442[A]	NCO	1	0
8	A	442[B]	NCO	1	0
2	B	401[A]	W88	5	0
2	B	401[B]	W88	3	0
3	B	402	GOL	2	0
3	B	408	GOL	2	0
3	B	409	GOL	1	0
3	B	410	GOL	2	0
3	B	412	GOL	5	0
6	B	416	EDO	6	0
6	B	418	EDO	4	0
6	B	419	EDO	2	0
6	B	420	EDO	1	0
6	B	421	EDO	2	0
6	B	422	EDO	1	0
6	B	423	EDO	1	0
6	B	424	EDO	4	0
6	B	425	EDO	1	0
6	B	426	EDO	3	0
6	B	427	EDO	1	0
6	B	429	EDO	3	0
6	B	430	EDO	2	0
7	B	431[B]	PEG	3	0
7	B	432	PEG	9	0
7	B	433	PEG	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	130[B]:CYS	C	131:PRO	N	1.73
1	A	130[A]:CYS	C	131:PRO	N	1.69

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	314/314 (100%)	-0.14	9 (2%)	52	51	4, 9, 26, 54	0
1	B	314/314 (100%)	-0.30	5 (1%)	72	72	4, 8, 20, 45	0
All	All	628/628 (100%)	-0.22	14 (2%)	62	62	4, 8, 23, 54	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	PRO	7.4
1	A	133	VAL	7.2
1	A	-1	SER	5.7
1	A	134	PRO	5.1
1	A	135	GLY	5.1
1	B	130[A]	CYS	4.7
1	A	130[A]	CYS	4.6
1	B	-1	SER	3.6
1	A	132	ASN	3.0
1	B	312	GLU	2.8
1	B	131	PRO	2.8
1	B	134	PRO	2.6
1	A	312[A]	GLU	2.4
1	A	0	MET	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	410	6/6	0.84	0.29	24.77	26,30,33,37	0
4	CAC	A	415	5/5	0.92	0.27	21.38	11,17,21,22	0
6	EDO	A	434	4/4	0.88	0.25	20.83	25,25,26,29	0
6	EDO	A	435	4/4	0.74	0.42	19.24	33,37,38,44	0
3	GOL	B	412	6/6	0.90	0.30	18.82	22,32,36,49	0
3	GOL	B	409	6/6	0.90	0.34	18.76	22,37,39,40	0
3	GOL	A	406	6/6	0.82	0.18	14.48	21,27,27,30	0
6	EDO	B	418	4/4	0.95	0.18	14.36	19,20,22,22	0
4	CAC	B	413	5/5	0.95	0.23	14.27	12,16,18,20	0
7	PEG	B	433	7/7	0.92	0.33	12.77	19,29,39,46	0
3	GOL	B	408	6/6	0.65	0.18	12.72	30,34,38,47	0
6	EDO	A	422	4/4	0.50	0.31	11.41	39,56,57,59	0
6	EDO	A	423	4/4	0.86	0.25	11.18	20,23,27,38	0
7	PEG	A	438	7/7	0.90	0.46	9.90	29,32,34,34	0
6	EDO	B	422	4/4	0.85	0.29	9.54	27,32,34,35	0
3	GOL	A	409	6/6	0.66	0.24	9.38	30,34,38,51	0
6	EDO	B	416	4/4	0.86	0.21	8.22	18,23,24,35	0
3	GOL	A	414	6/6	0.77	0.24	7.65	39,50,52,56	0
3	GOL	B	404[A]	6/6	0.82	0.18	7.26	16,18,21,25	6
6	EDO	B	426	4/4	0.84	0.22	6.82	26,34,35,39	0
7	PEG	A	436	7/7	0.93	0.16	6.14	13,25,28,33	0
3	GOL	A	412	6/6	0.86	0.23	5.84	29,40,43,44	0
6	EDO	A	418	4/4	0.85	0.26	5.82	17,24,29,30	0
6	EDO	B	425	4/4	0.88	0.21	5.79	24,29,30,30	0
6	EDO	B	424	4/4	0.96	0.22	5.65	16,22,22,27	0
6	EDO	B	421	4/4	0.80	0.18	5.42	37,38,45,47	0
6	EDO	A	432	4/4	0.82	0.17	5.36	34,40,41,42	0
7	PEG	B	432	7/7	0.83	0.23	5.11	22,26,30,34	0
3	GOL	A	410	6/6	0.89	0.13	4.51	24,27,28,41	0
3	GOL	B	406	6/6	0.90	0.17	4.44	29,40,44,54	0
3	GOL	B	403	6/6	0.89	0.13	4.41	22,24,26,26	0
8	NCO	A	442[A]	7/7	0.95	0.16	4.34	16,17,19,21	7
6	EDO	A	424	4/4	0.85	0.21	3.99	33,34,40,42	0
6	EDO	B	427	4/4	0.88	0.23	3.91	20,28,34,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NCO	A	442[B]	7/7	0.95	0.16	3.32	15,16,18,20	7
3	GOL	B	407	6/6	0.85	0.18	2.94	25,40,41,45	0
3	GOL	B	402	6/6	0.79	0.23	2.76	23,33,39,39	0
3	GOL	A	407[A]	6/6	0.81	0.20	2.19	37,41,42,48	6
8	NCO	A	441	7/7	0.99	0.09	2.15	6,6,7,7	0
3	GOL	A	402[B]	6/6	0.97	0.07	1.47	9,10,11,12	6
7	PEG	A	437[B]	7/7	0.77	0.23	1.46	20,21,26,27	7
7	PEG	A	437[A]	7/7	0.77	0.23	1.46	21,21,28,28	7
3	GOL	A	403	6/6	0.82	0.12	1.28	23,23,25,29	0
3	GOL	A	402[A]	6/6	0.97	0.07	1.25	9,9,10,10	6
3	GOL	B	405	6/6	0.85	0.17	1.20	17,22,23,26	0
2	W88	B	401[A]	28/28	0.95	0.15	1.05	6,13,34,36	28
2	W88	B	401[B]	28/28	0.95	0.15	1.01	6,14,26,29	28
6	EDO	A	430	4/4	0.17	0.30	0.99	63,68,70,72	0
3	GOL	A	405	6/6	0.92	0.12	0.81	17,21,32,32	0
6	EDO	A	433	4/4	0.87	0.13	0.80	20,25,30,36	0
2	W88	A	401	28/28	0.94	0.14	0.45	7,22,61,70	0
5	FMN	B	415	31/31	0.98	0.07	0.26	3,4,5,6	0
5	FMN	A	417	31/31	0.99	0.07	-0.17	3,4,6,6	0
3	GOL	A	404	6/6	0.95	0.07	-0.23	16,18,19,22	0
6	EDO	A	431	4/4	0.70	0.28	-	40,52,52,58	0
3	GOL	A	407[B]	6/6	0.81	0.20	-	20,28,29,30	6
6	EDO	A	421	4/4	0.91	0.14	-	29,30,34,38	0
6	EDO	B	419	4/4	0.81	0.21	-	27,31,34,35	0
6	EDO	B	428	4/4	0.71	0.25	-	50,52,54,56	0
6	EDO	B	430	4/4	0.77	0.31	-	35,37,39,44	0
7	PEG	B	431[A]	7/7	0.71	0.53	-	61,80,102,108	7
7	PEG	A	440	7/7	0.84	0.29	-	27,33,36,43	0
6	EDO	A	428	4/4	0.58	0.17	-	48,50,51,56	0
6	EDO	B	423	4/4	0.62	0.21	-	39,46,46,49	0
3	GOL	B	404[B]	6/6	0.82	0.18	-	21,26,27,28	6
6	EDO	A	427	4/4	0.70	0.43	-	52,53,56,58	0
6	EDO	A	425	4/4	0.69	0.26	-	31,35,41,41	0
6	EDO	A	429	4/4	0.74	0.16	-	36,39,40,44	0
7	PEG	B	431[B]	7/7	0.71	0.53	-	23,26,27,29	7
3	GOL	A	408	6/6	0.67	0.26	-	46,51,62,64	0
3	GOL	A	411	6/6	0.52	0.23	-	46,61,66,74	0
6	EDO	A	419	4/4	0.41	0.18	-	57,59,64,65	0
6	EDO	A	420	4/4	0.92	0.24	-	24,29,30,31	0
6	EDO	B	429	4/4	0.83	0.22	-	33,40,45,55	0
7	PEG	A	439	7/7	0.71	0.37	-	24,31,37,38	0
6	EDO	A	426	4/4	0.73	0.30	-	54,57,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	413	6/6	0.79	0.18	-	29,37,39,40	0
6	EDO	B	417	4/4	0.81	0.18	-	32,35,35,41	0
4	CAC	B	414	5/5	0.75	0.25	-	142,150,164,166	0
3	GOL	B	411	6/6	0.59	0.26	-	51,52,54,55	0
4	CAC	A	416	5/5	0.95	0.33	-	30,34,39,43	0
6	EDO	B	420	4/4	0.60	0.41	-	56,61,62,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.