



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 12:01 pm BST

PDB ID : 5M1E
Title : Crystal structure of N-terminally tagged UbiD from E. coli reconstituted with prFMN cofactor
Authors : Marshall, S.A.; Leys, D.
Deposited on : 2016-10-07
Resolution : 2.62 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

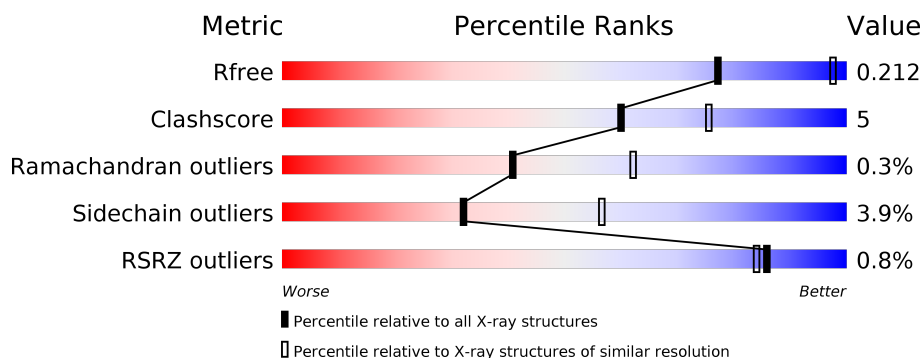
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	517	
1	B	517	
1	C	517	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11162 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 3-octaprenyl-4-hydroxybenzoate carboxy-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	1
			3667	2343	625	681	18			
1	B	465	Total	C	N	O	S	0	0	0
			3651	2333	622	678	18			
1	C	459	Total	C	N	O	S	2	0	0
			3588	2293	609	669	17			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0AAB5
A	-18	GLY	-	expression tag	UNP P0AAB5
A	-17	SER	-	expression tag	UNP P0AAB5
A	-16	SER	-	expression tag	UNP P0AAB5
A	-15	HIS	-	expression tag	UNP P0AAB5
A	-14	HIS	-	expression tag	UNP P0AAB5
A	-13	HIS	-	expression tag	UNP P0AAB5
A	-12	HIS	-	expression tag	UNP P0AAB5
A	-11	HIS	-	expression tag	UNP P0AAB5
A	-10	HIS	-	expression tag	UNP P0AAB5
A	-9	SER	-	expression tag	UNP P0AAB5
A	-8	SER	-	expression tag	UNP P0AAB5
A	-7	GLY	-	expression tag	UNP P0AAB5
A	-6	LEU	-	expression tag	UNP P0AAB5
A	-5	VAL	-	expression tag	UNP P0AAB5
A	-4	PRO	-	expression tag	UNP P0AAB5
A	-3	ARG	-	expression tag	UNP P0AAB5
A	-2	GLY	-	expression tag	UNP P0AAB5
A	-1	SER	-	expression tag	UNP P0AAB5
A	0	HIS	-	expression tag	UNP P0AAB5
B	-19	MET	-	initiating methionine	UNP P0AAB5
B	-18	GLY	-	expression tag	UNP P0AAB5
B	-17	SER	-	expression tag	UNP P0AAB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P0AAB5
B	-15	HIS	-	expression tag	UNP P0AAB5
B	-14	HIS	-	expression tag	UNP P0AAB5
B	-13	HIS	-	expression tag	UNP P0AAB5
B	-12	HIS	-	expression tag	UNP P0AAB5
B	-11	HIS	-	expression tag	UNP P0AAB5
B	-10	HIS	-	expression tag	UNP P0AAB5
B	-9	SER	-	expression tag	UNP P0AAB5
B	-8	SER	-	expression tag	UNP P0AAB5
B	-7	GLY	-	expression tag	UNP P0AAB5
B	-6	LEU	-	expression tag	UNP P0AAB5
B	-5	VAL	-	expression tag	UNP P0AAB5
B	-4	PRO	-	expression tag	UNP P0AAB5
B	-3	ARG	-	expression tag	UNP P0AAB5
B	-2	GLY	-	expression tag	UNP P0AAB5
B	-1	SER	-	expression tag	UNP P0AAB5
B	0	HIS	-	expression tag	UNP P0AAB5
C	-19	MET	-	initiating methionine	UNP P0AAB5
C	-18	GLY	-	expression tag	UNP P0AAB5
C	-17	SER	-	expression tag	UNP P0AAB5
C	-16	SER	-	expression tag	UNP P0AAB5
C	-15	HIS	-	expression tag	UNP P0AAB5
C	-14	HIS	-	expression tag	UNP P0AAB5
C	-13	HIS	-	expression tag	UNP P0AAB5
C	-12	HIS	-	expression tag	UNP P0AAB5
C	-11	HIS	-	expression tag	UNP P0AAB5
C	-10	HIS	-	expression tag	UNP P0AAB5
C	-9	SER	-	expression tag	UNP P0AAB5
C	-8	SER	-	expression tag	UNP P0AAB5
C	-7	GLY	-	expression tag	UNP P0AAB5
C	-6	LEU	-	expression tag	UNP P0AAB5
C	-5	VAL	-	expression tag	UNP P0AAB5
C	-4	PRO	-	expression tag	UNP P0AAB5
C	-3	ARG	-	expression tag	UNP P0AAB5
C	-2	GLY	-	expression tag	UNP P0AAB5
C	-1	SER	-	expression tag	UNP P0AAB5
C	0	HIS	-	expression tag	UNP P0AAB5

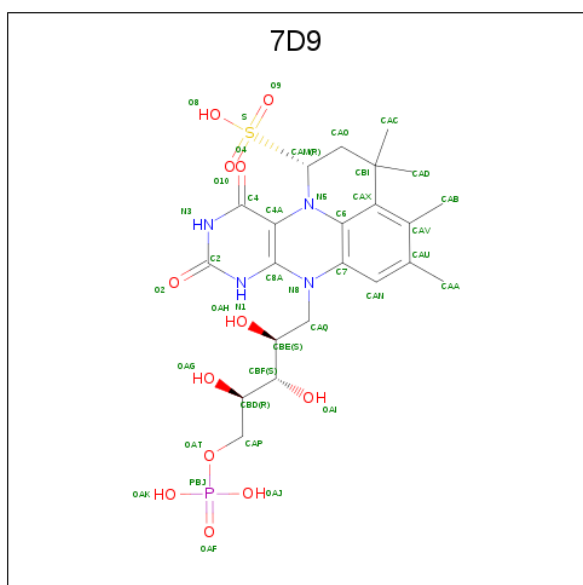
- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is (16 {R})-11,12,14,14-tetramethyl-3,5-bis(oxidanylidene)-8-[(2 {S},3 {S},4 {R})-2,3,4-tris(oxidanyl)-5-phosphonooxy-pentyl]-1,4,6,8-tetrazatetracyclo[7.7.1.0^{2,7}.0^{4,13}]-heptadeca-2(7),9(17),10,12-tetraene-16-sulfonic acid (three-letter code: 7D9) (formula: C₂₂H₃₁N₄O₁₂PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 40	C 22	N 4	O 12	P 1	S 1	0	0
3	B	1	Total 40	C 22	N 4	O 12	P 1	S 1	0	0
3	C	1	Total 40	C 22	N 4	O 12	P 1	S 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0

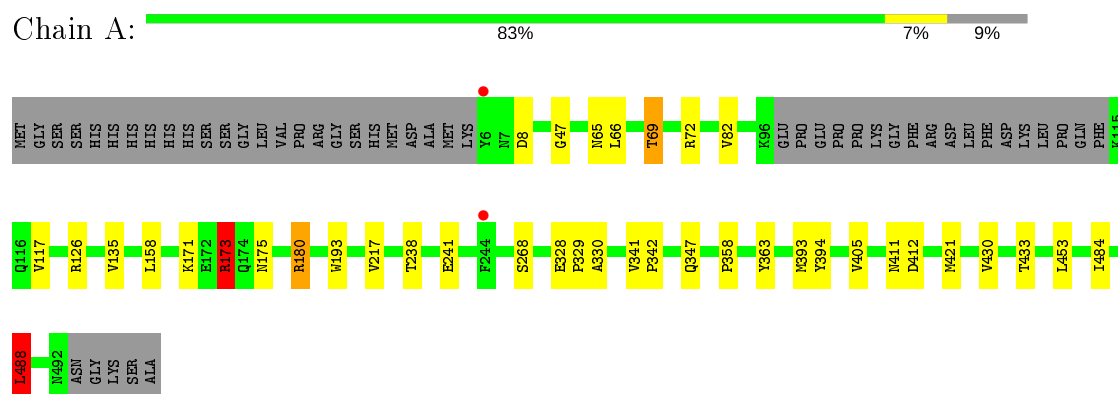
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total 37	O 37	0	0
5	B	60	Total 60	O 60	0	0
5	C	33	Total 33	O 33	0	0

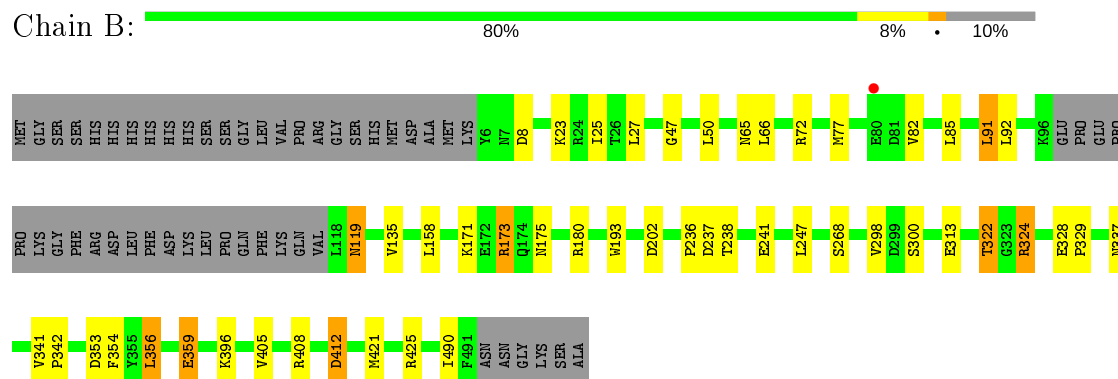
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

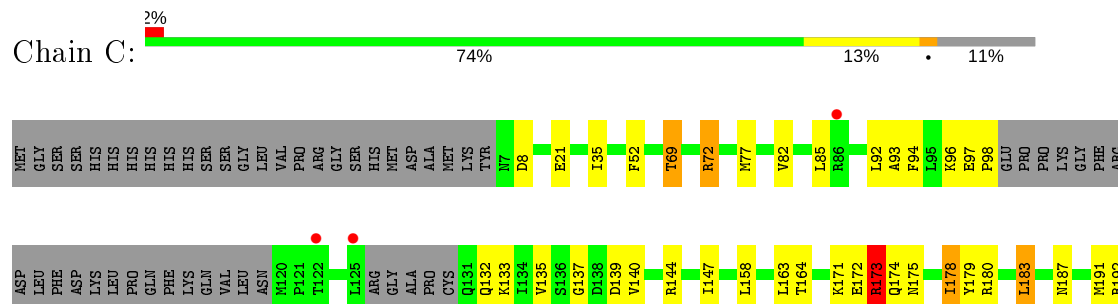
- Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase

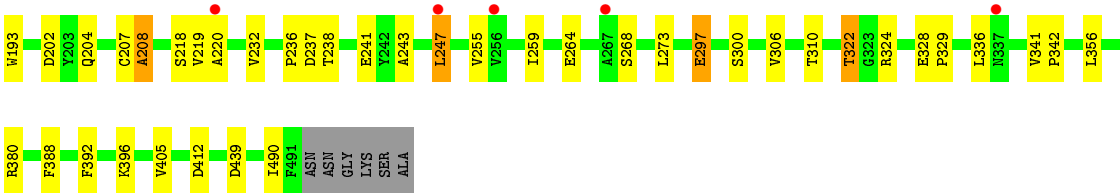


- Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase



- Molecule 1: 3-octaprenyl-4-hydroxybenzoate carboxy-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	194.52Å 194.52Å 107.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.03 – 2.62 94.03 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.2 (94.03-2.62) 99.2 (94.03-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.212 0.179 , 0.212	Depositor DCC
R_{free} test set	3085 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11162	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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: 7D9, MN, NA

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	0.75	2/3759 (0.1%)	0.85	4/5125 (0.1%)
1	B	0.77	0/3743	0.85	6/5101 (0.1%)
1	C	2.64	5/3677 (0.1%)	1.15	16/5013 (0.3%)
All	All	1.64	7/11179 (0.1%)	0.96	26/15239 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	GLU	CD-OE1	131.46	2.70	1.25
1	C	297	GLU	CD-OE2	-59.55	0.60	1.25
1	C	173	ARG	CA-CB	46.77	2.56	1.53
1	C	297	GLU	CG-CD	24.45	1.88	1.51
1	C	173	ARG	CB-CG	-10.54	1.24	1.52
1	A	175	ASN	CB-CG	5.48	1.63	1.51
1	A	363	TYR	CE1-CZ	5.21	1.45	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	GLU	OE1-CD-OE2	-35.88	80.25	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	GLU	CG-CD-OE2	19.96	158.23	118.30
1	C	297	GLU	CG-CD-OE1	-19.18	79.95	118.30
1	C	173	ARG	CB-CG-CD	-18.37	63.83	111.60
1	C	173	ARG	CA-CB-CG	-14.14	82.29	113.40
1	C	173	ARG	CB-CA-C	-12.79	84.81	110.40
1	A	241	GLU	OE1-CD-OE2	-12.38	108.44	123.30
1	B	241	GLU	OE1-CD-OE2	-9.98	111.33	123.30
1	C	241	GLU	OE1-CD-OE2	-8.28	113.36	123.30
1	C	178	ILE	CG1-CB-CG2	-8.05	93.69	111.40
1	A	173	ARG	CG-CD-NE	7.94	128.48	111.80
1	C	72	ARG	CG-CD-NE	7.64	127.84	111.80
1	C	297	GLU	CB-CG-CD	-7.28	94.53	114.20
1	B	241	GLU	CG-CD-OE2	6.55	131.40	118.30
1	A	241	GLU	CG-CD-OE1	6.39	131.08	118.30
1	A	488	LEU	CA-CB-CG	6.29	129.77	115.30
1	B	324	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	C	192	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	192	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	324	ARG	CG-CD-NE	-5.46	100.33	111.80
1	B	425	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	C	98	PRO	N-CA-CB	5.32	109.68	103.30
1	B	359	GLU	CB-CA-C	-5.28	99.85	110.40
1	C	241	GLU	CG-CD-OE1	5.22	128.73	118.30
1	C	324	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	412	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	421	MET	Peptide
1	B	421	MET	Peptide

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	3667	0	3617	26	0
1	B	3651	0	3612	26	0
1	C	3588	0	3527	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	40	0	0	2	0
3	B	40	0	0	1	0
3	C	40	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	37	0	0	0	0
5	B	60	0	0	2	0
5	C	33	0	0	1	1
All	All	11162	0	10756	100	1

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 5.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:THR:HG21	1:C:191:MET:HE2	1.46	0.97
1:C:140:VAL:HG11	1:C:306:VAL:HG13	1.52	0.89
1:A:158:LEU:HD11	1:A:180:ARG:HG3	1.54	0.89
1:C:174:GLN:HE22	1:C:264:GLU:H	1.29	0.79
1:C:158:LEU:HD11	1:C:180:ARG:HG3	1.70	0.73
1:B:158:LEU:HD11	1:B:180:ARG:HG3	1.72	0.72
1:C:179:TYR:HD2	1:C:191:MET:CE	2.02	0.71
1:C:173:ARG:NH2	1:C:202:ASP:OD2	2.23	0.71
1:B:173:ARG:NH2	1:B:202:ASP:OD2	2.23	0.70
1:C:173:ARG:CG	1:C:173:ARG:CA	2.69	0.70
1:B:47:GLY:O	1:B:72:ARG:NH2	2.25	0.69
1:A:47:GLY:O	1:A:72:ARG:NH2	2.27	0.68
1:C:396:LYS:NZ	1:C:439:ASP:OD2	2.28	0.67
1:A:484:ILE:HG13	1:A:488:LEU:HD22	1.78	0.65
3:B:502:7D9:CAB	3:B:502:7D9:CAD	2.75	0.65
1:C:297:GLU:CG	1:C:297:GLU:OE2	2.45	0.65
1:C:173:ARG:HD3	1:C:237:ASP:O	1.97	0.64
1:B:91:LEU:HD21	1:B:247:LEU:HD13	1.80	0.64
1:A:8:ASP:HB2	1:A:268:SER:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:HD3	1:B:237:ASP:O	1.99	0.62
1:B:353:ASP:OD2	1:B:408:ARG:NH1	2.32	0.62
1:B:8:ASP:HB2	1:B:268:SER:HB2	1.82	0.62
1:C:140:VAL:HG11	1:C:306:VAL:CG1	2.29	0.61
1:C:179:TYR:CD2	1:C:191:MET:CE	2.84	0.61
1:C:8:ASP:HB2	1:C:268:SER:HB2	1.82	0.61
1:C:219:VAL:HG22	1:C:273:LEU:HB2	1.82	0.61
1:B:236:PRO:HB2	1:B:238:THR:HG22	1.85	0.59
1:C:207:CYS:O	1:C:208:ALA:HB3	2.03	0.59
1:C:219:VAL:CG2	1:C:273:LEU:HB2	2.34	0.57
1:C:179:TYR:HD2	1:C:191:MET:HE1	1.66	0.57
1:A:180:ARG:HB3	3:A:502:7D9:O4	2.03	0.57
1:C:174:GLN:NE2	1:C:264:GLU:H	2.00	0.57
1:C:204:GLN:O	1:C:207:CYS:O	2.23	0.56
3:C:502:7D9:CAB	3:C:502:7D9:CAD	2.83	0.56
1:C:173:ARG:HG2	1:C:173:ARG:CA	2.35	0.56
1:C:236:PRO:HB2	1:C:238:THR:HG22	1.87	0.56
1:B:298:VAL:HG23	5:B:640:HOH:O	2.06	0.55
1:C:174:GLN:HE22	1:C:264:GLU:HG2	1.71	0.55
1:A:488:LEU:HD13	1:B:27:LEU:HD12	1.88	0.55
1:B:173:ARG:HH22	1:B:202:ASP:CG	2.10	0.55
1:A:330:ALA:HB1	1:A:358:PRO:HB3	1.88	0.55
1:A:173:ARG:C	1:A:173:ARG:HD2	2.27	0.55
1:C:207:CYS:O	1:C:208:ALA:CB	2.54	0.55
1:C:77:MET:SD	1:C:85:LEU:HD21	2.47	0.54
1:C:164:THR:HG21	1:C:191:MET:CE	2.29	0.54
1:C:147:ILE:HD12	1:C:183:LEU:HD13	1.89	0.53
1:A:66:LEU:O	1:A:72:ARG:HD2	2.10	0.52
1:B:77:MET:SD	1:B:85:LEU:HD21	2.49	0.52
1:C:243:ALA:O	1:C:247:LEU:HD22	2.09	0.52
1:C:219:VAL:HG21	1:C:273:LEU:HD12	1.91	0.52
1:A:411:ASN:OD1	1:B:359:GLU:CG	2.58	0.51
1:C:173:ARG:HH22	1:C:202:ASP:CG	2.13	0.51
1:B:405:VAL:HG13	1:B:412:ASP:HB3	1.93	0.51
1:A:411:ASN:HA	1:B:359:GLU:HG2	1.91	0.51
1:A:394:TYR:CD1	1:A:394:TYR:N	2.78	0.51
1:B:354:PHE:CE2	1:B:356:LEU:HD21	2.46	0.51
1:C:219:VAL:CG2	1:C:273:LEU:HD12	2.42	0.50
1:B:66:LEU:O	1:B:72:ARG:HD2	2.10	0.50
1:C:163:LEU:HD12	1:C:220:ALA:O	2.12	0.49
1:C:93:ALA:O	1:C:94:PHE:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:O	1:A:72:ARG:NH1	2.46	0.49
1:A:173:ARG:O	1:A:173:ARG:HD2	2.12	0.49
1:A:69:THR:HG22	1:A:72:ARG:H	1.80	0.47
3:A:502:7D9:CAD	3:A:502:7D9:CAB	2.92	0.47
1:C:179:TYR:CD2	1:C:191:MET:HE3	2.50	0.47
1:C:356:LEU:HD11	1:C:392:PHE:CE1	2.50	0.47
1:A:117:VAL:O	1:A:117:VAL:HG22	2.15	0.47
1:C:35:ILE:HG23	1:C:52:PHE:CE2	2.50	0.47
1:C:21:GLU:OE1	1:C:72:ARG:NH1	2.49	0.46
1:B:328:GLU:HB3	1:B:329:PRO:HD3	1.98	0.46
1:C:405:VAL:HG13	1:C:412:ASP:HB3	1.97	0.46
1:A:347:GLN:NE2	1:C:388:PHE:O	2.49	0.46
1:A:411:ASN:OD1	1:B:359:GLU:HG3	2.14	0.46
1:B:65:ASN:O	1:B:72:ARG:NH1	2.50	0.45
1:A:405:VAL:HG13	1:A:412:ASP:HB3	1.98	0.45
1:B:341:VAL:HB	1:B:342:PRO:HD3	1.99	0.45
1:B:396:LYS:NZ	5:B:608:HOH:O	2.50	0.45
1:C:328:GLU:HB3	1:C:329:PRO:HD3	1.98	0.45
1:C:306:VAL:O	1:C:306:VAL:HG13	2.18	0.44
1:C:341:VAL:HB	1:C:342:PRO:HD3	2.00	0.44
1:C:388:PHE:HB3	5:C:622:HOH:O	2.18	0.44
1:C:69:THR:HG22	1:C:72:ARG:H	1.83	0.44
1:B:119:ASN:ND2	1:B:119:ASN:O	2.51	0.44
1:B:322:THR:HG23	1:B:329:PRO:HG2	1.99	0.44
1:C:132:GLN:HB3	1:C:310:THR:HG22	1.99	0.43
1:C:322:THR:HG23	1:C:329:PRO:HG2	2.00	0.43
1:C:173:ARG:CZ	1:C:175:ASN:HB2	2.48	0.43
1:A:393:MET:SD	1:C:380:ARG:HD2	2.59	0.43
1:A:430:VAL:HG23	1:A:433:THR:HG21	2.01	0.42
1:A:453:LEU:N	1:A:453:LEU:HD12	2.34	0.42
1:A:484:ILE:HG13	1:A:488:LEU:CD2	2.49	0.41
1:C:178:ILE:HD13	1:C:232:VAL:HG12	2.02	0.41
1:A:393:MET:SD	1:C:380:ARG:CD	3.09	0.41
1:A:328:GLU:HB3	1:A:329:PRO:HD3	2.03	0.41
1:C:232:VAL:HG23	1:C:336:LEU:HD11	2.01	0.41
1:A:341:VAL:HB	1:A:342:PRO:HD3	2.04	0.40
1:B:173:ARG:CZ	1:B:175:ASN:HB2	2.51	0.40
1:B:25:ILE:HD11	1:B:50:LEU:HD22	2.02	0.40
1:C:187:ASN:CA	1:C:306:VAL:HG12	2.51	0.40
1:C:259:ILE:HD12	1:C:259:ILE:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:604:HOH:O	5:C:607:HOH:O[8_554]	1.07	1.13

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	465/517 (90%)	453 (97%)	12 (3%)	0	100	100
1	B	461/517 (89%)	452 (98%)	9 (2%)	0	100	100
1	C	453/517 (88%)	439 (97%)	10 (2%)	4 (1%)	17	33
All	All	1379/1551 (89%)	1344 (98%)	31 (2%)	4 (0%)	41	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	GLU
1	C	208	ALA
1	C	96	LYS
1	C	137	GLY

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	392/439 (89%)	381 (97%)	11 (3%)	43	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	392/439 (89%)	376 (96%)	16 (4%)	30	55
1	C	383/439 (87%)	365 (95%)	18 (5%)	26	49
All	All	1167/1317 (89%)	1122 (96%)	45 (4%)	32	56

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	A	82	VAL
1	A	126	ARG
1	A	135	VAL
1	A	171	LYS
1	A	173	ARG
1	A	180	ARG
1	A	193	TRP
1	A	217	VAL
1	A	238	THR
1	A	488	LEU
1	B	23	LYS
1	B	82	VAL
1	B	91	LEU
1	B	92	LEU
1	B	119	ASN
1	B	135	VAL
1	B	171	LYS
1	B	173	ARG
1	B	193	TRP
1	B	300	SER
1	B	313	GLU
1	B	322	THR
1	B	324	ARG
1	B	337	ASN
1	B	356	LEU
1	B	490	ILE
1	C	69	THR
1	C	82	VAL
1	C	92	LEU
1	C	133	LYS
1	C	135	VAL
1	C	139	ASP
1	C	144	ARG

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Mol	Chain	Res	Type
1	C	171	LYS
1	C	172	GLU
1	C	173	ARG
1	C	183	LEU
1	C	193	TRP
1	C	218	SER
1	C	247	LEU
1	C	255	VAL
1	C	300	SER
1	C	322	THR
1	C	490	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	B	18	GLN
1	B	119	ASN
1	B	131	GLN
1	C	174	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	7D9	B	502	2,4	36,43,43	1.20	4 (11%)	49,70,70	2.27	13 (26%)
3	7D9	A	502	2,4	36,43,43	1.19	4 (11%)	49,70,70	2.23	12 (24%)
3	7D9	C	502	2,4	36,43,43	1.19	5 (13%)	49,70,70	2.02	12 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	7D9	B	502	2,4	-	0/18/39/39	0/3/4/4
3	7D9	A	502	2,4	-	0/18/39/39	0/3/4/4
3	7D9	C	502	2,4	-	5/18/39/39	0/3/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	7D9	C4A-N5	3.26	1.44	1.39
3	C	502	7D9	C7-N8	3.17	1.42	1.38
3	A	502	7D9	C4A-N5	3.05	1.44	1.39
3	C	502	7D9	C8A-N1	3.00	1.37	1.33
3	A	502	7D9	C8A-N1	2.52	1.36	1.33
3	A	502	7D9	C6-N5	2.40	1.43	1.39
3	C	502	7D9	C6-N5	2.31	1.43	1.39
3	A	502	7D9	C7-N8	2.23	1.41	1.38
3	B	502	7D9	C7-N8	2.18	1.41	1.38
3	C	502	7D9	C4A-N5	2.16	1.42	1.39
3	C	502	7D9	O10-S	2.13	1.52	1.44
3	B	502	7D9	CAP-CBD	2.08	1.54	1.51
3	B	502	7D9	O9-S	2.02	1.52	1.44

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	7D9	C4-N3-C2	7.75	121.68	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	7D9	C4A-N5-C6	-7.32	114.97	121.75
3	A	502	7D9	C4-N3-C2	7.25	121.26	115.14
3	B	502	7D9	C4-N3-C2	7.01	121.06	115.14
3	B	502	7D9	C4A-N5-C6	-6.85	115.40	121.75
3	A	502	7D9	C4-C4A-C8A	-5.36	116.40	119.95
3	B	502	7D9	CAD-CBI-CAX	5.36	116.96	111.72
3	A	502	7D9	CAQ-N8-C7	4.82	122.09	118.29
3	C	502	7D9	C4A-N5-C6	-4.71	117.39	121.75
3	C	502	7D9	OAJ-PBJ-OAT	-4.45	94.89	106.73
3	B	502	7D9	CAO-CBI-CAX	-4.25	101.42	111.14
3	C	502	7D9	C4-C4A-C8A	-4.15	117.21	119.95
3	B	502	7D9	C7-N8-C8A	-3.66	117.11	121.91
3	B	502	7D9	C4-C4A-C8A	-3.61	117.56	119.95
3	A	502	7D9	C7-N8-C8A	-3.57	117.24	121.91
3	B	502	7D9	CAC-CBI-CAX	3.54	115.19	111.72
3	B	502	7D9	OAJ-PBJ-OAT	-3.39	97.70	106.73
3	C	502	7D9	C6-C7-N8	-3.39	117.72	120.43
3	C	502	7D9	CAD-CBI-CAX	3.34	114.98	111.72
3	B	502	7D9	C4A-C4-N3	-3.09	119.20	123.43
3	C	502	7D9	O9-S-O10	-2.85	105.28	116.52
3	B	502	7D9	O9-S-O10	-2.78	105.54	116.52
3	C	502	7D9	C4A-C4-N3	-2.65	119.81	123.43
3	A	502	7D9	OAH-CBE-CAQ	2.56	115.75	109.59
3	A	502	7D9	CAD-CBI-CAX	2.44	114.10	111.72
3	B	502	7D9	CAO-CAM-N5	-2.42	106.90	110.86
3	C	502	7D9	C7-N8-C8A	-2.39	118.77	121.91
3	C	502	7D9	OAJ-PBJ-OAF	2.34	119.82	110.68
3	A	502	7D9	CAA-CAU-CAV	2.28	124.72	121.17
3	C	502	7D9	CAO-CBI-CAX	-2.27	105.94	111.14
3	A	502	7D9	CAQ-N8-C8A	-2.27	116.38	118.41
3	C	502	7D9	C4A-C8A-N8	-2.16	118.08	120.30
3	B	502	7D9	OAT-CAP-CBD	-2.13	103.69	109.36
3	A	502	7D9	CAB-CAV-CAU	-2.07	115.90	119.71
3	A	502	7D9	C4A-C4-N3	-2.03	120.66	123.43
3	B	502	7D9	C4A-C8A-N8	-2.03	118.22	120.30
3	A	502	7D9	CAA-CAU-CAN	-2.01	115.52	120.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	502	7D9	N8-CAQ-CBE-OAH

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Mol	Chain	Res	Type	Atoms
3	C	502	7D9	CAP-OAT-PBJ-OAK
3	C	502	7D9	CAP-OAT-PBJ-OAF
3	C	502	7D9	OAT-CAP-CBD-CBF
3	C	502	7D9	OAT-CAP-CBD-OAG

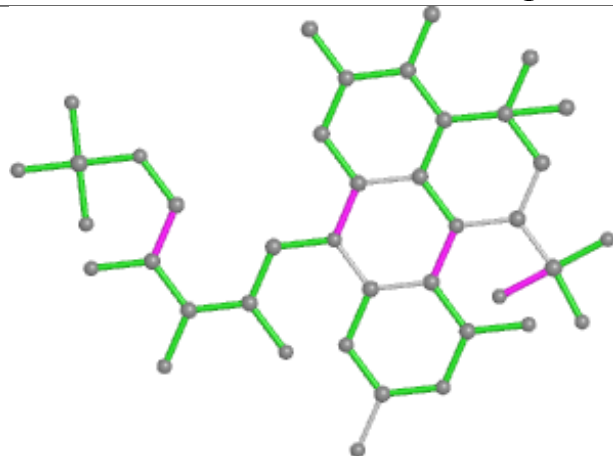
There are no ring outliers.

3 monomers are involved in 4 short contacts:

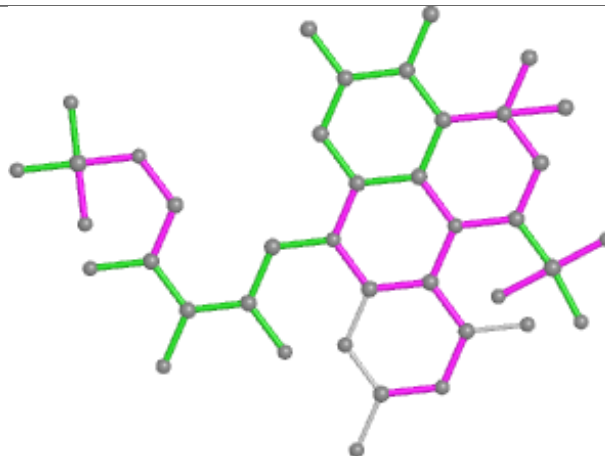
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	7D9	1	0
3	A	502	7D9	2	0
3	C	502	7D9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

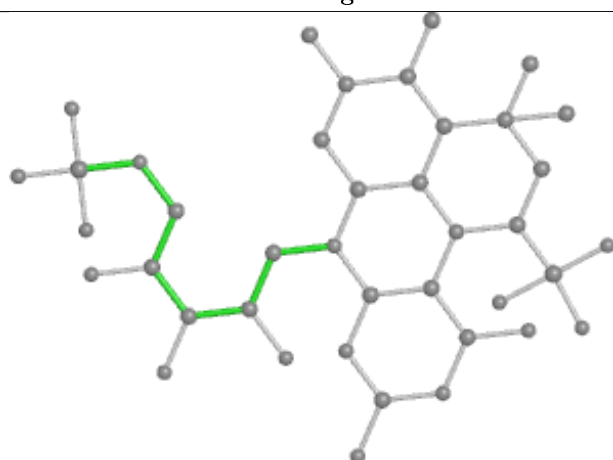
Ligand 7D9 B 502



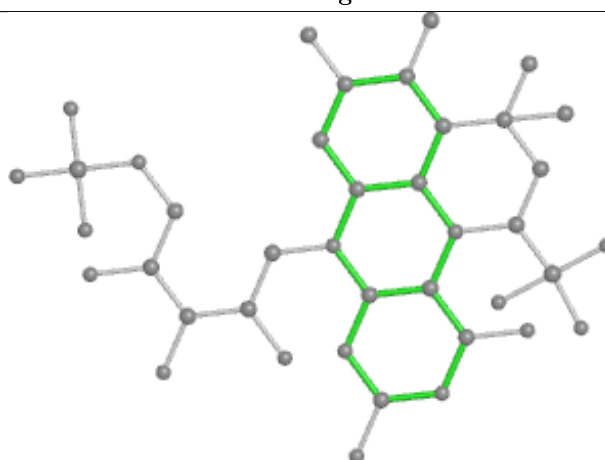
Bond lengths



Bond angles

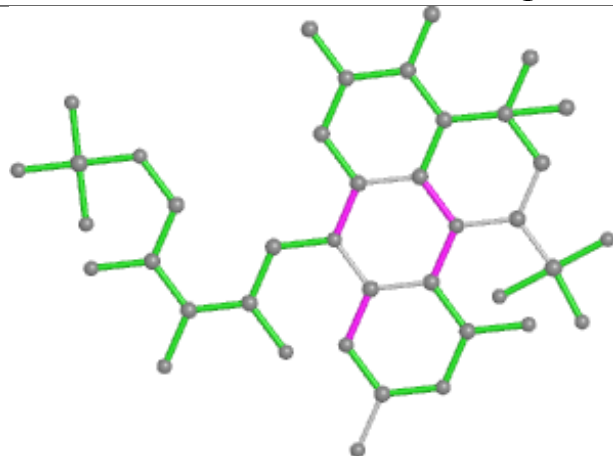


Torsions

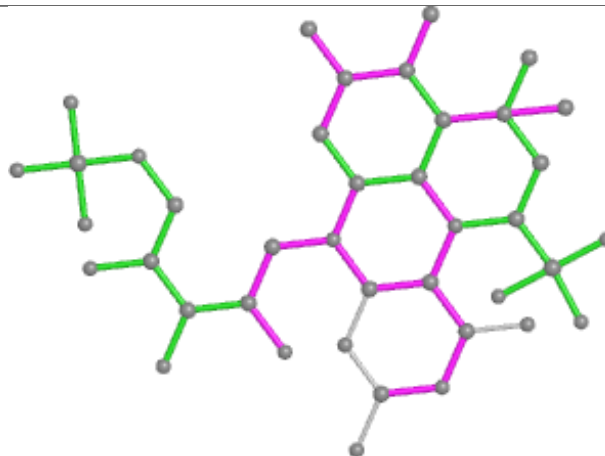


Rings

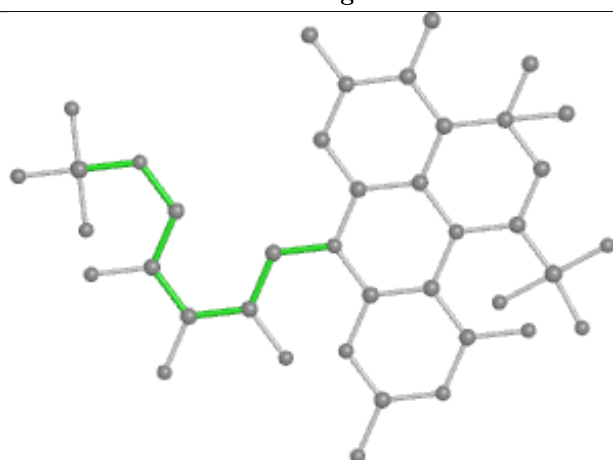
Ligand 7D9 A 502



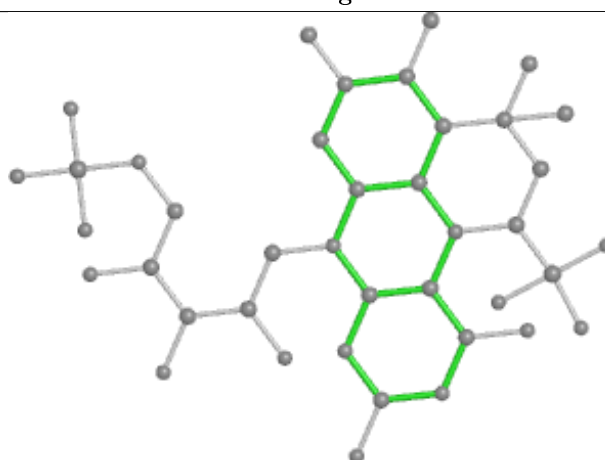
Bond lengths



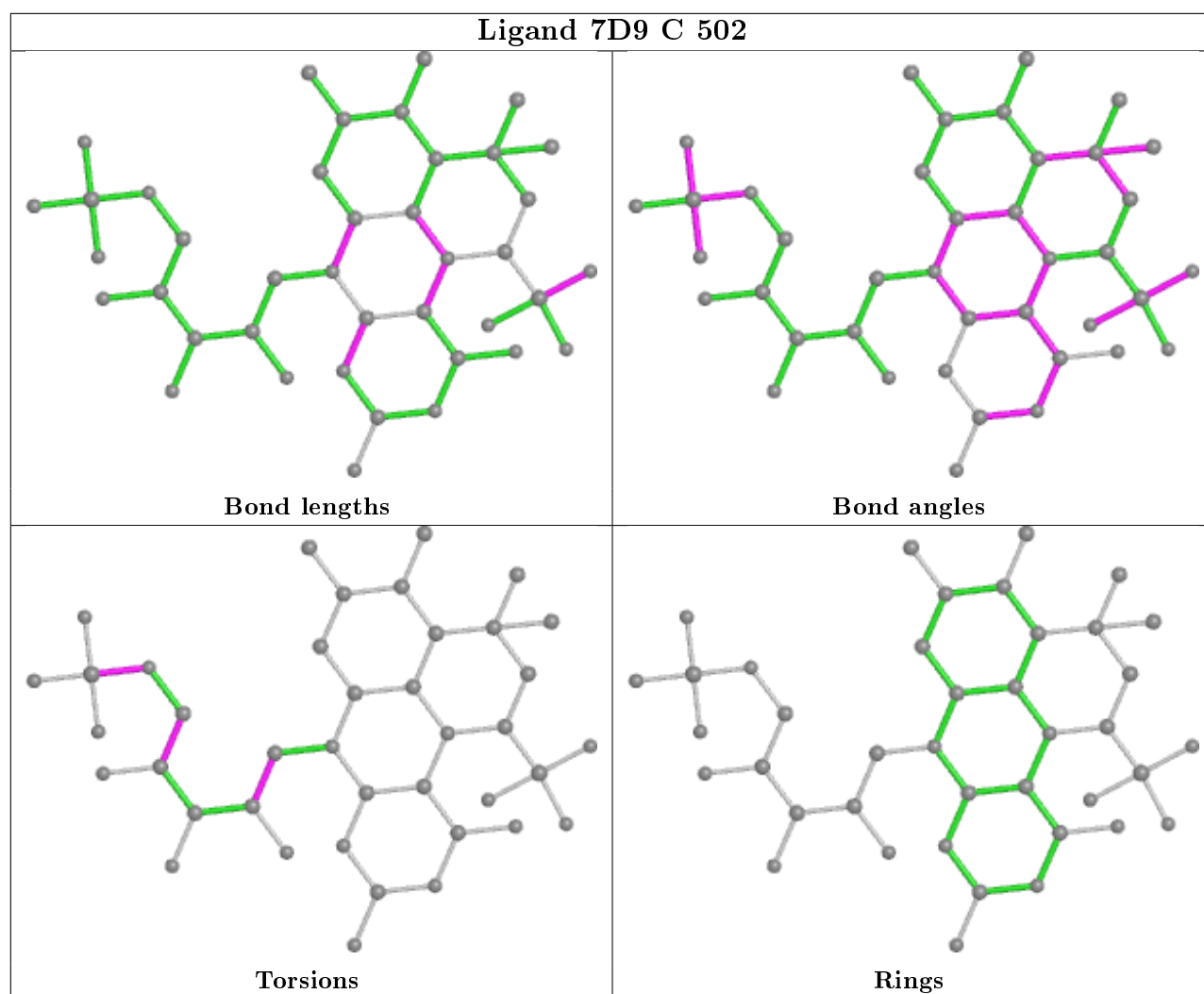
Bond angles



Torsions



Rings



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	469/517 (90%)	-0.25	2 (0%) 92 91	36, 62, 98, 139	0
1	B	465/517 (89%)	-0.28	1 (0%) 95 95	38, 55, 94, 152	0
1	C	459/517 (88%)	-0.05	8 (1%) 70 66	37, 76, 128, 154	1 (0%)
All	All	1393/1551 (89%)	-0.19	11 (0%) 86 84	36, 62, 118, 154	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	125	LEU	2.9
1	C	220	ALA	2.9
1	B	80	GLU	2.7
1	C	86	ARG	2.5
1	C	247	LEU	2.4
1	A	244	PHE	2.4
1	C	122	THR	2.4
1	A	6	TYR	2.3
1	C	256	VAL	2.3
1	C	337	ASN	2.1
1	C	267	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

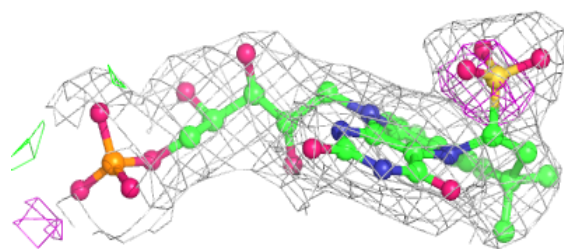
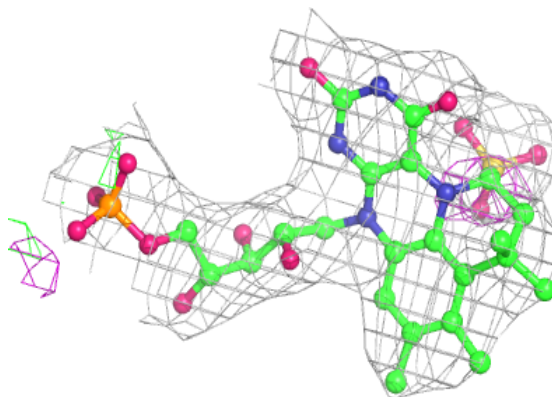
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MN	A	501	1/1	0.83	0.08	69,69,69,69	0
2	MN	C	501	1/1	0.94	0.13	102,102,102,102	0
4	NA	C	503	1/1	0.94	0.05	75,75,75,75	0
2	MN	B	501	1/1	0.95	0.07	64,64,64,64	0
3	7D9	A	502	40/40	0.96	0.14	54,62,84,101	0
3	7D9	C	502	40/40	0.96	0.13	52,70,85,91	0
3	7D9	B	502	40/40	0.97	0.14	41,49,66,80	0
4	NA	A	503	1/1	0.97	0.12	60,60,60,60	0
4	NA	B	503	1/1	0.99	0.08	64,64,64,64	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.

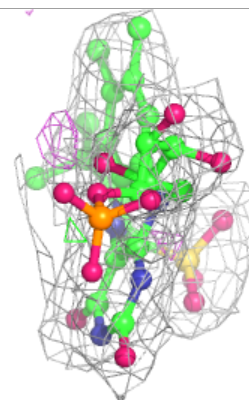
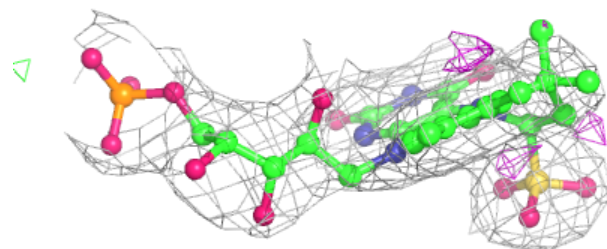
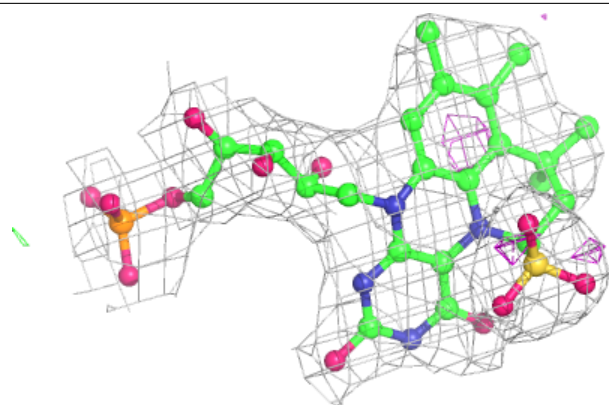
Electron density around 7D9 A 502:

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

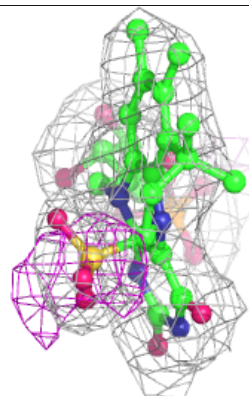
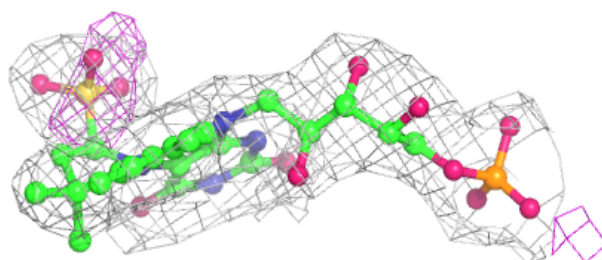
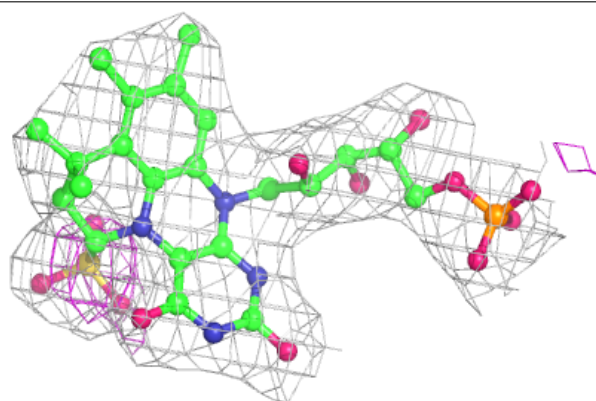


Electron density around 7D9 C 502:

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

**Electron density around 7D9 B 502:**

$2mF_o-DF_c$ (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.