



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:23 AM UTC

PDB ID : 7KK3 / pdb_00007kk3
Title : Structure of the catalytic domain of PARP1 in complex with talazoparib
Authors : Gajiwala, K.S.; Ryan, K.
Deposited on : 2020-10-27
Resolution : 2.06 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

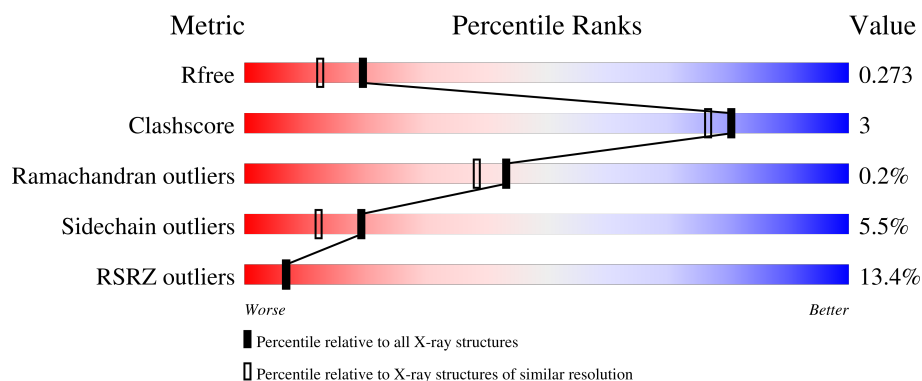
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	352	12% 83% 11% 5%
1	B	352	9% 83% 12% •
1	C	352	7% 84% 12% •
1	D	352	24% 80% 13% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10984 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.

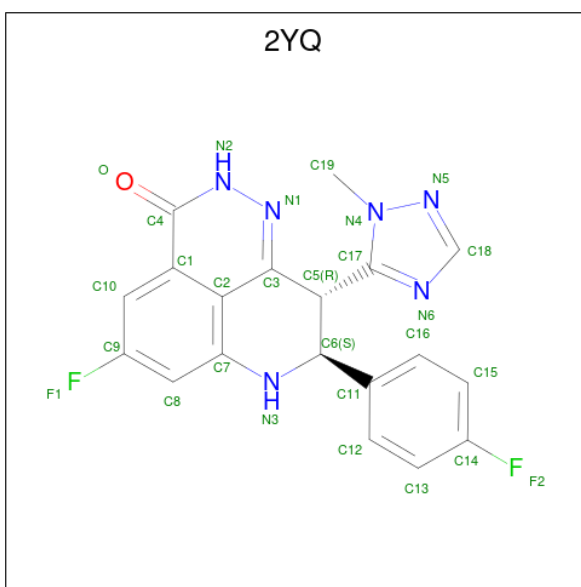
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2661	1699	450	502	10			
1	B	337	Total	C	N	O	S	0	0	0
			2661	1701	447	503	10			
1	C	340	Total	C	N	O	S	0	0	0
			2675	1701	451	513	10			
1	D	328	Total	C	N	O	S	0	0	0
			2594	1660	437	487	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	660	GLY	-	expression tag	UNP P09874
A	661	SER	-	expression tag	UNP P09874
B	660	GLY	-	expression tag	UNP P09874
B	661	SER	-	expression tag	UNP P09874
C	660	GLY	-	expression tag	UNP P09874
C	661	SER	-	expression tag	UNP P09874
D	660	GLY	-	expression tag	UNP P09874
D	661	SER	-	expression tag	UNP P09874

- Molecule 2 is (8S,9R)-5-fluoro-8-(4-fluorophenyl)-9-(1-methyl-1H-1,2,4-triazol-5-yl)-2,7,8,9-tetrahydro-3H-pyrido[4,3,2-de]phthalazin-3-one (CCD ID: 2YQ) (formula: C₁₉H₁₄F₂N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
2	B	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
2	C	1	Total	C	F	N	O	0	0
			28	19	2	6	1		
2	D	1	Total	C	F	N	O	0	0
			28	19	2	6	1		

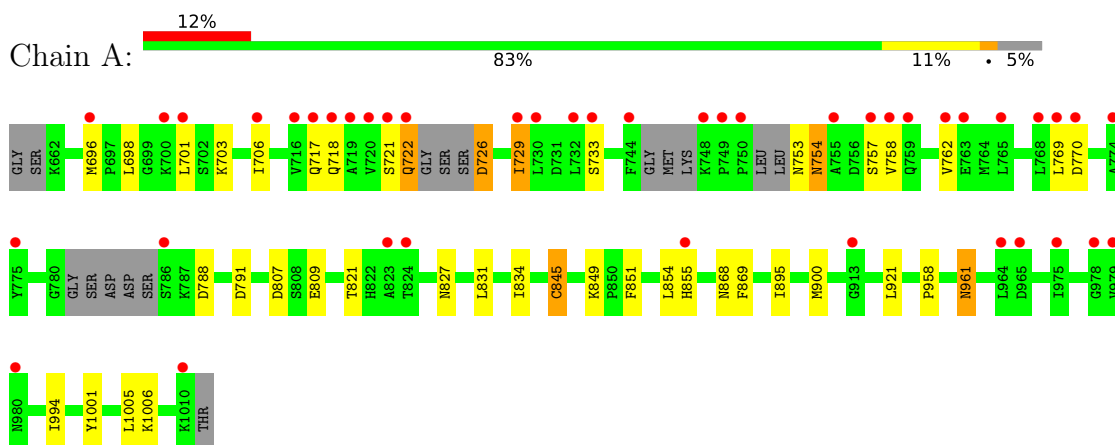
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	56	Total	O	0	0
			56	56		
3	C	92	Total	O	0	0
			92	92		
3	D	54	Total	O	0	0
			54	54		

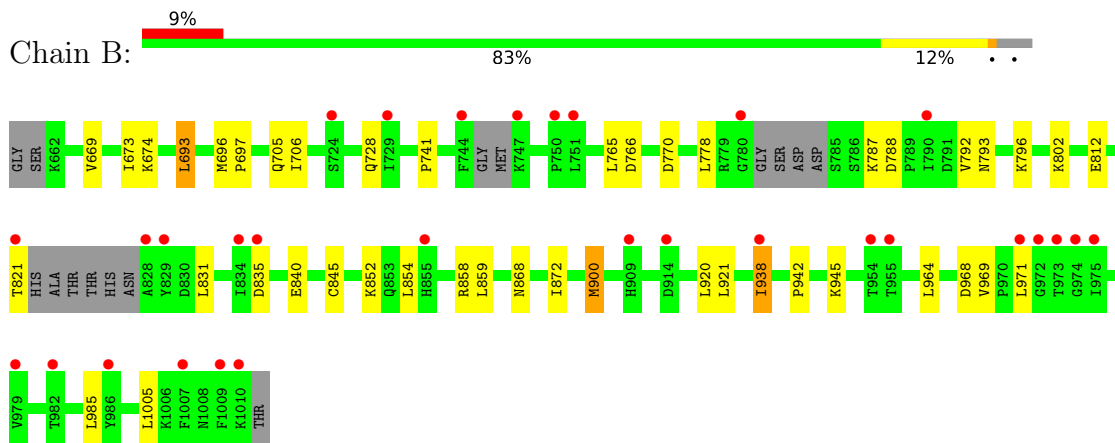
3 Residue-property plots

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.

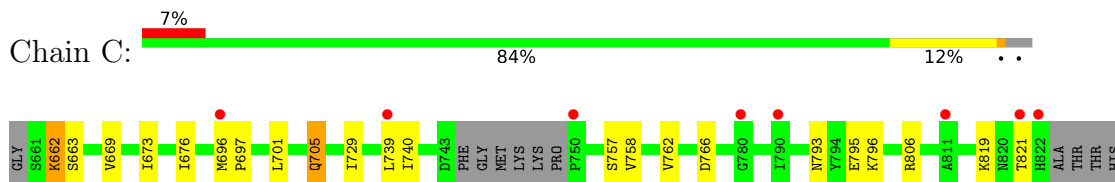
• Molecule 1: Poly [ADP-ribose] polymerase 1

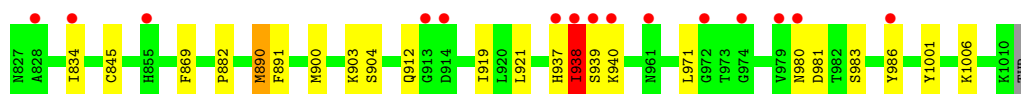


• Molecule 1: Poly [ADP-ribose] polymerase 1

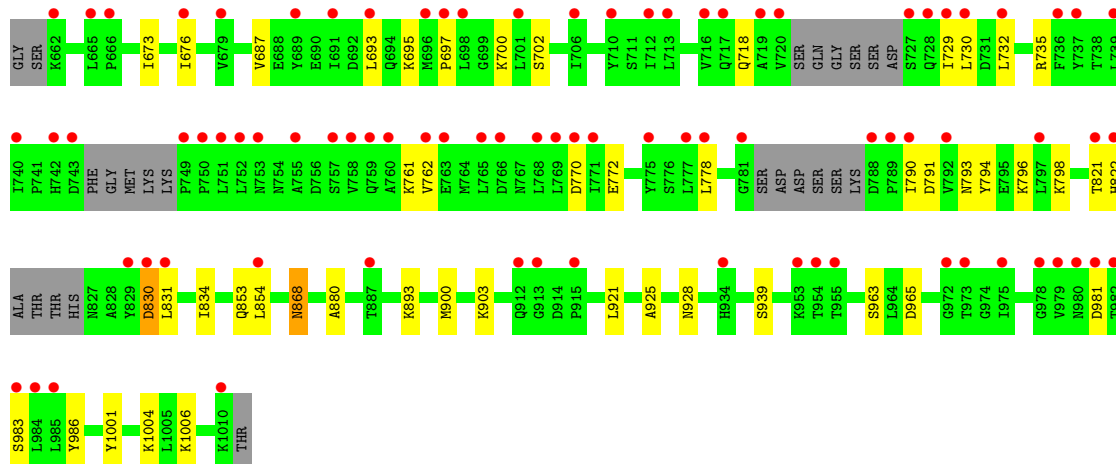
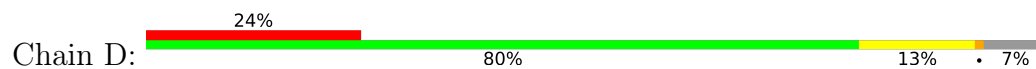


• Molecule 1: Poly [ADP-ribose] polymerase 1





● Molecule 1: Poly [ADP-ribose] polymerase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.48Å 107.68Å 143.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.12 – 2.06 86.12 – 2.06	Depositor EDS
% Data completeness (in resolution range)	79.1 (86.12-2.06) 79.1 (86.12-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.07Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.213 , 0.259 0.218 , 0.273	Depositor DCC
R_{free} test set	4066 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10984	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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: 2YQ

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	0.86	0/2709	1.31	10/3652 (0.3%)
1	B	0.86	0/2708	1.30	6/3649 (0.2%)
1	C	0.89	0/2722	1.36	17/3670 (0.5%)
1	D	0.84	0/2640	1.35	4/3559 (0.1%)
All	All	0.86	0/10779	1.33	37/14530 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	939	SER	N-CA-C	-8.55	101.64	114.64
1	C	937	HIS	CA-C-N	7.66	135.75	121.97
1	C	937	HIS	C-N-CA	7.66	135.75	121.97
1	D	830	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	869	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	827	ASN	CA-CB-CG	5.90	118.50	112.60
1	C	938	ILE	CA-C-N	5.85	132.12	121.41
1	C	938	ILE	C-N-CA	5.85	132.12	121.41
1	D	762	VAL	CA-C-N	5.81	128.06	120.28
1	D	762	VAL	C-N-CA	5.81	128.06	120.28
1	C	766	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	851	PHE	CA-C-N	5.66	128.14	120.38
1	A	851	PHE	C-N-CA	5.66	128.14	120.38
1	C	845	CYS	CA-C-N	5.53	127.63	120.44
1	C	845	CYS	C-N-CA	5.53	127.63	120.44
1	B	835	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	697	PRO	CA-C-N	5.49	127.90	120.38
1	C	697	PRO	C-N-CA	5.49	127.90	120.38
1	A	845	CYS	CA-C-N	5.46	127.86	120.44
1	A	845	CYS	C-N-CA	5.46	127.86	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	788	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	787	LYS	CA-C-N	5.39	127.89	120.39
1	B	787	LYS	C-N-CA	5.39	127.89	120.39
1	C	757	SER	CA-C-N	5.32	127.26	120.56
1	C	757	SER	C-N-CA	5.32	127.26	120.56
1	C	980	ASN	CA-C-N	5.26	130.93	122.83
1	C	980	ASN	C-N-CA	5.26	130.93	122.83
1	D	939	SER	N-CA-C	-5.10	106.75	113.12
1	A	807	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	753	ASN	CA-C-N	5.07	131.22	121.54
1	A	753	ASN	C-N-CA	5.07	131.22	121.54
1	B	674	LYS	CA-C-N	5.07	127.03	120.44
1	B	674	LYS	C-N-CA	5.07	127.03	120.44
1	B	766	ASP	CA-CB-CG	5.06	117.66	112.60
1	C	869	PHE	CA-CB-CG	-5.05	108.75	113.80
1	C	882	PRO	CA-C-N	5.05	127.99	120.31
1	C	882	PRO	C-N-CA	5.05	127.99	120.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2661	0	2703	15	0
1	B	2661	0	2718	16	0
1	C	2675	0	2712	13	0
1	D	2594	0	2646	12	0
2	A	28	0	14	0	0
2	B	28	0	14	0	0
2	C	28	0	14	0	0
2	D	28	0	14	0	0
3	A	79	0	0	0	0
3	B	56	0	0	0	0
3	C	92	0	0	0	0
3	D	54	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10984	0	10835	54	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 3.

All (54) 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:821:THR:HB	1:C:900:MET:HA	1.63	0.78
1:B:821:THR:HB	1:B:900:MET:HA	1.72	0.72
1:A:696:MET:HE2	1:A:701:LEU:HD23	1.73	0.71
1:B:942:PRO:HG2	1:B:945:LYS:HG3	1.75	0.68
1:C:903:LYS:HD2	1:C:986:TYR:HB2	1.75	0.68
1:D:697:PRO:HD2	1:D:700:LYS:HB2	1.77	0.66
1:C:834:ILE:HD11	1:C:1006:LYS:HB2	1.81	0.61
1:A:821:THR:HB	1:A:900:MET:HA	1.83	0.60
1:C:669:VAL:O	1:C:673:ILE:HG12	2.01	0.60
1:A:758:VAL:O	1:A:762:VAL:HG23	2.02	0.59
1:D:821:THR:HB	1:D:900:MET:HA	1.85	0.59
1:D:903:LYS:HD2	1:D:986:TYR:HB2	1.83	0.58
1:C:890:MET:HG2	1:C:891:PHE:CE2	2.39	0.58
1:D:921:LEU:HB2	1:D:1001:TYR:HB2	1.86	0.57
1:B:858:ARG:HG2	1:B:968:ASP:HB2	1.86	0.56
1:A:921:LEU:HB2	1:A:1001:TYR:HB2	1.88	0.55
1:C:758:VAL:O	1:C:762:VAL:HG23	2.07	0.54
1:A:845:CYS:HG	1:B:845:CYS:HG	1.33	0.53
1:C:696:MET:HE1	1:C:740:ILE:HG23	1.92	0.52
1:C:921:LEU:HB2	1:C:1001:TYR:HB2	1.92	0.51
1:B:831:LEU:HD22	1:B:1005:LEU:HD13	1.92	0.51
1:C:662:LYS:HE2	1:C:663:SER:H	1.76	0.50
1:B:693:LEU:HD23	1:B:697:PRO:HA	1.93	0.50
1:A:726:ASP:HA	1:A:729:ILE:HG23	1.94	0.49
1:A:754:ASN:HD22	1:A:757:SER:HB3	1.78	0.49
1:C:904:SER:HB3	1:C:919:ILE:HD11	1.95	0.49
1:A:696:MET:HE2	1:A:701:LEU:CD2	2.43	0.48
1:D:822:HIS:HE1	1:D:831:LEU:H	1.60	0.48
1:B:669:VAL:O	1:B:673:ILE:HG12	2.13	0.47
1:B:696:MET:HB2	1:B:741:PRO:HD2	1.96	0.47
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.97	0.46
1:A:958:PRO:O	1:A:961:ASN:HB2	2.15	0.46
1:A:770:ASP:HB3	1:A:868:ASN:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:ILE:HD11	1:D:794:TYR:HD1	1.80	0.46
1:D:834:ILE:HD11	1:D:1006:LYS:HB2	1.98	0.45
1:A:706:ILE:HG21	1:A:769:LEU:HG	1.99	0.45
1:B:793:ASN:HA	1:B:796:LYS:HD2	1.99	0.45
1:B:706:ILE:HG23	1:B:765:LEU:HD22	1.99	0.45
1:D:880:ALA:HB3	1:D:893:LYS:HG2	1.99	0.45
1:B:964:LEU:HD12	1:B:969:VAL:HG21	1.99	0.44
1:A:718:GLN:O	1:A:722:GLN:HB2	2.18	0.44
1:A:895:ILE:HD11	1:A:994:ILE:HG22	2.00	0.44
1:D:793:ASN:HA	1:D:796:LYS:HD2	2.00	0.43
1:B:770:ASP:HB2	1:B:868:ASN:HD22	1.82	0.43
1:C:793:ASN:HA	1:C:796:LYS:HD2	2.01	0.43
1:B:872:ILE:HG21	1:B:920:LEU:HD11	1.99	0.43
1:B:938:ILE:HD12	1:D:965:ASP:HA	2.01	0.43
1:C:701:LEU:HA	1:C:705:GLN:HE22	1.83	0.42
1:D:854:LEU:HD23	1:D:925:ALA:HB1	2.01	0.42
1:B:788:ASP:O	1:B:792:VAL:HG23	2.19	0.42
1:D:770:ASP:HB3	1:D:868:ASN:HA	2.01	0.42
1:A:831:LEU:HD22	1:A:1005:LEU:HD13	2.01	0.41
1:B:859:LEU:HG	1:B:921:LEU:HD22	2.02	0.41
1:C:938:ILE:HB	1:C:940:LYS:H	1.85	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/352 (93%)	317 (97%)	8 (2%)	1 (0%)	36	30
1	B	329/352 (94%)	317 (96%)	12 (4%)	0	100	100
1	C	334/352 (95%)	327 (98%)	6 (2%)	1 (0%)	36	30
1	D	318/352 (90%)	311 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1307/1408 (93%)	1272 (97%)	33 (2%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	754	ASN
1	C	938	ILE

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	297/309 (96%)	283 (95%)	14 (5%)	23	16
1	B	298/309 (96%)	285 (96%)	13 (4%)	25	19
1	C	300/309 (97%)	286 (95%)	14 (5%)	23	16
1	D	289/309 (94%)	265 (92%)	24 (8%)	10	4
All	All	1184/1236 (96%)	1119 (94%)	65 (6%)	19	12

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	698	LEU
1	A	703	LYS
1	A	717	GLN
1	A	721	SER
1	A	722	GLN
1	A	726	ASP
1	A	729	ILE
1	A	733	SER
1	A	791	ASP
1	A	809	GLU
1	A	849	LYS
1	A	854	LEU
1	A	855	HIS

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Mol	Chain	Res	Type
1	A	961	ASN
1	B	693	LEU
1	B	705	GLN
1	B	728	GLN
1	B	778	LEU
1	B	802	LYS
1	B	812	GLU
1	B	840	GLU
1	B	852	LYS
1	B	854	LEU
1	B	900	MET
1	B	938	ILE
1	B	971	LEU
1	B	985	LEU
1	C	662	LYS
1	C	676	ILE
1	C	705	GLN
1	C	729	ILE
1	C	739	LEU
1	C	795	GLU
1	C	806	ARG
1	C	819	LYS
1	C	890	MET
1	C	912	GLN
1	C	938	ILE
1	C	971	LEU
1	C	981	ASP
1	C	983	SER
1	D	676	ILE
1	D	687	VAL
1	D	693	LEU
1	D	695	LYS
1	D	702	SER
1	D	718	GLN
1	D	729	ILE
1	D	730	LEU
1	D	732	LEU
1	D	735	ARG
1	D	761	LYS
1	D	772	GLU
1	D	778	LEU
1	D	790	ILE

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Mol	Chain	Res	Type
1	D	791	ASP
1	D	798	LYS
1	D	830	ASP
1	D	853	GLN
1	D	868	ASN
1	D	928	ASN
1	D	963	SER
1	D	981	ASP
1	D	983	SER
1	D	1004	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	705	GLN
1	A	718	GLN
1	A	734	ASN
1	A	754	ASN
1	A	875	GLN
1	A	934	HIS
1	A	1008	ASN
1	B	767	ASN
1	B	868	ASN
1	B	875	GLN
1	B	937	HIS
1	B	998	ASN
1	C	670	GLN
1	C	705	GLN
1	C	718	GLN
1	C	722	GLN
1	C	754	ASN
1	C	875	GLN
1	D	705	GLN
1	D	753	ASN
1	D	767	ASN
1	D	822	HIS
1	D	928	ASN
1	D	934	HIS
1	D	998	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	2YQ	C	9001	-	31,32,32	0.66	1 (3%)	34,48,48	0.68	1 (2%)
2	2YQ	D	9001	-	31,32,32	0.30	0	34,48,48	0.76	1 (2%)
2	2YQ	B	9001	-	31,32,32	0.27	0	34,48,48	0.80	1 (2%)
2	2YQ	A	9001	-	31,32,32	0.52	1 (3%)	34,48,48	0.72	1 (2%)

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	2YQ	C	9001	-	-	0/6/20/20	0/5/5/5
2	2YQ	D	9001	-	-	0/6/20/20	0/5/5/5
2	2YQ	B	9001	-	-	0/6/20/20	0/5/5/5
2	2YQ	A	9001	-	-	0/6/20/20	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	9001	2YQ	C5-C3	-3.15	1.48	1.51
2	A	9001	2YQ	C5-C3	-2.26	1.49	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	9001	2YQ	C2-C3-N1	-3.68	120.40	122.78
2	D	9001	2YQ	C2-C3-N1	-3.36	120.60	122.78
2	A	9001	2YQ	C2-C3-N1	-2.69	121.04	122.78
2	C	9001	2YQ	C2-C3-N1	-2.21	121.35	122.78

There are no chirality outliers.

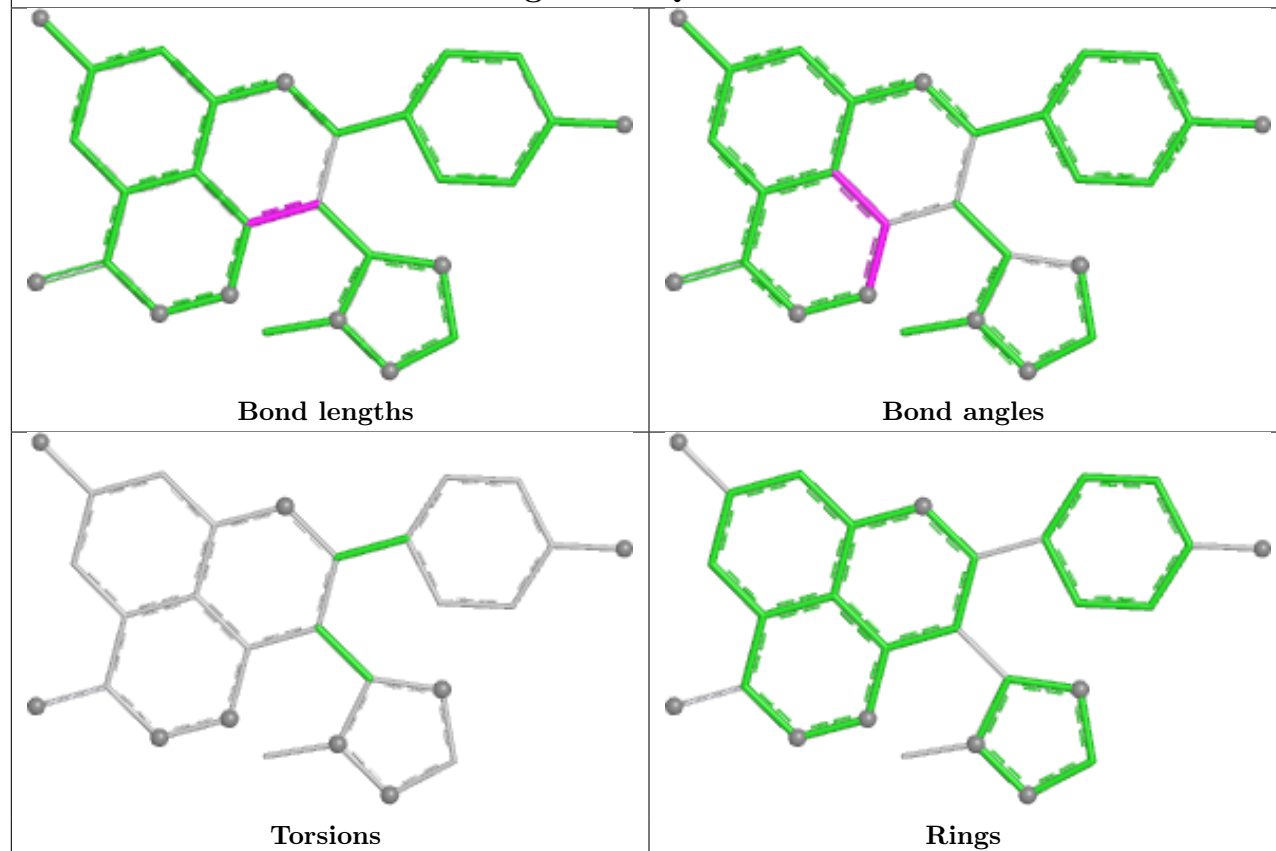
There are no torsion outliers.

There are no ring outliers.

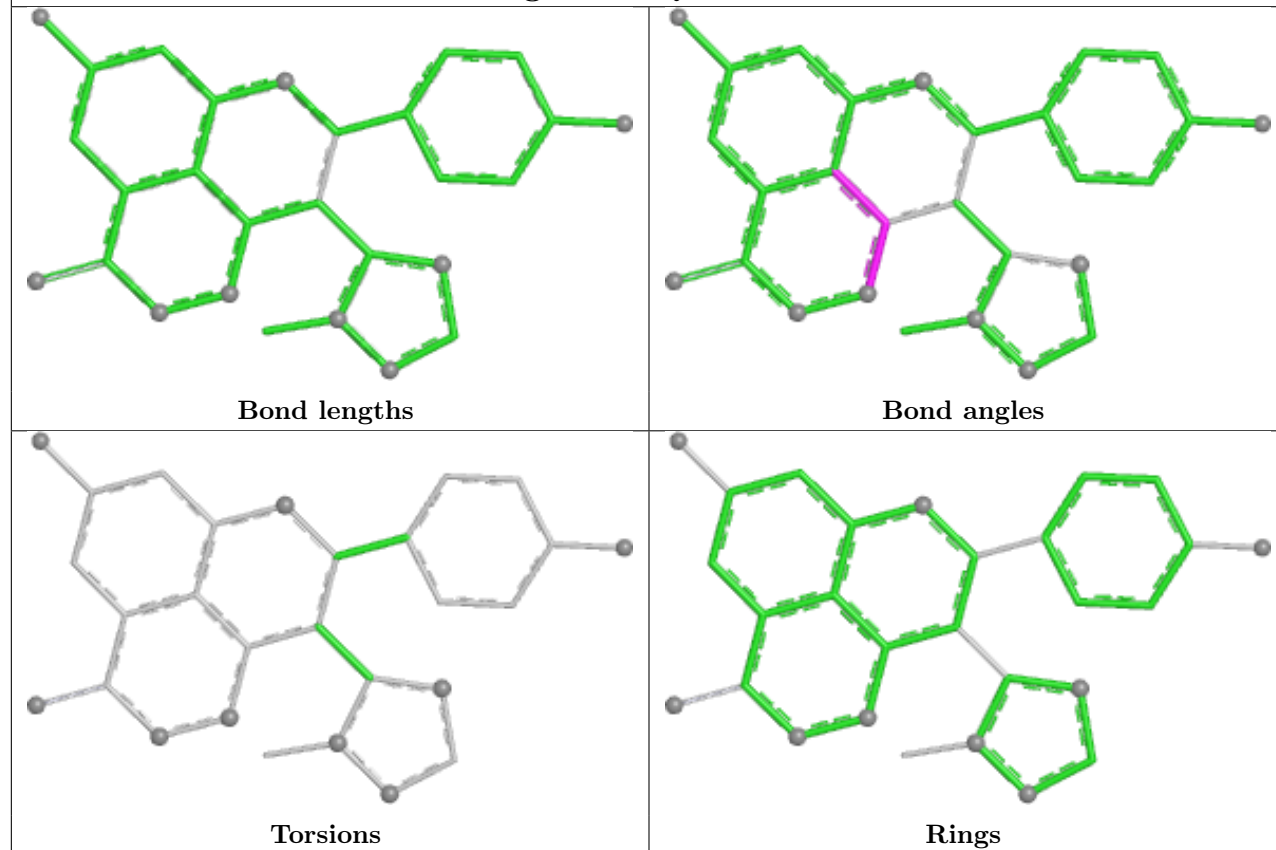
No monomer is involved in short contacts.

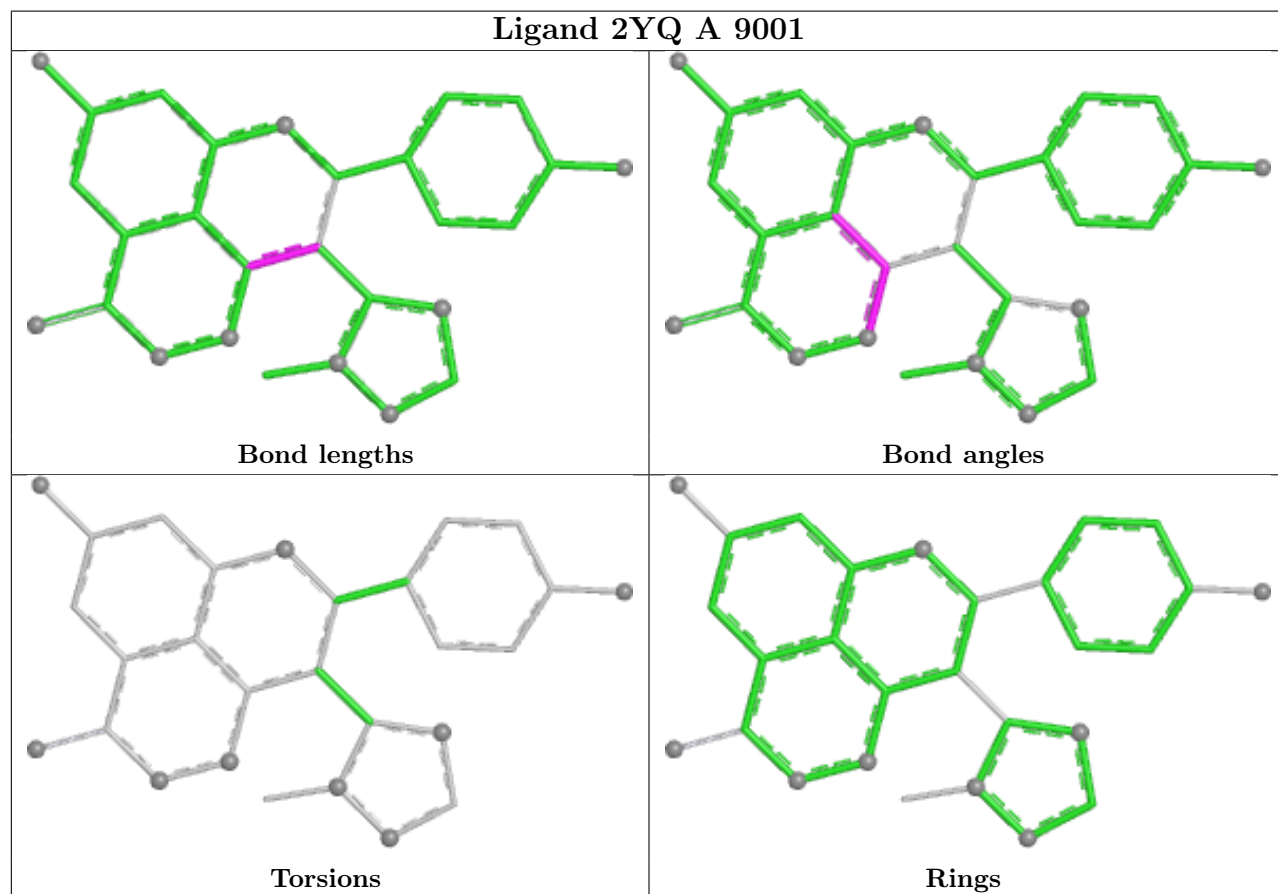
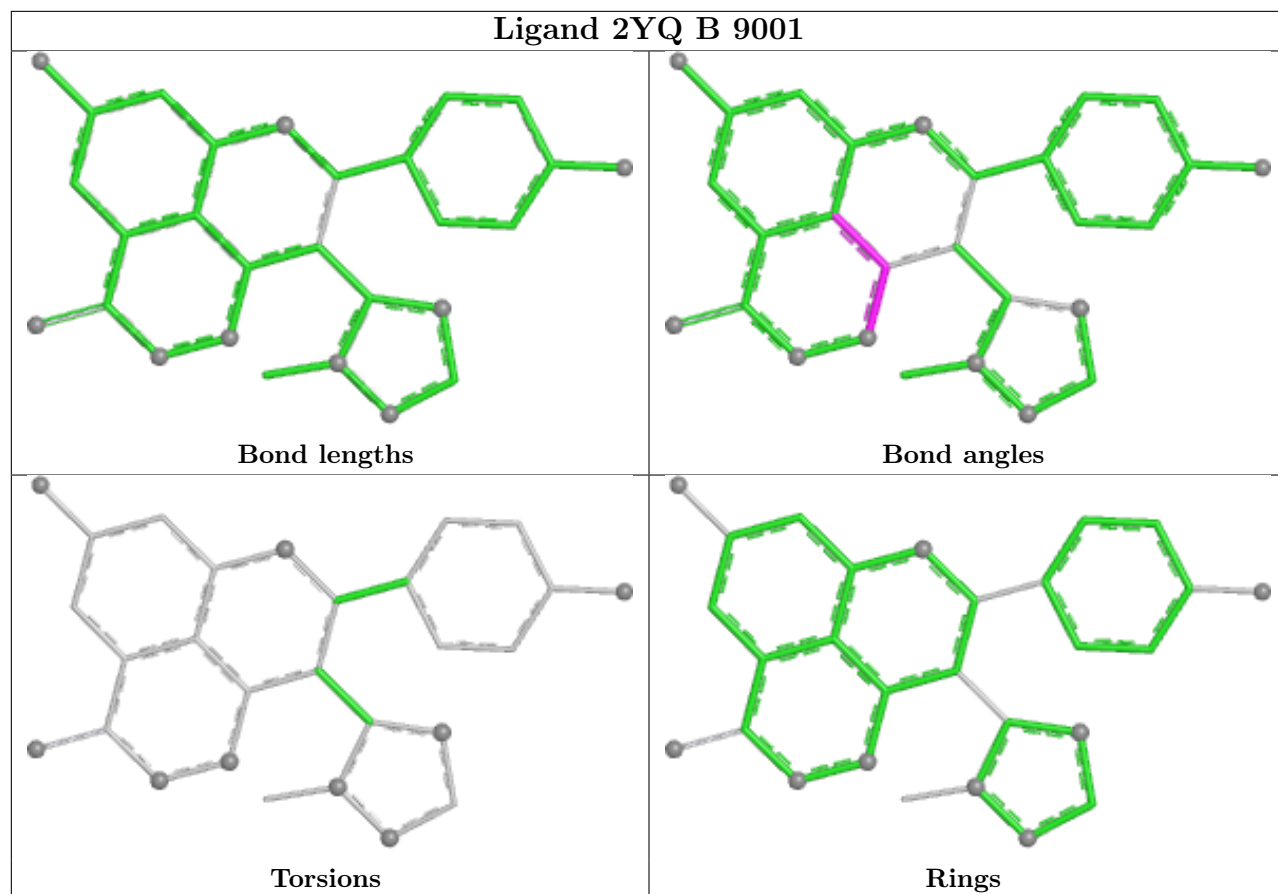
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 2YQ C 9001



Ligand 2YQ D 9001





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	336/352 (95%)	0.73	43 (12%) 7 7	31, 54, 92, 115	0
1	B	337/352 (95%)	0.75	30 (8%) 15 16	36, 58, 90, 117	0
1	C	340/352 (96%)	0.48	23 (6%) 23 23	31, 50, 83, 118	0
1	D	328/352 (93%)	1.26	84 (25%) 1 1	38, 67, 121, 149	0
All	All	1341/1408 (95%)	0.80	180 (13%) 7 7	31, 56, 102, 149	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	729	ILE	5.7
1	D	752	LEU	4.9
1	C	938	ILE	4.7
1	A	755	ALA	4.6
1	D	751	LEU	4.5
1	D	706	ILE	4.4
1	A	729	ILE	4.2
1	B	821	THR	4.2
1	D	954	THR	4.1
1	C	939	SER	4.1
1	B	780	GLY	4.1
1	B	828	ALA	4.1
1	D	720	VAL	3.9
1	A	716	VAL	3.9
1	A	758	VAL	3.9
1	A	964	LEU	3.9
1	B	744	PHE	3.8
1	D	693	LEU	3.8
1	A	720	VAL	3.8
1	D	749	PRO	3.8
1	D	983	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	985	LEU	3.7
1	A	759	GLN	3.6
1	D	665	LEU	3.6
1	D	755	ALA	3.5
1	D	887	THR	3.5
1	A	750	PRO	3.5
1	B	855	HIS	3.5
1	D	777	LEU	3.5
1	C	822	HIS	3.4
1	D	822	HIS	3.4
1	B	973	THR	3.4
1	D	691	ILE	3.4
1	B	974	GLY	3.4
1	A	732	LEU	3.4
1	D	979	VAL	3.4
1	D	831	LEU	3.4
1	D	732	LEU	3.3
1	A	744	PHE	3.3
1	B	751	LEU	3.2
1	D	736	PHE	3.2
1	A	717	GLN	3.2
1	D	781	GLY	3.2
1	C	937	HIS	3.2
1	D	698	LEU	3.1
1	B	790	ILE	3.1
1	D	730	LEU	3.0
1	D	753	ASN	3.0
1	D	763	GLU	3.0
1	D	975	ILE	3.0
1	B	750	PRO	3.0
1	B	835	ASP	3.0
1	D	759	GLN	2.9
1	D	719	ALA	2.9
1	D	984	LEU	2.9
1	A	979	VAL	2.9
1	D	821	THR	2.9
1	D	762	VAL	2.9
1	C	828	ALA	2.9
1	B	834	ILE	2.8
1	D	765	LEU	2.8
1	D	769	LEU	2.8
1	B	938	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	730	LEU	2.8
1	D	701	LEU	2.8
1	D	934	HIS	2.8
1	C	979	VAL	2.8
1	D	740	ILE	2.8
1	D	727	SER	2.7
1	B	914	ASP	2.7
1	D	710	TYR	2.7
1	D	679	VAL	2.7
1	D	758	VAL	2.7
1	A	855	HIS	2.7
1	A	824	THR	2.7
1	D	912	GLN	2.7
1	D	750	PRO	2.7
1	A	965	ASP	2.7
1	B	975	ILE	2.7
1	C	790	ILE	2.7
1	C	811	ALA	2.6
1	D	696	MET	2.6
1	D	713	LEU	2.6
1	B	955	THR	2.6
1	D	973	THR	2.6
1	B	1010	LYS	2.6
1	C	914	ASP	2.6
1	D	697	PRO	2.6
1	A	757	SER	2.6
1	D	778	LEU	2.6
1	A	975	ILE	2.5
1	D	676	ILE	2.5
1	B	986	TYR	2.5
1	A	721	SER	2.5
1	A	733	SER	2.5
1	D	790	ILE	2.5
1	A	749	PRO	2.5
1	A	823	ALA	2.5
1	D	717	GLN	2.5
1	D	728	GLN	2.5
1	D	757	SER	2.5
1	A	748	LYS	2.5
1	A	978	GLY	2.5
1	A	786	SER	2.4
1	B	982	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	979	VAL	2.4
1	D	712	ILE	2.4
1	D	915	PRO	2.4
1	C	961	ASN	2.4
1	A	763	GLU	2.4
1	C	696	MET	2.4
1	A	701	LEU	2.4
1	A	722	GLN	2.4
1	A	696	MET	2.4
1	B	909	HIS	2.4
1	D	982	THR	2.4
1	D	739	LEU	2.3
1	D	1010	LYS	2.3
1	B	729	ILE	2.3
1	C	855	HIS	2.3
1	B	972	GLY	2.3
1	A	1010	LYS	2.3
1	D	662	LYS	2.3
1	B	1007	PHE	2.3
1	D	955	THR	2.3
1	C	974	GLY	2.3
1	C	986	TYR	2.3
1	D	788	ASP	2.3
1	B	724	SER	2.3
1	D	743	ASP	2.3
1	D	760	ALA	2.3
1	D	766	ASP	2.3
1	D	770	ASP	2.3
1	A	762	VAL	2.2
1	A	774	ALA	2.2
1	A	765	LEU	2.2
1	B	971	LEU	2.2
1	A	706	ILE	2.2
1	C	980	ASN	2.2
1	D	771	ILE	2.2
1	D	716	VAL	2.2
1	D	953	LYS	2.2
1	A	770	ASP	2.2
1	D	854	LEU	2.2
1	B	829	TYR	2.2
1	D	737	TYR	2.2
1	D	775	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	768	LEU	2.2
1	A	775	TYR	2.2
1	D	972	GLY	2.1
1	D	978	GLY	2.1
1	A	719	ALA	2.1
1	A	980	ASN	2.1
1	B	954	THR	2.1
1	C	834	ILE	2.1
1	D	913	GLY	2.1
1	D	792	VAL	2.1
1	A	768	LEU	2.1
1	D	797	LEU	2.1
1	D	980	ASN	2.1
1	D	981	ASP	2.1
1	C	821	THR	2.1
1	D	789	PRO	2.1
1	A	913	GLY	2.1
1	C	780	GLY	2.1
1	C	913	GLY	2.1
1	C	972	GLY	2.1
1	A	700	LYS	2.1
1	B	747	LYS	2.1
1	C	739	LEU	2.0
1	D	742	HIS	2.0
1	C	750	PRO	2.0
1	D	829	TYR	2.0
1	B	1009	PHE	2.0
1	A	718	GLN	2.0
1	A	769	LEU	2.0
1	D	830	ASP	2.0
1	C	940	LYS	2.0
1	D	666	PRO	2.0
1	D	689	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

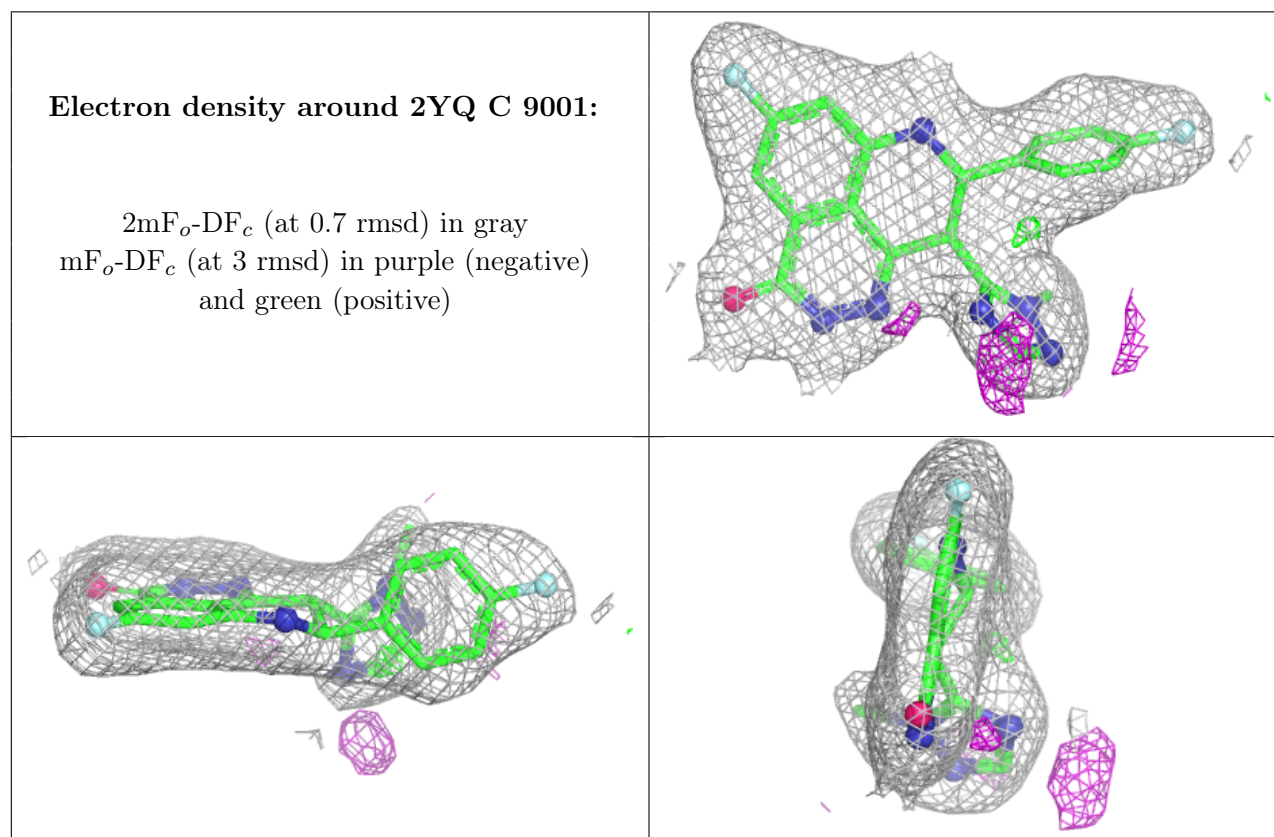
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

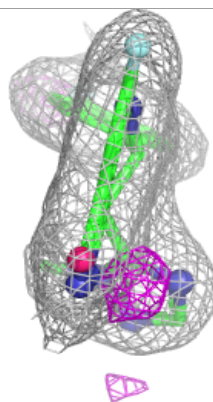
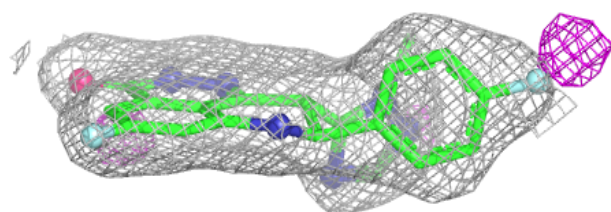
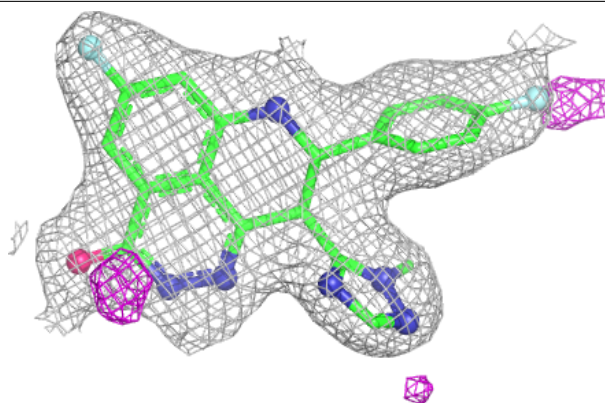
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2YQ	C	9001	28/28	0.94	0.08	31,41,54,57	0
2	2YQ	D	9001	28/28	0.94	0.08	43,45,54,61	0
2	2YQ	B	9001	28/28	0.95	0.08	35,44,64,68	0
2	2YQ	A	9001	28/28	0.96	0.06	28,35,42,45	0

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.

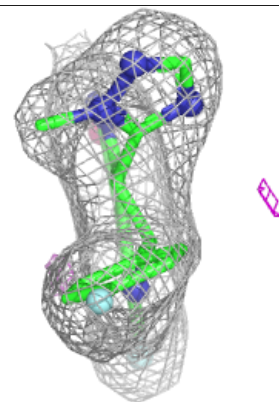
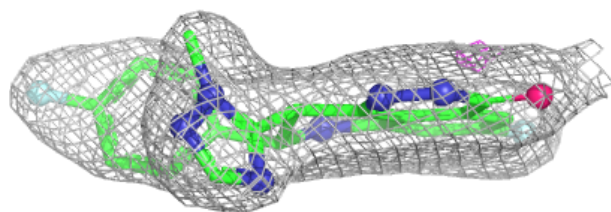
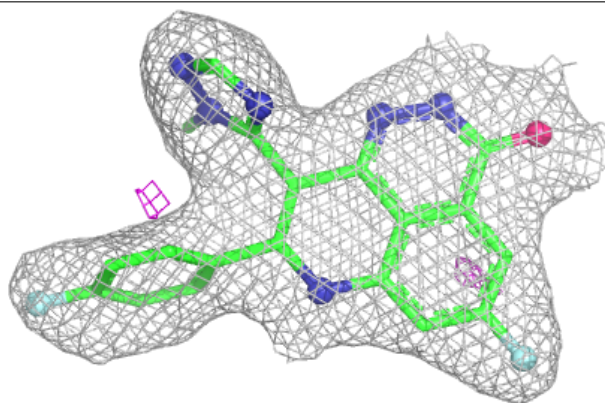


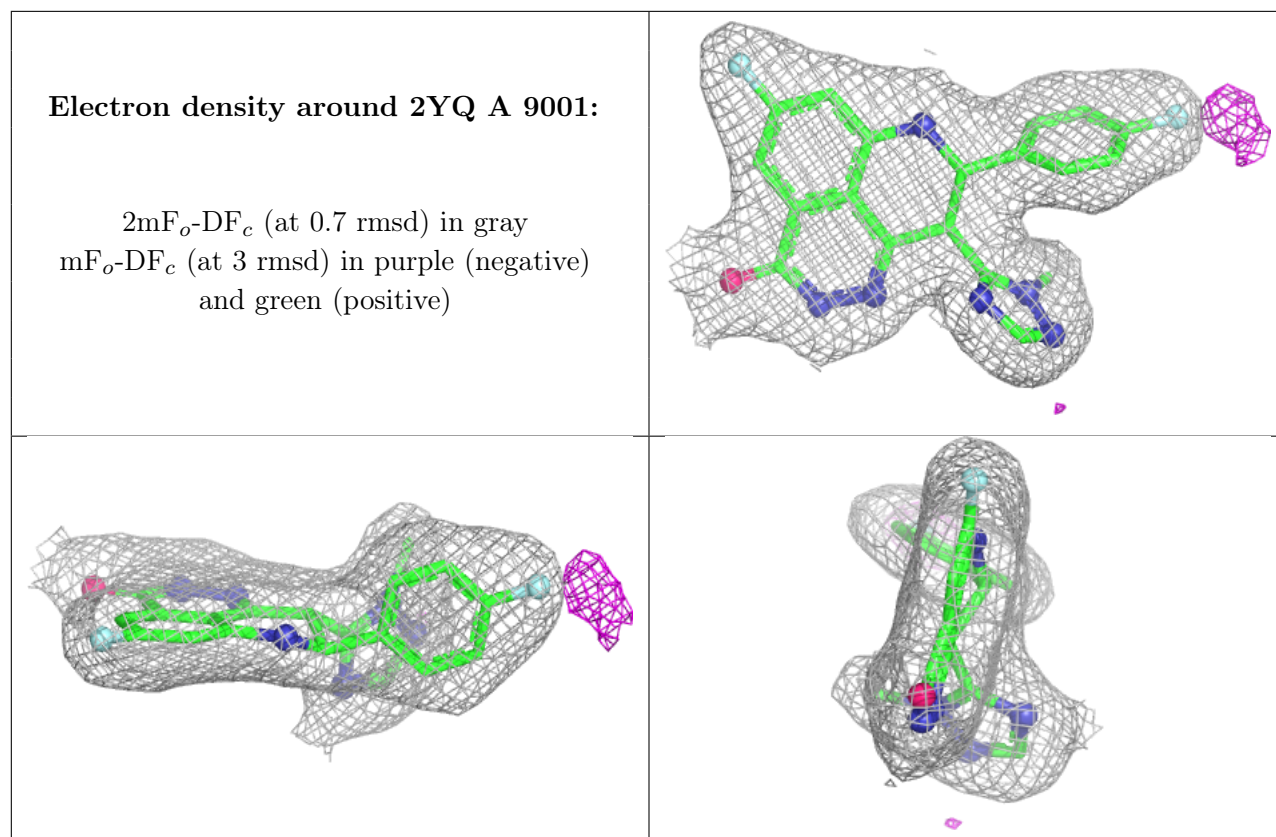
Electron density around 2YQ D 9001:

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

**Electron density around 2YQ B 9001:**

$2mF_o-DF_c$ (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.