



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:33 PM EDT

PDB ID : 4R6E / pdb_00004r6e
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 : 4-5-2 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

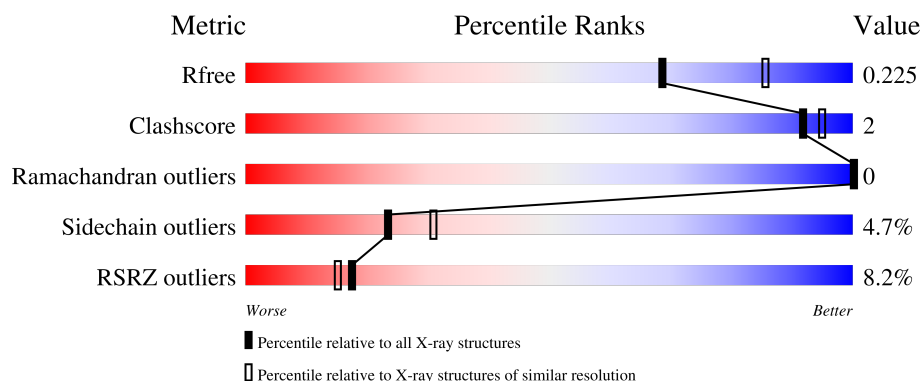
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	6% 89% 8% ..
1	B	358	5% 90% 8% .
1	C	358	9% 88% 9% .
1	D	358	12% 87% 9% ..

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:

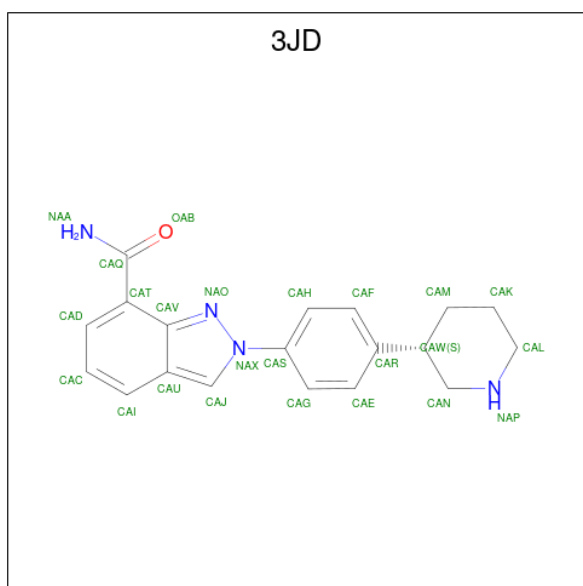
Chain	Residue	Modelled	Actual	Comment	Reference
A	661	MET	-	initiating methionine	UNP P09874
A	762	ALA	VAL	variant	UNP P09874
A	1012	ALA	-	expression tag	UNP P09874
A	1013	HIS	-	expression tag	UNP P09874
A	1014	HIS	-	expression tag	UNP P09874
A	1015	HIS	-	expression tag	UNP P09874
A	1016	HIS	-	expression 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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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		

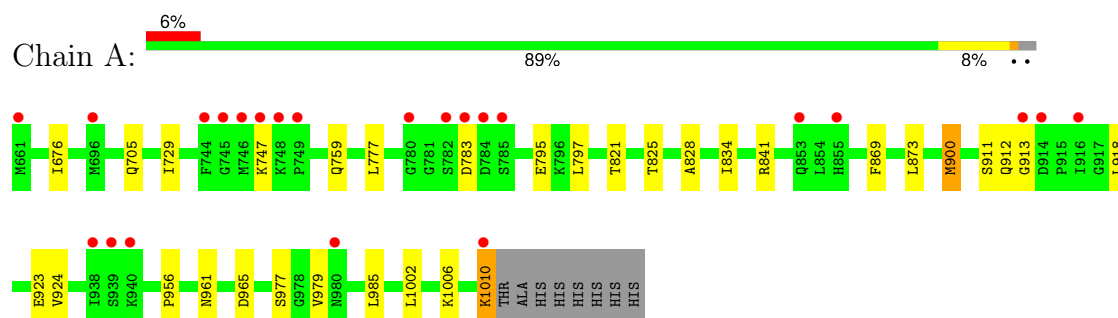
- Molecule 5 is water.

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		

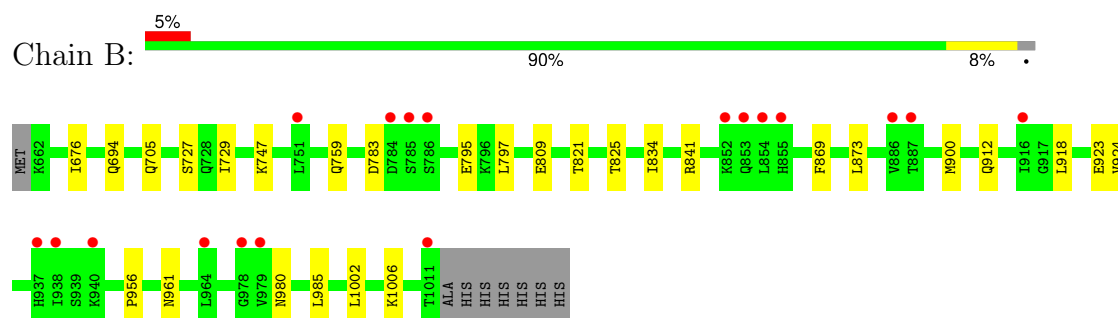
3 Residue-property plots [i](#)

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.

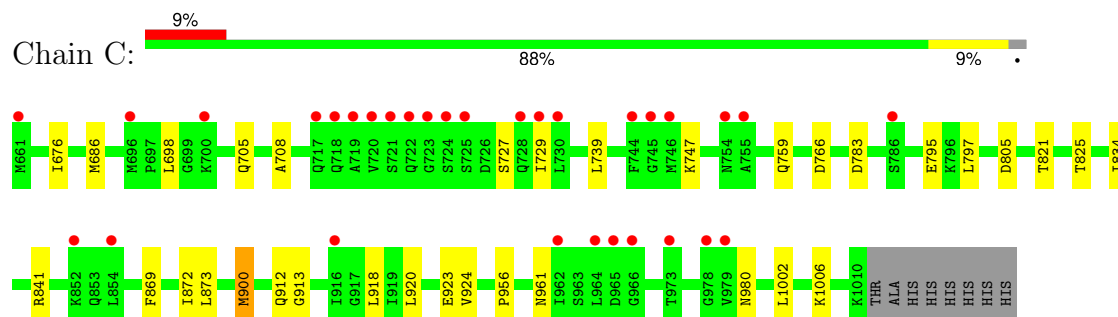
- Molecule 1: Poly [ADP-ribose] polymerase 1



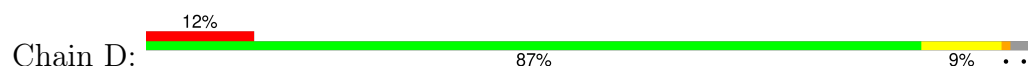
- Molecule 1: Poly [ADP-ribose] polymerase 1



- 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 86.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (86.30-2.20) 100.0 (86.30-2.20)	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 (4.98%)	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 , 39.0	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: GOL, 3JD, SO4

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	1/2804 (0.0%)	1.20	9/3783 (0.2%)
1	B	0.85	0/2803	1.17	3/3783 (0.1%)
1	C	0.84	1/2815 (0.0%)	1.19	4/3798 (0.1%)
1	D	0.82	1/2787 (0.0%)	1.20	10/3762 (0.3%)
All	All	0.84	3/11209 (0.0%)	1.19	26/15126 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	696	MET	SD-CE	-11.67	1.50	1.79
1	C	900	MET	SD-CE	-6.06	1.64	1.79
1	A	900	MET	SD-CE	-5.29	1.66	1.79

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	754	ASN	CA-CB-CG	7.76	120.36	112.60
1	C	869	PHE	CA-CB-CG	-6.94	106.86	113.80
1	A	869	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	979	VAL	N-CA-CB	6.17	117.45	110.72
1	B	869	PHE	CA-CB-CG	-5.98	107.82	113.80
1	D	923	GLU	CA-C-N	-5.96	115.33	123.14
1	D	923	GLU	C-N-CA	-5.96	115.33	123.14
1	C	923	GLU	CA-C-N	-5.92	115.39	123.14
1	C	923	GLU	C-N-CA	-5.92	115.39	123.14
1	D	869	PHE	CA-CB-CG	-5.88	107.92	113.80
1	D	718	GLN	CB-CG-CD	5.86	122.56	112.60
1	B	923	GLU	CA-C-N	-5.85	115.47	123.14
1	B	923	GLU	C-N-CA	-5.85	115.47	123.14
1	D	766	ASP	CA-CB-CG	5.56	118.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	965	ASP	CA-CB-CG	5.52	118.12	112.60
1	C	766	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	923	GLU	CA-C-N	-5.36	116.12	123.14
1	A	923	GLU	C-N-CA	-5.36	116.12	123.14
1	D	777	LEU	CA-C-N	5.22	127.28	120.28
1	D	777	LEU	C-N-CA	5.22	127.28	120.28
1	D	809	GLU	CA-C-N	5.17	127.16	120.44
1	D	809	GLU	C-N-CA	5.17	127.16	120.44
1	A	777	LEU	CA-C-N	5.08	127.09	120.28
1	A	777	LEU	C-N-CA	5.08	127.09	120.28
1	A	977	SER	CA-C-N	-5.01	117.48	123.44
1	A	977	SER	C-N-CA	-5.01	117.48	123.44

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	2752	0	2792	10	0
1	B	2751	0	2791	6	0
1	C	2759	0	2800	13	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	54	0	0	0	0
5	D	8	0	0	0	0
All	All	11285	0	11257	35	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 2.

All (35) 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:900:MET:HE3	1:D:956:PRO:HG3	1.89	0.53
1:A:900:MET:HE3	1:A:956:PRO:HG3	1.92	0.51
1:B:900:MET:HE3	1:B:956:PRO:HG3	1.91	0.51
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:900:MET:HE3	1:C:956:PRO:HG3	1.94	0.50
1:C:821:THR:HB	1:C:900:MET: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
1:A:676:ILE:HD11	1:A:797:LEU:HD11	1.97	0.47
1:D:676:ILE:HD11	1:D:797:LEU:HD11	1.95	0.47
1:C:686:MET:HE1	1:C:698:LEU:HB2	1.97	0.46
1:D:696:MET:HE1	1:D:701:LEU:HA	1.98	0.45
1:B:676:ILE:HD11	1:B:797:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:ILE:HD11	1:C:797:LEU:HD11	2.00	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: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%)	294 (96%)	13 (4%)	26	36
1	B	307/314 (98%)	292 (95%)	15 (5%)	22	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	308/314 (98%)	295 (96%)	13 (4%)	26	36
1	D	305/314 (97%)	288 (94%)	17 (6%)	19	24
All	All	1227/1256 (98%)	1169 (95%)	58 (5%)	23	31

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	705	GLN
1	A	729	ILE
1	A	747	LYS
1	A	759	GLN
1	A	783	ASP
1	A	795	GLU
1	A	825	THR
1	A	911	SER
1	A	912	GLN
1	A	924	VAL
1	A	961	ASN
1	A	985	LEU
1	A	1010	LYS
1	B	694	GLN
1	B	705	GLN
1	B	727	SER
1	B	729	ILE
1	B	747	LYS
1	B	759	GLN
1	B	783	ASP
1	B	795	GLU
1	B	809	GLU
1	B	825	THR
1	B	912	GLN
1	B	924	VAL
1	B	961	ASN
1	B	980	ASN
1	B	985	LEU
1	C	705	GLN
1	C	727	SER
1	C	729	ILE
1	C	747	LYS
1	C	759	GLN
1	C	783	ASP

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Mol	Chain	Res	Type
1	C	795	GLU
1	C	805	ASP
1	C	825	THR
1	C	912	GLN
1	C	924	VAL
1	C	961	ASN
1	C	980	ASN
1	D	694	GLN
1	D	705	GLN
1	D	718	GLN
1	D	729	ILE
1	D	747	LYS
1	D	754	ASN
1	D	756	ASP
1	D	759	GLN
1	D	783	ASP
1	D	795	GLU
1	D	805	ASP
1	D	825	THR
1	D	912	GLN
1	D	924	VAL
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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	717	GLN
1	A	793	ASN
1	A	909	HIS
1	A	912	GLN
1	A	1008	ASN
1	B	717	GLN
1	B	728	GLN
1	B	793	ASN
1	B	909	HIS
1	B	912	GLN
1	B	1008	ASN
1	C	694	GLN
1	C	728	GLN
1	C	909	HIS

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Mol	Chain	Res	Type
1	C	912	GLN
1	C	937	HIS
1	C	998	ASN
1	C	1008	ASN
1	D	728	GLN
1	D	742	HIS
1	D	793	ASN
1	D	820	ASN
1	D	822	HIS
1	D	909	HIS
1	D	912	GLN
1	D	998	ASN
1	D	1008	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	25,27,27	3.19	10 (40%)	29,38,38	3.01	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	3JD	A	1101	-	25,27,27	2.71	10 (40%)	29,38,38	2.72	9 (31%)
3	SO4	D	1102	-	4,4,4	0.26	0	6,6,6	0.16	0
4	GOL	B	1103	-	5,5,5	0.13	0	5,5,5	0.24	0
4	GOL	C	1103	-	5,5,5	0.15	0	5,5,5	0.17	0
2	3JD	C	1101	-	25,27,27	3.40	13 (52%)	29,38,38	2.63	5 (17%)
3	SO4	C	1102	-	4,4,4	0.13	0	6,6,6	0.36	0
3	SO4	A	1102	-	4,4,4	0.40	0	6,6,6	0.42	0
3	SO4	B	1102	-	4,4,4	0.50	0	6,6,6	0.27	0
2	3JD	D	1101	-	25,27,27	3.52	13 (52%)	29,38,38	3.18	7 (24%)
4	GOL	A	1103	-	5,5,5	0.14	0	5,5,5	0.28	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	B	1101	-	-	0/12/20/20	0/4/4/4
2	3JD	A	1101	-	-	0/12/20/20	0/4/4/4
4	GOL	B	1103	-	-	0/4/4/4	-
4	GOL	C	1103	-	-	0/4/4/4	-
2	3JD	C	1101	-	-	1/12/20/20	0/4/4/4
2	3JD	D	1101	-	-	1/12/20/20	0/4/4/4
4	GOL	A	1103	-	-	2/4/4/4	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	3JD	NAX-NAO	-11.80	1.22	1.36
2	C	1101	3JD	NAX-NAO	-11.59	1.22	1.36
2	B	1101	3JD	NAX-NAO	-10.88	1.23	1.36
2	A	1101	3JD	NAX-NAO	-7.37	1.27	1.36
2	C	1101	3JD	CAT-CAV	-5.44	1.37	1.43
2	D	1101	3JD	CAT-CAQ	-5.37	1.42	1.50
2	B	1101	3JD	CAT-CAV	-4.98	1.38	1.43
2	D	1101	3JD	CAG-CAS	4.56	1.47	1.39
2	B	1101	3JD	CAE-CAR	4.52	1.46	1.39
2	D	1101	3JD	CAC-CAD	4.32	1.46	1.38
2	A	1101	3JD	CAT-CAQ	-4.26	1.44	1.50
2	A	1101	3JD	CAG-CAE	4.14	1.45	1.38
2	A	1101	3JD	CAC-CAD	4.06	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	3JD	CAE-CAR	3.96	1.45	1.39
2	D	1101	3JD	CAT-CAV	-3.95	1.39	1.43
2	C	1101	3JD	CAC-CAD	3.86	1.45	1.38
2	A	1101	3JD	CAG-CAS	3.85	1.46	1.39
2	B	1101	3JD	CAG-CAE	3.76	1.44	1.38
2	B	1101	3JD	CAC-CAD	3.73	1.45	1.38
2	C	1101	3JD	CAR-CAW	-3.64	1.45	1.52
2	C	1101	3JD	CAS-NAX	-3.58	1.36	1.43
2	D	1101	3JD	CAR-CAW	-3.56	1.45	1.52
2	D	1101	3JD	CAF-CAR	3.45	1.44	1.39
2	D	1101	3JD	CAS-NAX	-3.45	1.36	1.43
2	A	1101	3JD	CAE-CAR	3.44	1.44	1.39
2	D	1101	3JD	CAG-CAE	3.44	1.44	1.38
2	C	1101	3JD	CAG-CAS	3.43	1.45	1.39
2	B	1101	3JD	CAR-CAW	-3.34	1.45	1.52
2	C	1101	3JD	CAC-CAI	3.27	1.44	1.38
2	B	1101	3JD	CAT-CAQ	-3.24	1.45	1.50
2	C	1101	3JD	CAT-CAQ	-3.19	1.45	1.50
2	C	1101	3JD	CAJ-NAX	3.13	1.41	1.35
2	C	1101	3JD	CAF-CAR	3.06	1.43	1.39
2	D	1101	3JD	CAH-CAS	3.00	1.45	1.39
2	A	1101	3JD	CAC-CAI	2.91	1.43	1.38
2	B	1101	3JD	CAG-CAS	2.79	1.44	1.39
2	A	1101	3JD	CAT-CAV	-2.78	1.40	1.43
2	A	1101	3JD	CAS-NAX	-2.75	1.38	1.43
2	D	1101	3JD	CAE-CAR	2.58	1.43	1.39
2	B	1101	3JD	CAS-NAX	-2.55	1.38	1.43
2	D	1101	3JD	CAC-CAI	2.53	1.43	1.38
2	A	1101	3JD	CAN-NAP	2.43	1.53	1.47
2	C	1101	3JD	CAH-CAS	2.43	1.43	1.39
2	B	1101	3JD	CAM-CAW	2.42	1.59	1.53
2	C	1101	3JD	CAG-CAE	2.20	1.42	1.38
2	D	1101	3JD	CAH-CAF	2.18	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	3JD	CAV-NAO-NAX	13.53	115.76	104.89
2	B	1101	3JD	CAV-NAO-NAX	11.25	113.93	104.89
2	C	1101	3JD	CAV-NAO-NAX	11.01	113.73	104.89
2	A	1101	3JD	CAV-NAO-NAX	10.14	113.03	104.89
2	B	1101	3JD	CAJ-NAX-NAO	-5.74	106.40	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	3JD	CAS-NAX-NAO	5.24	126.29	119.93
2	D	1101	3JD	CAJ-NAX-NAO	-5.04	107.12	112.31
2	D	1101	3JD	CAS-NAX-NAO	4.91	125.89	119.93
2	D	1101	3JD	CAM-CAW-CAR	4.54	123.43	112.67
2	C	1101	3JD	CAS-NAX-NAO	4.52	125.42	119.93
2	A	1101	3JD	CAS-NAX-NAO	4.50	125.40	119.93
2	A	1101	3JD	OAB-CAQ-NAA	-4.39	116.27	122.62
2	B	1101	3JD	OAB-CAQ-NAA	-4.10	116.70	122.62
2	C	1101	3JD	CAJ-NAX-NAO	-3.62	108.59	112.31
2	D	1101	3JD	OAB-CAQ-NAA	-3.50	117.56	122.62
2	A	1101	3JD	CAF-CAH-CAS	3.46	124.69	120.30
2	C	1101	3JD	CAK-CAM-CAW	-3.45	105.47	111.56
2	B	1101	3JD	CAD-CAT-CAV	-3.45	114.66	117.52
2	A	1101	3JD	CAJ-NAX-NAO	-3.34	108.88	112.31
2	C	1101	3JD	CAS-NAX-CAJ	-3.08	124.67	129.12
2	B	1101	3JD	CAG-CAE-CAR	-2.97	118.22	121.18
2	A	1101	3JD	CAS-NAX-CAJ	-2.83	125.03	129.12
2	A	1101	3JD	CAT-CAQ-NAA	2.68	122.42	118.27
2	A	1101	3JD	CAD-CAT-CAV	-2.66	115.31	117.52
2	A	1101	3JD	CAC-CAI-CAU	-2.48	116.79	120.16
2	B	1101	3JD	CAG-CAS-NAX	2.43	122.55	119.58
2	D	1101	3JD	CAS-NAX-CAJ	-2.33	125.75	129.12
2	B	1101	3JD	OAB-CAQ-CAT	2.06	122.66	120.23
2	B	1101	3JD	CAS-NAX-CAJ	-2.04	126.17	129.12
2	D	1101	3JD	CAG-CAS-NAX	2.03	122.06	119.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

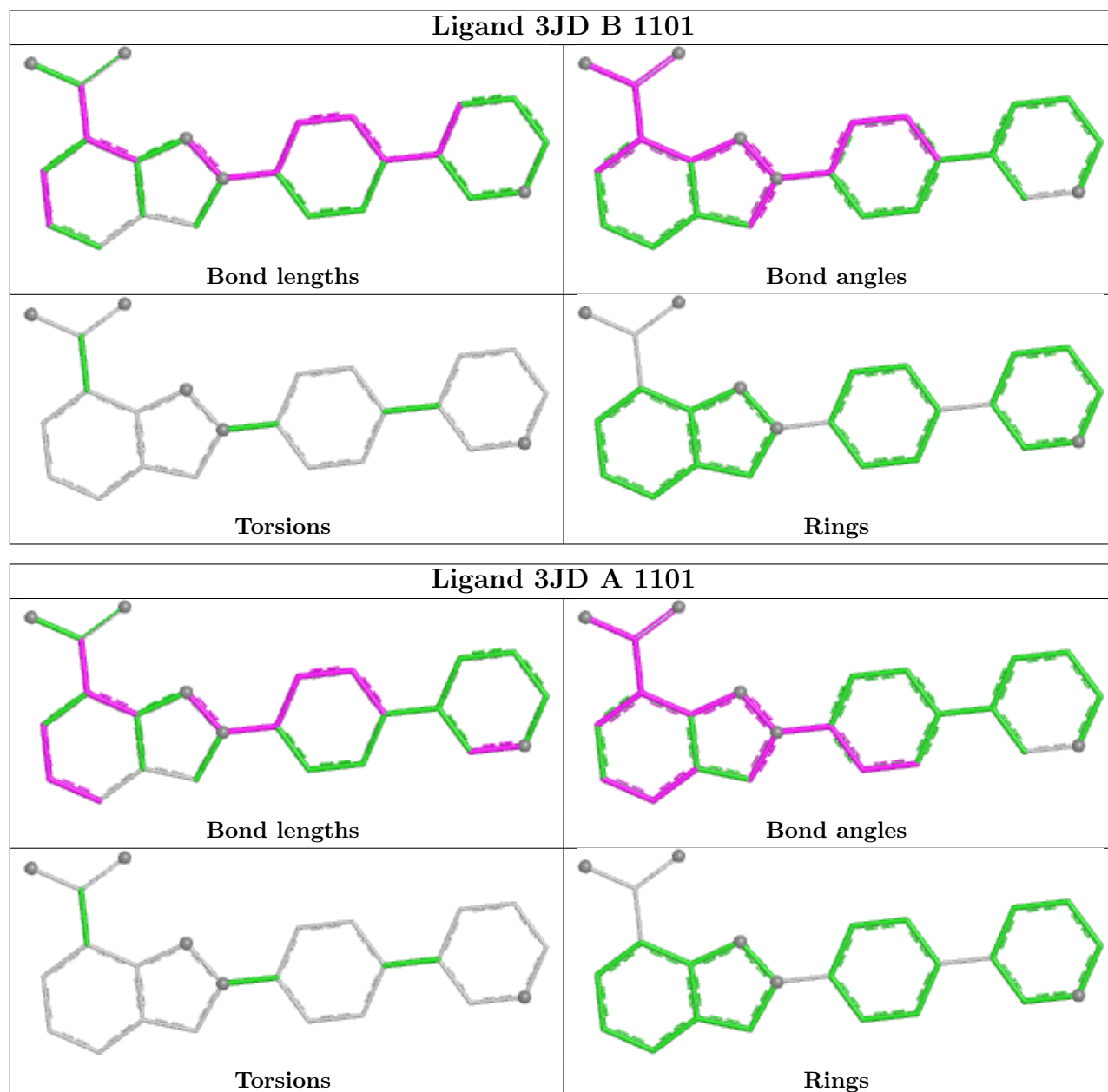
Mol	Chain	Res	Type	Atoms
4	A	1103	GOL	C1-C2-C3-O3
2	C	1101	3JD	CAE-CAR-CAW-CAN
2	D	1101	3JD	CAE-CAR-CAW-CAN
4	A	1103	GOL	O2-C2-C3-O3

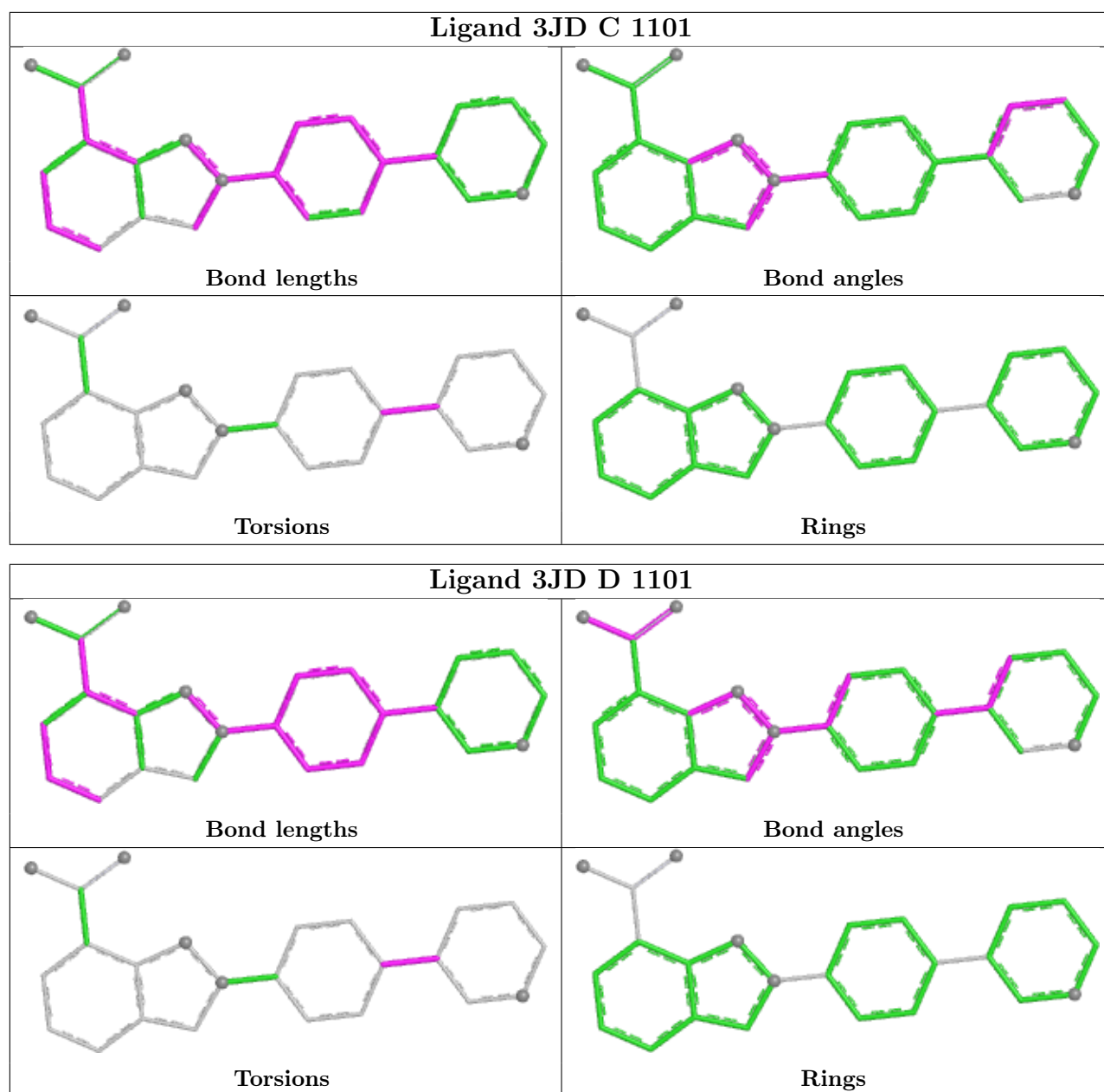
There are no ring outliers.

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.20	23 (6%)	24 21	24, 46, 88, 125	0
1	B	350/358 (97%)	0.25	18 (5%)	33 30	26, 49, 86, 116	0
1	C	350/358 (97%)	0.40	31 (8%)	15 13	25, 49, 104, 126	1 (0%)
1	D	348/358 (97%)	0.86	42 (12%)	8 6	35, 72, 137, 168	0
All	All	1398/1432 (97%)	0.43	114 (8%)	17 15	24, 52, 110, 168	1 (0%)

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	938	ILE	5.8
1	C	964	LEU	5.3
1	D	964	LEU	4.9
1	D	965	ASP	4.1
1	A	853	GLN	3.9
1	A	746	MET	3.8
1	D	706	ILE	3.7
1	A	749	PRO	3.7
1	C	720	VAL	3.6
1	A	939	SER	3.6
1	B	853	GLN	3.5
1	A	938	ILE	3.4
1	A	784	ASP	3.4
1	C	721	SER	3.4
1	A	745	GLY	3.3
1	B	937	HIS	3.2
1	B	916	ILE	3.2
1	C	717	GLN	3.2
1	D	963	SER	3.2
1	C	852	LYS	3.1
1	A	747	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	780	GLY	3.0
1	A	916	ILE	3.0
1	D	717	GLN	3.0
1	D	728	GLN	3.0
1	C	962	ILE	3.0
1	D	751	LEU	3.0
1	C	722	GLN	3.0
1	B	751	LEU	2.9
1	C	719	ALA	2.9
1	A	1010	LYS	2.9
1	B	1011	THR	2.9
1	A	661	MET	2.9
1	C	979	VAL	2.8
1	C	729	ILE	2.8
1	B	784	ASP	2.8
1	D	781	GLY	2.8
1	D	973	THR	2.7
1	D	720	VAL	2.7
1	B	855	HIS	2.7
1	C	755	ALA	2.7
1	A	913	GLY	2.7
1	C	725	SER	2.7
1	A	748	LYS	2.6
1	C	661	MET	2.6
1	D	732	LEU	2.6
1	D	852	LYS	2.6
1	C	696	MET	2.6
1	C	978	GLY	2.6
1	D	916	ILE	2.6
1	D	959	SER	2.6
1	D	752	LEU	2.5
1	D	962	ILE	2.5
1	D	739	LEU	2.5
1	C	723	GLY	2.5
1	A	744	PHE	2.5
1	D	730	LEU	2.5
1	B	978	GLY	2.5
1	D	966	GLY	2.5
1	A	785	SER	2.5
1	B	786	SER	2.5
1	D	749	PRO	2.5
1	D	913	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	809	GLU	2.4
1	D	833	VAL	2.4
1	D	755	ALA	2.4
1	D	701	LEU	2.4
1	A	980	ASN	2.4
1	C	728	GLN	2.4
1	B	887	THR	2.4
1	D	696	MET	2.4
1	C	718	GLN	2.4
1	D	747	LYS	2.3
1	D	748	LYS	2.3
1	A	855	HIS	2.3
1	C	700	LYS	2.3
1	D	1010	LYS	2.3
1	D	722	GLN	2.3
1	A	940	LYS	2.3
1	D	750	PRO	2.3
1	D	746	MET	2.3
1	C	973	THR	2.3
1	B	979	VAL	2.3
1	A	783	ASP	2.3
1	A	782	SER	2.3
1	B	964	LEU	2.2
1	D	828	ALA	2.2
1	D	705	GLN	2.2
1	C	744	PHE	2.2
1	B	886	VAL	2.2
1	C	965	ASP	2.2
1	D	745	GLY	2.2
1	B	940	LYS	2.2
1	C	746	MET	2.2
1	C	916	ILE	2.1
1	B	785	SER	2.1
1	D	960	ALA	2.1
1	A	914	ASP	2.1
1	D	976	SER	2.1
1	C	754	ASN	2.1
1	C	745	GLY	2.1
1	C	786	SER	2.1
1	D	721	SER	2.1
1	C	966	GLY	2.1
1	D	736	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	693	LEU	2.0
1	A	696	MET	2.0
1	C	724	SER	2.0
1	B	854	LEU	2.0
1	C	730	LEU	2.0
1	C	854	LEU	2.0
1	D	1008	ASN	2.0
1	D	691	ILE	2.0
1	B	852	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

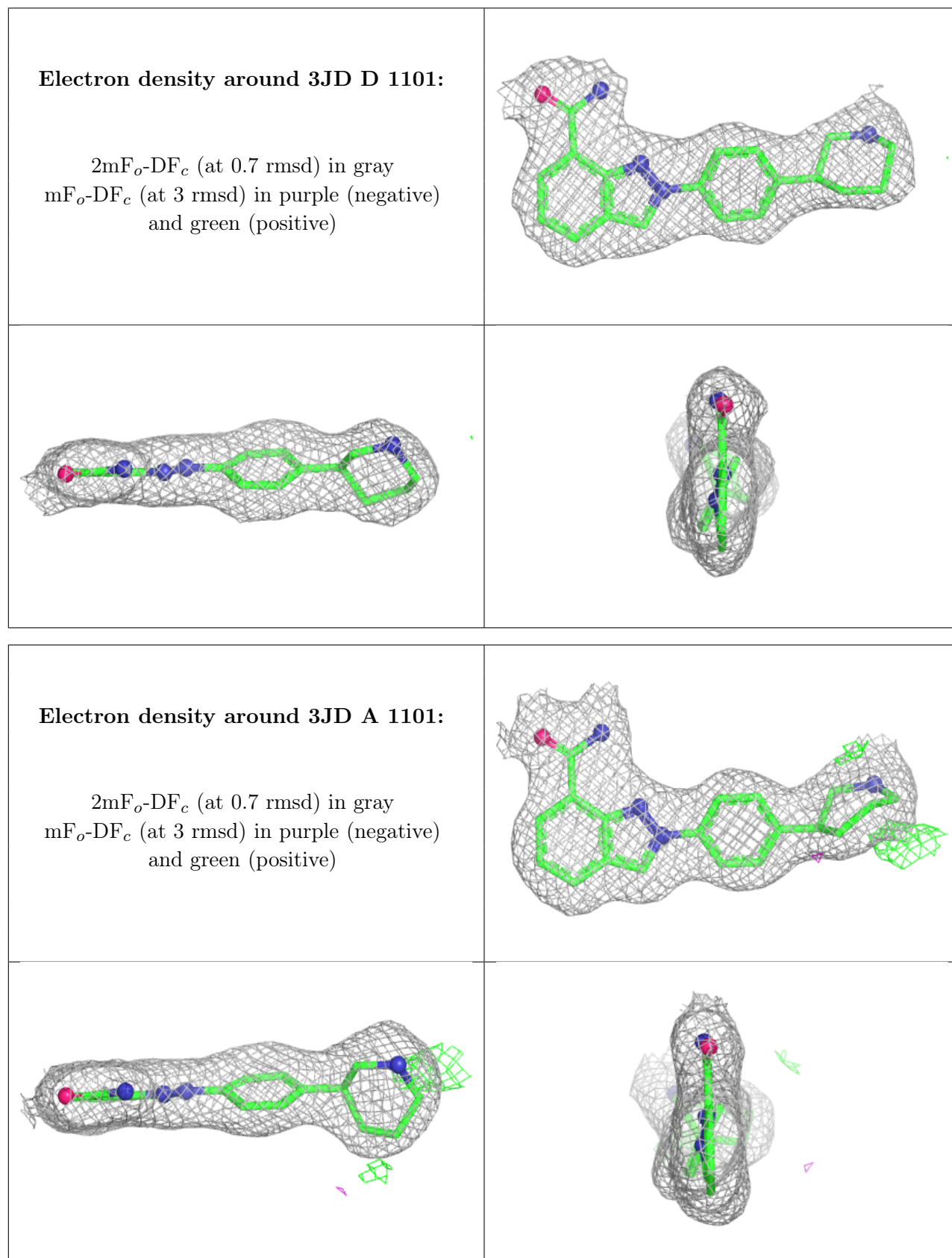
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	1102	5/5	0.74	0.13	98,98,99,100	0
3	SO4	B	1102	5/5	0.82	0.12	66,74,75,77	0
4	GOL	A	1103	6/6	0.86	0.15	33,50,58,63	0
3	SO4	A	1102	5/5	0.87	0.11	59,63,63,70	0
3	SO4	C	1102	5/5	0.91	0.13	19,33,34,36	5
4	GOL	B	1103	6/6	0.91	0.11	35,57,62,65	0
4	GOL	C	1103	6/6	0.91	0.12	38,52,58,62	0
2	3JD	D	1101	24/24	0.95	0.07	31,35,51,52	0
2	3JD	A	1101	24/24	0.96	0.07	23,29,39,41	0
2	3JD	B	1101	24/24	0.97	0.05	23,30,44,45	0
2	3JD	C	1101	24/24	0.97	0.06	18,29,44,47	0

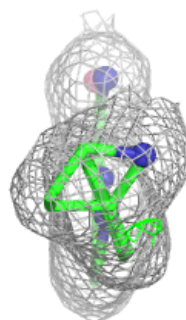
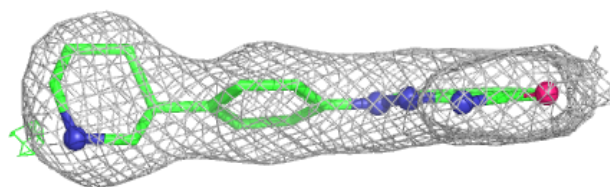
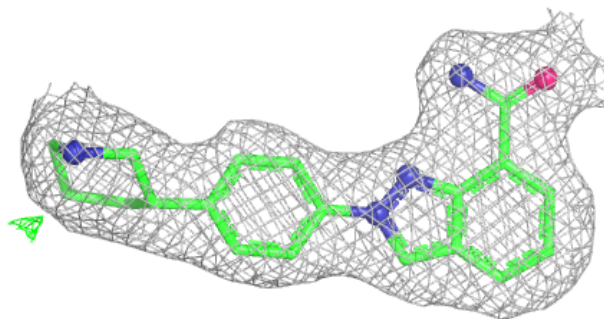
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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

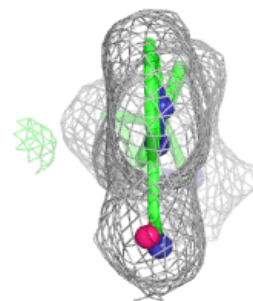
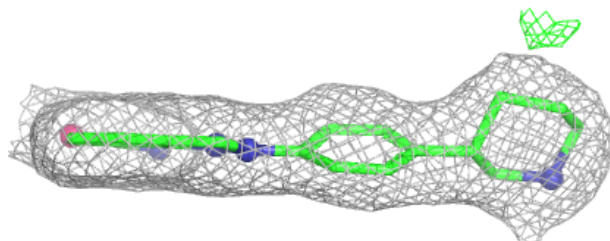
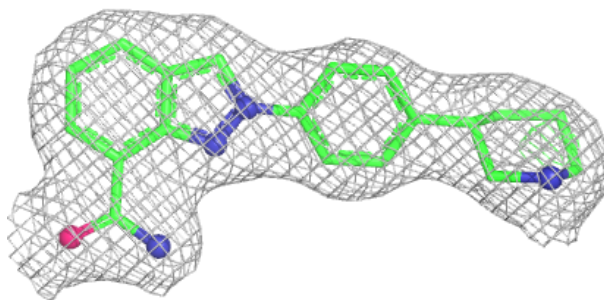


Electron density around 3JD B 1101:

$2mF_o-DF_c$ (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.