



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:26 am BST

PDB ID : 2F1T
Title : Outer membrane protein OmpW
Authors : van den Berg, B.
Deposited on : 2005-11-15
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
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

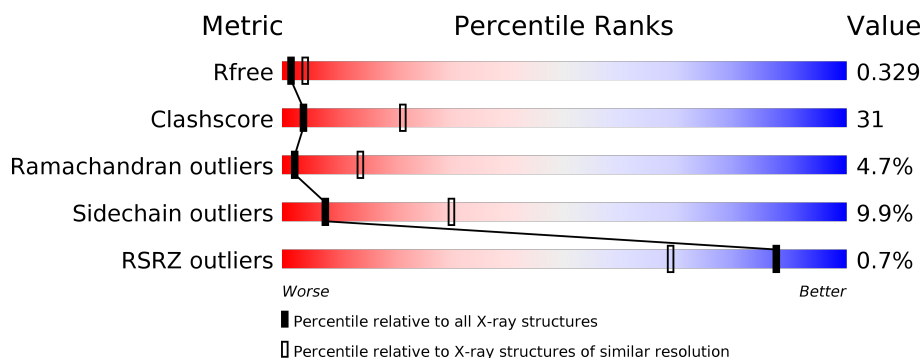
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	197	<div> <div style="width: 45%; background-color: green;"></div> <div style="width: 41%; background-color: yellow;"></div> <div style="width: 6%; background-color: orange;"></div> <div style="width: 7%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	B	197	<div> <div style="width: 47%; background-color: green;"></div> <div style="width: 38%; background-color: yellow;"></div> <div style="width: 8%; background-color: orange;"></div> <div style="width: 7%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div>
1	C	197	<div> <div style="width: 43%; background-color: green;"></div> <div style="width: 42%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 7%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></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
2	LDA	A	301	-	-	-	X
2	LDA	B	302	-	-	-	X
2	LDA	C	303	-	-	-	X
3	C8E	A	402	-	-	-	X
3	C8E	A	403	-	-	-	X
4	GOL	A	200	-	-	X	-
4	GOL	C	202	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4518 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.

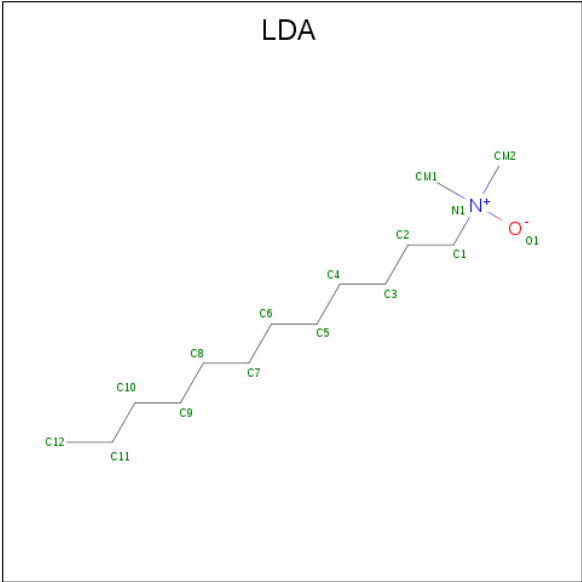
- Molecule 1 is a protein called Outer membrane protein W.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	69	0	0
			1428	912	243	267	6			
1	B	183	Total	C	N	O	S	69	0	0
			1428	912	243	267	6			
1	C	183	Total	C	N	O	S	69	0	0
			1428	912	243	267	6			

There are 18 discrepancies between the modelled and reference sequences:

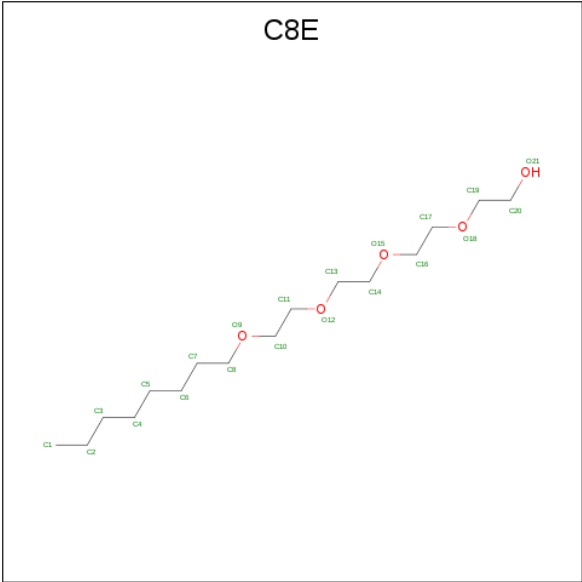
Chain	Residue	Modelled	Actual	Comment	Reference
A	192	HIS	-	EXPRESSION TAG	UNP P0A915
A	193	HIS	-	EXPRESSION TAG	UNP P0A915
A	194	HIS	-	EXPRESSION TAG	UNP P0A915
A	195	HIS	-	EXPRESSION TAG	UNP P0A915
A	196	HIS	-	EXPRESSION TAG	UNP P0A915
A	197	HIS	-	EXPRESSION TAG	UNP P0A915
B	192	HIS	-	EXPRESSION TAG	UNP P0A915
B	193	HIS	-	EXPRESSION TAG	UNP P0A915
B	194	HIS	-	EXPRESSION TAG	UNP P0A915
B	195	HIS	-	EXPRESSION TAG	UNP P0A915
B	196	HIS	-	EXPRESSION TAG	UNP P0A915
B	197	HIS	-	EXPRESSION TAG	UNP P0A915
C	192	HIS	-	EXPRESSION TAG	UNP P0A915
C	193	HIS	-	EXPRESSION TAG	UNP P0A915
C	194	HIS	-	EXPRESSION TAG	UNP P0A915
C	195	HIS	-	EXPRESSION TAG	UNP P0A915
C	196	HIS	-	EXPRESSION TAG	UNP P0A915
C	197	HIS	-	EXPRESSION TAG	UNP P0A915

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



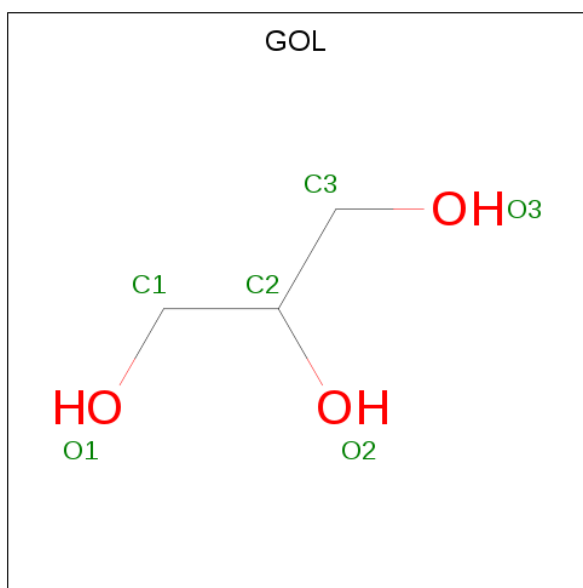
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

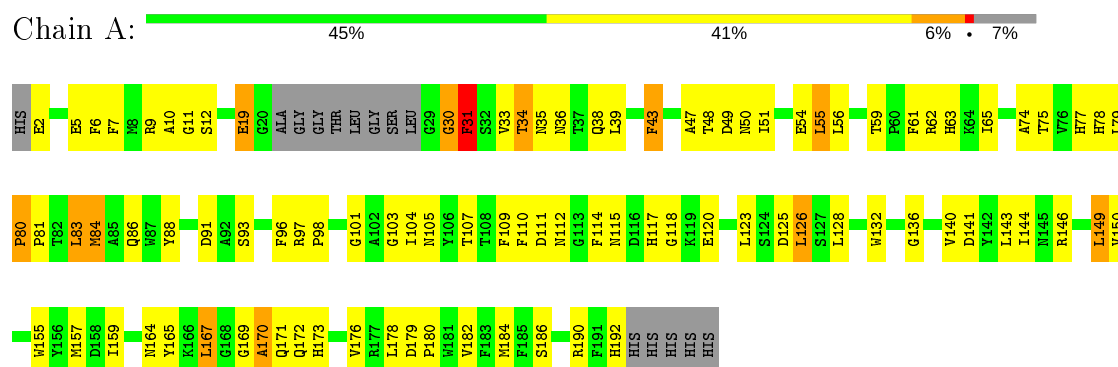


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

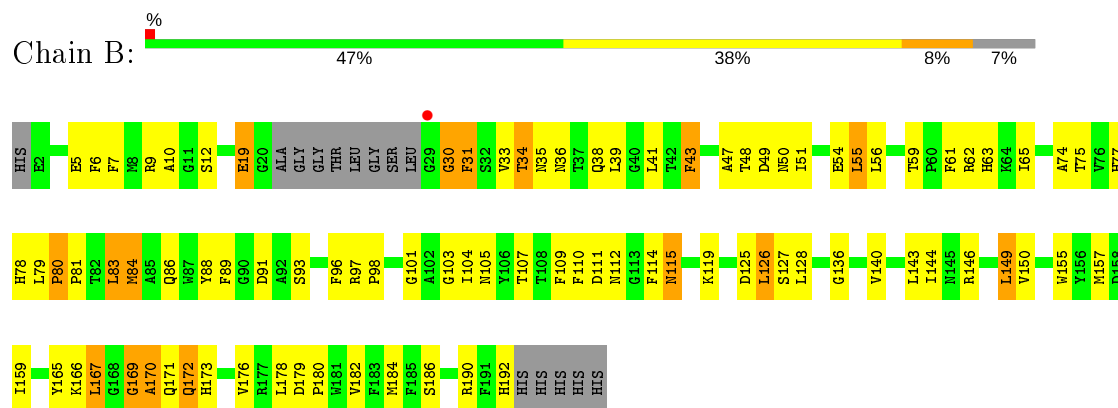
3 Residue-property plots [i](#)

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

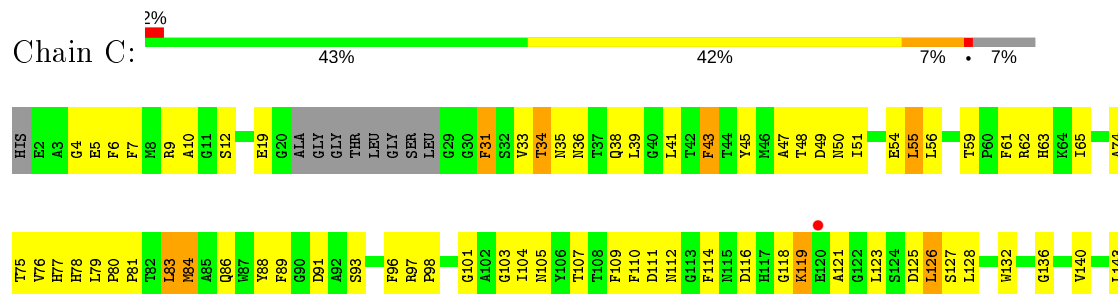
• Molecule 1: Outer membrane protein W



• Molecule 1: Outer membrane protein W



• Molecule 1: Outer membrane protein W





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.16 Å 82.16 Å 186.23 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00 46.78 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.7 (8.00-3.00) 98.2 (46.78-2.44)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.45 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.274 , 0.329 0.274 , 0.329	Depositor DCC
R_{free} test set	733 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.697	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 77.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4518	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.91 % 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 1.4306e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: 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	0.48	0/1469	0.79	1/1995 (0.1%)
1	B	0.43	0/1469	0.73	0/1995
1	C	0.42	0/1469	0.77	1/1995 (0.1%)
All	All	0.44	0/4407	0.76	2/5985 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	174	ASP	N-CA-C	5.57	126.04	111.00
1	A	126	LEU	CA-CB-CG	5.46	127.87	115.30

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	1428	0	1338	83	0
1	B	1428	0	1338	86	0
1	C	1428	0	1338	91	0
2	A	16	0	31	4	0
2	B	16	0	31	1	0
2	C	16	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	105	0	170	3	0
3	B	42	0	68	2	0
3	C	21	0	34	0	0
4	A	6	0	8	5	0
4	B	6	0	8	3	0
4	C	6	0	8	1	0
All	All	4518	0	4403	259	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 31.

All (259) 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:165:TYR:O	1:A:172:GLN:HB3	1.52	1.09
1:C:175:SER:O	1:C:176:VAL:HG23	1.54	1.05
1:C:62:ARG:HE	1:C:77:HIS:HE1	1.08	0.96
1:A:62:ARG:HE	1:A:77:HIS:HE1	1.09	0.95
1:B:62:ARG:HE	1:B:77:HIS:HE1	1.09	0.95
1:B:165:TYR:O	1:B:172:GLN:HB3	1.69	0.92
1:C:165:TYR:O	1:C:172:GLN:HG2	1.71	0.91
1:C:62:ARG:HE	1:C:77:HIS:CE1	1.90	0.90
1:C:105:ASN:HD22	1:C:157:MET:HE3	1.35	0.90
1:A:62:ARG:HE	1:A:77:HIS:CE1	1.90	0.90
1:B:62:ARG:HE	1:B:77:HIS:CE1	1.90	0.89
1:B:105:ASN:HD22	1:B:157:MET:HE3	1.38	0.88
1:B:7:PHE:CE2	4:B:201:GOL:H31	2.10	0.87
1:A:7:PHE:CE2	4:A:200:GOL:H12	2.14	0.82
1:A:105:ASN:HD22	1:A:157:MET:HE3	1.45	0.81
1:C:170:ALA:O	1:C:172:GLN:HG3	1.82	0.79
1:A:54:GLU:HB2	1:A:86:GLN:NE2	1.98	0.79
1:C:173:HIS:O	1:C:174:ASP:HB2	1.83	0.78
1:C:54:GLU:HB2	1:C:86:GLN:NE2	1.97	0.78
1:C:62:ARG:NE	1:C:77:HIS:HE1	1.82	0.78
1:B:54:GLU:HB2	1:B:86:GLN:NE2	1.98	0.78
1:B:62:ARG:NE	1:B:77:HIS:HE1	1.83	0.76
1:B:112:ASN:HB3	1:B:126:LEU:HD13	1.68	0.75
1:A:62:ARG:NE	1:A:77:HIS:HE1	1.82	0.74
1:A:91:ASP:OD2	1:A:93:SER:HB3	1.87	0.74
1:A:155:TRP:HB2	1:A:182:VAL:HB	1.68	0.74
1:B:176:VAL:HG21	2:B:302:LDA:H122	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:CZ	4:A:200:GOL:H32	2.23	0.73
1:C:155:TRP:HB2	1:C:182:VAL:HB	1.71	0.73
1:C:91:ASP:OD2	1:C:93:SER:HB3	1.89	0.73
1:C:10:ALA:O	1:C:186:SER:HB2	1.89	0.72
1:B:155:TRP:HB2	1:B:182:VAL:HB	1.69	0.72
1:B:91:ASP:OD2	1:B:93:SER:HB3	1.89	0.72
1:C:149:LEU:HD22	1:C:149:LEU:O	1.90	0.70
1:B:149:LEU:HD22	1:B:149:LEU:O	1.93	0.69
1:B:10:ALA:O	1:B:186:SER:HB2	1.93	0.69
1:A:125:ASP:O	1:A:165:TYR:HA	1.93	0.69
1:B:19:GLU:OE2	1:B:19:GLU:N	2.24	0.68
1:C:105:ASN:HD22	1:C:157:MET:CE	2.07	0.68
1:A:10:ALA:O	1:A:186:SER:HB2	1.94	0.68
1:A:48:THR:O	1:A:50:ASN:N	2.26	0.67
1:C:7:PHE:CZ	4:C:202:GOL:H11	2.30	0.66
1:A:105:ASN:HD22	1:A:157:MET:CE	2.10	0.65
1:B:48:THR:O	1:B:50:ASN:N	2.28	0.65
1:C:48:THR:O	1:C:50:ASN:N	2.29	0.65
1:B:30:GLY:O	1:B:31:PHE:HB3	1.98	0.64
1:B:105:ASN:HD22	1:B:157:MET:CE	2.09	0.63
1:C:5:GLU:OE2	1:C:190:ARG:HD3	1.99	0.63
1:B:165:TYR:O	1:B:172:GLN:CB	2.43	0.63
1:C:31:PHE:HD2	1:C:31:PHE:O	1.82	0.63
1:B:96:PHE:CE1	1:C:89:PHE:HE2	2.18	0.62
1:A:149:LEU:O	1:A:149:LEU:HD22	1.99	0.62
1:C:159:ILE:HD12	1:C:180:PRO:HG3	1.83	0.61
1:B:170:ALA:HB1	1:B:172:GLN:NE2	2.15	0.61
1:A:5:GLU:OE2	1:A:190:ARG:HD3	2.01	0.60
1:C:126:LEU:HD23	1:C:127:SER:H	1.65	0.60
1:B:7:PHE:CZ	4:B:201:GOL:H11	2.36	0.60
1:B:5:GLU:OE2	1:B:190:ARG:HD3	2.01	0.60
1:B:178:LEU:O	1:B:179:ASP:C	2.40	0.59
1:C:178:LEU:O	1:C:179:ASP:C	2.40	0.59
1:C:165:TYR:O	1:C:166:LYS:HG3	2.03	0.59
1:A:38:GLN:HE21	1:A:59:THR:HB	1.67	0.59
1:B:96:PHE:CZ	1:C:89:PHE:HE2	2.20	0.59
1:A:170:ALA:O	1:A:172:GLN:HG2	2.02	0.58
1:A:65:ILE:HG13	2:A:301:LDA:H102	1.86	0.58
1:A:112:ASN:HB3	1:A:126:LEU:CD1	2.33	0.58
1:B:159:ILE:HD12	1:B:180:PRO:HG3	1.85	0.58
1:C:77:HIS:HD2	1:C:111:ASP:O	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HG21	2:A:301:LDA:H112	1.86	0.57
1:A:178:LEU:O	1:A:179:ASP:C	2.42	0.57
1:A:141:ASP:OD1	4:A:200:GOL:O3	2.21	0.57
1:A:164:ASN:HD22	1:A:173:HIS:CE1	2.22	0.57
1:C:38:GLN:HE21	1:C:59:THR:HB	1.68	0.57
1:A:159:ILE:HD12	1:A:180:PRO:HG3	1.85	0.57
1:B:115:ASN:O	1:B:119:LYS:HG3	2.05	0.57
1:A:74:ALA:HB2	1:A:114:PHE:CD2	2.40	0.57
1:C:170:ALA:O	1:C:171:GLN:C	2.41	0.57
1:A:164:ASN:HA	1:A:172:GLN:O	2.04	0.56
1:A:77:HIS:HD2	1:A:111:ASP:O	1.88	0.56
1:B:36:ASN:ND2	1:B:62:ARG:H	2.03	0.56
1:C:61:PHE:O	1:C:77:HIS:HA	2.05	0.56
1:A:19:GLU:CD	1:A:19:GLU:H	2.09	0.56
1:B:38:GLN:HE21	1:B:59:THR:HB	1.69	0.56
1:B:170:ALA:O	1:B:172:GLN:N	2.36	0.56
1:C:33:VAL:HG22	1:C:65:ILE:HD12	1.87	0.56
1:A:61:PHE:O	1:A:77:HIS:HA	2.06	0.56
1:B:170:ALA:HB1	1:B:172:GLN:HE22	1.71	0.56
1:A:88:TYR:O	1:A:97:ARG:NH2	2.38	0.55
1:A:33:VAL:HG22	1:A:65:ILE:HD12	1.89	0.55
1:B:33:VAL:HG22	1:B:65:ILE:HD12	1.88	0.55
1:B:89:PHE:HD2	3:B:408:C8E:H101	1.71	0.55
1:C:170:ALA:O	1:C:172:GLN:CG	2.51	0.55
1:A:55:LEU:HD22	1:A:56:LEU:N	2.21	0.55
1:B:61:PHE:O	1:B:77:HIS:HA	2.06	0.55
1:C:149:LEU:HD22	1:C:149:LEU:C	2.26	0.55
1:B:77:HIS:HD2	1:B:111:ASP:O	1.88	0.55
1:C:36:ASN:ND2	1:C:62:ARG:H	2.05	0.55
1:C:76:VAL:HG21	2:C:303:LDA:H101	1.89	0.54
1:B:74:ALA:HA	1:B:114:PHE:HA	1.88	0.54
1:B:79:LEU:O	1:B:81:PRO:HD2	2.07	0.54
1:C:96:PHE:O	1:C:98:PRO:HD3	2.08	0.54
1:B:34:THR:HG23	1:B:35:ASN:O	2.06	0.54
1:B:88:TYR:O	1:B:97:ARG:NH2	2.38	0.54
1:C:34:THR:HG23	1:C:35:ASN:O	2.08	0.54
1:C:55:LEU:HD22	1:C:56:LEU:N	2.23	0.54
1:C:5:GLU:HG2	1:C:6:PHE:N	2.23	0.54
1:B:5:GLU:HG2	1:B:6:PHE:N	2.23	0.54
1:B:105:ASN:ND2	1:B:157:MET:HE3	2.17	0.54
1:A:43:PHE:CD1	1:A:43:PHE:N	2.76	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HG23	1:A:35:ASN:O	2.08	0.53
1:B:43:PHE:CD1	1:B:43:PHE:N	2.76	0.53
1:C:79:LEU:O	1:C:81:PRO:HD2	2.09	0.53
1:A:96:PHE:O	1:A:98:PRO:HD3	2.09	0.53
1:B:149:LEU:HD22	1:B:149:LEU:C	2.29	0.53
1:C:105:ASN:ND2	1:C:157:MET:HE3	2.14	0.53
1:A:79:LEU:O	1:A:81:PRO:HD2	2.09	0.53
1:A:36:ASN:ND2	1:A:62:ARG:H	2.06	0.52
1:C:43:PHE:N	1:C:43:PHE:CD1	2.77	0.52
1:A:109:PHE:O	1:A:110:PHE:HB3	2.09	0.52
1:B:7:PHE:CE2	4:B:201:GOL:C3	2.90	0.52
1:C:74:ALA:HA	1:C:114:PHE:HA	1.91	0.52
1:A:30:GLY:O	1:A:31:PHE:HB3	2.10	0.52
1:C:83:LEU:C	1:C:84:MET:HG2	2.30	0.52
1:A:5:GLU:HG2	1:A:6:PHE:N	2.24	0.52
1:B:83:LEU:C	1:B:84:MET:HG2	2.30	0.52
1:C:65:ILE:HG13	2:C:303:LDA:H102	1.92	0.52
1:B:74:ALA:HB2	1:B:114:PHE:CD2	2.46	0.51
1:C:88:TYR:O	1:C:97:ARG:NH2	2.40	0.51
1:A:2:GLU:OE1	4:A:200:GOL:O1	2.21	0.51
1:B:167:LEU:C	1:B:169:GLY:H	2.12	0.51
1:B:55:LEU:HD22	1:B:56:LEU:N	2.26	0.51
1:C:118:GLY:O	1:C:121:ALA:HB3	2.09	0.51
1:B:96:PHE:O	1:B:98:PRO:HD3	2.10	0.51
1:C:173:HIS:O	1:C:174:ASP:CB	2.54	0.50
1:A:118:GLY:O	1:A:123:LEU:HD23	2.11	0.50
1:A:123:LEU:HD11	2:A:301:LDA:H11	1.91	0.50
1:C:126:LEU:CD2	1:C:127:SER:H	2.25	0.50
3:A:402:C8E:H191	3:A:402:C8E:H141	1.94	0.50
1:B:105:ASN:ND2	1:B:157:MET:CE	2.74	0.50
1:B:109:PHE:O	1:B:110:PHE:HB3	2.12	0.50
1:C:109:PHE:O	1:C:110:PHE:HB3	2.12	0.50
1:C:62:ARG:NE	1:C:77:HIS:CE1	2.67	0.50
1:B:127:SER:C	1:B:128:LEU:HD12	2.31	0.50
1:A:165:TYR:O	1:A:172:GLN:CB	2.43	0.50
1:C:116:ASP:O	1:C:119:LYS:HG2	2.11	0.49
1:C:174:ASP:O	1:C:175:SER:O	2.29	0.49
1:C:65:ILE:HG13	2:C:303:LDA:H82	1.93	0.49
1:A:83:LEU:C	1:A:84:MET:HG2	2.32	0.49
1:B:165:TYR:O	1:B:172:GLN:CA	2.61	0.49
1:A:112:ASN:HB3	1:A:126:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PHE:CE1	1:A:126:LEU:HB2	2.47	0.49
1:B:165:TYR:N	1:B:172:GLN:HB2	2.28	0.49
1:A:7:PHE:CD2	4:A:200:GOL:H12	2.47	0.49
1:C:31:PHE:CZ	1:C:176:VAL:HG22	2.48	0.49
1:A:105:ASN:ND2	1:A:157:MET:CE	2.75	0.48
1:A:79:LEU:O	1:A:107:THR:HA	2.14	0.48
1:B:79:LEU:O	1:B:107:THR:HA	2.13	0.48
1:C:83:LEU:O	1:C:84:MET:HG2	2.13	0.48
1:A:7:PHE:HE1	1:A:9:ARG:NH2	2.10	0.48
1:A:74:ALA:HA	1:A:114:PHE:HA	1.95	0.48
1:A:11:GLY:HA2	3:A:401:C8E:H192	1.95	0.48
1:A:167:LEU:HD22	1:A:167:LEU:C	2.34	0.48
1:B:7:PHE:HE1	1:B:9:ARG:NH2	2.12	0.48
1:C:118:GLY:O	1:C:121:ALA:N	2.43	0.48
1:A:149:LEU:C	1:A:149:LEU:HD22	2.33	0.48
1:C:56:LEU:HB2	1:C:155:TRP:CH2	2.49	0.48
1:B:172:GLN:O	1:B:173:HIS:CG	2.67	0.47
1:C:105:ASN:ND2	1:C:157:MET:CE	2.73	0.47
1:B:83:LEU:O	1:B:84:MET:HG2	2.14	0.47
1:C:112:ASN:HB3	1:C:126:LEU:HD13	1.95	0.47
1:C:149:LEU:C	1:C:149:LEU:CD2	2.83	0.47
1:C:79:LEU:O	1:C:107:THR:HA	2.14	0.47
1:A:164:ASN:ND2	1:A:173:HIS:CE1	2.82	0.47
1:A:56:LEU:HB2	1:A:155:TRP:CH2	2.50	0.47
1:B:165:TYR:H	1:B:172:GLN:HA	1.80	0.47
1:C:7:PHE:HE1	1:C:9:ARG:NH2	2.13	0.47
1:B:51:ILE:HA	1:B:86:GLN:O	2.14	0.46
1:A:51:ILE:HA	1:A:86:GLN:O	2.14	0.46
1:B:56:LEU:HB2	1:B:155:TRP:CH2	2.50	0.46
1:C:31:PHE:C	1:C:31:PHE:CD2	2.89	0.46
1:A:83:LEU:O	1:A:84:MET:HG2	2.15	0.46
1:A:38:GLN:NE2	1:A:59:THR:HB	2.31	0.46
1:A:146:ARG:O	1:A:192:HIS:HE1	1.99	0.46
1:C:51:ILE:HA	1:C:86:GLN:O	2.16	0.46
1:C:109:PHE:CD2	1:C:128:LEU:HD22	2.51	0.46
1:B:109:PHE:CD2	1:B:128:LEU:HD22	2.51	0.45
1:B:63:HIS:NE2	1:B:78:HIS:HE1	2.14	0.45
1:B:146:ARG:O	1:B:192:HIS:HE1	2.00	0.45
1:B:149:LEU:C	1:B:149:LEU:CD2	2.85	0.45
1:C:146:ARG:O	1:C:192:HIS:HE1	1.99	0.45
1:B:125:ASP:OD2	1:B:166:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:NE2	1:A:78:HIS:HE1	2.15	0.45
1:C:38:GLN:NE2	1:C:59:THR:HB	2.31	0.45
1:A:123:LEU:N	1:A:123:LEU:HD22	2.32	0.45
1:C:47:ALA:N	1:C:51:ILE:O	2.49	0.44
1:C:63:HIS:NE2	1:C:78:HIS:HE1	2.15	0.44
1:A:48:THR:C	1:A:50:ASN:H	2.20	0.44
1:C:125:ASP:O	1:C:165:TYR:HA	2.18	0.44
1:C:144:ILE:HD11	1:C:150:VAL:HG23	1.99	0.44
1:B:167:LEU:C	1:B:169:GLY:N	2.70	0.44
1:B:38:GLN:NE2	1:B:59:THR:HB	2.31	0.44
1:C:9:ARG:NH1	1:C:54:GLU:OE2	2.45	0.44
1:A:109:PHE:CD2	1:A:128:LEU:HD22	2.53	0.44
1:B:165:TYR:N	1:B:172:GLN:CB	2.81	0.44
1:B:47:ALA:N	1:B:51:ILE:O	2.50	0.44
1:C:12:SER:O	1:C:184:MET:HG3	2.17	0.44
1:A:56:LEU:O	1:A:81:PRO:HA	2.17	0.43
1:B:165:TYR:H	1:B:172:GLN:CB	2.31	0.43
1:C:143:LEU:HD13	1:C:190:ARG:NH2	2.33	0.43
1:C:48:THR:C	1:C:50:ASN:H	2.21	0.43
1:A:62:ARG:NE	1:A:77:HIS:CE1	2.67	0.43
1:A:144:ILE:HD11	1:A:150:VAL:HG23	2.00	0.43
1:B:172:GLN:O	1:B:173:HIS:ND1	2.51	0.43
1:B:62:ARG:NE	1:B:77:HIS:CE1	2.68	0.43
1:A:117:HIS:O	1:A:120:GLU:HB2	2.19	0.43
1:C:116:ASP:HA	1:C:119:LYS:CD	2.48	0.43
1:B:12:SER:O	1:B:184:MET:HG3	2.18	0.43
1:C:83:LEU:O	1:C:103:GLY:HA3	2.19	0.43
1:A:12:SER:O	1:A:184:MET:HG3	2.18	0.43
3:A:401:C8E:O21	3:A:402:C8E:H51	2.19	0.43
1:B:143:LEU:HD13	1:B:190:ARG:NH2	2.34	0.43
1:A:128:LEU:HD21	2:A:301:LDA:H122	2.00	0.43
1:A:47:ALA:N	1:A:51:ILE:O	2.51	0.43
1:C:114:PHE:CE2	1:C:123:LEU:HG	2.53	0.43
1:C:65:ILE:CD1	2:C:303:LDA:H102	2.48	0.43
1:A:30:GLY:O	1:A:31:PHE:CB	2.66	0.42
1:B:83:LEU:O	1:B:103:GLY:HA3	2.19	0.42
1:B:41:LEU:HD11	3:B:405:C8E:H31	2.00	0.42
1:B:56:LEU:O	1:B:81:PRO:HA	2.18	0.42
1:C:101:GLY:O	1:C:136:GLY:HA2	2.19	0.42
1:A:83:LEU:O	1:A:103:GLY:HA3	2.20	0.42
1:C:31:PHE:CD2	1:C:31:PHE:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:O	1:C:81:PRO:HA	2.20	0.42
1:A:101:GLY:O	1:A:136:GLY:HA2	2.18	0.42
1:B:143:LEU:HB3	1:B:190:ARG:NH2	2.35	0.42
1:B:48:THR:C	1:B:50:ASN:H	2.20	0.42
1:B:165:TYR:H	1:B:172:GLN:CA	2.32	0.42
1:A:143:LEU:HB3	1:A:190:ARG:NH2	2.35	0.42
1:A:31:PHE:HD2	1:A:31:PHE:C	2.23	0.42
1:B:30:GLY:O	1:B:31:PHE:CB	2.66	0.42
1:C:159:ILE:HD12	1:C:180:PRO:CG	2.49	0.42
1:C:127:SER:C	1:C:128:LEU:HD12	2.39	0.41
1:A:143:LEU:HD13	1:A:190:ARG:NH2	2.35	0.41
1:A:105:ASN:O	1:A:132:TRP:HA	2.21	0.41
1:B:96:PHE:CZ	1:C:89:PHE:CE2	3.06	0.41
1:C:98:PRO:HA	1:C:140:VAL:HA	2.02	0.41
1:A:149:LEU:C	1:A:149:LEU:CD2	2.89	0.41
1:B:101:GLY:O	1:B:136:GLY:HA2	2.21	0.41
1:C:143:LEU:HB3	1:C:190:ARG:NH2	2.36	0.41
1:B:7:PHE:HE1	1:B:9:ARG:CZ	2.34	0.41
1:A:98:PRO:HA	1:A:140:VAL:HA	2.03	0.41
1:B:98:PRO:HA	1:B:140:VAL:HA	2.01	0.41
1:C:116:ASP:HA	1:C:119:LYS:HD3	2.03	0.41
1:C:74:ALA:HB2	1:C:114:PHE:CD2	2.55	0.40
1:C:10:ALA:HA	1:C:41:LEU:HD23	2.03	0.40
1:C:4:GLY:HA2	1:C:45:TYR:OH	2.21	0.40
1:C:105:ASN:O	1:C:132:TRP:HA	2.21	0.40
1:A:144:ILE:HG13	1:A:144:ILE:H	1.76	0.40
1:B:144:ILE:HD11	1:B:150:VAL:HG23	2.02	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	179/197 (91%)	155 (87%)	16 (9%)	8 (4%)	2	14
1	B	179/197 (91%)	158 (88%)	14 (8%)	7 (4%)	3	17
1	C	179/197 (91%)	152 (85%)	17 (10%)	10 (6%)	2	10
All	All	537/591 (91%)	465 (87%)	47 (9%)	25 (5%)	2	14

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	49	ASP
1	A	170	ALA
1	B	19	GLU
1	B	30	GLY
1	B	49	ASP
1	C	19	GLU
1	C	49	ASP
1	C	174	ASP
1	C	175	SER
1	C	176	VAL
1	A	19	GLU
1	A	30	GLY
1	B	115	ASN
1	B	170	ALA
1	C	166	LYS
1	C	167	LEU
1	C	169	GLY
1	A	169	GLY
1	C	171	GLN
1	A	80	PRO
1	A	115	ASN
1	B	80	PRO
1	C	80	PRO
1	B	169	GLY

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	145/155 (94%)	132 (91%)	13 (9%)	9	35
1	B	145/155 (94%)	130 (90%)	15 (10%)	7	28
1	C	145/155 (94%)	130 (90%)	15 (10%)	7	28
All	All	435/465 (94%)	392 (90%)	43 (10%)	8	30

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	PHE
1	A	34	THR
1	A	39	LEU
1	A	43	PHE
1	A	55	LEU
1	A	75	THR
1	A	80	PRO
1	A	83	LEU
1	A	84	MET
1	A	104	ILE
1	A	149	LEU
1	A	167	LEU
1	A	171	GLN
1	B	31	PHE
1	B	34	THR
1	B	39	LEU
1	B	43	PHE
1	B	55	LEU
1	B	75	THR
1	B	80	PRO
1	B	83	LEU
1	B	84	MET
1	B	104	ILE
1	B	126	LEU
1	B	149	LEU
1	B	167	LEU
1	B	171	GLN
1	B	172	GLN
1	C	31	PHE
1	C	34	THR
1	C	39	LEU
1	C	43	PHE
1	C	55	LEU
1	C	75	THR

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Mol	Chain	Res	Type
1	C	83	LEU
1	C	84	MET
1	C	104	ILE
1	C	119	LYS
1	C	126	LEU
1	C	149	LEU
1	C	171	GLN
1	C	172	GLN
1	C	174	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	38	GLN
1	A	77	HIS
1	A	78	HIS
1	A	86	GLN
1	A	105	ASN
1	A	137	GLN
1	A	164	ASN
1	A	171	GLN
1	A	192	HIS
1	B	36	ASN
1	B	38	GLN
1	B	77	HIS
1	B	78	HIS
1	B	86	GLN
1	B	105	ASN
1	B	137	GLN
1	B	171	GLN
1	B	172	GLN
1	B	192	HIS
1	C	36	ASN
1	C	38	GLN
1	C	77	HIS
1	C	78	HIS
1	C	86	GLN
1	C	105	ASN
1	C	137	GLN
1	C	171	GLN
1	C	192	HIS

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 ⓘ

14 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$
3	C8E	A	404	-	20,20,20	0.92	0	19,19,19	2.08	6 (31%)
3	C8E	B	405	-	20,20,20	0.87	0	19,19,19	2.02	6 (31%)
4	GOL	C	202	-	5,5,5	0.86	0	5,5,5	0.57	0
2	LDA	C	303	-	12,15,15	2.02	1 (8%)	14,17,17	1.72	4 (28%)
3	C8E	A	403	-	20,20,20	0.89	0	19,19,19	2.02	6 (31%)
4	GOL	B	201	-	5,5,5	1.47	1 (20%)	5,5,5	0.38	0
3	C8E	A	402	-	20,20,20	0.91	0	19,19,19	2.08	6 (31%)
2	LDA	B	302	-	12,15,15	2.04	1 (8%)	14,17,17	1.70	4 (28%)
3	C8E	A	407	-	20,20,20	0.88	0	19,19,19	2.01	6 (31%)
3	C8E	C	406	-	20,20,20	0.89	0	19,19,19	2.05	6 (31%)
4	GOL	A	200	-	5,5,5	1.61	1 (20%)	5,5,5	0.53	0
2	LDA	A	301	-	12,15,15	2.07	1 (8%)	14,17,17	1.70	4 (28%)
3	C8E	A	401	-	20,20,20	0.80	0	19,19,19	2.05	6 (31%)
3	C8E	B	408	-	20,20,20	0.78	0	19,19,19	1.96	6 (31%)

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
3	C8E	A	404	-	-	7/18/18/18	-
3	C8E	B	405	-	-	9/18/18/18	-
4	GOL	C	202	-	-	0/4/4/4	-
2	LDA	C	303	-	-	5/13/13/13	-
3	C8E	A	403	-	-	8/18/18/18	-
4	GOL	B	201	-	-	0/4/4/4	-
3	C8E	A	402	-	-	11/18/18/18	-
2	LDA	B	302	-	-	2/13/13/13	-
3	C8E	A	407	-	-	11/18/18/18	-
3	C8E	C	406	-	-	10/18/18/18	-
4	GOL	A	200	-	-	0/4/4/4	-
2	LDA	A	301	-	-	5/13/13/13	-
3	C8E	A	401	-	-	14/18/18/18	-
3	C8E	B	408	-	-	5/18/18/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	LDA	O1-N1	-6.99	1.25	1.42
2	B	302	LDA	O1-N1	-6.81	1.26	1.42
2	C	303	LDA	O1-N1	-6.74	1.26	1.42
4	A	200	GOL	C3-C2	-3.26	1.38	1.51
4	B	201	GOL	C3-C2	-3.16	1.38	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	C8E	O15-C14-C13	4.82	132.12	110.39
3	A	401	C8E	O15-C14-C13	4.78	131.96	110.39
3	A	403	C8E	O15-C14-C13	4.77	131.91	110.39
3	A	404	C8E	O15-C14-C13	4.66	131.40	110.39
3	B	405	C8E	O15-C14-C13	4.59	131.09	110.39
3	A	407	C8E	O15-C14-C13	4.58	131.06	110.39
3	C	406	C8E	O15-C14-C13	4.38	130.15	110.39
3	B	408	C8E	O15-C14-C13	4.35	129.99	110.39
2	C	303	LDA	CM1-N1-C1	-4.15	101.52	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	LDA	CM1-N1-C1	-4.04	101.75	110.23
2	A	301	LDA	CM1-N1-C1	-4.02	101.79	110.23
3	C	406	C8E	O12-C13-C14	3.61	126.66	110.39
3	B	405	C8E	O12-C13-C14	3.57	126.50	110.39
3	A	407	C8E	O12-C13-C14	3.55	126.40	110.39
3	A	402	C8E	O12-C13-C14	3.47	126.05	110.39
3	A	404	C8E	O12-C13-C14	3.36	125.56	110.39
3	A	401	C8E	O12-C13-C14	3.33	125.39	110.39
3	A	402	C8E	O9-C8-C7	3.32	127.73	110.26
3	C	406	C8E	O18-C19-C20	3.28	124.49	110.07
3	C	406	C8E	O9-C8-C7	3.28	127.51	110.26
3	A	404	C8E	O9-C8-C7	3.26	127.38	110.26
3	A	407	C8E	O18-C19-C20	3.22	124.21	110.07
3	A	403	C8E	O9-C8-C7	3.21	127.12	110.26
3	A	401	C8E	O9-C8-C7	3.18	126.96	110.26
3	B	408	C8E	O12-C13-C14	3.16	124.66	110.39
3	A	404	C8E	O18-C19-C20	3.14	123.87	110.07
3	A	403	C8E	O18-C19-C20	3.14	123.86	110.07
3	A	402	C8E	O18-C19-C20	3.14	123.86	110.07
3	A	403	C8E	O12-C13-C14	3.12	124.44	110.39
3	B	405	C8E	O9-C8-C7	3.11	126.63	110.26
3	A	407	C8E	O9-C8-C7	3.05	126.27	110.26
3	A	404	C8E	O18-C17-C16	3.04	124.09	110.39
3	A	401	C8E	C7-C6-C5	-3.03	99.05	114.42
3	B	405	C8E	O18-C19-C20	3.02	123.35	110.07
3	B	408	C8E	O9-C8-C7	3.01	126.08	110.26
3	A	401	C8E	O18-C17-C16	2.91	123.50	110.39
3	A	401	C8E	O18-C19-C20	2.91	122.84	110.07
3	C	406	C8E	C7-C6-C5	-2.88	99.81	114.42
3	A	402	C8E	C7-C6-C5	-2.86	99.91	114.42
3	B	408	C8E	O18-C19-C20	2.84	122.55	110.07
3	B	405	C8E	C7-C6-C5	-2.84	100.02	114.42
3	A	403	C8E	C7-C6-C5	-2.83	100.04	114.42
3	A	403	C8E	O18-C17-C16	2.83	123.14	110.39
3	A	404	C8E	C7-C6-C5	-2.81	100.14	114.42
3	B	408	C8E	C7-C6-C5	-2.78	100.30	114.42
3	A	407	C8E	O18-C17-C16	2.76	122.83	110.39
3	B	405	C8E	O18-C17-C16	2.71	122.63	110.39
3	B	408	C8E	O18-C17-C16	2.68	122.49	110.39
3	C	406	C8E	O18-C17-C16	2.66	122.41	110.39
3	A	407	C8E	C7-C6-C5	-2.66	100.94	114.42
3	A	402	C8E	O18-C17-C16	2.65	122.33	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	LDA	O1-N1-C1	2.29	114.88	109.27
2	B	302	LDA	CM2-N1-C1	2.22	114.89	110.23
2	A	301	LDA	C9-C8-C7	-2.20	103.25	114.42
2	B	302	LDA	C9-C8-C7	-2.19	103.29	114.42
2	C	303	LDA	C9-C8-C7	-2.19	103.32	114.42
2	A	301	LDA	C6-C5-C4	-2.13	103.60	114.42
2	B	302	LDA	O1-N1-C1	2.13	114.49	109.27
2	A	301	LDA	O1-N1-C1	2.08	114.38	109.27
2	C	303	LDA	CM2-N1-C1	2.00	114.44	110.23

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	303	LDA	N1-C1-C2-C3
2	B	302	LDA	N1-C1-C2-C3
3	B	405	C8E	O9-C10-C11-O12
3	A	407	C8E	O15-C16-C17-O18
3	A	401	C8E	O12-C13-C14-O15
3	C	406	C8E	O15-C16-C17-O18
3	A	402	C8E	O12-C13-C14-O15
3	B	408	C8E	O12-C13-C14-O15
3	B	405	C8E	O12-C13-C14-O15
3	C	406	C8E	O9-C10-C11-O12
3	A	402	C8E	O15-C16-C17-O18
3	A	403	C8E	O12-C13-C14-O15
3	A	402	C8E	O9-C10-C11-O12
3	B	408	C8E	O15-C16-C17-O18
3	A	403	C8E	O18-C19-C20-O21
3	A	401	C8E	O18-C19-C20-O21
3	A	401	C8E	C4-C5-C6-C7
3	B	405	C8E	C2-C3-C4-C5
2	A	301	LDA	C6-C7-C8-C9
3	A	407	C8E	C2-C3-C4-C5
3	B	405	C8E	C6-C7-C8-O9
3	B	405	C8E	C3-C4-C5-C6
3	A	401	C8E	C2-C3-C4-C5
3	A	402	C8E	C4-C5-C6-C7
3	A	401	C8E	C6-C7-C8-O9
3	A	403	C8E	O15-C16-C17-O18
3	A	402	C8E	C6-C7-C8-O9
2	A	301	LDA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	402	C8E	C5-C6-C7-C8
3	C	406	C8E	C2-C3-C4-C5
3	A	407	C8E	C4-C5-C6-C7
3	A	401	C8E	C3-C4-C5-C6
3	A	407	C8E	C3-C4-C5-C6
3	A	402	C8E	C2-C3-C4-C5
3	C	406	C8E	C5-C6-C7-C8
3	B	405	C8E	C1-C2-C3-C4
3	A	407	C8E	O12-C13-C14-O15
3	A	401	C8E	O9-C10-C11-O12
3	C	406	C8E	C1-C2-C3-C4
3	A	404	C8E	C3-C4-C5-C6
2	C	303	LDA	C1-C2-C3-C4
2	C	303	LDA	C6-C7-C8-C9
2	B	302	LDA	C7-C8-C9-C10
3	C	406	C8E	C4-C5-C6-C7
3	A	401	C8E	C1-C2-C3-C4
3	A	402	C8E	C3-C4-C5-C6
2	C	303	LDA	C3-C4-C5-C6
3	B	405	C8E	C4-C5-C6-C7
3	A	404	C8E	O18-C19-C20-O21
3	C	406	C8E	C10-C11-O12-C13
2	C	303	LDA	C2-C1-N1-CM2
2	A	301	LDA	C2-C1-N1-CM2
3	A	404	C8E	C10-C11-O12-C13
3	A	401	C8E	C20-C19-O18-C17
3	A	404	C8E	C14-C13-O12-C11
3	A	407	C8E	C1-C2-C3-C4
3	A	403	C8E	C10-C11-O12-C13
3	A	402	C8E	C1-C2-C3-C4
3	A	401	C8E	C14-C13-O12-C11
3	A	403	C8E	C20-C19-O18-C17
3	A	401	C8E	C5-C6-C7-C8
3	A	403	C8E	C7-C8-O9-C10
3	A	407	C8E	C7-C8-O9-C10
3	A	402	C8E	C7-C8-O9-C10
3	A	401	C8E	C7-C8-O9-C10
3	A	401	C8E	C10-C11-O12-C13
3	C	406	C8E	C3-C4-C5-C6
3	B	408	C8E	C14-C13-O12-C11
3	A	404	C8E	C7-C8-O9-C10
3	B	405	C8E	C7-C8-O9-C10

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Mol	Chain	Res	Type	Atoms
3	C	406	C8E	C7-C8-O9-C10
3	A	407	C8E	C5-C6-C7-C8
3	A	407	C8E	C20-C19-O18-C17
3	B	408	C8E	C7-C8-O9-C10
2	A	301	LDA	C1-C2-C3-C4
3	A	402	C8E	C10-C11-O12-C13
3	C	406	C8E	C20-C19-O18-C17
3	A	407	C8E	C6-C7-C8-O9
3	B	408	C8E	C4-C5-C6-C7
3	A	404	C8E	O12-C13-C14-O15
3	A	404	C8E	C20-C19-O18-C17
3	B	405	C8E	C14-C13-O12-C11
3	A	403	C8E	O9-C10-C11-O12
2	A	301	LDA	C11-C10-C9-C8
3	A	403	C8E	C1-C2-C3-C4
3	A	401	C8E	O15-C16-C17-O18
3	A	407	C8E	O9-C10-C11-O12

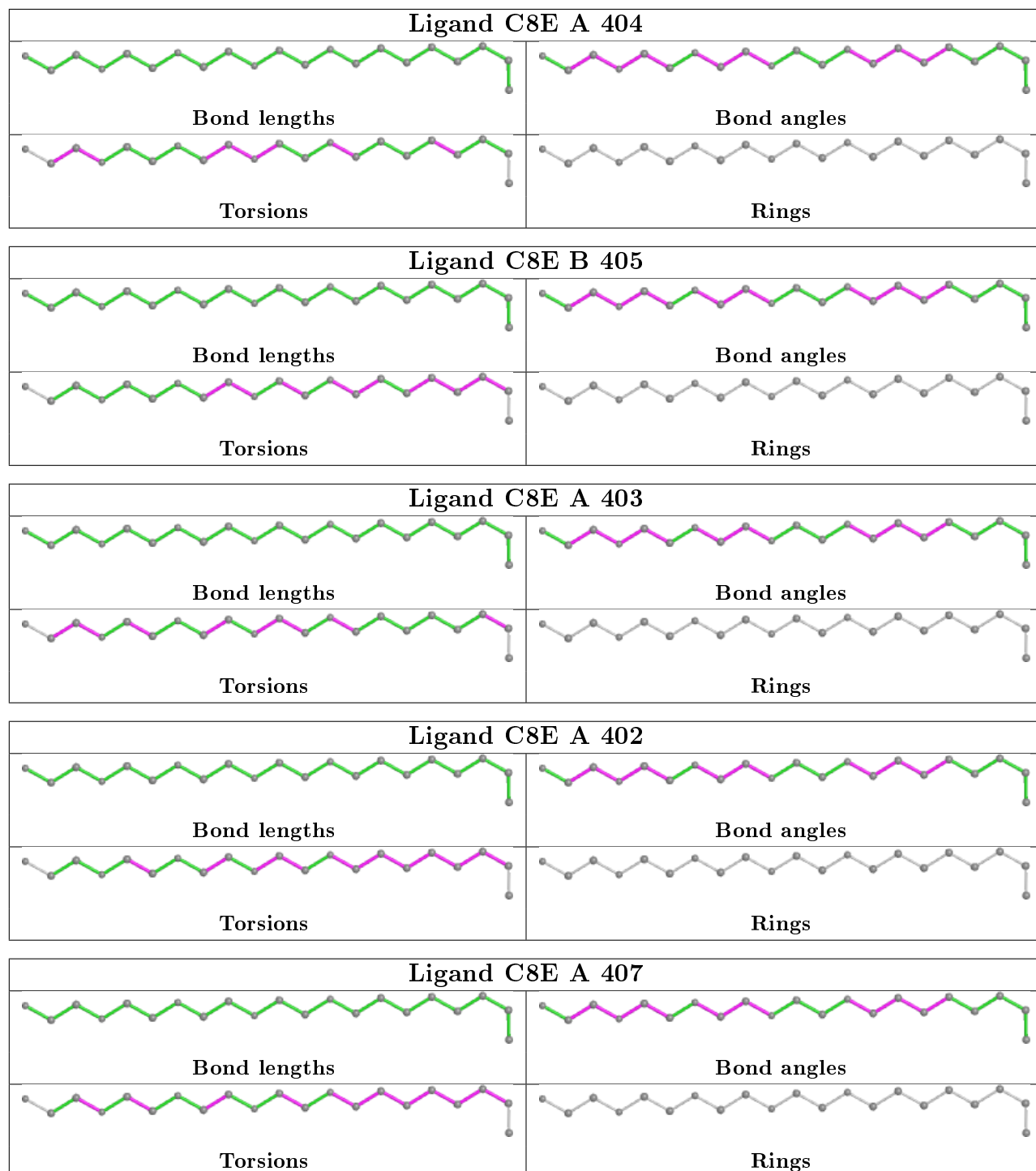
There are no ring outliers.

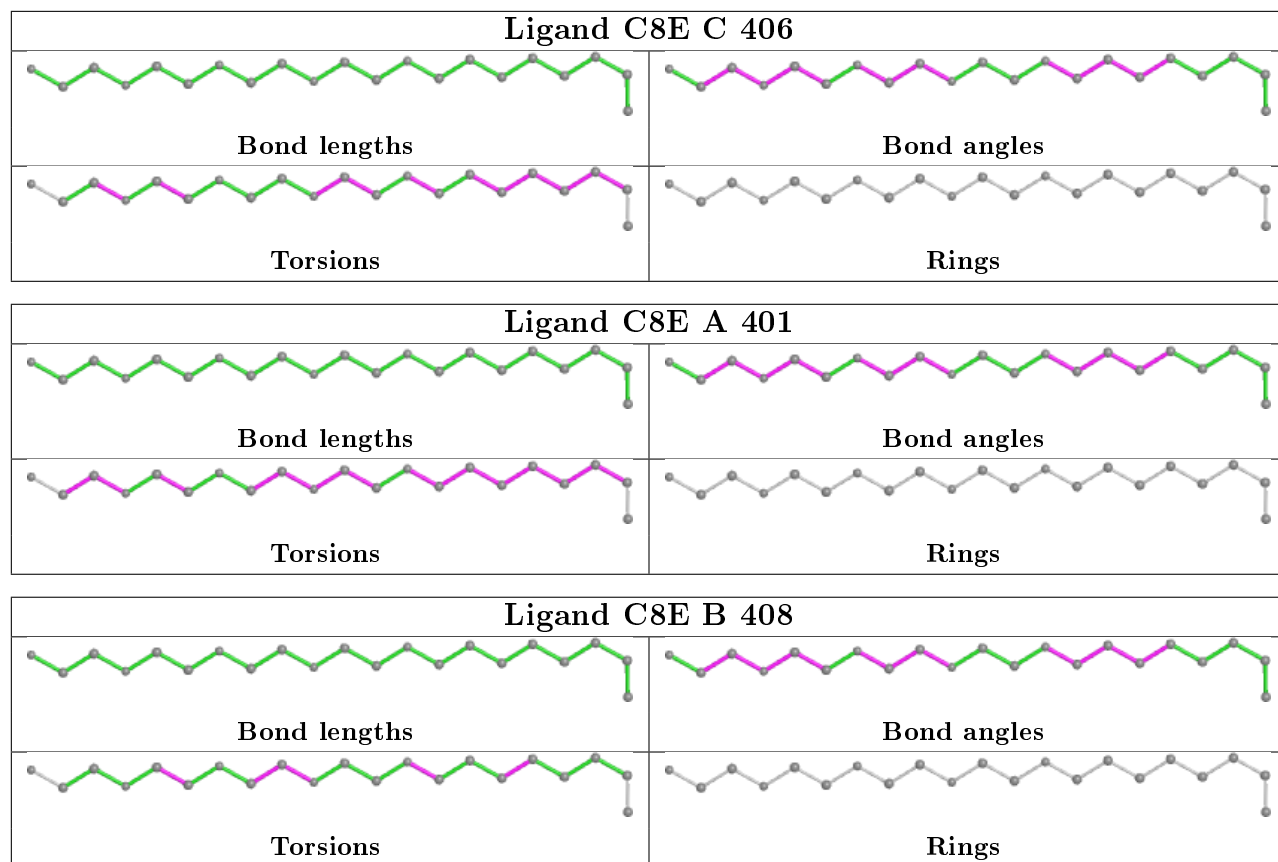
10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	405	C8E	1	0
4	C	202	GOL	1	0
2	C	303	LDA	4	0
4	B	201	GOL	3	0
3	A	402	C8E	2	0
2	B	302	LDA	1	0
4	A	200	GOL	5	0
2	A	301	LDA	4	0
3	A	401	C8E	2	0
3	B	408	C8E	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 [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	183/197 (92%)	-0.62	0 100 100	29, 56, 82, 97	45 (24%)
1	B	183/197 (92%)	-0.57	1 (0%) 91 75	41, 67, 85, 96	45 (24%)
1	C	183/197 (92%)	-0.39	3 (1%) 72 44	45, 80, 117, 128	45 (24%)
All	All	549/591 (92%)	-0.53	4 (0%) 87 69	29, 67, 99, 128	135 (24%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	GLY	5.6
1	C	159	ILE	3.6
1	C	173	HIS	2.1
1	C	120	GLU	2.1

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](#)

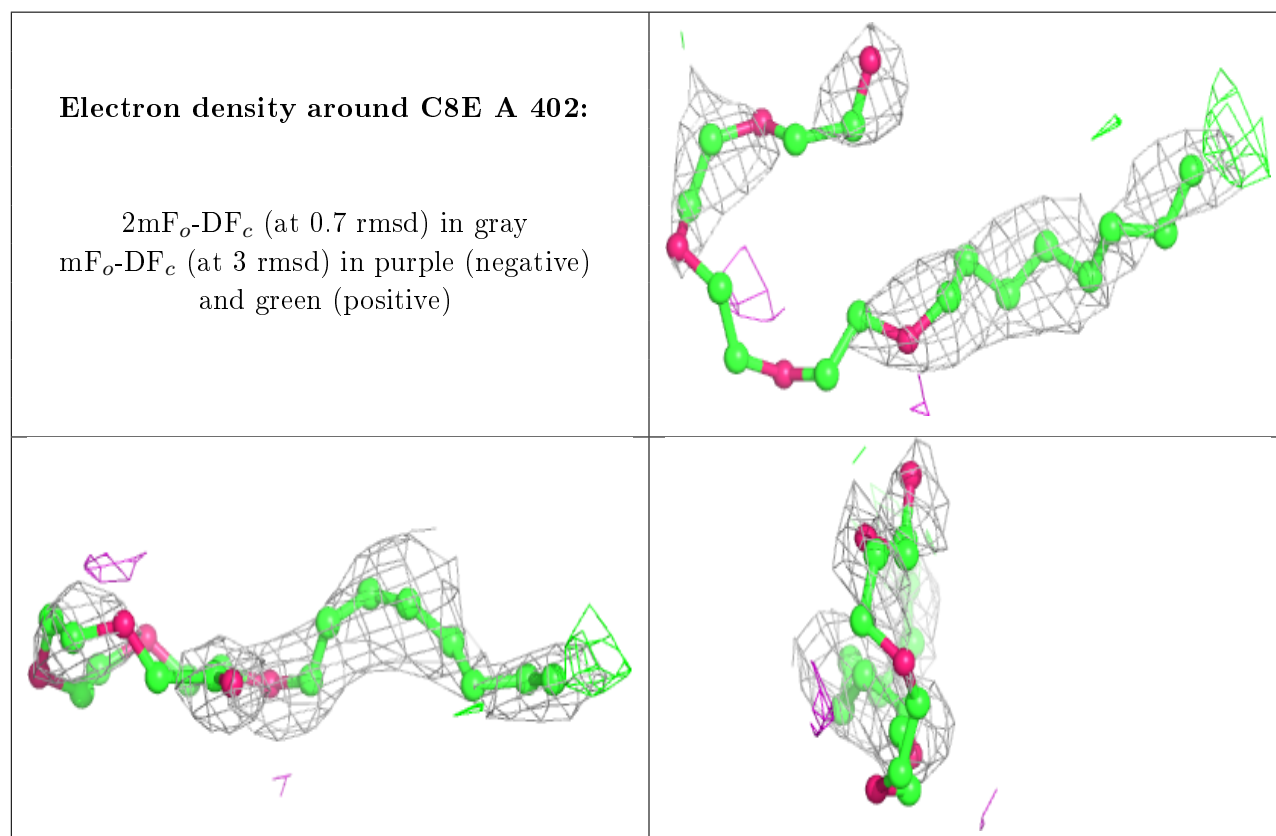
There are no carbohydrates in this entry.

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.

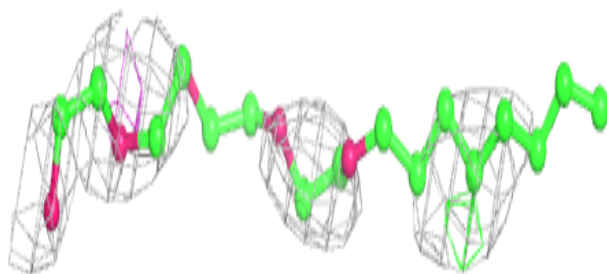
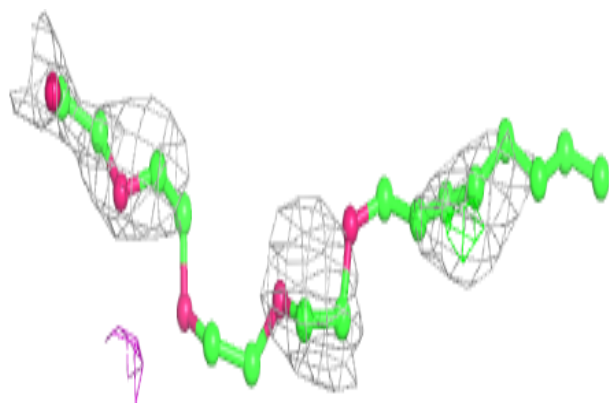
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LDA	C	303	16/16	0.28	1.36	134,142,147,150	0
3	C8E	A	402	21/21	0.47	0.46	64,85,102,104	0
3	C8E	A	404	21/21	0.58	0.34	83,106,128,136	0
4	GOL	B	201	6/6	0.60	0.32	63,64,65,65	0
3	C8E	B	408	21/21	0.60	0.31	76,85,98,102	0
4	GOL	C	202	6/6	0.64	0.61	61,62,64,65	0
3	C8E	A	407	21/21	0.65	0.36	90,100,108,109	0
3	C8E	B	405	21/21	0.66	0.28	66,80,88,94	0
3	C8E	A	401	21/21	0.70	0.32	44,69,86,98	0
3	C8E	A	403	21/21	0.71	0.41	76,85,98,102	0
2	LDA	B	302	16/16	0.77	0.54	72,89,123,124	0
2	LDA	A	301	16/16	0.78	0.45	56,77,98,104	0
3	C8E	C	406	21/21	0.79	0.32	58,81,92,97	0
4	GOL	A	200	6/6	0.88	0.17	54,56,58,59	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.



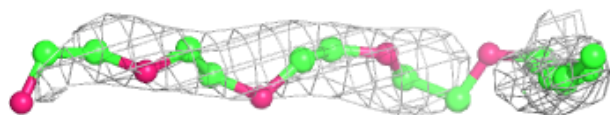
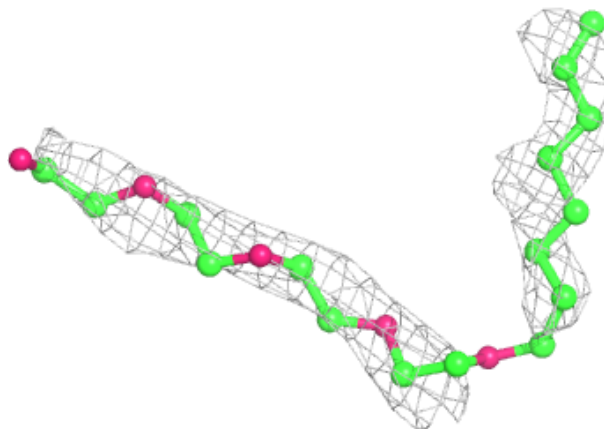
Electron density around C8E A 404:

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



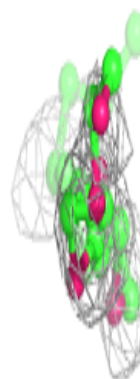
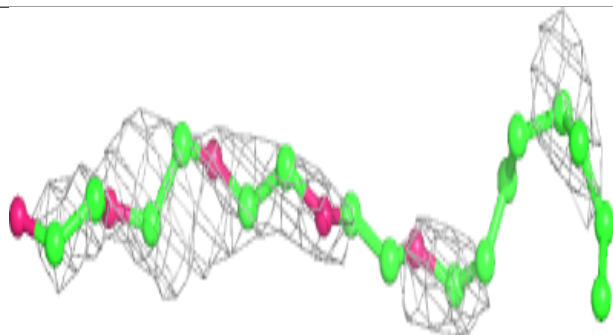
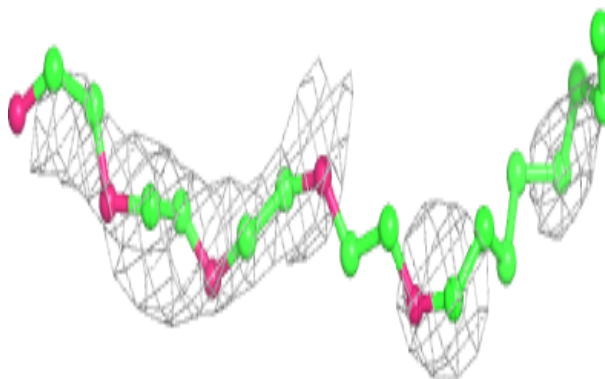
Electron density around C8E B 408:

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

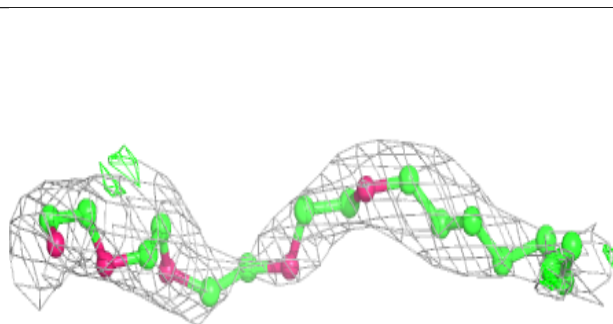
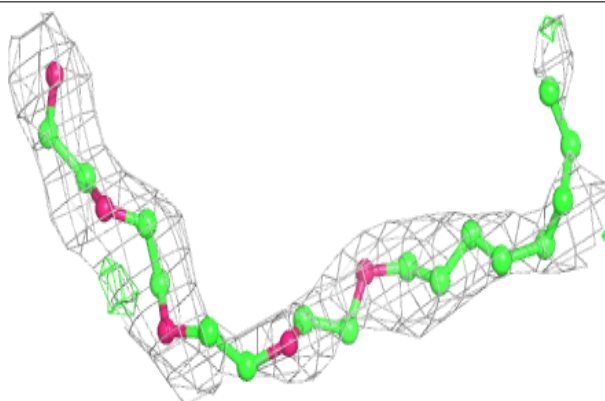


Electron density around C8E A 407:

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

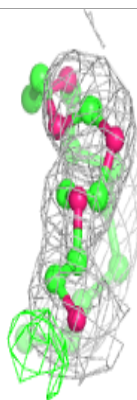
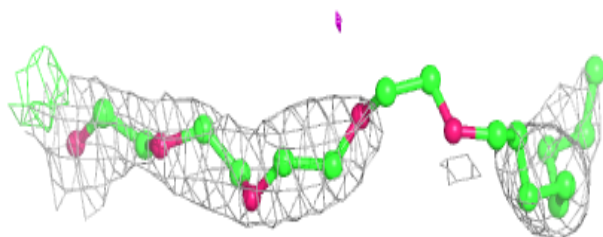
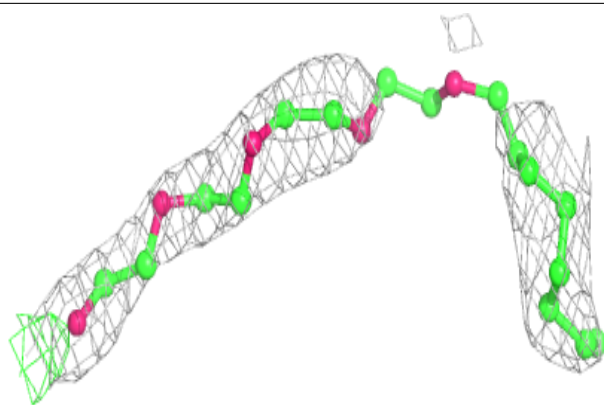
**Electron density around C8E B 405:**

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

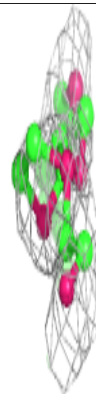
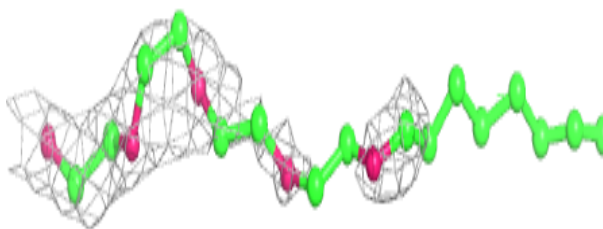
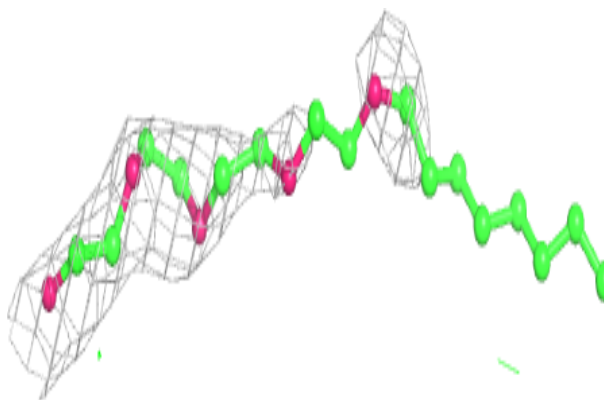


Electron density around C8E A 401:

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

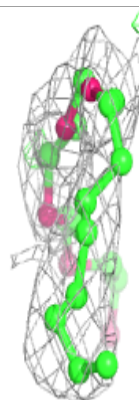
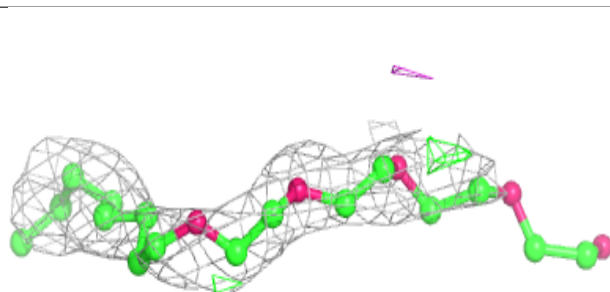
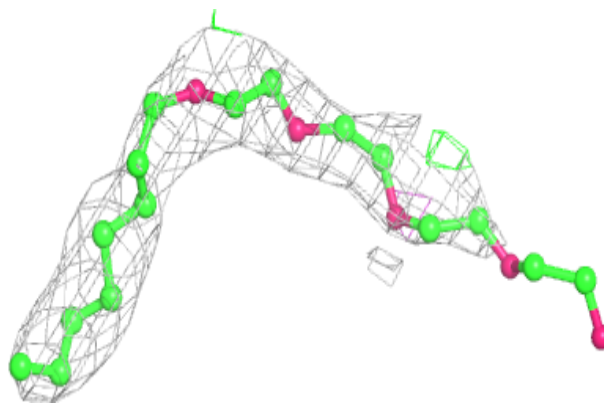
**Electron density around C8E A 403:**

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



Electron density around C8E C 406:

$2mF_o - DF_c$ (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.