



## Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:00 am BST

PDB ID : 1KCZ  
Title : Crystal Structure of beta-methylaspartase from Clostridium tetanomorphum.  
Mg-complex.  
Authors : Asuncion, M.; Blankenfeldt, W.; Barlow, J.N.; Gani, D.; Naismith, J.H.  
Deposited on : 2001-11-12  
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

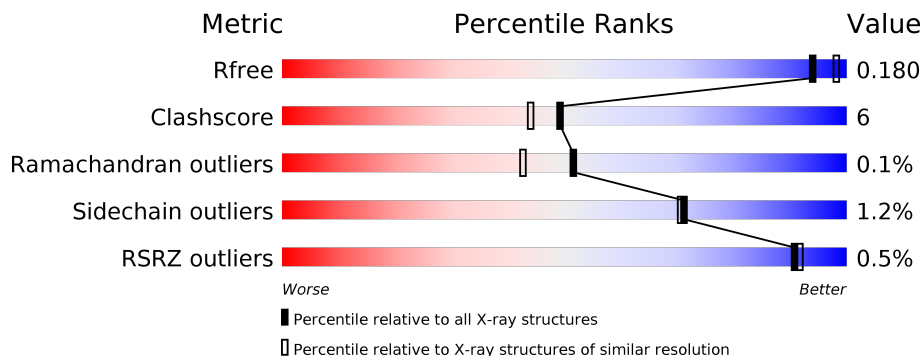
# 1 Overall quality at a glance

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	413	 85% 14%
1	B	413	 87% 11%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7293 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 beta-methylaspartase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3206	2010	558	612	26	0	2	0
1	B	413	3222	2020	559	615	28	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	OCS	CYS	MODIFIED RESIDUE	UNP Q05514
B	361	OCS	CYS	MODIFIED RESIDUE	UNP Q05514

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 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
3	A	1	Total C O 8 4 4	0	1
3	B	1	Total C O 8 4 4	0	1

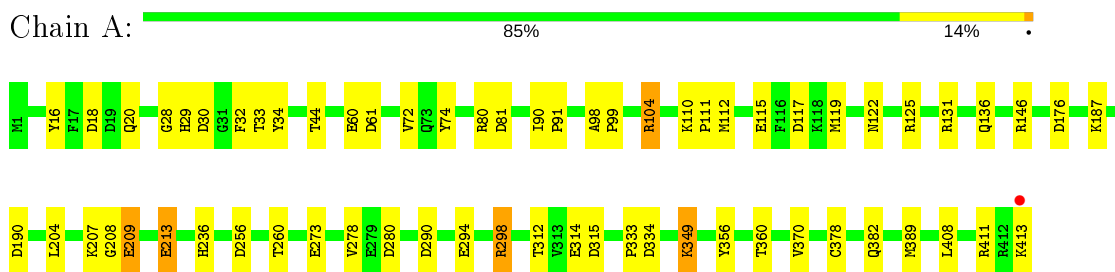
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	399	Total O 399 399	0	0
4	B	448	Total O 448 448	0	0

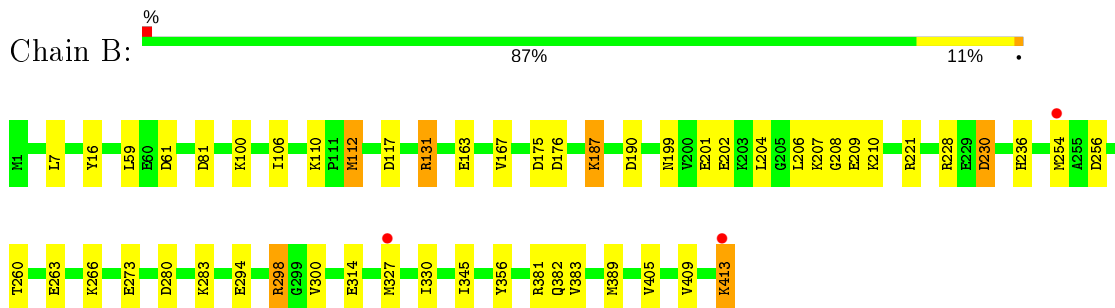
### 3 Residue-property plots [i](#)

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



- Molecule 1: beta-methylaspartase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.02Å 108.78Å 109.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.70 – 1.90 54.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (76.70-1.90) 99.5 (54.78-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.48 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.135 , 0.175 0.140 , 0.180	Depositor DCC
$R_{free}$ test set	3210 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.31 % 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 4.7817e-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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, MG, 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	0.94	4/3245 (0.1%)	0.98	15/4373 (0.3%)
1	B	0.91	4/3262 (0.1%)	1.02	12/4393 (0.3%)
All	All	0.93	8/6507 (0.1%)	1.00	27/8766 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	GLU	CD-OE1	8.20	1.34	1.25
1	B	112	MET	SD-CE	5.89	2.10	1.77
1	A	209	GLU	CD-OE2	-5.85	1.19	1.25
1	B	100	LYS	CD-CE	5.49	1.65	1.51
1	B	254[A]	MET	SD-CE	-5.47	1.47	1.77
1	B	254[B]	MET	SD-CE	-5.47	1.47	1.77
1	A	213	GLU	CD-OE1	5.24	1.31	1.25
1	A	213	GLU	CG-CD	5.01	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	B	413	LYS	N-CA-C	-11.68	79.47	111.00
1	B	131	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	B	298	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	298	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	81	ASP	CB-CG-OD2	7.57	125.11	118.30
1	A	298	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	280	ASP	CB-CG-OD2	7.30	124.87	118.30
1	B	190	ASP	CB-CG-OD2	7.20	124.78	118.30
1	B	176	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	334	ASP	CB-CG-OD2	6.83	124.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ARG	CG-CD-NE	-6.79	97.55	111.80
1	B	298	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	81	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	190	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	61	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	119	MET	CG-SD-CE	-5.76	90.98	100.20
1	B	280	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	61	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	104	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	60	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	A	349	LYS	CD-CE-NZ	-5.51	99.03	111.70
1	A	146	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	221	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	230	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	131	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	18	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3206	0	3206	39	0
1	B	3222	0	3222	40	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	12	1	0
3	B	8	0	12	0	0
4	A	399	0	0	10	8
4	B	448	0	0	12	8
All	All	7293	0	6452	76	9

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 6.

All (76) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:CE	1:A:112:MET:SD	2.02	1.48
1:B:112:MET:CE	1:B:112:MET:SD	2.10	1.38
1:B:283:LYS:HD2	4:B:1050:HOH:O	1.77	0.84
4:A:1222:HOH:O	1:B:389[A]:MET:CE	2.31	0.78
1:B:381:ARG:NH1	4:B:1292:HOH:O	2.17	0.78
1:A:349:LYS:HD2	1:A:378:CYS:O	1.85	0.77
4:A:1222:HOH:O	1:B:389[A]:MET:HE1	1.87	0.74
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.52	0.74
1:B:117:ASP:O	1:B:131:ARG:HD3	1.88	0.73
1:B:389[B]:MET:SD	4:B:1261:HOH:O	2.46	0.71
1:A:413:LYS:O	4:A:1169:HOH:O	2.07	0.71
1:A:176:ASP:OD1	4:A:1255:HOH:O	2.09	0.70
1:A:117:ASP:O	1:A:125:ARG:NH2	2.21	0.69
1:B:236:HIS:CD2	1:B:382:GLN:HE22	2.12	0.68
1:A:80:ARG:HG2	1:A:80:ARG:NH1	2.06	0.68
1:B:327[A]:MET:CG	4:B:1292:HOH:O	2.42	0.66
1:B:263:GLU:OE2	4:B:1089:HOH:O	2.13	0.66
1:B:294:GLU:O	1:B:298:ARG:HG3	1.97	0.65
1:A:290:ASP:OD2	4:A:1275:HOH:O	2.15	0.65
1:B:327[A]:MET:HG2	4:B:1292:HOH:O	1.98	0.64
1:B:294:GLU:OE2	1:B:298:ARG:HD3	1.97	0.64
1:A:236:HIS:CD2	1:A:382:GLN:HE22	2.16	0.63
1:A:294:GLU:OE2	1:A:298:ARG:HD2	2.00	0.62
1:A:207:LYS:HD2	4:A:1047:HOH:O	2.01	0.60
1:A:236:HIS:HD2	1:A:382:GLN:HE22	1.49	0.58
1:B:236:HIS:HD2	1:B:382:GLN:HE22	1.49	0.57
1:A:122:ASN:HA	4:A:1233:HOH:O	2.05	0.57
1:B:266:LYS:HE3	4:B:1244:HOH:O	2.07	0.54
1:A:408:LEU:HD12	3:A:903[B]:EDO:H21	1.88	0.54
1:B:298:ARG:HB2	1:B:300:VAL:HG23	1.90	0.54
1:B:117:ASP:OD1	1:B:131:ARG:HD2	2.08	0.53
1:B:314:GLU:HG2	4:B:1327:HOH:O	2.09	0.53
1:B:199:ASN:OD1	1:B:202:GLU:HG3	2.10	0.52
1:B:263:GLU:HG3	4:B:1089:HOH:O	2.09	0.52
1:A:236:HIS:HE1	1:A:273:GLU:OE1	1.94	0.51
1:B:163:GLU:HG2	1:B:413:LYS:NZ	2.26	0.51
1:A:110:LYS:HB3	1:A:111:PRO:HD3	1.92	0.50
1:A:314:GLU:HG2	1:A:315:ASP:N	2.26	0.50
1:B:110:LYS:HE2	4:B:1351:HOH:O	2.11	0.50
1:A:112:MET:CB	1:A:112:MET:CE	2.90	0.50
1:A:389[A]:MET:HE1	4:A:1279:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:HG2	1:B:413:LYS:HZ3	1.78	0.48
1:A:16:TYR:CE2	1:B:187:LYS:HE3	2.48	0.48
1:A:312:THR:OG1	1:A:314:GLU:HG2	2.14	0.48
1:A:30:ASP:O	1:A:33:THR:HG22	2.15	0.47
1:A:28:GLY:O	1:A:34:TYR:HA	2.14	0.47
1:B:256:ASP:O	1:B:260:THR:HG23	2.14	0.47
1:A:204:LEU:HG	1:A:208:GLY:HA2	1.97	0.46
1:A:20:GLN:HB2	1:A:74:TYR:CD2	2.50	0.46
1:A:112:MET:HB2	1:A:112:MET:CE	2.45	0.46
1:A:207:LYS:N	1:A:209:GLU:OE2	2.45	0.46
1:B:209:GLU:HG2	1:B:210:LYS:N	2.30	0.46
1:B:330:ILE:HD13	1:B:345:ILE:HG13	1.98	0.45
1:A:411:ARG:HD2	1:B:7:LEU:HD11	1.98	0.45
1:A:213:GLU:HB2	4:A:1166:HOH:O	2.15	0.45
1:B:201:GLU:HG3	4:B:1112:HOH:O	2.16	0.45
1:A:256:ASP:O	1:A:260:THR:HG23	2.18	0.44
1:A:104:ARG:NH2	1:A:115:GLU:OE1	2.37	0.44
1:B:228:ARG:HG3	1:B:230:ASP:OD1	2.18	0.44
1:A:333:PRO:HG3	1:A:360:THR:HG22	2.00	0.44
1:B:283:LYS:HD3	4:B:1018:HOH:O	2.18	0.44
1:A:98:ALA:N	1:A:99:PRO:CD	2.81	0.44
1:B:236:HIS:HE1	1:B:273:GLU:OE1	2.01	0.43
1:A:112:MET:CE	1:A:112:MET:CG	2.93	0.43
1:B:405:VAL:O	1:B:409:VAL:HG23	2.18	0.43
1:B:112:MET:CE	1:B:112:MET:HB2	2.48	0.43
1:B:112:MET:CB	1:B:112:MET:CE	2.97	0.42
1:A:90:ILE:HB	1:A:91:PRO:HD3	2.02	0.41
1:A:207:LYS:HG2	4:A:1059:HOH:O	2.20	0.41
1:A:136:GLN:HG2	1:A:370:VAL:HG11	2.01	0.41
1:B:201:GLU:HG2	1:B:206:LEU:HD21	2.03	0.41
1:A:187:LYS:HE3	1:B:16:TYR:CZ	2.55	0.41
1:B:167:VAL:HG11	1:B:383:VAL:HG13	2.03	0.41
1:B:204:LEU:HG	1:B:208:GLY:HA2	2.02	0.41
1:A:72:VAL:HG21	1:A:80:ARG:CZ	2.52	0.40
1:B:59:LEU:HD22	1:B:106:ILE:HD11	2.02	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1297:HOH:O	4:B:1342:HOH:O[1_655]	1.14	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1290:HOH:O	4:B:986:HOH:O[3_645]	1.66	0.54
1:B:413:LYS:O	4:A:1289:HOH:O[3_655]	1.76	0.44
4:A:1108:HOH:O	4:B:1306:HOH:O[3_645]	1.77	0.43
4:A:932:HOH:O	4:B:1293:HOH:O[2_554]	1.79	0.41
4:A:1290:HOH:O	4:B:1306:HOH:O[3_645]	2.01	0.19
4:A:1209:HOH:O	4:B:1021:HOH:O[2_554]	2.02	0.18
4:B:1163:HOH:O	4:B:1184:HOH:O[2_555]	2.04	0.16
4:A:1250:HOH:O	4:B:1142:HOH:O[2_554]	2.18	0.02

## 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	412/413 (100%)	398 (97%)	13 (3%)	1 (0%)	47	38
1	B	414/413 (100%)	400 (97%)	14 (3%)	0	100	100
All	All	826/826 (100%)	798 (97%)	27 (3%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	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	335/333 (101%)	331 (99%)	4 (1%)	71	70
1	B	337/333 (101%)	333 (99%)	4 (1%)	71	70
All	All	672/666 (101%)	664 (99%)	8 (1%)	71	70

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

Mol	Chain	Res	Type
1	A	29	HIS
1	A	32	PHE
1	A	44	THR
1	A	356	TYR
1	B	175	ASP
1	B	187	LYS
1	B	207	LYS
1	B	356	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	HIS
1	A	329	GLN
1	B	236	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	OCS	A	361	1	7,8,9	1.63	1 (14%)	6,11,13	1.94	2 (33%)
1	OCS	B	361	1	7,8,9	1.57	1 (14%)	6,11,13	2.04	3 (50%)

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
1	OCS	A	361	1	-	0/4/7/9	-
1	OCS	B	361	1	-	0/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	OCS	OD2-SG	-3.92	1.33	1.47
1	B	361	OCS	OD2-SG	-3.44	1.35	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	OCS	OD2-SG-CB	3.38	111.12	105.74
1	B	361	OCS	OD3-SG-CB	2.85	110.32	106.94
1	B	361	OCS	OD2-SG-CB	2.75	110.13	105.74
1	B	361	OCS	OD1-SG-CB	-2.11	104.43	106.94
1	A	361	OCS	OD2-SG-OD1	-2.09	106.16	111.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	EDO	A	903[A]	-	3,3,3	0.53	0	2,2,2	0.34	0
3	EDO	A	903[B]	-	3,3,3	0.48	0	2,2,2	0.37	0
3	EDO	B	904[A]	-	3,3,3	0.52	0	2,2,2	0.68	0
3	EDO	B	904[B]	-	3,3,3	0.46	0	2,2,2	0.21	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
3	EDO	A	903[A]	-	-	1/1/1/1	-
3	EDO	A	903[B]	-	-	0/1/1/1	-
3	EDO	B	904[A]	-	-	1/1/1/1	-
3	EDO	B	904[B]	-	-	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
3	B	904[A]	EDO	O1-C1-C2-O2
3	B	904[B]	EDO	O1-C1-C2-O2
3	A	903[A]	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903[B]	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	412/413 (99%)	-0.49	1 (0%) 95   95	3, 7, 17, 36	0
1	B	412/413 (99%)	-0.45	3 (0%) 87   88	3, 7, 17, 28	1 (0%)
All	All	824/826 (99%)	-0.47	4 (0%) 91   92	3, 7, 17, 36	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	254[A]	MET	13.6
1	B	327[A]	MET	2.6
1	A	413	LYS	2.3
1	B	413	LYS	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<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
1	OCS	A	361	9/10	0.97	0.10	5,8,18,19	0
1	OCS	B	361	9/10	0.97	0.10	5,6,17,18	0

### 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. 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
3	EDO	A	903[A]	4/4	0.91	0.25	3,4,5,9	4
3	EDO	A	903[B]	4/4	0.91	0.25	2,2,6,7	4
3	EDO	B	904[B]	4/4	0.93	0.21	3,4,5,6	4
3	EDO	B	904[A]	4/4	0.93	0.21	3,3,5,9	4
2	MG	B	902	1/1	0.99	0.07	6,6,6,6	0
2	MG	A	901	1/1	0.99	0.05	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.