



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:14 am BST

PDB ID : 5VAG  
Title : Crystal structure of H7-specific antibody m826 in complex with the HA1 domain of hemagglutinin from H7N9 influenza virus  
Authors : Song, H.; Ying, T.; Ji, X.  
Deposited on : 2017-03-26  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

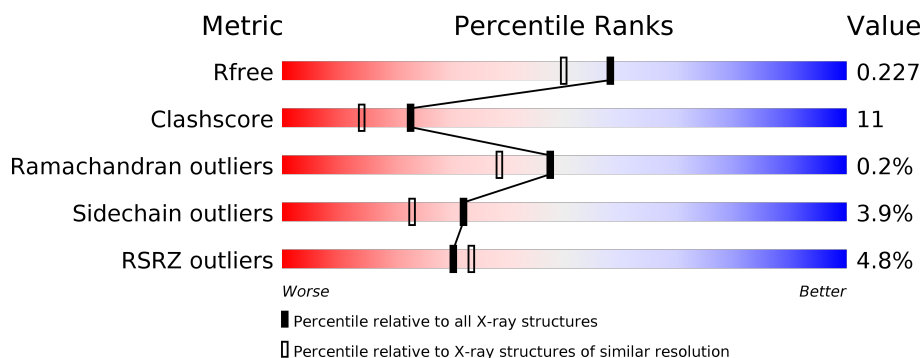
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	
2	B	215	
3	C	247	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5510 atoms, of which 60 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	5	0
			1641	1029	292	312	8			

- Molecule 2 is a protein called Light chain of antibody m826.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	7	0
			1669	1046	277	342	4			

- Molecule 3 is a protein called Heavy chain of antibody m826.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	221	Total	C	N	O	S	0	9	0
			1690	1071	278	335	6			

- Molecule 4 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
4	A	1	Total C H O 10 2 6 2	0	0
4	A	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	B	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C H O 10 2 6 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	103	Total O 103 103	0	0
5	B	150	Total O 150 150	0	0
5	C	157	Total O 157 157	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.33Å 101.33Å 136.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.72 – 1.90 37.72 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (37.72-1.90) 96.5 (37.72-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 1.89Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.191 , 0.227 0.191 , 0.227	Depositor DCC
$R_{free}$ test set	1000 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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.*

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

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

## 5 Model quality [i](#)

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

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

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	0.40	0/1692	0.63	4/2285 (0.2%)
2	B	0.46	0/1724	0.68	3/2340 (0.1%)
3	C	0.40	0/1753	0.59	0/2388
All	All	0.42	0/5169	0.63	7/7013 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148[A]	ARG	CA-C-O	7.08	134.97	120.10
1	A	148[B]	ARG	CA-C-O	7.08	134.97	120.10
2	B	11	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	211	ARG	N-CA-C	6.38	128.24	111.00
2	B	212	GLY	N-CA-C	-6.21	97.57	113.10
1	A	148[A]	ARG	CA-C-N	-5.55	104.99	117.20
1	A	148[B]	ARG	CA-C-N	-5.55	104.99	117.20

There are no chirality outliers.

There are no planarity outliers.

### 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	1641	0	1608	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1669	0	1650	53	0
3	C	1690	0	1665	21	0
4	A	8	12	12	0	0
4	B	20	30	30	4	0
4	C	12	18	18	1	0
5	A	103	0	0	6	0
5	B	150	0	0	8	0
5	C	157	0	0	2	0
All	All	5450	60	4983	115	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 11.

All (115) 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)
2:B:130:ALA:HB3	2:B:181[B]:LEU:HD11	1.27	1.14
2:B:181[B]:LEU:HD13	2:B:186:TYR:HB2	1.44	0.98
2:B:130:ALA:HB3	2:B:181[B]:LEU:CD1	1.95	0.96
2:B:181[B]:LEU:CD1	2:B:186:TYR:HB2	2.02	0.89
1:A:195:VAL:CG2	1:A:236:SER:HB2	2.08	0.84
3:C:30:SER:HB3	5:C:416:HOH:O	1.81	0.80
2:B:210:ASN:C	2:B:212:GLY:HA3	2.06	0.76
1:A:106:TYR:CE2	1:A:235:LEU:HD13	2.20	0.76
1:A:114[B]:GLU:OE2	2:B:94:THR:HB	1.89	0.71
2:B:144:ALA:O	2:B:145:LYS:HD2	1.90	0.71
2:B:151:ASP:OD1	2:B:190:LYS:HG2	1.92	0.69
2:B:18:ARG:HD2	5:B:410:HOH:O	1.92	0.69
3:C:32:TYR:CG	3:C:98[A]:ARG:HD2	2.29	0.68
3:C:207:ASN:ND2	3:C:214:LYS:HG2	2.09	0.67
1:A:173:MET:HE2	1:A:175:LYS:HE2	1.77	0.67
2:B:191:VAL:HG13	5:B:518:HOH:O	1.95	0.65
2:B:181[B]:LEU:HD21	2:B:186:TYR:HD1	1.63	0.64
1:A:235:LEU:HD23	1:A:237:GLY:H	1.63	0.63
1:A:195:VAL:HB	1:A:236:SER:HB2	1.80	0.63
1:A:196:SER:OG	1:A:199:GLU:HG2	1.99	0.62
3:C:98[A]:ARG:NH1	3:C:100:PRO:HG3	2.14	0.62
3:C:98[A]:ARG:NH2	3:C:109:GLN:OE1	2.32	0.62
3:C:151:LYS:HG3	3:C:185[B]:SER:OG	2.00	0.61
1:A:106:TYR:HE2	1:A:235:LEU:HD13	1.63	0.60
2:B:41:GLY:H	4:B:304:EDO:H21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:HG23	1:A:236:SER:HB2	1.81	0.59
1:A:67:VAL:CG2	1:A:92:ALA:HB2	2.32	0.58
1:A:67:VAL:HG23	1:A:92:ALA:HB2	1.85	0.58
1:A:145:SER:HB2	1:A:148[A]:ARG:HH21	1.69	0.58
2:B:110:VAL:HG21	2:B:199:GLN:NE2	2.18	0.58
1:A:195:VAL:CB	1:A:236:SER:HB2	2.34	0.58
1:A:123:SER:HB2	1:A:269:LEU:HG	1.86	0.57
2:B:150:VAL:HG13	2:B:192:TYR:CE2	2.39	0.57
1:A:217:ASN:HB3	5:A:600:HOH:O	2.03	0.57
3:C:32:TYR:CD2	3:C:98[A]:ARG:HD2	2.40	0.57
1:A:264:ASP:OD1	5:A:501:HOH:O	2.17	0.56
1:A:173:MET:CE	1:A:175:LYS:HE2	2.36	0.55
2:B:100:GLN:HG3	5:B:428:HOH:O	2.07	0.55
2:B:181[B]:LEU:HD11	2:B:186:TYR:HB2	1.89	0.54
2:B:207:LYS:HE2	5:B:493:HOH:O	2.08	0.54
1:A:138:ILE:HB	1:A:162:LEU:O	2.08	0.53
1:A:187:ILE:HD12	1:A:246:LEU:HB2	1.91	0.52
2:B:130:ALA:CB	2:B:181[B]:LEU:HD11	2.19	0.52
2:B:181[B]:LEU:HD13	2:B:182:SER:O	2.10	0.51
2:B:142:ARG:HH11	2:B:142:ARG:CG	2.23	0.51
2:B:150:VAL:O	2:B:151:ASP:C	2.46	0.51
2:B:155:GLN:CG	2:B:158:ASN:HD21	2.22	0.51
1:A:107:PRO:HG3	1:A:232:VAL:O	2.10	0.51
2:B:149:LYS:HE3	5:B:423:HOH:O	2.11	0.51
2:B:155:GLN:OE1	4:B:305:EDO:H21	2.10	0.50
1:A:235:LEU:CD2	1:A:237:GLY:H	2.25	0.50
1:A:96:ILE:N	1:A:96:ILE:HD12	2.25	0.50
3:C:68:VAL:HG22	3:C:83:LEU:HD13	1.92	0.50
2:B:158:ASN:HD22	2:B:181[A]:LEU:HD21	1.75	0.50
3:C:62[A]:GLN:HG3	3:C:63:LYS:N	2.24	0.50
3:C:67:ARG:NH2	3:C:90:ASP:OD2	2.40	0.48
2:B:158:ASN:ND2	2:B:179:LEU:HD11	2.28	0.48
2:B:110:VAL:HG21	2:B:199:GLN:HE21	1.78	0.48
1:A:195:VAL:HA	1:A:227:GLY:O	2.13	0.48
2:B:142:ARG:HH11	2:B:142:ARG:CB	2.27	0.48
2:B:62:PHE:CZ	4:B:302:EDO:H11	2.48	0.48
2:B:211:ARG:N	2:B:212:GLY:HA3	2.29	0.48
3:C:186:LEU:HD12	3:C:186:LEU:C	2.33	0.48
1:A:118:GLN:NE2	5:A:510:HOH:O	2.47	0.47
1:A:231:GLN:HB2	1:A:233:ASN:O	2.14	0.47
2:B:151:ASP:HA	2:B:191:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LYS:HE2	3:C:17:SER:O	2.15	0.47
3:C:11:VAL:HG21	3:C:155:PRO:HG3	1.97	0.47
2:B:144:ALA:C	2:B:145:LYS:HD2	2.35	0.47
1:A:195:VAL:HB	1:A:236:SER:C	2.36	0.46
1:A:106:TYR:OH	1:A:235:LEU:HD22	2.15	0.46
1:A:186:LEU:HB2	1:A:245:MET:HE1	1.98	0.46
2:B:181[B]:LEU:HD22	2:B:186:TYR:HA	1.98	0.45
2:B:210:ASN:O	2:B:212:GLY:HA3	2.15	0.45
2:B:212:GLY:O	2:B:213:GLU:HG2	2.17	0.44
1:A:261:ILE:HD12	1:A:261:ILE:N	2.32	0.44
2:B:41:GLY:H	4:B:304:EDO:C2	2.30	0.44
1:A:162:LEU:HD22	1:A:203:LEU:HD22	1.99	0.44
1:A:244:LEU:HD12	1:A:244:LEU:C	2.38	0.44
2:B:175:LEU:HD23	2:B:175:LEU:C	2.38	0.44
1:A:173:MET:HE2	1:A:175:LYS:CE	2.47	0.44
1:A:193:HIS:HE1	5:A:515:HOH:O	2.00	0.43
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.53	0.43
2:B:213:GLU:OE1	2:B:213:GLU:HA	2.18	0.43
2:B:72[B]:THR:HG23	5:B:536:HOH:O	2.18	0.43
2:B:54:LEU:HD22	2:B:58:VAL:HB	2.01	0.43
2:B:151:ASP:OD2	2:B:189:HIS:HB3	2.18	0.42
1:A:109:LYS:HE2	2:B:92:TYR:OH	2.18	0.42
3:C:32:TYR:CD1	3:C:98[B]:ARG:HG3	2.55	0.42
1:A:138:ILE:O	5:A:502:HOH:O	2.21	0.42
1:A:122[A]:GLU:HG3	5:A:526:HOH:O	2.20	0.42
1:A:229:ARG:HB3	1:A:230:PRO:HD2	2.01	0.42
2:B:145:LYS:HA	2:B:145:LYS:HD2	1.73	0.42
2:B:211:ARG:HH11	2:B:211:ARG:HD2	1.68	0.42
2:B:155:GLN:HG2	2:B:158:ASN:HD21	1.85	0.41
3:C:127:PRO:HB3	3:C:153:TYR:HB3	2.02	0.41
1:A:181[B]:ARG:HB3	1:A:181[B]:ARG:HE	1.58	0.41
1:A:188:VAL:O	1:A:263:PRO:HB3	2.21	0.41
3:C:2:VAL:HG21	3:C:98[B]:ARG:NH1	2.36	0.41
2:B:22[A]:THR:HG22	5:B:464:HOH:O	2.20	0.41
3:C:89[A]:GLU:H	3:C:89[A]:GLU:CD	2.24	0.41
1:A:171:PRO:O	1:A:173:MET:HG3	2.21	0.41
3:C:3:GLN:HB2	3:C:25:SER:OG	2.21	0.41
3:C:36:TRP:CE2	3:C:81:MET:HB2	2.56	0.41
2:B:158:ASN:OD1	2:B:158:ASN:N	2.53	0.41
2:B:187:GLU:OE1	2:B:211:ARG:NH1	2.54	0.41
1:A:235:LEU:HD23	1:A:236:SER:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:OG1	5:B:402:HOH:O	2.22	0.40
4:C:303:EDO:H12	5:C:527:HOH:O	2.21	0.40
2:B:190:LYS:HG3	2:B:191:VAL:N	2.37	0.40
2:B:160:GLN:HE22	3:C:179:GLN:HG2	1.86	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	212/322 (66%)	208 (98%)	3 (1%)	1 (0%)	29	18
2	B	219/215 (102%)	213 (97%)	6 (3%)	0	100	100
3	C	228/247 (92%)	224 (98%)	4 (2%)	0	100	100
All	All	659/784 (84%)	645 (98%)	13 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	VAL

### 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	179/269 (66%)	169 (94%)	10 (6%)	21	11
2	B	195/189 (103%)	188 (96%)	7 (4%)	35	26
3	C	192/205 (94%)	185 (96%)	7 (4%)	35	26
All	All	566/663 (85%)	542 (96%)	24 (4%)	32	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	148[A]	ARG
1	A	148[B]	ARG
1	A	163	SER
1	A	165	THR
1	A	195	VAL
1	A	229	ARG
1	A	231	GLN
1	A	235	LEU
1	A	249	ASN
2	B	12	SER
2	B	24	ARG
2	B	54	LEU
2	B	105	GLU
2	B	142	ARG
2	B	145	LYS
2	B	213	GLU
3	C	28	THR
3	C	62[A]	GLN
3	C	62[B]	GLN
3	C	63	LYS
3	C	98[A]	ARG
3	C	98[B]	ARG
3	C	146	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	ASN
2	B	199	GLN
3	C	110	HIS
3	C	207	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 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	402	-	3,3,3	0.24	0	2,2,2	0.64	0
4	EDO	C	301	-	3,3,3	0.61	0	2,2,2	0.07	0
4	EDO	A	401	-	3,3,3	0.52	0	2,2,2	0.10	0
4	EDO	B	303	-	3,3,3	0.56	0	2,2,2	0.22	0
4	EDO	C	302	-	3,3,3	0.47	0	2,2,2	0.25	0
4	EDO	B	302	-	3,3,3	0.54	0	2,2,2	0.52	0
4	EDO	B	305	-	3,3,3	0.33	0	2,2,2	0.20	0
4	EDO	B	304	-	3,3,3	0.52	0	2,2,2	0.58	0
4	EDO	B	301	-	3,3,3	0.62	0	2,2,2	0.12	0
4	EDO	C	303	-	3,3,3	0.25	0	2,2,2	0.23	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	402	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
4	EDO	A	401	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	C	302	-	-	1/1/1/1	-
4	EDO	B	302	-	-	0/1/1/1	-
4	EDO	B	305	-	-	0/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	B	301	-	-	1/1/1/1	-
4	EDO	C	303	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	EDO	O1-C1-C2-O2
4	C	302	EDO	O1-C1-C2-O2
4	B	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	302	EDO	1	0
4	B	305	EDO	1	0
4	B	304	EDO	2	0
4	C	303	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<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	209/322 (64%)	0.65	26 (12%) <span>4</span> <span>4</span>	30, 45, 72, 97	0
2	B	214/215 (99%)	-0.04	0 <span>100</span> <span>100</span>	29, 41, 67, 90	0
3	C	221/247 (89%)	-0.06	5 (2%) <span>60</span> <span>63</span>	29, 41, 57, 81	0
All	All	644/784 (82%)	0.18	31 (4%) <span>30</span> <span>33</span>	29, 42, 67, 97	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	VAL	6.2
1	A	232	VAL	6.2
1	A	199	GLU	5.0
1	A	233	ASN	5.0
1	A	234	GLY	4.7
1	A	227	GLY	4.5
1	A	231	GLN	4.0
1	A	228	ALA	3.9
1	A	165	THR	3.7
1	A	230	PRO	3.7
3	C	65	GLN	3.5
3	C	26	GLY	3.5
1	A	203	LEU	3.5
1	A	235	LEU	3.3
1	A	138	ILE	3.0
1	A	115	ALA	2.9
3	C	28	THR	2.7
3	C	27	GLY	2.4
1	A	99	ARG	2.4
1	A	229	ARG	2.4
1	A	135	TYR	2.4
1	A	119	ILE	2.4
1	A	166	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	114[A]	GLU	2.3
3	C	103	TRP	2.2
1	A	148[A]	ARG	2.1
1	A	164	ASN	2.1
1	A	116	LEU	2.1
1	A	198	ALA	2.0
1	A	78	ILE	2.0
1	A	163	SER	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	B	305	4/4	0.74	0.37	64,76,86,86	0
4	EDO	B	301	4/4	0.81	0.24	45,58,66,72	0
4	EDO	C	302	4/4	0.85	0.30	53,64,74,79	0
4	EDO	B	302	4/4	0.88	0.19	33,55,57,66	0
4	EDO	A	402	4/4	0.90	0.17	50,60,72,77	0
4	EDO	B	304	4/4	0.91	0.29	47,57,68,68	0
4	EDO	B	303	4/4	0.92	0.30	37,57,74,82	0
4	EDO	A	401	4/4	0.93	0.29	57,69,76,76	0
4	EDO	C	303	4/4	0.93	0.22	35,56,80,80	0
4	EDO	C	301	4/4	0.94	0.20	42,51,61,62	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.