Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:31 am BST

PDB ID	:	3BYV
Title	:	Crystal structure of Toxoplasma gondii specific rhoptry antigen kinase domain
Authors	:	Wernimont, A.K.; Lunin, V.V.; Yang, C.; Lew, J.; Kozieradzki, I.; Lin, Y.H.; Sun, X.; Khuu, C.; Zhao, Y.; Schapira, M.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bochkarev, A.; Hui, R.; Sibley, D.; Qiu, W.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-01-16
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

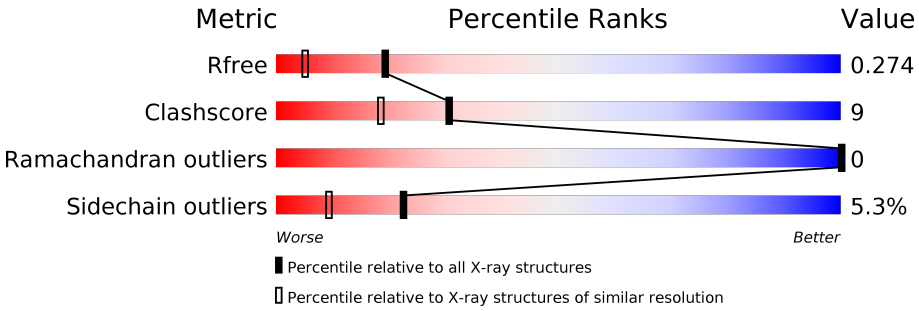
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	377	68% 20% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3023 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 Rhoptry kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	8	0
			2846	1839	498	500	9			

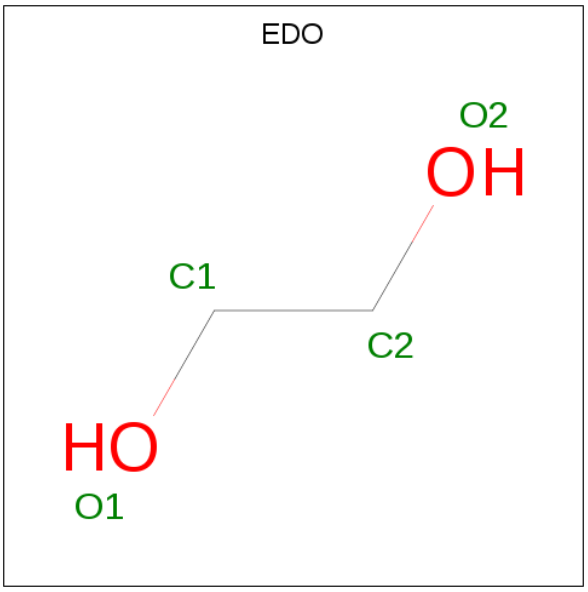
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	MET	-	EXPRESSION TAG	PDB 3BYV
A	193	HIS	-	EXPRESSION TAG	PDB 3BYV
A	194	HIS	-	EXPRESSION TAG	PDB 3BYV
A	195	HIS	-	EXPRESSION TAG	PDB 3BYV
A	196	HIS	-	EXPRESSION TAG	PDB 3BYV
A	197	HIS	-	EXPRESSION TAG	PDB 3BYV
A	198	HIS	-	EXPRESSION TAG	PDB 3BYV
A	199	SER	-	EXPRESSION TAG	PDB 3BYV
A	200	SER	-	EXPRESSION TAG	PDB 3BYV
A	201	GLY	-	EXPRESSION TAG	PDB 3BYV
A	202	ARG	-	EXPRESSION TAG	PDB 3BYV
A	203	GLU	-	EXPRESSION TAG	PDB 3BYV
A	204	ASN	-	EXPRESSION TAG	PDB 3BYV
A	205	LEU	-	EXPRESSION TAG	PDB 3BYV
A	206	TYR	-	EXPRESSION TAG	PDB 3BYV
A	207	PHE	-	EXPRESSION TAG	PDB 3BYV
A	208	GLN	-	EXPRESSION TAG	PDB 3BYV
A	209	GLY	-	EXPRESSION TAG	PDB 3BYV

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

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

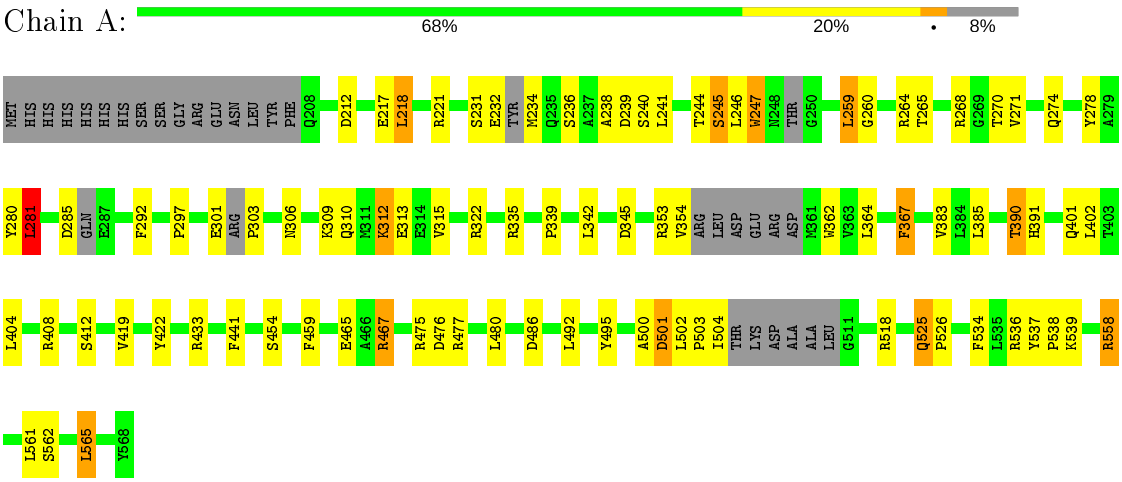
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	164	Total O 164 164	0	0

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. 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. 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: Rhoptry kinase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.07Å 69.82Å 85.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.44 – 1.80 36.43 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.44-1.80) 99.9 (36.43-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.233 0.245 , 0.274	Depositor DCC
R_{free} test set	1692 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3023	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.33	10/2935 (0.3%)	1.25	26/3976 (0.7%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	354	VAL	C-O	10.18	1.42	1.23
1	A	412	SER	CB-OG	-6.94	1.33	1.42
1	A	280	TYR	CD1-CE1	6.37	1.49	1.39
1	A	422	TYR	CE1-CZ	5.82	1.46	1.38
1	A	422	TYR	CG-CD2	5.67	1.46	1.39
1	A	467[A]	ARG	CG-CD	5.61	1.66	1.51
1	A	467[B]	ARG	CG-CD	5.61	1.66	1.51
1	A	419	VAL	CB-CG2	5.47	1.64	1.52
1	A	441	PHE	CD2-CE2	5.42	1.50	1.39
1	A	534	PHE	CD1-CE1	5.02	1.49	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	477	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	A	260	GLY	N-CA-C	-10.35	87.23	113.10
1	A	477	ARG	NE-CZ-NH2	-8.92	115.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	345	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	212	ASP	CB-CG-OD2	-7.27	111.76	118.30
1	A	281	LEU	CA-CB-CG	7.15	131.75	115.30
1	A	502	LEU	CB-CG-CD2	6.44	121.94	111.00
1	A	486	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	345	ASP	CB-CG-OD1	-6.15	112.76	118.30
1	A	480	LEU	CB-CG-CD2	-6.15	100.54	111.00
1	A	539	LYS	CD-CE-NZ	-6.13	97.59	111.70
1	A	558	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	492	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	A	476	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	501	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	475	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	558	ARG	CG-CD-NE	5.61	123.57	111.80
1	A	322	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	502	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	459	PHE	CB-CG-CD1	-5.44	116.99	120.80
1	A	486	ASP	CB-CG-OD1	5.36	123.13	118.30
1	A	218	LEU	CA-CB-CG	-5.31	103.09	115.30
1	A	335	ARG	CG-CD-NE	-5.09	101.10	111.80
1	A	402	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	A	383	VAL	CG1-CB-CG2	-5.04	102.84	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	259	LEU	Peptide
1	A	292	PHE	Peptide

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	2846	0	2861	53	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	18	1	0
4	A	164	0	0	6	2
All	All	3023	0	2879	53	2

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 9.

All (53) 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:390:THR:HG22	1:A:391:HIS:CD2	1.65	1.32
1:A:467[A]:ARG:HD3	4:A:836:HOH:O	1.30	1.28
1:A:390:THR:CG2	1:A:391:HIS:CD2	2.28	1.17
1:A:390:THR:HG22	1:A:391:HIS:HD2	0.92	1.07
1:A:303:PRO:HD2	1:A:362[A]:TRP:HE3	1.22	1.03
1:A:303:PRO:HD2	1:A:362[A]:TRP:CE3	1.94	1.02
1:A:433:ARG:HG2	4:A:829:HOH:O	1.61	0.99
1:A:217:GLU:OE2	1:A:221:ARG:HD2	1.62	0.97
1:A:390:THR:CG2	1:A:391:HIS:HD2	1.71	0.93
1:A:303:PRO:CD	1:A:362[A]:TRP:CE3	2.57	0.87
1:A:558:ARG:NH2	4:A:810:HOH:O	2.08	0.86
1:A:303:PRO:CD	1:A:362[A]:TRP:HE3	1.95	0.79
1:A:231:SER:CB	4:A:858:HOH:O	2.30	0.79
1:A:312:LYS:HD2	1:A:342:LEU:HD23	1.67	0.77
1:A:312:LYS:HD2	1:A:342:LEU:CD2	2.16	0.76
1:A:404:LEU:HD12	1:A:561:LEU:HD23	1.71	0.73
1:A:306:ASN:O	1:A:310:GLN:HG2	1.91	0.70
1:A:301:GLU:HA	1:A:362[B]:TRP:CZ3	2.32	0.64
1:A:390:THR:HG23	1:A:391:HIS:CD2	2.27	0.64
1:A:408:ARG:HH21	1:A:558:ARG:HH12	1.48	0.60
1:A:217:GLU:OE2	1:A:221:ARG:CD	2.46	0.59
1:A:309:LYS:HE2	1:A:313:GLU:OE1	2.04	0.58
1:A:247:TRP:HZ2	1:A:367:PHE:CZ	2.22	0.58
1:A:264:ARG:NH2	1:A:285:ASP:OD2	2.37	0.57
1:A:404:LEU:CD1	1:A:561:LEU:HD23	2.35	0.56
1:A:537[B]:TYR:HB3	1:A:538:PRO:HD3	1.87	0.56
1:A:247:TRP:CZ2	1:A:367:PHE:CZ	2.93	0.55
1:A:303:PRO:HD3	1:A:362[A]:TRP:CE3	2.41	0.55
1:A:238:ALA:HB2	1:A:274:GLN:HE21	1.75	0.52
1:A:401:GLN:OE1	1:A:561:LEU:HD21	2.10	0.51
1:A:268:ARG:HG2	1:A:281:LEU:HD23	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HG22	1:A:339:PRO:HG2	1.94	0.50
1:A:245:SER:HB3	1:A:246:LEU:HG	1.93	0.49
1:A:238:ALA:HB2	1:A:274:GLN:NE2	2.27	0.48
1:A:241:LEU:O	1:A:245:SER:HB2	2.14	0.48
1:A:353:ARG:HG3	1:A:362[A]:TRP:NE1	2.28	0.48
1:A:525:GLN:HG3	1:A:526:PRO:HD3	1.96	0.48
1:A:562[B]:SER:HA	1:A:565:LEU:HD22	1.96	0.47
1:A:562[A]:SER:HA	1:A:565:LEU:HD22	1.97	0.47
1:A:217:GLU:HG3	1:A:221:ARG:HD3	1.98	0.46
1:A:495:TYR:CD2	1:A:503:PRO:HD3	2.51	0.45
1:A:500:ALA:O	1:A:501:ASP:HB2	2.15	0.45
1:A:518:ARG:NH2	4:A:844:HOH:O	2.49	0.45
1:A:467[A]:ARG:NH1	4:A:804:HOH:O	2.51	0.44
1:A:536:ARG:HG2	1:A:538:PRO:HD2	1.98	0.44
1:A:467[A]:ARG:HG3	1:A:467[A]:ARG:NH1	2.33	0.43
1:A:278:TYR:OH	3:A:604:EDO:H22	2.18	0.43
1:A:467[A]:ARG:NH1	1:A:467[A]:ARG:CG	2.80	0.43
1:A:240:SER:O	1:A:244:THR:HG23	2.19	0.42
1:A:232:GLU:O	1:A:234:MET:N	2.52	0.42
1:A:297:PRO:HG2	1:A:364:LEU:HB2	2.03	0.41
1:A:385:LEU:HD22	1:A:500:ALA:HB3	2.02	0.41
1:A:239:ASP:HA	1:A:271:VAL:HG21	2.03	0.40

All (2) 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:740:HOH:O	4:A:855:HOH:O[4_455]	1.99	0.21
4:A:819:HOH:O	4:A:855:HOH:O[4_455]	2.19	0.01

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	339/377 (90%)	330 (97%)	9 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	310/336 (92%)	294 (95%)	16 (5%)	23 10

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	LEU
1	A	236	SER
1	A	245	SER
1	A	247	TRP
1	A	259	LEU
1	A	265	THR
1	A	270	THR
1	A	281	LEU
1	A	312	LYS
1	A	367	PHE
1	A	390	THR
1	A	454	SER
1	A	465	GLU
1	A	504	ILE
1	A	525	GLN
1	A	565	LEU

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	274	GLN
1	A	391	HIS

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

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	603	-	3,3,3	0.68	0	2,2,2	0.37	0
3	EDO	A	604	-	3,3,3	0.64	0	2,2,2	0.23	0
3	EDO	A	602	-	3,3,3	0.78	0	2,2,2	0.24	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	603	-	-	1/1/1/1	-
3	EDO	A	604	-	-	1/1/1/1	-
3	EDO	A	602	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	EDO	O1-C1-C2-O2
3	A	603	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	604	EDO	1	0

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.