



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 12:35 PM EDT

PDB ID : 4R6E
Title : Human artd1 (parp1) - catalytic domain in complex with inhibitor niraparib
Authors : Karlberg, T.; Thorsell, A.G.; Brock, J.; Schuler, H.
Deposited on : 2014-08-25
Resolution : 2.20 Å(reported)

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

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

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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

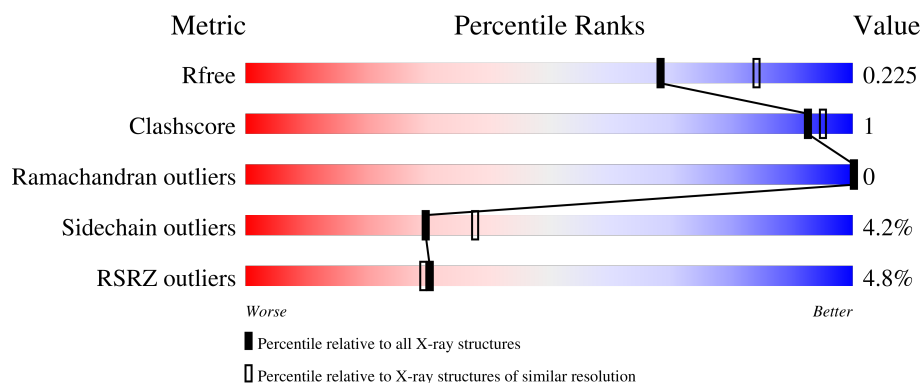
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	358	<div> <div>4%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	B	358	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	C	358	<div> <div>4%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	D	358	<div> <div>9%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11285 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	350	Total	C	N	O	S	0	0	0
			2752	1751	465	524	12			
1	B	350	Total	C	N	O	S	0	0	0
			2751	1750	465	525	11			
1	C	350	Total	C	N	O	S	0	1	0
			2759	1756	467	524	12			
1	D	348	Total	C	N	O	S	0	0	0
			2735	1740	462	522	11			

There are 36 discrepancies between the modelled and reference sequences:

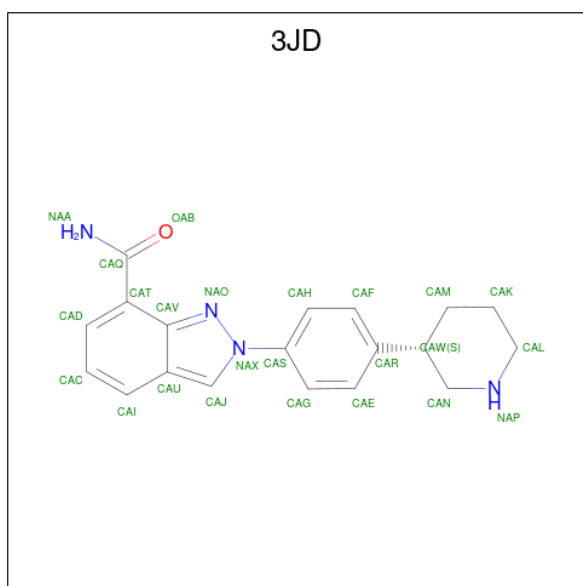
Chain	Residue	Modelled	Actual	Comment	Reference
A	661	MET	-	initiating methionine	UNP P09874
A	762	ALA	VAL	variant	UNP P09874
A	1012	ALA	-	expression tag	UNP P09874
A	1013	HIS	-	expression tag	UNP P09874
A	1014	HIS	-	expression tag	UNP P09874
A	1015	HIS	-	expression tag	UNP P09874
A	1016	HIS	-	expression tag	UNP P09874
A	1017	HIS	-	expression tag	UNP P09874
A	1018	HIS	-	expression tag	UNP P09874
B	661	MET	-	initiating methionine	UNP P09874
B	762	ALA	VAL	variant	UNP P09874
B	1012	ALA	-	expression tag	UNP P09874
B	1013	HIS	-	expression tag	UNP P09874
B	1014	HIS	-	expression tag	UNP P09874
B	1015	HIS	-	expression tag	UNP P09874
B	1016	HIS	-	expression tag	UNP P09874
B	1017	HIS	-	expression tag	UNP P09874
B	1018	HIS	-	expression tag	UNP P09874
C	661	MET	-	initiating methionine	UNP P09874
C	762	ALA	VAL	variant	UNP P09874
C	1012	ALA	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1013	HIS	-	expression tag	UNP P09874
C	1014	HIS	-	expression tag	UNP P09874
C	1015	HIS	-	expression tag	UNP P09874
C	1016	HIS	-	expression tag	UNP P09874
C	1017	HIS	-	expression tag	UNP P09874
C	1018	HIS	-	expression tag	UNP P09874
D	661	MET	-	initiating methionine	UNP P09874
D	762	ALA	VAL	variant	UNP P09874
D	1012	ALA	-	expression tag	UNP P09874
D	1013	HIS	-	expression tag	UNP P09874
D	1014	HIS	-	expression tag	UNP P09874
D	1015	HIS	-	expression tag	UNP P09874
D	1016	HIS	-	expression tag	UNP P09874
D	1017	HIS	-	expression tag	UNP P09874
D	1018	HIS	-	expression tag	UNP P09874

- Molecule 2 is 2-{4-[(3S)-piperidin-3-yl]phenyl}-2H-indazole-7-carboxamide (three-letter code: 3JD) (formula: C₁₉H₂₀N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	19	4	1		
2	B	1	Total	C	N	O	0	0
			24	19	4	1		
2	C	1	Total	C	N	O	0	0
			24	19	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			24	19	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

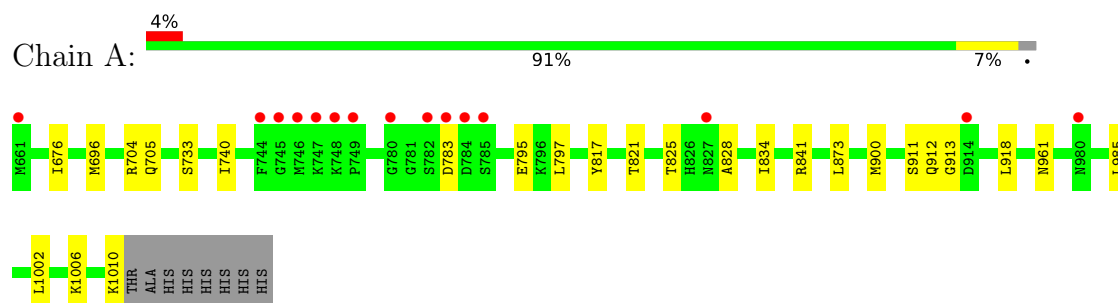
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	41	Total	O	0	0
			41	41		
5	C	54	Total	O	0	0
			54	54		
5	D	8	Total	O	0	0
			8	8		

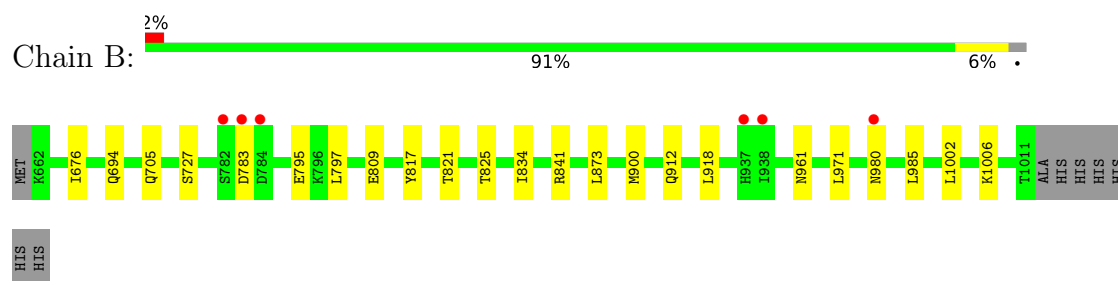
3 Residue-property plots [i](#)

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.

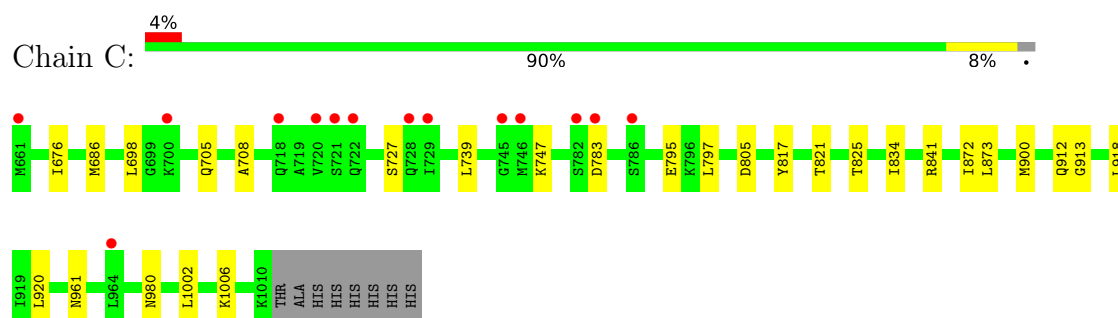
- Molecule 1: Poly [ADP-ribose] polymerase 1



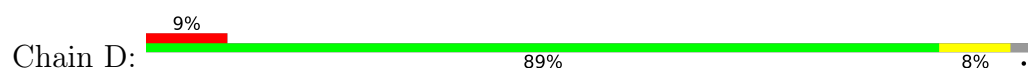
- Molecule 1: Poly [ADP-ribose] polymerase 1

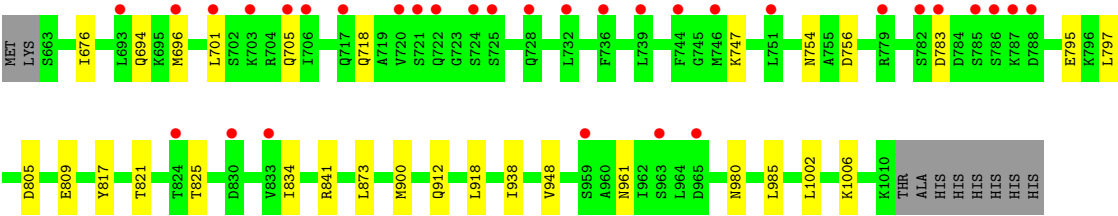


- Molecule 1: Poly [ADP-ribose] polymerase 1



- 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	104.40Å 108.63Å 142.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.30 – 2.20 86.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.30-2.20) 100.0 (86.32-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.79 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.202 , 0.218 0.208 , 0.225	Depositor DCC
R_{free} test set	4123 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11285	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: SO4, 3JD, GOL

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	0.50	0/2804	0.63	0/3783
1	B	0.50	0/2803	0.63	0/3783
1	C	0.49	0/2815	0.62	0/3798
1	D	0.46	0/2787	0.62	0/3762
All	All	0.49	0/11209	0.63	0/15126

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2752	0	2792	10	0
1	B	2751	0	2791	5	0
1	C	2759	0	2800	12	0
1	D	2735	0	2770	9	0
2	A	24	0	20	0	0
2	B	24	0	20	0	0
2	C	24	0	20	0	0
2	D	24	0	20	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	A	51	0	0	0	0
5	B	41	0	0	0	0
5	C	54	0	0	0	0
5	D	8	0	0	0	0
All	All	11285	0	11257	33	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 1.

All (33) 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:913:GLY:HA2	1:C:913:GLY:CA	2.30	0.61
1:B:841:ARG:HD2	1:B:873:LEU:O	2.01	0.60
1:C:918:LEU:HD22	1:C:1002:LEU:HD21	1.83	0.60
1:A:913:GLY:HA2	1:C:913:GLY:HA2	1.84	0.60
1:C:841:ARG:HD2	1:C:873:LEU:O	2.02	0.60
1:A:913:GLY:CA	1:C:913:GLY:HA2	2.34	0.58
1:A:841:ARG:HD2	1:A:873:LEU:O	2.03	0.57
1:D:841:ARG:HD2	1:D:873:LEU:O	2.04	0.57
1:A:918:LEU:HD22	1:A:1002:LEU:HD21	1.87	0.57
1:B:918:LEU:HD22	1:B:1002:LEU:HD21	1.88	0.55
1:D:918:LEU:HD22	1:D:1002:LEU:HD21	1.89	0.54
1:D:938:ILE:HD13	1:D:948:VAL:HG21	1.91	0.51
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.92	0.51
1:C:821:THR:HB	1:C:900:MET:HA	1.94	0.49
1:A:696:MET:HE3	1:A:740:ILE:HA	1.94	0.49
1:C:834:ILE:HD11	1:C:1006:LYS:HB2	1.94	0.49
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	1.94	0.49
1:D:696:MET:CE	1:D:701:LEU:HA	2.44	0.47
1:D:834:ILE:HD11	1:D:1006:LYS:HB2	1.96	0.47
1:B:821:THR:HB	1:B:900:MET:HA	1.96	0.47
1:C:686:MET:CE	1:C:698:LEU:HD13	2.44	0.47
1:A:821:THR:HB	1:A:900:MET:HA	1.95	0.47
1:D:821:THR:HB	1:D:900:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ILE:HD11	1:A:797:LEU:HD11	1.97	0.47
1:D:696:MET:HE1	1:D:701:LEU:HA	1.97	0.47
1:D:676:ILE:HD11	1:D:797:LEU:HD11	1.95	0.47
1:B:676:ILE:HD11	1:B:797:LEU:HD11	1.98	0.44
1:C:676:ILE:HD11	1:C:797:LEU:HD11	2.00	0.44
1:C:686:MET:HE1	1:C:698:LEU:HB2	1.98	0.44
1:C:708:ALA:HB3	1:C:739:LEU:HD21	1.99	0.44
1:A:828:ALA:O	1:A:1010:LYS:HG2	2.19	0.42
1:D:696:MET:HE2	1:D:701:LEU:HD23	2.01	0.41
1:C:872:ILE:HG21	1:C:920:LEU:HD11	2.03	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	348/358 (97%)	341 (98%)	7 (2%)	0	100	100
1	B	348/358 (97%)	342 (98%)	6 (2%)	0	100	100
1	C	349/358 (98%)	344 (99%)	5 (1%)	0	100	100
1	D	346/358 (97%)	341 (99%)	5 (1%)	0	100	100
All	All	1391/1432 (97%)	1368 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	307/314 (98%)	296 (96%)	11 (4%)	35	45
1	B	307/314 (98%)	294 (96%)	13 (4%)	30	38
1	C	308/314 (98%)	297 (96%)	11 (4%)	35	45
1	D	305/314 (97%)	289 (95%)	16 (5%)	23	28
All	All	1227/1256 (98%)	1176 (96%)	51 (4%)	30	38

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	704	ARG
1	A	705	GLN
1	A	733	SER
1	A	783	ASP
1	A	795	GLU
1	A	817	TYR
1	A	825	THR
1	A	911	SER
1	A	912	GLN
1	A	961	ASN
1	A	985	LEU
1	B	694	GLN
1	B	705	GLN
1	B	727	SER
1	B	783	ASP
1	B	795	GLU
1	B	809	GLU
1	B	817	TYR
1	B	825	THR
1	B	912	GLN
1	B	961	ASN
1	B	971	LEU
1	B	980	ASN
1	B	985	LEU
1	C	705	GLN
1	C	727	SER
1	C	747	LYS
1	C	783	ASP
1	C	795	GLU
1	C	805	ASP

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Mol	Chain	Res	Type
1	C	817	TYR
1	C	825	THR
1	C	912	GLN
1	C	961	ASN
1	C	980	ASN
1	D	694	GLN
1	D	705	GLN
1	D	718	GLN
1	D	747	LYS
1	D	754	ASN
1	D	756	ASP
1	D	783	ASP
1	D	795	GLU
1	D	805	ASP
1	D	809	GLU
1	D	817	TYR
1	D	825	THR
1	D	912	GLN
1	D	961	ASN
1	D	980	ASN
1	D	985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	912	GLN
1	A	998	ASN
1	B	912	GLN
1	B	998	ASN
1	C	694	GLN
1	C	912	GLN
1	C	961	ASN
1	C	998	ASN
1	D	742	HIS
1	D	820	ASN
1	D	826	HIS
1	D	912	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	3JD	B	1101	-	26,27,27	2.80	12 (46%)	26,38,38	2.25	9 (34%)
2	3JD	D	1101	-	26,27,27	3.06	13 (50%)	26,38,38	1.96	5 (19%)
3	SO4	C	1102	-	4,4,4	0.11	0	6,6,6	0.39	0
3	SO4	B	1102	-	4,4,4	0.40	0	6,6,6	0.24	0
4	GOL	A	1103	-	5,5,5	0.13	0	5,5,5	0.29	0
2	3JD	C	1101	-	26,27,27	3.00	15 (57%)	26,38,38	1.51	2 (7%)
3	SO4	D	1102	-	4,4,4	0.14	0	6,6,6	0.14	0
4	GOL	B	1103	-	5,5,5	0.13	0	5,5,5	0.24	0
3	SO4	A	1102	-	4,4,4	0.33	0	6,6,6	0.41	0
2	3JD	A	1101	-	26,27,27	2.62	10 (38%)	26,38,38	2.05	9 (34%)
4	GOL	C	1103	-	5,5,5	0.14	0	5,5,5	0.18	0

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	3JD	D	1101	-	-	4/12/20/20	0/4/4/4
4	GOL	A	1103	-	-	2/4/4/4	-
2	3JD	C	1101	-	-	3/12/20/20	0/4/4/4
4	GOL	B	1103	-	-	0/4/4/4	-
2	3JD	B	1101	-	-	2/12/20/20	0/4/4/4
2	3JD	A	1101	-	-	2/12/20/20	0/4/4/4
4	GOL	C	1103	-	-	0/4/4/4	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	3JD	NAO-NAX	-9.02	1.22	1.39
2	C	1101	3JD	NAO-NAX	-8.88	1.22	1.39
2	B	1101	3JD	NAO-NAX	-8.42	1.23	1.39
2	A	1101	3JD	NAO-NAX	-6.14	1.27	1.39
2	D	1101	3JD	CAG-CAS	4.81	1.47	1.38
2	D	1101	3JD	CAT-CAQ	-4.74	1.42	1.50
2	B	1101	3JD	CAE-CAR	4.45	1.46	1.39
2	A	1101	3JD	CAN-NAP	4.19	1.53	1.46
2	A	1101	3JD	CAG-CAS	4.14	1.46	1.38
2	A	1101	3JD	CAD-CAT	3.95	1.45	1.38
2	C	1101	3JD	CAE-CAR	3.91	1.45	1.39
2	C	1101	3JD	CAJ-NAX	3.77	1.41	1.36
2	A	1101	3JD	CAT-CAQ	-3.75	1.44	1.50
2	C	1101	3JD	CAG-CAS	3.74	1.45	1.38
2	A	1101	3JD	CAG-CAE	3.71	1.45	1.38
2	D	1101	3JD	CAD-CAT	3.66	1.44	1.38
2	C	1101	3JD	CAT-CAV	-3.66	1.37	1.43
2	C	1101	3JD	CAR-CAW	-3.55	1.45	1.52
2	D	1101	3JD	CAC-CAD	3.50	1.46	1.38
2	D	1101	3JD	CAR-CAW	-3.47	1.45	1.52
2	C	1101	3JD	CAC-CAI	3.42	1.44	1.36
2	D	1101	3JD	CAF-CAR	3.42	1.44	1.39
2	A	1101	3JD	CAE-CAR	3.40	1.44	1.39
2	B	1101	3JD	CAG-CAE	3.37	1.44	1.38
2	B	1101	3JD	CAT-CAV	-3.35	1.38	1.43
2	D	1101	3JD	CAH-CAS	3.33	1.45	1.38
2	C	1101	3JD	CAJ-CAU	-3.32	1.33	1.40
2	A	1101	3JD	CAC-CAD	3.29	1.45	1.38
2	B	1101	3JD	CAR-CAW	-3.26	1.45	1.52
2	B	1101	3JD	CAJ-CAU	-3.20	1.34	1.40
2	A	1101	3JD	CAC-CAI	3.15	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	3JD	CAG-CAS	3.13	1.44	1.38
2	C	1101	3JD	CAC-CAD	3.13	1.45	1.38
2	D	1101	3JD	CAG-CAE	3.09	1.44	1.38
2	C	1101	3JD	CAF-CAR	3.03	1.43	1.39
2	B	1101	3JD	CAC-CAD	3.02	1.45	1.38
2	D	1101	3JD	CAC-CAI	2.87	1.43	1.36
2	B	1101	3JD	CAT-CAQ	-2.84	1.45	1.50
2	C	1101	3JD	CAT-CAQ	-2.80	1.45	1.50
2	C	1101	3JD	CAH-CAS	2.78	1.43	1.38
2	C	1101	3JD	CAS-NAX	-2.69	1.36	1.44
2	D	1101	3JD	CAT-CAV	-2.65	1.39	1.43
2	D	1101	3JD	CAS-NAX	-2.61	1.36	1.44
2	D	1101	3JD	CAE-CAR	2.57	1.43	1.39
2	C	1101	3JD	CAI-CAU	-2.46	1.36	1.41
2	C	1101	3JD	CAD-CAT	2.46	1.42	1.38
2	B	1101	3JD	CAH-CAS	2.34	1.43	1.38
2	B	1101	3JD	CAM-CAW	2.29	1.59	1.53
2	B	1101	3JD	CAN-CAW	2.27	1.56	1.53
2	A	1101	3JD	CAS-NAX	-2.13	1.38	1.44

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	3JD	CAJ-NAX-NAO	-6.20	106.40	112.72
2	D	1101	3JD	CAJ-NAX-NAO	-5.49	107.12	112.72
2	D	1101	3JD	CAM-CAW-CAR	4.54	123.43	112.79
2	A	1101	3JD	OAB-CAQ-NAA	-4.44	116.27	122.58
2	B	1101	3JD	OAB-CAQ-NAA	-4.14	116.70	122.58
2	C	1101	3JD	CAJ-NAX-NAO	-4.05	108.59	112.72
2	B	1101	3JD	CAG-CAS-NAX	3.89	122.55	119.15
2	A	1101	3JD	CAF-CAH-CAS	3.86	124.69	119.07
2	A	1101	3JD	CAJ-NAX-NAO	-3.77	108.88	112.72
2	B	1101	3JD	CAG-CAS-CAH	-3.59	116.01	121.33
2	A	1101	3JD	CAG-CAS-CAH	-3.54	116.09	121.33
2	D	1101	3JD	OAB-CAQ-NAA	-3.54	117.56	122.58
2	D	1101	3JD	CAG-CAS-NAX	3.33	122.06	119.15
2	C	1101	3JD	CAK-CAM-CAW	-3.06	105.47	111.47
2	B	1101	3JD	CAD-CAT-CAV	-3.02	114.66	118.37
2	B	1101	3JD	CAG-CAE-CAR	-2.96	118.22	121.20
2	A	1101	3JD	CAG-CAS-NAX	2.95	121.73	119.15
2	A	1101	3JD	CAT-CAQ-NAA	2.71	122.42	118.28
2	A	1101	3JD	CAH-CAS-NAX	2.63	121.45	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	3JD	CAD-CAT-CAV	-2.49	115.31	118.37
2	B	1101	3JD	CAE-CAG-CAS	2.37	122.51	119.07
2	A	1101	3JD	CAC-CAI-CAU	-2.34	116.79	120.44
2	D	1101	3JD	CAG-CAS-CAH	-2.28	117.96	121.33
2	B	1101	3JD	CAH-CAS-NAX	2.09	120.98	119.15
2	B	1101	3JD	OAB-CAQ-CAT	2.07	122.66	120.22

There are no chirality outliers.

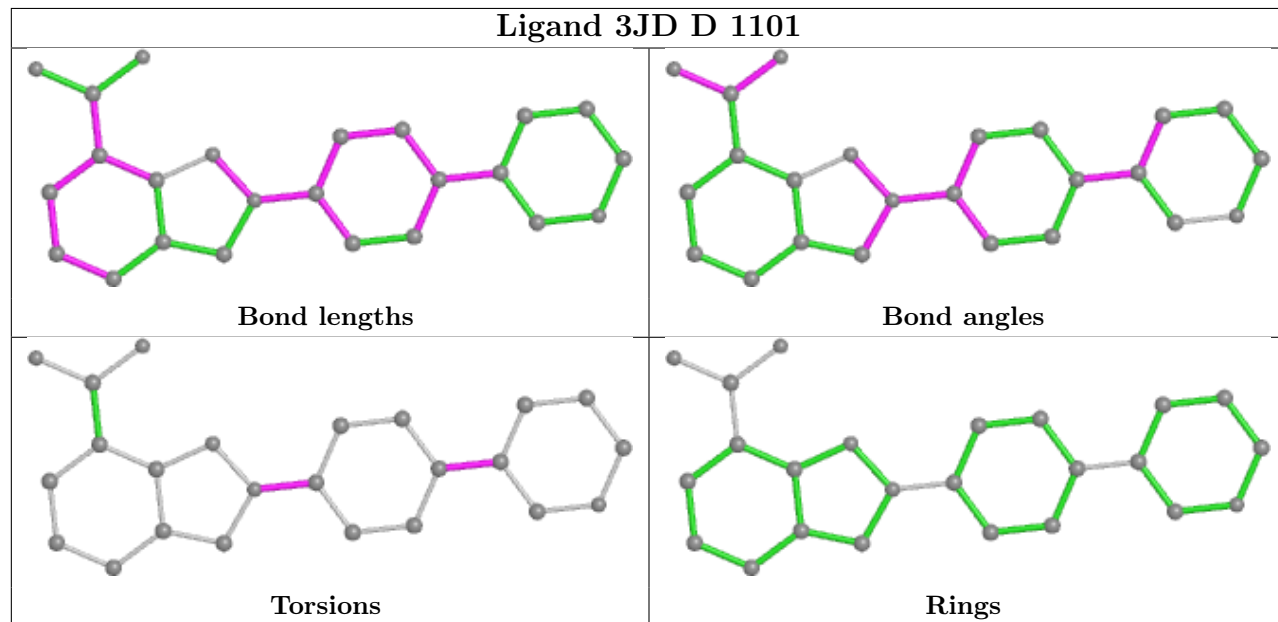
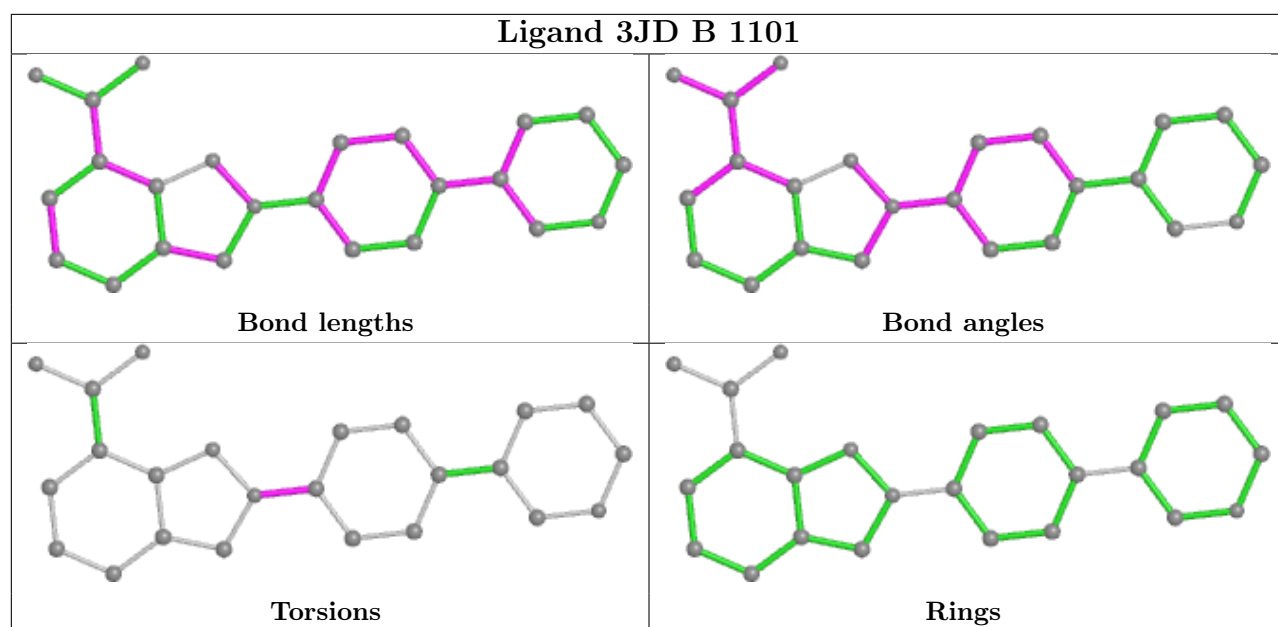
All (13) torsion outliers are listed below:

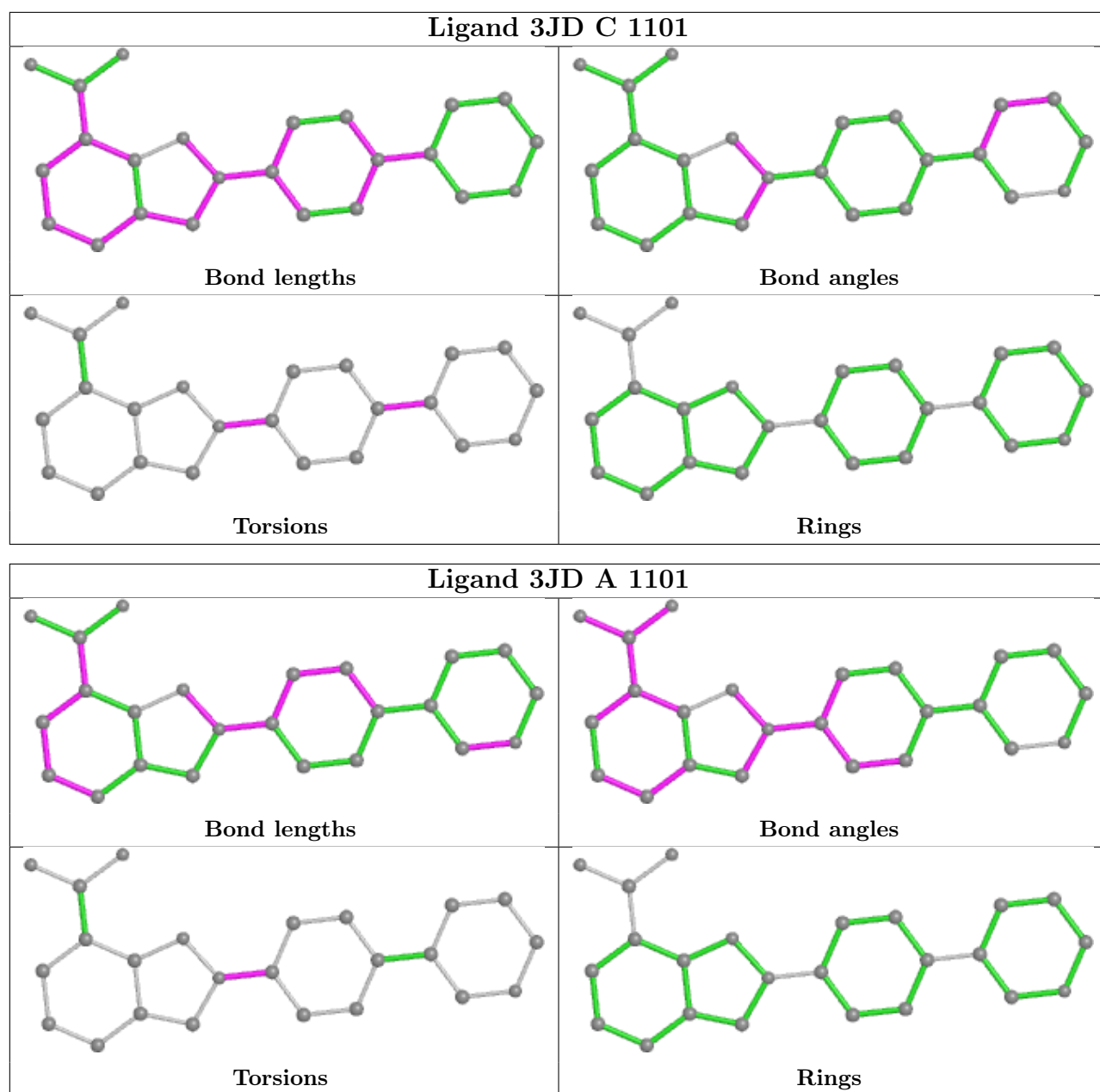
Mol	Chain	Res	Type	Atoms
2	B	1101	3JD	CAH-CAS-NAX-CAJ
2	C	1101	3JD	CAH-CAS-NAX-CAJ
2	D	1101	3JD	CAH-CAS-NAX-CAJ
2	A	1101	3JD	CAH-CAS-NAX-CAJ
4	A	1103	GOL	C1-C2-C3-O3
2	C	1101	3JD	CAF-CAR-CAW-CAN
2	C	1101	3JD	CAE-CAR-CAW-CAN
2	D	1101	3JD	CAF-CAR-CAW-CAN
2	D	1101	3JD	CAE-CAR-CAW-CAN
2	A	1101	3JD	CAG-CAS-NAX-CAJ
2	B	1101	3JD	CAG-CAS-NAX-CAJ
2	D	1101	3JD	CAG-CAS-NAX-CAJ
4	A	1103	GOL	O2-C2-C3-O3

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.





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	350/358 (97%)	-0.03	15 (4%) 35 33	24, 46, 88, 125	0
1	B	350/358 (97%)	-0.12	6 (1%) 70 68	26, 49, 86, 116	0
1	C	350/358 (97%)	0.01	14 (4%) 38 36	25, 49, 104, 126	0
1	D	348/358 (97%)	0.43	32 (9%) 9 7	35, 72, 137, 168	0
All	All	1398/1432 (97%)	0.07	67 (4%) 30 29	24, 52, 110, 168	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	783	ASP	7.5
1	A	661	MET	6.5
1	A	746	MET	5.9
1	A	782	SER	5.6
1	A	748	LYS	5.5
1	D	782	SER	5.5
1	D	785	SER	5.4
1	D	787	LYS	5.1
1	C	746	MET	4.7
1	D	696	MET	4.6
1	C	721	SER	4.5
1	A	783	ASP	4.5
1	A	749	PRO	4.4
1	A	785	SER	4.2
1	D	717	GLN	4.1
1	A	784	ASP	4.1
1	B	784	ASP	4.0
1	D	744	PHE	3.9
1	B	783	ASP	3.9
1	D	965	ASP	3.7
1	D	706	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	746	MET	3.6
1	D	705	GLN	3.5
1	B	782	SER	3.5
1	D	728	GLN	3.4
1	C	745	GLY	3.3
1	C	964	LEU	3.3
1	C	718	GLN	3.2
1	D	732	LEU	3.2
1	D	701	LEU	3.1
1	D	693	LEU	3.1
1	C	661	MET	3.1
1	B	980	ASN	3.0
1	D	720	VAL	2.9
1	B	937	HIS	2.9
1	D	786	SER	2.9
1	D	833	VAL	2.9
1	D	721	SER	2.8
1	D	959	SER	2.8
1	C	728	GLN	2.8
1	C	782	SER	2.8
1	A	744	PHE	2.8
1	C	720	VAL	2.8
1	A	745	GLY	2.8
1	A	747	LYS	2.7
1	C	729	ILE	2.7
1	D	724	SER	2.7
1	D	739	LEU	2.7
1	A	914	ASP	2.6
1	C	700	LYS	2.5
1	C	786	SER	2.4
1	A	780	GLY	2.4
1	D	751	LEU	2.4
1	D	725	SER	2.4
1	D	779	ARG	2.3
1	C	722	GLN	2.3
1	D	703	LYS	2.3
1	D	736	PHE	2.3
1	D	788	ASP	2.3
1	D	722	GLN	2.1
1	B	938	ILE	2.1
1	D	824	THR	2.1
1	A	827	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	783	ASP	2.1
1	D	963	SER	2.1
1	A	980	ASN	2.0
1	D	830	ASP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

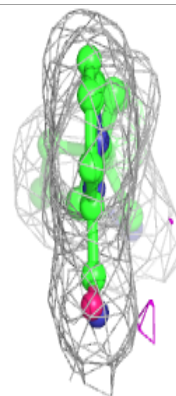
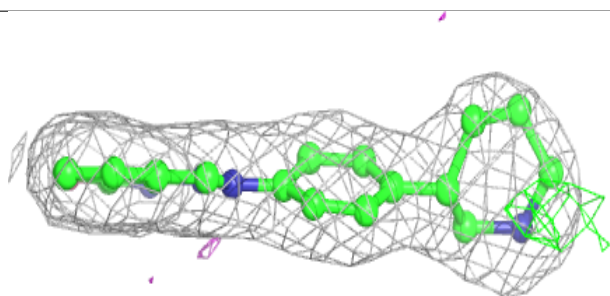
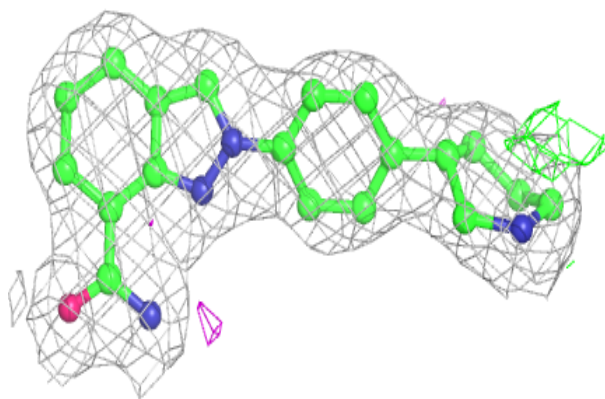
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	1103	6/6	0.92	0.17	33,50,58,63	0
3	SO4	D	1102	5/5	0.93	0.21	98,98,99,100	0
4	GOL	C	1103	6/6	0.93	0.17	38,52,58,62	0
3	SO4	A	1102	5/5	0.94	0.12	59,63,63,70	0
3	SO4	B	1102	5/5	0.94	0.20	66,74,75,77	0
4	GOL	B	1103	6/6	0.94	0.13	35,57,62,65	0
3	SO4	C	1102	5/5	0.94	0.15	19,33,34,36	5
2	3JD	A	1101	24/24	0.96	0.11	23,29,39,41	0
2	3JD	D	1101	24/24	0.97	0.10	31,35,51,52	0
2	3JD	B	1101	24/24	0.98	0.10	23,30,44,45	0
2	3JD	C	1101	24/24	0.98	0.10	18,29,44,47	0

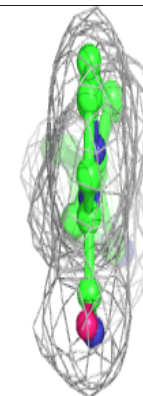
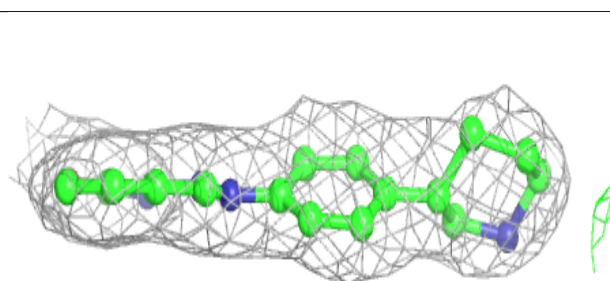
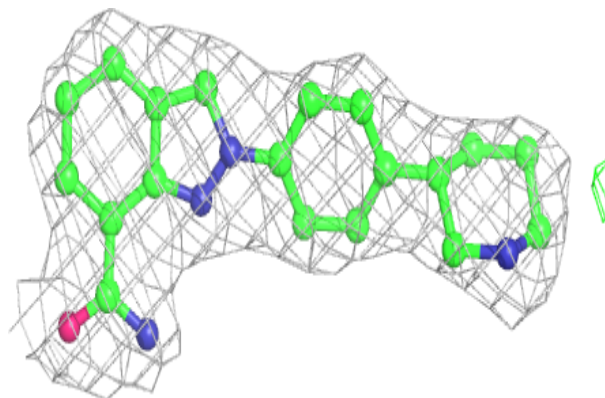
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3JD A 1101:

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

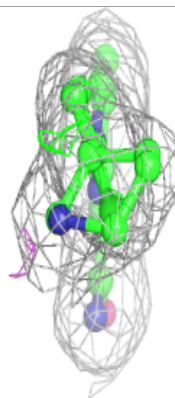
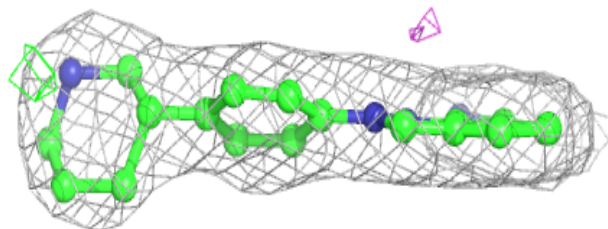
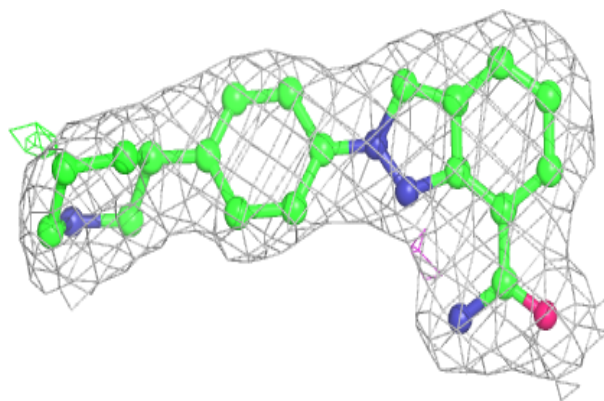
**Electron density around 3JD D 1101:**

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

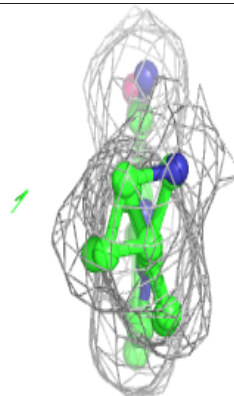
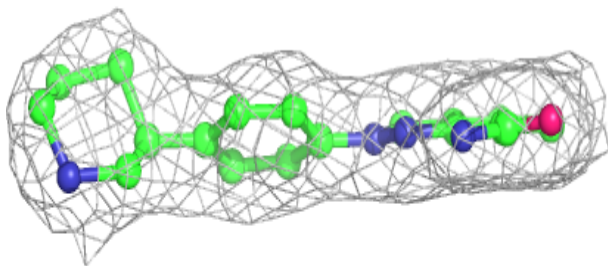
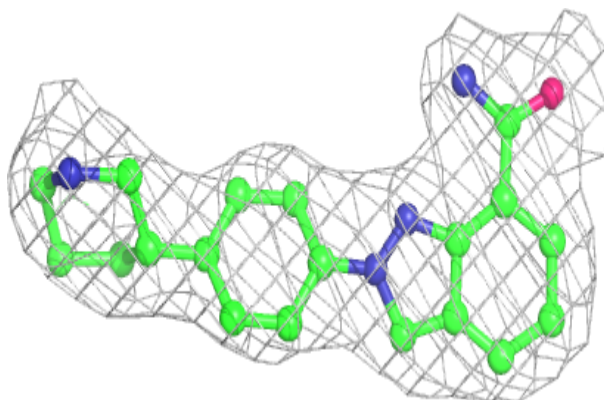


Electron density around 3JD B 1101:

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

**Electron density around 3JD C 1101:**

$2mF_o-DF_c$ (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.