



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 02:47 am BST

PDB ID : 6O9B
Title : Crystal structure of HLA-A3*01 in complex with a wild-type beta-catenin peptide
Authors : Miller, M.S.; Gabelli, S.B.
Deposited on : 2019-03-13
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

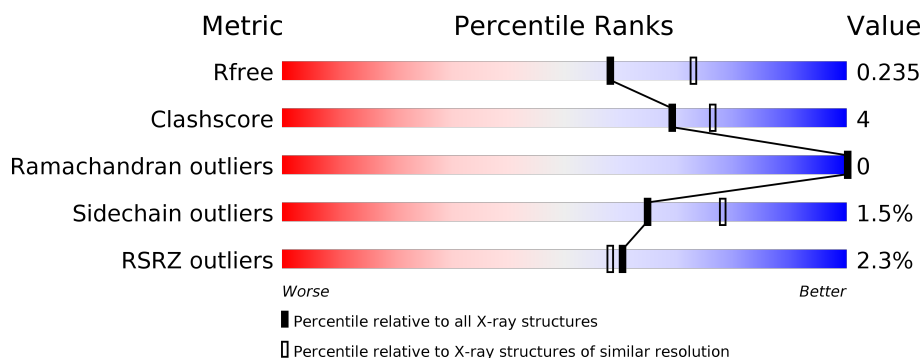
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 $\leq 5\%$. 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	300	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
2	B	119	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>10%</div> <div>15%</div> </div> </div>
3	C	9	<div> <div></div> <div>100%</div> </div>

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
7	PEG	B	205	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3479 atoms, of which 10 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 HLA class I histocompatibility antigen, A-3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	1	0
			2265	1408	410	438	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	cloning artifact	UNP P04439
A	-1	ALA	-	cloning artifact	UNP P04439
A	0	SER	-	cloning artifact	UNP P04439
A	281	GLY	-	expression tag	UNP P04439
A	282	SER	-	expression tag	UNP P04439
A	283	LEU	-	expression tag	UNP P04439
A	284	HIS	-	expression tag	UNP P04439
A	285	HIS	-	expression tag	UNP P04439
A	286	ILE	-	expression tag	UNP P04439
A	287	LEU	-	expression tag	UNP P04439
A	288	ASP	-	expression tag	UNP P04439
A	289	ALA	-	expression tag	UNP P04439
A	290	GLN	-	expression tag	UNP P04439
A	291	LYS	-	expression tag	UNP P04439
A	292	MET	-	expression tag	UNP P04439
A	293	VAL	-	expression tag	UNP P04439
A	294	TRP	-	expression tag	UNP P04439
A	295	ASN	-	expression tag	UNP P04439
A	296	HIS	-	expression tag	UNP P04439
A	297	ARG	-	expression tag	UNP P04439

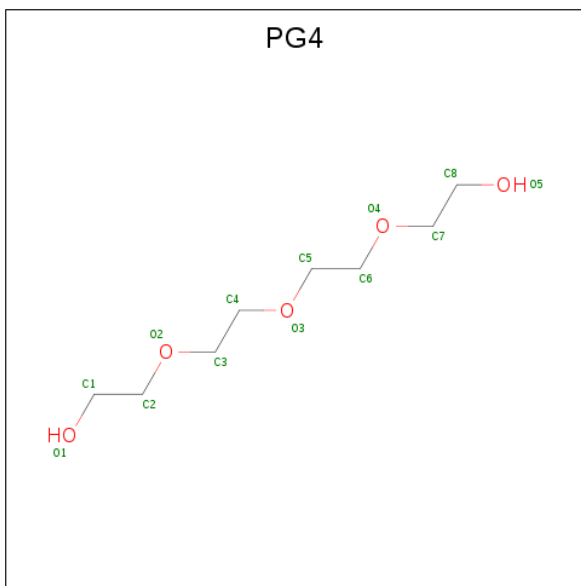
- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	1	0
			850	541	145	161	3			

- Molecule 3 is a protein called Catenin beta-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			60	36	10	14			

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



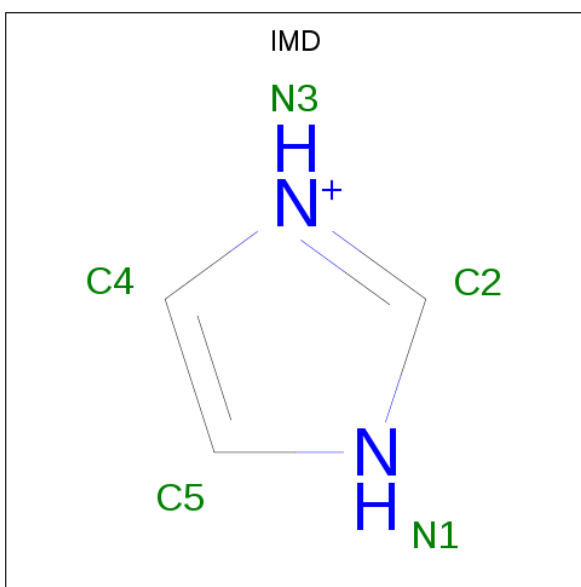
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	3	2		

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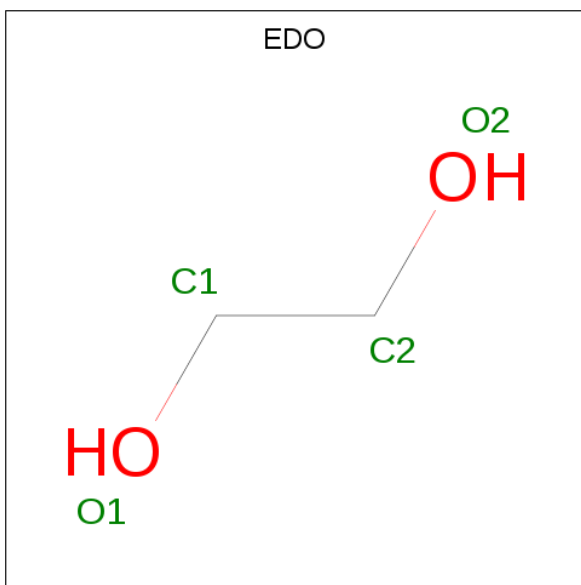
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O		0	0
			7	4	3			
7	A	1	Total	C	O		0	0
			7	4	3			
7	B	1	Total	C	O		0	0
			7	4	3			
7	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	117	Total O 117 117	0	0
9	B	43	Total O 43 43	0	0
9	C	6	Total O 6 6	0	0

- Molecule 1: HLA class I histocompatibility antigen, A-3 alpha chain



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.77Å 152.77Å 84.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.87 – 2.20 28.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.87-2.20) 99.3 (28.87-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.227 0.193 , 0.235	Depositor DCC
R_{free} test set	1452 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3479	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PG4, PEG, IMD, MES, 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	0.89	0/2328	0.94	0/3159
2	B	0.86	0/876	0.97	0/1185
3	C	1.18	0/60	0.81	0/79
All	All	0.89	0/3264	0.95	0/4423

There are no bond length outliers.

There are no bond angle outliers.

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	2265	0	2120	14	0
2	B	850	0	815	13	0
3	C	60	0	65	0	0
4	A	13	0	18	0	0
4	B	13	0	18	1	0
5	A	12	0	13	0	0
5	B	24	0	26	2	0
6	A	10	0	10	0	0
7	A	14	0	20	0	0
7	B	14	10	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	16	0	24	0	0
8	B	12	0	18	2	0
9	A	117	0	0	1	0
9	B	43	0	0	0	0
9	C	6	0	0	0	0
All	All	3469	10	3167	24	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 4.

The worst 5 of 24 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:77:SER:HB3	5:B:203:MES:H32	1.70	0.74
2:B:101:ARG:HE	8:B:206:EDO:H12	1.61	0.66
2:B:21:ILE:HD13	2:B:23[B]:ARG:HE	1.63	0.63
1:A:192:HIS:CE1	2:B:118:ASP:HB3	2.40	0.57
1:A:230:LEU:HD23	1:A:245:ALA:HB2	1.87	0.55

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	277/300 (92%)	271 (98%)	6 (2%)	0	100	100
2	B	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
All	All	384/428 (90%)	375 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	236/254 (93%)	233 (99%)	3 (1%)	69	81
2	B	96/109 (88%)	94 (98%)	2 (2%)	53	67
3	C	7/7 (100%)	7 (100%)	0	100	100
All	All	339/370 (92%)	334 (98%)	5 (2%)	65	78

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	67	VAL
1	A	116	ASP
2	B	78	LYS
2	B	90	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

18 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
8	EDO	A	310	-	3,3,3	0.16	0	2,2,2	0.47	0
8	EDO	A	308	-	3,3,3	0.66	0	2,2,2	0.59	0
8	EDO	B	207	-	3,3,3	0.43	0	2,2,2	0.54	0
4	PG4	B	201	-	12,12,12	0.72	0	11,11,11	0.79	0
8	EDO	A	307	-	3,3,3	0.43	0	2,2,2	0.32	0
4	PG4	A	301	-	12,12,12	0.24	0	11,11,11	0.48	0
5	MES	B	202	-	12,12,12	0.71	0	14,16,16	0.37	0
6	IMD	A	303	-	3,5,5	0.15	0	4,5,5	0.64	0
7	PEG	A	306	-	6,6,6	0.18	0	5,5,5	0.37	0
7	PEG	B	205	-	6,6,6	0.11	0	5,5,5	0.13	0
8	EDO	B	206	-	3,3,3	0.42	0	2,2,2	0.52	0
7	PEG	A	305	-	6,6,6	0.51	0	5,5,5	0.56	0
5	MES	B	203	-	12,12,12	0.74	0	14,16,16	0.43	0
5	MES	A	302	-	12,12,12	0.72	0	14,16,16	0.38	0
8	EDO	A	309	-	3,3,3	0.37	0	2,2,2	0.30	0
8	EDO	B	208	-	3,3,3	0.20	0	2,2,2	0.58	0
7	PEG	B	204	-	6,6,6	0.29	0	5,5,5	0.19	0
6	IMD	A	304	-	3,5,5	0.24	0	4,5,5	0.62	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
8	EDO	A	310	-	-	1/1/1/1	-
8	EDO	A	308	-	-	1/1/1/1	-
8	EDO	B	207	-	-	1/1/1/1	-
4	PG4	B	201	-	-	4/10/10/10	-
8	EDO	A	307	-	-	1/1/1/1	-
4	PG4	A	301	-	-	3/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	B	202	-	-	0/6/14/14	0/1/1/1
6	IMD	A	303	-	-	-	0/1/1/1
7	PEG	A	306	-	-	2/4/4/4	-
7	PEG	B	205	-	-	1/4/4/4	-
8	EDO	B	206	-	-	1/1/1/1	-
7	PEG	A	305	-	-	2/4/4/4	-
5	MES	B	203	-	-	5/6/14/14	0/1/1/1
5	MES	A	302	-	-	0/6/14/14	0/1/1/1
8	EDO	A	309	-	-	1/1/1/1	-
8	EDO	B	208	-	-	0/1/1/1	-
7	PEG	B	204	-	-	0/4/4/4	-
6	IMD	A	304	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	203	MES	C7-C8-S-O1S
5	B	203	MES	C7-C8-S-O2S
4	B	201	PG4	O2-C3-C4-O3
4	A	301	PG4	O3-C5-C6-O4
7	A	305	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	PG4	1	0
8	B	206	EDO	2	0
5	B	203	MES	2	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 [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, 95th 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 ²)	Q<0.9
1	A	278/300 (92%)	-0.37	6 (2%) 62 59	21, 35, 68, 98	0
2	B	101/119 (84%)	-0.17	3 (2%) 50 48	23, 37, 69, 89	0
3	C	9/9 (100%)	-0.62	0 100 100	26, 31, 33, 34	0
All	All	388/428 (90%)	-0.32	9 (2%) 60 58	21, 36, 69, 98	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	GLU	4.9
1	A	226	GLN	4.3
1	A	197	HIS	3.8
1	A	223	ASP	3.1
1	A	0	SER	2.6

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. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
8	EDO	B	207	4/4	0.41	0.23	69,72,79,83	0
8	EDO	A	307	4/4	0.65	0.21	62,65,68,68	0
7	PEG	A	305	7/7	0.70	0.34	53,58,66,66	0
7	PEG	B	205	7/7	0.80	0.44	20,20,20,20	0
8	EDO	B	208	4/4	0.81	0.16	65,66,67,69	0
7	PEG	B	204	7/7	0.81	0.23	59,65,69,71	0
8	EDO	A	310	4/4	0.84	0.20	58,60,69,74	0
6	IMD	A	304	5/5	0.85	0.17	59,61,65,68	0
8	EDO	A	308	4/4	0.86	0.14	48,53,57,63	0
4	PG4	A	301	13/13	0.89	0.14	46,52,63,65	0
8	EDO	A	309	4/4	0.90	0.17	54,59,59,71	0
5	MES	B	202	12/12	0.90	0.19	45,60,66,67	0
5	MES	A	302	12/12	0.91	0.15	45,53,73,74	0
7	PEG	A	306	7/7	0.92	0.09	55,58,61,64	0
4	PG4	B	201	13/13	0.92	0.17	35,40,58,67	0
6	IMD	A	303	5/5	0.93	0.14	56,61,66,70	0
8	EDO	B	206	4/4	0.94	0.13	46,57,63,71	0
5	MES	B	203	12/12	0.95	0.15	50,60,69,74	0

6.5 Other polymers ⓘ

There are no such residues in this entry.