



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2024 – 10:03 AM EDT

PDB ID : 9CM8  
Title : UDP-GlcNAc 2-epimerase MnaA of Paenibacillus alvei  
Authors : Legg, M.S.G.; Mateyko, N.; Evans, S.V.  
Deposited on : 2024-07-13  
Resolution : 2.20 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

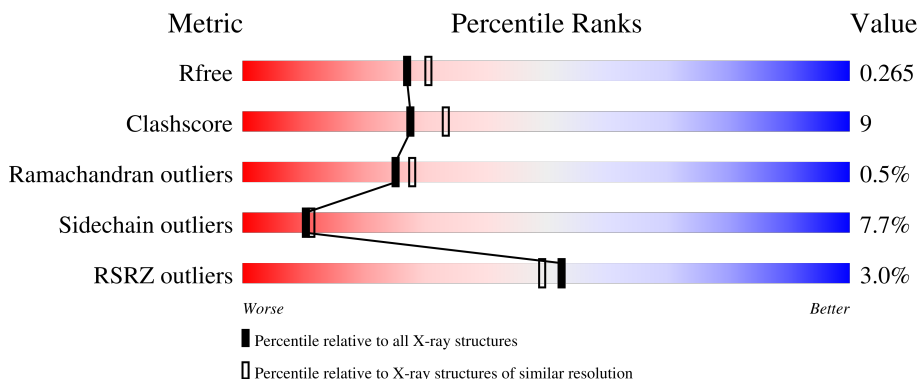
# 1 Overall quality at a glance

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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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 of 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	392	 3% 73% 19% • 6%
1	B	392	 3% 73% 17% • 5%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5855 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 UDP-N-acetylglucosamine 2-epimerase (non-hydrolyzing).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	2850	1817	493	532	8	0	2	0
1	B	371	2808	1795	479	525	9	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP A0A8I2FAI9
A	386	GLU	-	expression tag	UNP A0A8I2FAI9
A	387	HIS	-	expression tag	UNP A0A8I2FAI9
A	388	HIS	-	expression tag	UNP A0A8I2FAI9
A	389	HIS	-	expression tag	UNP A0A8I2FAI9
A	390	HIS	-	expression tag	UNP A0A8I2FAI9
A	391	HIS	-	expression tag	UNP A0A8I2FAI9
A	392	HIS	-	expression tag	UNP A0A8I2FAI9
B	385	LEU	-	expression tag	UNP A0A8I2FAI9
B	386	GLU	-	expression tag	UNP A0A8I2FAI9
B	387	HIS	-	expression tag	UNP A0A8I2FAI9
B	388	HIS	-	expression tag	UNP A0A8I2FAI9
B	389	HIS	-	expression tag	UNP A0A8I2FAI9
B	390	HIS	-	expression tag	UNP A0A8I2FAI9
B	391	HIS	-	expression tag	UNP A0A8I2FAI9
B	392	HIS	-	expression tag	UNP A0A8I2FAI9

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



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

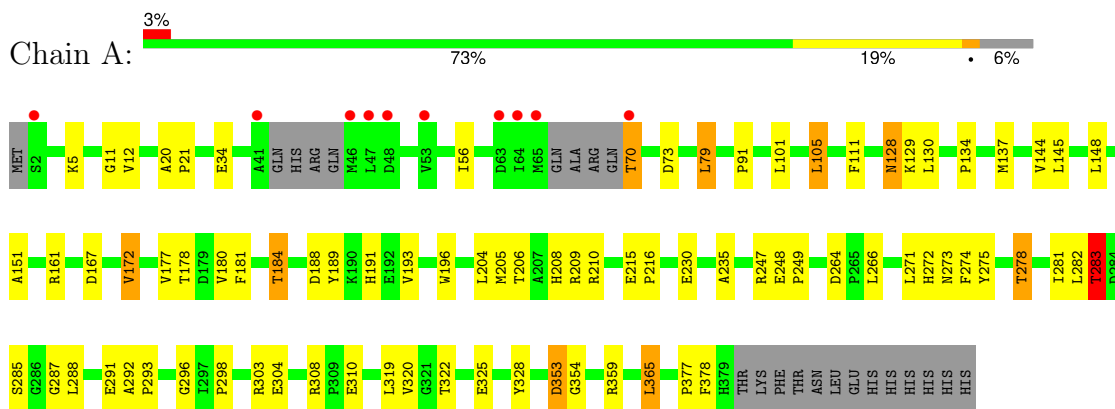
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	118	Total O 118 118	0	0
3	B	65	Total O 65 65	0	0

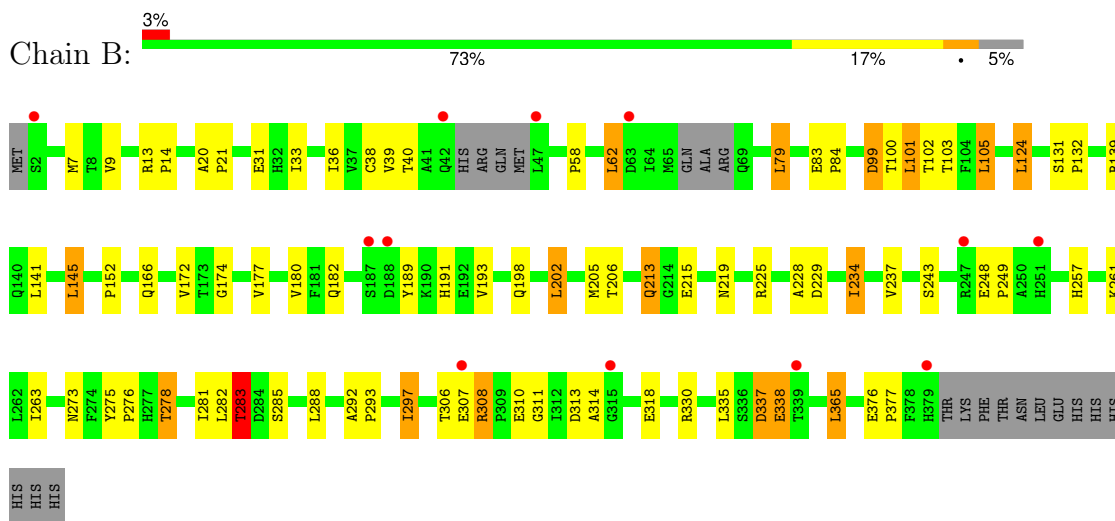
### 3 Residue-property plots

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: UDP-N-acetylglucosamine 2-epimerase (non-hydrolyzing)



- Molecule 1: UDP-N-acetylglucosamine 2-epimerase (non-hydrolyzing)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.82Å 81.76Å 107.72Å 90.00° 97.14° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.20) 99.2 (50.00-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.210 , 0.263 0.215 , 0.265	Depositor DCC
$R_{free}$ test set	2031 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.9	Xtrriage
Anisotropy	0.638	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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 28.80 % 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 1.7294e-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: PEG

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	0.71	0/2921	0.89	2/3985 (0.1%)
1	B	0.71	0/2872	0.89	2/3926 (0.1%)
All	All	0.71	0/5793	0.89	4/7911 (0.1%)

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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	283	THR	CB-CA-C	-7.41	91.58	111.60
1	B	283	THR	CB-CA-C	-6.28	94.65	111.60
1	A	353	ASP	CB-CA-C	-6.20	98.01	110.40
1	B	182	GLN	CB-CA-C	-5.67	99.05	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	ASP	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	2850	0	2770	47	0
1	B	2808	0	2689	52	0
2	A	7	0	10	0	0
2	B	7	0	10	1	0
3	A	118	0	0	2	0
3	B	65	0	0	0	0
All	All	5855	0	5479	99	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 9.

All (99) 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:B:281:ILE:CD1	1:B:297:ILE:HD11	1.88	1.01
1:B:206:THR:OG1	1:B:283:THR:CG2	2.26	0.83
1:B:281:ILE:HD12	1:B:297:ILE:HD11	1.61	0.80
1:A:184:THR:HG21	1:A:272:HIS:ND1	1.97	0.79
1:B:281:ILE:HD11	1:B:297:ILE:HD11	1.66	0.78
1:A:283:THR:HG21	1:A:285:SER:HB3	1.72	0.70
1:B:206:THR:OG1	1:B:283:THR:HG22	1.92	0.67
1:B:234:ILE:HD11	1:B:335:LEU:HD22	1.77	0.66
1:B:318:GLU:OE1	1:B:330:ARG:HD3	1.95	0.65
1:B:206:THR:OG1	1:B:283:THR:HG23	1.97	0.63
1:B:278:THR:OG1	1:B:297:ILE:HD12	1.99	0.63
1:A:205:MET:HA	1:A:282:LEU:O	1.99	0.62
1:A:181:PHE:HA	1:A:184:THR:HG22	1.81	0.61
1:A:353:ASP:OD2	1:A:359:ARG:NH2	2.25	0.61
1:A:248:GLU:HB2	1:A:249:PRO:HD3	1.83	0.61
1:A:274:PHE:O	1:A:278:THR:HG22	2.01	0.59
1:A:101:LEU:HG	1:A:105:LEU:CD2	2.32	0.59
1:A:196:TRP:CZ3	1:A:235:ALA:HB1	2.38	0.58
1:B:31:GLU:O	2:B:401:PEG:H11	2.03	0.57
1:A:230:GLU:OE1	1:A:328:TYR:OH	2.15	0.57
1:A:177:VAL:O	1:A:180:VAL:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:VAL:O	1:A:377:PRO:O	2.23	0.56
1:A:206:THR:OG1	1:A:283:THR:CG2	2.54	0.56
1:A:274:PHE:O	1:A:278:THR:CG2	2.54	0.56
1:B:101:LEU:O	1:B:105:LEU:HD22	2.06	0.56
1:B:177:VAL:O	1:B:180:VAL:HG13	2.06	0.55
1:A:292:ALA:N	1:A:293:PRO:CD	2.70	0.55
1:B:205:MET:HA	1:B:282:LEU:O	2.08	0.53
1:A:206:THR:OG1	1:A:283:THR:HG22	2.10	0.52
1:B:99:ASP:HB3	1:B:139:ARG:HB3	1.92	0.52
1:A:151:ALA:O	1:A:172:VAL:HA	2.10	0.52
1:A:191:HIS:HD2	1:A:193:VAL:H	1.57	0.51
1:A:204:LEU:O	1:A:281:ILE:HA	2.11	0.51
1:B:202:LEU:C	1:B:202:LEU:HD12	2.32	0.50
1:A:215:GLU:HB3	1:A:216:PRO:HD3	1.92	0.49
1:A:56:ILE:HA	3:A:553:HOH:O	2.11	0.49
1:B:213:GLN:O	1:B:213:GLN:HG2	2.12	0.49
1:A:178:THR:HG22	1:A:354:GLY:N	2.27	0.49
1:B:100:THR:HG23	1:B:103:THR:H	1.78	0.49
1:A:128:ASN:ND2	1:A:130:LEU:H	2.11	0.48
1:B:337:ASP:C	1:B:338:GLU:O	2.48	0.48
1:B:40:THR:HG22	1:B:62:LEU:HD11	1.97	0.47
1:B:83:GLU:HB3	1:B:84:PRO:HD3	1.96	0.47
1:A:111:PHE:HB2	1:A:145:LEU:HD22	1.97	0.47
1:A:5:LYS:HB3	1:A:91:PRO:HA	1.97	0.46
1:A:296:GLY:O	1:A:298:PRO:HD3	2.14	0.46
1:B:189:TYR:CD2	1:B:273:ASN:HB3	2.50	0.46
1:A:271:LEU:HD21	1:A:288:LEU:CD2	2.46	0.46
1:B:202:LEU:HD13	1:B:237:VAL:HG23	1.98	0.46
1:A:70:THR:HG22	1:A:73:ASP:CG	2.36	0.46
1:B:39:VAL:HG23	1:B:58:PRO:HB3	1.98	0.46
1:B:215:GLU:O	1:B:219:ASN:ND2	2.49	0.45
1:B:124:LEU:HD23	1:B:124:LEU:N	2.32	0.45
1:B:311:GLY:O	1:B:314:ALA:O	2.34	0.45
1:A:137:MET:HA	1:A:137:MET:HE2	1.98	0.45
1:A:20:ALA:N	1:A:21:PRO:CD	2.81	0.44
1:A:189:TYR:CD2	1:A:273:ASN:HB3	2.53	0.44
1:B:152:PRO:O	1:B:174:GLY:HA2	2.18	0.44
1:B:141:LEU:O	1:B:145:LEU:HD12	2.17	0.43
1:B:229:ASP:OD1	1:B:257:HIS:NE2	2.50	0.43
1:A:303:ARG:NH1	3:A:515:HOH:O	2.43	0.43
1:B:307:GLU:O	1:B:308:ARG:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ALA:HB1	1:B:257:HIS:CE1	2.54	0.43
1:B:13:ARG:N	1:B:14:PRO:HD2	2.34	0.42
1:B:292:ALA:HB1	1:B:297:ILE:HG12	2.00	0.42
1:B:308:ARG:HD2	1:B:310:GLU:OE2	2.18	0.42
1:A:283:THR:HB	1:A:285:SER:H	1.85	0.42
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.95	0.42
1:A:230:GLU:OE1	1:A:328:TYR:CE1	2.73	0.42
1:B:213:GLN:O	1:B:213:GLN:CG	2.67	0.42
1:B:33:ILE:HD11	1:B:365:LEU:HD13	2.00	0.42
1:B:40:THR:OG1	1:B:102:THR:HG21	2.19	0.42
1:B:7:MET:HA	1:B:36:ILE:O	2.20	0.42
1:B:292:ALA:N	1:B:293:PRO:CD	2.83	0.42
1:A:11:GLY:O	1:A:12:VAL:HG13	2.20	0.42
1:B:191:HIS:HD2	1:B:193:VAL:H	1.66	0.42
1:A:283:THR:CG2	1:A:285:SER:HB3	2.44	0.41
1:A:308:ARG:NH1	1:A:310:GLU:OE2	2.53	0.41
1:B:20:ALA:HB3	1:B:21:PRO:HD3	2.01	0.41
1:A:5:LYS:HE2	1:A:34:GLU:OE2	2.20	0.41
1:B:40:THR:HG22	1:B:62:LEU:CD1	2.50	0.41
1:A:128:ASN:C	1:A:128:ASN:HD22	2.23	0.41
1:B:100:THR:HG22	1:B:103:THR:OG1	2.21	0.41
1:B:283:THR:HB	1:B:285:SER:H	1.86	0.41
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.89	0.41
1:A:128:ASN:HD22	1:A:130:LEU:H	1.69	0.41
1:B:285:SER:HB3	1:B:288:LEU:HG	2.03	0.41
1:B:281:ILE:HD12	1:B:297:ILE:CD1	2.40	0.41
1:A:247:ARG:NH2	1:A:264:ASP:OD1	2.54	0.41
1:A:287:GLY:O	1:A:291:GLU:HG3	2.21	0.41
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.89	0.41
1:B:275:TYR:N	1:B:276:PRO:CD	2.83	0.41
1:B:376:GLU:HA	1:B:377:PRO:HD3	1.91	0.41
1:B:131:SER:HA	1:B:132:PRO:HA	1.69	0.41
1:A:275:TYR:HA	1:A:278:THR:HG23	2.03	0.40
1:B:9:VAL:HA	1:B:38:CYS:O	2.22	0.40
1:B:248:GLU:HB2	1:B:249:PRO:HD3	2.03	0.40
1:A:161:ARG:NE	1:A:167:ASP:OD1	2.43	0.40
1:A:206:THR:OG1	1:A:283:THR:HG23	2.21	0.40

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	366/392 (93%)	345 (94%)	19 (5%)	2 (0%)	25	28
1	B	365/392 (93%)	347 (95%)	16 (4%)	2 (0%)	25	28
All	All	731/784 (93%)	692 (95%)	35 (5%)	4 (0%)	25	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	PHE
1	B	308	ARG
1	B	338	GLU
1	A	188	ASP

### 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	301/343 (88%)	278 (92%)	23 (8%)	11	12
1	B	289/343 (84%)	266 (92%)	23 (8%)	10	10
All	All	590/686 (86%)	544 (92%)	46 (8%)	10	11

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	THR
1	A	79	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	105	LEU
1	A	128	ASN
1	A	129	LYS
1	A	134	PRO
1	A	144	VAL
1	A	148	LEU
1	A	172	VAL
1	A	184	THR
1	A	208[A]	HIS
1	A	208[B]	HIS
1	A	209	ARG
1	A	210	ARG
1	A	266	LEU
1	A	278	THR
1	A	283	THR
1	A	304	GLU
1	A	319	LEU
1	A	320	VAL
1	A	322	THR
1	A	325	GLU
1	A	365	LEU
1	B	62	LEU
1	B	79	LEU
1	B	99	ASP
1	B	101	LEU
1	B	105	LEU
1	B	124	LEU
1	B	145	LEU
1	B	166	GLN
1	B	172	VAL
1	B	198	GLN
1	B	202	LEU
1	B	213	GLN
1	B	225	ARG
1	B	234	ILE
1	B	243	SER
1	B	261	LYS
1	B	263	ILE
1	B	278	THR
1	B	283	THR
1	B	297	ILE
1	B	306	THR

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Mol	Chain	Res	Type
1	B	313	ASP
1	B	365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	128	ASN
1	A	166	GLN
1	A	191	HIS
1	B	113	GLN
1	B	166	GLN
1	B	191	HIS
1	B	198	GLN
1	B	219	ASN
1	B	277	HIS
1	B	358	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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$
2	PEG	A	401	-	6,6,6	0.38	0	5,5,5	0.39	0
2	PEG	B	401	-	6,6,6	0.38	0	5,5,5	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
2	PEG	A	401	-	-	2/4/4/4	-
2	PEG	B	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	PEG	O1-C1-C2-O2
2	A	401	PEG	C1-C2-O2-C3
2	B	401	PEG	C1-C2-O2-C3
2	A	401	PEG	O2-C3-C4-O4

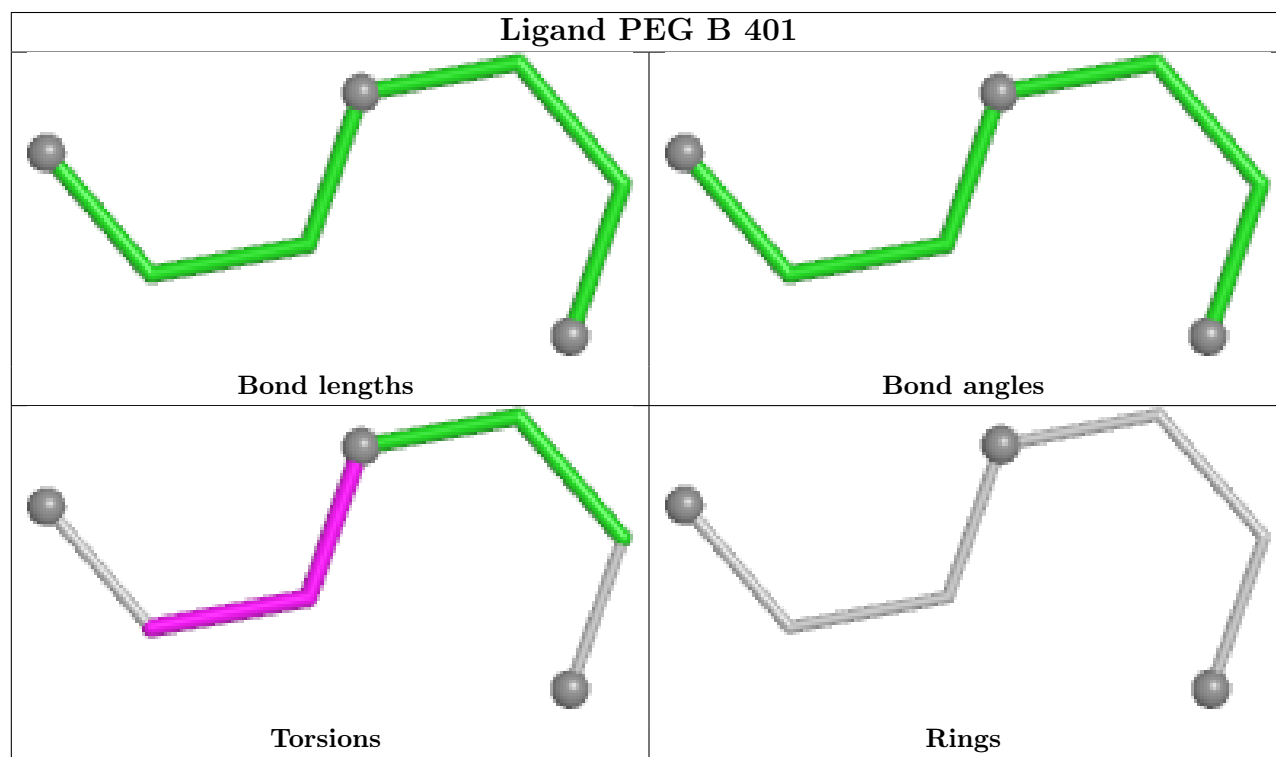
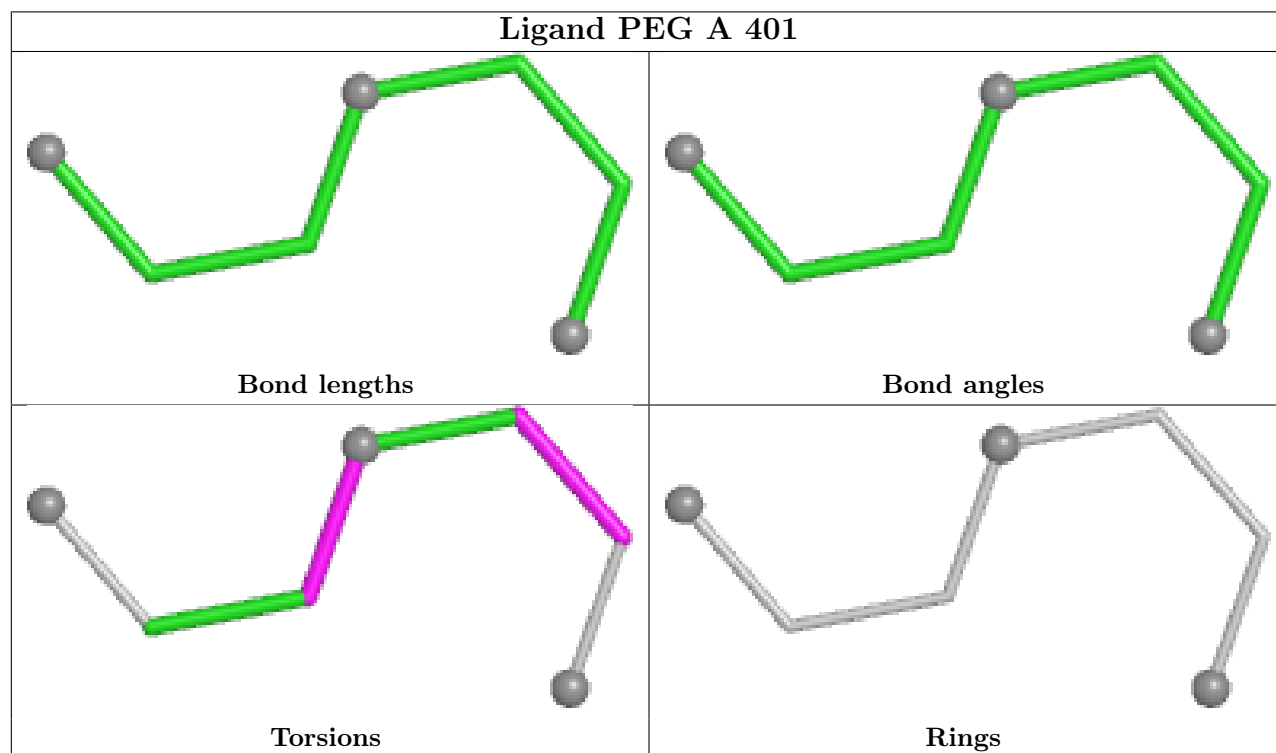
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PEG	1	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 than 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

### 6.1 Protein, DNA and RNA chains

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	370/392 (94%)	-0.03	10 (2%) 56 53	17, 33, 58, 88	2 (0%)
1	B	371/392 (94%)	0.04	12 (3%) 50 47	15, 34, 63, 88	0
All	All	741/784 (94%)	0.01	22 (2%) 52 49	15, 33, 61, 88	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	LEU	3.6
1	A	65	MET	3.4
1	B	307	GLU	3.3
1	B	42	GLN	2.9
1	B	47	LEU	2.8
1	B	315	GLY	2.6
1	B	2	SER	2.6
1	B	187	SER	2.6
1	A	48	ASP	2.6
1	B	251	HIS	2.5
1	A	70	THR	2.5
1	A	64	ILE	2.5
1	B	339	THR	2.4
1	A	46	MET	2.3
1	A	2	SER	2.3
1	B	247	ARG	2.3
1	A	41	ALA	2.2
1	B	63	ASP	2.2
1	A	63	ASP	2.2
1	A	53	VAL	2.1
1	B	379	HIS	2.1
1	B	188	ASP	2.0

## 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](#)

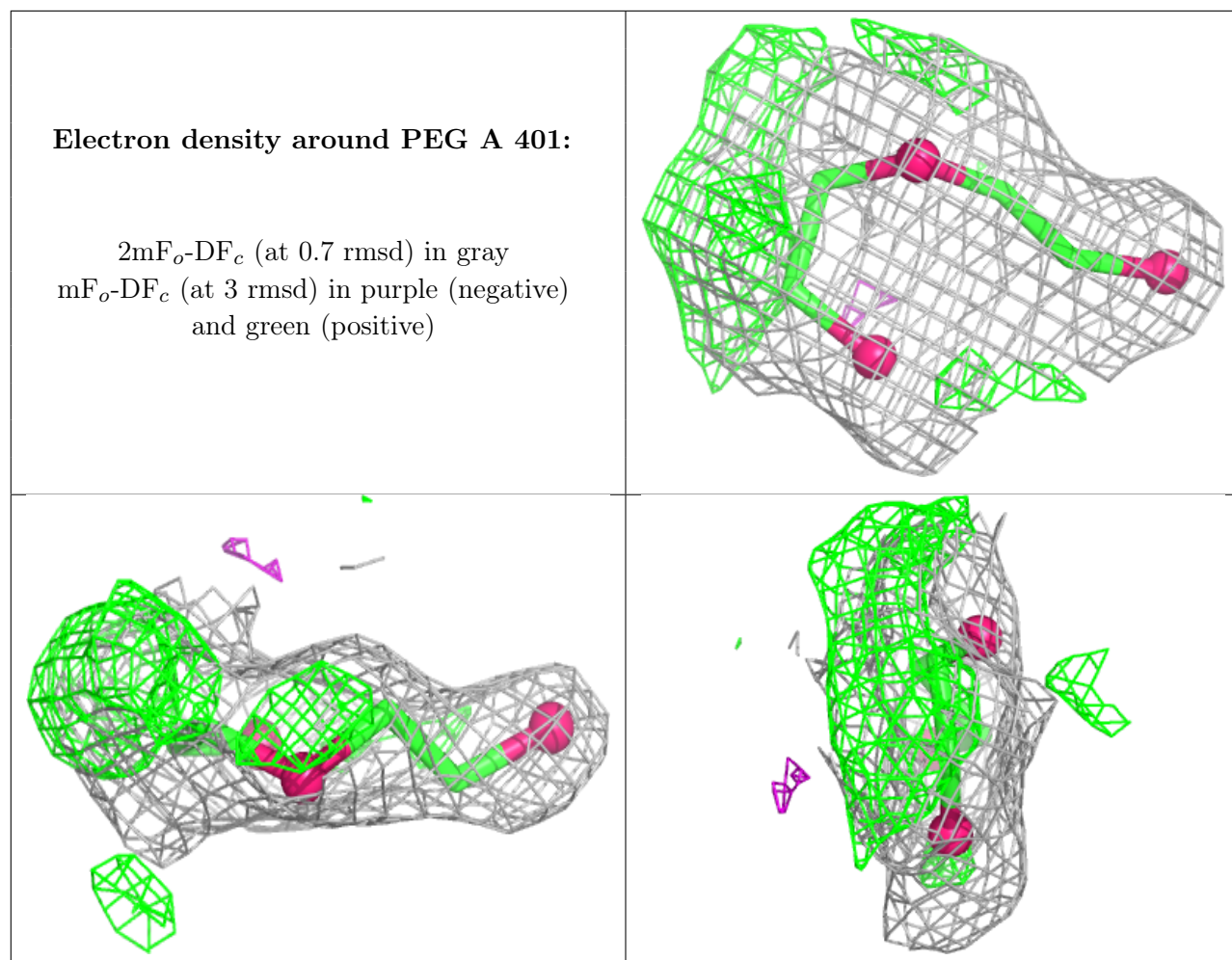
There are no monosaccharides in this entry.

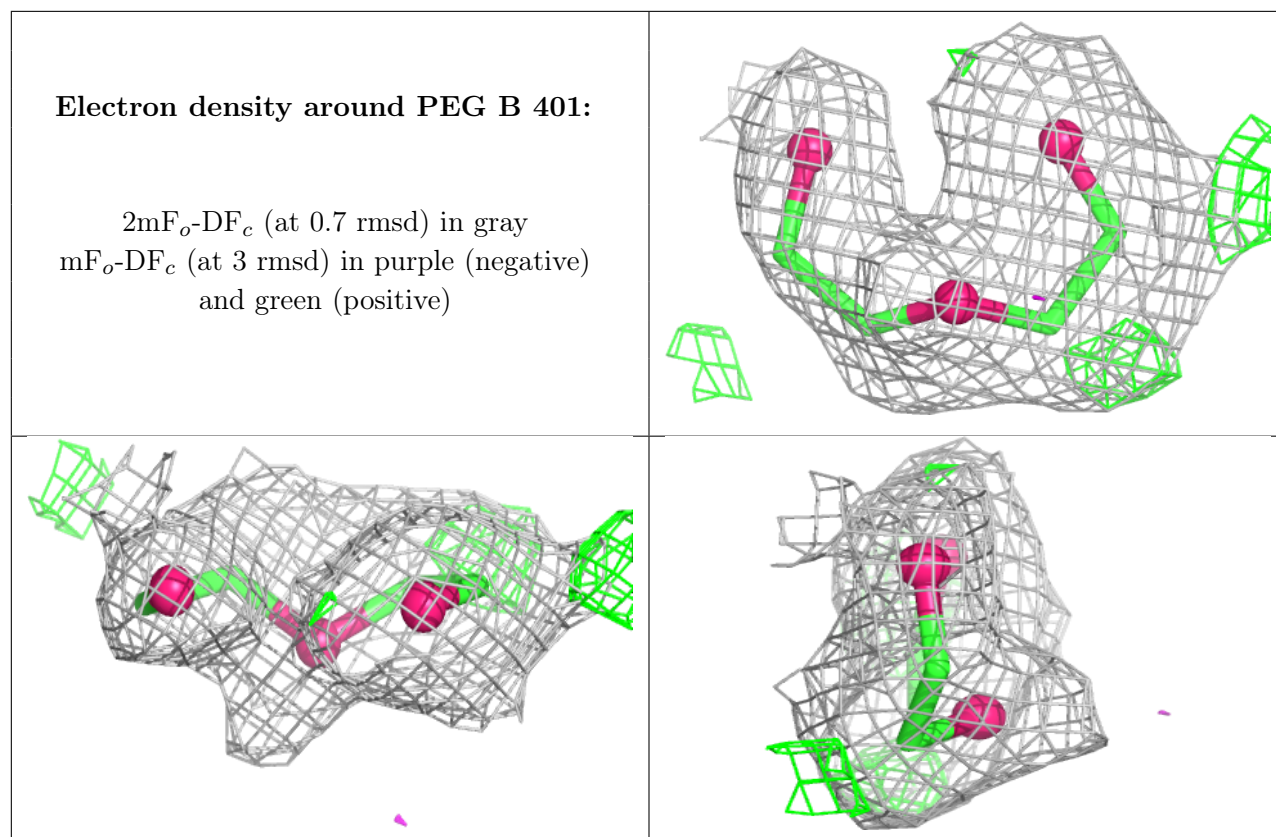
## 6.4 Ligands [i](#)

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, 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
2	PEG	A	401	7/7	0.52	0.21	47,52,58,59	0
2	PEG	B	401	7/7	0.80	0.14	35,46,55,57	0

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.