



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:04 PM UTC

PDB ID : 5ONU / pdb_00005onu
Title : Trimeric OmpU structure
Authors : Li, H.Y.; Dong, C.J.
Deposited on : 2017-08-04
Resolution : 2.22 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

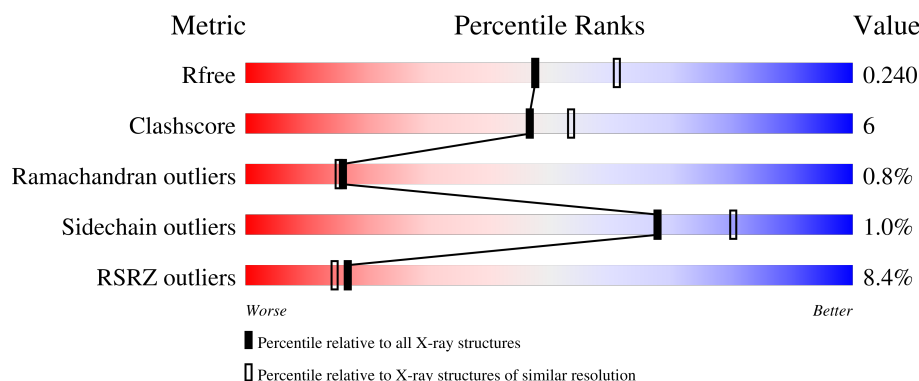
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

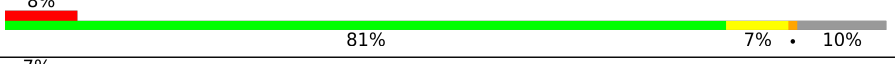
The reported resolution of this entry is 2.22 Å.

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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 ≥ 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	356	
1	B	356	
1	C	356	

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
4	LDA	A	405	-	-	-	X
4	LDA	B	405	-	-	X	-
4	LDA	B	406	-	-	X	-
4	LDA	C	404	-	-	X	-
4	LDA	C	405	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8240 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.

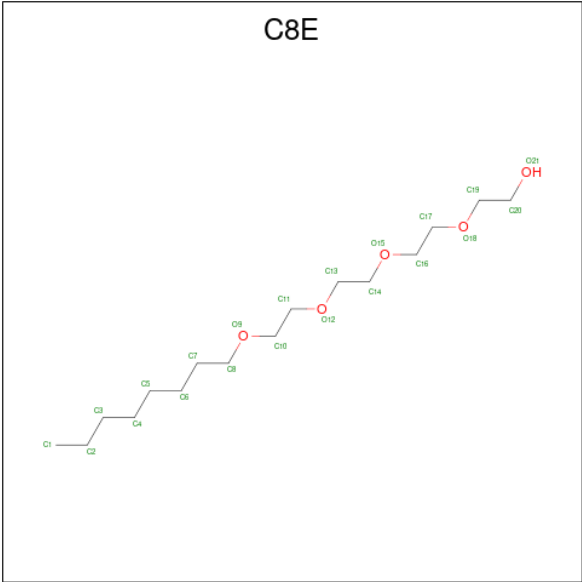
- Molecule 1 is a protein called Outer membrane protein OmpU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2448	1526	406	511	5			
1	B	320	Total	C	N	O	S	0	0	0
			2448	1526	406	511	5			
1	C	320	Total	C	N	O	S	0	0	0
			2448	1526	406	511	5			

There are 18 discrepancies between the modelled and reference sequences:

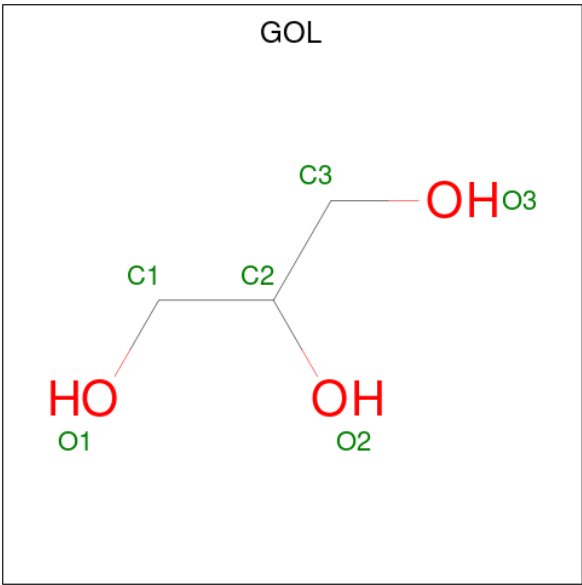
Chain	Residue	Modelled	Actual	Comment	Reference
A	351	HIS	-	expression tag	UNP A0A1V9N7P1
A	352	HIS	-	expression tag	UNP A0A1V9N7P1
A	353	HIS	-	expression tag	UNP A0A1V9N7P1
A	354	HIS	-	expression tag	UNP A0A1V9N7P1
A	355	HIS	-	expression tag	UNP A0A1V9N7P1
A	356	HIS	-	expression tag	UNP A0A1V9N7P1
B	351	HIS	-	expression tag	UNP A0A1V9N7P1
B	352	HIS	-	expression tag	UNP A0A1V9N7P1
B	353	HIS	-	expression tag	UNP A0A1V9N7P1
B	354	HIS	-	expression tag	UNP A0A1V9N7P1
B	355	HIS	-	expression tag	UNP A0A1V9N7P1
B	356	HIS	-	expression tag	UNP A0A1V9N7P1
C	351	HIS	-	expression tag	UNP A0A1V9N7P1
C	352	HIS	-	expression tag	UNP A0A1V9N7P1
C	353	HIS	-	expression tag	UNP A0A1V9N7P1
C	354	HIS	-	expression tag	UNP A0A1V9N7P1
C	355	HIS	-	expression tag	UNP A0A1V9N7P1
C	356	HIS	-	expression tag	UNP A0A1V9N7P1

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



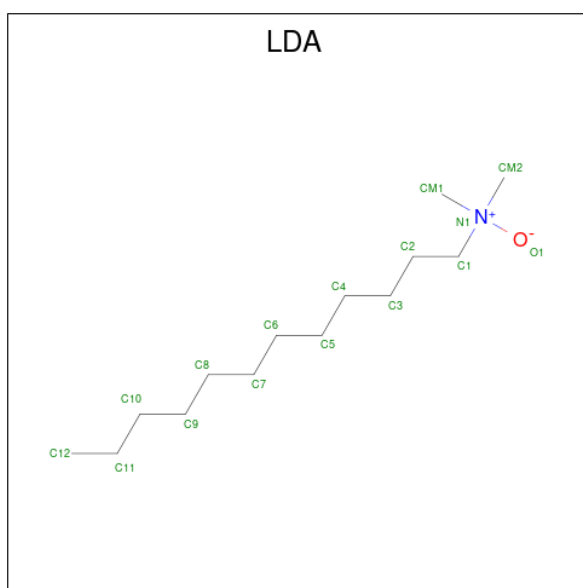
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		

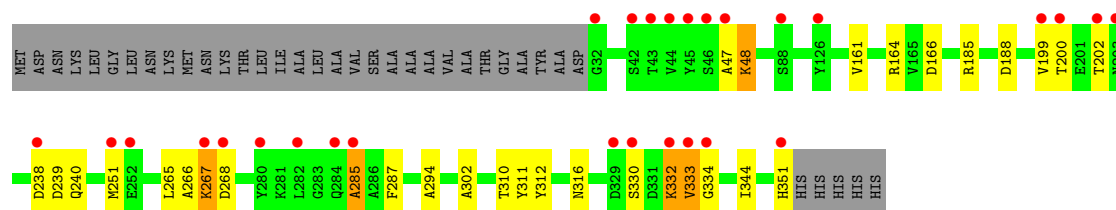
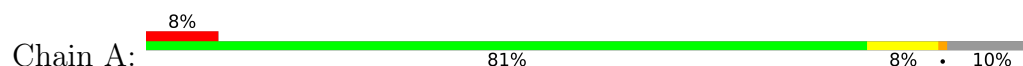
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	204	Total	O	0	0
			204	204		
5	B	208	Total	O	0	0
			208	208		
5	C	225	Total	O	0	0
			225	225		

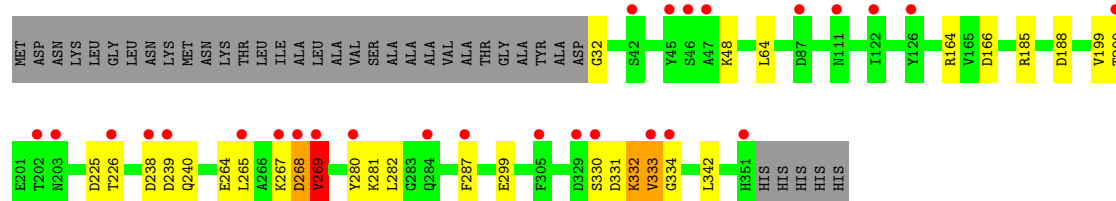
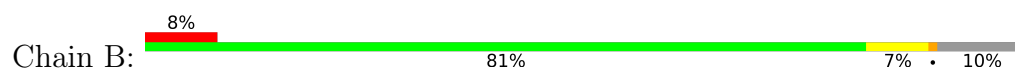
3 Residue-property plots [i](#)

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.

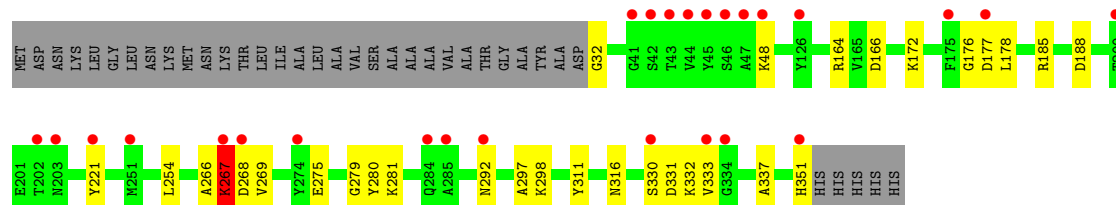
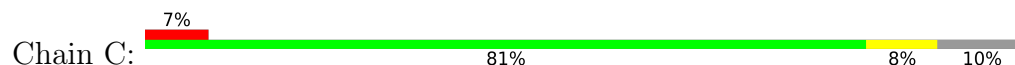
• Molecule 1: Outer membrane protein OmpU



• Molecule 1: Outer membrane protein OmpU



• Molecule 1: Outer membrane protein OmpU



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.88Å 153.47Å 81.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.73 – 2.22 62.73 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.7 (62.73-2.22) 99.7 (62.73-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.236 0.216 , 0.240	Depositor DCC
R_{free} test set	4020 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8240	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: GOL, LDA, C8E

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	0.36	0/2492	0.78	1/3366 (0.0%)
1	B	0.40	1/2492 (0.0%)	0.83	4/3366 (0.1%)
1	C	0.34	0/2492	0.79	1/3366 (0.0%)
All	All	0.37	1/7476 (0.0%)	0.80	6/10098 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	VAL	CA-CB	6.36	1.62	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ASP	N-CA-C	-6.03	105.58	113.12
1	B	332	LYS	N-CA-C	-5.92	101.71	110.48
1	B	268	ASP	CA-C-N	-5.69	115.53	123.10
1	B	268	ASP	C-N-CA	-5.69	115.53	123.10
1	A	332	LYS	N-CA-C	-5.67	102.12	110.52
1	C	331	ASP	N-CA-C	-5.63	106.08	113.12

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	2448	0	2271	25	0
1	B	2448	0	2271	24	0
1	C	2448	0	2271	26	0
2	A	21	0	34	1	0
2	B	21	0	34	1	0
2	C	21	0	34	5	0
3	A	12	0	16	1	0
3	B	12	0	16	1	0
3	C	12	0	16	1	0
4	A	48	0	93	3	0
4	B	64	0	124	3	108
4	C	48	0	93	8	108
5	A	204	0	0	1	0
5	B	208	0	0	1	0
5	C	225	0	0	9	0
All	All	8240	0	7273	85	108

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.

All (85) 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:C:176:GLY:HA2	4:C:405:LDA:HM13	1.30	1.12
1:B:267:LYS:HG2	1:B:268:ASP:H	1.25	1.01
4:C:404:LDA:H122	4:C:404:LDA:H81	1.59	0.85
1:B:267:LYS:HE3	1:B:269:VAL:HG12	1.61	0.83
1:C:178:LEU:HD13	1:C:221:TYR:CE2	2.14	0.81
4:C:404:LDA:H81	4:C:404:LDA:C12	2.10	0.81
1:A:238:ASP:OD1	1:A:239:ASP:N	2.15	0.79
1:B:238:ASP:OD1	1:B:239:ASP:N	2.19	0.76
1:B:166:ASP:O	1:B:185:ARG:NH1	2.19	0.75
1:C:176:GLY:HA2	4:C:405:LDA:CM1	2.14	0.72
1:A:47:ALA:O	1:A:48:LYS:HB2	1.88	0.72
4:B:405:LDA:O1	4:B:405:LDA:H42	1.91	0.71
1:C:185:ARG:NH2	1:C:188:ASP:OD2	2.26	0.68
1:A:185:ARG:NH2	1:A:188:ASP:OD2	2.27	0.68
4:C:404:LDA:H122	4:C:404:LDA:C8	2.24	0.66
1:A:267:LYS:HG3	1:A:268:ASP:N	2.09	0.66
2:C:401:C8E:H52	5:C:504:HOH:O	1.95	0.65
1:B:32:GLY:N	5:B:502:HOH:O	2.30	0.65
1:C:177:ASP:H	4:C:405:LDA:H62	1.62	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:GLY:N	5:C:506:HOH:O	2.32	0.63
1:B:164:ARG:HH22	3:B:403:GOL:H12	1.64	0.63
1:B:267:LYS:CG	1:B:268:ASP:H	2.07	0.63
1:A:267:LYS:HG3	1:A:268:ASP:H	1.65	0.60
1:A:333:VAL:HG12	1:A:334:GLY:N	2.17	0.59
1:B:267:LYS:HG2	1:B:268:ASP:N	2.08	0.58
1:A:267:LYS:CG	1:A:268:ASP:H	2.18	0.56
1:C:275:GLU:OE2	1:C:292:ASN:ND2	2.38	0.56
1:B:185:ARG:NH2	1:B:188:ASP:OD2	2.40	0.55
1:B:333:VAL:HG12	1:B:334:GLY:N	2.23	0.53
1:A:285:ALA:HB2	1:A:311:TYR:HD2	1.72	0.53
1:A:285:ALA:HA	1:A:310:THR:O	2.08	0.53
1:C:275:GLU:CD	1:C:292:ASN:ND2	2.66	0.53
1:B:280:TYR:HE2	1:B:282:LEU:HG	1.73	0.53
1:A:166:ASP:O	1:A:185:ARG:NH1	2.42	0.52
1:B:287:PHE:HB3	4:B:405:LDA:H41	1.92	0.52
1:B:64:LEU:HD12	1:B:342:LEU:HD23	1.92	0.51
1:A:238:ASP:CG	1:A:239:ASP:H	2.18	0.51
1:B:240:GLN:HG2	1:B:265:LEU:O	2.12	0.50
1:B:281:LYS:HE2	2:B:401:C8E:H142	1.93	0.50
1:B:280:TYR:CE2	1:B:282:LEU:HG	2.47	0.50
1:C:281:LYS:NZ	5:C:507:HOH:O	2.36	0.50
2:C:401:C8E:H62	5:C:527:HOH:O	2.13	0.49
1:A:287:PHE:HB3	4:A:405:LDA:H42	1.95	0.49
1:A:164:ARG:HH12	3:A:403:GOL:H31	1.78	0.49
1:B:238:ASP:CG	1:B:239:ASP:H	2.20	0.49
1:A:251:MET:O	1:A:251:MET:HG3	2.13	0.48
1:C:48:LYS:HE3	1:C:48:LYS:HB2	1.54	0.47
1:C:297:ALA:O	1:C:298:LYS:HG2	2.14	0.47
1:A:164:ARG:NH1	5:A:506:HOH:O	2.47	0.47
1:C:176:GLY:CA	4:C:405:LDA:HM13	2.23	0.47
1:C:275:GLU:CD	1:C:292:ASN:HD21	2.23	0.47
2:C:401:C8E:H42	5:C:711:HOH:O	2.15	0.47
1:A:312:TYR:CE1	2:A:401:C8E:H171	2.50	0.46
4:A:405:LDA:HM11	4:A:405:LDA:H22	1.55	0.46
1:A:332:LYS:O	1:A:333:VAL:HB	2.16	0.45
2:C:401:C8E:H71	5:C:504:HOH:O	2.15	0.45
1:A:294:ALA:HB3	1:A:302:ALA:HB3	1.99	0.45
1:C:164:ARG:HH12	3:C:403:GOL:H31	1.82	0.45
1:C:280:TYR:HA	5:C:504:HOH:O	2.17	0.45
1:B:267:LYS:HE3	1:B:269:VAL:CG1	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASP:O	1:C:185:ARG:NH1	2.50	0.45
1:C:316:ASN:HB3	1:C:351:HIS:CE1	2.52	0.45
1:C:332:LYS:O	1:C:333:VAL:HB	2.17	0.45
1:C:279:GLY:HA3	2:C:401:C8E:H41	2.00	0.44
1:A:199:VAL:HG22	1:A:200:THR:H	1.82	0.43
1:C:172:LYS:NZ	5:C:517:HOH:O	2.50	0.43
1:A:266:ALA:O	1:A:267:LYS:C	2.62	0.43
1:A:316:ASN:HB3	1:A:351:HIS:CE1	2.53	0.43
4:B:407:LDA:HM13	4:B:407:LDA:H22	1.54	0.42
1:A:200:THR:HG22	1:A:202:THR:H	1.84	0.42
1:C:266:ALA:O	1:C:267:LYS:C	2.62	0.42
1:B:332:LYS:O	1:B:333:VAL:HB	2.19	0.42
1:C:311:TYR:HB2	4:C:406:LDA:H101	2.01	0.42
1:C:267:LYS:HB2	1:C:268:ASP:H	1.62	0.42
1:C:178:LEU:HD22	1:C:221:TYR:OH	2.19	0.42
1:B:264:GLU:HA	1:B:269:VAL:O	2.20	0.42
1:B:199:VAL:HG22	1:B:200:THR:H	1.85	0.41
1:B:333:VAL:HG12	1:B:334:GLY:H	1.85	0.41
1:B:267:LYS:HB3	1:B:269:VAL:HG12	2.03	0.41
1:A:285:ALA:HB2	1:A:311:TYR:CD2	2.52	0.41
1:A:344:ILE:HD11	4:A:406:LDA:HM21	2.02	0.41
1:B:225:ASP:O	1:B:226:THR:OG1	2.25	0.41
1:A:240:GLN:HG2	1:A:265:LEU:O	2.20	0.41
1:C:254:LEU:HA	5:C:504:HOH:O	2.21	0.40
1:C:333:VAL:HG13	1:C:337:ALA:HB3	2.02	0.40

All (108) 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:B:405:LDA:C8	4:C:404:LDA:C3[3_455]	0.16	2.04
4:B:405:LDA:C9	4:C:404:LDA:C2[3_455]	0.20	2.00
4:B:405:LDA:C7	4:C:404:LDA:C4[3_455]	0.23	1.97
4:B:406:LDA:C8	4:C:405:LDA:C8[3_455]	0.23	1.97
4:B:405:LDA:C10	4:C:404:LDA:C1[3_455]	0.25	1.95
4:B:406:LDA:C12	4:C:405:LDA:C12[3_455]	0.34	1.86
4:B:405:LDA:O1	4:C:404:LDA:C12[3_455]	0.39	1.81
4:B:405:LDA:C11	4:C:404:LDA:N1[3_455]	0.40	1.80
4:B:406:LDA:O1	4:C:405:LDA:CM2[3_455]	0.42	1.78
4:B:406:LDA:CM1	4:C:405:LDA:O1[3_455]	0.42	1.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:405:LDA:C12	4:C:404:LDA:CM2[3_455]	0.45	1.75
4:B:406:LDA:C9	4:C:405:LDA:C9[3_455]	0.46	1.74
4:B:406:LDA:C7	4:C:405:LDA:C7[3_455]	0.47	1.73
4:B:406:LDA:N1	4:C:405:LDA:N1[3_455]	0.49	1.71
4:B:405:LDA:N1	4:C:404:LDA:C11[3_455]	0.53	1.67
4:B:405:LDA:C2	4:C:404:LDA:C9[3_455]	0.55	1.65
4:B:405:LDA:C5	4:C:404:LDA:C6[3_455]	0.65	1.55
4:B:406:LDA:C5	4:C:405:LDA:C4[3_455]	0.67	1.53
4:B:406:LDA:C6	4:C:405:LDA:C6[3_455]	0.67	1.53
4:B:406:LDA:C4	4:C:405:LDA:C3[3_455]	0.67	1.53
4:B:406:LDA:C2	4:C:405:LDA:C1[3_455]	0.70	1.50
4:B:405:LDA:C1	4:C:404:LDA:C10[3_455]	0.76	1.44
4:B:406:LDA:C3	4:C:405:LDA:C2[3_455]	0.76	1.44
4:B:406:LDA:C10	4:C:405:LDA:C10[3_455]	0.90	1.30
4:B:406:LDA:C6	4:C:405:LDA:C5[3_455]	0.90	1.30
4:B:406:LDA:C2	4:C:405:LDA:C2[3_455]	0.92	1.28
4:B:405:LDA:C6	4:C:404:LDA:C5[3_455]	0.93	1.27
4:B:405:LDA:C1	4:C:404:LDA:C9[3_455]	0.97	1.23
4:B:406:LDA:C3	4:C:405:LDA:C3[3_455]	0.98	1.22
4:B:405:LDA:C4	4:C:404:LDA:C7[3_455]	0.99	1.21
4:B:405:LDA:C3	4:C:404:LDA:C7[3_455]	1.00	1.20
4:B:406:LDA:C10	4:C:405:LDA:C11[3_455]	1.01	1.19
4:B:406:LDA:C5	4:C:405:LDA:C5[3_455]	1.01	1.19
4:B:405:LDA:C3	4:C:404:LDA:C8[3_455]	1.03	1.17
4:B:406:LDA:O1	4:C:405:LDA:N1[3_455]	1.06	1.14
4:B:406:LDA:C4	4:C:405:LDA:C4[3_455]	1.07	1.13
4:B:405:LDA:N1	4:C:404:LDA:C10[3_455]	1.08	1.12
4:B:406:LDA:CM2	4:C:405:LDA:CM1[3_455]	1.08	1.12
4:B:405:LDA:C11	4:C:404:LDA:CM1[3_455]	1.09	1.11
4:B:406:LDA:C11	4:C:405:LDA:C11[3_455]	1.10	1.10
4:B:406:LDA:C7	4:C:405:LDA:C6[3_455]	1.13	1.07
4:B:406:LDA:N1	4:C:405:LDA:O1[3_455]	1.14	1.06
4:B:405:LDA:C5	4:C:404:LDA:C5[3_455]	1.15	1.05
4:B:406:LDA:N1	4:C:405:LDA:CM1[3_455]	1.18	1.02
4:B:405:LDA:C4	4:C:404:LDA:C6[3_455]	1.19	1.01
4:B:406:LDA:C1	4:C:405:LDA:C1[3_455]	1.20	1.00
4:B:405:LDA:CM2	4:C:404:LDA:C11[3_455]	1.21	0.99
4:B:405:LDA:O1	4:C:404:LDA:C11[3_455]	1.25	0.95
4:B:406:LDA:C11	4:C:405:LDA:C12[3_455]	1.25	0.95
4:B:405:LDA:C12	4:C:404:LDA:N1[3_455]	1.27	0.93
4:B:405:LDA:C11	4:C:404:LDA:O1[3_455]	1.27	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:406:LDA:C1	4:C:405:LDA:N1[3_455]	1.27	0.93
4:B:405:LDA:C4	4:C:404:LDA:C8[3_455]	1.30	0.90
4:B:406:LDA:C11	4:C:405:LDA:C10[3_455]	1.30	0.90
4:B:406:LDA:C9	4:C:405:LDA:C8[3_455]	1.31	0.89
4:B:405:LDA:C6	4:C:404:LDA:C4[3_455]	1.35	0.85
4:B:406:LDA:C9	4:C:405:LDA:C10[3_455]	1.36	0.84
4:B:405:LDA:C10	4:C:404:LDA:C2[3_455]	1.37	0.83
4:B:405:LDA:C10	4:C:404:LDA:N1[3_455]	1.38	0.82
4:B:406:LDA:C8	4:C:405:LDA:C7[3_455]	1.38	0.82
4:B:405:LDA:CM1	4:C:404:LDA:C11[3_455]	1.45	0.75
4:B:406:LDA:C1	4:C:405:LDA:CM1[3_455]	1.45	0.75
4:B:405:LDA:C8	4:C:404:LDA:C2[3_455]	1.46	0.74
4:B:405:LDA:C2	4:C:404:LDA:C8[3_455]	1.47	0.73
4:B:405:LDA:C5	4:C:404:LDA:C7[3_455]	1.47	0.73
4:B:405:LDA:C6	4:C:404:LDA:C6[3_455]	1.49	0.71
4:B:405:LDA:C8	4:C:404:LDA:C4[3_455]	1.51	0.69
4:B:405:LDA:C7	4:C:404:LDA:C3[3_455]	1.53	0.67
4:B:406:LDA:C12	4:C:405:LDA:C11[3_455]	1.54	0.66
4:B:405:LDA:C7	4:C:404:LDA:C5[3_455]	1.55	0.65
4:B:405:LDA:N1	4:C:404:LDA:C12[3_455]	1.55	0.65
4:B:406:LDA:N1	4:C:405:LDA:CM2[3_455]	1.59	0.61
4:B:405:LDA:C9	4:C:404:LDA:C3[3_455]	1.60	0.60
4:B:406:LDA:CM1	4:C:405:LDA:N1[3_455]	1.63	0.57
4:B:405:LDA:C11	4:C:404:LDA:C1[3_455]	1.65	0.55
4:B:406:LDA:C10	4:C:405:LDA:C9[3_455]	1.65	0.55
4:B:405:LDA:C9	4:C:404:LDA:C1[3_455]	1.67	0.53
4:B:406:LDA:C7	4:C:405:LDA:C8[3_455]	1.67	0.53
4:B:406:LDA:C8	4:C:405:LDA:C9[3_455]	1.70	0.50
4:B:405:LDA:C11	4:C:404:LDA:CM2[3_455]	1.73	0.47
4:B:406:LDA:C6	4:C:405:LDA:C7[3_455]	1.73	0.47
4:B:405:LDA:CM1	4:C:404:LDA:C10[3_455]	1.75	0.45
4:B:405:LDA:C1	4:C:404:LDA:C8[3_455]	1.79	0.41
4:B:405:LDA:C12	4:C:404:LDA:O1[3_455]	1.80	0.40
4:B:406:LDA:C4	4:C:405:LDA:C5[3_455]	1.81	0.39
4:B:406:LDA:C3	4:C:405:LDA:C4[3_455]	1.81	0.39
4:B:406:LDA:C2	4:C:405:LDA:C3[3_455]	1.82	0.38
4:B:406:LDA:C1	4:C:405:LDA:C2[3_455]	1.84	0.36
4:B:405:LDA:CM2	4:C:404:LDA:C10[3_455]	1.86	0.34
4:B:405:LDA:C3	4:C:404:LDA:C9[3_455]	1.86	0.34
4:B:406:LDA:O1	4:C:405:LDA:O1[3_455]	1.86	0.34
4:B:406:LDA:CM2	4:C:405:LDA:N1[3_455]	1.90	0.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:406:LDA:N1	4:C:405:LDA:C1[3_455]	1.93	0.27
4:B:406:LDA:C5	4:C:405:LDA:C6[3_455]	1.93	0.27
4:B:405:LDA:C1	4:C:404:LDA:C11[3_455]	1.97	0.23
4:B:405:LDA:N1	4:C:404:LDA:C9[3_455]	2.03	0.17
4:B:406:LDA:O1	4:C:405:LDA:C1[3_455]	2.04	0.16
4:B:405:LDA:C2	4:C:404:LDA:C10[3_455]	2.05	0.15
4:B:406:LDA:C2	4:C:405:LDA:N1[3_455]	2.05	0.15
4:B:406:LDA:C5	4:C:405:LDA:C3[3_455]	2.06	0.14
4:B:406:LDA:C1	4:C:405:LDA:O1[3_455]	2.08	0.12
4:B:406:LDA:O1	4:C:405:LDA:CM1[3_455]	2.10	0.10
4:B:406:LDA:C4	4:C:405:LDA:C2[3_455]	2.11	0.09
4:B:405:LDA:C10	4:C:404:LDA:O1[3_455]	2.12	0.08
4:B:406:LDA:C6	4:C:405:LDA:C4[3_455]	2.12	0.08
4:B:405:LDA:C2	4:C:404:LDA:C7[3_455]	2.15	0.05
4:B:405:LDA:C12	4:C:404:LDA:CM1[3_455]	2.18	0.02
4:B:406:LDA:C3	4:C:405:LDA:C1[3_455]	2.18	0.02

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	318/356 (89%)	295 (93%)	19 (6%)	4 (1%)	9	7
1	B	318/356 (89%)	296 (93%)	20 (6%)	2 (1%)	21	22
1	C	318/356 (89%)	297 (93%)	19 (6%)	2 (1%)	21	22
All	All	954/1068 (89%)	888 (93%)	58 (6%)	8 (1%)	16	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	285	ALA
1	A	330	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	333	VAL
1	B	330	SER
1	B	333	VAL
1	C	267	LYS
1	C	330	SER

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	244/270 (90%)	242 (99%)	2 (1%)	73	84
1	B	244/270 (90%)	241 (99%)	3 (1%)	63	76
1	C	244/270 (90%)	242 (99%)	2 (1%)	73	84
All	All	732/810 (90%)	725 (99%)	7 (1%)	68	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	VAL
1	A	267	LYS
1	B	48	LYS
1	B	269	VAL
1	B	299	GLU
1	C	267	LYS
1	C	269	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	B	34	ASN
1	B	35	GLN
1	B	115	ASN
1	B	292	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	304	ASN
1	C	34	ASN
1	C	70	GLN
1	C	167	ASN
1	C	240	GLN
1	C	292	ASN
1	C	304	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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
4	LDA	B	405	-	13,15,15	2.38	2 (15%)	14,17,17	1.10	2 (14%)
2	C8E	B	401	-	20,20,20	0.39	0	19,19,19	0.41	0
4	LDA	A	405	-	13,15,15	2.38	2 (15%)	14,17,17	0.56	0
2	C8E	C	401	-	20,20,20	0.37	0	19,19,19	0.54	0
4	LDA	C	405	-	13,15,15	2.17	2 (15%)	14,17,17	0.80	0
4	LDA	A	404	-	13,15,15	2.40	2 (15%)	14,17,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	C	406	-	13,15,15	2.41	2 (15%)	14,17,17	0.58	0
4	LDA	C	404	-	13,15,15	2.47	2 (15%)	14,17,17	0.50	0
3	GOL	B	402	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	A	402	-	5,5,5	0.37	0	5,5,5	0.31	0
3	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.35	0
3	GOL	C	402	-	5,5,5	0.38	0	5,5,5	0.34	0
4	LDA	B	404	-	13,15,15	2.44	2 (15%)	14,17,17	0.63	0
4	LDA	B	406	-	13,15,15	2.39	2 (15%)	14,17,17	0.55	0
2	C8E	A	401	-	20,20,20	0.38	0	19,19,19	0.40	0
3	GOL	A	403	-	5,5,5	0.39	0	5,5,5	0.29	0
4	LDA	B	407	-	13,15,15	2.35	2 (15%)	14,17,17	0.64	0
4	LDA	A	406	-	13,15,15	2.43	2 (15%)	14,17,17	0.47	0
3	GOL	C	403	-	5,5,5	0.37	0	5,5,5	0.22	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
4	LDA	B	405	-	-	4/13/13/13	-
2	C8E	B	401	-	-	11/18/18/18	-
4	LDA	A	405	-	-	9/13/13/13	-
2	C8E	C	401	-	-	8/18/18/18	-
4	LDA	C	405	-	-	10/13/13/13	-
4	LDA	A	404	-	-	8/13/13/13	-
4	LDA	C	406	-	-	7/13/13/13	-
4	LDA	C	404	-	-	5/13/13/13	-
3	GOL	B	402	-	-	2/4/4/4	-
3	GOL	A	402	-	-	2/4/4/4	-
3	GOL	B	403	-	-	1/4/4/4	-
3	GOL	C	402	-	-	4/4/4/4	-
4	LDA	B	404	-	-	10/13/13/13	-
4	LDA	B	406	-	-	6/13/13/13	-
2	C8E	A	401	-	-	10/18/18/18	-
3	GOL	A	403	-	-	2/4/4/4	-
4	LDA	B	407	-	-	9/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	A	406	-	-	4/13/13/13	-
3	GOL	C	403	-	-	2/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	404	LDA	O1-N1	-7.73	1.23	1.42
4	B	406	LDA	O1-N1	-7.23	1.24	1.42
4	C	405	LDA	O1-N1	-7.19	1.24	1.42
4	B	405	LDA	O1-N1	-6.95	1.25	1.42
4	A	405	LDA	O1-N1	-6.81	1.25	1.42
4	A	406	LDA	O1-N1	-6.80	1.25	1.42
4	B	404	LDA	O1-N1	-6.79	1.25	1.42
4	C	406	LDA	O1-N1	-6.79	1.25	1.42
4	B	407	LDA	O1-N1	-6.77	1.25	1.42
4	A	404	LDA	O1-N1	-6.76	1.25	1.42
4	B	404	LDA	C1-N1	-5.54	1.45	1.51
4	A	406	LDA	C1-N1	-5.43	1.45	1.51
4	C	406	LDA	C1-N1	-5.36	1.45	1.51
4	A	404	LDA	C1-N1	-5.34	1.46	1.51
4	A	405	LDA	C1-N1	-5.13	1.46	1.51
4	B	405	LDA	C1-N1	-5.04	1.46	1.51
4	B	407	LDA	C1-N1	-5.04	1.46	1.51
4	B	406	LDA	C1-N1	-4.66	1.46	1.51
4	C	404	LDA	C1-N1	-4.42	1.46	1.51
4	C	405	LDA	C1-N1	-3.07	1.48	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	LDA	CM1-N1-C1	-2.59	104.80	110.23
4	B	405	LDA	O1-N1-C1	2.03	114.26	109.27

There are no chirality outliers.

All (114) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-C3
3	B	402	GOL	C1-C2-C3-O3
3	C	402	GOL	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	403	GOL	C1-C2-C3-O3
3	C	403	GOL	O2-C2-C3-O3
4	A	404	LDA	C2-C1-N1-CM1
4	A	404	LDA	N1-C1-C2-C3
4	A	405	LDA	C2-C1-N1-O1
4	A	405	LDA	C2-C1-N1-CM1
4	A	405	LDA	N1-C1-C2-C3
4	B	404	LDA	C2-C1-N1-CM1
4	B	404	LDA	C2-C1-N1-CM2
4	B	404	LDA	N1-C1-C2-C3
4	B	405	LDA	N1-C1-C2-C3
4	B	406	LDA	N1-C1-C2-C3
4	B	407	LDA	C2-C1-N1-O1
4	B	407	LDA	C2-C1-N1-CM1
4	B	407	LDA	C2-C1-N1-CM2
4	B	407	LDA	N1-C1-C2-C3
4	C	405	LDA	C2-C1-N1-CM2
4	C	406	LDA	C2-C1-N1-CM1
4	C	406	LDA	C2-C1-N1-CM2
2	B	401	C8E	O12-C13-C14-O15
2	B	401	C8E	O15-C16-C17-O18
2	A	401	C8E	O12-C13-C14-O15
3	B	403	GOL	C1-C2-C3-O3
3	C	402	GOL	O1-C1-C2-C3
2	A	401	C8E	O18-C19-C20-O21
2	A	401	C8E	C5-C6-C7-C8
2	A	401	C8E	C6-C7-C8-O9
2	C	401	C8E	C5-C6-C7-C8
4	C	406	LDA	C4-C5-C6-C7
4	C	405	LDA	C3-C4-C5-C6
3	A	402	GOL	O1-C1-C2-O2
3	A	403	GOL	O1-C1-C2-O2
3	B	402	GOL	O2-C2-C3-O3
3	C	402	GOL	O1-C1-C2-O2
4	C	405	LDA	C7-C8-C9-C10
4	B	405	LDA	C5-C6-C7-C8
4	B	407	LDA	C5-C6-C7-C8
4	B	407	LDA	C7-C8-C9-C10
4	B	405	LDA	C2-C3-C4-C5
4	B	407	LDA	C2-C3-C4-C5
4	A	406	LDA	C11-C10-C9-C8
4	C	405	LDA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	404	LDA	C4-C5-C6-C7
4	B	404	LDA	C7-C8-C9-C10
4	C	404	LDA	C5-C6-C7-C8
4	C	406	LDA	C1-C2-C3-C4
4	A	405	LDA	C6-C7-C8-C9
2	B	401	C8E	C2-C3-C4-C5
2	C	401	C8E	C4-C5-C6-C7
4	B	404	LDA	C2-C3-C4-C5
4	A	405	LDA	C2-C3-C4-C5
4	C	404	LDA	C2-C3-C4-C5
4	A	406	LDA	C3-C4-C5-C6
4	C	406	LDA	C7-C8-C9-C10
2	C	401	C8E	C2-C3-C4-C5
3	C	402	GOL	O2-C2-C3-O3
4	C	406	LDA	C3-C4-C5-C6
4	A	405	LDA	C1-C2-C3-C4
4	A	404	LDA	C3-C4-C5-C6
4	B	406	LDA	C1-C2-C3-C4
4	B	404	LDA	C6-C7-C8-C9
4	C	405	LDA	C9-C10-C11-C12
2	B	401	C8E	C4-C5-C6-C7
4	B	406	LDA	C2-C3-C4-C5
4	A	406	LDA	C9-C10-C11-C12
4	C	405	LDA	C6-C7-C8-C9
4	A	404	LDA	C4-C5-C6-C7
2	B	401	C8E	C1-C2-C3-C4
4	A	405	LDA	C9-C10-C11-C12
2	C	401	C8E	C1-C2-C3-C4
4	B	407	LDA	C1-C2-C3-C4
4	C	405	LDA	C4-C5-C6-C7
4	C	405	LDA	C1-C2-C3-C4
4	B	405	LDA	C6-C7-C8-C9
2	C	401	C8E	O18-C19-C20-O21
2	B	401	C8E	C10-C11-O12-C13
4	A	406	LDA	C1-C2-C3-C4
4	C	404	LDA	C7-C8-C9-C10
2	C	401	C8E	C3-C4-C5-C6
2	A	401	C8E	C11-C10-O9-C8
4	B	406	LDA	C4-C5-C6-C7
4	C	405	LDA	C11-C10-C9-C8
2	C	401	C8E	C10-C11-O12-C13
2	A	401	C8E	C17-C16-O15-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	404	LDA	C2-C1-N1-CM2
4	C	405	LDA	C2-C1-N1-CM1
4	A	405	LDA	C5-C6-C7-C8
4	B	406	LDA	C5-C6-C7-C8
2	A	401	C8E	C10-C11-O12-C13
4	B	404	LDA	C2-C1-N1-O1
4	C	406	LDA	C2-C1-N1-O1
2	A	401	C8E	C2-C3-C4-C5
4	B	407	LDA	C9-C10-C11-C12
4	A	404	LDA	C2-C3-C4-C5
4	A	404	LDA	C7-C8-C9-C10
2	A	401	C8E	O15-C16-C17-O18
2	B	401	C8E	C20-C19-O18-C17
4	B	404	LDA	C4-C5-C6-C7
4	B	406	LDA	C9-C10-C11-C12
4	C	404	LDA	C6-C7-C8-C9
4	B	404	LDA	C3-C4-C5-C6
2	B	401	C8E	C13-C14-O15-C16
2	B	401	C8E	C17-C16-O15-C14
4	B	404	LDA	C11-C10-C9-C8
2	C	401	C8E	C17-C16-O15-C14
2	A	401	C8E	O9-C10-C11-O12
2	B	401	C8E	C16-C17-O18-C19
4	A	405	LDA	C2-C1-N1-CM2
4	A	404	LDA	C2-C1-N1-O1
2	B	401	C8E	C5-C6-C7-C8

There are no ring outliers.

14 monomers are involved in 132 short contacts:

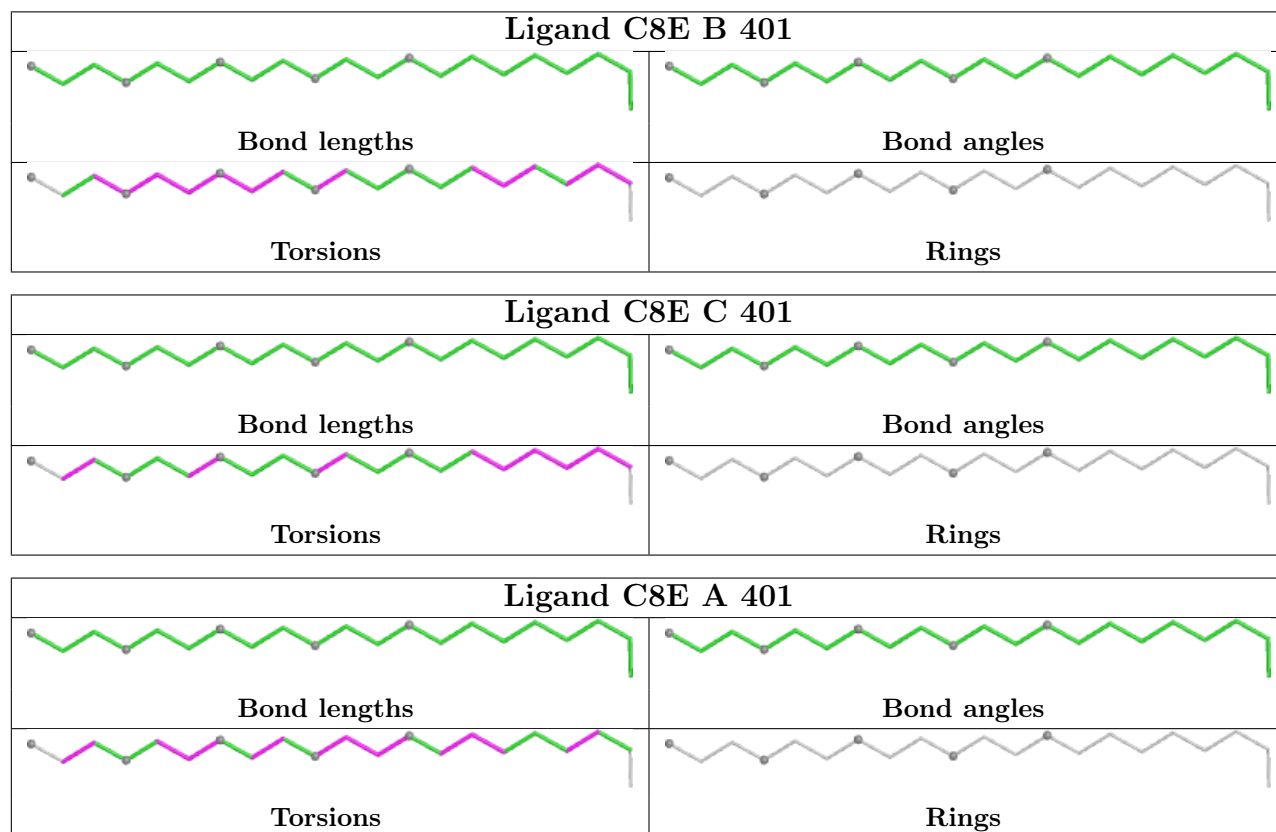
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	405	LDA	2	52
2	B	401	C8E	1	0
4	A	405	LDA	2	0
2	C	401	C8E	5	0
4	C	405	LDA	4	56
4	C	406	LDA	1	0
4	C	404	LDA	3	52
3	B	403	GOL	1	0
4	B	406	LDA	0	56
2	A	401	C8E	1	0
3	A	403	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	407	LDA	1	0
4	A	406	LDA	1	0
3	C	403	GOL	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 ⓘ

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

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	320/356 (89%)	0.49	28 (8%)	15 13	27, 38, 76, 102	0
1	B	320/356 (89%)	0.44	27 (8%)	17 15	25, 37, 75, 136	0
1	C	320/356 (89%)	0.44	26 (8%)	18 15	26, 37, 69, 95	0
All	All	960/1068 (89%)	0.46	81 (8%)	17 15	25, 37, 73, 136	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	TYR	6.7
1	B	126	TYR	6.4
1	C	333	VAL	5.8
1	C	221	TYR	5.6
1	A	126	TYR	5.2
1	A	285	ALA	5.1
1	C	351	HIS	5.1
1	B	333	VAL	4.9
1	A	45	TYR	4.8
1	B	269	VAL	4.8
1	C	45	TYR	4.7
1	A	333	VAL	4.6
1	B	280	TYR	4.5
1	C	44	VAL	4.5
1	B	351	HIS	4.2
1	B	267	LYS	4.2
1	A	351	HIS	4.1
1	B	334	GLY	4.0
1	C	175	PHE	3.9
1	C	42	SER	3.8
1	A	238	ASP	3.8
1	A	47	ALA	3.7
1	C	267	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	3.5
1	A	42	SER	3.4
1	B	226	THR	3.3
1	B	46	SER	3.3
1	A	88	SER	3.3
1	A	44	VAL	3.3
1	A	251	MET	3.2
1	B	284	GLN	3.2
1	A	32	GLY	3.2
1	A	334	GLY	3.2
1	A	203	ASN	3.2
1	A	268	ASP	3.2
1	A	200	THR	3.2
1	B	330	SER	3.1
1	C	46	SER	3.0
1	C	43	THR	3.0
1	A	284	GLN	2.9
1	B	203	ASN	2.9
1	B	268	ASP	2.9
1	B	305	PHE	2.8
1	C	126	TYR	2.7
1	A	329	ASP	2.7
1	B	111	ASN	2.7
1	C	274	TYR	2.7
1	C	177	ASP	2.6
1	B	202	THR	2.6
1	A	267	LYS	2.6
1	A	282	LEU	2.5
1	B	287	PHE	2.5
1	B	42	SER	2.5
1	C	41	GLY	2.5
1	B	87	ASP	2.5
1	C	292	ASN	2.5
1	B	265	LEU	2.4
1	B	239	ASP	2.4
1	C	284	GLN	2.4
1	A	252	GLU	2.4
1	A	46	SER	2.4
1	B	238	ASP	2.4
1	B	47	ALA	2.4
1	C	251	MET	2.4
1	A	280	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	202	THR	2.3
1	B	122	ILE	2.3
1	C	330	SER	2.3
1	A	43	THR	2.3
1	A	202	THR	2.3
1	C	200	THR	2.2
1	C	334	GLY	2.1
1	C	47	ALA	2.1
1	C	285	ALA	2.1
1	A	199	VAL	2.1
1	B	200	THR	2.1
1	A	332	LYS	2.1
1	B	329	ASP	2.1
1	C	268	ASP	2.0
1	C	203	ASN	2.0
1	C	48	LYS	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 oligosaccharides 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(Å ²)	Q<0.9
4	LDA	C	405	16/16	0.69	0.26	122,130,163,163	0
4	LDA	B	406	16/16	0.75	0.27	152,180,196,196	0
4	LDA	A	405	16/16	0.75	0.41	103,114,129,130	0
4	LDA	C	404	16/16	0.77	0.34	142,158,194,194	0
4	LDA	A	404	16/16	0.77	0.32	58,90,132,132	0
4	LDA	A	406	16/16	0.79	0.27	53,72,103,104	0
3	GOL	A	403	6/6	0.79	0.20	60,69,71,74	0

Continued on next page...

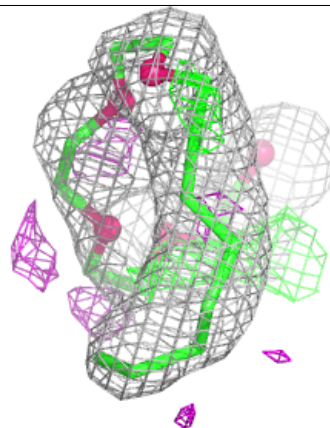
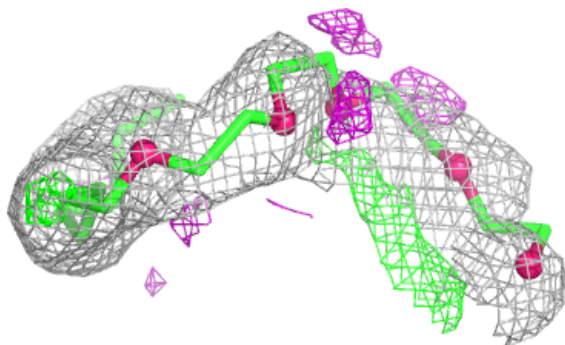
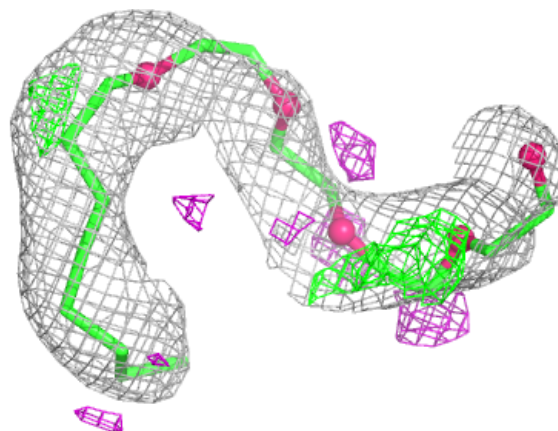
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	LDA	C	406	16/16	0.80	0.31	45,60,96,98	0
2	C8E	C	401	21/21	0.81	0.26	66,91,97,99	0
4	LDA	B	404	16/16	0.82	0.21	49,57,100,102	0
4	LDA	B	405	16/16	0.82	0.32	174,177,187,187	0
3	GOL	C	403	6/6	0.82	0.21	64,67,68,69	0
4	LDA	B	407	16/16	0.84	0.31	66,76,114,116	0
3	GOL	B	403	6/6	0.86	0.22	62,68,72,74	0
2	C8E	B	401	21/21	0.87	0.18	44,53,68,80	0
3	GOL	C	402	6/6	0.88	0.16	58,61,62,62	0
2	C8E	A	401	21/21	0.89	0.17	56,74,82,83	0
3	GOL	B	402	6/6	0.91	0.19	46,51,52,54	0
3	GOL	A	402	6/6	0.93	0.10	47,56,57,57	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.

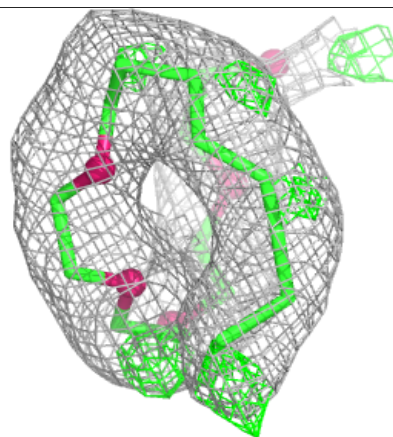
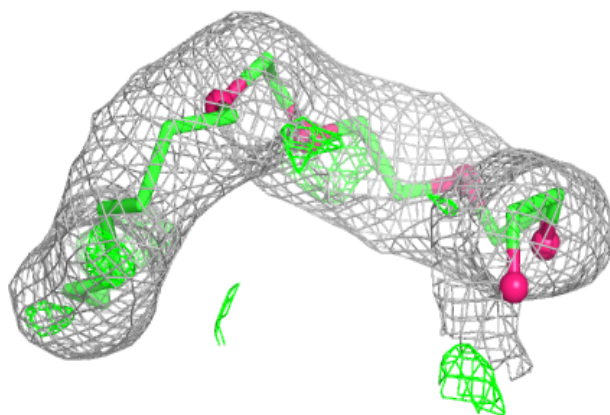
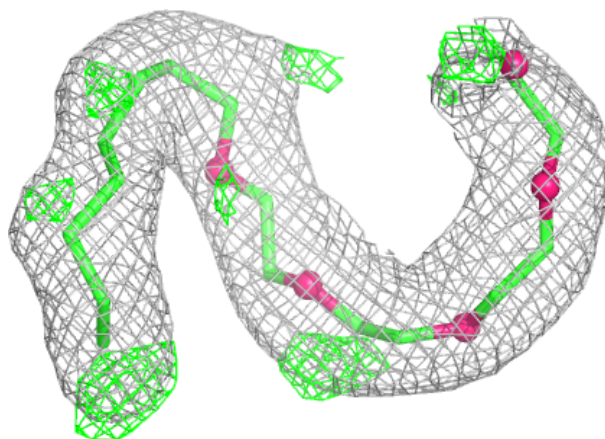
Electron density around C8E C 401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

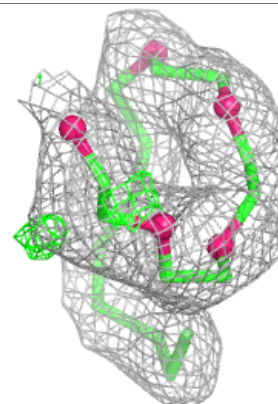
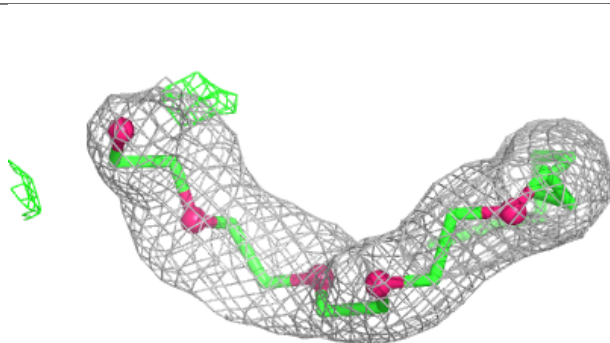
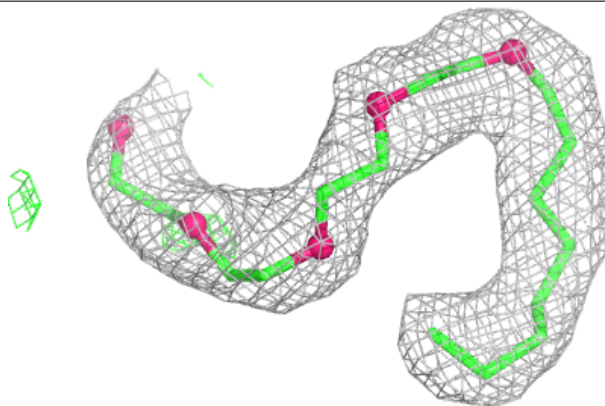


Electron density around C8E B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around C8E A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.