

wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2022 – 05:50 pm BST

PDB ID	:	7NMG
Title	:	Human MHC Class I, A24 Allele presenting LWM, Complex with 4C6 TCR
Authors	:	Rizkallah, P.J.; Sewell, A.K.; Cole, D.K.; Wall, A.
Deposited on		
Resolution	:	2.48 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

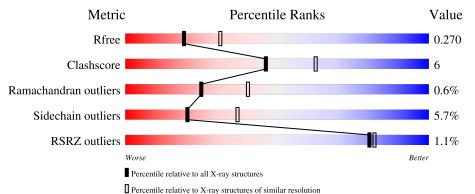
MolProbity		4 09b 467
•		
Mogul	:	1.8.4, CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.48 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 of 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% 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	А	276	82%	17%	•
2	В	100	81%	18%	•
3	С	9	89%	119	%
4	D	192	4%	18%	•
5	Е	240	82%	17%	•



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
6	SO4	А	301	-	-	-	Х
6	SO4	С	102	-	-	Х	-



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6763 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 antigen.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	276	Total 2238	C 1392	N 405	0 431	S 10	0	0	0

• Molecule 2 is a protein called Human MHC Class I, beta 2 microglobulin.

Mo	l Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 837	C 533	N 141	O 159	$\frac{S}{4}$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called Diabetes epitope LWMRLLPLL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	9	Total 81	C 57	N 13	O 10	S 1	0	0	0

• Molecule 4 is a protein called Human 4C6 T-cell Receptor, alpha Chain.

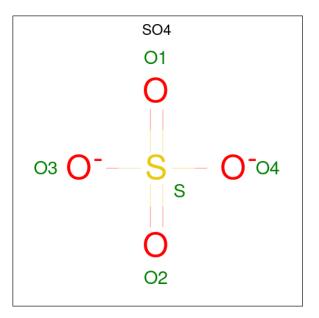
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	192	Total 1510	C 943	N 248	O 310	S 9	0	1	0

• Molecule 5 is a protein called Human 4C6 T-cell Receptor, beta Chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
5	Е	240	Total 1943	C 1218	N 347	0 372	S 6	0	0	0

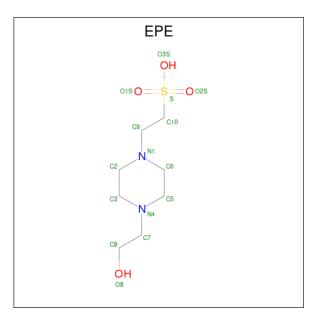


• Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

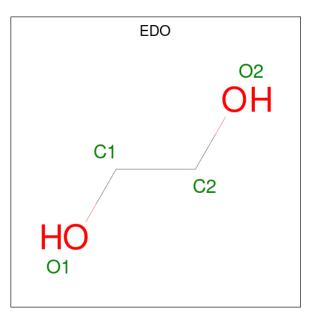
• Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	Λ	1	Total	С	Ν	0	S	0	0
1	A	1	15	8	2	4	1		U

• Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
8	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
8	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

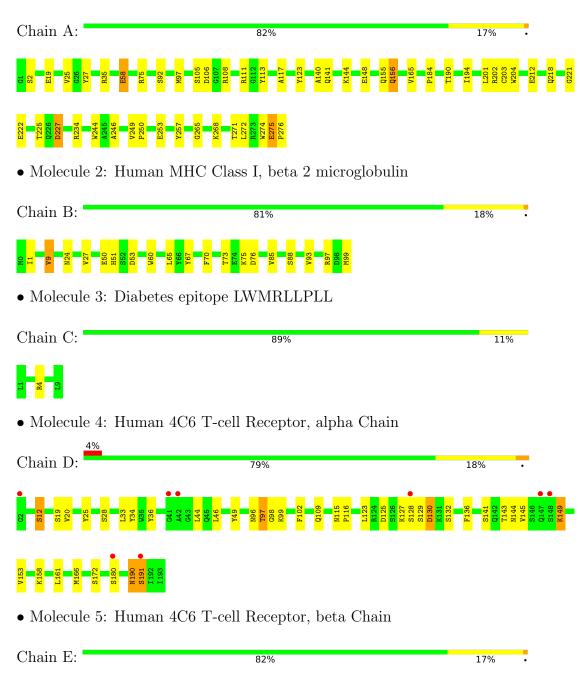
• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	40	Total O 40 40	0	0
9	В	20	TotalO2020	0	0
9	С	2	Total O 2 2	0	0
9	D	25	TotalO2525	0	0
9	Е	25	TotalO2525	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: MHC class I antigen



P179 T3 L1811 D8 L1812 D8 L1813 P9 L1814 P13 R191 R16 D201 V20 D24 P44 V229 F45 V229 F44 V229 F45 V229 F45 V229 F46 V229 F46 V229 F46 V229 F46 V20 F46 V20 F46 V20 F46 P34 F46 P34 F46 P34 F46 P34 F46 P34 F47 P34 F46 P46 P64 P64 P64 P34 F13 F13</



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	54.32Å 72.13Å 230.65Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.93 - 2.48	Depositor
Resolution (A)	52.87 - 2.48	EDS
% Data completeness	99.7 (52.93-2.48)	Depositor
(in resolution range)	99.7(52.87-2.48)	EDS
R _{merge}	0.10	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.52 (at 2.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D.	0.198 , 0.271	Depositor
R, R_{free}	0.202 , 0.270	DCC
R_{free} test set	1616 reflections (4.90%)	wwPDB-VP
Wilson B-factor $(Å^2)$	49.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ L > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6763	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: EPE, SO4, 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	Bo	nd lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.79	2/2299~(0.1%)	0.84	0/3116
2	В	0.74	0/860	0.81	0/1162
3	С	0.67	0/83	0.77	0/111
4	D	0.76	0/1537	0.82	0/2079
5	Ε	0.73	1/1996~(0.1%)	0.79	0/2712
All	All	0.76	3/6775~(0.0%)	0.82	0/9180

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
4	D	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	Ε	100	GLU	CD-OE2	5.56	1.31	1.25
1	А	58	GLU	CD-OE1	5.37	1.31	1.25
1	А	212	GLU	CD-OE2	5.10	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	149	LYS	Peptide
4	D	96	ASN	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	А	2238	0	2095	30	0
2	В	837	0	803	13	0
3	С	81	0	96	1	0
4	D	1510	0	1447	27	0
5	Е	1943	0	1838	21	0
6	А	5	0	0	0	0
6	С	5	0	0	2	0
6	D	5	0	0	0	0
7	А	15	0	17	2	0
8	В	8	0	12	0	0
8	С	4	0	6	0	0
9	А	40	0	0	2	0
9	В	20	0	0	0	0
9	С	2	0	0	0	0
9	D	25	0	0	0	0
9	Е	25	0	0	0	0
All	All	6763	0	6314	82	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 6.

The worst 5 of 82 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:156:GLN:HE21	1:A:156:GLN:HA	1.38	0.88
4:D:97:THR:OG1	4:D:98:GLY:N	2.13	0.80
4:D:149:LYS:HD2	4:D:153:VAL:O	1.85	0.77
5:E:16:ARG:NH2	5:E:113:GLU:OE1	2.18	0.76
5:E:176:LYS:NZ	5:E:181:LEU:O	2.22	0.72

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	Percen	tiles
1	А	274/276~(99%)	263~(96%)	8~(3%)	3~(1%)	14	23
2	В	98/100~(98%)	95~(97%)	3~(3%)	0	100	100
3	С	7/9~(78%)	6 (86%)	1 (14%)	0	100	100
4	D	191/192~(100%)	175~(92%)	14 (7%)	2(1%)	15	26
5	Е	238/240~(99%)	226~(95%)	12~(5%)	0	100	100
All	All	808/817~(99%)	765~(95%)	38~(5%)	5 (1%)	25	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	128	SER
1	А	225	THR
1	А	274	TRP
1	А	275	GLU
4	D	190	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Percer	ntiles
1	А	232/232~(100%)	220~(95%)	12~(5%)	23	41
2	В	95/95~(100%)	88~(93%)	7 (7%)	13	25
3	С	9/9~(100%)	9 (100%)	0	100	100
4	D	174/173~(101%)	166~(95%)	8 (5%)	27	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	Е	212/212~(100%)	198~(93%)	14 (7%)	16 30
All	All	722/721 (100%)	681 (94%)	41 (6%)	20 37

5 of 41 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
5	Е	10	ARG
5	Е	79	GLU
5	Е	13	ILE
5	Е	59	SER
5	Е	183	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	45	GLN
4	D	109	GLN
5	Е	99	HIS
1	А	226	GLN
1	А	156	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

7 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	Turne	Chain	hain Res		Bond lengths			Bond angles		
NIOI	Type	Unam	nes	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
6	SO4	D	201	-	4,4,4	0.36	0	6,6,6	0.05	0
8	EDO	В	102	-	3,3,3	0.10	0	2,2,2	0.10	0
8	EDO	В	101	-	3,3,3	0.41	0	2,2,2	0.44	0
7	EPE	А	302	-	$15,\!15,\!15$	0.99	1 (6%)	18,20,20	1.11	2 (11%)
8	EDO	С	101	-	3,3,3	0.36	0	2,2,2	0.34	0
6	SO4	С	102	-	4,4,4	0.38	0	6,6,6	0.10	0
6	SO4	А	301	-	4,4,4	0.37	0	6,6,6	0.06	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	С	101	-	-	1/1/1/1	-
8	EDO	В	101	-	-	0/1/1/1	-
8	EDO	В	102	-	-	1/1/1/1	-
7	EPE	А	302	-	-	3/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	А	302	EPE	O2S-S	3.61	1.55	1.45

All (2) bond angle outliers are listed below:

Mo	l Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	А	302	EPE	03S-S-01S	3.20	119.10	111.27
7	А	302	EPE	O2S-S-C10	-2.95	103.36	106.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

7 A 302 EPE C8-C7-N4-C5	Mol	Chain	Res	Type	Atoms
	7	А	302	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
8	В	102	EDO	O1-C1-C2-O2
8	С	101	EDO	O1-C1-C2-O2
7	А	302	EPE	C8-C7-N4-C3
7	А	302	EPE	C9-C10-S-O3S

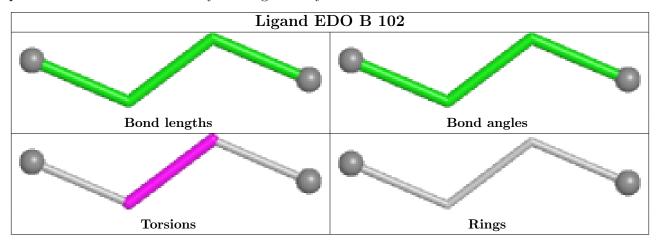
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There are no ring outliers.

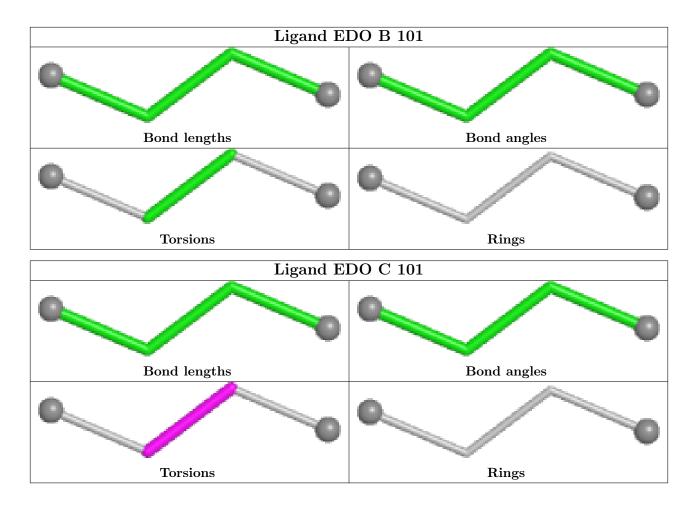
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	302	EPE	2	0
6	С	102	SO4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q < 0.9
1	А	276/276~(100%)	-0.06	0 100 100	28, 47, 79, 121	0
2	В	100/100~(100%)	-0.08	0 100 100	31, 50, 76, 88	0
3	С	9/9~(100%)	0.03	0 100 100	38, 40, 49, 49	0
4	D	192/192~(100%)	0.10	8 (4%) 36 38	36, 54, 102, 129	0
5	Ε	240/240~(100%)	-0.03	1 (0%) 92 93	36, 57, 84, 95	0
All	All	817/817~(100%)	-0.02	9 (1%) 80 82	28, 52, 88, 129	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	2	GLY	5.5
4	D	191	SER	4.1
4	D	128	SER	3.6
4	D	180	SER	2.9
4	D	148	SER	2.9

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 monosaccharides in this entry.

6.4 Ligands (i)

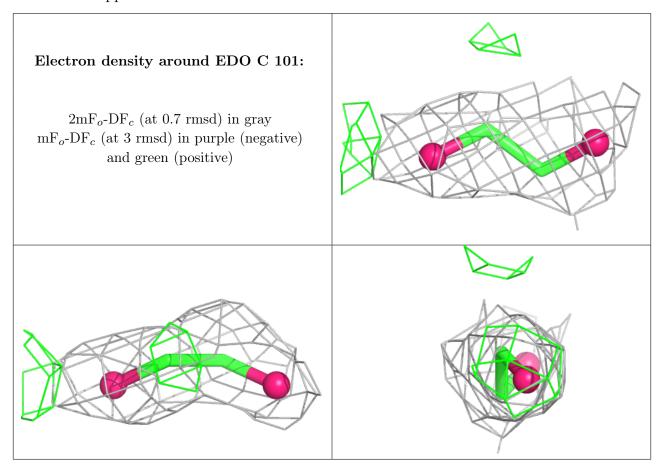
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



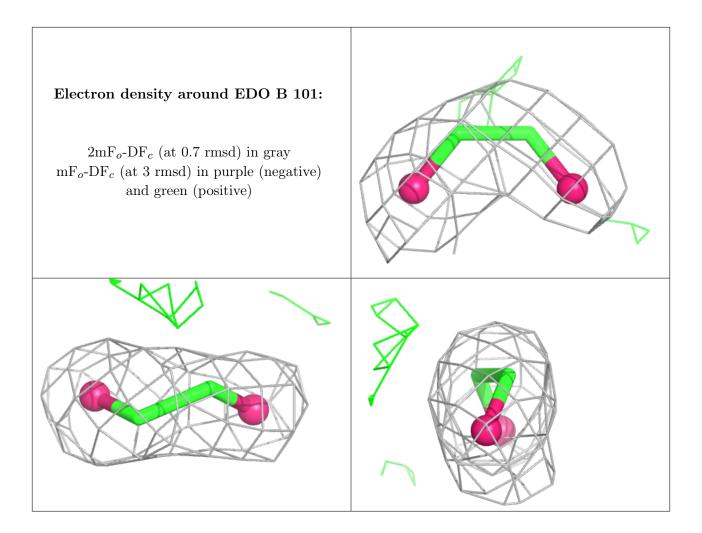
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	$\mathbf{Q} < 0.9$
6	SO4	А	301	5/5	0.61	0.47	138,141,146,151	0
7	EPE	А	302	15/15	0.70	0.28	74,109,118,119	0
6	SO4	D	201	5/5	0.84	0.27	58,59,61,64	5
6	SO4	С	102	5/5	0.89	0.31	31,36,39,39	5
8	EDO	С	101	4/4	0.90	0.22	43,49,50,61	0
8	EDO	В	101	4/4	0.91	0.20	45,45,49,51	0
8	EDO	В	102	4/4	0.96	0.16	47,49,50,51	0

median, 95^{th} 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.

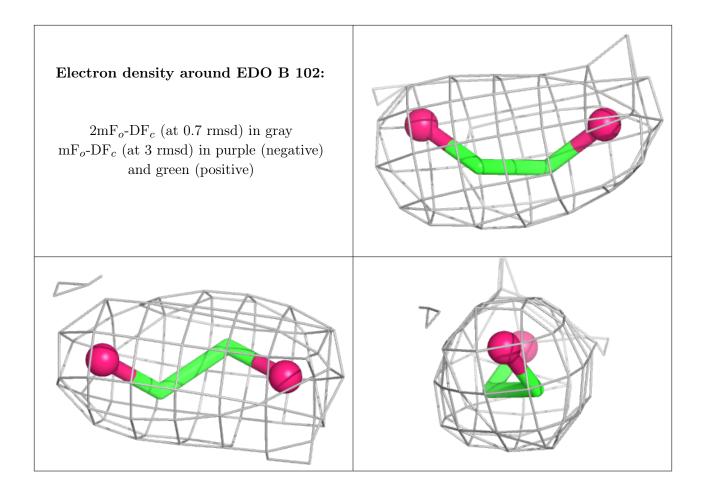
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.











6.5 Other polymers (i)

There are no such residues in this entry.

