



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:22 pm BST

PDB ID : 4NJA  
Title : Crystal structure of Fab 6C8 in complex with MPTS  
Authors : Stanfield, R.L.; Romesberg, F.E.; Zimmermann, J.; Wilson, I.A.  
Deposited on : 2013-11-08  
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](mailto: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

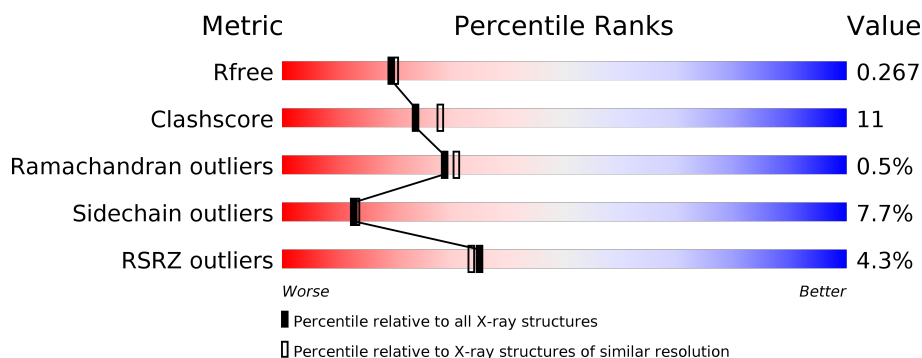
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	L	218	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
2	H	233	<div> <div>6%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>• 5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	H	502	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3519 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 6C8 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	217	Total	C	N	O	S	0	0	0
			1681	1041	289	345	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	96	ARG	TYR	conflict	UNP P01660

- Molecule 2 is a protein called 6C8 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1657	1045	271	332	9			

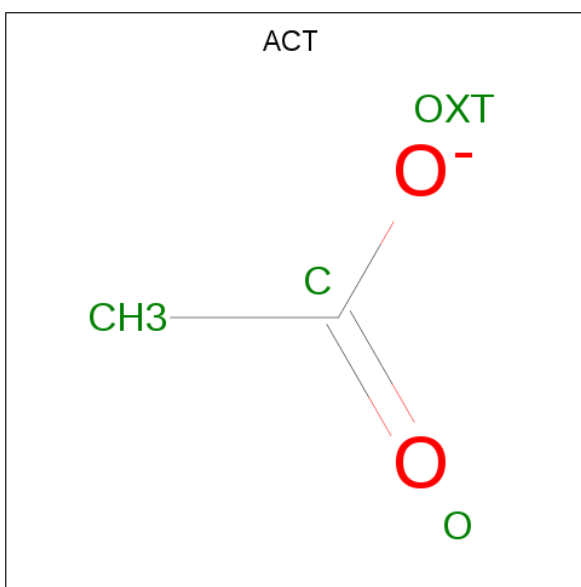
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	140	SER	LEU	conflict	UNP A0A0F7R1P3
H	151	PRO	SER	conflict	UNP A0A0F7R1P3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

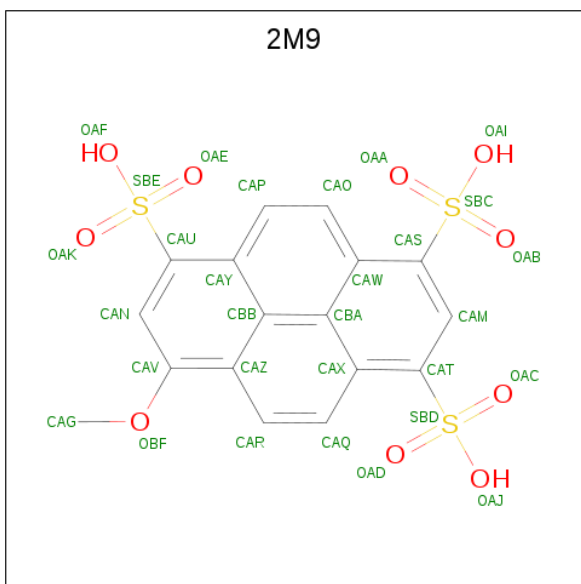
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 8-methoxypyrene-1,3,6-trisulfonic acid (three-letter code: 2M9) (formula:  $C_{17}H_{12}O_{10}S_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	O	S	0	0
			30	17	10	3		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	O	P	0	0
			5	4	1		

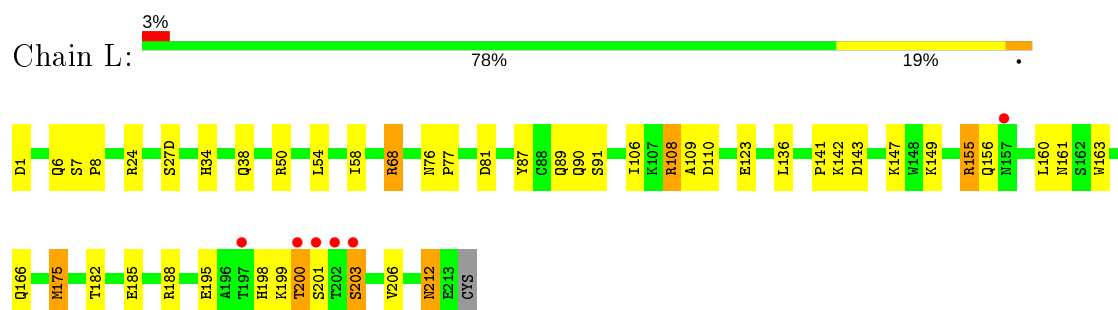
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	82	Total	O	0	0
			82	82		
7	H	54	Total	O	0	0
			54	54		

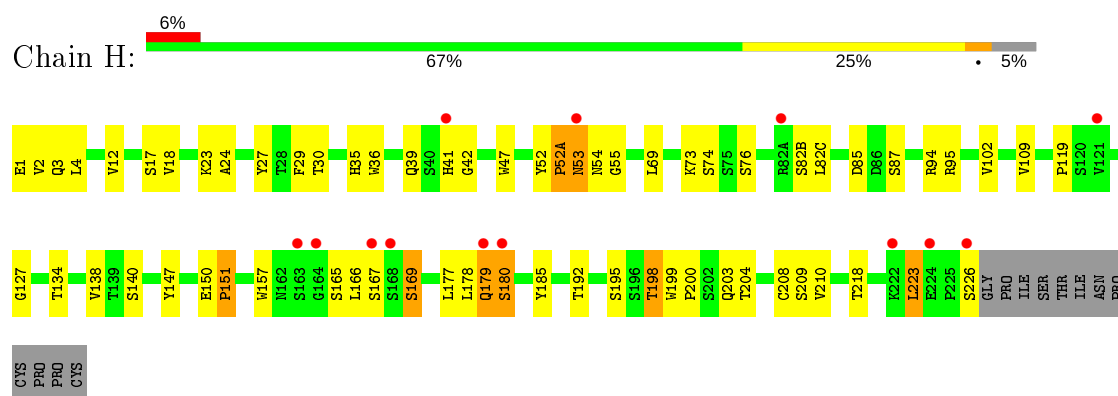
### 3 Residue-property plots [i](#)

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: 6C8 light chain



- Molecule 2: 6C8 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.66 Å 127.84 Å 47.78 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.51 – 2.20 42.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (42.51-2.20) 96.8 (42.47-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.216 , 0.265 0.217 , 0.267	Depositor DCC
$R_{free}$ test set	1446 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2M9, PO4, ACT

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	L	0.78	0/1718	0.87	2/2334 (0.1%)
2	H	0.76	2/1703 (0.1%)	0.84	6/2324 (0.3%)
All	All	0.77	2/3421 (0.1%)	0.85	8/4658 (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	L	0	1
2	H	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	74	SER	CB-OG	9.12	1.54	1.42
2	H	74	SER	CA-CB	6.64	1.62	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	95	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	H	95	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	H	94	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	L	1	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	L	1	ASP	CB-CG-OD1	5.55	123.29	118.30
2	H	94	ARG	NE-CZ-NH1	5.35	122.97	120.30
2	H	223	LEU	CB-CG-CD1	-5.25	102.08	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	127	GLY	N-CA-C	-5.01	100.56	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	134	THR	Peptide
1	L	155	ARG	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	L	1681	0	1606	38	0
2	H	1657	0	1599	38	0
3	H	1	0	0	0	0
3	L	1	0	0	0	0
4	L	8	0	6	0	0
5	H	30	0	11	2	0
6	H	5	0	0	0	0
7	H	54	0	0	0	0
7	L	82	0	0	3	0
All	All	3519	0	3222	74	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 11.

All (74) 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:L:68:ARG:HG2	1:L:68:ARG:HH11	1.01	1.17
2:H:54:ASN:CB	2:H:55:GLY:HA2	1.79	1.12
2:H:54:ASN:HB3	2:H:55:GLY:CA	1.84	1.07
1:L:68:ARG:HG2	1:L:68:ARG:NH1	1.75	0.87
2:H:54:ASN:HB3	2:H:55:GLY:HA2	0.89	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:160:LEU:HD21	2:H:179:GLN:HG2	1.57	0.86
2:H:140:SER:HB3	2:H:223:LEU:HD13	1.61	0.81
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.31	0.76
2:H:30:THR:HB	2:H:53:ASN:HB2	1.68	0.76
1:L:68:ARG:CG	1:L:68:ARG:HH11	1.90	0.75
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.34	0.75
1:L:34:HIS:HD2	1:L:50:ARG:H	1.38	0.70
1:L:142:LYS:HE3	7:L:477:HOH:O	1.90	0.70
1:L:106:ILE:H	1:L:166:GLN:HE22	1.39	0.69
1:L:81:ASP:HB2	7:L:448:HOH:O	1.92	0.69
1:L:6:GLN:HE22	1:L:87:TYR:HA	1.57	0.69
1:L:182:THR:HG23	7:L:480:HOH:O	1.94	0.67
1:L:34:HIS:CD2	1:L:50:ARG:H	2.13	0.65
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.81	0.64
1:L:68:ARG:CG	1:L:68:ARG:NH1	2.55	0.63
1:L:147:LYS:HE2	1:L:149:LYS:CE	2.28	0.62
1:L:147:LYS:HE2	1:L:149:LYS:HE3	1.82	0.60
2:H:150:GLU:HG3	2:H:151:PRO:HB3	1.83	0.60
2:H:29:PHE:CD2	2:H:76:SER:HA	2.36	0.60
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.19	0.59
1:L:141:PRO:HG3	1:L:199:LYS:HD3	1.86	0.56
1:L:34:HIS:HE1	1:L:91:SER:OG	1.89	0.55
2:H:18:VAL:HG12	2:H:82(C):LEU:HD11	1.88	0.54
1:L:110:ASP:HB3	1:L:200:THR:HG23	1.91	0.51
2:H:157:TRP:CZ3	2:H:223:LEU:HD11	2.47	0.50
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.93	0.50
2:H:53:ASN:HA	2:H:73:LYS:HE3	1.95	0.49
1:L:147:LYS:HE2	1:L:149:LYS:HE2	1.93	0.49
2:H:41:HIS:HA	2:H:42:GLY:HA2	1.59	0.49
1:L:89:GLN:HG2	1:L:90:GLN:N	2.28	0.48
1:L:108:ARG:NH1	1:L:109:ALA:O	2.43	0.48
1:L:141:PRO:O	1:L:198:HIS:HE1	1.96	0.48
1:L:201:SER:C	1:L:203:SER:H	2.16	0.48
2:H:3:GLN:C	2:H:4:LEU:HD12	2.35	0.48
1:L:106:ILE:H	1:L:166:GLN:NE2	2.08	0.47
1:L:198:HIS:CD2	1:L:200:THR:OG1	2.66	0.47
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.95	0.47
2:H:157:TRP:HZ3	2:H:223:LEU:HD11	1.80	0.46
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.50	0.46
2:H:87:SER:HA	2:H:109:VAL:O	2.16	0.46
2:H:36:TRP:CD1	2:H:69:LEU:HD22	2.51	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:LEU:N	1:L:136:LEU:HD12	2.30	0.46
1:L:54:LEU:HD11	1:L:58:ILE:HG22	1.98	0.46
2:H:210:VAL:O	2:H:218:THR:HA	2.16	0.45
2:H:52(A):PRO:O	2:H:53:ASN:C	2.54	0.45
1:L:50:ARG:HD3	5:H:501:2M9:OAB	2.15	0.45
1:L:161:ASN:O	2:H:177:LEU:HD11	2.15	0.45
2:H:150:GLU:HG3	2:H:151:PRO:CB	2.47	0.45
5:H:501:2M9:OAC	5:H:501:2M9:H4	2.17	0.45
1:L:163:TRP:CH2	1:L:175:MET:HE2	2.52	0.45
2:H:199:TRP:CG	2:H:200:PRO:HA	2.53	0.44
2:H:150:GLU:HG3	2:H:151:PRO:CA	2.48	0.43
2:H:180:SER:O	2:H:180:SER:OG	2.35	0.43
1:L:155:ARG:NH2	1:L:185:GLU:OE2	2.51	0.43
2:H:2:VAL:HG11	2:H:102:VAL:HG21	2.00	0.42
2:H:29:PHE:HB2	2:H:76:SER:HB3	2.02	0.42
2:H:195:SER:C	2:H:198:THR:H	2.23	0.42
2:H:140:SER:HB3	2:H:223:LEU:CD1	2.41	0.42
2:H:178:LEU:HD13	2:H:185:TYR:CZ	2.55	0.41
2:H:3:GLN:O	2:H:4:LEU:HD12	2.20	0.41
1:L:201:SER:C	1:L:203:SER:N	2.74	0.41
1:L:24:ARG:HB2	1:L:24:ARG:HE	1.50	0.41
1:L:212:ASN:C	1:L:212:ASN:HD22	2.23	0.41
1:L:76:ASN:HA	1:L:77:PRO:HA	1.95	0.41
1:L:7:SER:HA	1:L:8:PRO:C	2.42	0.40
2:H:23:LYS:HE3	2:H:23:LYS:HB3	1.88	0.40
2:H:208:CYS:O	2:H:208:CYS:SG	2.79	0.40
2:H:169:SER:HB2	2:H:192:THR:H	1.86	0.40
2:H:52:TYR:CE2	2:H:53:ASN:HB3	2.57	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	L	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	H	219/233 (94%)	206 (94%)	11 (5%)	2 (1%)	17	16
All	All	434/451 (96%)	413 (95%)	19 (4%)	2 (0%)	29	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	52(A)	PRO
2	H	151	PRO

### 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	L	191/192 (100%)	180 (94%)	11 (6%)	20	23
2	H	188/199 (94%)	170 (90%)	18 (10%)	8	8
All	All	379/391 (97%)	350 (92%)	29 (8%)	13	13

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	27(D)	SER
1	L	68	ARG
1	L	108	ARG
1	L	123	GLU
1	L	143	ASP
1	L	156	GLN
1	L	175	MET
1	L	188	ARG
1	L	200	THR
1	L	203	SER
1	L	212	ASN
2	H	1	GLU
2	H	12	VAL
2	H	17	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	53	ASN
2	H	82(B)	SER
2	H	85	ASP
2	H	138	VAL
2	H	165	SER
2	H	166	LEU
2	H	167	SER
2	H	169	SER
2	H	179	GLN
2	H	180	SER
2	H	198	THR
2	H	203	GLN
2	H	204	THR
2	H	209	SER
2	H	226	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	34	HIS
1	L	42	GLN
1	L	161	ASN
1	L	166	GLN
1	L	198	HIS
1	L	212	ASN
2	H	3	GLN
2	H	35	HIS
2	H	39	GLN
2	H	53	ASN
2	H	203	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	ACT	L	302	-	1,3,3	1.60	0	0,3,3	0.00	-
4	ACT	L	303	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-
6	PO4	H	502	-	4,4,4	1.92	2 (50%)	6,6,6	2.05	2 (33%)
5	2M9	H	501	-	30,33,33	1.18	2 (6%)	46,55,55	1.86	9 (19%)

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
5	2M9	H	501	-	-	0/20/20/20	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	502	PO4	P-O4	-2.97	1.45	1.54
5	H	501	2M9	CAT-CAX	-2.82	1.38	1.43
5	H	501	2M9	CAR-CAQ	2.50	1.42	1.35
6	H	502	PO4	P-O3	-2.43	1.47	1.54
4	L	303	ACT	CH3-C	2.30	1.51	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	501	2M9	OBF-CAV-CAZ	7.31	121.60	114.46
5	H	501	2M9	CAQ-CAX-CAT	-3.84	118.56	123.60
6	H	502	PO4	O4-P-O3	3.71	119.86	107.97
5	H	501	2M9	CAP-CAY-CAU	-3.11	119.53	123.60
5	H	501	2M9	OAE-SBE-CAU	2.97	115.29	106.43
5	H	501	2M9	CAG-OBF-CAV	2.82	121.69	117.75
5	H	501	2M9	OBF-CAV-CAN	-2.64	118.64	123.34
6	H	502	PO4	O4-P-O1	-2.46	101.90	110.89
5	H	501	2M9	CAR-CAQ-CAX	-2.27	118.16	121.61
5	H	501	2M9	CAO-CAP-CAY	-2.19	118.27	121.61
5	H	501	2M9	CAO-CAW-CAS	-2.19	120.73	123.60

There are no chirality outliers.

There are no torsion outliers.

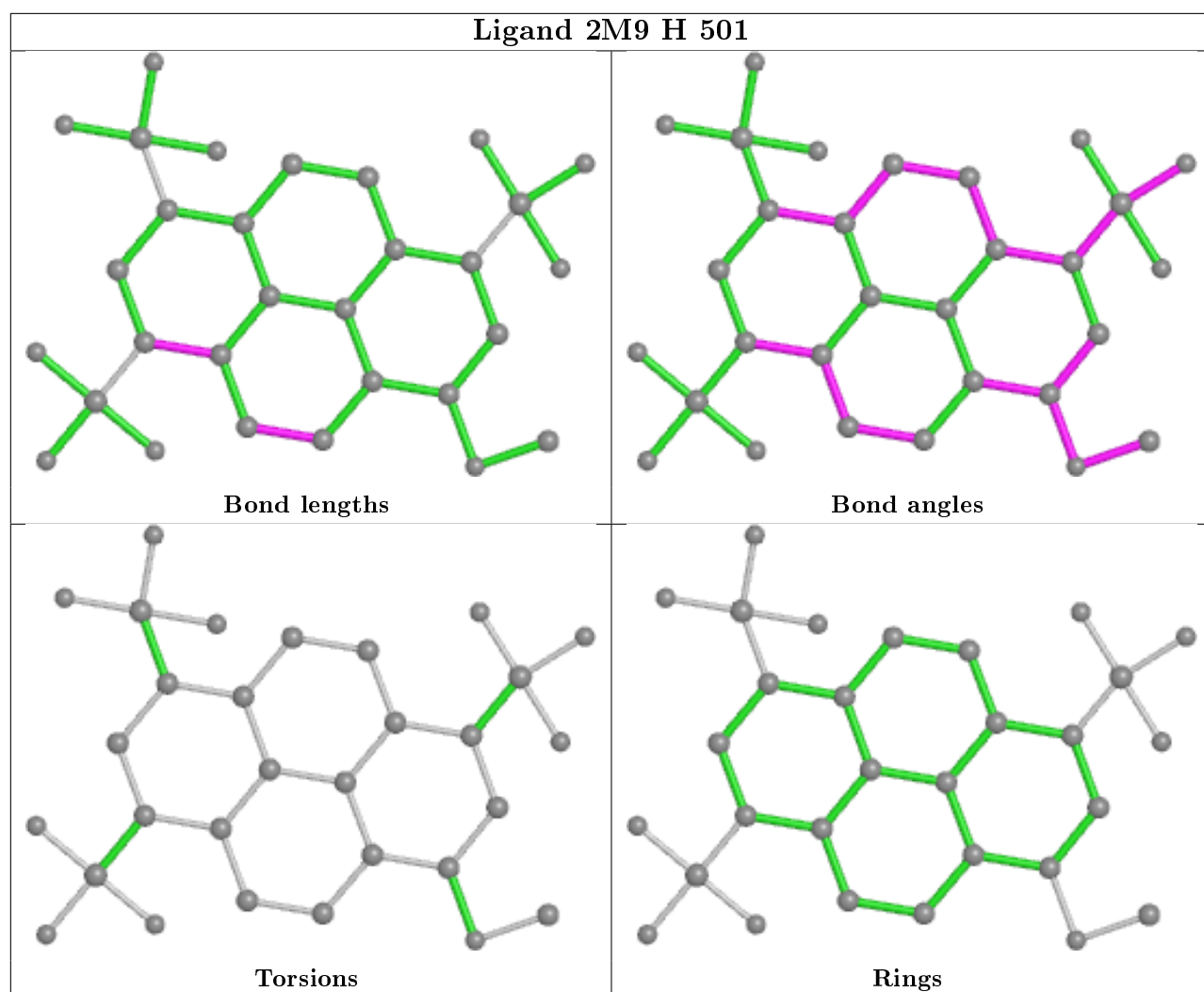
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	501	2M9	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	217/218 (99%)	-0.00	6 (2%) 53 51	21, 40, 76, 106	0
2	H	221/233 (94%)	0.17	13 (5%) 22 21	20, 55, 84, 115	0
All	All	438/451 (97%)	0.09	19 (4%) 35 33	20, 47, 81, 115	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	168	SER	4.6
1	L	202	THR	4.1
2	H	179	GLN	3.9
1	L	203	SER	3.5
1	L	157	ASN	3.3
2	H	180	SER	2.9
1	L	201	SER	2.8
2	H	167	SER	2.8
2	H	224	GLU	2.6
2	H	164	GLY	2.4
2	H	121	VAL	2.4
2	H	163	SER	2.3
1	L	200	THR	2.2
2	H	226	SER	2.2
2	H	222	LYS	2.2
2	H	53	ASN	2.2
2	H	82(A)	ARG	2.1
2	H	41	HIS	2.0
1	L	197	THR	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

There are no carbohydrates in this entry.

### 6.4 Ligands

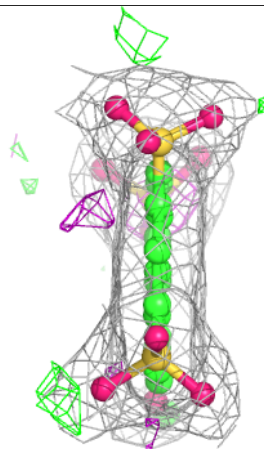
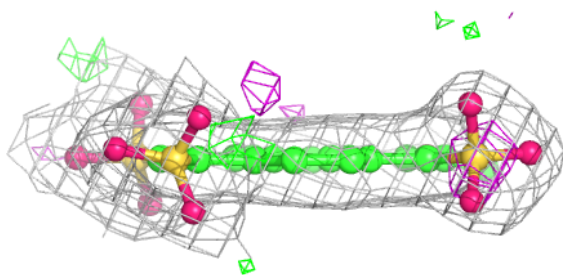
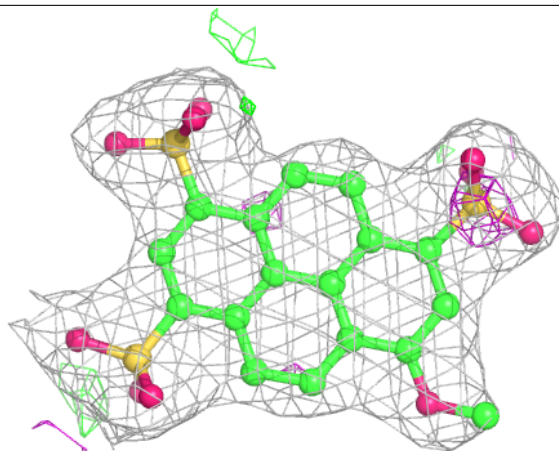
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	ACT	L	302	4/4	0.66	0.20	41,46,48,55	0
4	ACT	L	303	4/4	0.81	0.20	52,54,58,64	0
5	2M9	H	501	30/30	0.96	0.16	26,34,46,48	0
3	ZN	H	503	1/1	0.97	0.03	56,56,56,56	0
6	PO4	H	502	5/5	0.98	0.19	34,38,40,46	0
3	ZN	L	301	1/1	0.99	0.09	43,43,43,43	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 2M9 H 501:**

$2mF_o-DF_c$  (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.