



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:21 AM UTC

PDB ID : 5D7Y / pdb_00005d7y
Title : Crystal structure of Hepatitis B virus T=4 capsid in complex with the allosteric modulator HAP18
Authors : Venkatakrishnan, B.; Katen, S.P.; Zlotnick, A.
Deposited on : 2015-08-14
Resolution : 3.89 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

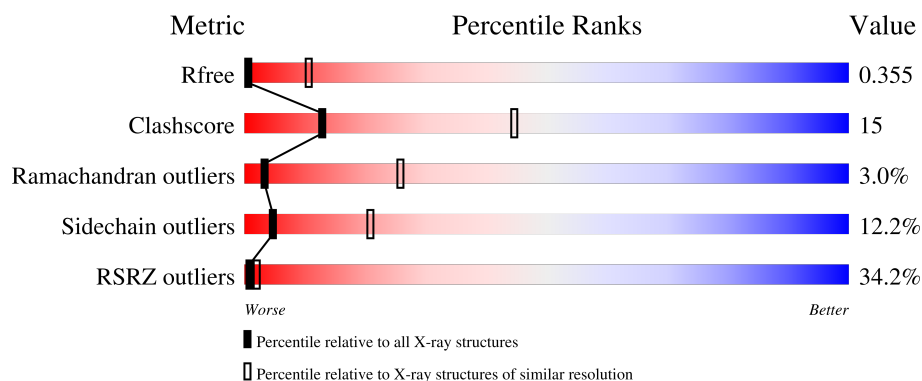
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	150	
1	B	150	
1	C	150	
1	D	150	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4610 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.

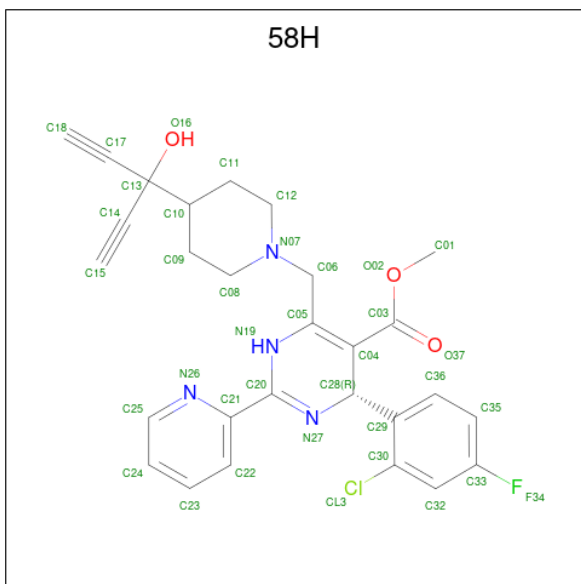
- Molecule 1 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1130	735	186	206	3			
1	B	143	Total	C	N	O	S	0	0	0
			1138	741	187	207	3			
1	C	142	Total	C	N	O	S	0	0	0
			1130	735	186	206	3			
1	D	143	Total	C	N	O	S	0	0	0
			1138	741	187	207	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	CYS	engineered mutation	UNP P03147
A	61	ALA	CYS	engineered mutation	UNP P03147
A	93	MET	VAL	engineered mutation	UNP P03147
A	107	ALA	CYS	engineered mutation	UNP P03147
A	150	CYS	-	expression tag	UNP P03147
B	48	ALA	CYS	engineered mutation	UNP P03147
B	61	ALA	CYS	engineered mutation	UNP P03147
B	93	MET	VAL	engineered mutation	UNP P03147
B	107	ALA	CYS	engineered mutation	UNP P03147
B	150	CYS	-	expression tag	UNP P03147
C	48	ALA	CYS	engineered mutation	UNP P03147
C	61	ALA	CYS	engineered mutation	UNP P03147
C	93	MET	VAL	engineered mutation	UNP P03147
C	107	ALA	CYS	engineered mutation	UNP P03147
C	150	CYS	-	expression tag	UNP P03147
D	48	ALA	CYS	engineered mutation	UNP P03147
D	61	ALA	CYS	engineered mutation	UNP P03147
D	93	MET	VAL	engineered mutation	UNP P03147
D	107	ALA	CYS	engineered mutation	UNP P03147
D	150	CYS	-	expression tag	UNP P03147

- Molecule 2 is methyl (4R)-4-(2-chloro-4-fluorophenyl)-6-{[4-(3-hydroxypenta-1,4-diyn-3-yl)piperidin-1-yl]methyl}-2-(pyridin-2-yl)-1,4-dihydropyrimidine-5-carboxylate (CCD ID: 58H) (formula: C₂₈H₂₆ClFN₄O₃).

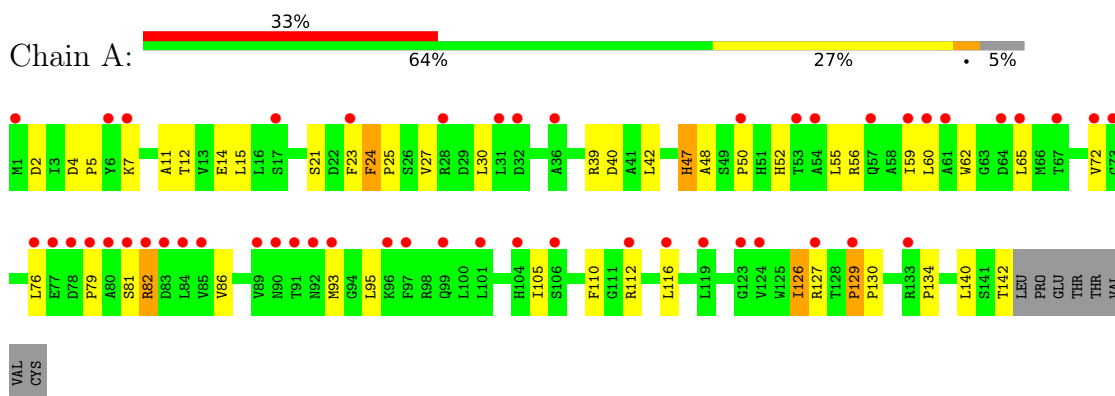


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 37	C 28	Cl 1	F 1	N 4	O 3	0	0
2	C	1	Total 37	C 28	Cl 1	F 1	N 4	O 3	0	0

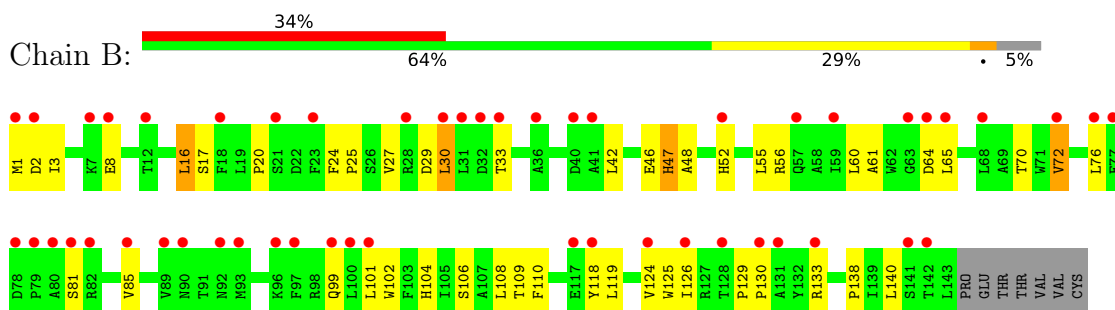
3 Residue-property plots [i](#)

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.

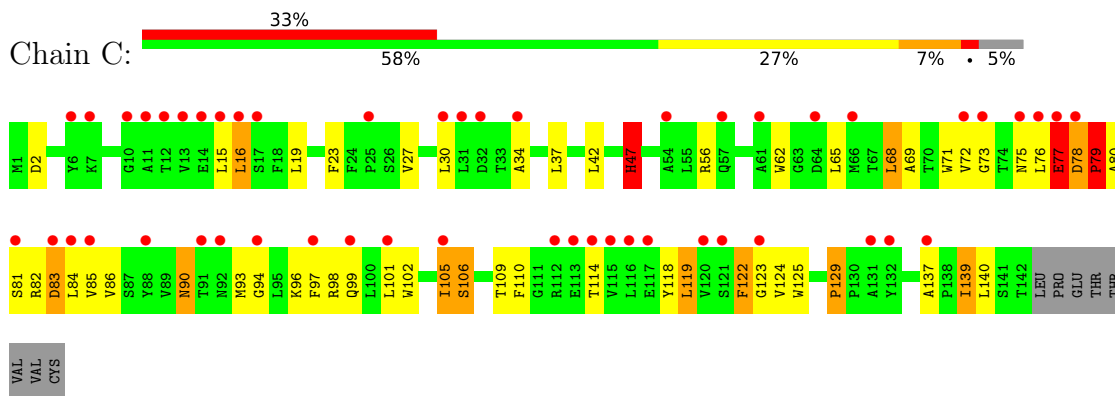
• Molecule 1: Capsid protein



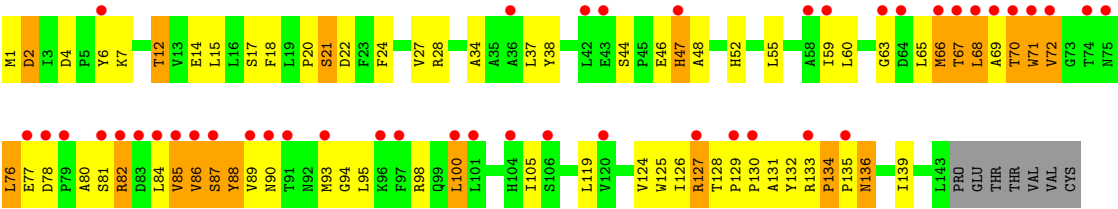
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



• Molecule 1: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	529.38Å 367.41Å 542.00Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	35.68 – 3.89 35.68 – 3.89	Depositor EDS
% Data completeness (in resolution range)	89.1 (35.68-3.89) 75.2 (35.68-3.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.18 (at 3.87Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.263 , 0.273 0.363 , 0.355	Depositor DCC
R_{free} test set	2000 reflections (0.15%)	wwPDB-VP
Wilson B-factor (Å ²)	133.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.55	EDS
Total number of atoms	4610	wwPDB-VP
Average B, all atoms (Å ²)	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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: 58H

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	0.30	0/1165	0.80	4/1597 (0.3%)
1	B	0.33	0/1173	0.79	2/1608 (0.1%)
1	C	0.38	1/1165 (0.1%)	0.87	4/1597 (0.3%)
1	D	0.35	0/1173	0.91	5/1608 (0.3%)
All	All	0.34	1/4676 (0.0%)	0.84	15/6410 (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	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	79	PRO	N-CD	5.19	1.55	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	129	PRO	CA-C-N	5.97	125.67	119.05
1	C	129	PRO	C-N-CA	5.97	125.67	119.05
1	A	129	PRO	CA-C-N	5.74	126.12	119.47
1	A	129	PRO	C-N-CA	5.74	126.12	119.47
1	D	86	VAL	CA-C-N	5.65	131.86	121.70
1	D	86	VAL	C-N-CA	5.65	131.86	121.70
1	A	134	PRO	CA-C-N	5.60	125.70	119.32
1	A	134	PRO	C-N-CA	5.60	125.70	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	ASP	CA-C-N	-5.29	113.22	119.84
1	C	78	ASP	C-N-CA	-5.29	113.22	119.84
1	D	66	MET	N-CA-C	5.28	121.40	114.75
1	B	129	PRO	CA-C-N	5.26	125.58	119.47
1	B	129	PRO	C-N-CA	5.26	125.58	119.47
1	D	66	MET	CA-C-N	5.22	131.10	121.70
1	D	66	MET	C-N-CA	5.22	131.10	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	85	VAL	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	1130	0	1110	25	0
1	B	1138	0	1121	34	0
1	C	1130	0	1110	44	0
1	D	1138	0	1121	50	0
2	B	37	0	26	0	0
2	C	37	0	26	1	0
All	All	4610	0	4514	138	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 15.

All (138) 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:79:PRO:HG2	1:C:81:SER:HB3	1.55	0.85
1:C:79:PRO:HD2	1:C:81:SER:HB3	1.58	0.85
1:C:79:PRO:HG2	1:C:81:SER:CB	2.06	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:H	1:D:87:SER:C	1.88	0.80
1:D:128:THR:OG1	1:D:133:ARG:NH2	2.15	0.80
1:C:80:ALA:H	1:C:81:SER:HB3	1.47	0.78
1:C:90:ASN:O	1:C:90:ASN:ND2	2.15	0.77
1:C:79:PRO:CG	1:C:81:SER:HB3	2.15	0.76
1:C:79:PRO:CD	1:C:81:SER:HB3	2.15	0.76
1:C:65:LEU:HD21	1:D:65:LEU:HD11	1.68	0.74
1:C:93:MET:HE1	1:D:68:LEU:HD22	1.70	0.71
1:D:133:ARG:HH11	1:D:134:PRO:HD3	1.57	0.70
1:C:72:VAL:HG11	1:C:85:VAL:HG11	1.72	0.69
1:A:59:ILE:HD13	1:B:1:MET:HE1	1.73	0.68
1:D:68:LEU:HA	1:D:71:TRP:HB2	1.76	0.68
1:D:69:ALA:H	1:D:70:THR:C	2.00	0.68
1:C:69:ALA:HB1	1:C:86:VAL:HG13	1.74	0.68
1:C:79:PRO:HB2	1:C:83:ASP:OD2	1.95	0.66
1:C:122:PHE:O	1:C:124:VAL:N	2.28	0.66
1:A:56:ARG:NH1	1:B:8:GLU:OE2	2.28	0.65
1:B:47:HIS:H	1:B:47:HIS:HD1	1.45	0.64
1:D:87:SER:OG	1:D:88:TYR:N	2.27	0.63
1:A:76:LEU:HD12	1:B:81:SER:HB2	1.81	0.63
1:D:89:VAL:O	1:D:94:GLY:N	2.31	0.62
1:C:118:TYR:CG	1:C:140:LEU:HG	2.35	0.62
1:C:78:ASP:HB2	1:C:79:PRO:HD3	1.81	0.61
1:C:82:ARG:H	1:C:86:VAL:HG23	1.65	0.61
1:B:29:ASP:O	1:B:33:THR:OG1	2.17	0.61
1:C:122:PHE:O	1:C:125:TRP:N	2.26	0.61
1:C:79:PRO:HG2	1:C:81:SER:HB2	1.82	0.61
1:D:87:SER:O	1:D:89:VAL:N	2.34	0.61
1:D:129:PRO:O	1:D:131:ALA:N	2.34	0.60
1:A:81:SER:HB2	1:B:76:LEU:HG	1.84	0.60
1:C:68:LEU:HD12	1:D:89:VAL:HG21	1.83	0.59
1:D:24:PHE:O	1:D:98:ARG:NH1	2.34	0.59
1:A:50:PRO:HG3	1:B:47:HIS:CD2	2.38	0.59
1:C:16:LEU:HD12	1:C:99:GLN:HB3	1.84	0.59
1:C:90:ASN:HD22	1:C:90:ASN:C	2.07	0.58
1:B:30:LEU:HD12	1:B:101:LEU:HB3	1.86	0.58
1:D:82:ARG:HB2	1:D:86:VAL:HG22	1.84	0.58
1:B:102:TRP:HH2	1:B:119:LEU:HD21	1.69	0.57
1:C:80:ALA:O	1:C:82:ARG:NH1	2.37	0.57
1:A:12:THR:HG23	1:A:15:LEU:H	1.69	0.57
1:B:25:PRO:HB3	1:C:129:PRO:HD3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:THR:HG23	1:D:15:LEU:HD13	1.87	0.56
1:D:85:VAL:N	1:D:86:VAL:HG23	2.21	0.56
1:A:21:SER:HB3	1:A:95:LEU:HD11	1.86	0.56
1:A:39:ARG:HD2	1:B:1:MET:HG2	1.88	0.55
1:C:34:ALA:HB2	1:C:105:ILE:HD11	1.89	0.55
1:B:42:LEU:O	1:B:56:ARG:NH1	2.40	0.54
1:D:21:SER:HB2	1:D:95:LEU:HD11	1.88	0.54
1:D:133:ARG:HG2	1:D:134:PRO:HB3	1.90	0.54
1:D:133:ARG:HD2	1:D:134:PRO:HG3	1.90	0.54
1:D:78:ASP:OD2	1:D:81:SER:OG	2.26	0.53
1:B:125:TRP:CE2	1:B:133:ARG:HD2	2.44	0.53
1:D:6:TYR:CZ	1:D:100:LEU:HD12	2.44	0.53
1:A:42:LEU:HD21	1:A:55:LEU:HD23	1.91	0.52
1:A:72:VAL:HA	1:A:76:LEU:HD23	1.91	0.52
1:C:73:GLY:O	1:C:82:ARG:NH2	2.42	0.52
1:A:65:LEU:HD21	1:B:65:LEU:HD21	1.92	0.52
1:C:110:PHE:CE1	1:C:140:LEU:HB3	2.44	0.51
1:D:46:GLU:O	1:D:48:ALA:N	2.44	0.51
1:D:134:PRO:HG2	1:D:136:ASN:O	2.11	0.51
1:A:5:PRO:HG3	1:B:60:LEU:HD13	1.92	0.51
1:D:2:ASP:N	1:D:2:ASP:OD1	2.42	0.51
1:D:86:VAL:HB	1:D:87:SER:CB	2.41	0.51
1:D:66:MET:H	1:D:67:THR:HG22	1.75	0.50
1:B:16:LEU:HD21	1:B:102:TRP:HZ3	1.76	0.50
1:D:4:ASP:HB3	1:D:7:LYS:HB2	1.91	0.50
1:D:66:MET:N	1:D:68:LEU:H	2.09	0.50
1:C:79:PRO:CG	1:C:81:SER:CB	2.80	0.49
1:C:79:PRO:HB2	1:C:83:ASP:CG	2.37	0.49
1:C:15:LEU:HD23	1:C:119:LEU:HD22	1.95	0.49
1:B:130:PRO:HA	1:B:133:ARG:HB3	1.94	0.49
1:A:110:PHE:CE2	1:A:140:LEU:HB3	2.48	0.49
1:B:104:HIS:O	1:B:108:LEU:HG	2.13	0.49
1:B:24:PHE:CZ	1:B:99:GLN:HG2	2.48	0.48
1:C:79:PRO:CG	1:C:80:ALA:H	2.26	0.48
1:C:23:PHE:CZ	2:C:201:58H:H20	2.49	0.48
1:D:67:THR:O	1:D:68:LEU:HB2	2.12	0.48
1:A:11:ALA:HB2	1:A:116:LEU:HD21	1.96	0.47
1:C:34:ALA:HB3	1:D:1:MET:HE1	1.95	0.47
1:D:93:MET:C	1:D:95:LEU:H	2.23	0.47
1:A:24:PHE:HA	1:A:25:PRO:HD2	1.75	0.47
1:C:19:LEU:HD13	1:C:23:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:VAL:HG22	1:D:76:LEU:HB2	1.97	0.47
1:D:86:VAL:N	1:D:87:SER:O	2.46	0.47
1:B:42:LEU:HD21	1:B:55:LEU:HD23	1.97	0.46
1:D:48:ALA:HB3	1:D:52:HIS:CG	2.51	0.46
1:A:79:PRO:HA	1:A:82:ARG:HB3	1.97	0.46
1:C:27:VAL:HG11	1:C:62:TRP:CE2	2.51	0.46
1:C:79:PRO:HG2	1:C:80:ALA:H	1.79	0.46
1:C:102:TRP:O	1:C:106:SER:OG	2.34	0.46
1:D:20:PRO:O	1:D:22:ASP:N	2.49	0.45
1:A:60:LEU:HD21	1:B:3:ILE:HB	1.98	0.45
1:C:42:LEU:O	1:C:56:ARG:HD3	2.16	0.45
1:B:102:TRP:O	1:B:106:SER:OG	2.32	0.45
1:C:80:ALA:HB3	1:C:81:SER:HA	1.99	0.45
1:D:86:VAL:HB	1:D:87:SER:HB3	1.98	0.45
1:A:129:PRO:HA	1:A:130:PRO:HD3	1.83	0.45
1:B:72:VAL:HG21	1:B:85:VAL:HG11	1.98	0.45
1:D:18:PHE:HZ	1:D:127:ARG:CZ	2.30	0.45
1:D:60:LEU:HD23	1:D:60:LEU:HA	1.87	0.45
1:C:137:ALA:O	1:C:139:ILE:HD12	2.18	0.44
1:D:133:ARG:NH1	1:D:134:PRO:HD3	2.27	0.44
1:B:20:PRO:HD3	1:B:126:ILE:HD12	1.99	0.44
1:B:52:HIS:O	1:B:56:ARG:HG3	2.18	0.44
1:D:34:ALA:HB2	1:D:105:ILE:HD11	2.00	0.44
1:D:71:TRP:CE2	1:D:72:VAL:HG23	2.52	0.44
1:A:48:ALA:HB3	1:A:52:HIS:CG	2.52	0.43
1:A:93:MET:HE1	1:B:64:ASP:HB3	2.00	0.43
1:A:4:ASP:HB3	1:A:7:LYS:HB2	2.01	0.43
1:D:14:GLU:O	1:D:17:SER:OG	2.35	0.43
1:C:79:PRO:HD2	1:C:81:SER:CB	2.40	0.43
1:C:97:PHE:O	1:C:101:LEU:HB2	2.19	0.43
1:D:72:VAL:HG22	1:D:76:LEU:HD13	2.01	0.42
1:C:47:HIS:HA	1:C:56:ARG:NH2	2.35	0.42
1:A:30:LEU:HD12	1:A:105:ILE:HD12	2.00	0.42
1:B:48:ALA:HB3	1:B:52:HIS:CG	2.54	0.42
1:D:66:MET:N	1:D:68:LEU:N	2.68	0.42
1:B:1:MET:HE3	1:B:1:MET:HB2	1.93	0.42
1:B:47:HIS:ND1	1:B:47:HIS:N	2.59	0.41
1:D:65:LEU:HG	1:D:68:LEU:O	2.21	0.41
1:D:80:ALA:C	1:D:82:ARG:H	2.28	0.41
1:B:61:ALA:O	1:B:65:LEU:HD23	2.20	0.41
1:C:76:LEU:O	1:C:77:GLU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG11	1:A:62:TRP:CZ2	2.55	0.41
1:A:126:ILE:HG22	1:A:127:ARG:HG3	2.03	0.41
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.94	0.41
1:D:37:LEU:HB2	1:D:38:TYR:CD1	2.56	0.41
1:D:85:VAL:HB	1:D:86:VAL:HA	2.03	0.41
1:A:82:ARG:O	1:A:86:VAL:HG23	2.21	0.41
1:D:125:TRP:HE1	1:D:134:PRO:HG2	1.86	0.41
1:B:110:PHE:CG	1:B:140:LEU:HD21	2.56	0.40
1:D:59:ILE:O	1:D:63:GLY:N	2.55	0.40
1:B:46:GLU:O	1:B:48:ALA:N	2.54	0.40
1:B:118:TYR:OH	1:B:138:PRO:O	2.32	0.40
1:C:94:GLY:O	1:C:98:ARG:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	140/150 (93%)	133 (95%)	4 (3%)	3 (2%)	5	31
1	B	141/150 (94%)	132 (94%)	9 (6%)	0	100	100
1	C	140/150 (93%)	117 (84%)	18 (13%)	5 (4%)	2	23
1	D	141/150 (94%)	113 (80%)	19 (14%)	9 (6%)	1	15
All	All	562/600 (94%)	495 (88%)	50 (9%)	17 (3%)	3	26

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	77	GLU
1	C	123	GLY
1	D	47	HIS

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Mol	Chain	Res	Type
1	D	68	LEU
1	D	88	TYR
1	D	134	PRO
1	C	47	HIS
1	C	79	PRO
1	C	122	PHE
1	D	21	SER
1	A	23	PHE
1	A	24	PHE
1	D	72	VAL
1	D	135	PRO
1	A	47	HIS
1	D	132	TYR
1	D	130	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	A	122/130 (94%)	114 (93%)	8 (7%)	15	41
1	B	123/130 (95%)	113 (92%)	10 (8%)	11	35
1	C	122/130 (94%)	103 (84%)	19 (16%)	2	15
1	D	123/130 (95%)	100 (81%)	23 (19%)	1	10
All	All	490/520 (94%)	430 (88%)	60 (12%)	5	21

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	14	GLU
1	A	40	ASP
1	A	47	HIS
1	A	82	ARG
1	A	112	ARG
1	A	126	ILE

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Mol	Chain	Res	Type
1	A	142	THR
1	B	2	ASP
1	B	16	LEU
1	B	17	SER
1	B	27	VAL
1	B	30	LEU
1	B	47	HIS
1	B	70	THR
1	B	72	VAL
1	B	109	THR
1	B	124	VAL
1	C	2	ASP
1	C	16	LEU
1	C	30	LEU
1	C	37	LEU
1	C	47	HIS
1	C	68	LEU
1	C	71	TRP
1	C	75	ASN
1	C	77	GLU
1	C	83	ASP
1	C	84	LEU
1	C	90	ASN
1	C	96	LYS
1	C	105	ILE
1	C	106	SER
1	C	109	THR
1	C	114	THR
1	C	119	LEU
1	C	139	ILE
1	D	2	ASP
1	D	12	THR
1	D	27	VAL
1	D	28	ARG
1	D	44	SER
1	D	47	HIS
1	D	55	LEU
1	D	67	THR
1	D	70	THR
1	D	71	TRP
1	D	76	LEU
1	D	77	GLU

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Mol	Chain	Res	Type
1	D	82	ARG
1	D	84	LEU
1	D	87	SER
1	D	90	ASN
1	D	100	LEU
1	D	119	LEU
1	D	124	VAL
1	D	126	ILE
1	D	127	ARG
1	D	136	ASN
1	D	139	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	B	51	HIS
1	B	75	ASN
1	C	75	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	58H	B	201	-	36,40,40	1.05	2 (5%)	42,57,57	1.59	7 (16%)
2	58H	C	201	-	36,40,40	0.78	0	42,57,57	1.47	6 (14%)

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	58H	B	201	-	-	10/24/56/56	0/4/4/4
2	58H	C	201	-	-	9/24/56/56	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	58H	C06-N07	2.76	1.52	1.47
2	B	201	58H	C08-N07	2.49	1.53	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	58H	C04-C05-N19	-4.47	115.84	120.49
2	C	201	58H	C04-C05-N19	-4.17	116.14	120.49
2	B	201	58H	C29-C30-CL3	3.76	124.26	120.41
2	C	201	58H	C06-N07-C12	2.86	115.59	111.14
2	C	201	58H	C29-C30-CL3	2.70	123.18	120.41
2	B	201	58H	C03-C04-C05	2.54	124.91	121.32
2	B	201	58H	C11-C12-N07	-2.39	107.21	111.08
2	B	201	58H	C06-N07-C12	2.27	114.67	111.14
2	C	201	58H	C03-C04-C05	-2.19	118.23	121.32
2	C	201	58H	C23-C22-C21	-2.17	116.04	118.63
2	B	201	58H	C22-C21-N26	2.14	125.63	122.74
2	B	201	58H	C32-C30-CL3	-2.07	115.06	118.45
2	C	201	58H	O02-C03-O37	2.03	127.39	123.50

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	58H	C11-C10-C13-O16
2	C	201	58H	O02-C03-C04-C05
2	C	201	58H	N19-C05-C06-N07
2	C	201	58H	N19-C20-C21-C22
2	C	201	58H	N19-C20-C21-N26
2	C	201	58H	N27-C20-C21-C22
2	C	201	58H	N27-C20-C21-N26
2	C	201	58H	O37-C03-C04-C05
2	C	201	58H	O37-C03-C04-C28
2	C	201	58H	O02-C03-C04-C28
2	B	201	58H	O02-C03-C04-C28
2	B	201	58H	O37-C03-C04-C28
2	B	201	58H	O02-C03-C04-C05
2	B	201	58H	O37-C03-C04-C05
2	B	201	58H	C09-C10-C13-O16
2	B	201	58H	C11-C10-C13-C14
2	B	201	58H	C11-C10-C13-C17
2	B	201	58H	C09-C10-C13-C17
2	B	201	58H	C04-C28-C29-C36

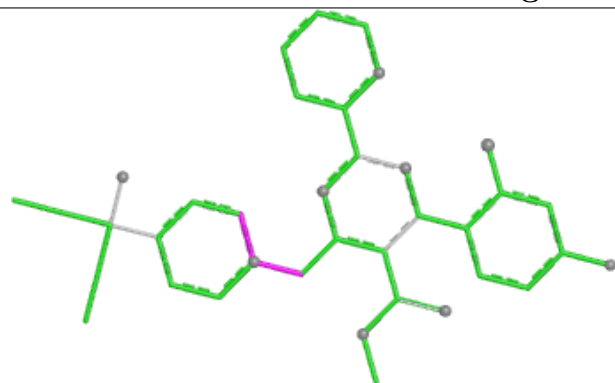
There are no ring outliers.

1 monomer is involved in 1 short contact:

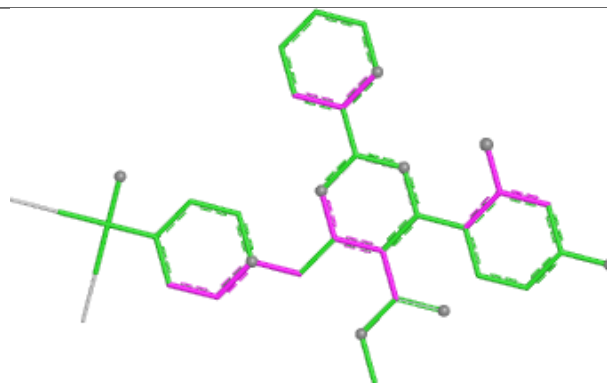
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	201	58H	1	0

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.

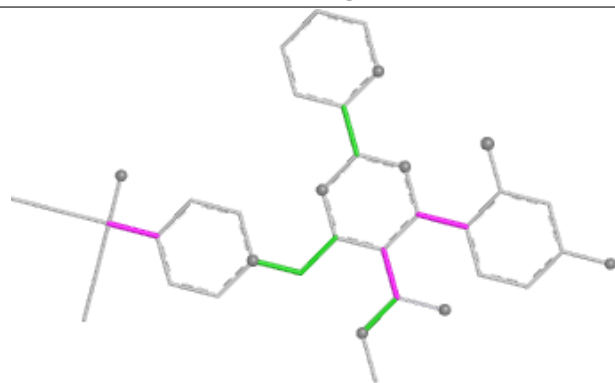
Ligand 58H B 201



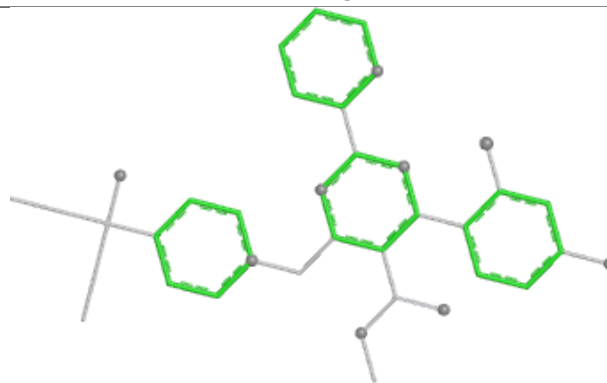
Bond lengths



Bond angles

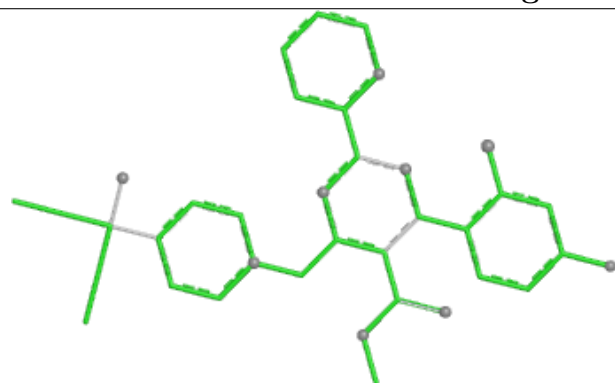


Torsions

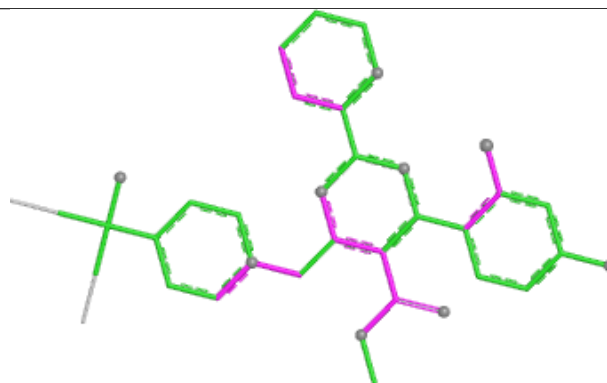


Rings

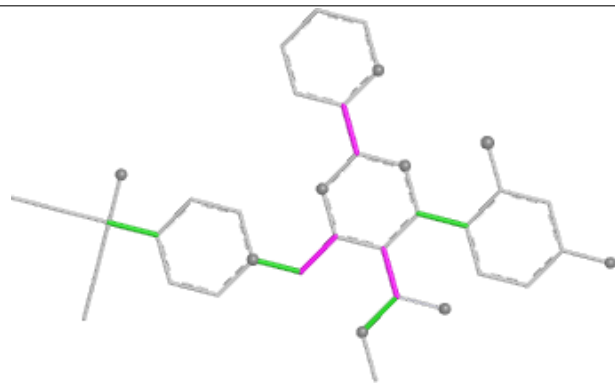
Ligand 58H C 201



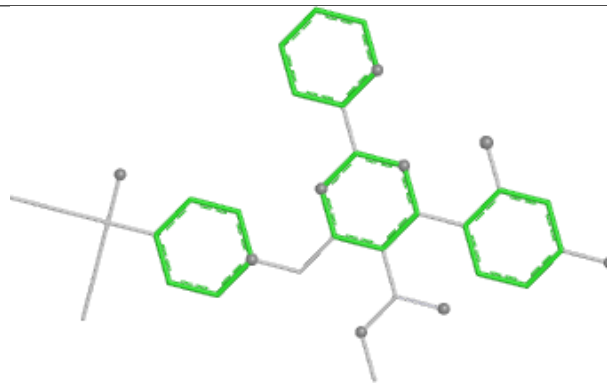
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	142/150 (94%)	1.56	50 (35%) 1 2	110, 174, 236, 332	0
1	B	143/150 (95%)	1.71	51 (35%) 1 2	100, 164, 241, 291	0
1	C	142/150 (94%)	1.74	50 (35%) 1 2	101, 159, 290, 467	0
1	D	143/150 (95%)	1.69	44 (30%) 1 3	106, 170, 346, 529	0
All	All	570/600 (95%)	1.68	195 (34%) 1 2	100, 167, 290, 529	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	84	LEU	7.9
1	D	69	ALA	6.8
1	D	66	MET	6.2
1	D	77	GLU	6.1
1	D	64	ASP	5.5
1	D	70	THR	5.5
1	D	130	PRO	5.2
1	B	99	GLN	5.1
1	C	88	TYR	5.1
1	B	96	LYS	4.9
1	C	72	VAL	4.7
1	C	99	GLN	4.7
1	A	85	VAL	4.5
1	D	93	MET	4.4
1	C	78	ASP	4.3
1	B	93	MET	4.3
1	C	113	GLU	4.3
1	C	121	SER	4.1
1	B	85	VAL	4.1
1	C	83	ASP	4.0
1	C	12	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	40	ASP	3.9
1	D	83	ASP	3.9
1	C	77	GLU	3.9
1	C	97	PHE	3.9
1	A	77	GLU	3.8
1	D	85	VAL	3.8
1	D	67	THR	3.8
1	D	6	TYR	3.8
1	A	81	SER	3.8
1	B	80	ALA	3.7
1	B	79	PRO	3.7
1	B	21	SER	3.7
1	D	71	TRP	3.6
1	C	75	ASN	3.6
1	A	80	ALA	3.6
1	C	31	LEU	3.6
1	C	10	GLY	3.6
1	B	31	LEU	3.5
1	C	14	GLU	3.5
1	B	32	ASP	3.5
1	B	8	GLU	3.5
1	A	93	MET	3.5
1	C	76	LEU	3.5
1	D	84	LEU	3.5
1	D	91	THR	3.5
1	B	65	LEU	3.4
1	B	72	VAL	3.4
1	C	85	VAL	3.4
1	D	79	PRO	3.4
1	D	75	ASN	3.4
1	A	76	LEU	3.4
1	D	96	LYS	3.4
1	A	67	THR	3.3
1	B	101	LEU	3.3
1	D	74	THR	3.3
1	A	72	VAL	3.3
1	A	97	PHE	3.3
1	B	78	ASP	3.3
1	B	76	LEU	3.2
1	D	89	VAL	3.2
1	B	23	PHE	3.2
1	D	129	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	127	ARG	3.2
1	C	7	LYS	3.2
1	A	99	GLN	3.1
1	D	59	ILE	3.1
1	B	41	ALA	3.1
1	A	79	PRO	3.1
1	A	64	ASP	3.1
1	B	59	ILE	3.0
1	A	28	ARG	3.0
1	D	120	VAL	3.0
1	D	97	PHE	3.0
1	B	90	ASN	3.0
1	B	124	VAL	3.0
1	D	106	SER	2.9
1	D	133	ARG	2.9
1	A	60	LEU	2.9
1	D	82	ARG	2.9
1	C	64	ASP	2.9
1	A	124	VAL	2.9
1	D	86	VAL	2.9
1	D	100	LEU	2.9
1	C	117	GLU	2.9
1	A	36	ALA	2.8
1	B	118	TYR	2.8
1	C	73	GLY	2.8
1	D	104	HIS	2.8
1	A	23	PHE	2.8
1	B	133	ARG	2.8
1	B	30	LEU	2.8
1	C	105	ILE	2.8
1	B	92	ASN	2.8
1	C	13	VAL	2.8
1	A	78	ASP	2.8
1	B	28	ARG	2.7
1	C	25	PRO	2.7
1	A	73	GLY	2.7
1	C	11	ALA	2.7
1	B	117	GLU	2.7
1	B	128	THR	2.7
1	D	81	SER	2.7
1	C	137	ALA	2.7
1	B	81	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	64	ASP	2.7
1	B	63	GLY	2.7
1	C	132	TYR	2.7
1	C	101	LEU	2.7
1	C	6	TYR	2.6
1	A	31	LEU	2.6
1	C	120	VAL	2.6
1	A	6	TYR	2.6
1	B	141	SER	2.6
1	B	52	HIS	2.6
1	C	17	SER	2.6
1	B	33	THR	2.6
1	B	77	GLU	2.6
1	D	43	GLU	2.6
1	C	15	LEU	2.6
1	A	104	HIS	2.5
1	B	131	ALA	2.5
1	A	57	GLN	2.5
1	C	81	SER	2.5
1	C	115	VAL	2.5
1	D	135	PRO	2.5
1	A	84	LEU	2.5
1	C	114	THR	2.5
1	A	59	ILE	2.5
1	C	34	ALA	2.5
1	A	54	ALA	2.4
1	D	90	ASN	2.4
1	A	65	LEU	2.4
1	A	129	PRO	2.4
1	B	7	LYS	2.4
1	A	7	LYS	2.4
1	B	89	VAL	2.4
1	D	72	VAL	2.4
1	B	126	ILE	2.4
1	C	91	THR	2.4
1	B	82	ARG	2.4
1	A	116	LEU	2.4
1	B	68	LEU	2.4
1	A	90	ASN	2.3
1	A	92	ASN	2.3
1	B	18	PHE	2.3
1	A	91	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	32	ASP	2.3
1	C	94	GLY	2.3
1	C	92	ASN	2.3
1	D	68	LEU	2.3
1	A	83	ASP	2.3
1	C	116	LEU	2.3
1	D	42	LEU	2.3
1	B	12	THR	2.3
1	A	61	ALA	2.3
1	D	36	ALA	2.3
1	B	57	GLN	2.3
1	B	2	ASP	2.3
1	A	17	SER	2.2
1	C	66	MET	2.2
1	A	112	ARG	2.2
1	B	1	MET	2.2
1	A	82	ARG	2.2
1	C	112	ARG	2.2
1	A	50	PRO	2.2
1	B	36	ALA	2.2
1	C	131	ALA	2.1
1	D	78	ASP	2.1
1	A	123	GLY	2.1
1	C	57	GLN	2.1
1	D	87	SER	2.1
1	A	53	THR	2.1
1	B	142	THR	2.1
1	A	119	LEU	2.1
1	A	127	ARG	2.1
1	D	63	GLY	2.1
1	B	130	PRO	2.1
1	A	101	LEU	2.1
1	B	100	LEU	2.1
1	C	54	ALA	2.1
1	C	61	ALA	2.1
1	A	96	LYS	2.1
1	C	30	LEU	2.1
1	C	32	ASP	2.1
1	A	1	MET	2.1
1	A	133	ARG	2.1
1	B	97	PHE	2.1
1	D	47	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	106	SER	2.0
1	C	16	LEU	2.0
1	D	101	LEU	2.0
1	C	123	GLY	2.0
1	A	89	VAL	2.0
1	D	58	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

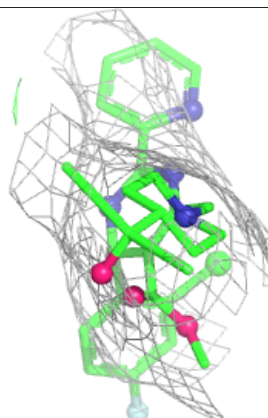
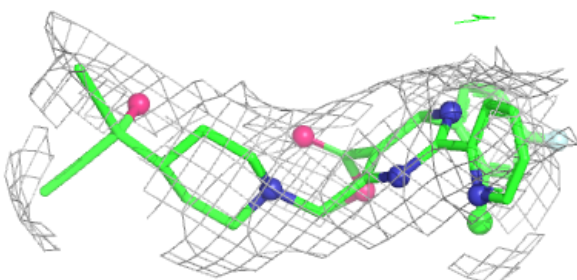
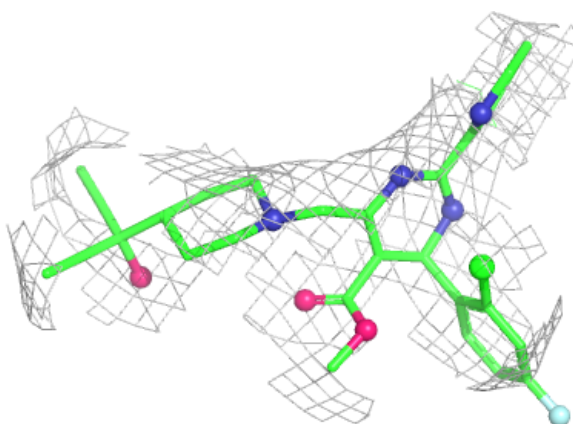
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	58H	C	201	37/37	0.87	0.24	274,274,274,274	0
2	58H	B	201	37/37	0.95	0.18	260,260,260,260	0

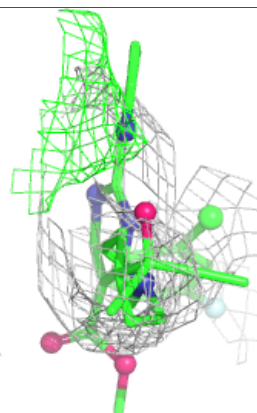
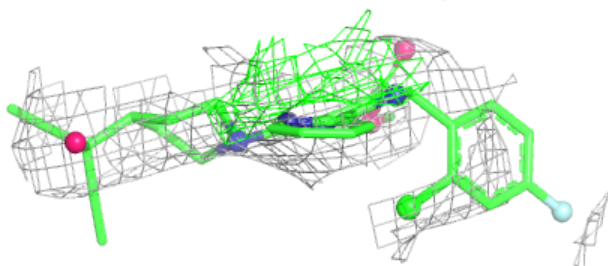
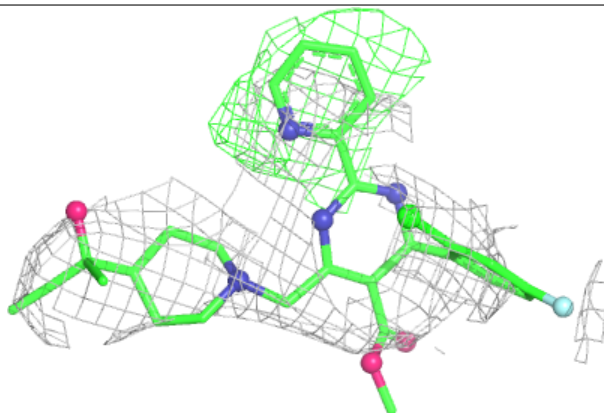
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 58H C 201:

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

**Electron density around 58H B 201:**

$2mF_o-DF_c$ (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.