



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:54 AM UTC

PDB ID : 3LJ0 / pdb_00003lj0
Title : IRE1 complexed with ADP and Quercetin
Authors : Lee, K.P.K.; Sicheri, F.
Deposited on : 2010-01-25
Resolution : 3.20 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

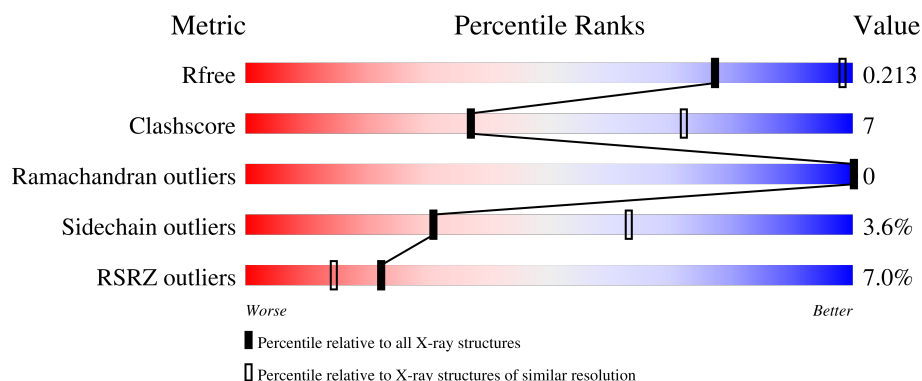
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	434	7% 81% 11% • 6%
1	B	434	6% 82% 9% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6363 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	P	S	0	0	0
			3158	2018	541	582	3	14			
1	B	402	Total	C	N	O	P	S	0	0	0
			3103	1983	530	572	3	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	deletion	UNP P32361
A	?	-	GLN	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	GLU	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	ARG	deletion	UNP P32361
A	?	-	HIS	deletion	UNP P32361
A	?	-	THR	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	VAL	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	SER	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
A	?	-	TYR	deletion	UNP P32361
A	?	-	ASP	deletion	UNP P32361
A	?	-	PRO	deletion	UNP P32361
A	?	-	PHE	deletion	UNP P32361
B	?	-	CYS	deletion	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	GLU	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ARG	deletion	UNP P32361
B	?	-	HIS	deletion	UNP P32361
B	?	-	THR	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	VAL	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	SER	deletion	UNP P32361
B	?	-	PHE	deletion	UNP P32361
B	?	-	TYR	deletion	UNP P32361
B	?	-	ASP	deletion	UNP P32361
B	?	-	PRO	deletion	UNP P32361
B	?	-	PHE	deletion	UNP P32361

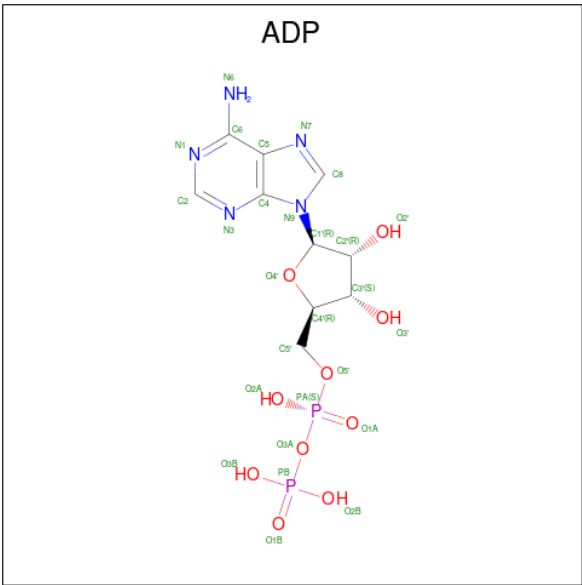
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

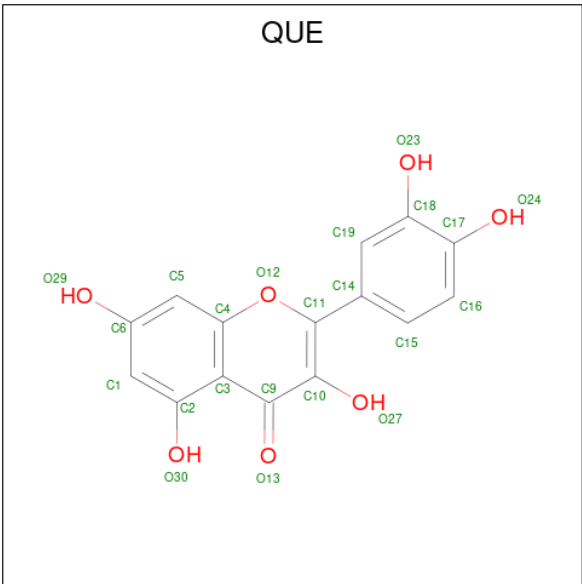
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Sr 1 1	0	0
3	B	1	Total Sr 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (CCD ID: QUE) (formula: C₁₅H₁₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			22	15	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			22	15	7		

- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	131.02Å 131.02Å 175.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.51 – 3.20 65.51 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (65.51-3.20) 98.0 (65.51-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.217 , 0.224 0.204 , 0.213	Depositor DCC
R_{free} test set	1389 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6363	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 4.90% 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: MG, ADP, TPO, SR, SEP, QUE

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	0.46	1/3193 (0.0%)	0.87	10/4323 (0.2%)
1	B	0.44	0/3138	0.86	5/4254 (0.1%)
All	All	0.45	1/6331 (0.0%)	0.87	15/8577 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	712	ALA	CA-CB	-5.16	1.46	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1046	SER	N-CA-CB	-10.71	94.86	110.40
1	A	1046	SER	N-CA-CB	-9.41	97.60	110.67
1	B	1047	LYS	N-CA-C	9.18	123.54	110.23
1	B	1046	SER	CB-CA-C	9.12	123.48	109.34
1	B	1078	ASP	N-CA-C	8.81	121.99	111.33
1	A	925	TYR	N-CA-C	7.49	119.22	111.14
1	A	697	ARG	NE-CZ-NH2	5.94	124.54	119.20
1	A	893	THR	N-CA-C	-5.80	101.81	110.23
1	A	1078	ASP	N-CA-C	5.67	120.33	113.41
1	B	1073	MET	N-CA-C	-5.61	105.26	111.71
1	A	856	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	A	712	ALA	N-CA-C	-5.33	107.33	113.88
1	A	697	ARG	NE-CZ-NH1	-5.24	116.27	121.50
1	A	856	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	1076	VAL	C-N-CD	5.16	131.96	120.60

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	3158	0	3025	48	0
1	B	3103	0	2955	46	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
5	A	22	0	5	2	0
5	B	22	0	5	0	0
All	All	6363	0	6014	88	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 7.

All (88) 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:B:1044:HIS:CG	1:B:1047:LYS:HZ1	1.15	1.59
1:A:1104:SER:O	1:A:1110:ARG:CD	1.65	1.44
1:B:1044:HIS:CG	1:B:1047:LYS:NZ	1.87	1.41
1:B:1044:HIS:CD2	1:B:1047:LYS:NZ	1.88	1.38
1:B:1003:ASP:OD1	1:B:1004:PRO:CD	1.75	1.34
1:B:1003:ASP:CG	1:B:1004:PRO:HD3	1.59	1.27
1:B:1106:ASP:O	1:B:1110:ARG:HG2	1.38	1.22
1:B:1003:ASP:OD1	1:B:1004:PRO:HD2	1.31	1.18
1:A:1104:SER:O	1:A:1110:ARG:HD3	1.24	1.17
1:B:794:ILE:HG21	1:B:901:ILE:HD11	1.17	1.17
1:A:1106:ASP:O	1:A:1110:ARG:HG2	1.44	1.16
1:A:1104:SER:C	1:A:1110:ARG:HD3	1.73	1.12
1:B:1003:ASP:CG	1:B:1004:PRO:CD	2.26	1.04
1:B:1107:GLN:HA	1:B:1110:ARG:HE	1.14	1.04
1:B:794:ILE:CG2	1:B:901:ILE:HD11	1.89	1.02
1:A:1104:SER:O	1:A:1110:ARG:NE	1.92	1.01
1:B:1107:GLN:HG2	1:B:1110:ARG:HH21	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1044:HIS:CD2	1:B:1047:LYS:HZ3	1.77	0.94
1:A:860:LEU:HD12	1:A:901:ILE:HD11	1.48	0.92
1:B:1044:HIS:CD2	1:B:1047:LYS:HZ2	1.88	0.90
1:B:725:HIS:HD2	1:B:727:ASN:H	1.20	0.89
1:A:725:HIS:HD2	1:A:727:ASN:H	1.20	0.88
1:A:857:ALA:CB	1:A:901:ILE:HD12	2.10	0.82
1:A:1105:ASP:HA	1:A:1110:ARG:HH11	1.47	0.80
1:A:857:ALA:HB3	1:A:901:ILE:CD1	2.12	0.79
1:A:1104:SER:C	1:A:1110:ARG:CD	2.42	0.79
1:A:857:ALA:HB3	1:A:901:ILE:HD12	1.62	0.79
1:A:860:LEU:CD1	1:A:901:ILE:HD11	2.13	0.78
1:B:1107:GLN:HG2	1:B:1110:ARG:NH2	1.99	0.78
1:B:1044:HIS:CB	1:B:1047:LYS:HZ1	1.94	0.77
1:B:725:HIS:CD2	1:B:727:ASN:H	2.04	0.76
1:B:1106:ASP:O	1:B:1110:ARG:CG	2.29	0.76
1:A:895:ARG:HG2	1:A:895:ARG:O	1.84	0.75
1:B:1107:GLN:HA	1:B:1110:ARG:NE	1.98	0.75
1:A:757:GLU:O	1:A:758:SER:C	2.30	0.74
1:A:725:HIS:CD2	1:A:727:ASN:H	2.04	0.72
1:B:898:THR:O	1:B:901:ILE:HG12	1.89	0.71
1:A:1106:ASP:O	1:A:1110:ARG:CG	2.32	0.70
1:A:1104:SER:O	1:A:1110:ARG:HD2	1.86	0.69
1:B:1044:HIS:CB	1:B:1047:LYS:NZ	2.53	0.68
1:A:1105:ASP:HA	1:A:1110:ARG:NH1	2.11	0.65
1:B:859:GLU:HB2	1:B:895:ARG:HD2	1.78	0.64
1:B:1001:ASN:OD1	1:B:1003:ASP:OD1	2.17	0.63
1:A:860:LEU:CD1	1:A:901:ILE:CD1	2.78	0.62
1:A:1104:SER:O	1:A:1110:ARG:CZ	2.48	0.62
1:A:1063:MET:HE2	1:B:999:ILE:HD13	1.84	0.59
1:A:857:ALA:HB2	1:A:901:ILE:HD12	1.84	0.59
1:A:1025:TRP:CD1	1:A:1045:SER:O	2.57	0.58
1:A:1075:PRO:HB3	1:B:1107:GLN:NE2	2.19	0.57
1:A:1075:PRO:CB	1:B:1107:GLN:NE2	2.67	0.57
1:A:752:LEU:HD21	1:A:913:ILE:HD11	1.88	0.55
1:A:999:ILE:HD13	1:B:1063:MET:HE2	1.88	0.55
1:A:1075:PRO:HB3	1:B:1107:GLN:HE22	1.70	0.55
1:B:794:ILE:CG2	1:B:901:ILE:CD1	2.75	0.53
1:A:1105:ASP:N	1:A:1110:ARG:HD3	2.23	0.53
1:B:752:LEU:HD21	1:B:913:ILE:HD11	1.91	0.53
1:A:1105:ASP:CA	1:A:1110:ARG:HD3	2.40	0.52
1:A:777:LEU:HD11	1:A:822:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:GLU:O	1:B:758:SER:C	2.54	0.51
1:A:1003:ASP:CB	1:A:1004:PRO:HD3	2.42	0.50
1:B:777:LEU:HD11	1:B:822:LEU:HD12	1.94	0.49
1:A:1075:PRO:HB2	1:B:1107:GLN:NE2	2.28	0.48
1:B:773:ASN:HD22	1:B:774:PRO:HD2	1.78	0.48
1:A:865:ASN:HB3	1:A:868:GLN:HB2	1.95	0.47
1:A:773:ASN:HD22	1:A:774:PRO:HD2	1.79	0.47
5:A:1:QUE:H19	5:A:1:QUE:O27	2.13	0.47
1:B:1003:ASP:CB	1:B:1004:PRO:HD3	2.41	0.47
1:B:785:VAL:HG11	1:B:906:MET:HE2	1.97	0.46
1:B:725:HIS:HD2	1:B:727:ASN:N	2.01	0.46
1:B:1044:HIS:CG	1:B:1047:LYS:HZ2	2.05	0.46
1:B:796:ARG:HD3	1:B:831:LEU:O	2.17	0.45
1:A:901:ILE:HG23	1:A:902:ASP:N	2.31	0.44
1:A:785:VAL:HG11	1:A:906:MET:HE2	1.98	0.44
1:A:1063:MET:HG2	1:B:999:ILE:HG21	2.00	0.44
1:A:977:HIS:CG	1:A:978:PRO:HD2	2.53	0.44
1:B:977:HIS:CG	1:B:978:PRO:HD2	2.53	0.44
1:A:796:ARG:HD3	1:A:831:LEU:O	2.17	0.43
1:A:1028:LYS:HB3	1:A:1087:ARG:HG2	2.00	0.43
1:A:667:GLU:HB3	1:A:675:VAL:HB	2.02	0.42
1:A:725:HIS:HD2	1:A:727:ASN:N	2.01	0.42
1:A:862:GLU:CB	1:A:895:ARG:HH12	2.33	0.42
5:A:1:QUE:O29	1:B:988:GLU:OE1	2.38	0.41
1:B:719:LEU:HD13	1:B:731:TYR:HB2	2.02	0.41
1:B:723:ASP:HB2	1:B:730:ARG:HA	2.01	0.41
1:B:1028:LYS:HB3	1:B:1087:ARG:HG2	2.02	0.40
1:A:1076:VAL:H	1:A:1076:VAL:HG22	1.61	0.40
1:A:860:LEU:HD11	1:A:901:ILE:HG12	2.04	0.40
1:A:719:LEU:HD13	1:A:731:TYR:HB2	2.04	0.40

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	399/434 (92%)	383 (96%)	16 (4%)	0	100	100
1	B	394/434 (91%)	377 (96%)	17 (4%)	0	100	100
All	All	793/868 (91%)	760 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/395 (82%)	313 (96%)	12 (4%)	30	63
1	B	318/395 (80%)	307 (96%)	11 (4%)	32	64
All	All	643/790 (81%)	620 (96%)	23 (4%)	31	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	796	ARG
1	A	856	ARG
1	A	895	ARG
1	A	942	LYS
1	A	949	LEU
1	A	1046	SER
1	A	1053	ARG
1	A	1063	MET
1	A	1077	PRO
1	A	1078	ASP
1	A	1087	ARG
1	A	1109	LEU
1	B	796	ARG
1	B	895	ARG
1	B	949	LEU

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Mol	Chain	Res	Type
1	B	1046	SER
1	B	1049	MET
1	B	1053	ARG
1	B	1063	MET
1	B	1076	VAL
1	B	1087	ARG
1	B	1109	LEU
1	B	1110	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	725	HIS
1	A	727	ASN
1	A	773	ASN
1	A	801	GLN
1	A	816	GLN
1	A	1057	ASN
1	A	1060	HIS
1	A	1107	GLN
1	B	725	HIS
1	B	727	ASN
1	B	773	ASN
1	B	801	GLN
1	B	816	GLN
1	B	1044	HIS
1	B	1057	ASN
1	B	1060	HIS
1	B	1107	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	SEP	A	840	1	8,9,10	1.64	1 (12%)	7,12,14	1.67	1 (14%)
1	SEP	A	841	1	8,9,10	1.62	1 (12%)	7,12,14	1.59	1 (14%)
1	TPO	A	844	1	8,10,11	0.81	0	10,14,16	0.97	0
1	SEP	B	841	1	8,9,10	1.58	1 (12%)	7,12,14	1.60	1 (14%)
1	TPO	B	844	1	8,10,11	0.79	0	10,14,16	0.96	0
1	SEP	B	840	1	8,9,10	1.67	2 (25%)	7,12,14	1.68	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	840	1	-	0/6/8/10	-
1	SEP	A	841	1	-	2/6/8/10	-
1	TPO	A	844	1	-	5/9/11/13	-
1	SEP	B	841	1	-	2/6/8/10	-
1	TPO	B	844	1	-	5/9/11/13	-
1	SEP	B	840	1	-	0/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	840	SEP	P-O1P	3.58	1.61	1.50
1	B	841	SEP	P-O1P	3.58	1.61	1.50
1	A	841	SEP	P-O1P	3.55	1.61	1.50
1	B	840	SEP	P-O1P	3.55	1.61	1.50
1	B	840	SEP	P-O3P	2.01	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	840	SEP	OG-CB-CA	3.95	111.99	108.14
1	A	840	SEP	OG-CB-CA	3.92	111.96	108.14
1	B	841	SEP	OG-CB-CA	3.48	111.53	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	841	SEP	OG-CB-CA	3.48	111.53	108.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	841	SEP	C-CA-CB-OG
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1
1	A	844	TPO	C-CA-CB-CG2
1	B	841	SEP	C-CA-CB-OG
1	B	844	TPO	N-CA-CB-CG2
1	B	844	TPO	N-CA-CB-OG1
1	B	844	TPO	C-CA-CB-CG2
1	A	841	SEP	N-CA-CB-OG
1	B	841	SEP	N-CA-CB-OG
1	A	844	TPO	CB-OG1-P-O2P
1	B	844	TPO	CB-OG1-P-O2P
1	A	844	TPO	O-C-CA-CB
1	B	844	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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
5	QUE	B	1	-	24,24,24	3.27	4 (16%)	36,36,36	1.67	5 (13%)
4	ADP	A	2101	3,2	28,29,29	1.36	4 (14%)	43,45,45	1.78	8 (18%)
4	ADP	B	2101	3,2	28,29,29	1.41	4 (14%)	43,45,45	1.80	8 (18%)
5	QUE	A	1	-	24,24,24	3.30	4 (16%)	36,36,36	1.71	7 (19%)

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
5	QUE	B	1	-	-	0/4/4/4	0/3/3/3
4	ADP	A	2101	3,2	-	1/16/32/32	0/3/3/3
4	ADP	B	2101	3,2	-	2/16/32/32	0/3/3/3
5	QUE	A	1	-	-	0/4/4/4	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	QUE	C10-C11	13.65	1.49	1.36
5	B	1	QUE	C10-C11	13.64	1.49	1.36
5	A	1	QUE	C18-C17	5.52	1.49	1.40
5	B	1	QUE	C18-C17	5.08	1.48	1.40
4	B	2101	ADP	C5-C4	4.80	1.47	1.39
4	A	2101	ADP	C5-C4	4.63	1.47	1.39
5	A	1	QUE	C3-C4	4.49	1.48	1.40
5	B	1	QUE	C3-C4	4.40	1.48	1.40
5	B	1	QUE	C3-C2	4.28	1.48	1.41
5	A	1	QUE	C3-C2	4.27	1.48	1.41
4	B	2101	ADP	C5-C6	2.70	1.48	1.41
4	A	2101	ADP	C5-C6	2.56	1.48	1.41
4	B	2101	ADP	C5-N7	-2.30	1.34	1.39
4	B	2101	ADP	C8-N7	2.26	1.36	1.31
4	A	2101	ADP	C8-N7	2.20	1.35	1.31
4	A	2101	ADP	C5-N7	-2.11	1.35	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2101	ADP	C5-C4-N3	-5.80	118.73	126.72
4	A	2101	ADP	C5-C4-N3	-5.68	118.89	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2101	ADP	N3-C4-N9	4.73	135.21	127.17
4	B	2101	ADP	N3-C4-N9	4.72	135.20	127.17
5	B	1	QUE	C11-C10-C9	-4.71	118.16	121.52
5	A	1	QUE	C11-C10-C9	-4.33	118.43	121.52
5	A	1	QUE	O12-C11-C14	4.29	116.88	110.87
5	A	1	QUE	C14-C11-C10	-4.19	121.84	128.44
5	B	1	QUE	O12-C11-C14	4.05	116.54	110.87
4	B	2101	ADP	C2-N3-C4	3.71	120.90	111.83
5	B	1	QUE	C14-C11-C10	-3.69	122.63	128.44
4	A	2101	ADP	C2-N3-C4	3.69	120.84	111.83
5	B	1	QUE	O12-C4-C5	3.48	120.77	115.83
4	A	2101	ADP	N3-C2-N1	-3.38	123.47	128.58
4	B	2101	ADP	N3-C2-N1	-3.30	123.58	128.58
5	A	1	QUE	O12-C4-C5	3.13	120.27	115.83
4	B	2101	ADP	C4-C5-N7	-3.08	107.06	110.58
4	A	2101	ADP	C4-C5-N7	-3.05	107.09	110.58
5	A	1	QUE	C19-C14-C11	-2.93	116.52	120.65
4	A	2101	ADP	C4-N9-C8	2.75	108.63	105.74
4	B	2101	ADP	C3'-C2'-C1'	2.46	106.12	101.46
4	B	2101	ADP	C4-N9-C8	2.44	108.30	105.74
4	B	2101	ADP	C5-N7-C8	2.28	107.03	103.45
4	A	2101	ADP	C5-N7-C8	2.26	107.00	103.45
4	A	2101	ADP	C2'-C1'-N9	-2.13	108.02	113.30
5	B	1	QUE	C19-C14-C11	-2.09	117.70	120.65
5	A	1	QUE	C1-C2-C3	-2.07	118.59	120.92
5	A	1	QUE	C15-C14-C19	2.03	121.60	119.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

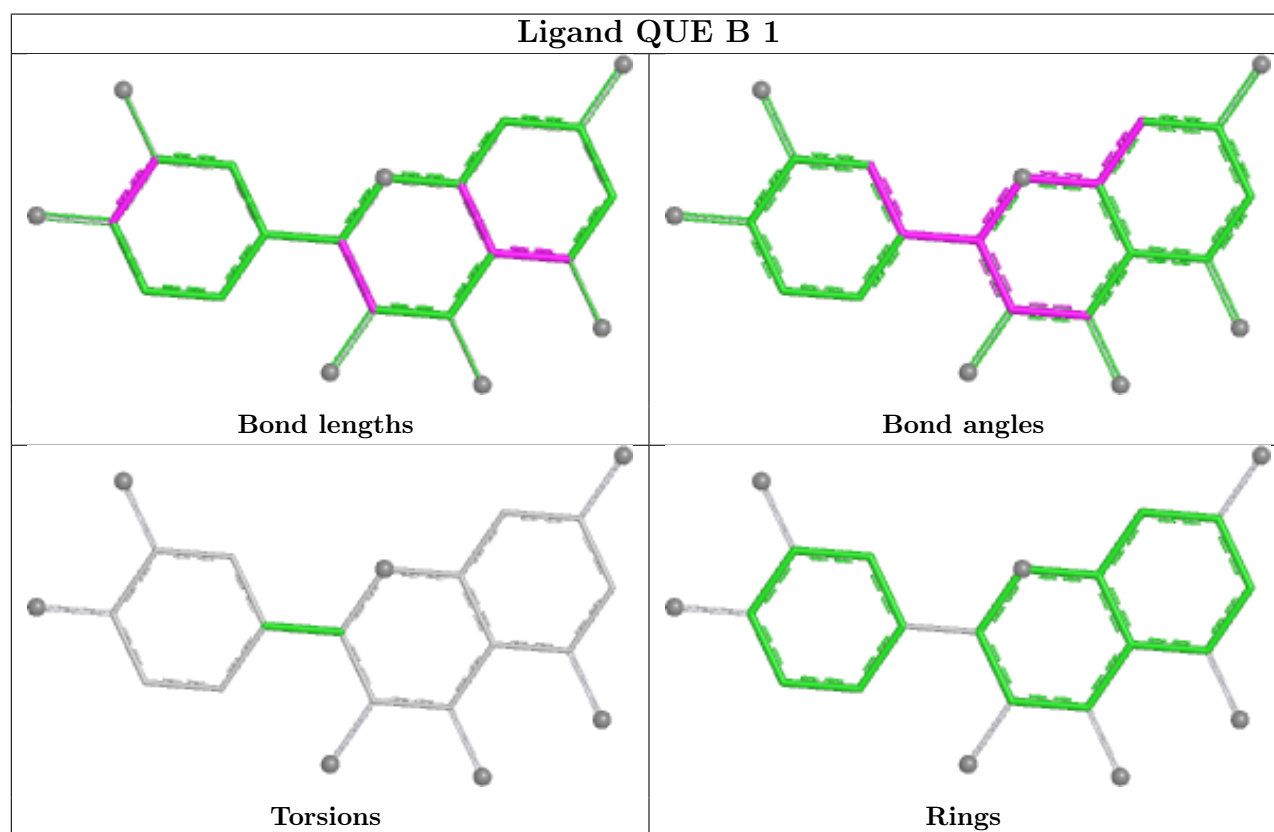
Mol	Chain	Res	Type	Atoms
4	A	2101	ADP	O4'-C4'-C5'-O5'
4	B	2101	ADP	O4'-C4'-C5'-O5'
4	B	2101	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

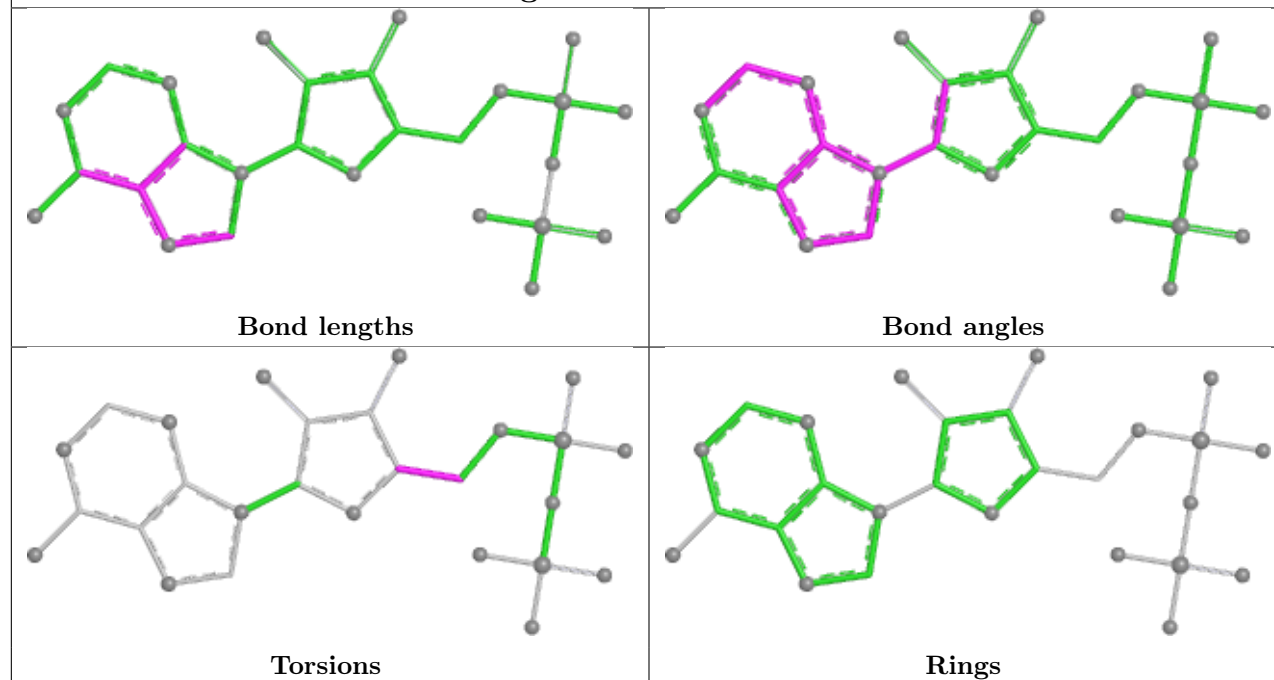
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	QUE	2	0

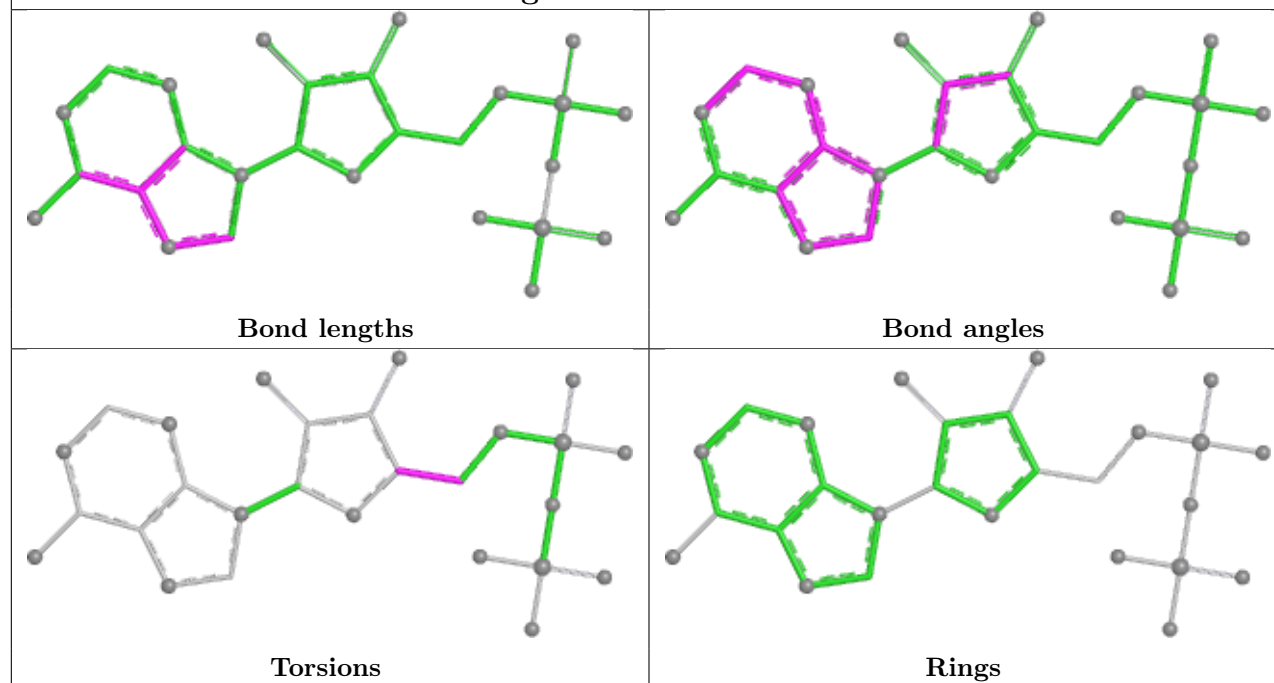
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

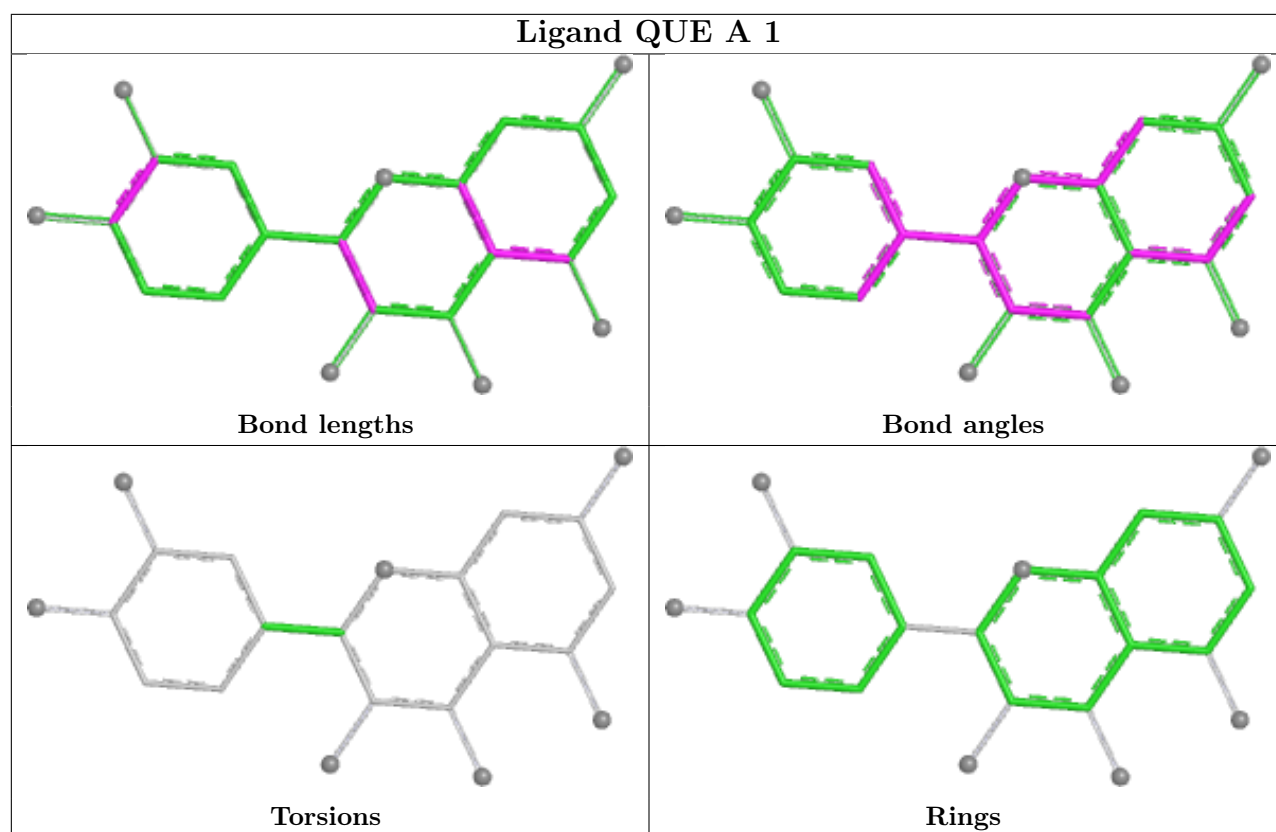


Ligand ADP A 2101



Ligand ADP B 2101





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	404/434 (93%)	0.34	31 (7%) 19 13	23, 53, 112, 155	0
1	B	399/434 (91%)	0.23	25 (6%) 26 17	20, 53, 107, 169	0
All	All	803/868 (92%)	0.29	56 (6%) 22 14	20, 53, 112, 169	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	852	THR	6.0
1	A	666	PHE	5.0
1	B	893	THR	5.0
1	A	836	ASP	4.6
1	A	758	SER	4.6
1	B	672	ASN	4.5
1	A	1003	ASP	4.5
1	A	709	CYS	4.2
1	A	714	MET	4.0
1	B	852	THR	3.7
1	A	843	ARG	3.6
1	B	1068	ASP	3.6
1	B	721	GLU	3.5
1	B	670	LEU	3.5
1	B	772	TYR	3.4
1	A	772	TYR	3.3
1	A	672	ASN	3.2
1	A	668	GLN	3.2
1	A	684	SER	3.2
1	A	839	GLN	3.1
1	A	711	ILE	2.9
1	A	1038	GLU	2.9
1	A	706	ILE	2.8
1	A	893	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1063	MET	2.8
1	A	1036	ASN	2.8
1	B	709	CYS	2.8
1	B	710	ASP	2.7
1	A	665	ASN	2.7
1	B	1035	ASP	2.6
1	A	818	GLY	2.6
1	A	707	ASP	2.5
1	A	842	PHE	2.5
1	B	1034	MET	2.5
1	A	671	LYS	2.4
1	A	817	THR	2.4
1	B	842	PHE	2.4
1	B	1022	SER	2.4
1	A	896	ARG	2.4
1	B	1101	GLU	2.3
1	A	1110	ARG	2.3
1	B	895	ARG	2.3
1	A	669	SER	2.3
1	B	832	CYS	2.3
1	B	1042	LYS	2.3
1	B	1063	MET	2.2
1	A	895	ARG	2.2
1	A	1037	LEU	2.2
1	B	1003	ASP	2.2
1	B	708	PHE	2.1
1	B	1001	ASN	2.1
1	B	1036	ASN	2.1
1	A	738	ASP	2.1
1	B	1026	THR	2.1
1	B	714	MET	2.0
1	B	1043	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	A	844	11/12	0.50	0.21	85,182,182,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	B	844	11/12	0.52	0.19	112,185,185,185	0
1	SEP	A	841	10/11	0.79	0.16	101,133,133,133	0
1	SEP	B	840	10/11	0.80	0.20	113,151,151,151	0
1	SEP	B	841	10/11	0.83	0.15	98,149,149,149	0
1	SEP	A	840	10/11	0.86	0.16	109,152,152,152	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

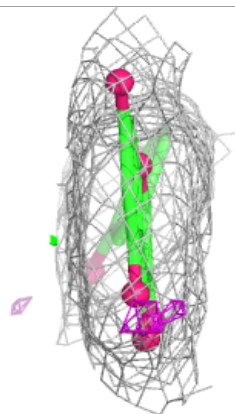
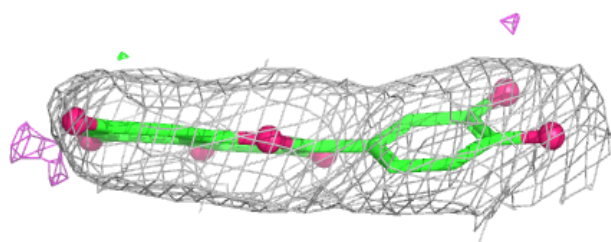
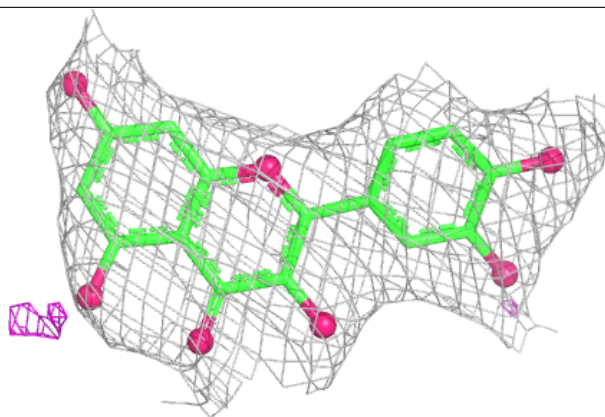
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	QUE	A	1	22/22	0.95	0.10	47,47,47,47	0
5	QUE	B	1	22/22	0.95	0.10	49,49,49,49	0
2	MG	A	2102	1/1	0.96	0.05	35,35,35,35	0
4	ADP	A	2101	27/27	0.96	0.09	51,51,51,51	0
4	ADP	B	2101	27/27	0.97	0.08	54,54,54,54	0
3	SR	B	2103	1/1	0.97	0.06	93,93,93,93	0
3	SR	A	2103	1/1	0.97	0.06	82,82,82,82	0
2	MG	B	2102	1/1	0.99	0.06	26,26,26,26	0

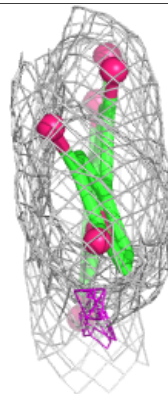
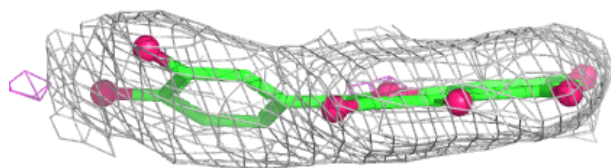
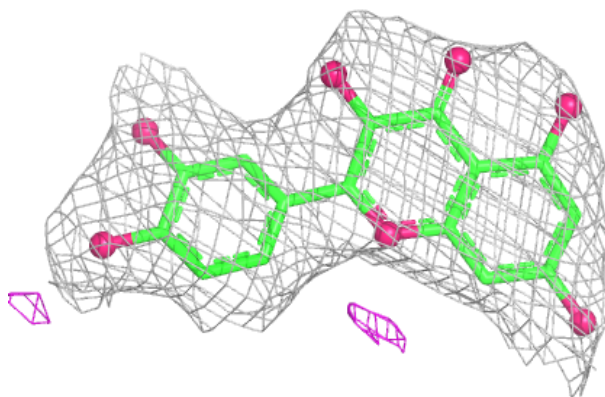
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QUE A 1:

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

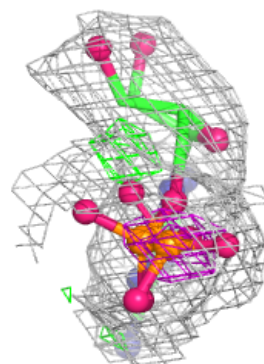
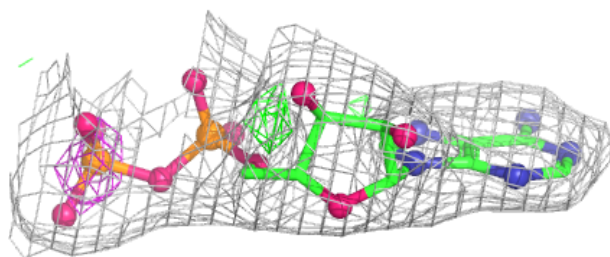
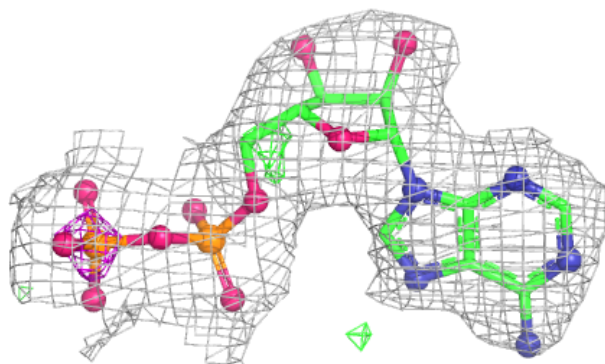
**Electron density around QUE B 1:**

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

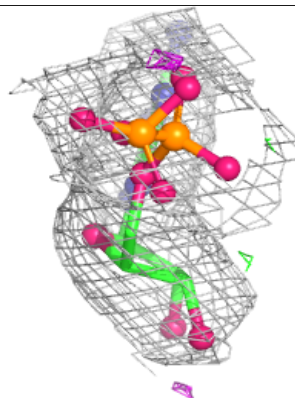
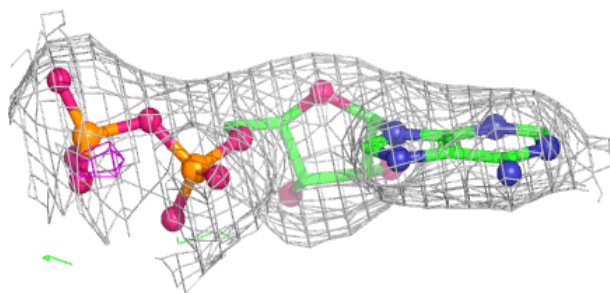
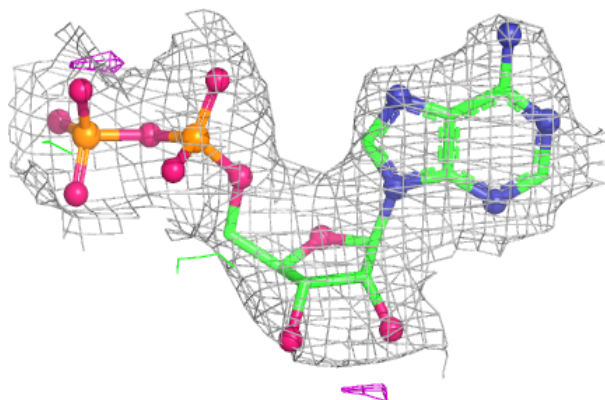


Electron density around ADP A 2101:

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

**Electron density around ADP B 2101:**

$2mF_o-DF_c$ (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.