



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:39 PM UTC

PDB ID : 4K8N / pdb_00004k8n
Title : Crystal structure of human ceramide-1-phosphate transfer protein (CPTP) in complex with 18:1 Ceramide-1-Phosphate (18:1-C1P)
Authors : Simanshu, D.K.; Brown, R.E.; Patel, D.J.
Deposited on : 2013-04-18
Resolution : 3.10 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

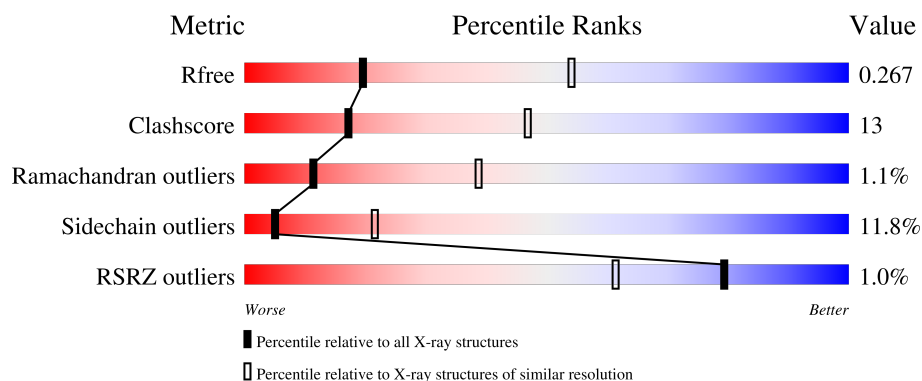
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	215	 70% 23% . .
1	B	215	 73% 19% . .
1	C	215	 51% 37% 7% .
1	D	215	 66% 26% . .
1	E	215	 67% 26% . .

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Mol	Chain	Length	Quality of chain
1	F	215	4% 53% 35% 7% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10099 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.

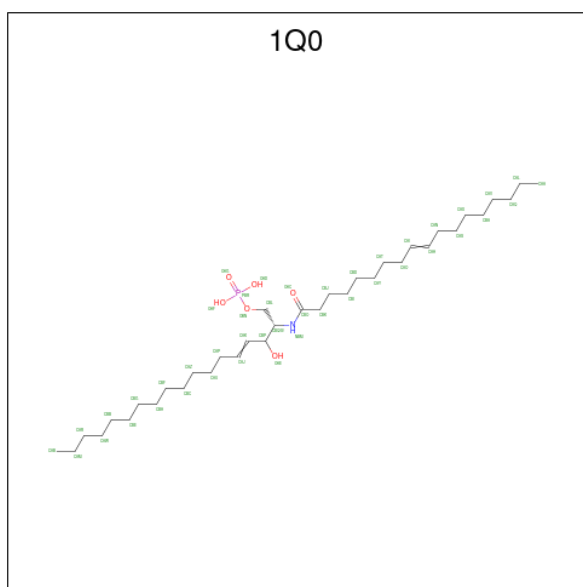
- Molecule 1 is a protein called Glycolipid transfer protein domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1659	1060	295	296	8			
1	B	206	Total	C	N	O	S	0	0	0
			1644	1048	293	295	8			
1	C	206	Total	C	N	O	S	0	0	0
			1637	1045	293	291	8			
1	D	206	Total	C	N	O	S	0	0	0
			1651	1051	297	295	8			
1	E	207	Total	C	N	O	S	0	0	0
			1653	1055	296	294	8			
1	F	205	Total	C	N	O	S	0	0	0
			1621	1037	288	288	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q5TA50
B	0	SER	-	expression tag	UNP Q5TA50
C	0	SER	-	expression tag	UNP Q5TA50
D	0	SER	-	expression tag	UNP Q5TA50
E	0	SER	-	expression tag	UNP Q5TA50
F	0	SER	-	expression tag	UNP Q5TA50

- Molecule 2 is (2S,3R,4Z)-3-hydroxy-2-[(9E)-octadec-9-enoylamino]octadec-4-en-1-yl dihydrogen phosphate (CCD ID: 1Q0) (formula: C₃₆H₇₀NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	36	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			27	19	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			44	36	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			44	36	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			44	36	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

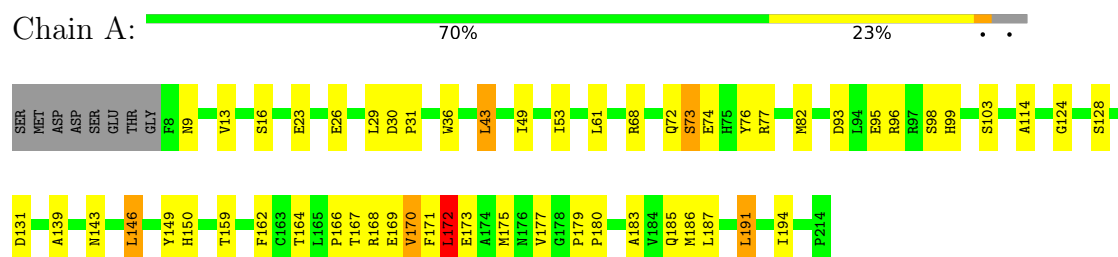
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		
3	C	3	Total	O	0	0
			3	3		
3	D	2	Total	O	0	0
			2	2		
3	E	3	Total	O	0	0
			3	3		

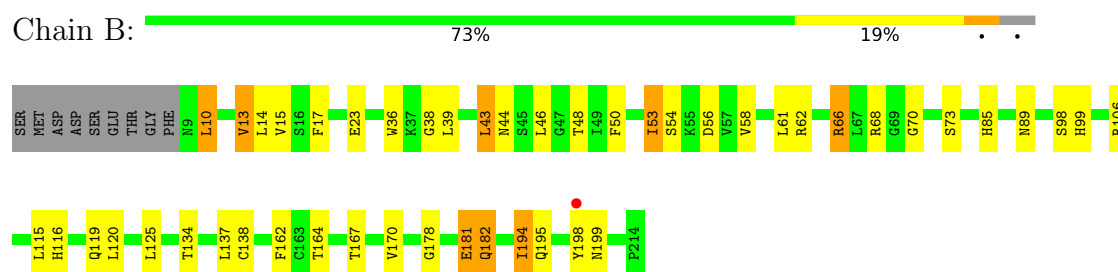
3 Residue-property plots [i](#)

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: Glycolipid transfer protein domain-containing protein 1



- Molecule 1: Glycolipid transfer protein domain-containing protein 1

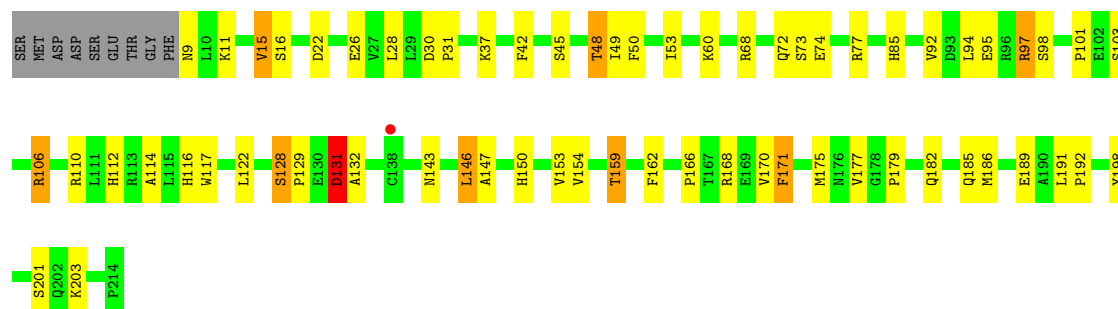


- Molecule 1: Glycolipid transfer protein domain-containing protein 1



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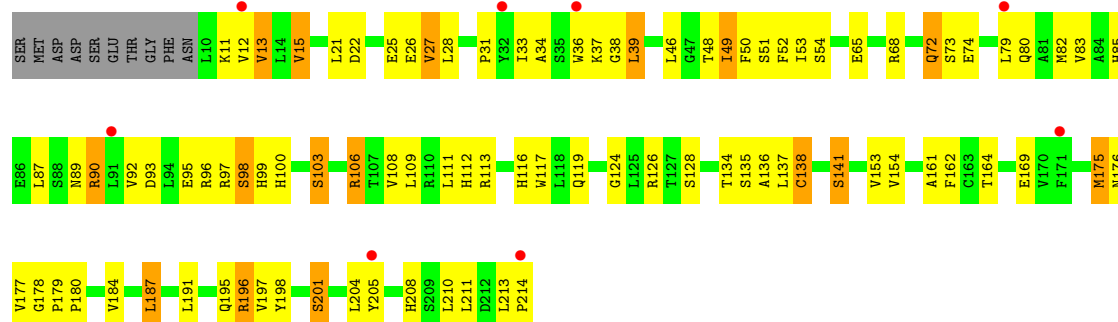




- Molecule 1: Glycolipid transfer protein domain-containing protein 1



- Molecule 1: Glycolipid transfer protein domain-containing protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	236.98Å 128.76Å 66.66Å 90.00° 93.53° 90.00°	Depositor
Resolution (Å)	30.05 – 3.10 30.05 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.05-3.10) 94.3 (30.05-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 3.11Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.225 , 0.263 0.231 , 0.267	Depositor DCC
R_{free} test set	1786 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	65.9	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10099	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: 1Q0

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	0.37	0/1697	0.82	3/2301 (0.1%)
1	B	0.37	0/1681	0.86	4/2281 (0.2%)
1	C	0.35	0/1674	0.86	4/2272 (0.2%)
1	D	0.35	0/1688	0.86	5/2288 (0.2%)
1	E	0.34	0/1691	0.82	0/2295
1	F	0.36	0/1658	0.92	3/2252 (0.1%)
All	All	0.36	0/10089	0.86	19/13689 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	48	THR	CB-CA-C	-7.93	106.36	115.79
1	C	165	LEU	CB-CA-C	7.46	122.96	109.45
1	D	177	VAL	N-CA-C	-7.45	105.45	112.83
1	F	178	GLY	CA-C-N	6.90	127.48	120.38
1	F	178	GLY	C-N-CA	6.90	127.48	120.38
1	D	131	ASP	CB-CA-C	-6.65	98.07	109.65
1	B	66	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	D	16	SER	N-CA-C	-6.51	105.34	113.28
1	C	98	SER	N-CA-C	5.89	123.35	110.80
1	B	178	GLY	CA-C-N	5.78	126.34	120.38
1	B	178	GLY	C-N-CA	5.78	126.34	120.38
1	C	137	LEU	N-CA-C	-5.68	106.99	114.04
1	B	66	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	D	179	PRO	CA-C-N	5.32	124.96	119.05
1	D	179	PRO	C-N-CA	5.32	124.96	119.05
1	A	179	PRO	CA-C-N	5.21	124.66	119.24
1	A	179	PRO	C-N-CA	5.21	124.66	119.24
1	A	172	LEU	N-CA-C	5.04	116.77	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	GLU	N-CA-C	-5.00	107.13	113.18

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	1659	0	1670	31	0
1	B	1644	0	1650	27	0
1	C	1637	0	1644	56	0
1	D	1651	0	1663	40	0
1	E	1653	0	1655	37	0
1	F	1621	0	1622	55	0
2	A	44	0	68	9	0
2	B	27	0	28	5	0
2	C	44	0	68	1	0
2	D	44	0	68	9	0
2	E	44	0	68	12	0
2	F	16	0	8	3	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	1	0
All	All	10099	0	10212	255	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 13.

All (255) 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)
2:E:301:1Q0:CAO	2:E:301:1Q0:H68	2.09	0.83
1:C:64:MET:HE1	1:C:104:GLY:HA2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:HD12	2:D:301:1Q0:H38	1.65	0.77
1:A:53:ILE:HD12	2:A:301:1Q0:H40	1.66	0.77
1:E:117:TRP:CH2	2:E:301:1Q0:H8	2.23	0.73
1:F:191:LEU:HG	1:F:195:GLN:HE22	1.53	0.73
1:C:25:GLU:OE1	1:C:196:ARG:NH2	2.23	0.70
1:B:58:VAL:HA	1:B:61:LEU:HD12	1.72	0.70
1:D:74:GLU:O	1:D:77:ARG:NH1	2.26	0.69
1:B:195:GLN:O	1:B:199:ASN:ND2	2.25	0.69
2:E:301:1Q0:H68	2:E:301:1Q0:H44	1.74	0.69
1:F:113:ARG:NH2	1:F:211:LEU:O	2.28	0.67
1:B:119:GLN:HG3	1:B:195:GLN:HG2	1.76	0.66
1:A:114:ALA:HB1	2:A:301:1Q0:H42	1.77	0.66
1:F:37:LYS:NZ	1:F:65:GLU:OE2	2.29	0.66
1:D:128:SER:HB3	1:D:168:ARG:HE	1.60	0.65
2:E:301:1Q0:H68	2:E:301:1Q0:H45	1.79	0.65
1:C:143:ASN:HA	1:C:147:ALA:HB3	1.78	0.65
2:A:301:1Q0:H55	2:A:301:1Q0:CAI	2.28	0.64
1:F:79:LEU:HA	1:F:82:MET:HB3	1.80	0.64
1:C:195:GLN:O	1:C:199:ASN:ND2	2.31	0.63
1:C:30:ASP:OD1	1:C:30:ASP:N	2.30	0.63
1:B:13:VAL:HG21	1:B:38:GLY:HA3	1.79	0.63
1:C:126:ARG:NH1	1:C:187:LEU:O	2.33	0.62
1:F:135:SER:HB2	1:F:162:PHE:HD1	1.63	0.62
1:D:48:THR:OG1	1:D:49:ILE:N	2.30	0.62
1:C:139:ALA:O	1:C:143:ASN:ND2	2.32	0.61
1:D:122:LEU:HD21	2:D:301:1Q0:H63	1.83	0.61
1:B:85:HIS:O	1:B:89:ASN:ND2	2.33	0.61
1:A:26:GLU:OE1	1:A:77:ARG:NH2	2.34	0.60
1:C:9:ASN:OD1	1:C:41:ARG:NH2	2.32	0.60
1:A:149:TYR:OH	1:B:182:GLN:NE2	2.25	0.60
2:F:301:1Q0:OAC	2:F:301:1Q0:H29	2.02	0.59
1:C:22:ASP:OD1	1:C:26:GLU:N	2.35	0.58
1:F:49:ILE:HG13	1:F:50:PHE:N	2.14	0.58
1:B:98:SER:OG	1:B:99:HIS:N	2.37	0.58
1:C:147:ALA:O	1:C:155:ARG:NE	2.21	0.58
1:B:116:HIS:HB2	1:B:198:TYR:CE1	2.39	0.57
1:C:98:SER:OG	1:C:99:HIS:N	2.30	0.57
1:E:150:HIS:HE1	2:E:301:1Q0:H16	1.69	0.57
1:B:70:GLY:O	1:B:73:SER:OG	2.23	0.57
1:E:175:MET:HE2	2:E:301:1Q0:H61	1.86	0.57
1:F:33:ILE:HD13	1:F:65:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:SER:O	1:F:54:SER:OG	2.23	0.56
1:F:93:ASP:HB3	1:F:96:ARG:O	2.04	0.56
1:E:116:HIS:HB2	1:E:198:TYR:CE1	2.40	0.56
1:C:40:VAL:HG13	1:C:54:SER:HB3	1.88	0.56
1:B:39:LEU:HD23	2:B:301:1Q0:H50	1.88	0.55
1:B:36:TRP:HB3	1:B:61:LEU:HD21	1.88	0.55
1:B:125:LEU:HA	1:B:137:LEU:HD13	1.88	0.55
2:B:301:1Q0:OBN	2:B:301:1Q0:OAE	2.22	0.55
1:C:13:VAL:O	1:C:16:SER:OG	2.25	0.55
1:D:30:ASP:OD1	1:D:68:ARG:NE	2.40	0.55
1:A:169:GLU:O	1:A:172:LEU:N	2.38	0.55
1:D:146:LEU:HG	1:D:150:HIS:HE1	1.71	0.55
1:D:146:LEU:O	1:D:150:HIS:ND1	2.37	0.55
1:F:72:GLN:HE21	1:F:85:HIS:CE1	2.25	0.54
2:A:301:1Q0:H55	2:A:301:1Q0:H46	1.89	0.54
1:D:97:ARG:HH21	1:D:106:ARG:HH12	1.53	0.54
2:A:301:1Q0:H46	2:A:301:1Q0:CAX	2.38	0.54
1:B:116:HIS:HB2	1:B:198:TYR:CZ	2.43	0.54
1:F:21:LEU:HB2	1:F:197:VAL:HG12	1.90	0.54
1:D:106:ARG:NH2	2:D:301:1Q0:OAF	2.40	0.54
1:A:114:ALA:HB2	2:A:301:1Q0:H70	1.90	0.54
1:A:13:VAL:O	1:A:16:SER:OG	2.25	0.53
1:C:126:ARG:HG3	1:C:187:LEU:HB2	1.90	0.53
1:A:146:LEU:HB3	1:A:150:HIS:CE1	2.44	0.53
1:E:14:LEU:HG	1:E:190:ALA:HB2	1.89	0.53
1:E:126:ARG:HG3	1:E:127:THR:H	1.73	0.53
1:A:68:ARG:NH1	1:A:73:SER:O	2.42	0.53
1:C:64:MET:HE2	1:C:64:MET:HA	1.90	0.53
1:A:187:LEU:O	1:A:191:LEU:HB2	2.09	0.53
1:F:25:GLU:OE2	1:F:196:ARG:NH2	2.42	0.53
2:A:301:1Q0:CAI	2:A:301:1Q0:CAX	2.87	0.52
1:F:68:ARG:NH1	1:F:73:SER:O	2.42	0.52
1:B:56:ASP:OD2	2:B:301:1Q0:H24	2.09	0.52
1:C:64:MET:HE2	1:C:67:LEU:HD12	1.92	0.52
1:C:9:ASN:N	1:C:175:MET:O	2.42	0.52
1:E:194:ILE:O	1:E:197:VAL:N	2.42	0.52
1:E:150:HIS:NE2	2:E:301:1Q0:OAC	2.24	0.51
1:C:14:LEU:HB3	1:C:190:ALA:HB1	1.92	0.51
1:E:195:GLN:O	1:E:199:ASN:ND2	2.43	0.51
1:B:56:ASP:OD2	2:B:301:1Q0:NBM	2.44	0.51
1:C:19:GLN:OE1	1:C:19:GLN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:HA	1:C:175:MET:HE3	1.91	0.51
1:E:129:PRO:HB3	3:E:402:HOH:O	2.10	0.51
1:A:128:SER:OG	1:A:168:ARG:NE	2.42	0.51
1:B:181:GLU:OE2	1:E:96:ARG:NH1	2.43	0.51
1:A:159:THR:HA	1:A:162:PHE:CD2	2.45	0.51
1:C:179:PRO:C	1:C:181:GLU:H	2.20	0.50
1:D:9:ASN:OD1	1:D:11:LYS:N	2.45	0.50
1:E:39:LEU:HB3	2:E:301:1Q0:H53	1.93	0.50
1:C:10:LEU:HD23	1:C:175:MET:SD	2.52	0.50
1:C:28:LEU:HB2	1:C:31:PRO:HG2	1.94	0.50
1:E:8:PHE:O	1:E:10:LEU:N	2.45	0.50
1:F:13:VAL:HG21	1:F:38:GLY:HA3	1.94	0.49
1:E:126:ARG:HH21	1:E:188:GLY:HA3	1.77	0.49
1:A:139:ALA:O	1:A:143:ASN:ND2	2.42	0.49
1:E:117:TRP:HH2	2:E:301:1Q0:H4	1.78	0.49
1:E:150:HIS:CE1	2:E:301:1Q0:H16	2.47	0.49
1:C:205:TYR:HB3	1:C:211:LEU:HD23	1.95	0.49
1:F:210:LEU:HD23	1:F:213:LEU:HD11	1.94	0.49
1:D:150:HIS:HB3	1:D:154:VAL:CG2	2.42	0.49
1:B:13:VAL:CG2	1:B:38:GLY:HA3	2.43	0.49
1:D:30:ASP:HB2	1:D:31:PRO:HD3	1.95	0.49
1:A:53:ILE:CD1	2:A:301:1Q0:H40	2.40	0.49
1:D:131:ASP:OD1	1:D:131:ASP:N	2.46	0.49
1:F:93:ASP:CG	1:F:100:HIS:H	2.21	0.48
1:B:43:LEU:HD22	1:B:50:PHE:HB3	1.95	0.48
1:F:112:HIS:CE1	1:F:201:SER:HB2	2.48	0.48
1:F:126:ARG:HD2	1:F:187:LEU:HD23	1.94	0.48
1:D:101:PRO:O	1:D:106:ARG:NH1	2.46	0.48
1:D:72:GLN:HG2	1:D:85:HIS:CE1	2.49	0.47
1:D:117:TRP:CH2	2:D:301:1Q0:H66	2.49	0.47
1:F:175:MET:H	1:F:175:MET:HG2	1.54	0.47
1:C:50:PHE:O	1:C:53:ILE:HG12	2.14	0.47
1:F:177:VAL:O	1:F:179:PRO:HD2	2.13	0.47
1:A:36:TRP:HB3	1:A:61:LEU:HD11	1.96	0.47
1:D:129:PRO:HG2	1:D:132:ALA:HB2	1.97	0.47
1:F:116:HIS:O	1:F:119:GLN:HG2	2.14	0.47
1:D:50:PHE:O	1:D:53:ILE:HG12	2.14	0.47
1:A:172:LEU:HD23	1:A:180:PRO:HB3	1.95	0.47
1:A:191:LEU:O	1:A:194:ILE:HG22	2.14	0.47
1:F:135:SER:HB2	1:F:162:PHE:CD1	2.48	0.47
1:A:166:PRO:HD2	1:A:171:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:VAL:O	1:E:16:SER:OG	2.32	0.47
1:C:41:ARG:HA	1:C:44:ASN:HB2	1.97	0.47
2:D:301:1Q0:H44	2:D:301:1Q0:H51	1.71	0.47
1:F:28:LEU:HB3	1:F:31:PRO:HD2	1.96	0.47
1:C:134:THR:HA	1:C:137:LEU:HD23	1.96	0.47
1:B:167:THR:OG1	1:B:170:VAL:HG23	2.15	0.46
1:C:141:SER:O	1:C:145:SER:OG	2.33	0.46
1:A:131:ASP:N	1:A:131:ASP:OD1	2.47	0.46
1:E:126:ARG:NH2	1:E:188:GLY:HA3	2.30	0.46
1:F:134:THR:O	1:F:138:CYS:HB2	2.15	0.46
1:C:62:ARG:O	1:C:66:ARG:HG2	2.15	0.46
1:D:153:VAL:HG21	2:F:301:1Q0:H26	1.97	0.46
1:F:87:LEU:HD12	1:F:92:VAL:HG21	1.98	0.46
1:F:205:TYR:CD1	1:F:210:LEU:HD22	2.51	0.46
1:A:74:GLU:HG3	1:D:74:GLU:HB2	1.97	0.46
1:C:138:CYS:O	1:C:142:TYR:N	2.46	0.46
1:E:125:LEU:HA	1:E:137:LEU:HD13	1.97	0.46
1:A:43:LEU:HG	2:A:301:1Q0:H54	1.98	0.46
1:D:60:LYS:CE	2:D:301:1Q0:H30	2.46	0.46
1:E:123:GLU:O	1:E:126:ARG:HG3	2.16	0.46
1:C:116:HIS:HB2	1:C:198:TYR:CE1	2.51	0.46
1:D:42:PHE:HZ	1:D:175:MET:HA	1.81	0.46
1:D:116:HIS:HB2	1:D:198:TYR:CE1	2.51	0.46
1:D:112:HIS:CE1	1:D:201:SER:HB2	2.52	0.45
1:F:137:LEU:O	1:F:141:SER:OG	2.33	0.45
1:F:187:LEU:HG	1:F:191:LEU:HB2	1.97	0.45
1:F:103:SER:O	1:F:106:ARG:HG3	2.15	0.45
1:F:50:PHE:CE1	1:F:161:ALA:HB1	2.51	0.45
1:C:115:LEU:HD12	1:C:115:LEU:HA	1.83	0.45
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.85	0.45
1:F:72:GLN:HE21	1:F:85:HIS:HE1	1.65	0.45
1:D:159:THR:O	1:D:162:PHE:HB2	2.17	0.45
1:B:53:ILE:HB	2:B:301:1Q0:CAU	2.46	0.44
1:E:63:ILE:HD13	1:E:102:GLU:HB3	1.98	0.44
1:F:22:ASP:HB3	1:F:26:GLU:HG3	1.99	0.44
2:F:301:1Q0:CAJ	2:F:301:1Q0:NBM	2.78	0.44
1:C:78:SER:OG	1:C:79:LEU:N	2.49	0.44
1:F:36:TRP:HA	1:F:39:LEU:HD22	1.99	0.44
2:D:301:1Q0:H36	2:D:301:1Q0:H20	2.00	0.44
1:E:12:VAL:HA	1:E:15:VAL:HG13	1.98	0.44
1:E:52:PHE:CE1	1:E:53:ILE:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ARG:NH2	1:F:214:PRO:OXT	2.36	0.44
1:A:124:GLY:O	1:A:128:SER:HB3	2.18	0.44
1:A:9:ASN:HB2	1:A:175:MET:O	2.18	0.44
1:A:23:GLU:CD	1:A:23:GLU:H	2.26	0.44
1:D:186:MET:HE3	1:D:186:MET:HB3	1.95	0.44
1:C:24:LYS:HE2	1:C:24:LYS:HB3	1.63	0.44
1:C:64:MET:CE	1:C:104:GLY:HA2	2.40	0.44
1:C:74:GLU:CD	1:C:74:GLU:H	2.26	0.44
1:D:146:LEU:HD12	1:D:146:LEU:HA	1.83	0.44
1:D:106:ARG:HE	1:D:106:ARG:HB2	1.60	0.44
1:E:146:LEU:HG	1:E:150:HIS:CE1	2.52	0.44
1:F:49:ILE:O	1:F:52:PHE:N	2.50	0.44
1:F:80:GLN:CD	1:F:204:LEU:HD21	2.43	0.44
1:F:169:GLU:OE1	1:F:169:GLU:N	2.48	0.44
1:E:179:PRO:HB2	1:E:182:GLN:OE1	2.18	0.43
1:C:112:HIS:CE1	1:C:201:SER:HB2	2.54	0.43
1:B:44:ASN:C	1:B:46:LEU:H	2.26	0.43
1:D:28:LEU:O	1:D:31:PRO:HD2	2.18	0.43
1:B:10:LEU:O	1:B:13:VAL:N	2.48	0.43
1:B:15:VAL:C	1:B:17:PHE:H	2.27	0.43
1:E:60:LYS:NZ	2:E:301:1Q0:OAF	2.52	0.43
1:C:80:GLN:HG3	1:C:204:LEU:HD22	1.99	0.43
1:F:27:VAL:HG13	1:F:79:LEU:HG	2.00	0.43
1:C:78:SER:OG	1:C:80:GLN:OE1	2.30	0.43
1:D:114:ALA:HB1	2:D:301:1Q0:H40	2.00	0.43
1:F:82:MET:O	1:F:85:HIS:N	2.51	0.43
1:C:43:LEU:HG	2:C:301:1Q0:H54	2.01	0.43
1:C:96:ARG:O	1:C:98:SER:N	2.52	0.43
1:D:117:TRP:CH2	2:D:301:1Q0:CAW	3.02	0.43
1:E:56:ASP:O	1:E:60:LYS:HG2	2.18	0.43
1:F:72:GLN:H	1:F:72:GLN:HG2	1.68	0.43
1:A:93:ASP:HB3	1:A:96:ARG:O	2.19	0.42
1:C:191:LEU:O	1:C:195:GLN:HB2	2.19	0.42
1:C:16:SER:C	1:C:18:LYS:H	2.27	0.42
1:A:167:THR:OG1	1:A:170:VAL:HG23	2.19	0.42
1:C:83:VAL:O	1:C:87:LEU:HB2	2.19	0.42
1:C:24:LYS:H	1:C:24:LYS:HG2	1.48	0.42
1:C:124:GLY:O	1:C:128:SER:HB3	2.20	0.42
1:D:60:LYS:HE3	1:D:110:ARG:HG2	2.02	0.42
1:C:62:ARG:HH11	1:C:62:ARG:HG3	1.85	0.42
1:A:172:LEU:HD12	1:A:175:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:LEU:HD22	1:F:213:LEU:HD13	2.02	0.42
1:F:179:PRO:HA	1:F:180:PRO:HD2	1.87	0.42
1:F:195:GLN:HA	1:F:198:TYR:HB3	2.02	0.42
1:C:36:TRP:CZ2	1:C:115:LEU:HD13	2.55	0.42
1:E:8:PHE:O	1:E:10:LEU:HD22	2.19	0.42
1:F:124:GLY:O	1:F:128:SER:HB3	2.19	0.42
1:D:143:ASN:HA	1:D:147:ALA:HB3	2.02	0.42
1:D:166:PRO:HD2	1:D:171:PHE:HE1	1.85	0.42
1:B:17:PHE:CD2	1:B:194:ILE:HG12	2.54	0.42
1:C:119:GLN:O	1:C:123:GLU:HB3	2.20	0.42
1:F:90:ARG:HD3	1:F:90:ARG:HA	1.72	0.42
1:C:90:ARG:HD3	1:E:208:HIS:O	2.20	0.41
1:C:116:HIS:O	1:C:120:LEU:HB2	2.19	0.41
2:E:301:1Q0:H42	2:E:301:1Q0:H50	2.02	0.41
1:A:98:SER:OG	1:A:99:HIS:N	2.53	0.41
1:D:182:GLN:HA	1:D:185:GLN:HB2	2.01	0.41
1:E:9:ASN:C	1:E:11:LYS:H	2.28	0.41
1:E:17:PHE:HD1	1:E:17:PHE:HA	1.73	0.41
1:D:128:SER:O	1:D:168:ARG:NH2	2.53	0.41
1:D:191:LEU:N	1:D:192:PRO:HD2	2.35	0.41
1:E:59:SER:O	1:E:62:ARG:HB2	2.21	0.41
1:F:79:LEU:O	1:F:83:VAL:HG23	2.21	0.41
1:F:187:LEU:HD21	1:F:191:LEU:HD22	2.01	0.41
1:F:135:SER:OG	1:F:136:ALA:N	2.53	0.41
1:A:76:TYR:CE1	1:A:82:MET:HG3	2.54	0.41
1:C:106:ARG:HG3	1:C:107:THR:N	2.34	0.41
1:E:190:ALA:O	1:E:194:ILE:HG13	2.20	0.41
1:A:30:ASP:HB2	1:A:31:PRO:HD3	2.01	0.41
1:C:142:TYR:O	1:C:145:SER:N	2.39	0.41
1:E:58:VAL:O	1:E:62:ARG:HG2	2.21	0.41
1:E:71:PRO:HB2	1:E:72:GLN:OE1	2.20	0.41
1:E:177:VAL:HG11	1:E:186:MET:SD	2.60	0.41
1:F:31:PRO:HA	1:F:34:ALA:HB3	2.02	0.41
1:F:117:TRP:NE1	1:F:141:SER:HB2	2.35	0.41
1:F:108:VAL:HA	1:F:111:LEU:HD12	2.02	0.41
1:B:53:ILE:HG13	1:B:54:SER:N	2.35	0.41
1:C:172:LEU:HD23	1:C:175:MET:HE3	2.03	0.41
1:D:22:ASP:OD1	1:D:26:GLU:N	2.45	0.41
1:E:87:LEU:HD23	1:E:87:LEU:HA	1.82	0.41
1:F:204:LEU:O	1:F:208:HIS:ND1	2.53	0.41
1:F:11:LYS:O	1:F:15:VAL:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:THR:O	1:F:164:THR:OG1	2.30	0.40
1:F:175:MET:O	1:F:176:ASN:HB2	2.19	0.40
1:C:76:TYR:CE1	1:C:82:MET:HG3	2.57	0.40
1:A:177:VAL:HG21	1:A:183:ALA:HA	2.04	0.40
1:B:138:CYS:HB3	1:B:162:PHE:CE2	2.56	0.40
1:D:11:LYS:O	1:D:15:VAL:HG23	2.21	0.40
1:C:49:ILE:H	1:C:49:ILE:HG12	1.58	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	205/215 (95%)	195 (95%)	9 (4%)	1 (0%)	24	57
1	B	204/215 (95%)	188 (92%)	15 (7%)	1 (0%)	24	57
1	C	204/215 (95%)	174 (85%)	23 (11%)	7 (3%)	3	16
1	D	204/215 (95%)	190 (93%)	13 (6%)	1 (0%)	24	57
1	E	205/215 (95%)	188 (92%)	14 (7%)	3 (2%)	8	32
1	F	203/215 (94%)	180 (89%)	22 (11%)	1 (0%)	24	57
All	All	1225/1290 (95%)	1115 (91%)	96 (8%)	14 (1%)	11	39

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	9	ASN
1	B	66	ARG
1	C	143	ASN
1	E	166	PRO
1	C	97	ARG

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Mol	Chain	Res	Type
1	C	186	MET
1	D	98	SER
1	C	17	PHE
1	C	166	PRO
1	C	188	GLY
1	F	98	SER
1	A	170	VAL
1	C	180	PRO
1	E	194	ILE

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	182/190 (96%)	168 (92%)	14 (8%)	12	38
1	B	180/190 (95%)	163 (91%)	17 (9%)	8	31
1	C	178/190 (94%)	150 (84%)	28 (16%)	2	12
1	D	181/190 (95%)	162 (90%)	19 (10%)	6	26
1	E	180/190 (95%)	158 (88%)	22 (12%)	5	20
1	F	175/190 (92%)	148 (85%)	27 (15%)	2	12
All	All	1076/1140 (94%)	949 (88%)	127 (12%)	5	21

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	43	LEU
1	A	49	ILE
1	A	72	GLN
1	A	73	SER
1	A	95	GLU
1	A	103	SER
1	A	146	LEU
1	A	164	THR

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Mol	Chain	Res	Type
1	A	172	LEU
1	A	173	GLU
1	A	185	GLN
1	A	186	MET
1	A	191	LEU
1	B	10	LEU
1	B	13	VAL
1	B	14	LEU
1	B	23	GLU
1	B	43	LEU
1	B	48	THR
1	B	53	ILE
1	B	62	ARG
1	B	68	ARG
1	B	106	ARG
1	B	115	LEU
1	B	120	LEU
1	B	134	THR
1	B	164	THR
1	B	181	GLU
1	B	182	GLN
1	B	194	ILE
1	C	14	LEU
1	C	23	GLU
1	C	24	LYS
1	C	25	GLU
1	C	26	GLU
1	C	30	ASP
1	C	43	LEU
1	C	48	THR
1	C	49	ILE
1	C	72	GLN
1	C	78	SER
1	C	95	GLU
1	C	115	LEU
1	C	120	LEU
1	C	134	THR
1	C	137	LEU
1	C	138	CYS
1	C	140	ASP
1	C	146	LEU
1	C	153	VAL

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Mol	Chain	Res	Type
1	C	164	THR
1	C	167	THR
1	C	182	GLN
1	C	184	VAL
1	C	191	LEU
1	C	195	GLN
1	C	197	VAL
1	C	200	VAL
1	D	15	VAL
1	D	37	LYS
1	D	45	SER
1	D	48	THR
1	D	73	SER
1	D	92	VAL
1	D	94	LEU
1	D	95	GLU
1	D	97	ARG
1	D	103	SER
1	D	106	ARG
1	D	128	SER
1	D	131	ASP
1	D	146	LEU
1	D	159	THR
1	D	170	VAL
1	D	171	PHE
1	D	189	GLU
1	D	203	LYS
1	E	10	LEU
1	E	15	VAL
1	E	16	SER
1	E	17	PHE
1	E	21	LEU
1	E	23	GLU
1	E	29	LEU
1	E	51	SER
1	E	53	ILE
1	E	78	SER
1	E	95	GLU
1	E	100	HIS
1	E	115	LEU
1	E	119	GLN
1	E	128	SER

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Mol	Chain	Res	Type
1	E	156	ARG
1	E	164	THR
1	E	168	ARG
1	E	170	VAL
1	E	186	MET
1	E	187	LEU
1	E	191	LEU
1	F	12	VAL
1	F	13	VAL
1	F	15	VAL
1	F	27	VAL
1	F	39	LEU
1	F	46	LEU
1	F	49	ILE
1	F	53	ILE
1	F	72	GLN
1	F	74	GLU
1	F	89	ASN
1	F	90	ARG
1	F	95	GLU
1	F	97	ARG
1	F	98	SER
1	F	99	HIS
1	F	103	SER
1	F	106	ARG
1	F	138	CYS
1	F	141	SER
1	F	153	VAL
1	F	154	VAL
1	F	175	MET
1	F	184	VAL
1	F	187	LEU
1	F	196	ARG
1	F	201	SER

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

Mol	Chain	Res	Type
1	A	100	HIS
1	B	19	GLN
1	C	112	HIS
1	C	185	GLN

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Mol	Chain	Res	Type
1	D	75	HIS
1	D	89	ASN
1	D	100	HIS
1	E	89	ASN
1	F	85	HIS
1	F	116	HIS
1	F	195	GLN

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 ⓘ

6 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	1Q0	F	301	-	14,15,43	1.13	2 (14%)	17,20,48	1.22	3 (17%)
2	1Q0	C	301	-	42,43,43	0.81	2 (4%)	45,48,48	0.83	3 (6%)
2	1Q0	A	301	-	42,43,43	0.82	2 (4%)	45,48,48	0.83	3 (6%)
2	1Q0	D	301	-	42,43,43	1.00	3 (7%)	45,48,48	1.04	4 (8%)
2	1Q0	B	301	-	25,26,43	1.06	2 (8%)	27,31,48	1.05	3 (11%)
2	1Q0	E	301	-	42,43,43	0.82	2 (4%)	45,48,48	0.83	3 (6%)

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	1Q0	F	301	-	-	11/17/17/46	-
2	1Q0	C	301	-	-	23/46/46/46	-
2	1Q0	A	301	-	-	19/46/46/46	-
2	1Q0	D	301	-	-	22/46/46/46	-
2	1Q0	B	301	-	-	13/29/29/46	-
2	1Q0	E	301	-	-	24/46/46/46	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	1Q0	CBO-NBM	3.95	1.42	1.34
2	E	301	1Q0	CBO-NBM	3.95	1.42	1.34
2	A	301	1Q0	CBO-NBM	3.94	1.42	1.34
2	C	301	1Q0	CBO-NBM	3.92	1.42	1.34
2	D	301	1Q0	CBQ-NBM	-3.44	1.40	1.46
2	D	301	1Q0	CBO-NBM	3.12	1.40	1.34
2	F	301	1Q0	CBO-NBM	2.47	1.42	1.34
2	E	301	1Q0	CBQ-NBM	-2.29	1.42	1.46
2	A	301	1Q0	CBQ-NBM	-2.29	1.42	1.46
2	B	301	1Q0	CBQ-NBM	-2.27	1.42	1.46
2	C	301	1Q0	CBQ-NBM	-2.22	1.42	1.46
2	F	301	1Q0	CBQ-NBM	-2.20	1.42	1.46
2	D	301	1Q0	OAE-CBP	-2.14	1.39	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	1Q0	CBP-CBQ-NBM	-3.10	104.41	109.66
2	F	301	1Q0	CBP-CAK-CAJ	-2.45	119.99	124.73
2	A	301	1Q0	CBK-CBO-NBM	2.36	120.02	115.86
2	D	301	1Q0	CBP-CAK-CAJ	-2.34	119.83	124.69
2	C	301	1Q0	CBK-CBO-NBM	2.34	119.99	115.86
2	E	301	1Q0	CBK-CBO-NBM	2.34	119.99	115.86
2	F	301	1Q0	CBK-CBO-NBM	2.34	119.99	116.12
2	B	301	1Q0	CBK-CBO-NBM	2.34	119.98	115.86
2	B	301	1Q0	CBP-CAK-CAJ	-2.29	119.94	124.69
2	A	301	1Q0	CBP-CAK-CAJ	-2.27	119.99	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	1Q0	CBP-CAK-CAJ	-2.27	119.99	124.69
2	E	301	1Q0	CBP-CAK-CAJ	-2.25	120.04	124.69
2	F	301	1Q0	CBQ-NBM-CBO	-2.17	119.99	122.90
2	D	301	1Q0	OAE-CBP-CAK	-2.15	105.31	110.88
2	D	301	1Q0	CBK-CBO-NBM	2.06	119.49	115.86
2	C	301	1Q0	CBQ-NBM-CBO	-2.05	119.99	123.40
2	E	301	1Q0	CBQ-NBM-CBO	-2.05	119.99	123.40
2	B	301	1Q0	CBQ-NBM-CBO	-2.05	119.99	123.40
2	A	301	1Q0	CBQ-NBM-CBO	-2.03	120.02	123.40

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	1Q0	CAK-CBP-CBQ-CBL
2	B	301	1Q0	OBN-CBL-CBQ-CBP
2	B	301	1Q0	OBN-CBL-CBQ-NBM
2	B	301	1Q0	CBL-OBN-PBR-OAG
2	C	301	1Q0	OBN-CBL-CBQ-NBM
2	C	301	1Q0	CBL-OBN-PBR-OAD
2	D	301	1Q0	OBN-CBL-CBQ-CBP
2	D	301	1Q0	OBN-CBL-CBQ-NBM
2	E	301	1Q0	CBL-OBN-PBR-OAF
2	E	301	1Q0	CBL-OBN-PBR-OAD
2	F	301	1Q0	CAP-CAJ-CAK-CBP
2	F	301	1Q0	CAJ-CAK-CBP-CBQ
2	F	301	1Q0	CBP-CBQ-NBM-CBO
2	F	301	1Q0	CBL-CBQ-NBM-CBO
2	F	301	1Q0	CBL-OBN-PBR-OAF
2	F	301	1Q0	CBL-OBN-PBR-OAD
2	E	301	1Q0	CBJ-CBK-CBO-NBM
2	E	301	1Q0	CBJ-CBK-CBO-OAC
2	F	301	1Q0	CAJ-CAK-CBP-OAE
2	D	301	1Q0	CBB-CBE-CBG-CBH
2	A	301	1Q0	CAM-CAR-CAW-CBB
2	C	301	1Q0	CAQ-CAV-CBA-CAX
2	A	301	1Q0	CAP-CAU-CAZ-CBC
2	D	301	1Q0	CAP-CAU-CAZ-CBC
2	C	301	1Q0	CAT-CAY-CBD-CBI
2	A	301	1Q0	CAZ-CBC-CBF-CBH
2	D	301	1Q0	CAQ-CAV-CBA-CAX
2	A	301	1Q0	CBB-CBE-CBG-CBH

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Mol	Chain	Res	Type	Atoms
2	D	301	1Q0	CAR-CAW-CBB-CBE
2	B	301	1Q0	CAT-CAY-CBD-CBI
2	C	301	1Q0	CBE-CBG-CBH-CBF
2	A	301	1Q0	CAL-CAQ-CAV-CBA
2	C	301	1Q0	CAL-CAQ-CAV-CBA
2	C	301	1Q0	CAU-CAZ-CBC-CBF
2	B	301	1Q0	CAI-CAH-CAN-CAS
2	C	301	1Q0	CBB-CBE-CBG-CBH
2	D	301	1Q0	CBC-CBF-CBH-CBG
2	D	301	1Q0	CAY-CBD-CBI-CBJ
2	D	301	1Q0	CAW-CBB-CBE-CBG
2	A	301	1Q0	CAK-CAJ-CAP-CAU
2	B	301	1Q0	CAH-CAI-CAO-CAT
2	D	301	1Q0	CAK-CAJ-CAP-CAU
2	E	301	1Q0	CAN-CAS-CAX-CBA
2	D	301	1Q0	CAZ-CBC-CBF-CBH
2	A	301	1Q0	CAU-CAZ-CBC-CBF
2	A	301	1Q0	CAI-CAO-CAT-CAY
2	E	301	1Q0	CAH-CAN-CAS-CAX
2	A	301	1Q0	CBD-CBI-CBJ-CBK
2	E	301	1Q0	CBB-CBE-CBG-CBH
2	D	301	1Q0	CBE-CBG-CBH-CBF
2	C	301	1Q0	CAI-CAO-CAT-CAY
2	C	301	1Q0	CAH-CAN-CAS-CAX
2	E	301	1Q0	CBL-OBN-PBR-OAG
2	C	301	1Q0	CAN-CAS-CAX-CBA
2	D	301	1Q0	CAT-CAY-CBD-CBI
2	C	301	1Q0	CBI-CBJ-CBK-CBO
2	E	301	1Q0	CAT-CAY-CBD-CBI
2	E	301	1Q0	CAB-CAM-CAR-CAW
2	A	301	1Q0	CAB-CAM-CAR-CAW
2	E	301	1Q0	CAK-CAJ-CAP-CAU
2	D	301	1Q0	CAN-CAS-CAX-CBA
2	D	301	1Q0	CAB-CAM-CAR-CAW
2	A	301	1Q0	CAY-CBD-CBI-CBJ
2	E	301	1Q0	CAO-CAT-CAY-CBD
2	E	301	1Q0	CAA-CAL-CAQ-CAV
2	C	301	1Q0	CAO-CAT-CAY-CBD
2	C	301	1Q0	CAB-CAM-CAR-CAW
2	E	301	1Q0	CAZ-CBC-CBF-CBH
2	E	301	1Q0	CAM-CAR-CAW-CBB
2	C	301	1Q0	CAY-CBD-CBI-CBJ

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Mol	Chain	Res	Type	Atoms
2	B	301	1Q0	CAO-CAT-CAY-CBD
2	C	301	1Q0	CAK-CAJ-CAP-CAU
2	C	301	1Q0	CBL-OBN-PBR-OAF
2	B	301	1Q0	OAE-CBP-CBQ-CBL
2	E	301	1Q0	OBN-CBL-CBQ-NBM
2	D	301	1Q0	CAU-CAZ-CBC-CBF
2	E	301	1Q0	CAS-CAX-CBA-CAV
2	B	301	1Q0	CAJ-CAK-CBP-OAE
2	F	301	1Q0	OBN-CBL-CBQ-CBP
2	C	301	1Q0	CBL-OBN-PBR-OAG
2	D	301	1Q0	CAO-CAT-CAY-CBD
2	D	301	1Q0	CAS-CAX-CBA-CAV
2	E	301	1Q0	CAH-CAI-CAO-CAT
2	A	301	1Q0	CAH-CAI-CAO-CAT
2	A	301	1Q0	CBC-CBF-CBH-CBG
2	A	301	1Q0	CAI-CAH-CAN-CAS
2	E	301	1Q0	CAJ-CAP-CAU-CAZ
2	C	301	1Q0	CAA-CAL-CAQ-CAV
2	C	301	1Q0	CAZ-CBC-CBF-CBH
2	A	301	1Q0	CBJ-CBK-CBO-OAC
2	E	301	1Q0	CBD-CBI-CBJ-CBK
2	D	301	1Q0	CBI-CBJ-CBK-CBO
2	B	301	1Q0	CAJ-CAK-CBP-CBQ
2	C	301	1Q0	CBJ-CBK-CBO-OAC
2	A	301	1Q0	OAE-CBP-CBQ-NBM
2	B	301	1Q0	OAE-CBP-CBQ-NBM
2	B	301	1Q0	CBL-OBN-PBR-OAD
2	D	301	1Q0	CBL-OBN-PBR-OAF
2	D	301	1Q0	CBL-OBN-PBR-OAD
2	E	301	1Q0	OAE-CBP-CBQ-NBM
2	F	301	1Q0	OAE-CBP-CBQ-NBM
2	F	301	1Q0	CBL-OBN-PBR-OAG
2	D	301	1Q0	CBD-CBI-CBJ-CBK
2	A	301	1Q0	OAE-CBP-CBQ-CBL
2	E	301	1Q0	OAE-CBP-CBQ-CBL
2	F	301	1Q0	OAE-CBP-CBQ-CBL
2	A	301	1Q0	CBJ-CBK-CBO-NBM
2	C	301	1Q0	CBJ-CBK-CBO-NBM
2	E	301	1Q0	CAI-CAH-CAN-CAS
2	E	301	1Q0	CAJ-CAK-CBP-OAE
2	A	301	1Q0	CBE-CBG-CBH-CBF
2	C	301	1Q0	OBN-CBL-CBQ-CBP

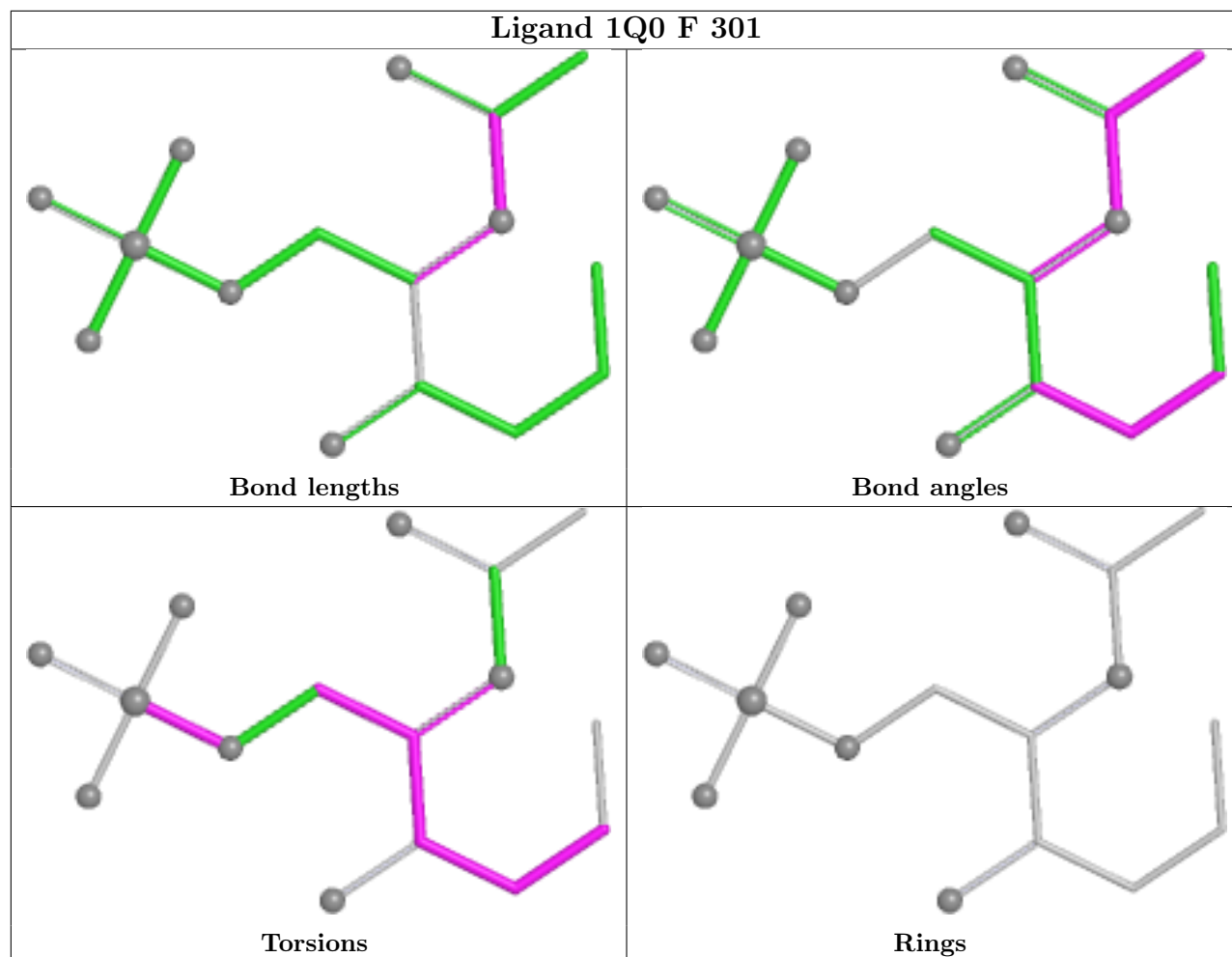
There are no ring outliers.

6 monomers are involved in 39 short contacts:

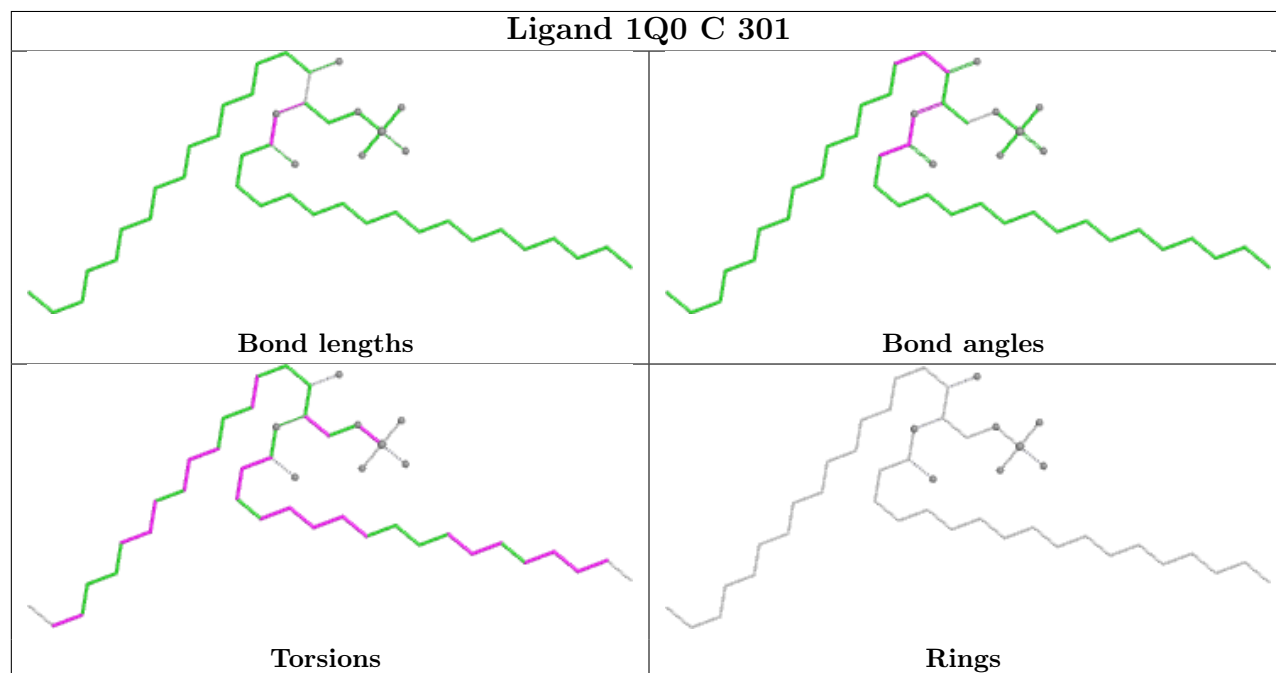
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	1Q0	3	0
2	C	301	1Q0	1	0
2	A	301	1Q0	9	0
2	D	301	1Q0	9	0
2	B	301	1Q0	5	0
2	E	301	1Q0	12	0

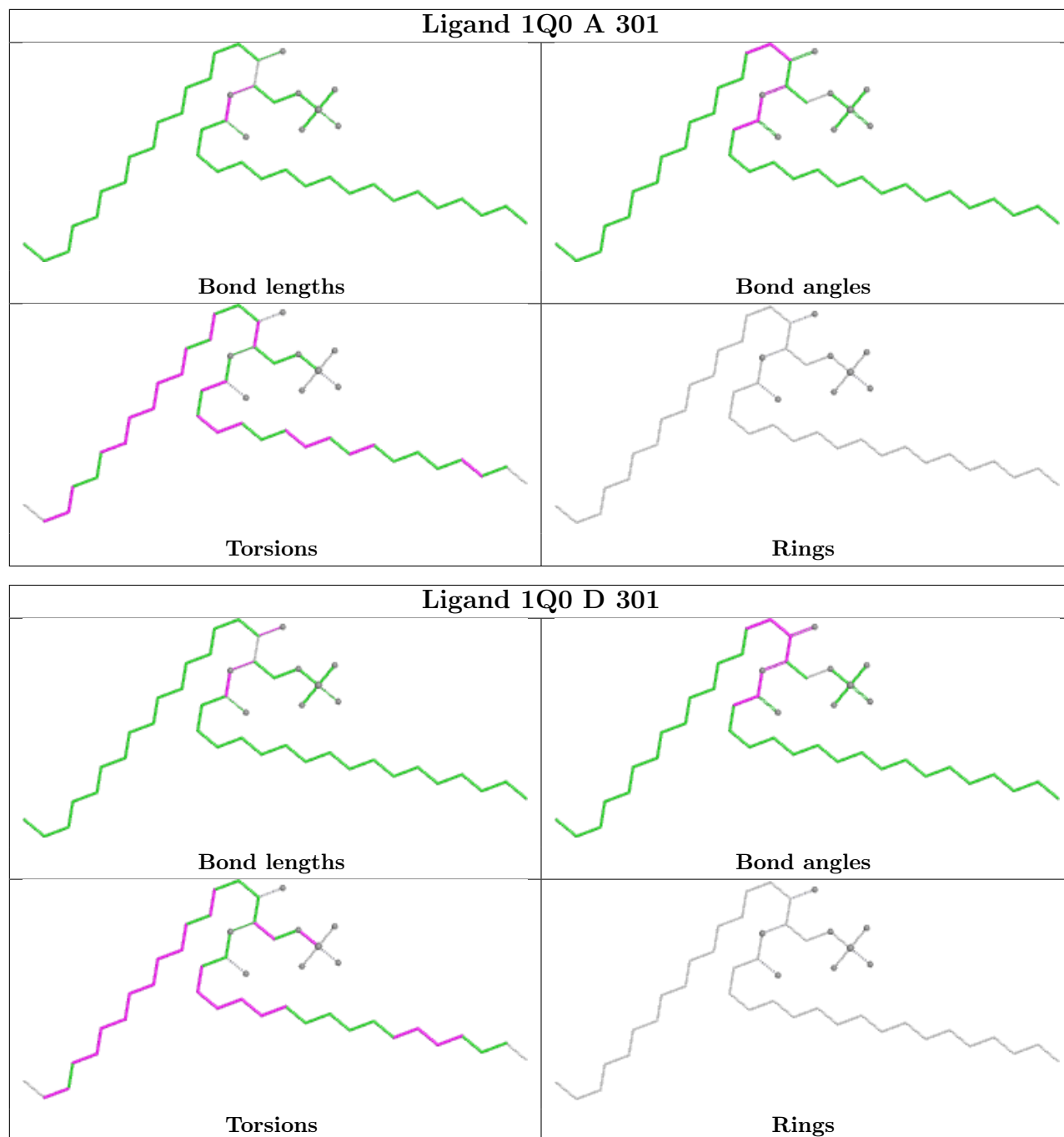
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

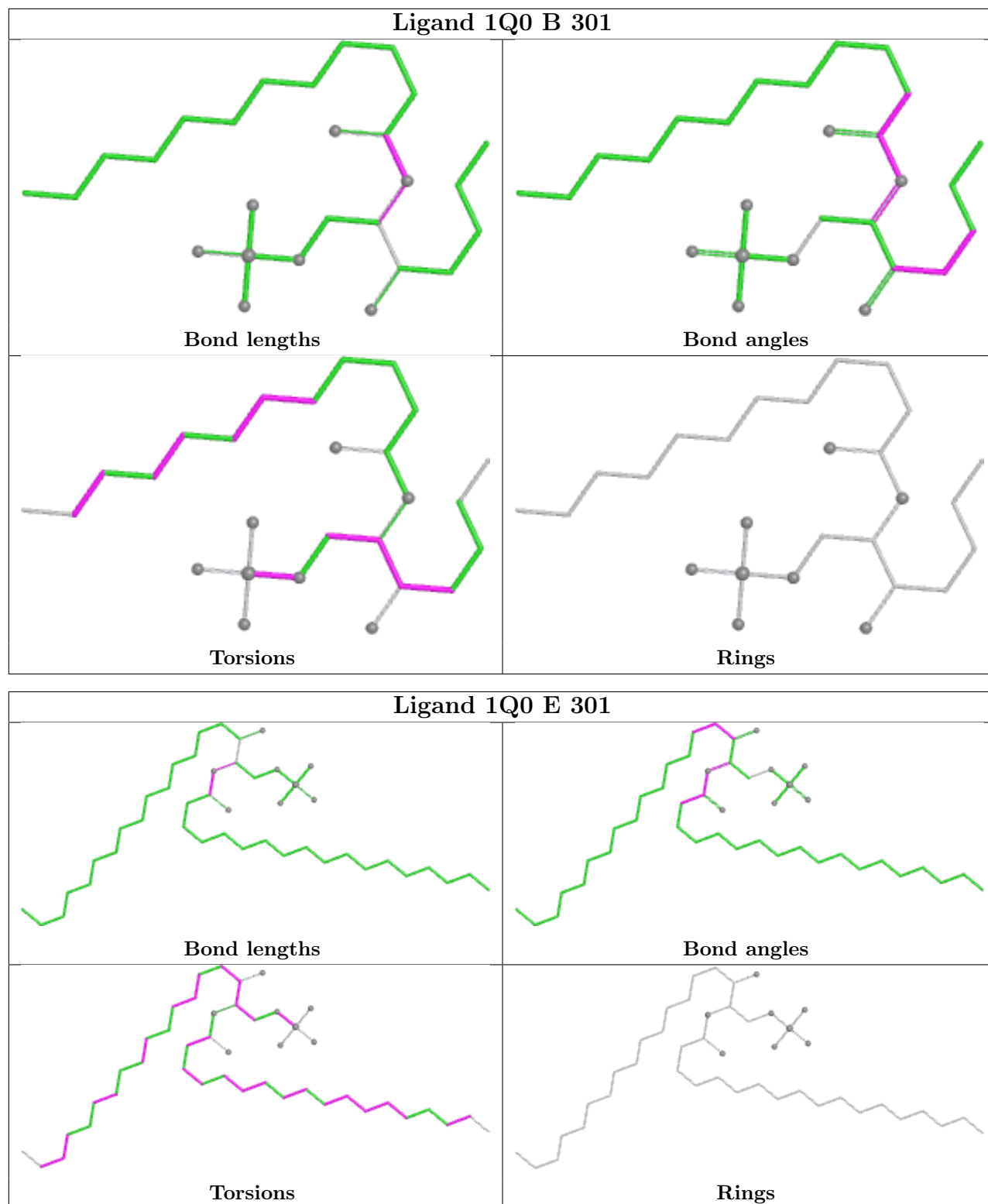
Ligand 1Q0 F 301



Ligand 1Q0 C 301







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	207/215 (96%)	-0.23	0 100 100	37, 63, 107, 132	0
1	B	206/215 (95%)	0.04	1 (0%) 87 73	44, 79, 118, 142	0
1	C	206/215 (95%)	0.21	1 (0%) 87 73	49, 95, 140, 191	0
1	D	206/215 (95%)	0.06	1 (0%) 87 73	47, 86, 130, 207	0
1	E	207/215 (96%)	-0.01	1 (0%) 87 73	44, 84, 129, 174	0
1	F	205/215 (95%)	0.62	8 (3%) 43 24	89, 149, 195, 226	0
All	All	1237/1290 (95%)	0.11	12 (0%) 79 61	37, 89, 165, 226	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	32	TYR	3.4
1	F	36	TRP	2.9
1	F	79	LEU	2.5
1	F	91	LEU	2.5
1	F	205	TYR	2.4
1	F	171	PHE	2.4
1	F	12	VAL	2.4
1	C	51	SER	2.3
1	E	126	ARG	2.1
1	D	138	CYS	2.1
1	B	198	TYR	2.0
1	F	214	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](#)

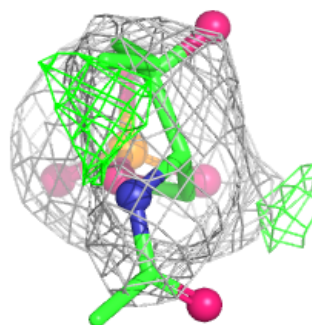
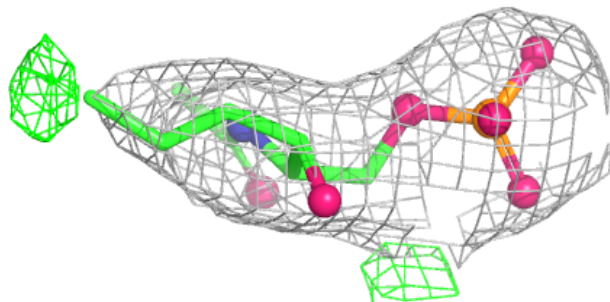
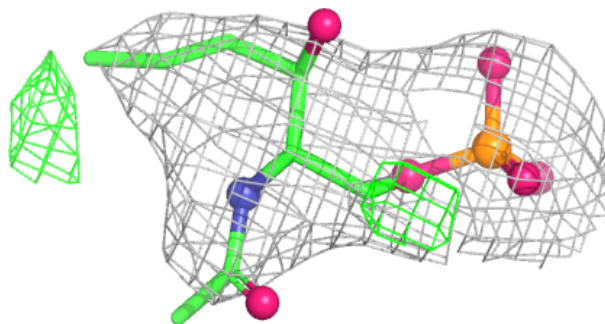
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	1Q0	F	301	16/44	0.86	0.18	94,96,98,100	16
2	1Q0	C	301	44/44	0.93	0.16	71,77,85,88	0
2	1Q0	A	301	44/44	0.94	0.14	66,66,68,69	0
2	1Q0	E	301	44/44	0.94	0.14	69,72,79,81	0
2	1Q0	B	301	27/44	0.94	0.14	49,57,61,62	27
2	1Q0	D	301	44/44	0.95	0.14	82,85,88,89	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.

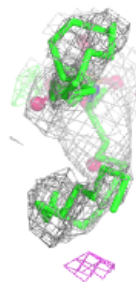
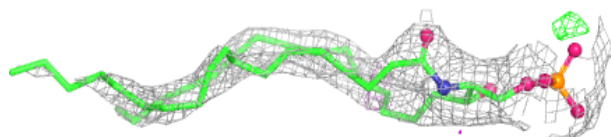
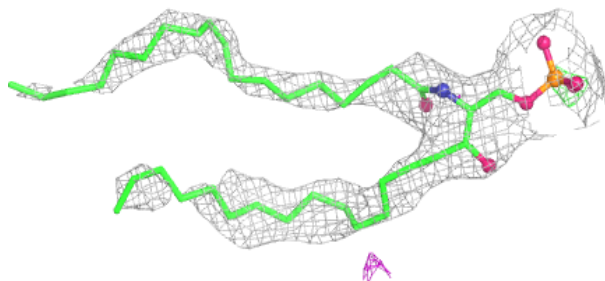
Electron density around 1Q0 F 301:

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

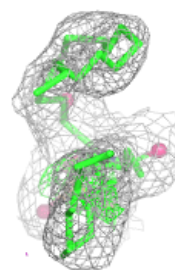
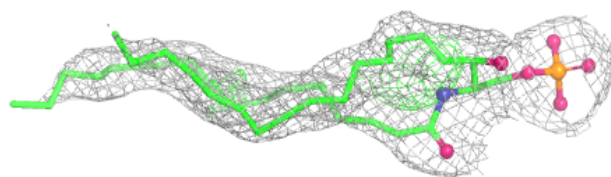
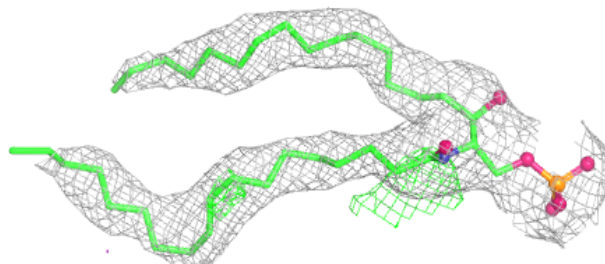


Electron density around 1Q0 C 301:

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

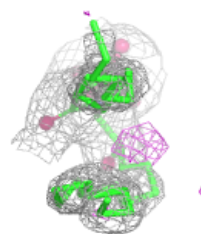
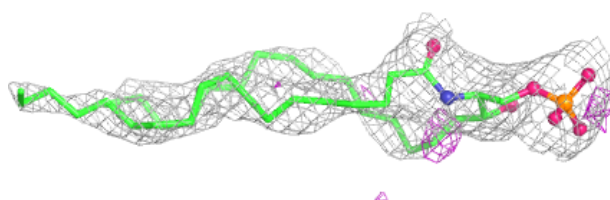
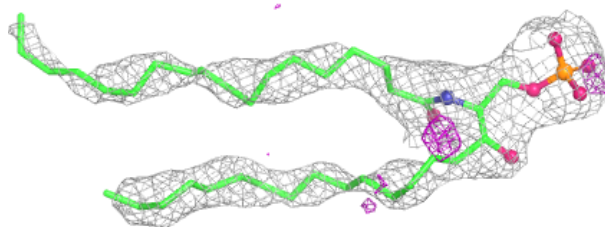
**Electron density around 1Q0 A 301:**

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

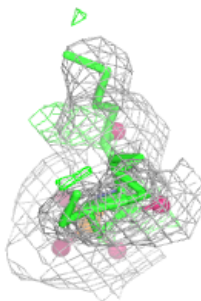
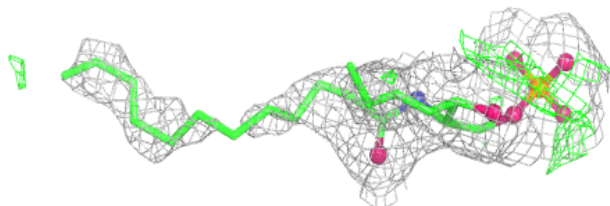
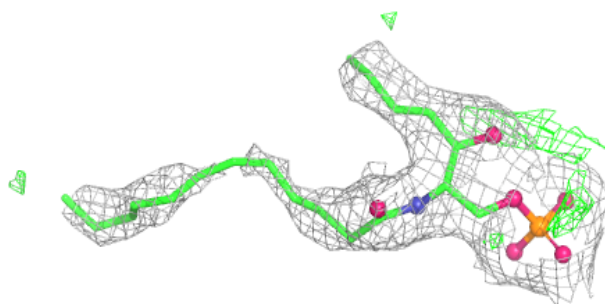


Electron density around 1Q0 E 301:

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

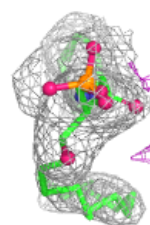
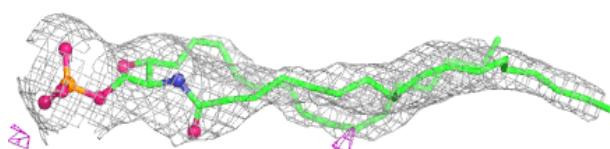
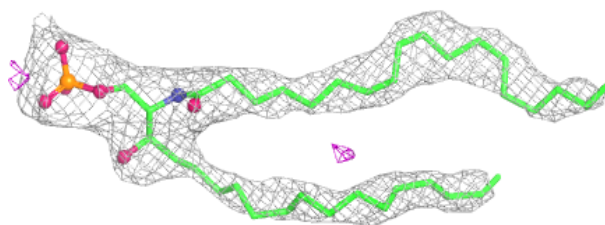
**Electron density around 1Q0 B 301:**

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



Electron density around 1Q0 D 301:

$2mF_o-DF_c$ (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.