



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:41 am BST

PDB ID : 2WRM
Title : Identification of Novel Allosteric Inhibitors of Hepatitis C Virus NS5B Polymerase Thumb Domain (Site II) by Structure-Based Design
Authors : Di Marco, S.
Deposited on : 2009-09-01
Resolution : 1.95 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

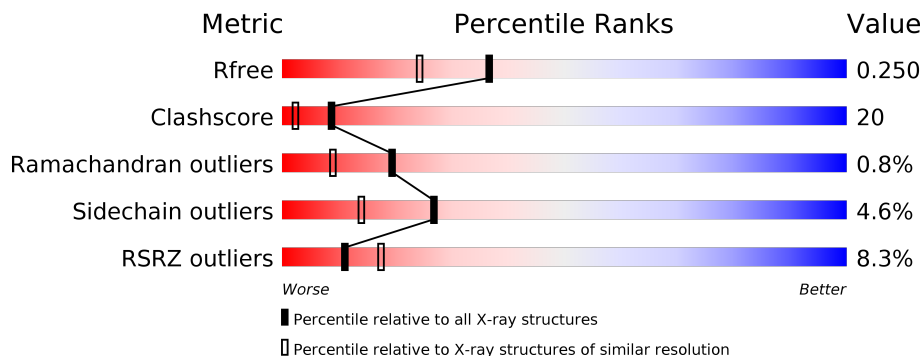
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

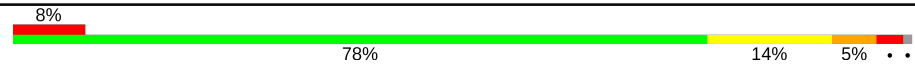
The reported resolution of this entry is 1.95 Å.

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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	536	

2 Entry composition [i](#)

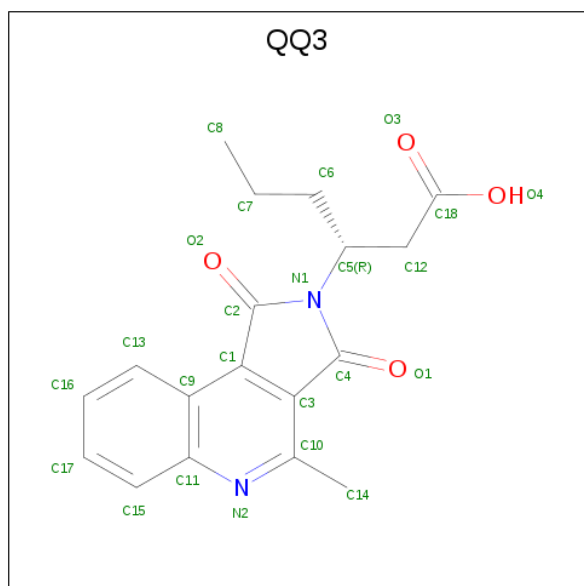
There are 3 unique types of molecules in this entry. The entry contains 4835 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	531	4137	2605	733	768	31	130	2	0

- Molecule 2 is (3R)-3-(4-METHYL-1,3-DIOXO-1,3-DIHYDRO-2H-PYRROLO[3,4-C]QUINOLIN-2-YL)HEXANOIC ACID (three-letter code: QQ3) (formula: C₁₈H₁₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	24	18	2	4	0	0
2	A	1	24	18	2	4	0	0
2	A	1	21	17	2	2	0	0

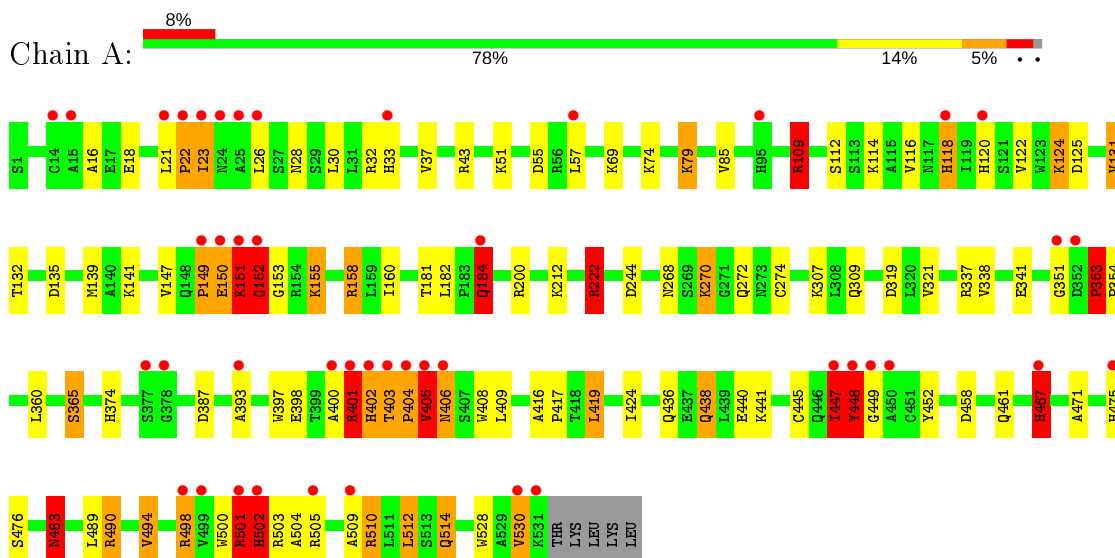
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	629	Total 629	O 629	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: RNA-DIRECTED RNA POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	66.76Å 96.17Å 95.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 19.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-1.95) 99.6 (19.76-1.95)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.01 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.189 , 0.244 0.199 , 0.250	Depositor DCC
R_{free} test set	1840 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.013 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4835	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: QQ3

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	15.47	80/4231 (1.9%)	5.09	132/5740 (2.3%)

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	23

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	405	VAL	CB-CG1	628.57	14.72	1.52
1	A	222	ARG	CD-NE	358.76	7.56	1.46
1	A	222	ARG	NE-CZ	311.01	5.37	1.33
1	A	502	HIS	CE1-NE2	283.58	7.84	1.32
1	A	401	ARG	CZ-NH1	280.68	4.97	1.33
1	A	502	HIS	ND1-CE1	228.85	7.06	1.34
1	A	152	GLY	N-CA	181.38	4.18	1.46
1	A	150	GLU	CA-C	152.45	5.49	1.52
1	A	448	TYR	CD1-CE1	138.56	3.47	1.39
1	A	448	TYR	CD2-CE2	137.09	3.44	1.39
1	A	124	LYS	CE-NZ	131.61	4.78	1.49
1	A	448	TYR	CZ-OH	97.19	3.03	1.37
1	A	184	GLN	CD-OE1	79.07	2.97	1.24
1	A	109	ARG	NE-CZ	71.15	2.25	1.33
1	A	404	PRO	N-CD	70.86	2.47	1.47
1	A	222	ARG	CZ-NH1	67.28	2.20	1.33
1	A	109	ARG	CG-CD	58.88	2.99	1.51
1	A	152	GLY	CA-C	58.84	2.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	GLN	CD-NE2	57.04	2.75	1.32
1	A	22	PRO	CA-C	54.61	2.62	1.52
1	A	404	PRO	CA-CB	45.14	2.43	1.53
1	A	32	ARG	NE-CZ	44.44	1.90	1.33
1	A	502	HIS	CD2-NE2	43.40	2.33	1.38
1	A	155	LYS	CD-CE	37.91	2.46	1.51
1	A	405	VAL	CA-CB	-37.33	0.76	1.54
1	A	28	ASN	CB-CG	35.21	2.32	1.51
1	A	402	HIS	CE1-NE2	32.33	2.07	1.32
1	A	483	ASN	CG-ND2	31.03	2.10	1.32
1	A	448	TYR	CG-CD2	30.41	1.78	1.39
1	A	32	ARG	CD-NE	-29.98	0.95	1.46
1	A	43	ARG	CG-CD	28.69	2.23	1.51
1	A	18	GLU	CG-CD	26.79	1.92	1.51
1	A	147	VAL	CB-CG1	-26.06	0.98	1.52
1	A	69	LYS	CE-NZ	-25.17	0.86	1.49
1	A	490	ARG	CD-NE	23.54	1.86	1.46
1	A	440	GLU	CD-OE1	-21.66	1.01	1.25
1	A	149	PRO	C-N	-21.04	0.85	1.34
1	A	151	LYS	CG-CD	18.73	2.16	1.52
1	A	23	ILE	CA-C	18.70	2.01	1.52
1	A	51	LYS	CE-NZ	17.87	1.93	1.49
1	A	402	HIS	CD2-NE2	-17.20	1.00	1.38
1	A	402	HIS	ND1-CE1	16.38	1.75	1.34
1	A	440	GLU	CD-OE2	15.81	1.43	1.25
1	A	502	HIS	CG-ND1	15.55	1.73	1.38
1	A	32	ARG	CZ-NH1	15.43	1.53	1.33
1	A	307	LYS	CE-NZ	-15.40	1.10	1.49
1	A	490	ARG	CZ-NH2	15.18	1.52	1.33
1	A	365	SER	CB-OG	-14.94	1.22	1.42
1	A	74	LYS	CE-NZ	14.64	1.85	1.49
1	A	212	LYS	CE-NZ	14.28	1.84	1.49
1	A	272	GLN	CD-NE2	13.84	1.67	1.32
1	A	270	LYS	CG-CD	-12.79	1.08	1.52
1	A	149	PRO	N-CD	-12.66	1.30	1.47
1	A	494	VAL	CB-CG2	12.37	1.78	1.52
1	A	438	GLN	CD-OE1	12.11	1.50	1.24
1	A	79	LYS	CD-CE	-11.36	1.22	1.51
1	A	51	LYS	CG-CD	-11.35	1.13	1.52
1	A	530	VAL	CB-CG2	-9.93	1.31	1.52
1	A	16	ALA	CA-CB	-9.88	1.31	1.52
1	A	149	PRO	CB-CG	-9.80	1.00	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	512	LEU	CG-CD1	-9.44	1.17	1.51
1	A	109	ARG	CZ-NH2	-9.16	1.21	1.33
1	A	270	LYS	CD-CE	8.90	1.73	1.51
1	A	353	PRO	CB-CG	-8.84	1.05	1.50
1	A	402	HIS	CG-ND1	8.08	1.56	1.38
1	A	440	GLU	CG-CD	-8.00	1.40	1.51
1	A	79	LYS	CG-CD	7.91	1.79	1.52
1	A	447	ILE	CB-CG2	7.79	1.76	1.52
1	A	530	VAL	CB-CG1	-7.75	1.36	1.52
1	A	158	ARG	NE-CZ	7.05	1.42	1.33
1	A	419	LEU	CG-CD1	6.86	1.77	1.51
1	A	436	GLN	CD-NE2	-6.77	1.16	1.32
1	A	467	HIS	CG-CD2	-6.72	1.24	1.35
1	A	502	HIS	CA-CB	6.41	1.68	1.53
1	A	514	GLN	CD-OE1	6.29	1.37	1.24
1	A	26	LEU	CG-CD1	-5.82	1.30	1.51
1	A	441	LYS	CG-CD	5.80	1.72	1.52
1	A	490	ARG	NE-CZ	-5.54	1.25	1.33
1	A	155	LYS	CG-CD	-5.52	1.33	1.52
1	A	158	ARG	CZ-NH1	5.21	1.39	1.33

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	ARG	NE-CZ-NH1	-176.30	32.15	120.30
1	A	448	TYR	CG-CD2-CE2	-140.69	8.75	121.30
1	A	222	ARG	NE-CZ-NH2	-116.01	62.30	120.30
1	A	222	ARG	NE-CZ-NH1	-109.34	65.63	120.30
1	A	448	TYR	CD1-CE1-CZ	-107.56	22.99	119.80
1	A	222	ARG	CD-NE-CZ	-81.94	8.89	123.60
1	A	109	ARG	CD-NE-CZ	-71.08	24.09	123.60
1	A	222	ARG	NH1-CZ-NH2	-61.07	52.22	119.40
1	A	448	TYR	CZ-CE2-CD2	58.51	172.45	119.80
1	A	502	HIS	ND1-CE1-NE2	-40.61	20.56	109.90
1	A	404	PRO	N-CA-CB	-40.58	54.60	103.30
1	A	158	ARG	NE-CZ-NH1	-39.67	100.47	120.30
1	A	23	ILE	CA-C-O	-39.44	37.28	120.10
1	A	152	GLY	CA-C-O	-39.01	50.38	120.60
1	A	405	VAL	O-C-N	-38.26	61.49	122.70
1	A	467	HIS	CG-ND1-CE1	-34.51	59.89	108.20
1	A	149	PRO	O-C-N	-34.37	67.71	122.70
1	A	184	GLN	OE1-CD-NE2	-32.88	46.29	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	LEU	CD1-CG-CD2	-31.94	14.67	110.50
1	A	124	LYS	CD-CE-NZ	-31.76	38.66	111.70
1	A	502	HIS	CG-ND1-CE1	-31.46	64.16	108.20
1	A	447	ILE	CG1-CB-CG2	-30.42	44.48	111.40
1	A	448	TYR	CG-CD1-CE1	-29.87	97.40	121.30
1	A	405	VAL	CA-CB-CG1	29.67	155.41	110.90
1	A	404	PRO	CA-N-CD	27.18	149.75	111.70
1	A	28	ASN	CB-CG-OD1	-26.91	67.78	121.60
1	A	222	ARG	CG-CD-NE	26.47	167.38	111.80
1	A	405	VAL	CG1-CB-CG2	-26.22	68.94	110.90
1	A	402	HIS	N-CA-CB	-25.45	64.79	110.60
1	A	28	ASN	CB-CG-ND2	-24.91	56.92	116.70
1	A	402	HIS	CA-CB-CG	-24.85	71.35	113.60
1	A	109	ARG	CG-CD-NE	-23.85	61.72	111.80
1	A	79	LYS	CD-CE-NZ	21.88	162.03	111.70
1	A	353	PRO	CA-CB-CG	21.82	146.26	104.80
1	A	353	PRO	N-CA-CB	-21.12	77.96	103.30
1	A	151	LYS	CG-CD-CE	-20.93	49.11	111.90
1	A	131	VAL	CG1-CB-CG2	19.97	142.86	110.90
1	A	155	LYS	CD-CE-NZ	-19.96	65.78	111.70
1	A	467	HIS	CG-CD2-NE2	-19.61	71.94	109.20
1	A	502	HIS	N-CA-CB	-19.58	75.36	110.60
1	A	158	ARG	NE-CZ-NH2	19.22	129.91	120.30
1	A	402	HIS	CG-ND1-CE1	-19.09	80.88	105.70
1	A	530	VAL	CA-CB-CG1	-18.90	82.56	110.90
1	A	109	ARG	NE-CZ-NH2	18.44	129.52	120.30
1	A	23	ILE	N-CA-C	18.39	160.66	111.00
1	A	490	ARG	NE-CZ-NH2	-18.31	111.15	120.30
1	A	184	GLN	CG-CD-OE1	-17.77	86.07	121.60
1	A	490	ARG	CD-NE-CZ	-16.24	100.86	123.60
1	A	405	VAL	CA-CB-CG2	16.11	135.07	110.90
1	A	530	VAL	CG1-CB-CG2	16.10	136.66	110.90
1	A	530	VAL	CA-CB-CG2	-15.94	87.00	110.90
1	A	405	VAL	CB-CA-C	15.91	141.63	111.40
1	A	447	ILE	CA-CB-CG2	-15.36	80.18	110.90
1	A	212	LYS	CD-CE-NZ	-15.27	76.57	111.70
1	A	18	GLU	CG-CD-OE1	14.95	148.20	118.30
1	A	270	LYS	CB-CG-CD	14.84	150.18	111.60
1	A	149	PRO	CA-C-N	14.78	149.71	117.20
1	A	403	THR	C-N-CD	-14.64	88.40	120.60
1	A	514	GLN	CG-CD-OE1	-14.41	92.78	121.60
1	A	404	PRO	N-CD-CG	-14.40	81.60	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLU	CB-CA-C	-13.96	82.47	110.40
1	A	490	ARG	NE-CZ-NH1	-13.65	113.47	120.30
1	A	147	VAL	CA-CB-CG1	13.55	131.22	110.90
1	A	23	ILE	CB-CA-C	-13.45	84.70	111.60
1	A	404	PRO	CA-CB-CG	13.22	129.92	104.80
1	A	16	ALA	CB-CA-C	13.12	129.78	110.10
1	A	109	ARG	CB-CG-CD	-12.67	78.67	111.60
1	A	494	VAL	CA-CB-CG2	-12.37	92.35	110.90
1	A	18	GLU	OE1-CD-OE2	-11.66	109.31	123.30
1	A	502	HIS	CG-CD2-NE2	-11.26	87.80	109.20
1	A	502	HIS	CE1-NE2-CD2	-11.22	78.54	106.60
1	A	32	ARG	NE-CZ-NH2	10.95	125.78	120.30
1	A	419	LEU	CB-CG-CD1	-10.77	92.69	111.00
1	A	79	LYS	CG-CD-CE	10.65	143.86	111.90
1	A	151	LYS	C-N-CA	10.38	144.10	122.30
1	A	22	PRO	CB-CA-C	10.34	137.86	112.00
1	A	448	TYR	CA-CB-CG	10.34	133.05	113.40
1	A	150	GLU	CA-C-O	-10.24	98.59	120.10
1	A	69	LYS	CD-CE-NZ	-10.16	88.34	111.70
1	A	402	HIS	CE1-NE2-CD2	-9.90	81.85	106.60
1	A	51	LYS	CB-CG-CD	9.70	136.82	111.60
1	A	32	ARG	NE-CZ-NH1	-9.50	115.55	120.30
1	A	483	ASN	CB-CG-ND2	-9.48	93.95	116.70
1	A	184	GLN	CG-CD-NE2	-9.48	93.95	116.70
1	A	448	TYR	OH-CZ-CE2	-9.47	94.53	120.10
1	A	448	TYR	CE1-CZ-OH	9.13	144.75	120.10
1	A	401	ARG	CA-CB-CG	8.89	132.96	113.40
1	A	467	HIS	CB-CG-ND1	-8.68	101.50	123.20
1	A	490	ARG	CG-CD-NE	8.62	129.91	111.80
1	A	182	LEU	CD1-CG-CD2	-8.56	84.83	110.50
1	A	151	LYS	CB-CG-CD	-8.54	89.40	111.60
1	A	109	ARG	NH1-CZ-NH2	-8.42	110.13	119.40
1	A	149	PRO	C-N-CA	8.29	142.43	121.70
1	A	272	GLN	CG-CD-NE2	8.27	136.55	116.70
1	A	149	PRO	CA-N-CD	-8.21	100.00	111.50
1	A	18	GLU	CG-CD-OE2	-8.18	101.94	118.30
1	A	405	VAL	N-CA-CB	-8.18	93.51	111.50
1	A	155	LYS	CB-CG-CD	7.89	132.11	111.60
1	A	502	HIS	CA-CB-CG	-7.86	100.25	113.60
1	A	32	ARG	CD-NE-CZ	-7.76	112.73	123.60
1	A	272	GLN	OE1-CD-NE2	-7.75	104.07	121.90
1	A	57	LEU	CB-CG-CD1	7.62	123.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	LEU	CB-CG-CD1	7.57	123.86	111.00
1	A	23	ILE	CA-C-N	7.49	133.69	117.20
1	A	467	HIS	CB-CG-CD2	-7.47	107.63	130.80
1	A	448	TYR	CB-CG-CD1	-7.36	116.58	121.00
1	A	69	LYS	CB-CG-CD	7.01	129.83	111.60
1	A	55	ASP	CB-CG-OD2	6.82	124.44	118.30
1	A	402	HIS	CG-CD2-NE2	6.76	122.05	109.20
1	A	353	PRO	CB-CG-CD	-6.50	81.14	106.50
1	A	307	LYS	CD-CE-NZ	6.34	126.28	111.70
1	A	22	PRO	N-CA-C	-6.11	96.22	112.10
1	A	404	PRO	CB-CA-C	6.03	127.08	112.00
1	A	149	PRO	CA-CB-CG	6.01	116.22	104.80
1	A	26	LEU	CB-CG-CD1	5.97	121.14	111.00
1	A	438	GLN	OE1-CD-NE2	-5.96	108.19	121.90
1	A	135	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	114	LYS	CD-CE-NZ	-5.86	98.22	111.70
1	A	43	ARG	CG-CD-NE	-5.64	99.95	111.80
1	A	18	GLU	CB-CG-CD	-5.62	99.01	114.20
1	A	319	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	402	HIS	CB-CG-ND1	-5.55	109.31	123.20
1	A	436	GLN	CG-CD-NE2	5.47	129.82	116.70
1	A	387	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	448	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	441	LYS	CB-CG-CD	5.30	125.39	111.60
1	A	502	HIS	N-CA-C	5.19	125.00	111.00
1	A	436	GLN	OE1-CD-NE2	-5.17	110.02	121.90
1	A	458	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	270	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	A	51	LYS	CD-CE-NZ	5.08	123.38	111.70
1	A	69	LYS	CG-CD-CE	5.00	126.92	111.90

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	149	PRO	Mainchain
1	A	150	GLU	Mainchain,Peptide
1	A	151	LYS	Peptide
1	A	152	GLY	Mainchain,Peptide
1	A	158	ARG	Sidechain
1	A	184	GLN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	23	ILE	Mainchain,Peptide
1	A	401	ARG	Sidechain
1	A	402	HIS	Sidechain
1	A	405	VAL	Mainchain
1	A	438	GLN	Sidechain
1	A	448	TYR	Sidechain
1	A	467	HIS	Sidechain
1	A	483	ASN	Sidechain
1	A	490	ARG	Sidechain
1	A	501	ARG	Peptide
1	A	502	HIS	Sidechain
1	A	514	GLN	Sidechain

5.2 Too-close contacts [i](#)

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	4137	0	4148	165	0
2	A	69	0	49	3	0
3	A	629	0	0	49	1
All	All	4835	0	4197	165	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 20.

All (165) 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:A:448:TYR:CG	1:A:448:TYR:CD2	1.78	1.66
1:A:502:HIS:CG	1:A:502:HIS:ND1	1.73	1.57
1:A:374:HIS:HB2	1:A:475:HIS:CE1	1.38	1.54
1:A:502:HIS:NE2	1:A:503:ARG:HB2	1.30	1.40
1:A:374:HIS:CB	1:A:475:HIS:CE1	2.08	1.33
1:A:374:HIS:CB	1:A:475:HIS:HE1	1.38	1.31
1:A:500:TRP:O	1:A:502:HIS:ND1	1.61	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:O	1:A:120:HIS:ND1	1.63	1.30
1:A:120:HIS:CD2	3:A:2213:HOH:O	1.73	1.28
1:A:467:HIS:CD2	3:A:2577:HOH:O	1.84	1.25
1:A:118:HIS:CD2	3:A:2209:HOH:O	1.93	1.17
1:A:118:HIS:HE1	1:A:122:VAL:CG2	1.59	1.16
1:A:118:HIS:CE1	1:A:122:VAL:HG23	1.85	1.10
1:A:116:VAL:HG13	1:A:120:HIS:CE1	1.85	1.10
1:A:500:TRP:C	1:A:502:HIS:ND1	2.05	1.09
1:A:120:HIS:CD2	3:A:2212:HOH:O	2.02	1.09
1:A:118:HIS:NE2	3:A:2209:HOH:O	1.84	1.08
1:A:501:ARG:C	1:A:502:HIS:ND1	2.07	1.06
1:A:500:TRP:HA	1:A:502:HIS:NE2	1.70	1.06
1:A:494:VAL:CB	3:A:2597:HOH:O	2.08	1.01
1:A:502:HIS:NE2	1:A:503:ARG:CB	2.22	1.01
1:A:501:ARG:N	1:A:502:HIS:CD2	2.22	1.01
1:A:467:HIS:CD2	3:A:2576:HOH:O	2.12	1.00
1:A:181:THR:HB	3:A:2298:HOH:O	1.62	0.99
1:A:118:HIS:CE1	1:A:122:VAL:CG2	2.44	0.98
1:A:445:CYS:HB2	3:A:2555:HOH:O	1.61	0.98
1:A:118:HIS:ND1	1:A:118:HIS:C	2.16	0.97
1:A:509:ALA:O	3:A:2607:HOH:O	1.82	0.97
1:A:141:LYS:HG3	1:A:405:VAL:CG1	1.94	0.96
1:A:21:LEU:HB3	3:A:2031:HOH:O	1.67	0.95
1:A:118:HIS:HE1	1:A:122:VAL:HG23	1.23	0.94
1:A:502:HIS:ND1	1:A:503:ARG:N	2.17	0.93
1:A:116:VAL:HG13	1:A:120:HIS:HE1	1.29	0.93
1:A:21:LEU:HD21	1:A:37:VAL:HG12	1.47	0.93
1:A:120:HIS:HD2	3:A:2213:HOH:O	1.18	0.92
1:A:502:HIS:CG	1:A:503:ARG:H	1.89	0.90
1:A:502:HIS:CD2	1:A:502:HIS:ND1	2.39	0.90
1:A:374:HIS:HB3	1:A:475:HIS:HE1	1.38	0.88
1:A:118:HIS:HE1	1:A:122:VAL:HG21	1.37	0.88
1:A:467:HIS:CE1	1:A:471:ALA:HB2	2.08	0.88
1:A:118:HIS:O	1:A:118:HIS:ND1	2.08	0.86
1:A:120:HIS:HD2	3:A:2212:HOH:O	1.46	0.86
1:A:419:LEU:HB2	3:A:2626:HOH:O	1.74	0.86
1:A:417:PRO:HG3	1:A:467:HIS:ND1	1.90	0.86
1:A:374:HIS:HB2	1:A:475:HIS:NE2	1.92	0.85
1:A:309:GLN:NE2	3:A:2430:HOH:O	2.10	0.84
1:A:21:LEU:HD22	1:A:397:TRP:CZ3	2.15	0.82
1:A:116:VAL:CG1	1:A:120:HIS:CE1	2.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ALA:HB2	3:A:2040:HOH:O	1.81	0.80
1:A:374:HIS:O	1:A:475:HIS:ND1	2.13	0.80
1:A:321:VAL:HG21	1:A:365:SER:HB3	1.61	0.80
1:A:500:TRP:CA	1:A:502:HIS:NE2	2.42	0.80
1:A:141:LYS:CG	1:A:405:VAL:CG1	2.59	0.79
1:A:498:ARG:O	1:A:502:HIS:HB3	1.83	0.79
1:A:21:LEU:CG	3:A:2031:HOH:O	2.32	0.78
1:A:374:HIS:CA	1:A:475:HIS:HE1	1.96	0.77
1:A:406:ASN:HB2	3:A:2533:HOH:O	1.84	0.76
1:A:22:PRO:CA	3:A:2032:HOH:O	2.34	0.76
1:A:374:HIS:HB3	1:A:475:HIS:CE1	2.17	0.75
1:A:502:HIS:CG	1:A:503:ARG:N	2.55	0.74
1:A:21:LEU:HD21	1:A:37:VAL:CG1	2.17	0.74
1:A:374:HIS:CA	1:A:475:HIS:CE1	2.71	0.73
1:A:374:HIS:C	1:A:475:HIS:CE1	2.62	0.73
1:A:85:VAL:HG11	1:A:120:HIS:CE1	2.25	0.72
1:A:498:ARG:O	1:A:502:HIS:CB	2.37	0.71
1:A:184:GLN:CB	3:A:2311:HOH:O	2.38	0.71
1:A:21:LEU:CD2	1:A:37:VAL:HG12	2.21	0.71
1:A:160:ILE:N	1:A:405:VAL:HG11	2.08	0.69
1:A:401:ARG:CB	3:A:2528:HOH:O	2.13	0.69
1:A:21:LEU:HD22	1:A:397:TRP:CE3	2.27	0.69
1:A:501:ARG:N	1:A:502:HIS:CG	2.61	0.68
1:A:184:GLN:HB2	3:A:2311:HOH:O	1.93	0.68
1:A:401:ARG:NH1	3:A:2528:HOH:O	2.27	0.68
1:A:21:LEU:CB	3:A:2031:HOH:O	2.30	0.67
1:A:447:ILE:HG13	3:A:2557:HOH:O	1.96	0.66
1:A:502:HIS:N	1:A:502:HIS:ND1	2.42	0.66
1:A:79:LYS:HG3	1:A:244:ASP:HB3	1.79	0.65
1:A:22:PRO:HB2	1:A:400:ALA:HB1	1.79	0.65
1:A:501:ARG:N	1:A:502:HIS:ND1	2.45	0.65
1:A:483:ASN:CG	3:A:2591:HOH:O	2.35	0.64
1:A:510:ARG:NH2	3:A:2609:HOH:O	2.31	0.63
1:A:337:ARG:O	1:A:341:GLU:HG2	1.99	0.63
1:A:467:HIS:HD2	3:A:2577:HOH:O	1.48	0.63
1:A:141:LYS:N	1:A:405:VAL:HG12	2.14	0.63
1:A:409:LEU:HD23	3:A:2555:HOH:O	1.99	0.63
1:A:118:HIS:CE1	1:A:122:VAL:HG21	2.25	0.62
1:A:509:ALA:HA	3:A:2607:HOH:O	1.98	0.62
1:A:397:TRP:CD1	1:A:401:ARG:NH1	2.67	0.62
1:A:116:VAL:O	1:A:120:HIS:CE1	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:PRO:CG	1:A:467:HIS:ND1	2.64	0.61
1:A:400:ALA:HB3	1:A:401:ARG:HH11	1.66	0.60
1:A:21:LEU:CD2	1:A:397:TRP:CE3	2.86	0.59
1:A:512:LEU:HB2	3:A:2607:HOH:O	2.02	0.59
1:A:21:LEU:HD12	3:A:2031:HOH:O	2.02	0.58
1:A:502:HIS:CA	1:A:502:HIS:ND1	2.66	0.58
1:A:406:ASN:CB	3:A:2533:HOH:O	2.47	0.58
1:A:501:ARG:O	1:A:505:ARG:HG3	2.04	0.58
1:A:374:HIS:C	1:A:475:HIS:HE1	2.04	0.58
1:A:502:HIS:C	1:A:502:HIS:ND1	2.57	0.58
1:A:467:HIS:HE1	1:A:471:ALA:HB2	1.66	0.57
1:A:502:HIS:NE2	1:A:503:ARG:HD2	2.19	0.57
1:A:406:ASN:HB3	1:A:408:TRP:CD1	2.40	0.57
1:A:448:TYR:C	3:A:2559:HOH:O	2.42	0.57
1:A:501:ARG:O	1:A:502:HIS:ND1	2.36	0.57
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.34	0.56
1:A:475:HIS:CD2	1:A:476:SER:OG	2.58	0.56
1:A:160:ILE:HG22	1:A:405:VAL:HG11	1.86	0.56
1:A:501:ARG:CA	1:A:502:HIS:ND1	2.69	0.56
1:A:21:LEU:HG	3:A:2031:HOH:O	2.02	0.55
1:A:124:LYS:HG2	1:A:125:ASP:N	2.22	0.55
1:A:502:HIS:CG	1:A:502:HIS:NE2	2.65	0.55
1:A:374:HIS:O	1:A:475:HIS:CE1	2.59	0.55
1:A:139[B]:MET:CE	1:A:139[B]:MET:CG	2.84	0.54
1:A:116:VAL:C	1:A:120:HIS:ND1	2.54	0.54
1:A:120:HIS:NE2	3:A:2213:HOH:O	2.14	0.54
1:A:21:LEU:CD1	3:A:2031:HOH:O	2.56	0.54
1:A:502:HIS:HD1	1:A:504:ALA:H	1.56	0.54
1:A:79:LYS:CE	1:A:79:LYS:CG	2.87	0.53
1:A:21:LEU:HD22	1:A:397:TRP:HZ3	1.72	0.52
1:A:120:HIS:CG	3:A:2212:HOH:O	2.49	0.52
1:A:21:LEU:CD2	1:A:37:VAL:CG1	2.84	0.52
1:A:501:ARG:HG2	1:A:502:HIS:H	1.73	0.52
1:A:501:ARG:CG	1:A:502:HIS:N	2.72	0.52
1:A:30:LEU:O	1:A:494:VAL:HG13	2.10	0.52
1:A:200:ARG:HH21	1:A:365:SER:CB	2.22	0.52
1:A:109:ARG:NE	3:A:2196:HOH:O	2.43	0.52
1:A:447:ILE:HB	1:A:452:TYR:HE1	1.73	0.52
1:A:160:ILE:CB	1:A:405:VAL:HG11	2.40	0.51
1:A:21:LEU:HD23	1:A:37:VAL:O	2.10	0.51
1:A:184:GLN:CG	3:A:2311:HOH:O	2.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLY:N	3:A:2559:HOH:O	2.44	0.49
1:A:124:LYS:HD2	3:A:2221:HOH:O	2.13	0.49
1:A:528:TRP:HB2	2:A:1532:QQ3:C6	2.43	0.49
1:A:33:HIS:HB2	3:A:2057:HOH:O	2.13	0.48
1:A:33:HIS:ND1	3:A:2057:HOH:O	2.34	0.48
1:A:447:ILE:CG1	3:A:2557:HOH:O	2.55	0.48
1:A:21:LEU:CD2	1:A:397:TRP:HE3	2.27	0.48
1:A:424:ILE:HD11	1:A:489:LEU:HD21	1.94	0.48
1:A:467:HIS:CE1	1:A:471:ALA:CB	2.90	0.48
1:A:131:VAL:CB	3:A:2243:HOH:O	2.62	0.47
1:A:528:TRP:HB2	2:A:1532:QQ3:H62C	1.96	0.47
1:A:338:VAL:HA	1:A:341:GLU:CG	2.43	0.47
1:A:501:ARG:HA	1:A:528:TRP:CZ3	2.49	0.47
1:A:160:ILE:CG2	1:A:405:VAL:HG11	2.46	0.46
1:A:155:LYS:CG	1:A:155:LYS:CE	2.93	0.46
1:A:502:HIS:NE2	1:A:503:ARG:CG	2.78	0.45
1:A:405:VAL:HA	3:A:2532:HOH:O	2.16	0.45
1:A:498:ARG:O	1:A:502:HIS:CD2	2.69	0.45
1:A:400:ALA:CB	3:A:2040:HOH:O	2.54	0.44
1:A:500:TRP:C	1:A:502:HIS:CG	2.55	0.44
1:A:152:GLY:O	2:A:1534:QQ3:H71C	2.16	0.44
1:A:448:TYR:CB	1:A:448:TYR:CD2	2.82	0.44
1:A:141:LYS:CD	1:A:405:VAL:CG1	2.96	0.44
1:A:37:VAL:HG13	1:A:393:ALA:HB1	1.99	0.43
1:A:501:ARG:HG2	1:A:502:HIS:N	2.33	0.43
1:A:353:PRO:HA	1:A:354:PRO:HD2	1.89	0.42
1:A:501:ARG:HA	1:A:528:TRP:HZ3	1.85	0.42
1:A:398:GLU:CD	1:A:406:ASN:HA	2.39	0.42
1:A:141:LYS:H	1:A:405:VAL:HG12	1.84	0.42
1:A:120:HIS:CB	3:A:2212:HOH:O	2.66	0.41
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.61	0.41
1:A:160:ILE:HB	1:A:405:VAL:HG11	2.02	0.41
1:A:416:ALA:N	1:A:417:PRO:CD	2.84	0.41
1:A:475:HIS:H	1:A:475:HIS:HD1	1.70	0.40
1:A:416:ALA:HB3	1:A:467:HIS:CD2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2167:HOH:O	3:A:2468:HOH:O[3_556]	2.17	0.03

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	531/536 (99%)	509 (96%)	18 (3%)	4 (1%)	19 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLY
1	A	502	HIS
1	A	351	GLY
1	A	501	ARG

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	454/459 (99%)	433 (95%)	21 (5%)	27 14

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	118	HIS
1	A	132	THR
1	A	151	LYS
1	A	184	GLN
1	A	222	ARG
1	A	270	LYS

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Mol	Chain	Res	Type
1	A	353	PRO
1	A	360	LEU
1	A	403	THR
1	A	404	PRO
1	A	405	VAL
1	A	406	ASN
1	A	447	ILE
1	A	448	TYR
1	A	461	GLN
1	A	467	HIS
1	A	498	ARG
1	A	502	HIS
1	A	510	ARG
1	A	530	VAL

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

Mol	Chain	Res	Type
1	A	34	HIS
1	A	35	ASN
1	A	49	GLN
1	A	58	GLN
1	A	110	ASN
1	A	273	ASN
1	A	309	GLN
1	A	374	HIS
1	A	461	GLN
1	A	467	HIS
1	A	475	HIS
1	A	502	HIS

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](#)

3 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	QQ3	A	1533	-	23,26,26	2.74	6 (26%)	31,38,38	2.14	11 (35%)
2	QQ3	A	1534	-	23,23,26	2.62	7 (30%)	32,34,38	2.04	11 (34%)
2	QQ3	A	1532	-	23,26,26	2.64	5 (21%)	31,38,38	2.18	12 (38%)

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	QQ3	A	1533	-	-	4/9/27/27	0/3/3/3
2	QQ3	A	1534	-	-	3/7/23/27	0/3/3/3
2	QQ3	A	1532	-	-	3/9/27/27	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1533	QQ3	C1-C2	-7.32	1.39	1.49
2	A	1532	QQ3	C1-C2	-6.78	1.40	1.49
2	A	1534	QQ3	C10-N2	6.67	1.40	1.32
2	A	1534	QQ3	C1-C2	-6.66	1.40	1.49
2	A	1533	QQ3	C10-N2	6.00	1.40	1.32
2	A	1532	QQ3	C3-C4	-6.00	1.38	1.49
2	A	1533	QQ3	C3-C4	-5.73	1.39	1.49
2	A	1532	QQ3	C10-N2	5.50	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1534	QQ3	C3-C4	-5.39	1.39	1.49
2	A	1533	QQ3	C4-N1	-4.22	1.31	1.40
2	A	1532	QQ3	C4-N1	-4.15	1.32	1.40
2	A	1532	QQ3	C2-N1	-3.06	1.34	1.40
2	A	1533	QQ3	C2-N1	-2.88	1.34	1.40
2	A	1534	QQ3	C2-N1	-2.83	1.34	1.40
2	A	1534	QQ3	C4-N1	-2.82	1.34	1.40
2	A	1533	QQ3	C14-C10	2.27	1.54	1.50
2	A	1534	QQ3	C14-C10	2.10	1.53	1.50
2	A	1534	QQ3	C1-C9	-2.06	1.40	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1533	QQ3	C3-C10-N2	-5.47	119.15	122.50
2	A	1534	QQ3	C3-C10-N2	-5.14	119.35	122.50
2	A	1532	QQ3	C3-C10-N2	-4.87	119.52	122.50
2	A	1532	QQ3	C5-N1-C2	4.22	133.27	124.19
2	A	1533	QQ3	C1-C2-N1	4.03	109.59	106.43
2	A	1534	QQ3	C1-C2-N1	3.87	109.47	106.43
2	A	1532	QQ3	O2-C2-C1	-3.78	124.57	129.02
2	A	1533	QQ3	O2-C2-C1	-3.70	124.66	129.02
2	A	1534	QQ3	O2-C2-C1	-3.67	124.70	129.02
2	A	1533	QQ3	C3-C1-C2	-3.56	105.07	108.14
2	A	1532	QQ3	C3-C4-N1	3.39	109.88	105.82
2	A	1534	QQ3	C3-C4-N1	3.29	109.75	105.82
2	A	1532	QQ3	C5-N1-C4	-3.19	117.33	124.19
2	A	1533	QQ3	C9-C1-C2	3.13	134.79	129.28
2	A	1532	QQ3	C1-C2-N1	3.13	108.89	106.43
2	A	1534	QQ3	C1-C3-C4	-3.03	106.09	108.12
2	A	1532	QQ3	C9-C1-C2	3.02	134.59	129.28
2	A	1534	QQ3	O1-C4-C3	-2.97	124.86	129.09
2	A	1532	QQ3	C1-C3-C4	-2.93	106.16	108.12
2	A	1533	QQ3	C9-C11-N2	-2.83	119.81	122.81
2	A	1532	QQ3	C3-C1-C2	-2.81	105.71	108.14
2	A	1534	QQ3	C9-C11-N2	-2.79	119.85	122.81
2	A	1534	QQ3	C2-N1-C4	-2.76	108.36	111.53
2	A	1533	QQ3	C3-C4-N1	2.68	109.03	105.82
2	A	1533	QQ3	C10-N2-C11	2.61	120.91	118.38
2	A	1533	QQ3	C5-N1-C2	2.59	129.76	124.19
2	A	1532	QQ3	C9-C11-N2	-2.40	120.27	122.81
2	A	1532	QQ3	C10-N2-C11	2.26	120.58	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1534	QQ3	C9-C1-C2	2.20	133.16	129.28
2	A	1533	QQ3	C14-C10-N2	2.16	120.21	116.97
2	A	1534	QQ3	C10-N2-C11	2.11	120.43	118.38
2	A	1534	QQ3	C3-C1-C2	-2.10	106.33	108.14
2	A	1533	QQ3	C2-N1-C4	-2.09	109.13	111.53
2	A	1532	QQ3	C18-C12-C5	2.06	117.15	113.22

There are no chirality outliers.

All (10) torsion outliers are listed below:

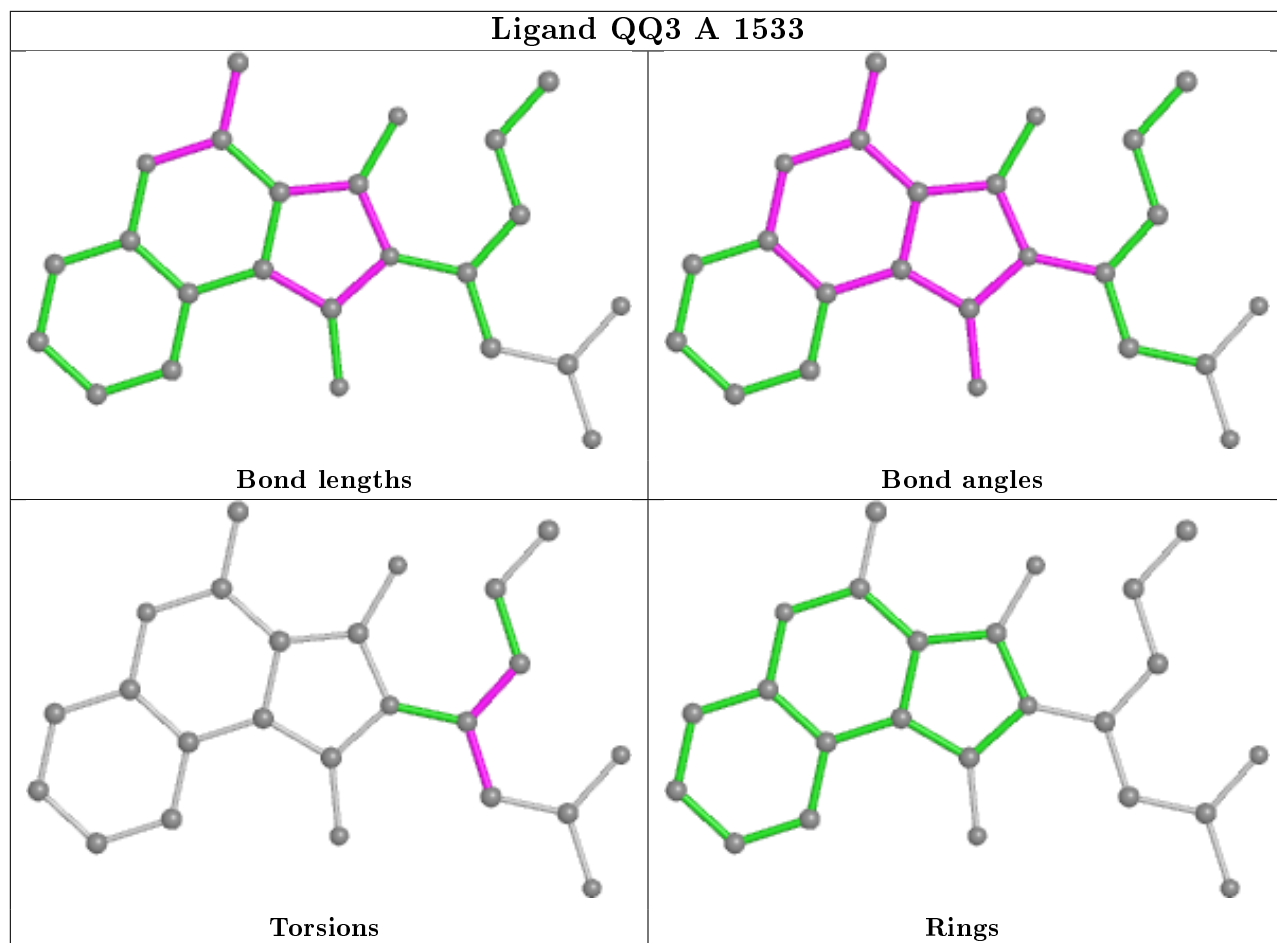
Mol	Chain	Res	Type	Atoms
2	A	1533	QQ3	C18-C12-C5-C6
2	A	1533	QQ3	C18-C12-C5-N1
2	A	1532	QQ3	C18-C12-C5-N1
2	A	1534	QQ3	C5-C6-C7-C8
2	A	1532	QQ3	C5-C6-C7-C8
2	A	1534	QQ3	N1-C5-C6-C7
2	A	1533	QQ3	N1-C5-C6-C7
2	A	1534	QQ3	C12-C5-C6-C7
2	A	1532	QQ3	C18-C12-C5-C6
2	A	1533	QQ3	C12-C5-C6-C7

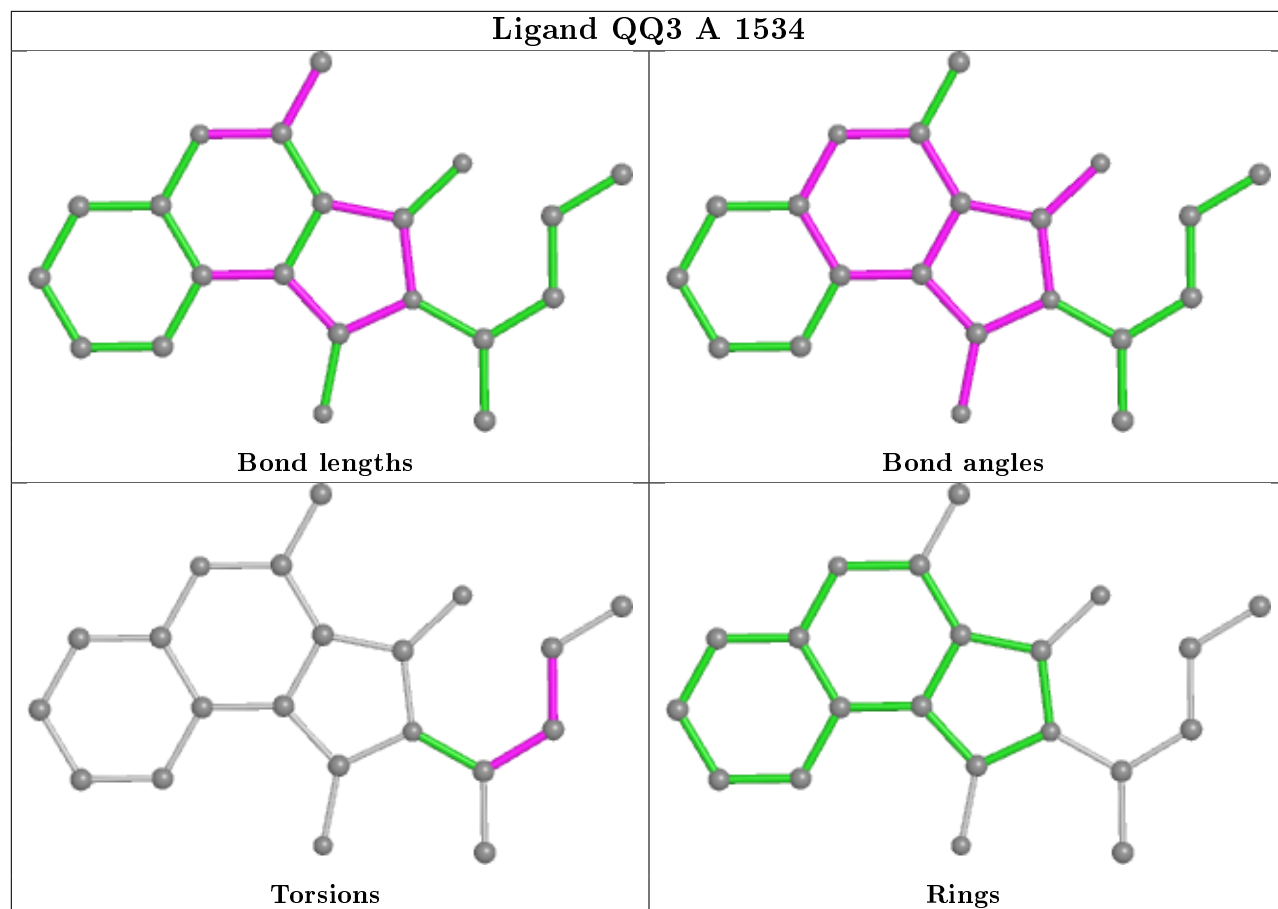
There are no ring outliers.

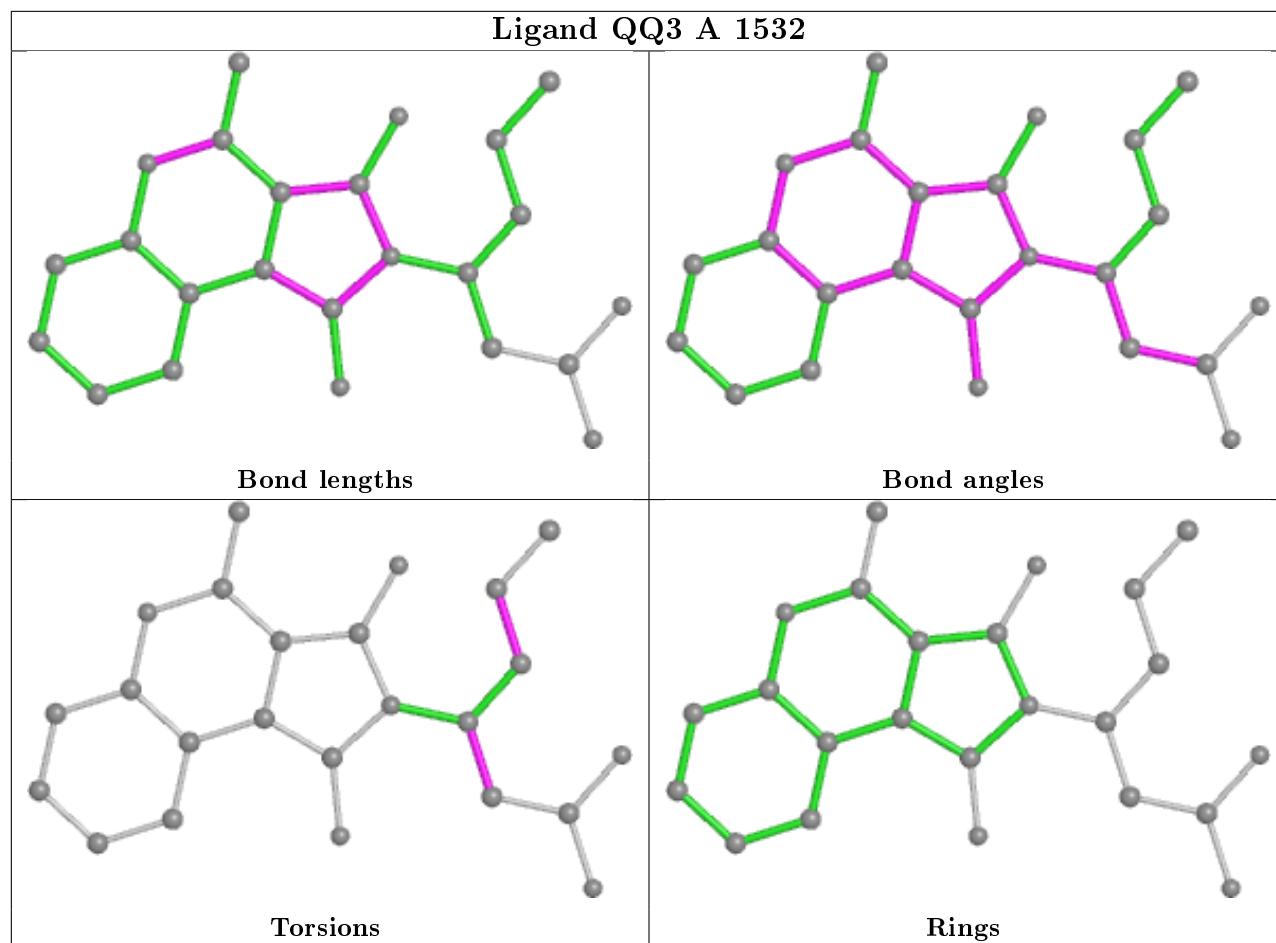
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1534	QQ3	1	0
2	A	1532	QQ3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	149:PRO	C	150:GLU	N	0.85

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	531/536 (99%)	0.38	44 (8%) 11 17	12, 20, 39, 65	58 (10%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	LYS	9.6
1	A	150	GLU	7.9
1	A	448	TYR	7.0
1	A	405	VAL	6.9
1	A	24	ASN	6.6
1	A	449	GLY	6.0
1	A	447	ILE	5.7
1	A	25	ALA	5.4
1	A	502	HIS	5.3
1	A	33	HIS	5.3
1	A	531	LYS	5.1
1	A	475	HIS	4.6
1	A	450	ALA	4.5
1	A	467	HIS	4.4
1	A	501	ARG	4.4
1	A	95	HIS	4.4
1	A	404	PRO	4.3
1	A	23	ILE	4.0
1	A	22	PRO	4.0
1	A	406	ASN	4.0
1	A	352	ASP	3.7
1	A	498	ARG	3.7
1	A	21	LEU	3.6
1	A	14	CYS	3.5
1	A	120	HIS	3.4
1	A	403	THR	3.2
1	A	152	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	15	ALA	3.1
1	A	505	ARG	3.1
1	A	149	PRO	3.0
1	A	402	HIS	3.0
1	A	400	ALA	3.0
1	A	351	GLY	2.9
1	A	184	GLN	2.8
1	A	378	GLY	2.7
1	A	401	ARG	2.5
1	A	530	VAL	2.4
1	A	509	ALA	2.3
1	A	377	SER	2.3
1	A	26	LEU	2.3
1	A	393	ALA	2.2
1	A	118	HIS	2.1
1	A	57	LEU	2.1
1	A	499	VAL	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 carbohydrates in this entry.

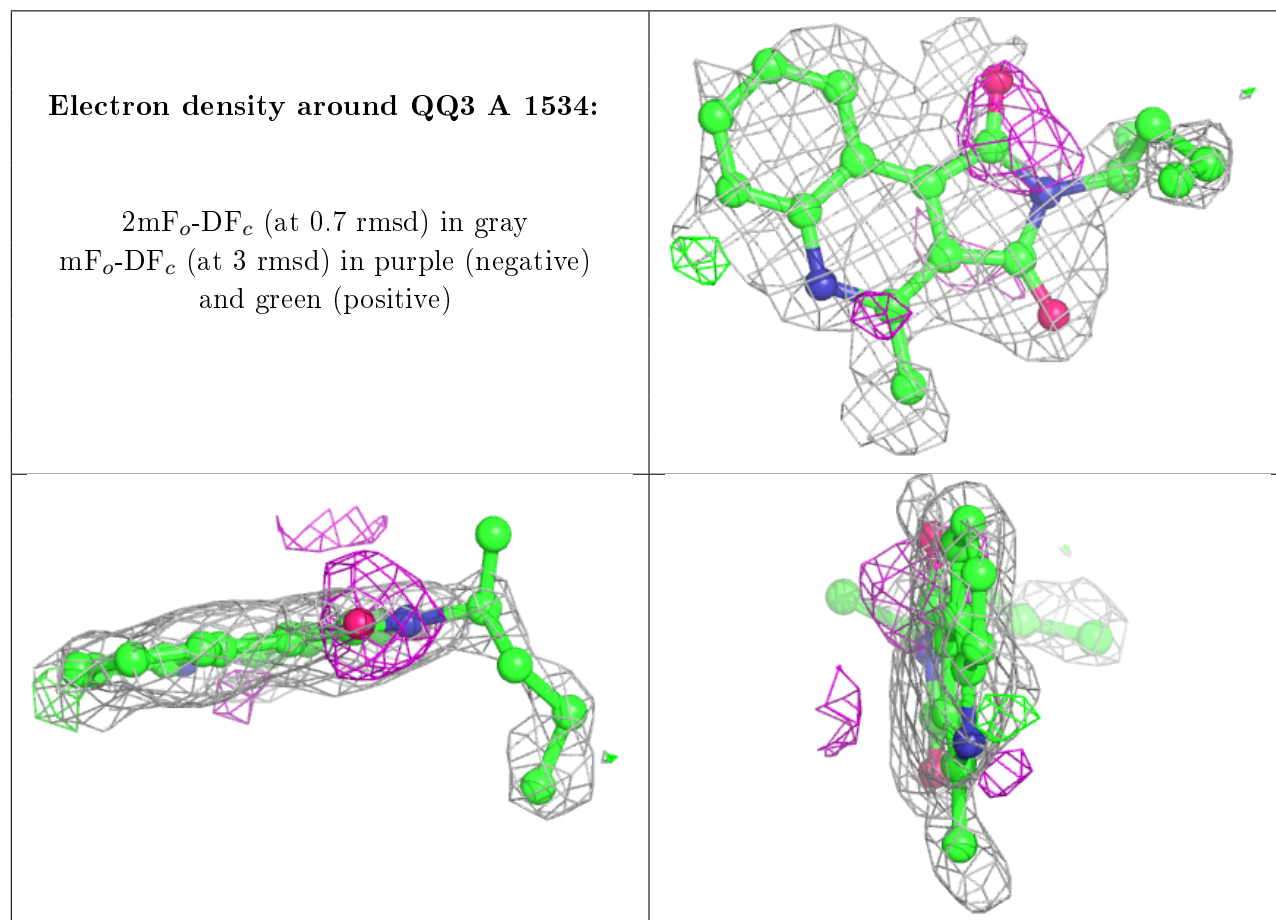
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	QQ3	A	1534	21/24	0.73	0.38	42,43,45,45	0
2	QQ3	A	1532	24/24	0.88	0.15	27,29,32,33	0
2	QQ3	A	1533	24/24	0.94	0.12	24,26,32,35	0

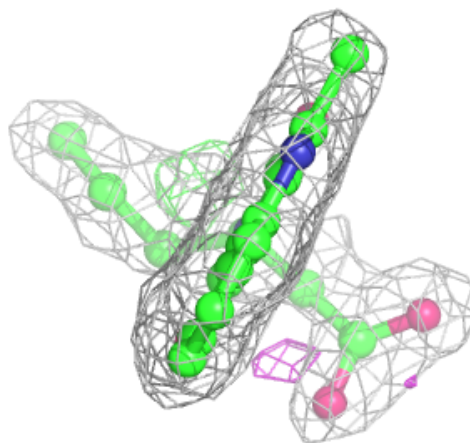
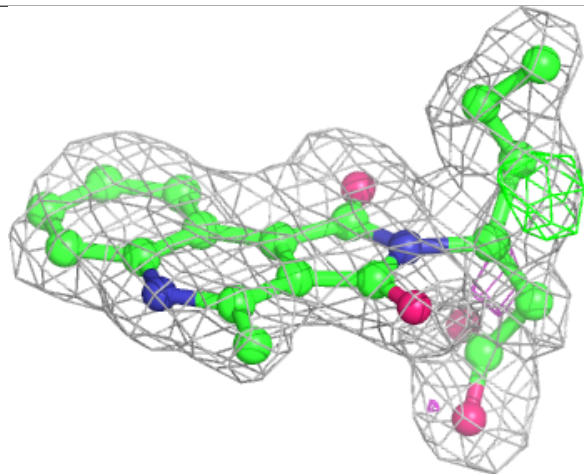
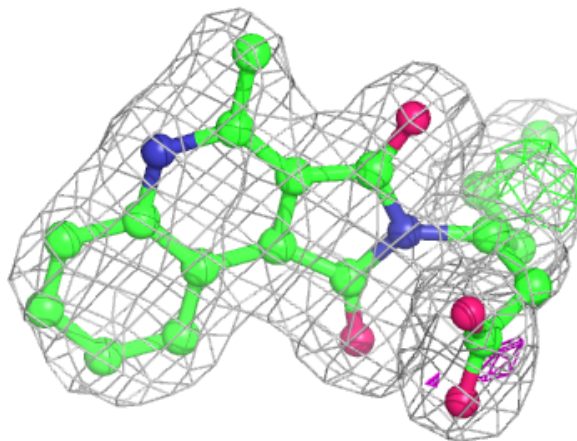
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

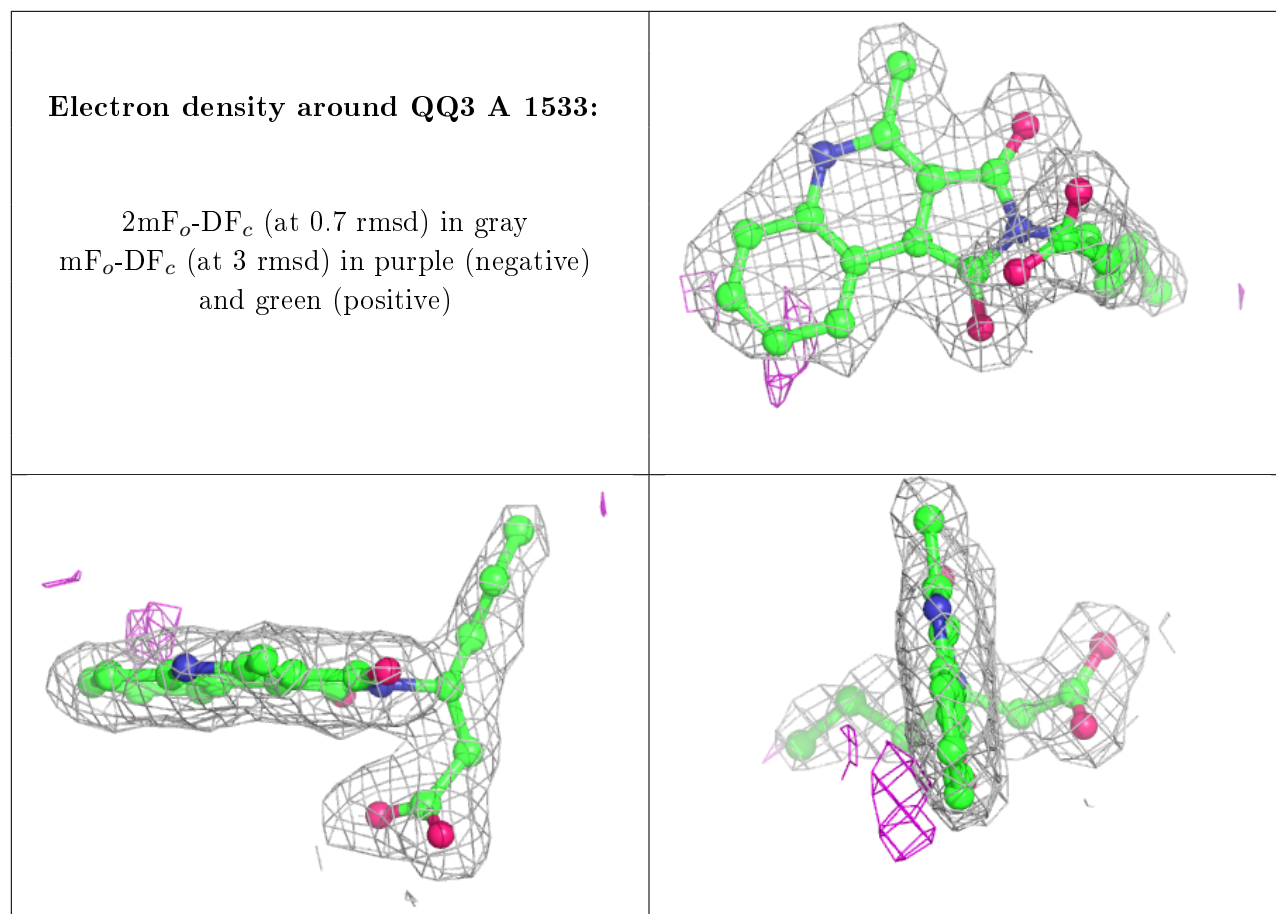
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around QQ3 A 1532:

$2mF_o-DF_c$ (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.