



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:53 PM GMT

PDB ID : 3VAV  
Title : Crystal structure of 3-methyl-2-oxobutanoate hydroxymethyltransferase from *Burkholderia thailandensis*  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2011-12-29  
Resolution : 1.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

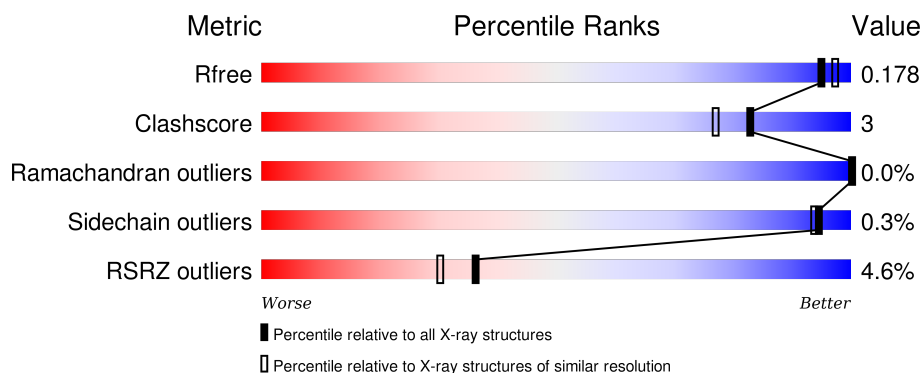
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	275	<div> <div>7%</div> <div>89% 5% 5%</div> </div>
1	B	275	<div> <div>6%</div> <div>88% 6% 5%</div> </div>
1	C	275	<div> <div>2%</div> <div>83% 5% 12%</div> </div>
1	D	275	<div> <div>5%</div> <div>91% • 6%</div> </div>
1	E	275	<div> <div>6%</div> <div>87% • 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	275	
1	G	275	
1	H	275	
1	I	275	
1	J	275	

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
2	EDO	A	272	-	-	-	X
2	EDO	B	272	-	-	-	X
2	EDO	D	272	-	-	-	X
2	EDO	E	272	-	-	-	X
2	EDO	G	272	-	-	-	X
2	EDO	H	272	-	-	-	X
2	EDO	I	272	-	-	-	X
2	EDO	J	272	-	-	-	X
2	EDO	J	273	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21566 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 3-methyl-2-oxobutanoate hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	7	0
			1947	1239	337	361	10			
1	B	260	Total	C	N	O	S	0	6	0
			1955	1250	337	358	10			
1	C	243	Total	C	N	O	S	0	4	0
			1828	1165	315	338	10			
1	D	259	Total	C	N	O	S	0	7	0
			1958	1247	341	360	10			
1	E	251	Total	C	N	O	S	0	9	0
			1897	1210	322	354	11			
1	F	253	Total	C	N	O	S	0	5	0
			1899	1205	334	350	10			
1	G	239	Total	C	N	O	S	0	4	0
			1793	1145	304	333	11			
1	H	263	Total	C	N	O	S	0	5	0
			1966	1251	339	366	10			
1	I	245	Total	C	N	O	S	0	9	0
			1861	1185	321	344	11			
1	J	263	Total	C	N	O	S	0	4	0
			1959	1247	338	364	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
A	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
A	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
A	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
B	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
B	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
B	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
B	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
C	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
C	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
C	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
D	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
D	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
D	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
D	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
E	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
E	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
E	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
E	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
F	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
F	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
F	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
F	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
G	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
G	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
G	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
G	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
H	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
H	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
H	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
H	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
I	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
I	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
I	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
I	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1
J	-3	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
J	-2	PRO	-	EXPRESSION TAG	UNP Q2SYZ1
J	-1	GLY	-	EXPRESSION TAG	UNP Q2SYZ1
J	0	SER	-	EXPRESSION TAG	UNP Q2SYZ1

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Cl	0	0
			1	1		

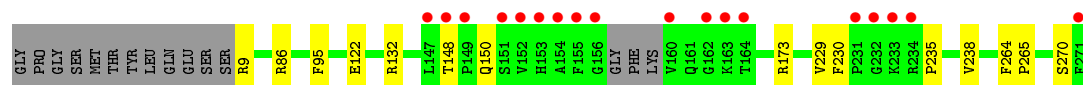
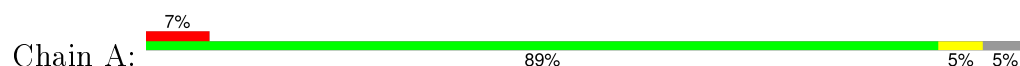
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	264	Total 264	O 264	0	0
4	B	245	Total 245	O 245	0	0
4	C	239	Total 239	O 239	0	0
4	D	264	Total 264	O 264	0	0
4	E	205	Total 205	O 205	0	0
4	F	248	Total 248	O 248	0	0
4	G	253	Total 253	O 253	0	0
4	H	287	Total 287	O 287	0	0
4	I	231	Total 231	O 231	0	0
4	J	222	Total 222	O 222	0	0

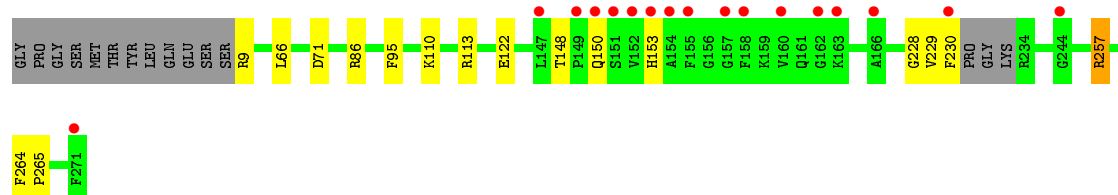
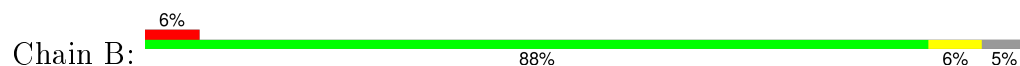
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

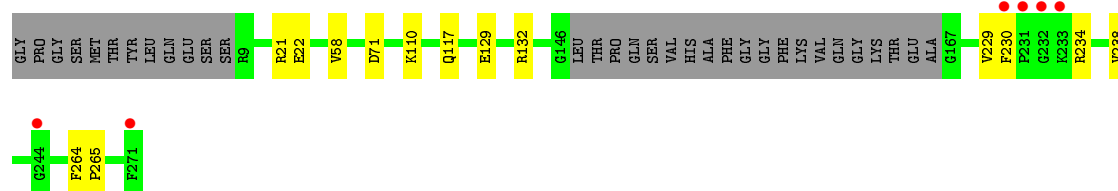
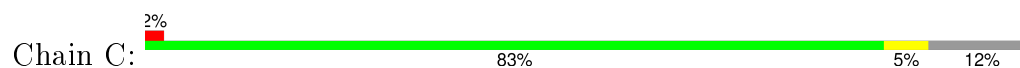
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



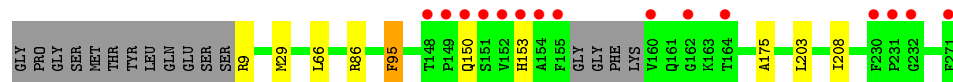
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



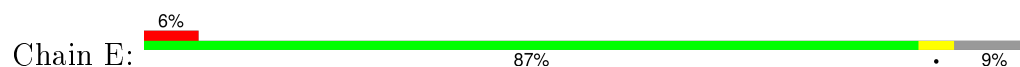
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



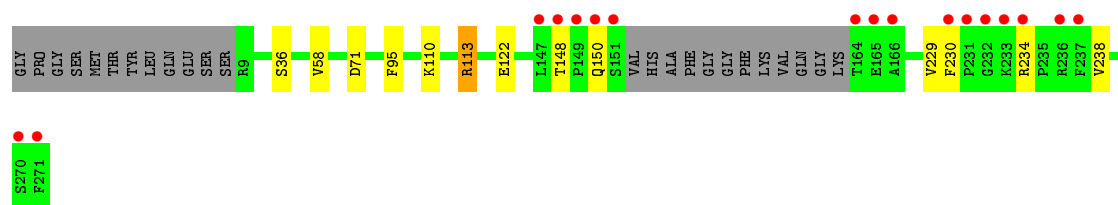
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



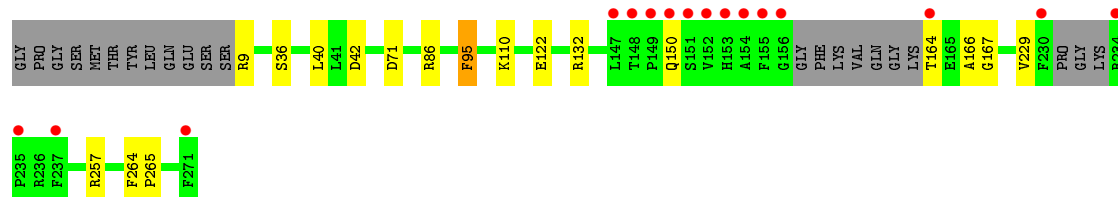
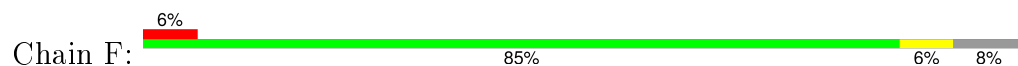
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



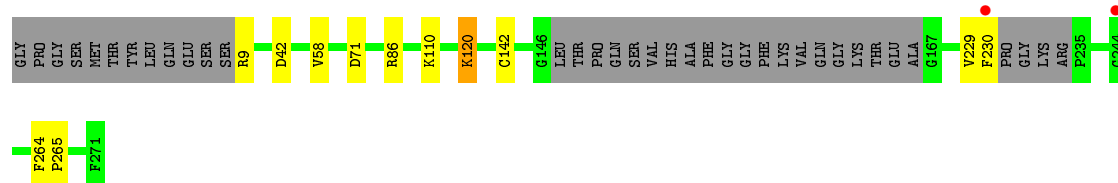
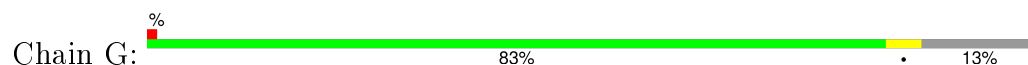




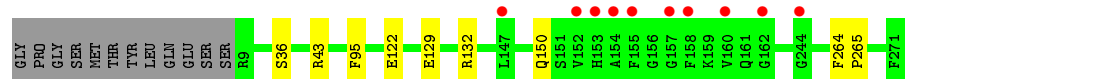
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



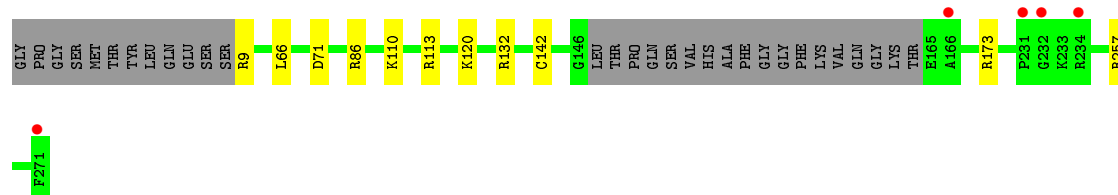
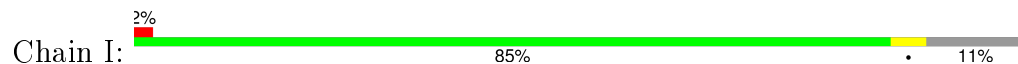
- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase

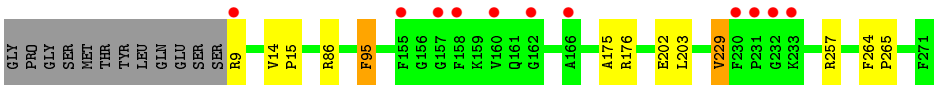


- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase



- Molecule 1: 3-methyl-2-oxobutanoate hydroxymethyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.71Å 174.75Å 104.58Å 90.00° 108.71° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 47.67 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.80) 100.0 (47.67-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.91 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.154 , 0.180 0.153 , 0.178	Depositor DCC
$R_{free}$ test set	12850 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 255850 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CL

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	0.65	0/2001	0.66	0/2723
1	B	0.65	0/2003	0.70	2/2723 (0.1%)
1	C	0.68	0/1868	0.73	1/2541 (0.0%)
1	D	0.66	0/2010	0.66	0/2734
1	E	0.57	0/1953	0.63	1/2657 (0.0%)
1	F	0.65	0/1944	0.69	0/2640
1	G	0.66	0/1833	0.69	0/2488
1	H	0.69	0/2019	0.69	1/2746 (0.0%)
1	I	0.64	0/1917	0.69	2/2601 (0.1%)
1	J	0.61	0/2006	0.65	0/2731
All	All	0.65	0/19554	0.68	7/26584 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	257	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	257[A]	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	257[B]	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	H	43	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	21	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	E	113	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	I	257	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1947	0	1957	22	0
1	B	1955	0	1971	14	0
1	C	1828	0	1842	9	0
1	D	1958	0	1966	12	0
1	E	1897	0	1908	12	0
1	F	1899	0	1913	20	0
1	G	1793	0	1806	7	0
1	H	1966	0	1970	9	0
1	I	1861	0	1889	14	0
1	J	1959	0	1960	10	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	G	8	0	12	0	0
2	H	4	0	6	0	0
2	I	4	0	6	0	0
2	J	8	0	12	0	0
3	I	1	0	0	0	0
4	A	264	0	0	4	0
4	B	245	0	0	2	0
4	C	239	0	0	2	0
4	D	264	0	0	2	0
4	E	205	0	0	3	0
4	F	248	0	0	2	0
4	G	253	0	0	0	0
4	H	287	0	0	4	0
4	I	231	0	0	2	0
4	J	222	0	0	1	0
All	All	21566	0	19248	120	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 3.

All (120) 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:F:229[A]:VAL:O	1:F:229[A]:VAL:HG12	1.63	0.96
1:H:129[A]:GLU:OE1	1:H:132[A]:ARG:NH2	2.01	0.93
1:I:173[B]:ARG:HH21	1:I:173[B]:ARG:CG	1.87	0.86
1:J:229[B]:VAL:O	1:J:229[B]:VAL:HG12	1.84	0.78
1:I:173[B]:ARG:HH21	1:I:173[B]:ARG:HG2	1.49	0.76
1:G:229:VAL:O	1:G:230[B]:PHE:CD2	2.38	0.76
1:F:229[A]:VAL:CG1	1:F:229[A]:VAL:O	2.37	0.72
1:I:9:ARG:HE	1:I:86:ARG:HE	1.37	0.72
4:H:1492:HOH:O	1:I:66:LEU:HD22	1.89	0.71
1:F:9:ARG:HE	1:F:86:ARG:HE	1.36	0.70
1:H:150:GLN:HG2	4:H:697:HOH:O	1.92	0.68
1:A:150:GLN:HG2	4:A:1283:HOH:O	1.94	0.66
1:I:113:ARG:NH1	1:J:95:PHE:O	2.26	0.66
1:J:9:ARG:HE	1:J:86:ARG:HE	1.46	0.64
1:E:71:ASP:OD2	1:E:110[B]:LYS:HE2	1.98	0.64
1:G:229:VAL:O	1:G:230[B]:PHE:CG	2.52	0.62
1:I:173[B]:ARG:NH2	1:I:173[B]:ARG:CG	2.53	0.61
1:C:132[A]:ARG:NH1	4:C:2104:HOH:O	2.33	0.61
1:A:9:ARG:HE	1:A:86:ARG:HE	1.47	0.61
1:G:71:ASP:OD2	1:G:110:LYS:HE2	2.01	0.61
1:D:9:ARG:HE	1:D:86:ARG:HE	1.47	0.61
1:B:150:GLN:HG2	4:B:1039:HOH:O	1.99	0.60
1:A:95:PHE:HB2	1:A:150:GLN:HB3	1.83	0.60
1:C:129[A]:GLU:OE2	1:C:132[A]:ARG:NH2	2.35	0.59
1:F:164:THR:HG22	1:F:167:GLY:H	1.67	0.59
1:A:229[B]:VAL:O	1:A:229[B]:VAL:HG12	2.00	0.59
1:E:229[B]:VAL:O	1:E:230[B]:PHE:CG	2.56	0.59
1:B:95:PHE:HB2	1:B:150:GLN:HB3	1.84	0.58
1:C:22:GLU:OE1	4:C:299:HOH:O	2.17	0.58
1:H:95:PHE:HB2	1:H:150:GLN:HB3	1.86	0.58
1:E:229[B]:VAL:HG12	1:E:229[B]:VAL:O	2.04	0.58
1:E:229[B]:VAL:O	1:E:230[B]:PHE:CD2	2.58	0.57
1:B:257[B]:ARG:CZ	1:B:257[B]:ARG:HB2	2.34	0.57
1:E:234:ARG:NE	1:E:238:VAL:O	2.37	0.56
1:A:229[B]:VAL:HG13	1:F:40:LEU:HD12	1.87	0.55
1:F:164:THR:HG22	1:F:166:ALA:N	2.21	0.55
1:E:122:GLU:OE1	1:E:148:THR:HB	2.06	0.55
1:A:270:SER:CB	4:A:2071:HOH:O	2.55	0.55
1:E:150:GLN:NE2	4:E:2034:HOH:O	2.40	0.55
1:E:36:SER:HB3	1:J:229[A]:VAL:HG11	1.89	0.54
1:F:257[A]:ARG:CZ	1:F:257[A]:ARG:HB2	2.37	0.53
1:I:173[B]:ARG:NH2	1:I:173[B]:ARG:HG3	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:71:ASP:OD2	1:I:110[A]:LYS:HE2	2.09	0.53
1:D:95:PHE:O	1:E:113:ARG:NH1	2.38	0.53
1:B:122:GLU:HB3	1:B:148:THR:HB	1.91	0.52
1:A:173[A]:ARG:NH2	4:A:2064:HOH:O	2.34	0.51
1:A:229[A]:VAL:HG11	1:F:36:SER:HB3	1.93	0.51
1:J:229[B]:VAL:O	1:J:229[B]:VAL:CG1	2.56	0.50
1:F:164:THR:HG22	1:F:166:ALA:H	1.74	0.50
1:E:58:VAL:HG12	1:E:230[B]:PHE:CZ	2.46	0.50
1:I:173[B]:ARG:HH21	1:I:173[B]:ARG:HG3	1.74	0.50
1:A:95:PHE:O	1:B:113:ARG:NH1	2.42	0.50
1:B:229[B]:VAL:HG12	1:B:229[B]:VAL:O	2.12	0.50
1:J:176:ARG:NH2	1:J:202:GLU:OE1	2.41	0.50
1:D:29:MET:HE3	1:D:208:ILE:HG13	1.94	0.49
1:F:122:GLU:HG3	4:F:1696:HOH:O	2.10	0.49
1:D:95:PHE:HB2	1:D:150:GLN:HB3	1.95	0.49
1:F:257[A]:ARG:NH1	1:F:257[A]:ARG:HB2	2.28	0.49
1:B:153:HIS:CE1	1:C:117:GLN:HG2	2.48	0.48
1:A:9:ARG:HG2	1:A:86:ARG:NE	2.29	0.48
1:B:71:ASP:OD2	1:B:110[A]:LYS:HE2	2.12	0.48
1:D:150:GLN:NE2	4:D:1924:HOH:O	2.46	0.48
1:F:95:PHE:HB2	1:F:150:GLN:HB3	1.94	0.48
1:A:132[A]:ARG:HD3	4:A:1331:HOH:O	2.14	0.48
1:D:153:HIS:CD2	4:E:1061:HOH:O	2.65	0.48
1:H:95:PHE:HB2	1:H:150:GLN:CG	2.44	0.47
1:E:95:PHE:HB2	1:E:150:GLN:HB3	1.97	0.47
1:F:150:GLN:HG2	4:F:926:HOH:O	2.14	0.47
1:J:175:ALA:HB1	1:J:203:LEU:HD11	1.96	0.47
1:J:257:ARG:NH1	4:J:1579:HOH:O	2.47	0.47
1:D:150:GLN:HG2	4:D:1505:HOH:O	2.14	0.46
1:E:58:VAL:HG12	1:E:230[B]:PHE:HZ	1.80	0.46
1:G:264:PHE:CD1	1:G:265:PRO:HA	2.51	0.46
1:F:9:ARG:HG3	1:F:86:ARG:HD2	1.98	0.45
1:C:234:ARG:HD3	1:C:238:VAL:O	2.16	0.45
1:H:122:GLU:HG3	4:H:2396:HOH:O	2.16	0.45
1:B:66[A]:LEU:HD22	4:B:1039:HOH:O	2.16	0.45
1:C:71:ASP:OD2	1:C:110:LYS:NZ	2.45	0.45
1:A:229[B]:VAL:HG13	1:F:40:LEU:CD1	2.47	0.45
1:C:58:VAL:HG12	1:C:230[B]:PHE:CZ	2.51	0.45
1:B:264:PHE:CD1	1:B:265:PRO:HA	2.52	0.44
1:F:9:ARG:HG2	1:F:86:ARG:NE	2.32	0.44
1:H:95:PHE:HB2	1:H:150:GLN:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PHE:CD1	1:C:265:PRO:HA	2.52	0.44
1:J:264:PHE:CD1	1:J:265:PRO:HA	2.53	0.44
1:A:9:ARG:HG3	1:A:86:ARG:HD2	1.99	0.43
1:D:9:ARG:HG3	1:D:86:ARG:HD2	1.99	0.43
1:D:9:ARG:CG	1:D:86:ARG:HE	2.30	0.43
1:C:229[B]:VAL:HG11	1:H:36:SER:HB3	1.99	0.43
1:F:132[B]:ARG:HG2	1:F:132[B]:ARG:NH2	2.32	0.43
1:D:66:LEU:HD22	4:E:1061:HOH:O	2.18	0.43
1:A:264:PHE:CD1	1:A:265:PRO:HA	2.54	0.43
1:I:173[B]:ARG:NH2	4:I:1879:HOH:O	2.52	0.43
1:A:229[B]:VAL:O	1:A:230:PHE:CG	2.72	0.43
1:H:264:PHE:CD1	1:H:265:PRO:HA	2.53	0.43
1:I:120:LYS:HA	1:I:142:CYS:O	2.19	0.42
1:A:9:ARG:NE	1:A:86:ARG:HE	2.14	0.42
1:A:9:ARG:O	1:A:86:ARG:HD2	2.19	0.42
1:B:95:PHE:HB2	1:B:150:GLN:CB	2.49	0.42
1:D:175:ALA:HB1	1:D:203:LEU:HD11	2.00	0.42
1:G:58:VAL:HG12	1:G:230[B]:PHE:CZ	2.55	0.42
1:D:9:ARG:O	1:D:86:ARG:HD2	2.19	0.42
1:B:66[A]:LEU:HD13	1:B:95:PHE:CD2	2.55	0.42
1:H:122:GLU:HG3	4:H:1068:HOH:O	2.21	0.41
1:B:9:ARG:O	1:B:86:ARG:HD2	2.21	0.41
1:J:14:VAL:HB	1:J:15:PRO:HD3	2.02	0.41
1:B:228:GLY:HA2	1:B:230[A]:PHE:CE2	2.55	0.41
1:A:235:PRO:O	1:A:238[B]:VAL:HG22	2.20	0.41
1:G:9:ARG:O	1:G:86:ARG:HD2	2.20	0.41
1:A:95:PHE:HB2	1:A:150:GLN:CG	2.50	0.41
1:I:9:ARG:O	1:I:86:ARG:HD2	2.21	0.41
1:F:164:THR:CG2	1:F:167:GLY:H	2.31	0.41
1:G:120:LYS:HA	1:G:142:CYS:O	2.21	0.41
1:F:264:PHE:CD1	1:F:265:PRO:HA	2.56	0.41
1:F:71:ASP:OD2	1:F:110[A]:LYS:HE2	2.22	0.40
1:A:95:PHE:HB2	1:A:150:GLN:CB	2.48	0.40
1:A:122:GLU:HB3	1:A:148:THR:HB	2.03	0.40
1:A:229[A]:VAL:O	1:A:229[A]:VAL:CG1	2.68	0.40
1:I:132:ARG:NH1	4:I:1865:HOH:O	2.39	0.40
1:I:9:ARG:NE	1:I:86:ARG:HE	2.14	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	263/275 (96%)	256 (97%)	7 (3%)	0	100	100
1	B	261/275 (95%)	259 (99%)	2 (1%)	0	100	100
1	C	243/275 (88%)	238 (98%)	5 (2%)	0	100	100
1	D	262/275 (95%)	259 (99%)	3 (1%)	0	100	100
1	E	256/275 (93%)	249 (97%)	7 (3%)	0	100	100
1	F	252/275 (92%)	248 (98%)	4 (2%)	0	100	100
1	G	236/275 (86%)	230 (98%)	6 (2%)	0	100	100
1	H	266/275 (97%)	263 (99%)	3 (1%)	0	100	100
1	I	249/275 (90%)	246 (99%)	3 (1%)	0	100	100
1	J	265/275 (96%)	259 (98%)	4 (2%)	2 (1%)	24	8
All	All	2553/2750 (93%)	2507 (98%)	44 (2%)	2 (0%)	100	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	229[A]	VAL
1	J	229[B]	VAL

### 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	198/209 (95%)	198 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/209 (95%)	198 (100%)	0	100	100
1	C	186/209 (89%)	186 (100%)	0	100	100
1	D	198/209 (95%)	197 (100%)	1 (0%)	92	91
1	E	194/209 (93%)	194 (100%)	0	100	100
1	F	192/209 (92%)	190 (99%)	2 (1%)	82	77
1	G	183/209 (88%)	181 (99%)	2 (1%)	80	74
1	H	199/209 (95%)	199 (100%)	0	100	100
1	I	190/209 (91%)	190 (100%)	0	100	100
1	J	198/209 (95%)	197 (100%)	1 (0%)	92	91
All	All	1936/2090 (93%)	1930 (100%)	6 (0%)	94	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	95	PHE
1	F	42	ASP
1	F	95	PHE
1	G	42	ASP
1	G	120	LYS
1	J	95	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	D	243	GLN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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	EDO	A	272	-	3,3,3	0.40	0	2,2,2	0.28	0
2	EDO	B	272	-	3,3,3	0.62	0	2,2,2	0.19	0
2	EDO	C	272	-	3,3,3	0.45	0	2,2,2	0.11	0
2	EDO	D	272	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	E	272	-	3,3,3	0.53	0	2,2,2	0.31	0
2	EDO	G	272	-	3,3,3	0.37	0	2,2,2	0.44	0
2	EDO	G	273	-	3,3,3	0.48	0	2,2,2	0.40	0
2	EDO	H	272	-	3,3,3	0.61	0	2,2,2	0.53	0
2	EDO	I	272	-	3,3,3	0.46	0	2,2,2	0.07	0
2	EDO	J	272	-	3,3,3	0.66	0	2,2,2	0.15	0
2	EDO	J	273	-	3,3,3	0.51	0	2,2,2	0.61	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	EDO	A	272	-	-	0/1/1/1	0/0/0/0
2	EDO	B	272	-	-	0/1/1/1	0/0/0/0
2	EDO	C	272	-	-	0/1/1/1	0/0/0/0
2	EDO	D	272	-	-	0/1/1/1	0/0/0/0
2	EDO	E	272	-	-	0/1/1/1	0/0/0/0
2	EDO	G	272	-	-	0/1/1/1	0/0/0/0
2	EDO	G	273	-	-	0/1/1/1	0/0/0/0
2	EDO	H	272	-	-	0/1/1/1	0/0/0/0
2	EDO	I	272	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	J	272	-	-	0/1/1/1	0/0/0/0
2	EDO	J	273	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	260/275 (94%)	-0.23	18 (6%) 20 16	8, 13, 37, 48	0
1	B	260/275 (94%)	-0.27	17 (6%) 22 18	8, 14, 37, 52	0
1	C	243/275 (88%)	-0.49	6 (2%) 61 56	7, 12, 27, 53	0
1	D	259/275 (94%)	-0.35	15 (5%) 26 21	8, 14, 41, 57	0
1	E	251/275 (91%)	-0.17	17 (6%) 20 16	9, 18, 42, 67	0
1	F	253/275 (92%)	-0.28	16 (6%) 23 19	8, 15, 37, 55	0
1	G	239/275 (86%)	-0.64	2 (0%) 87 85	7, 12, 24, 40	0
1	H	263/275 (95%)	-0.37	10 (3%) 44 38	7, 12, 31, 43	0
1	I	245/275 (89%)	-0.49	5 (2%) 68 64	8, 14, 29, 51	0
1	J	263/275 (95%)	-0.28	11 (4%) 40 34	9, 17, 36, 49	0
All	All	2536/2750 (92%)	-0.35	117 (4%) 36 30	7, 14, 35, 67	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	232	GLY	6.4
1	E	231	PRO	6.1
1	F	155	PHE	5.8
1	A	160	VAL	5.7
1	F	271	PHE	5.6
1	E	271	PHE	5.6
1	A	232	GLY	5.3
1	B	158	PHE	5.3
1	G	230[A]	PHE	5.1
1	B	162	GLY	5.0
1	I	232	GLY	5.0
1	E	230[A]	PHE	4.8
1	D	160	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	166	ALA	4.7
1	B	160	VAL	4.6
1	B	155	PHE	4.5
1	B	271	PHE	4.4
1	D	232	GLY	4.4
1	F	154	ALA	4.4
1	E	147	LEU	4.4
1	F	152	VAL	4.2
1	A	155	PHE	4.1
1	H	155	PHE	4.0
1	D	152	VAL	3.9
1	E	151	SER	3.8
1	D	154	ALA	3.8
1	F	147	LEU	3.8
1	D	231	PRO	3.8
1	J	158	PHE	3.7
1	F	235	PRO	3.7
1	J	166	ALA	3.7
1	D	230[A]	PHE	3.7
1	F	156	GLY	3.6
1	A	271	PHE	3.6
1	I	166	ALA	3.6
1	A	147	LEU	3.6
1	H	147	LEU	3.5
1	G	244	GLY	3.5
1	I	231	PRO	3.5
1	A	151	SER	3.4
1	D	151	SER	3.4
1	E	150	GLN	3.4
1	H	157	GLY	3.4
1	A	148	THR	3.4
1	C	230[A]	PHE	3.3
1	D	271	PHE	3.3
1	F	230	PHE	3.3
1	E	164	THR	3.3
1	E	270	SER	3.3
1	F	151	SER	3.3
1	J	233	LYS	3.2
1	E	149	PRO	3.2
1	H	162	GLY	3.2
1	C	232	GLY	3.2
1	F	150	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	152	VAL	3.2
1	A	233	LYS	3.2
1	F	153	HIS	3.2
1	D	148	THR	3.1
1	B	151	SER	3.1
1	F	149	PRO	3.1
1	B	230[A]	PHE	3.1
1	I	271	PHE	3.1
1	A	231	PRO	3.1
1	J	157	GLY	3.1
1	J	232	GLY	3.1
1	E	148	THR	3.1
1	A	163	LYS	3.1
1	J	162	GLY	3.0
1	F	164	THR	3.0
1	A	154	ALA	3.0
1	J	155	PHE	2.9
1	A	162	GLY	2.9
1	J	160	VAL	2.9
1	D	153	HIS	2.8
1	B	149	PRO	2.8
1	B	152	VAL	2.8
1	D	164	THR	2.8
1	E	233	LYS	2.8
1	A	153	HIS	2.7
1	H	153	HIS	2.7
1	H	154	ALA	2.7
1	C	244	GLY	2.7
1	D	162	GLY	2.7
1	B	147	LEU	2.7
1	A	156	GLY	2.7
1	D	155	PHE	2.7
1	C	231	PRO	2.7
1	H	244	GLY	2.6
1	C	233	LYS	2.6
1	B	163	LYS	2.6
1	E	165	GLU	2.6
1	D	150	GLN	2.6
1	B	157	GLY	2.5
1	B	166	ALA	2.5
1	J	231	PRO	2.5
1	F	234	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	9	ARG	2.4
1	A	149	PRO	2.4
1	E	236	ARG	2.4
1	A	164	THR	2.3
1	E	237	PHE	2.3
1	F	237	PHE	2.2
1	J	230	PHE	2.2
1	A	234	ARG	2.2
1	I	234	ARG	2.2
1	B	153	HIS	2.2
1	H	158	PHE	2.2
1	B	244	GLY	2.2
1	E	234	ARG	2.2
1	C	271	PHE	2.1
1	F	148	THR	2.1
1	H	152	VAL	2.1
1	B	150	GLN	2.1
1	B	154	ALA	2.0
1	D	149	PRO	2.0
1	H	160	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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
2	EDO	I	272	4/4	0.91	0.23	17.27	8,8,8,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	J	273	4/4	0.91	0.16	7.87	15,15,15,17	0
2	EDO	D	272	4/4	0.91	0.11	4.77	22,24,25,26	0
2	EDO	B	272	4/4	0.87	0.12	4.22	23,26,27,28	0
2	EDO	H	272	4/4	0.92	0.10	3.07	22,23,24,26	0
2	EDO	J	272	4/4	0.91	0.12	2.85	15,17,17,20	0
2	EDO	G	272	4/4	0.96	0.11	2.85	21,24,25,29	0
2	EDO	A	272	4/4	0.92	0.11	2.40	22,24,27,30	0
2	EDO	E	272	4/4	0.84	0.10	2.13	29,30,31,35	0
2	EDO	C	272	4/4	0.97	0.09	0.48	22,23,23,25	0
2	EDO	G	273	4/4	0.95	0.08	0.33	21,22,24,25	0
3	CL	I	273	1/1	0.96	0.10	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.