



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:29 pm BST

PDB ID : 1QO3
Title : Complex between NK cell receptor Ly49A and its MHC class I ligand H-2Dd
Authors : Tormo, J.; Mariuzza, R.A.
Deposited on : 1999-11-01
Resolution : 2.30 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

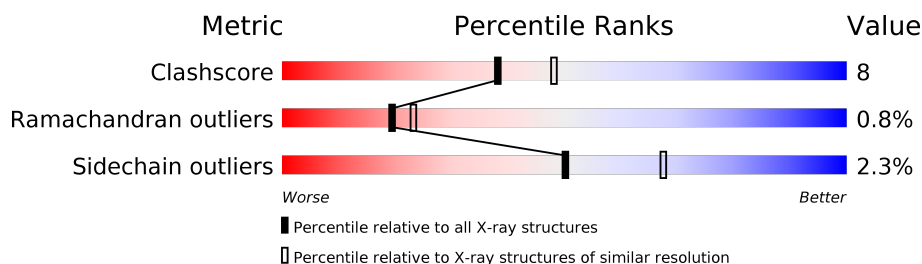
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	277	78% 19% ..
2	B	100	83% 16% .
3	C	137	79% 13% . 7%
3	D	137	74% 13% . 12%
4	P	10	80% 20%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5542 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 MHC CLASS I H-2DD HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2248	1411	407	421	9			

- Molecule 2 is a protein called BETA-2-MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			826	528	139	151	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	variant	UNP P01887

- Molecule 3 is a protein called LY49A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	128	Total	C	N	O	S	0	0	0
			1040	659	177	192	12			
3	D	121	Total	C	N	O	S	0	0	0
			988	627	168	181	12			

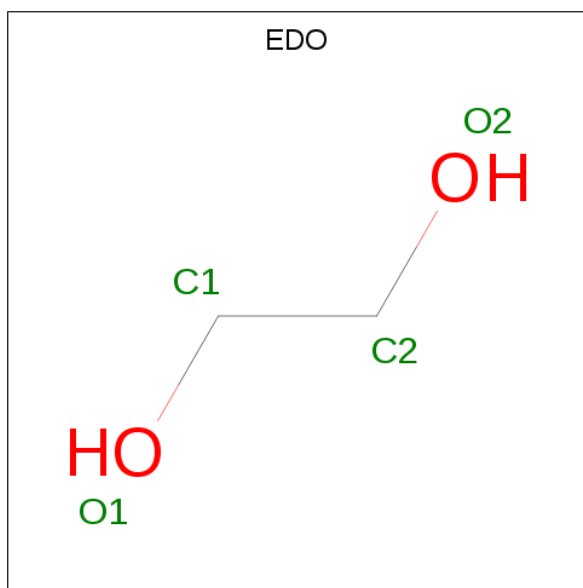
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	126	SER	LYS	engineered mutation	UNP P20937
C	166	THR	ALA	variant	UNP P20937
C	223	ARG	GLY	variant	UNP P20937
D	126	SER	LYS	engineered mutation	UNP P20937
D	166	THR	ALA	variant	UNP P20937
D	223	ARG	GLY	variant	UNP P20937

- Molecule 4 is a protein called HIV ENVELOPE GLYCOPROTEIN 120 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	10	Total	C	N	O	0	0	0
			76	48	16	12			

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 6 is water.

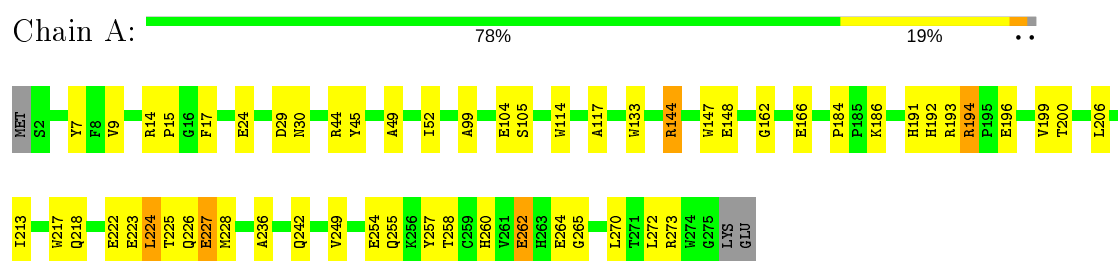
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total	O	0	0
			157	157		
6	B	64	Total	O	0	0
			64	64		
6	C	71	Total	O	0	0
			71	71		
6	D	57	Total	O	0	0
			57	57		
6	P	3	Total	O	0	0
			3	3		

3 Residue-property plots [i](#)

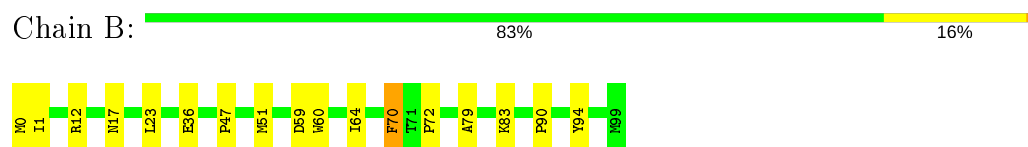
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

Note EDS was not executed.

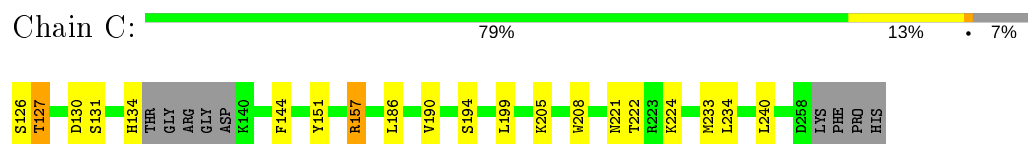
• Molecule 1: MHC CLASS I H-2DD HEAVY CHAIN



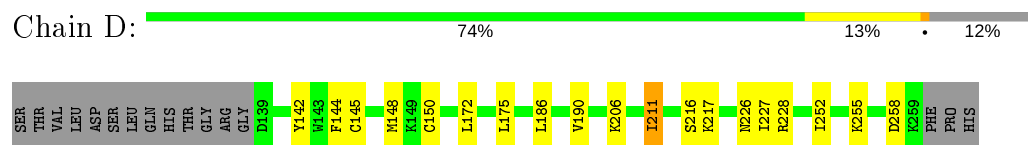
• Molecule 2: BETA-2-MICROGLOBULIN



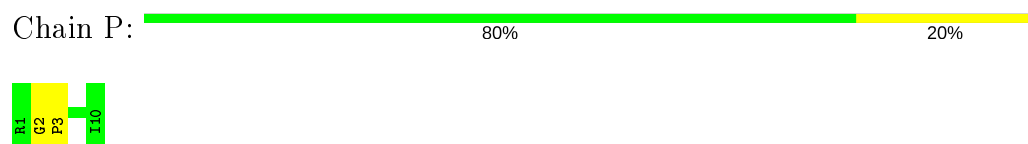
• Molecule 3: LY49A



• Molecule 3: LY49A



• Molecule 4: HIV ENVELOPE GLYCOPROTEIN 120 PEPTIDE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.96 Å 96.96 Å 99.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	95.5 (20.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.198 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5542	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	0.37	0/2311	0.62	0/3138
2	B	0.36	0/852	0.63	0/1154
3	C	0.38	0/1061	0.64	1/1427 (0.1%)
3	D	0.37	0/1009	0.69	0/1356
4	P	0.48	0/77	0.72	0/101
All	All	0.37	0/5310	0.64	1/7176 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	240	LEU	N-CA-C	-5.45	96.30	111.00

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	2248	0	2114	39	0
2	B	826	0	806	11	0
3	C	1040	0	1019	11	0
3	D	988	0	970	19	0
4	P	76	0	82	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	18	3	0
6	A	157	0	0	1	0
6	B	64	0	0	0	0
6	C	71	0	0	0	0
6	D	57	0	0	0	0
6	P	3	0	0	0	0
All	All	5542	0	5009	77	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 8.

All (77) 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:114:TRP:HE1	5:A:1277:EDO:H11	1.38	0.88
3:D:211:ILE:HD13	3:D:211:ILE:O	1.86	0.76
3:C:127:THR:HG23	3:C:130:ASP:OD2	1.88	0.72
1:A:206:LEU:HD22	1:A:242:GLN:HG3	1.71	0.71
1:A:206:LEU:CD2	1:A:242:GLN:HG3	2.22	0.69
1:A:114:TRP:NE1	5:A:1277:EDO:H11	2.06	0.69
2:B:17:ASN:HA	2:B:72:PRO:O	1.97	0.65
3:C:199:LEU:HD23	3:C:233:MET:HG2	1.79	0.65
3:D:148:MET:CE	3:D:258:ASP:HB3	2.28	0.64
3:D:217:LYS:HE2	3:D:217:LYS:N	2.14	0.62
1:A:9:VAL:HG22	1:A:24:GLU:HG2	1.81	0.62
1:A:218:GLN:HA	1:A:224:LEU:HB2	1.81	0.62
3:D:148:MET:HE2	3:D:258:ASP:HB3	1.81	0.61
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.20	0.56
1:A:104:GLU:HG3	1:A:105:SER:N	2.21	0.56
1:A:264:GLU:HB2	6:A:2155:HOH:O	2.07	0.55
3:C:221:ASN:O	3:C:224:LYS:HG2	2.08	0.53
3:D:175:LEU:HD22	3:D:252:ILE:HG21	1.88	0.53
1:A:15:PRO:O	1:A:17:PHE:HD1	1.93	0.52
2:B:36:GLU:HB3	2:B:83:LYS:HB2	1.92	0.52
3:C:157:ARG:HG2	3:C:157:ARG:HH11	1.75	0.51
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.50
3:D:211:ILE:HD13	3:D:211:ILE:C	2.32	0.50
3:C:186:LEU:O	3:C:190:VAL:HG13	2.11	0.50
1:A:162:GLY:O	1:A:166:GLU:HG2	2.12	0.49
1:A:196:GLU:OE1	1:A:196:GLU:N	2.45	0.49
1:A:217:TRP:O	1:A:224:LEU:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:O	1:A:148:GLU:HG3	2.13	0.48
1:A:254:GLU:N	1:A:254:GLU:OE1	2.46	0.48
1:A:193:ARG:O	1:A:193:ARG:HG3	2.13	0.48
3:D:175:LEU:HD21	3:D:186:LEU:CD1	2.44	0.48
2:B:0:MET:SD	2:B:1:ILE:N	2.87	0.48
3:C:126:SER:HB3	3:C:134:HIS:CE1	2.49	0.48
3:D:227:ILE:HG13	3:D:227:ILE:O	2.14	0.47
2:B:51:MET:HB3	2:B:64:ILE:HD11	1.95	0.47
1:A:14:ARG:N	1:A:15:PRO:HD3	2.30	0.47
1:A:225:THR:O	1:A:227:GLU:N	2.48	0.46
2:B:83:LYS:HG2	2:B:90:PRO:HG3	1.97	0.46
3:D:172:LEU:HD22	3:D:255:LYS:HB2	1.96	0.46
3:D:186:LEU:O	3:D:190:VAL:HG23	2.16	0.46
1:A:186:LYS:N	1:A:186:LYS:HD2	2.31	0.46
2:B:79:ALA:HB2	2:B:94:TYR:CD1	2.51	0.46
3:C:194:SER:HB3	3:C:234:LEU:HB3	1.98	0.46
3:D:145:CYS:HA	3:D:150:CYS:HA	1.98	0.46
1:A:236:ALA:HB1	2:B:12:ARG:HD3	1.98	0.45
1:A:213:ILE:HG13	1:A:262:GLU:O	2.16	0.45
3:C:151:TYR:CD1	3:C:151:TYR:N	2.84	0.45
3:D:226:ASN:C	3:D:228:ARG:N	2.70	0.45
2:B:23:LEU:HB2	2:B:70:PHE:CD1	2.52	0.44
3:C:208:TRP:CD1	3:C:222:THR:HB	2.53	0.44
3:D:216:SER:C	3:D:217:LYS:HE2	2.38	0.44
1:A:255:GLN:O	1:A:255:GLN:HG2	2.17	0.43
1:A:192:HIS:O	1:A:199:VAL:HG13	2.18	0.43
3:D:206:LYS:HB3	3:D:206:LYS:NZ	2.34	0.43
1:A:29:ASP:O	1:A:30:ASN:HB2	2.17	0.43
1:A:7:TYR:CE1	4:P:2:GLY:HA2	2.54	0.43
1:A:15:PRO:O	1:A:17:PHE:CD1	2.71	0.43
2:B:36:GLU:OE2	2:B:83:LYS:HD3	2.18	0.43
1:A:147:TRP:CZ2	5:A:1277:EDO:H21	2.53	0.43
1:A:222:GLU:O	1:A:224:LEU:N	2.50	0.43
3:D:148:MET:HE3	3:D:258:ASP:HB3	1.99	0.43
3:C:157:ARG:HG2	3:C:157:ARG:NH1	2.33	0.43
1:A:260:HIS:HA	1:A:270:LEU:O	2.20	0.42
1:A:191:HIS:CD2	1:A:199:VAL:HG11	2.54	0.42
3:D:226:ASN:C	3:D:228:ARG:H	2.23	0.42
1:A:272:LEU:N	1:A:272:LEU:HD12	2.34	0.42
2:B:59:ASP:O	2:B:60:TRP:HB2	2.20	0.42
1:A:249:VAL:HG12	1:A:257:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:HB3	4:P:3:PRO:HG3	2.02	0.41
1:A:194:ARG:HD3	1:A:200:THR:OG1	2.21	0.41
3:C:144:PHE:HA	3:D:144:PHE:HB3	2.02	0.41
3:D:217:LYS:HE2	3:D:217:LYS:CA	2.51	0.41
3:D:175:LEU:HD22	3:D:252:ILE:CG2	2.51	0.41
1:A:49:ALA:O	1:A:52:ILE:HG22	2.21	0.40
1:A:258:THR:HG22	1:A:273:ARG:HG2	2.03	0.40
1:A:133:TRP:HB2	1:A:144:ARG:HG3	2.04	0.40
1:A:184:PRO:HG3	1:A:265:GLY:O	2.21	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	272/277 (98%)	261 (96%)	8 (3%)	3 (1%)	14	15
2	B	98/100 (98%)	92 (94%)	5 (5%)	1 (1%)	15	17
3	C	124/137 (90%)	115 (93%)	8 (6%)	1 (1%)	19	23
3	D	119/137 (87%)	113 (95%)	6 (5%)	0	100	100
4	P	8/10 (80%)	8 (100%)	0	0	100	100
All	All	621/661 (94%)	589 (95%)	27 (4%)	5 (1%)	19	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	GLU
1	A	226	GLN
1	A	227	GLU
3	C	205	LYS
2	B	47	PRO

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	229/232 (99%)	222 (97%)	7 (3%)	40	55
2	B	94/94 (100%)	93 (99%)	1 (1%)	73	86
3	C	119/126 (94%)	116 (98%)	3 (2%)	47	65
3	D	112/126 (89%)	110 (98%)	2 (2%)	59	75
4	P	7/7 (100%)	7 (100%)	0	100	100
All	All	561/585 (96%)	548 (98%)	13 (2%)	50	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	45	TYR
1	A	144	ARG
1	A	194	ARG
1	A	224	LEU
1	A	228	MET
1	A	262	GLU
2	B	70	PHE
3	C	127	THR
3	C	131	SER
3	C	157	ARG
3	D	142	TYR
3	D	211	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	176	ASN
1	A	218	GLN
3	C	134	HIS
3	D	168	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	$\# Z > 2$
5	EDO	A	1278	-	3,3,3	0.50	0	2,2,2	0.67	0
5	EDO	A	1277	-	3,3,3	0.61	0	2,2,2	0.50	0
5	EDO	A	1276	-	3,3,3	0.66	0	2,2,2	0.57	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
5	EDO	A	1278	-	-	1/1/1/1	-
5	EDO	A	1277	-	-	1/1/1/1	-
5	EDO	A	1276	-	-	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
5	A	1277	EDO	O1-C1-C2-O2
5	A	1278	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1277	EDO	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.