



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:38 AM EDT

PDB ID : 1Y0G / pdb_00001y0g
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.;
New York SGX Research Center for Structural Genomics (NYSGXRC)
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	:	4-5-2 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

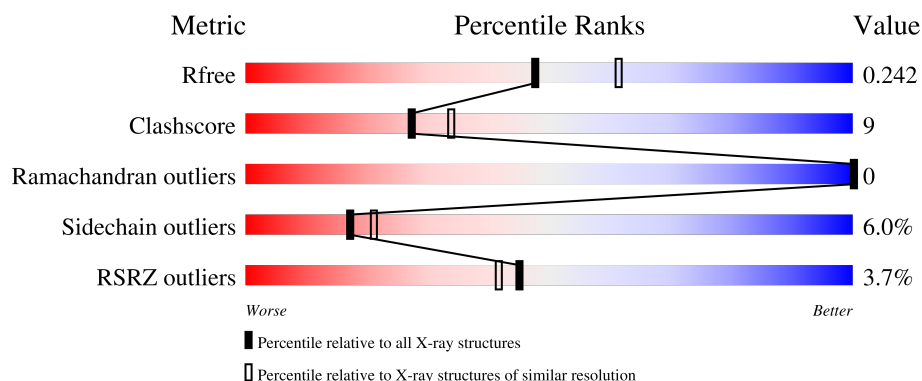
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	
1	B	191	
1	C	191	
1	D	191	

2 Entry composition [i](#)

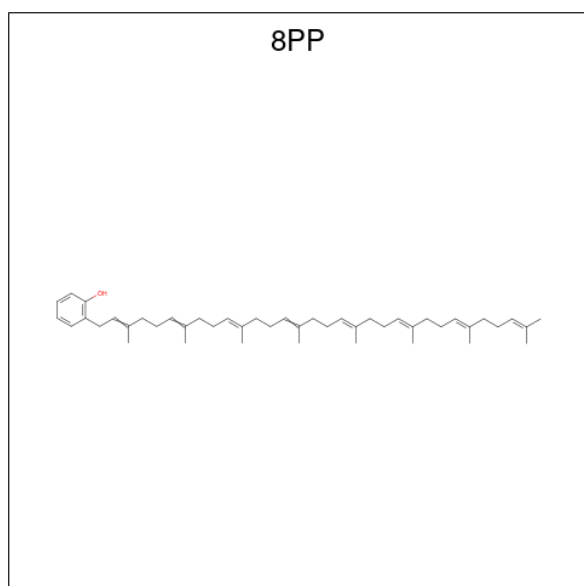
There are 3 unique types of molecules in this entry. The entry contains 5796 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	169	Total	C	N	O	0	0	0
			1323	834	223	266			
1	B	169	Total	C	N	O	0	0	0
			1323	834	223	266			
1	C	169	Total	C	N	O	0	0	0
			1323	834	223	266			
1	D	169	Total	C	N	O	0	0	0
			1323	834	223	266			

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



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

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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		

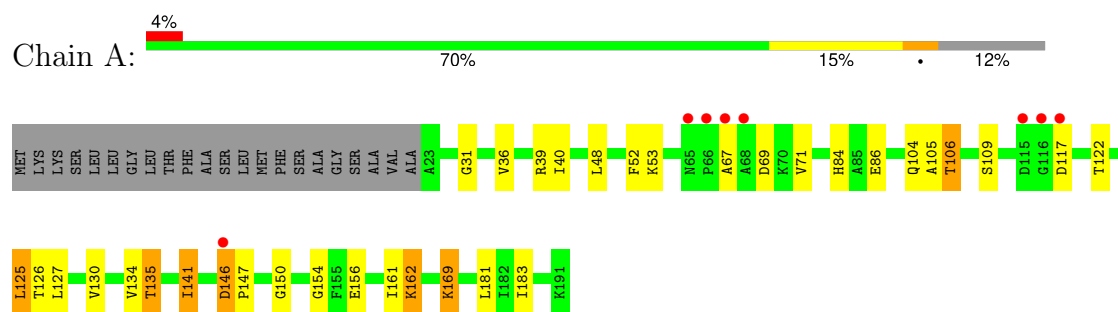
- Molecule 3 is water.

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		

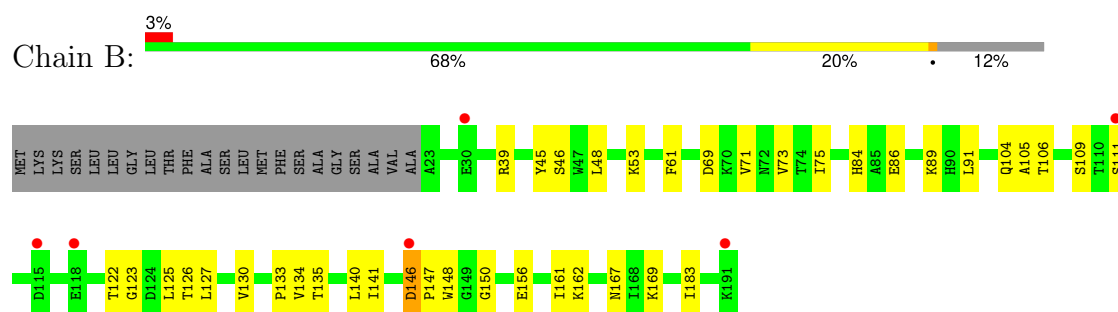
3 Residue-property plots [i](#)

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.

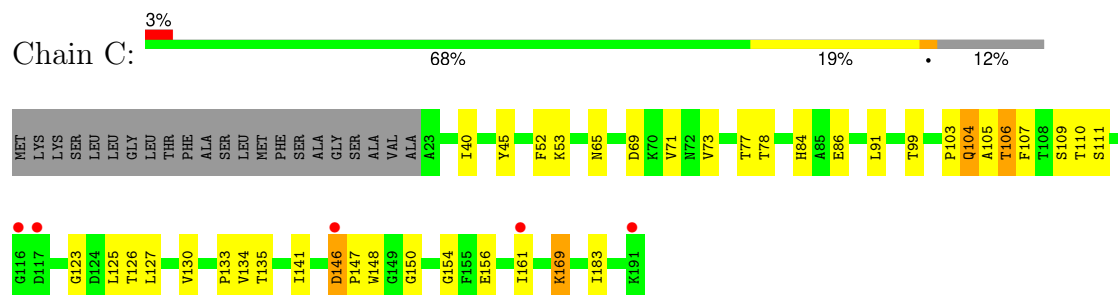
- Molecule 1: Protein yceI



- Molecule 1: Protein yceI

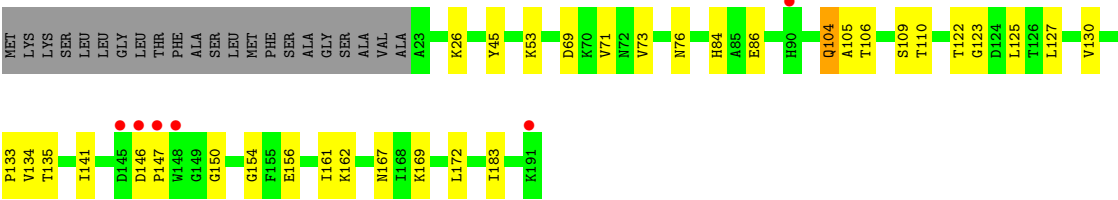


- Molecule 1: Protein yceI



- 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 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.1 (20.00-2.20) 96.3 (20.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.228 , 0.248 0.225 , 0.242	Depositor DCC
R_{free} test set	1234 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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	0.51	0/1349	0.99	7/1822 (0.4%)
1	B	0.50	0/1349	0.99	7/1822 (0.4%)
1	C	0.49	0/1349	0.96	9/1822 (0.5%)
1	D	0.53	0/1349	0.95	8/1822 (0.4%)
All	All	0.51	0/5396	0.97	31/7288 (0.4%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	LYS	N-CA-C	7.78	119.84	111.36
1	A	169	LYS	N-CA-C	7.58	119.62	111.36
1	C	147	PRO	N-CA-C	-7.14	105.63	114.20
1	B	104	GLN	N-CA-C	7.01	120.97	109.06
1	A	53	LYS	N-CA-C	6.78	120.65	112.38
1	C	53	LYS	N-CA-C	6.77	120.64	112.38
1	B	53	LYS	N-CA-C	6.62	120.46	112.38
1	D	169	LYS	N-CA-C	6.57	118.53	111.36
1	D	104	GLN	N-CA-C	6.53	119.34	109.23
1	A	147	PRO	N-CA-C	-6.42	106.50	114.20
1	C	104	GLN	N-CA-C	6.36	119.88	109.06
1	B	147	PRO	N-CA-C	-6.22	106.73	114.20
1	C	183	ILE	N-CA-C	6.12	118.19	108.89
1	B	169	LYS	N-CA-C	6.01	117.92	111.36
1	D	183	ILE	N-CA-C	5.89	117.07	108.53
1	C	110	THR	N-CA-C	-5.79	107.20	114.56
1	A	104	GLN	N-CA-C	5.78	118.89	109.06
1	D	53	LYS	N-CA-C	5.67	119.30	112.38
1	C	65	ASN	CA-C-N	5.64	125.31	119.56
1	C	65	ASN	C-N-CA	5.64	125.31	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	110	THR	N-CA-C	-5.53	107.54	114.56
1	D	167	ASN	N-CA-C	5.51	119.30	112.24
1	B	105	ALA	N-CA-C	-5.43	101.31	109.95
1	C	105	ALA	N-CA-C	-5.33	101.47	109.95
1	A	183	ILE	N-CA-C	5.33	116.99	108.89
1	D	105	ALA	N-CA-C	-5.20	101.68	109.95
1	D	147	PRO	N-CA-C	-5.19	107.27	114.27
1	B	183	ILE	N-CA-C	5.16	116.74	108.89
1	B	167	ASN	N-CA-C	5.16	118.84	112.24
1	A	141	ILE	N-CA-C	-5.07	106.21	111.58
1	A	105	ALA	N-CA-C	-5.03	101.96	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	24	0
1	C	1323	0	1284	29	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
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	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:146:ASP:C	1:B:148:TRP:H	2.27	0.42
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:C:146:ASP:C	1:C:148:TRP:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	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 ⓘ

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%)	14	16
1	B	142/158 (90%)	133 (94%)	9 (6%)	16	19
1	C	142/158 (90%)	135 (95%)	7 (5%)	22	29
1	D	142/158 (90%)	134 (94%)	8 (6%)	19	24
All	All	568/632 (90%)	534 (94%)	34 (6%)	17	21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	THR
1	A	117	ASP
1	A	125	LEU
1	A	127	LEU
1	A	130	VAL
1	A	134	VAL
1	A	135	THR
1	A	146	ASP
1	A	162	LYS
1	A	169	LYS
1	B	73	VAL
1	B	89	LYS
1	B	111	SER
1	B	125	LEU
1	B	127	LEU
1	B	130	VAL
1	B	134	VAL
1	B	146	ASP
1	B	162	LYS
1	C	106	THR
1	C	125	LEU
1	C	127	LEU
1	C	130	VAL
1	C	134	VAL

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Mol	Chain	Res	Type
1	C	135	THR
1	C	146	ASP
1	D	26	LYS
1	D	73	VAL
1	D	106	THR
1	D	125	LEU
1	D	127	LEU
1	D	130	VAL
1	D	134	VAL
1	D	162	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	32	GLN
1	B	37	ASN
1	B	76	ASN
1	B	90	HIS
1	B	98	ASN
1	B	104	GLN
1	B	189	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
1	D	167	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 ⓘ

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	D	323	-	47,47,47	2.07	10 (21%)	57,57,57	2.52	17 (29%)
2	8PP	A	320	-	47,47,47	2.35	10 (21%)	57,57,57	2.62	18 (31%)
2	8PP	B	321	-	47,47,47	2.03	11 (23%)	57,57,57	2.67	20 (35%)
2	8PP	C	322	-	47,47,47	1.96	8 (17%)	57,57,57	2.88	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	D	323	-	-	11/47/47/47	0/1/1/1
2	8PP	A	320	-	-	12/47/47/47	0/1/1/1
2	8PP	B	321	-	-	8/47/47/47	0/1/1/1
2	8PP	C	322	-	-	12/47/47/47	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	320	8PP	C8-C9	8.75	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	321	8PP	O-C1	-6.29	1.23	1.36
2	D	323	8PP	O-C1	-6.08	1.24	1.36
2	A	320	8PP	O-C1	-6.01	1.24	1.36
2	C	322	8PP	O-C1	-5.93	1.24	1.36
2	B	321	8PP	C6-C1	5.35	1.48	1.39
2	A	320	8PP	C6-C1	5.31	1.48	1.39
2	D	323	8PP	C6-C1	5.25	1.48	1.39
2	C	322	8PP	C4-C3	4.81	1.47	1.38
2	C	322	8PP	C6-C1	4.79	1.47	1.39
2	D	323	8PP	C4-C3	4.60	1.46	1.38
2	C	322	8PP	C5-C4	4.38	1.47	1.38
2	A	320	8PP	C4-C3	4.36	1.46	1.38
2	D	323	8PP	C5-C4	4.10	1.47	1.38
2	A	320	8PP	C5-C4	3.86	1.46	1.38
2	D	323	8PP	C1-C2	3.85	1.45	1.40
2	B	321	8PP	C4-C3	3.73	1.45	1.38
2	B	321	8PP	C3-C2	-3.53	1.33	1.39
2	B	321	8PP	C5-C4	3.43	1.45	1.38
2	A	320	8PP	C1-C2	3.32	1.44	1.40
2	D	323	8PP	C11-C9	3.13	1.57	1.51
2	B	321	8PP	C23-C24	3.08	1.40	1.33
2	C	322	8PP	C1-C2	2.94	1.44	1.40
2	D	323	8PP	C23-C24	2.91	1.39	1.33
2	A	320	8PP	C23-C24	2.90	1.39	1.33
2	C	322	8PP	C23-C24	2.89	1.39	1.33
2	A	320	8PP	C3-C2	-2.75	1.35	1.39
2	B	321	8PP	C1-C2	2.58	1.43	1.40
2	C	322	8PP	C42-C43	-2.50	1.42	1.50
2	B	321	8PP	C18-C19	2.50	1.38	1.33
2	C	322	8PP	C3-C2	-2.36	1.35	1.39
2	D	323	8PP	C42-C43	-2.35	1.43	1.50
2	B	321	8PP	C30-C29	2.22	1.56	1.50
2	B	321	8PP	C42-C43	-2.20	1.43	1.50
2	D	323	8PP	C18-C19	2.17	1.38	1.33
2	A	320	8PP	C42-C43	-2.12	1.44	1.50
2	A	320	8PP	C11-C9	2.10	1.55	1.51
2	B	321	8PP	C46-C44	2.08	1.56	1.50
2	D	323	8PP	C40-C39	2.04	1.55	1.51

All (75) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	320	8PP	C15-C14-C16	9.12	131.05	115.23
2	D	323	8PP	C15-C14-C16	9.06	130.95	115.23
2	C	322	8PP	C15-C14-C16	9.03	130.91	115.23
2	B	321	8PP	C15-C14-C16	7.47	128.19	115.23
2	C	322	8PP	C7-C8-C9	-6.82	117.64	127.42
2	C	322	8PP	C10-C9-C11	6.47	126.45	115.23
2	D	323	8PP	C7-C8-C9	-6.34	118.34	127.42
2	A	320	8PP	C7-C8-C9	-6.15	118.61	127.42
2	C	322	8PP	C32-C33-C34	-5.56	114.90	127.62
2	B	321	8PP	C41-C39-C40	-5.46	105.74	115.23
2	B	321	8PP	C32-C33-C34	-5.40	115.26	127.62
2	C	322	8PP	C12-C13-C14	-5.37	115.34	127.62
2	A	320	8PP	C41-C39-C40	-5.37	105.92	115.23
2	C	322	8PP	C17-C18-C19	-5.27	115.57	127.62
2	A	320	8PP	C32-C33-C34	-5.23	115.66	127.62
2	C	322	8PP	C41-C39-C40	-5.23	106.16	115.23
2	D	323	8PP	C32-C33-C34	-5.20	115.73	127.62
2	B	321	8PP	C12-C13-C14	-5.12	115.91	127.62
2	D	323	8PP	C41-C39-C40	-4.93	106.67	115.23
2	B	321	8PP	C10-C9-C11	4.90	123.73	115.23
2	B	321	8PP	C7-C8-C9	-4.87	120.45	127.42
2	C	322	8PP	C11-C9-C8	-4.84	110.30	121.17
2	D	323	8PP	C22-C23-C24	-4.65	116.98	127.62
2	A	320	8PP	C16-C14-C13	-4.62	110.81	121.17
2	A	320	8PP	C22-C23-C24	-4.61	117.08	127.62
2	B	321	8PP	C30-C29-C31	-4.40	107.58	115.23
2	C	322	8PP	C22-C23-C24	-4.40	117.55	127.62
2	B	321	8PP	C15-C14-C13	-4.39	112.34	123.63
2	B	321	8PP	C22-C23-C24	-4.35	117.66	127.62
2	A	320	8PP	C36-C34-C33	-4.33	111.44	121.17
2	B	321	8PP	C36-C34-C33	-4.16	111.84	121.17
2	D	323	8PP	C36-C34-C33	-4.15	111.85	121.17
2	A	320	8PP	C35-C34-C36	4.09	122.33	115.23
2	C	322	8PP	C36-C34-C33	-4.04	112.10	121.17
2	C	322	8PP	C35-C34-C36	3.91	122.01	115.23
2	A	320	8PP	C10-C9-C8	3.90	133.63	123.63
2	C	322	8PP	C37-C38-C39	-3.87	118.76	127.62
2	D	323	8PP	C15-C14-C13	-3.85	113.73	123.63
2	A	320	8PP	C41-C39-C38	3.85	133.52	123.63
2	B	321	8PP	C35-C34-C36	3.85	121.91	115.23
2	D	323	8PP	C35-C34-C36	3.83	121.87	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	321	8PP	C11-C9-C8	-3.77	112.71	121.17
2	A	320	8PP	C11-C9-C8	-3.76	112.72	121.17
2	D	323	8PP	C37-C38-C39	-3.69	119.17	127.62
2	B	321	8PP	C41-C39-C38	3.69	133.11	123.63
2	A	320	8PP	C17-C16-C14	3.66	125.30	113.19
2	C	322	8PP	C41-C39-C38	3.65	132.99	123.63
2	D	323	8PP	C10-C9-C8	3.61	132.91	123.63
2	C	322	8PP	C15-C14-C13	-3.61	114.37	123.63
2	A	320	8PP	C37-C38-C39	-3.58	119.44	127.62
2	B	321	8PP	C37-C38-C39	-3.55	119.49	127.62
2	D	323	8PP	C41-C39-C38	3.55	132.74	123.63
2	D	323	8PP	C11-C9-C8	-3.38	113.58	121.17
2	B	321	8PP	C2-C7-C8	3.29	119.77	112.67
2	B	321	8PP	C17-C18-C19	-3.15	120.41	127.62
2	D	323	8PP	C17-C18-C19	-3.08	120.58	127.62
2	A	320	8PP	C17-C18-C19	-2.97	120.83	127.62
2	B	321	8PP	C12-C11-C9	2.94	122.92	113.19
2	C	322	8PP	C16-C14-C13	-2.87	114.72	121.17
2	D	323	8PP	C26-C24-C23	2.75	127.35	121.17
2	C	322	8PP	C30-C29-C31	-2.73	110.48	115.23
2	D	323	8PP	C16-C14-C13	-2.70	115.09	121.17
2	B	321	8PP	C26-C24-C23	2.68	127.19	121.17
2	A	320	8PP	C26-C24-C23	2.63	127.08	121.17
2	C	322	8PP	C26-C24-C23	2.54	126.87	121.17
2	D	323	8PP	C30-C29-C31	-2.47	110.94	115.23
2	B	321	8PP	C4-C5-C6	-2.42	117.26	120.24
2	B	321	8PP	C30-C29-C28	2.21	129.31	123.63
2	C	322	8PP	C4-C5-C6	-2.21	117.51	120.24
2	C	322	8PP	C2-C7-C8	-2.20	107.93	112.67
2	A	320	8PP	C12-C13-C14	2.17	132.58	127.62
2	A	320	8PP	C15-C14-C13	-2.14	118.13	123.63
2	C	322	8PP	C20-C19-C18	-2.07	118.32	123.63
2	A	320	8PP	C4-C5-C6	-2.02	117.74	120.24
2	D	323	8PP	C4-C5-C6	-2.02	117.74	120.24

There are no chirality outliers.

All (43) 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

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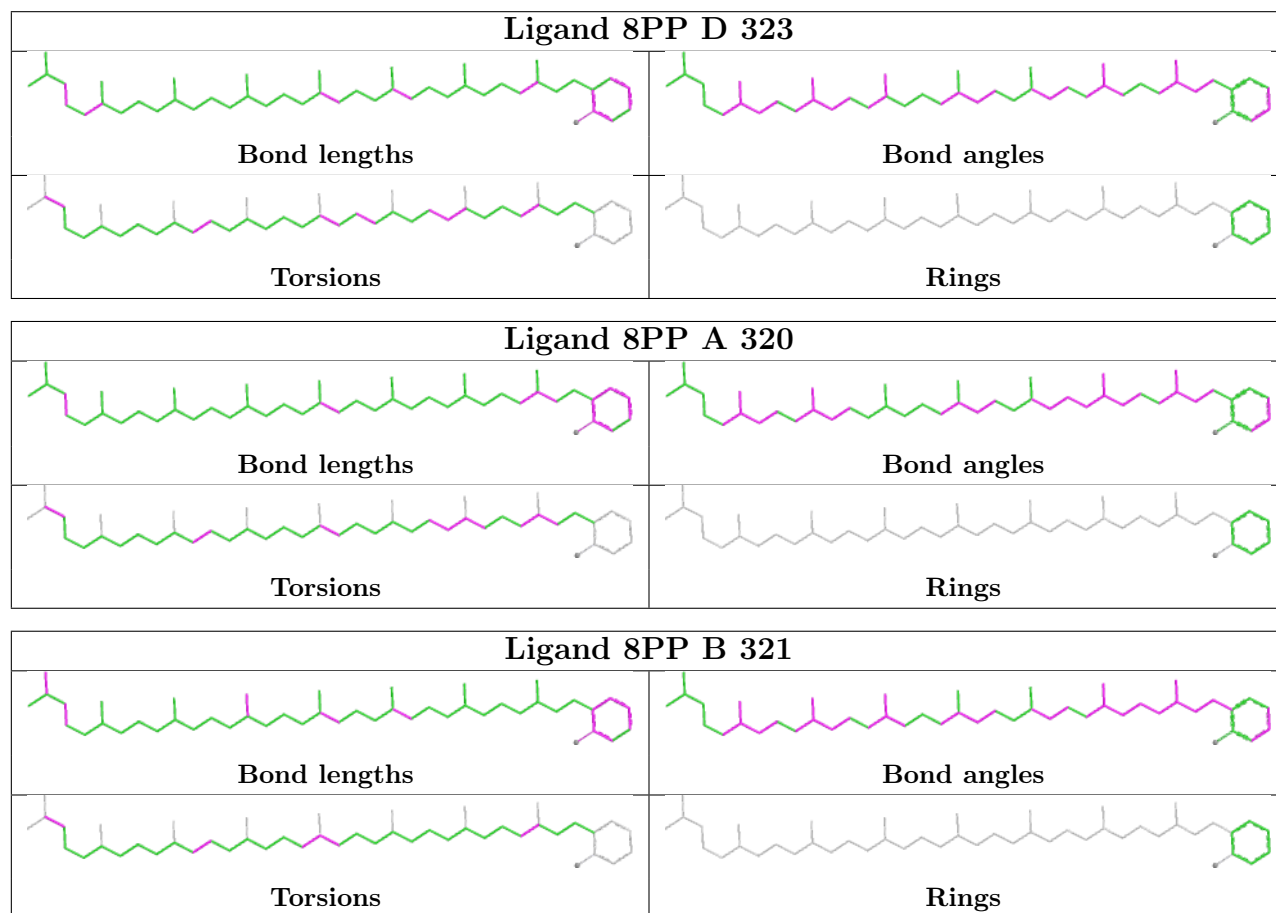
Mol	Chain	Res	Type	Atoms
2	B	321	8PP	C22-C23-C24-C25
2	B	321	8PP	C22-C23-C24-C26
2	C	322	8PP	C22-C23-C24-C25
2	C	322	8PP	C22-C23-C24-C26
2	D	323	8PP	C22-C23-C24-C25
2	D	323	8PP	C22-C23-C24-C26
2	A	320	8PP	C42-C43-C44-C45
2	C	322	8PP	C42-C43-C44-C45
2	A	320	8PP	C12-C13-C14-C15
2	C	322	8PP	C12-C13-C14-C15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

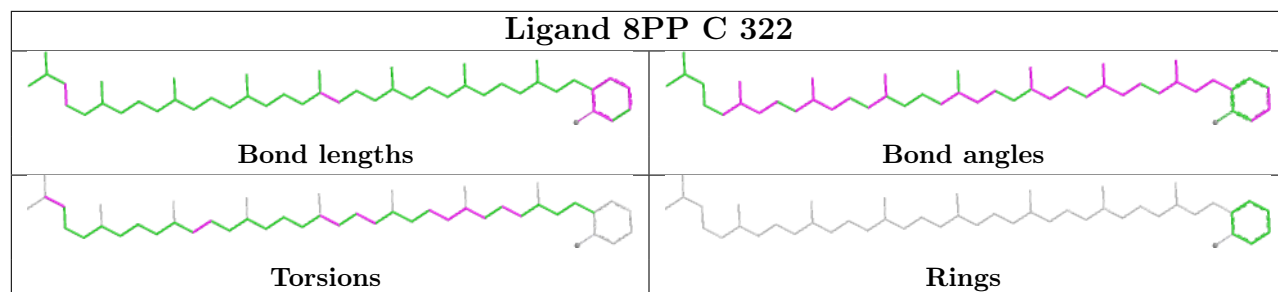
There are no ring outliers.

4 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	323	8PP	10	0
2	A	320	8PP	8	0
2	B	321	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

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	169/191 (88%)	0.09	8 (4%) 36 33	17, 32, 64, 75	0
1	B	169/191 (88%)	0.11	6 (3%) 46 43	18, 30, 50, 71	0
1	C	169/191 (88%)	-0.04	5 (2%) 52 49	16, 27, 44, 68	0
1	D	169/191 (88%)	0.15	6 (3%) 46 43	15, 33, 56, 69	0
All	All	676/764 (88%)	0.08	25 (3%) 45 42	15, 31, 54, 75	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	TRP	5.4
1	B	115	ASP	4.5
1	C	116	GLY	3.9
1	A	67	ALA	3.5
1	A	117	ASP	3.4
1	D	191	LYS	3.2
1	A	66	PRO	3.2
1	A	116	GLY	3.1
1	B	118	GLU	3.1
1	A	68	ALA	2.9
1	D	146	ASP	2.9
1	C	117	ASP	2.9
1	B	191	LYS	2.8
1	A	115	ASP	2.7
1	A	146	ASP	2.7
1	B	111	SER	2.7
1	A	65	ASN	2.5
1	D	145	ASP	2.4
1	B	146	ASP	2.3
1	C	191	LYS	2.3
1	B	30	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	90	HIS	2.1
1	C	146	ASP	2.0
1	C	161	ILE	2.0
1	D	147	PRO	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](#)

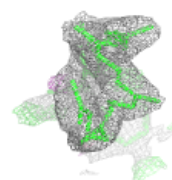
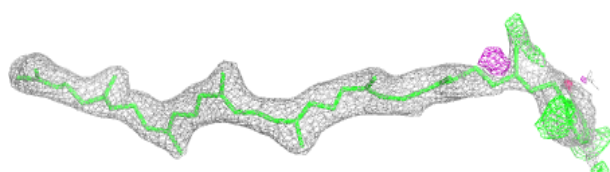
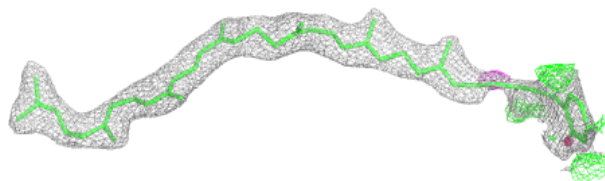
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	8PP	D	323	47/47	0.83	0.14	27,36,67,70	0
2	8PP	A	320	47/47	0.85	0.13	21,33,53,56	0
2	8PP	C	322	47/47	0.86	0.13	28,35,64,65	0
2	8PP	B	321	47/47	0.88	0.11	19,30,43,75	0

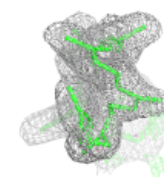
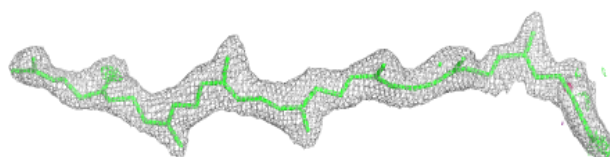
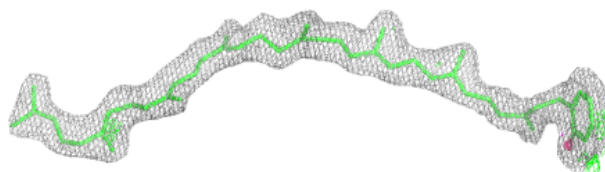
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8PP D 323:

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

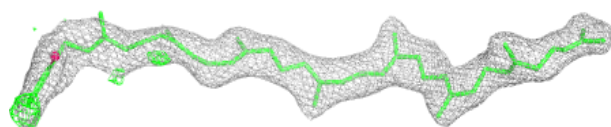
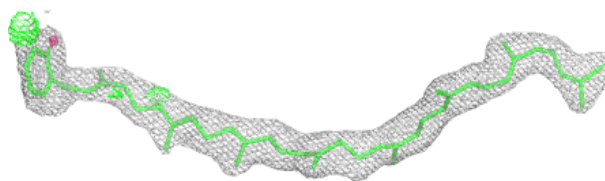
**Electron density around 8PP A 320:**

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

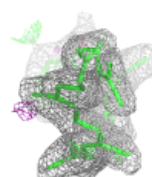
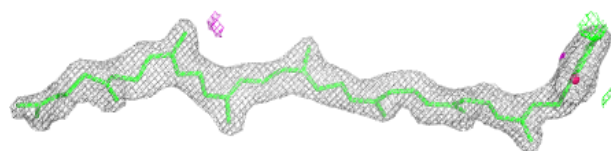
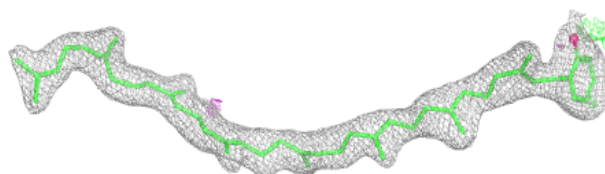


Electron density around 8PP C 322:

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

**Electron density around 8PP B 321:**

$2mF_o-DF_c$ (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.