



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 08:11 PM EDT

PDB ID : 1Y0G
Title : CRYSTAL STRUCTURE OF THE ESCHERICHIA COLI YCEI PROTEIN,
STRUCTURAL GENOMICS
Authors : Patskovsky, Y.V.; Strokopytov, B.; Ramagopal, U.; Almo, S.C.; Burley, S.K.;
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Deposited on : 2004-11-15
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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

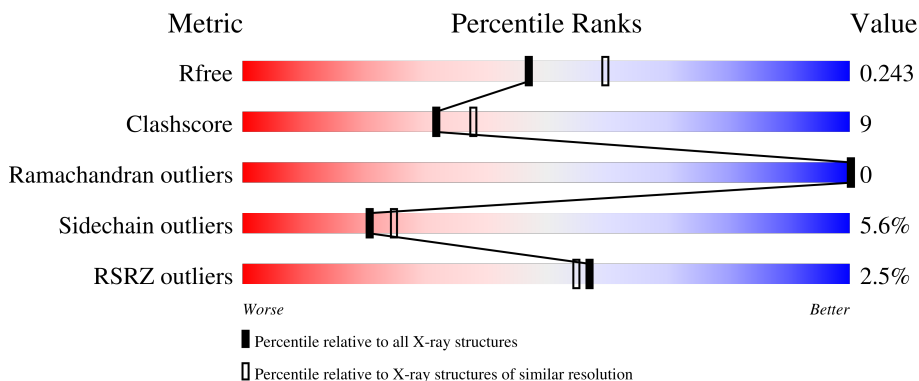
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	191	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">4% 73% 13% • 12%</p>
1	B	191	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">2% 73% 15% • 12%</p>
1	C	191	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">% 71% 16% • 12%</p>
1	D	191	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 75%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 40px;">3% 75% 13% • 12%</p>

2 Entry composition [i](#)

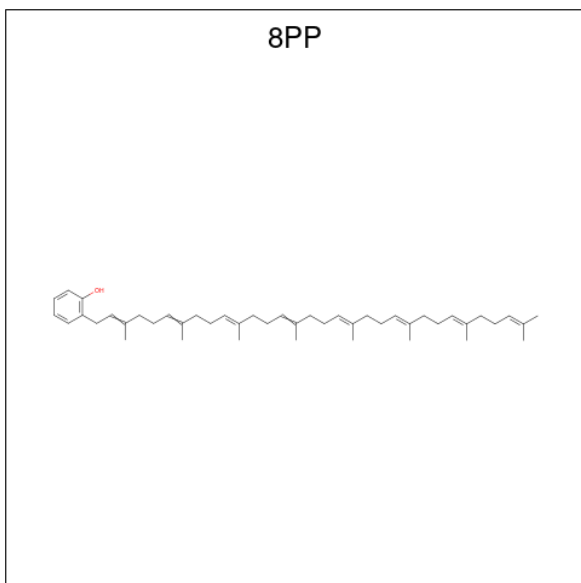
There are 3 unique types of molecules in this entry. The entry contains 5796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Protein yceI.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	169	1323	834	223	266	0	0	0
1	B	169	1323	834	223	266	0	0	0
1	C	169	1323	834	223	266	0	0	0
1	D	169	1323	834	223	266	0	0	0

- Molecule 2 is 2-[(2E,6E,10E,14E,18E,22E,26E)-3,7,11,15,19,23,27,31-OCTAMETHYL DOTRIACONTA-2,6,10,14,18,22,26,30-OCTAENYL]PHENOL (three-letter code: 8PP) (formula: C₄₆H₇₀O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	47	46	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			47	46	1		
2	C	1	Total	C	O	0	0
			47	46	1		
2	D	1	Total	C	O	0	0
			47	46	1		

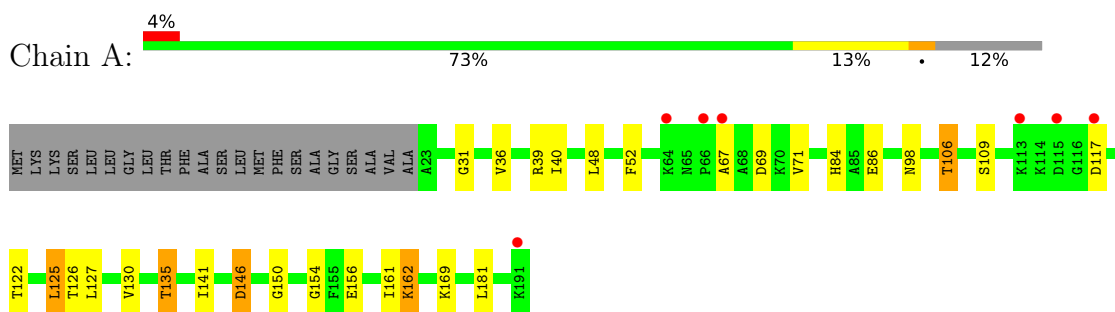
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total	O	0	0
			78	78		
3	B	88	Total	O	0	0
			88	88		
3	C	80	Total	O	0	0
			80	80		
3	D	70	Total	O	0	0
			70	70		

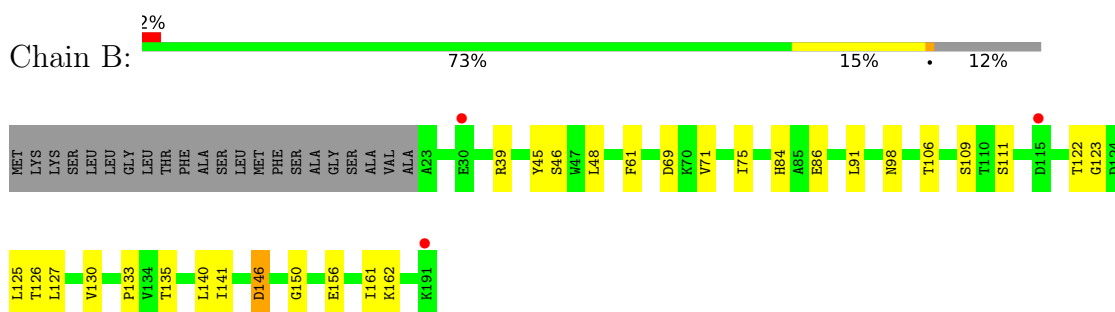
3 Residue-property plots [i](#)

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.

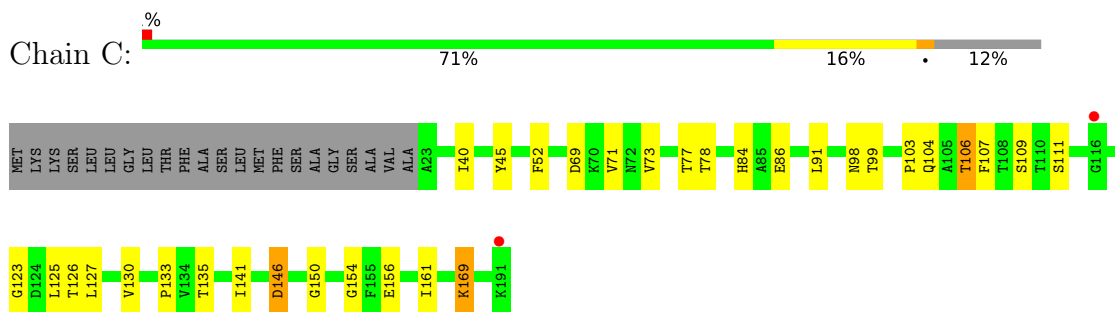
- Molecule 1: Protein yceI



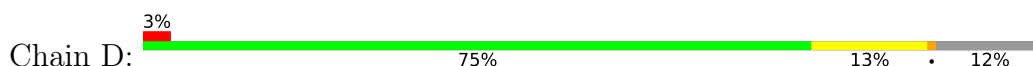
- Molecule 1: Protein yceI

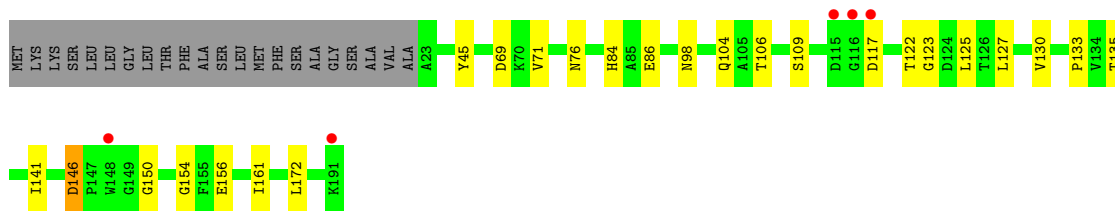


- Molecule 1: Protein yceI



- Molecule 1: Protein yceI





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.17Å 41.93Å 130.25Å 90.00° 126.33° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (20.00-2.20) 96.4 (19.96-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.19Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.248 0.225 , 0.243	Depositor DCC
R_{free} test set	1234 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtrriage
Anisotropy	0.324	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5796	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: 8PP

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	0.41	0/1349	0.71	0/1822
1	B	0.42	0/1349	0.71	0/1822
1	C	0.41	0/1349	0.68	0/1822
1	D	0.43	0/1349	0.68	0/1822
All	All	0.42	0/5396	0.69	0/7288

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1323	0	1284	27	0
1	B	1323	0	1284	23	0
1	C	1323	0	1284	28	0
1	D	1323	0	1284	22	0
2	A	47	0	69	8	0
2	B	47	0	69	8	0
2	C	47	0	69	6	0
2	D	47	0	69	10	0
3	A	78	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	88	0	0	2	0
3	C	80	0	0	5	0
3	D	70	0	0	0	0
All	All	5796	0	5412	97	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 (97) 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:D:172:LEU:HD22	2:D:323:8PP:H103	1.37	1.01
1:D:172:LEU:HD13	2:D:323:8PP:H101	1.56	0.84
1:B:71:VAL:HG12	1:B:109:SER:HB3	1.62	0.78
1:C:40:ILE:HG21	2:C:322:8PP:H13	1.65	0.77
1:A:67:ALA:HB1	1:C:104:GLN:OE1	1.89	0.72
1:D:71:VAL:HG12	1:D:109:SER:HB3	1.73	0.71
1:B:106:THR:HG22	1:B:126:THR:HB	1.71	0.71
1:C:91:LEU:HD21	2:C:322:8PP:H122	1.74	0.70
1:B:106:THR:HG23	3:B:362:HOH:O	1.93	0.69
1:D:69:ASP:HB3	2:D:323:8PP:H451	1.76	0.68
1:D:172:LEU:CD2	2:D:323:8PP:H103	2.21	0.67
1:D:84:HIS:CE1	1:D:86:GLU:HB3	2.31	0.65
1:B:146:ASP:HB2	1:B:150:GLY:H	1.60	0.65
1:C:71:VAL:HG12	1:C:109:SER:HB3	1.76	0.65
1:A:146:ASP:HB2	1:A:150:GLY:H	1.62	0.65
1:A:146:ASP:CB	1:A:150:GLY:H	2.11	0.63
1:D:172:LEU:HD13	2:D:323:8PP:C10	2.28	0.62
1:A:146:ASP:HB2	1:A:150:GLY:O	1.99	0.61
1:A:106:THR:HG22	1:A:126:THR:HB	1.83	0.61
1:B:69:ASP:HB3	2:B:321:8PP:H451	1.83	0.61
1:C:78:THR:HG22	3:C:357:HOH:O	2.00	0.60
1:B:84:HIS:CE1	1:B:86:GLU:HB2	2.37	0.60
1:A:84:HIS:CE1	1:A:86:GLU:HB2	2.36	0.59
1:B:146:ASP:CB	1:B:150:GLY:H	2.16	0.58
1:C:69:ASP:HB3	2:C:322:8PP:H451	1.86	0.57
1:C:154:GLY:HA3	1:D:45:TYR:O	2.04	0.56
1:D:141:ILE:HD11	1:D:156:GLU:HB3	1.86	0.56
1:B:71:VAL:HG21	2:B:321:8PP:H38	1.88	0.56
1:D:71:VAL:HG21	2:D:323:8PP:H38	1.87	0.56
1:C:146:ASP:CB	1:C:150:GLY:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ASP:HB2	1:C:150:GLY:H	1.70	0.55
1:A:40:ILE:HG21	2:A:320:8PP:H13	1.88	0.55
1:C:45:TYR:O	1:D:154:GLY:HA3	2.06	0.55
1:C:52:PHE:CE1	2:C:322:8PP:H222	2.42	0.54
1:A:161:ILE:CD1	2:A:320:8PP:H23	2.38	0.53
1:B:161:ILE:CD1	2:B:321:8PP:H23	2.39	0.52
1:D:161:ILE:CD1	2:D:323:8PP:H23	2.39	0.52
1:D:146:ASP:CB	1:D:150:GLY:H	2.23	0.52
1:B:146:ASP:HB2	1:B:150:GLY:O	2.10	0.52
1:B:61:PHE:CZ	1:B:140:LEU:HD13	2.45	0.50
1:A:71:VAL:HG12	1:A:109:SER:HB3	1.94	0.50
1:B:123:GLY:O	1:B:133:PRO:HA	2.11	0.49
1:B:146:ASP:HB2	1:B:150:GLY:N	2.26	0.49
1:C:169:LYS:N	1:C:169:LYS:HD2	2.26	0.49
1:B:141:ILE:HD11	1:B:156:GLU:HB3	1.94	0.49
1:C:146:ASP:HB2	1:C:150:GLY:O	2.12	0.49
1:A:69:ASP:HB3	2:A:320:8PP:H451	1.94	0.49
1:A:154:GLY:HA3	1:B:45:TYR:O	2.13	0.49
1:D:146:ASP:HB2	1:D:150:GLY:O	2.13	0.48
1:A:146:ASP:HB2	1:A:150:GLY:N	2.28	0.48
1:C:161:ILE:CD1	2:C:322:8PP:H23	2.44	0.48
1:A:31:GLY:HA2	3:B:322:HOH:O	2.14	0.47
1:C:123:GLY:O	1:C:133:PRO:HA	2.14	0.47
1:A:161:ILE:HD12	1:A:181:LEU:HD21	1.97	0.47
1:C:111:SER:HB2	3:C:377:HOH:O	2.14	0.47
1:B:122:THR:OG1	1:B:135:THR:HG22	2.15	0.47
1:D:122:THR:OG1	1:D:135:THR:HG22	2.15	0.47
1:A:36:VAL:HG22	2:A:320:8PP:H353	1.97	0.47
1:B:84:HIS:HE1	1:B:86:GLU:HB2	1.80	0.46
1:A:106:THR:HG23	3:A:372:HOH:O	2.16	0.46
1:C:106:THR:CG2	3:C:375:HOH:O	2.64	0.46
1:A:52:PHE:CE1	2:A:320:8PP:H222	2.50	0.46
1:C:141:ILE:HD11	1:C:156:GLU:HB3	1.98	0.46
1:C:73:VAL:HG21	2:C:322:8PP:H321	1.97	0.46
1:A:122:THR:OG1	1:A:135:THR:HG23	2.16	0.46
1:B:91:LEU:HD21	2:B:321:8PP:H122	1.99	0.45
1:D:146:ASP:HB2	1:D:150:GLY:H	1.81	0.45
1:D:76:ASN:HD22	1:D:104:GLN:HG2	1.82	0.44
1:C:73:VAL:HG22	1:C:107:PHE:HB3	1.99	0.44
1:D:122:THR:HA	1:D:135:THR:HG22	2.00	0.44
1:A:141:ILE:HD11	1:A:156:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:CD1	2:B:321:8PP:H261	2.49	0.43
1:A:71:VAL:HG21	2:A:320:8PP:H38	1.99	0.43
1:C:77:THR:HG21	3:C:372:HOH:O	2.18	0.43
1:A:161:ILE:HD12	2:A:320:8PP:H23	2.01	0.43
1:A:39:ARG:HA	1:A:48:LEU:O	2.19	0.42
1:A:84:HIS:HE1	1:A:86:GLU:HB2	1.83	0.42
1:C:106:THR:HG22	1:C:126:THR:HB	2.02	0.42
1:C:103:PRO:O	1:C:104:GLN:HG3	2.19	0.42
1:D:71:VAL:HG21	2:D:323:8PP:C38	2.47	0.42
1:B:39:ARG:HA	1:B:48:LEU:O	2.20	0.42
2:B:321:8PP:H152	2:B:321:8PP:H121	1.70	0.42
1:C:146:ASP:HB2	1:C:150:GLY:N	2.34	0.42
1:D:71:VAL:CG2	2:D:323:8PP:H38	2.49	0.41
1:A:146:ASP:HB3	1:A:150:GLY:H	1.85	0.41
1:C:77:THR:OG1	1:C:99:THR:HG22	2.20	0.41
1:B:71:VAL:HG21	2:B:321:8PP:C38	2.50	0.41
1:C:84:HIS:CE1	1:C:86:GLU:HB2	2.56	0.41
1:D:123:GLY:O	1:D:133:PRO:HA	2.21	0.41
1:A:125:LEU:HG	2:A:320:8PP:H303	2.02	0.40
2:D:323:8PP:H101	2:D:323:8PP:H122	1.95	0.40
1:B:71:VAL:CG2	2:B:321:8PP:H38	2.50	0.40
1:D:146:ASP:HB3	1:D:150:GLY:H	1.87	0.40
1:A:141:ILE:HD12	1:B:46:SER:HA	2.03	0.40
1:A:162:LYS:HE3	1:A:162:LYS:HB2	1.88	0.40
1:C:106:THR:HG23	3:C:375:HOH:O	2.22	0.40
1:C:71:VAL:HG12	1:C:109:SER:CB	2.50	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	167/191 (87%)	158 (95%)	9 (5%)	0	100	100
1	B	167/191 (87%)	157 (94%)	10 (6%)	0	100	100
1	C	167/191 (87%)	155 (93%)	12 (7%)	0	100	100
1	D	167/191 (87%)	156 (93%)	11 (7%)	0	100	100
All	All	668/764 (87%)	626 (94%)	42 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	142/158 (90%)	132 (93%)	10 (7%)	15	16
1	B	142/158 (90%)	135 (95%)	7 (5%)	25	31
1	C	142/158 (90%)	134 (94%)	8 (6%)	21	25
1	D	142/158 (90%)	135 (95%)	7 (5%)	25	31
All	All	568/632 (90%)	536 (94%)	32 (6%)	21	25

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	106	THR
1	A	117	ASP
1	A	125	LEU
1	A	127	LEU
1	A	130	VAL
1	A	135	THR
1	A	146	ASP
1	A	162	LYS
1	A	169	LYS
1	B	98	ASN
1	B	111	SER
1	B	125	LEU

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Mol	Chain	Res	Type
1	B	127	LEU
1	B	130	VAL
1	B	146	ASP
1	B	162	LYS
1	C	98	ASN
1	C	106	THR
1	C	125	LEU
1	C	127	LEU
1	C	130	VAL
1	C	135	THR
1	C	146	ASP
1	C	169	LYS
1	D	98	ASN
1	D	106	THR
1	D	117	ASP
1	D	125	LEU
1	D	127	LEU
1	D	130	VAL
1	D	146	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	76	ASN
1	A	98	ASN
1	A	104	GLN
1	B	37	ASN
1	B	76	ASN
1	B	90	HIS
1	B	98	ASN
1	B	104	GLN
1	C	37	ASN
1	C	76	ASN
1	C	98	ASN
1	D	37	ASN
1	D	76	ASN
1	D	98	ASN
1	D	104	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	8PP	B	321	-	47,47,47	1.94	11 (23%)	57,57,57	2.72	20 (35%)
2	8PP	D	323	-	47,47,47	1.97	10 (21%)	57,57,57	2.54	16 (28%)
2	8PP	A	320	-	47,47,47	2.24	9 (19%)	57,57,57	2.67	18 (31%)
2	8PP	C	322	-	47,47,47	1.85	8 (17%)	57,57,57	2.91	20 (35%)

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	8PP	B	321	-	-	9/47/47/47	0/1/1/1
2	8PP	D	323	-	-	11/47/47/47	0/1/1/1
2	8PP	A	320	-	-	15/47/47/47	0/1/1/1
2	8PP	C	322	-	-	12/47/47/47	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	320	8PP	C8-C9	8.43	1.53	1.33
2	B	321	8PP	O-C1	-6.23	1.23	1.36
2	D	323	8PP	O-C1	-6.03	1.24	1.36
2	A	320	8PP	O-C1	-5.96	1.24	1.36
2	C	322	8PP	O-C1	-5.88	1.24	1.36
2	B	321	8PP	C6-C1	5.22	1.48	1.39
2	A	320	8PP	C6-C1	5.18	1.48	1.39
2	D	323	8PP	C6-C1	5.12	1.48	1.39
2	C	322	8PP	C6-C1	4.67	1.47	1.39
2	C	322	8PP	C4-C3	3.90	1.47	1.38
2	D	323	8PP	C4-C3	3.73	1.46	1.38
2	C	322	8PP	C5-C4	3.72	1.47	1.38
2	D	323	8PP	C1-C2	3.69	1.45	1.40
2	A	320	8PP	C4-C3	3.54	1.46	1.38
2	D	323	8PP	C5-C4	3.49	1.47	1.38
2	B	321	8PP	C3-C2	-3.38	1.33	1.39
2	A	320	8PP	C5-C4	3.29	1.46	1.38
2	A	320	8PP	C1-C2	3.17	1.44	1.40
2	D	323	8PP	C11-C9	3.11	1.57	1.51
2	B	321	8PP	C4-C3	3.02	1.45	1.38
2	B	321	8PP	C23-C24	2.99	1.40	1.33
2	B	321	8PP	C5-C4	2.93	1.45	1.38
2	D	323	8PP	C23-C24	2.83	1.39	1.33
2	A	320	8PP	C23-C24	2.81	1.39	1.33
2	C	322	8PP	C23-C24	2.81	1.39	1.33
2	C	322	8PP	C1-C2	2.81	1.44	1.40
2	A	320	8PP	C3-C2	-2.63	1.35	1.39
2	B	321	8PP	C1-C2	2.47	1.43	1.40
2	B	321	8PP	C18-C19	2.43	1.38	1.33
2	C	322	8PP	C42-C43	-2.31	1.42	1.50
2	C	322	8PP	C3-C2	-2.26	1.35	1.39
2	D	323	8PP	C42-C43	-2.16	1.43	1.50
2	B	321	8PP	C30-C29	2.12	1.56	1.50
2	D	323	8PP	C18-C19	2.12	1.38	1.33
2	B	321	8PP	C46-C44	2.08	1.56	1.50
2	A	320	8PP	C11-C9	2.08	1.55	1.51
2	B	321	8PP	C42-C43	-2.03	1.43	1.50
2	D	323	8PP	C40-C39	2.02	1.55	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	320	8PP	C15-C14-C16	9.38	131.05	115.27
2	D	323	8PP	C15-C14-C16	9.32	130.95	115.27
2	C	322	8PP	C15-C14-C16	9.30	130.91	115.27
2	B	321	8PP	C15-C14-C16	7.68	128.19	115.27
2	C	322	8PP	C10-C9-C11	6.65	126.45	115.27
2	C	322	8PP	C7-C8-C9	-6.19	117.64	127.24
2	D	323	8PP	C7-C8-C9	-5.74	118.34	127.24
2	B	321	8PP	C41-C39-C40	-5.66	105.74	115.27
2	A	320	8PP	C7-C8-C9	-5.56	118.61	127.24
2	A	320	8PP	C41-C39-C40	-5.56	105.92	115.27
2	C	322	8PP	C41-C39-C40	-5.42	106.16	115.27
2	C	322	8PP	C11-C9-C8	-5.35	110.30	121.12
2	C	322	8PP	C32-C33-C34	-5.30	114.90	127.66
2	B	321	8PP	C32-C33-C34	-5.15	115.26	127.66
2	C	322	8PP	C12-C13-C14	-5.12	115.34	127.66
2	D	323	8PP	C41-C39-C40	-5.11	106.67	115.27
2	A	320	8PP	C16-C14-C13	-5.10	110.81	121.12
2	B	321	8PP	C10-C9-C11	5.03	123.73	115.27
2	C	322	8PP	C17-C18-C19	-5.02	115.57	127.66
2	A	320	8PP	C32-C33-C34	-4.99	115.66	127.66
2	D	323	8PP	C32-C33-C34	-4.95	115.73	127.66
2	B	321	8PP	C12-C13-C14	-4.88	115.91	127.66
2	A	320	8PP	C36-C34-C33	-4.78	111.44	121.12
2	B	321	8PP	C36-C34-C33	-4.58	111.84	121.12
2	D	323	8PP	C36-C34-C33	-4.58	111.85	121.12
2	B	321	8PP	C30-C29-C31	-4.57	107.58	115.27
2	C	322	8PP	C36-C34-C33	-4.46	112.10	121.12
2	D	323	8PP	C22-C23-C24	-4.43	116.98	127.66
2	B	321	8PP	C15-C14-C13	-4.42	112.34	123.68
2	A	320	8PP	C22-C23-C24	-4.39	117.08	127.66
2	B	321	8PP	C7-C8-C9	-4.38	120.45	127.24
2	C	322	8PP	C22-C23-C24	-4.20	117.55	127.66
2	A	320	8PP	C35-C34-C36	4.19	122.33	115.27
2	B	321	8PP	C11-C9-C8	-4.15	112.71	121.12
2	B	321	8PP	C22-C23-C24	-4.15	117.66	127.66
2	A	320	8PP	C11-C9-C8	-4.15	112.72	121.12
2	C	322	8PP	C35-C34-C36	4.01	122.01	115.27
2	B	321	8PP	C35-C34-C36	3.94	121.91	115.27
2	D	323	8PP	C35-C34-C36	3.92	121.87	115.27
2	B	321	8PP	C2-C7-C8	3.91	119.77	112.36
2	A	320	8PP	C10-C9-C8	3.88	133.63	123.68
2	D	323	8PP	C15-C14-C13	-3.88	113.73	123.68
2	A	320	8PP	C41-C39-C38	3.84	133.52	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	320	8PP	C17-C16-C14	3.75	125.30	112.98
2	D	323	8PP	C11-C9-C8	-3.73	113.58	121.12
2	C	322	8PP	C37-C38-C39	-3.69	118.76	127.66
2	B	321	8PP	C41-C39-C38	3.68	133.11	123.68
2	C	322	8PP	C41-C39-C38	3.63	132.99	123.68
2	C	322	8PP	C15-C14-C13	-3.63	114.37	123.68
2	D	323	8PP	C10-C9-C8	3.60	132.91	123.68
2	D	323	8PP	C41-C39-C38	3.53	132.74	123.68
2	D	323	8PP	C37-C38-C39	-3.53	119.17	127.66
2	A	320	8PP	C37-C38-C39	-3.41	119.44	127.66
2	B	321	8PP	C37-C38-C39	-3.39	119.49	127.66
2	C	322	8PP	C16-C14-C13	-3.16	114.72	121.12
2	D	323	8PP	C26-C24-C23	3.08	127.35	121.12
2	B	321	8PP	C12-C11-C9	3.02	122.92	112.98
2	B	321	8PP	C17-C18-C19	-3.01	120.41	127.66
2	B	321	8PP	C26-C24-C23	3.00	127.19	121.12
2	D	323	8PP	C16-C14-C13	-2.98	115.09	121.12
2	A	320	8PP	C26-C24-C23	2.95	127.08	121.12
2	D	323	8PP	C17-C18-C19	-2.94	120.58	127.66
2	C	322	8PP	C30-C29-C31	-2.85	110.48	115.27
2	C	322	8PP	C26-C24-C23	2.84	126.87	121.12
2	A	320	8PP	C17-C18-C19	-2.84	120.83	127.66
2	D	323	8PP	C30-C29-C31	-2.57	110.94	115.27
2	A	320	8PP	C16-C17-C18	2.51	120.14	111.88
2	C	322	8PP	C2-C7-C8	-2.34	107.93	112.36
2	B	321	8PP	C7-C2-C1	2.32	124.34	120.49
2	B	321	8PP	C30-C29-C28	2.20	129.31	123.68
2	A	320	8PP	C15-C14-C13	-2.16	118.13	123.68
2	C	322	8PP	C20-C19-C18	-2.09	118.32	123.68
2	C	322	8PP	C7-C2-C1	2.05	123.89	120.49
2	A	320	8PP	C12-C13-C14	2.04	132.58	127.66

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	320	8PP	C7-C8-C9-C10
2	A	320	8PP	C22-C23-C24-C25
2	A	320	8PP	C22-C23-C24-C26
2	A	320	8PP	C42-C43-C44-C45
2	B	321	8PP	C22-C23-C24-C25
2	B	321	8PP	C22-C23-C24-C26

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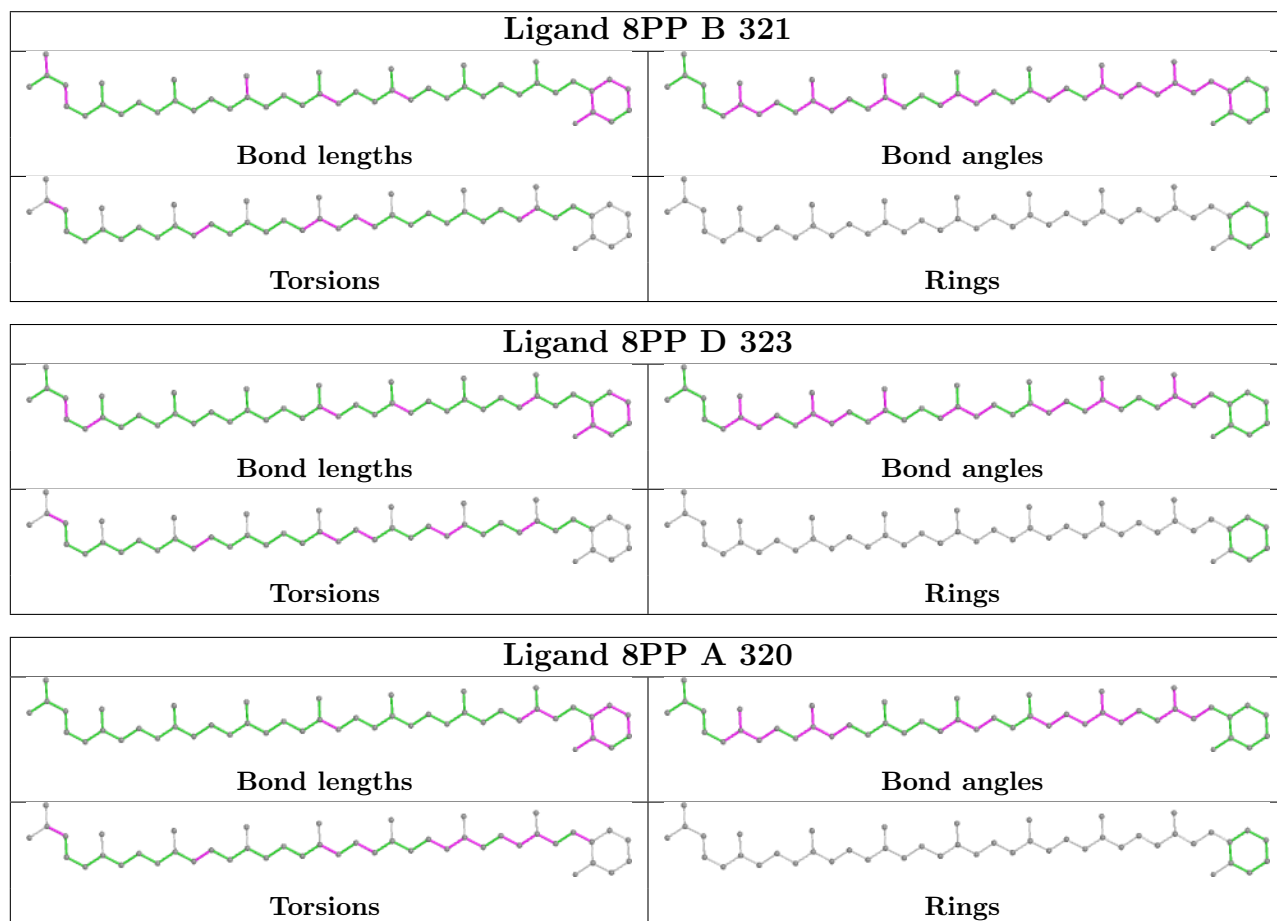
Mol	Chain	Res	Type	Atoms
2	C	322	8PP	C22-C23-C24-C25
2	C	322	8PP	C22-C23-C24-C26
2	C	322	8PP	C42-C43-C44-C45
2	D	323	8PP	C22-C23-C24-C25
2	D	323	8PP	C22-C23-C24-C26
2	D	323	8PP	C42-C43-C44-C45
2	D	323	8PP	C12-C11-C9-C8
2	B	321	8PP	C42-C43-C44-C45
2	A	320	8PP	C12-C13-C14-C15
2	C	322	8PP	C12-C13-C14-C15
2	A	320	8PP	C12-C13-C14-C16
2	C	322	8PP	C12-C13-C14-C16
2	A	320	8PP	C42-C43-C44-C46
2	C	322	8PP	C42-C43-C44-C46
2	D	323	8PP	C42-C43-C44-C46
2	A	320	8PP	C15-C14-C16-C17
2	C	322	8PP	C15-C14-C16-C17
2	D	323	8PP	C12-C11-C9-C10
2	D	323	8PP	C15-C14-C16-C17
2	A	320	8PP	C13-C14-C16-C17
2	C	322	8PP	C13-C14-C16-C17
2	D	323	8PP	C13-C14-C16-C17
2	C	322	8PP	C9-C11-C12-C13
2	D	323	8PP	C14-C16-C17-C18
2	B	321	8PP	C42-C43-C44-C46
2	A	320	8PP	C14-C16-C17-C18
2	C	322	8PP	C14-C16-C17-C18
2	B	321	8PP	C12-C11-C9-C10
2	B	321	8PP	C12-C11-C9-C8
2	A	320	8PP	C12-C11-C9-C8
2	C	322	8PP	C19-C21-C22-C23
2	D	323	8PP	C19-C21-C22-C23
2	A	320	8PP	C1-C2-C7-C8
2	A	320	8PP	C31-C32-C33-C34
2	B	321	8PP	C31-C32-C33-C34
2	C	322	8PP	C31-C32-C33-C34
2	D	323	8PP	C31-C32-C33-C34
2	B	321	8PP	C25-C24-C26-C27
2	A	320	8PP	C9-C11-C12-C13
2	A	320	8PP	C19-C21-C22-C23
2	B	321	8PP	C19-C21-C22-C23

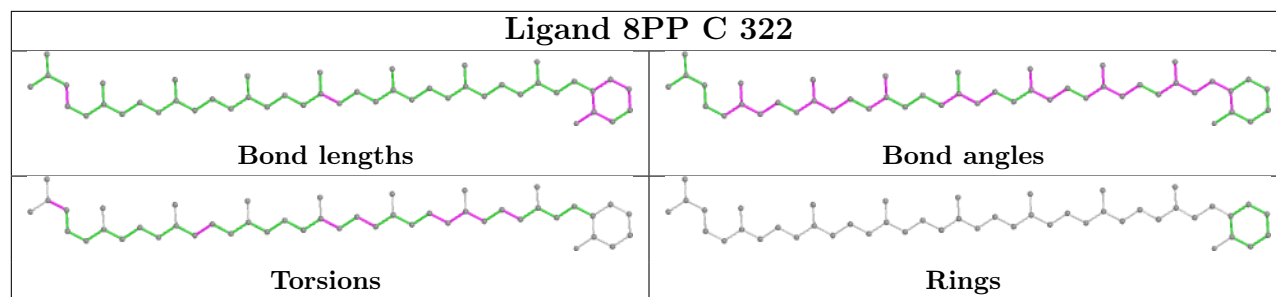
There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	321	8PP	8	0
2	D	323	8PP	10	0
2	A	320	8PP	8	0
2	C	322	8PP	6	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	169/191 (88%)	-0.11	7 (4%) 37 35	17, 32, 64, 75	0
1	B	169/191 (88%)	-0.19	3 (1%) 68 66	18, 30, 50, 71	0
1	C	169/191 (88%)	-0.28	2 (1%) 79 77	16, 27, 44, 68	0
1	D	169/191 (88%)	-0.06	5 (2%) 50 48	15, 33, 56, 69	0
All	All	676/764 (88%)	-0.16	17 (2%) 57 55	15, 31, 54, 75	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	ASP	5.2
1	D	148	TRP	4.6
1	A	191	LYS	3.9
1	D	117	ASP	3.6
1	A	115	ASP	3.3
1	B	191	LYS	3.3
1	A	67	ALA	3.1
1	D	191	LYS	2.6
1	D	115	ASP	2.6
1	B	115	ASP	2.5
1	A	66	PRO	2.4
1	C	116	GLY	2.4
1	C	191	LYS	2.3
1	A	64	LYS	2.2
1	B	30	GLU	2.1
1	D	116	GLY	2.0
1	A	113	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](#)

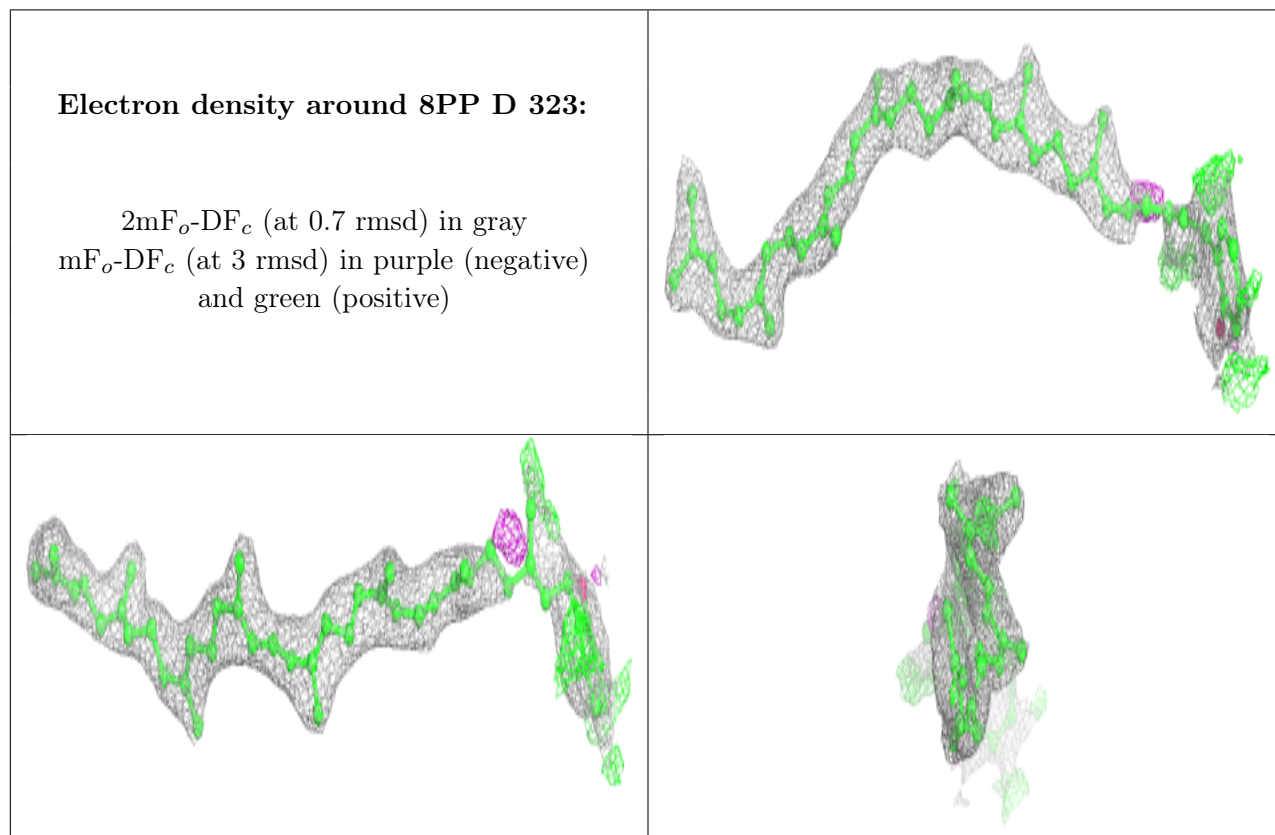
There are no monosaccharides in this entry.

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, 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.

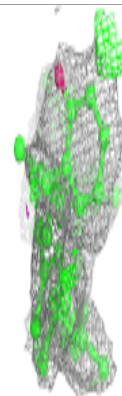
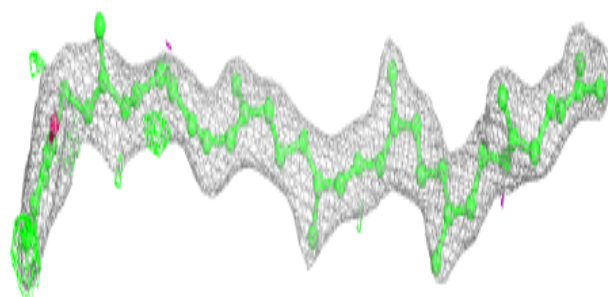
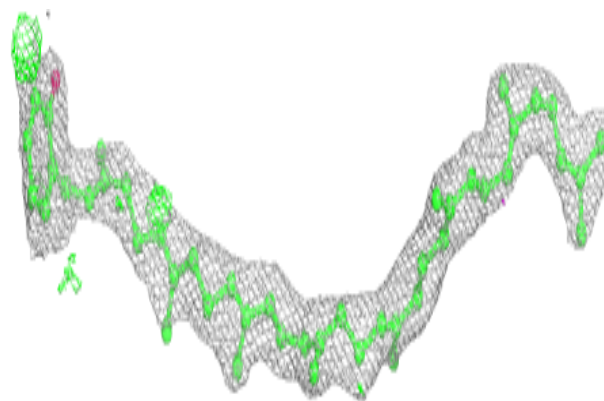
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8PP	D	323	47/47	0.83	0.26	27,36,67,70	0
2	8PP	C	322	47/47	0.86	0.24	28,35,64,65	0
2	8PP	A	320	47/47	0.86	0.25	21,33,53,56	0
2	8PP	B	321	47/47	0.90	0.22	19,30,43,75	0

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.

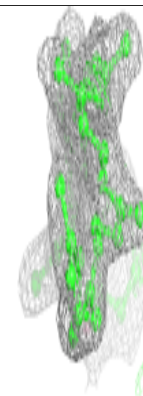
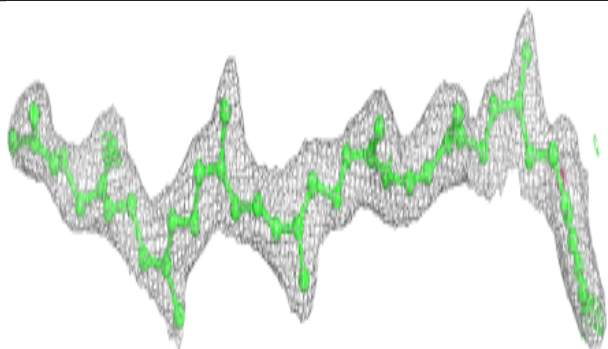
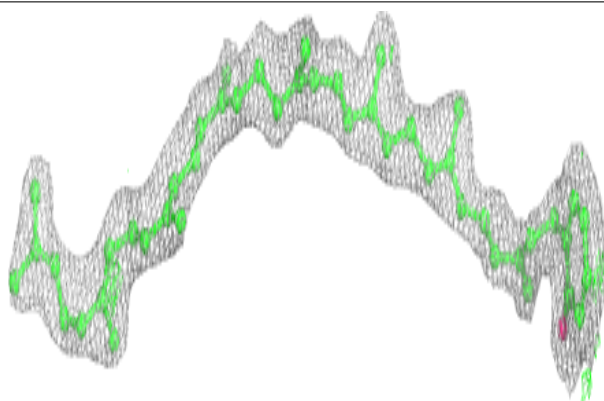


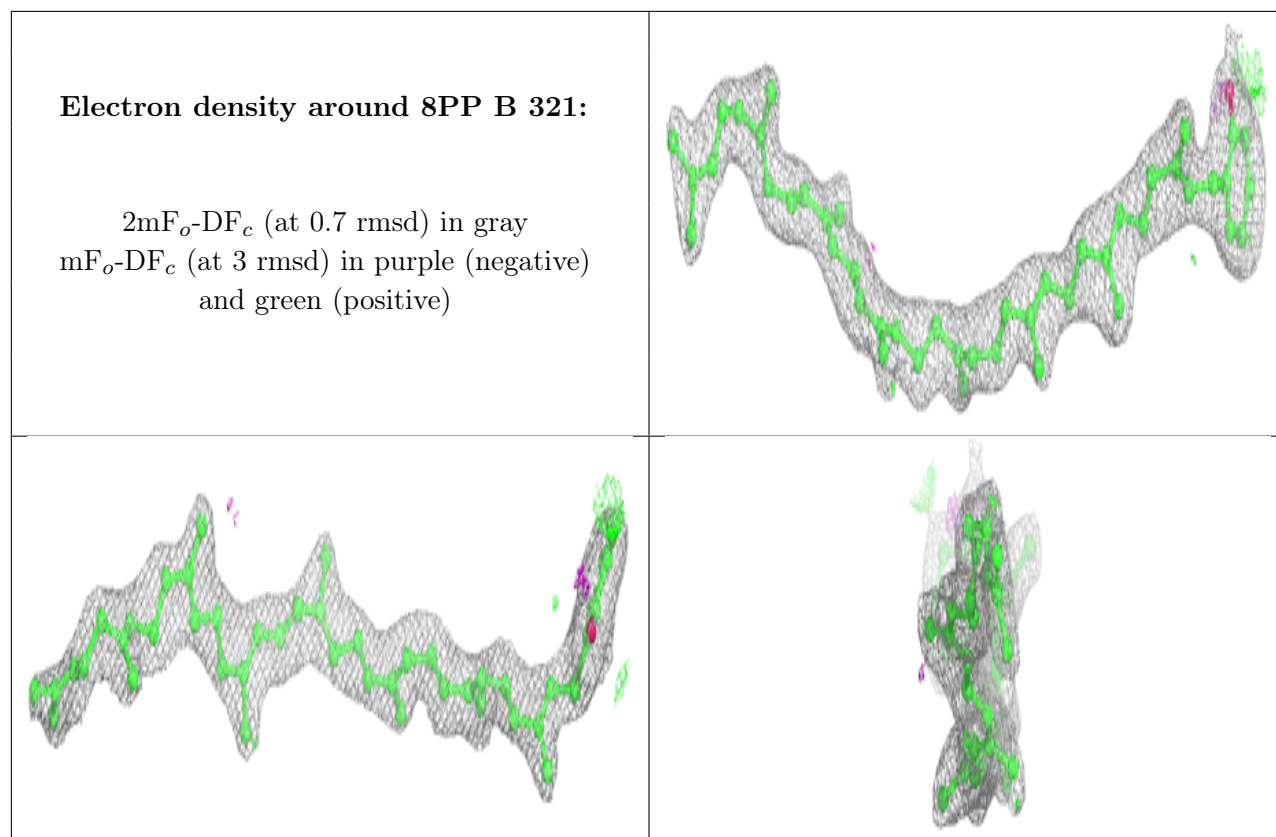
Electron density around 8PP C 322:

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

**Electron density around 8PP A 320:**

$2mF_o-DF_c$ (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.