



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:49 PM UTC

PDB ID : 8DSH / pdb_00008dsh
Title : Human NAMPT in complex with quercitrin and AMPcP
Authors : Ratia, K.; Xiong, R.; Shen, Z.; Thatcher, G.R.
Deposited on : 2022-07-22
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

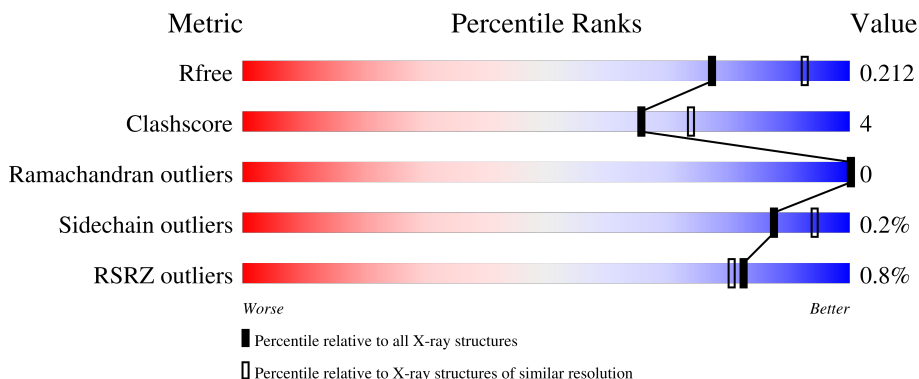
1 Overall quality at a glance

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	499	
1	B	499	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8254 atoms, of which 40 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.

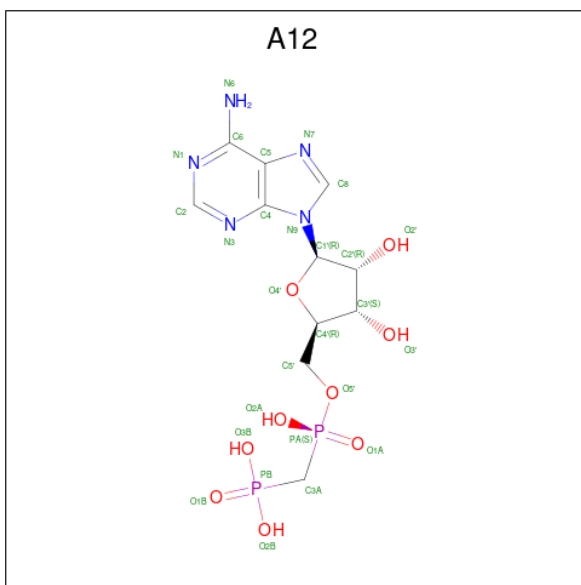
- Molecule 1 is a protein called Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	2	0
			3756	2416	617	716	7			
1	B	473	Total	C	N	O	S	0	1	0
			3786	2434	625	720	7			

There are 16 discrepancies between the modelled and reference sequences:

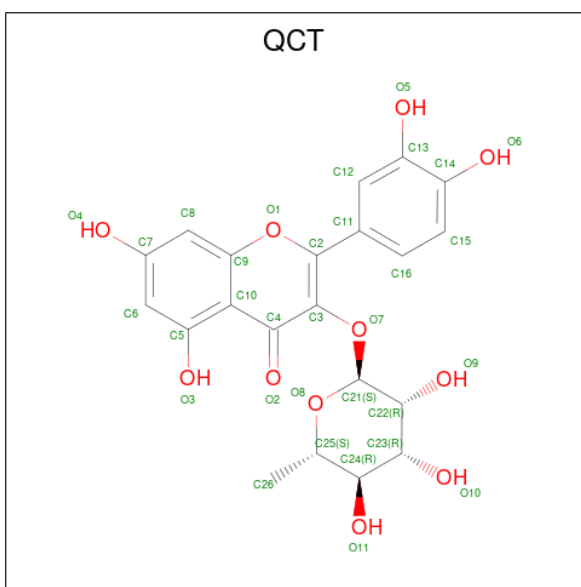
Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP P43490
A	493	GLU	-	expression tag	UNP P43490
A	494	HIS	-	expression tag	UNP P43490
A	495	HIS	-	expression tag	UNP P43490
A	496	HIS	-	expression tag	UNP P43490
A	497	HIS	-	expression tag	UNP P43490
A	498	HIS	-	expression tag	UNP P43490
A	499	HIS	-	expression tag	UNP P43490
B	492	LEU	-	expression tag	UNP P43490
B	493	GLU	-	expression tag	UNP P43490
B	494	HIS	-	expression tag	UNP P43490
B	495	HIS	-	expression tag	UNP P43490
B	496	HIS	-	expression tag	UNP P43490
B	497	HIS	-	expression tag	UNP P43490
B	498	HIS	-	expression tag	UNP P43490
B	499	HIS	-	expression tag	UNP P43490

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: A12) (formula: $C_{11}H_{17}N_5O_9P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 11	N 5	O 9	P 2	0	0
2	B	1	Total 27	C 11	N 5	O 9	P 2	0	0

- Molecule 3 is 2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxo-4H-chromen-3-yl 6-deoxy-alpha-L-mannopyranoside (CCD ID: QCT) (formula: C₂₁H₂₀O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			52	21	20	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			52	21	20	11		

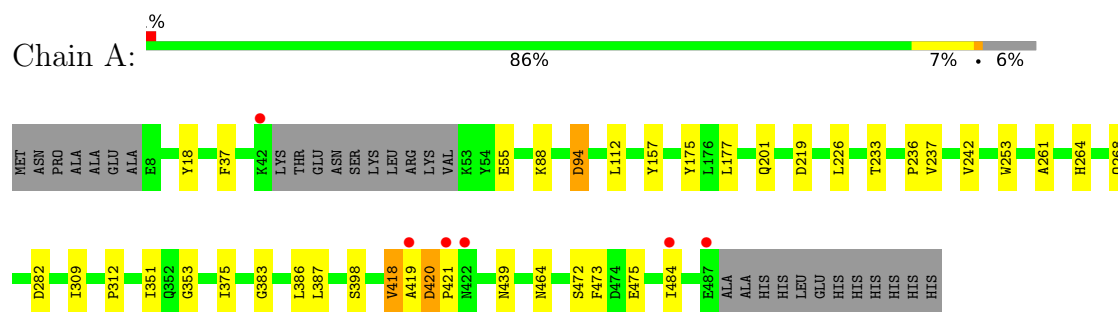
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	272	Total	O	0	0
			272	272		
4	B	282	Total	O	0	0
			282	282		

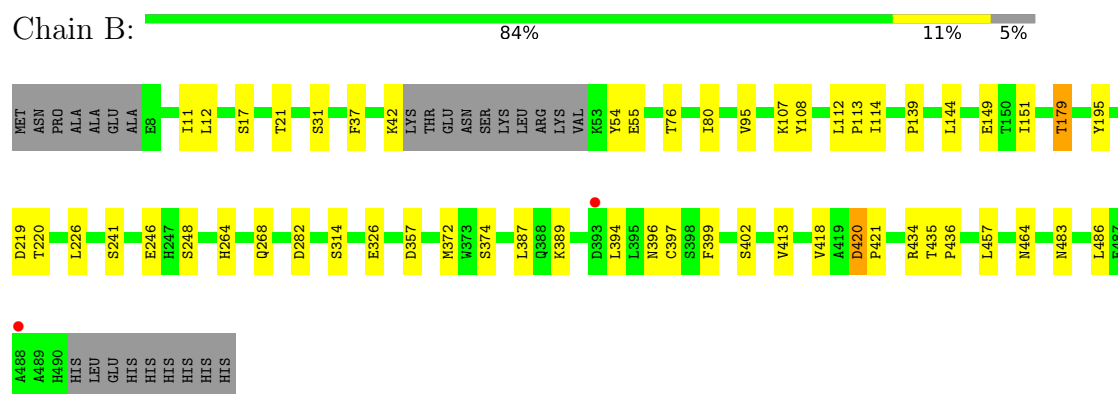
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.86Å 107.27Å 83.52Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	45.04 – 2.20 45.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.3 (45.04-2.20) 97.3 (45.04-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.165 , 0.211 0.168 , 0.212	Depositor DCC
R_{free} test set	2557 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8254	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: QCT, A12

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	0.62	0/3850	0.78	9/5220 (0.2%)
1	B	0.60	0/3878	0.76	6/5255 (0.1%)
All	All	0.61	0/7728	0.77	15/10475 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	ASP	CA-C-N	8.02	128.10	119.28
1	B	420	ASP	C-N-CA	8.02	128.10	119.28
1	A	237	VAL	CA-C-N	7.14	126.64	118.85
1	A	237	VAL	C-N-CA	7.14	126.64	118.85
1	B	387	LEU	N-CA-C	6.59	122.41	113.97
1	B	179	THR	N-CA-C	5.86	117.75	111.36
1	A	420	ASP	CA-C-N	5.85	125.22	118.85
1	A	420	ASP	C-N-CA	5.85	125.22	118.85
1	A	387	LEU	N-CA-C	5.72	121.29	113.97
1	A	157	TYR	CA-C-N	-5.62	113.24	119.19
1	A	157	TYR	C-N-CA	-5.62	113.24	119.19
1	A	386	LEU	N-CA-C	5.58	117.16	111.14
1	B	55	GLU	N-CA-C	5.54	117.40	111.36
1	A	55	GLU	N-CA-C	5.39	117.15	111.28
1	B	314	SER	N-CA-C	5.17	116.69	108.79

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	3756	0	3710	27	0
1	B	3786	0	3753	34	0
2	A	27	0	14	3	0
2	B	27	0	14	2	0
3	A	32	20	17	2	0
3	B	32	20	15	1	0
4	A	272	0	0	2	0
4	B	282	0	0	4	0
All	All	8214	40	7523	58	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 4.

All (58) 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:236:PRO:HD2	4:A:1407:HOH:O	1.79	0.81
1:A:177:LEU:HD22	1:A:484:ILE:HD11	1.67	0.75
1:B:21:THR:HG22	1:B:95:VAL:HG21	1.83	0.61
1:B:434:ARG:HG2	1:B:457:LEU:HD11	1.87	0.57
1:A:353:GLY:O	2:A:1301:A12:H1'	2.05	0.56
2:A:1301:A12:H5'2	2:A:1301:A12:H8	1.87	0.55
1:B:114:ILE:HD11	1:B:144:LEU:HG	1.88	0.54
1:B:326[A]:GLU:HG2	4:B:1651:HOH:O	2.08	0.54
1:B:483:ASN:HA	1:B:486:LEU:HD12	1.90	0.53
1:B:435:THR:HB	1:B:436:PRO:HD2	1.92	0.51
1:A:472:SER:OG	1:A:475:GLU:HG3	2.11	0.51
1:A:439:ASN:HB3	4:A:1587:HOH:O	2.11	0.51
1:B:37:PHE:CZ	1:B:397:CYS:HB3	2.46	0.50
1:B:107:LYS:HD3	1:B:108:TYR:CZ	2.47	0.49
1:B:42:LYS:HE3	1:B:396:ASN:OD1	2.13	0.49
1:B:246:GLU:OE2	1:B:248:SER:OG	2.31	0.49
1:B:76:THR:O	1:B:80:ILE:HG13	2.14	0.48
1:A:219:ASP:CG	1:B:17:SER:HB2	2.39	0.47
1:A:418:VAL:HG12	1:B:282:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLN:NE2	1:B:151:ILE:HD12	2.30	0.47
1:B:357:ASP:OD2	1:B:389:LYS:NZ	2.47	0.47
1:B:241:SER:HA	3:B:1502:QCT:O3	2.15	0.47
1:B:11:ILE:HG23	1:B:12:LEU:HD12	1.96	0.47
1:A:233:THR:CG2	1:A:473:PHE:HB3	2.45	0.47
1:A:419:ALA:HB3	4:B:1682:HOH:O	2.15	0.47
1:A:419:ALA:CB	4:B:1682:HOH:O	2.63	0.46
1:A:420:ASP:HA	1:A:421:PRO:HD3	1.80	0.46
1:A:312:PRO:HD2	1:A:351:ILE:O	2.15	0.46
1:A:383:GLY:HA3	2:A:1301:A12:O3'	2.16	0.46
1:B:435:THR:HB	1:B:436:PRO:CD	2.46	0.46
2:B:1501:A12:H8	2:B:1501:A12:H5'2	1.97	0.46
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.97	0.46
1:B:95:VAL:HG22	1:B:95:VAL:O	2.14	0.46
1:B:420:ASP:HA	1:B:421:PRO:HD2	1.66	0.45
1:A:88:LYS:HD2	1:A:94:ASP:OD2	2.16	0.45
1:B:113:PRO:HD2	1:B:144:LEU:CD2	2.47	0.45
1:B:195:TYR:CG	1:B:220:THR:HG23	2.52	0.44
1:B:54:TYR:CE2	1:B:394:LEU:HD11	2.53	0.44
1:B:112:LEU:O	1:B:464:ASN:HA	2.17	0.44
1:B:402:SER:HA	1:B:413:VAL:O	2.18	0.43
1:B:372:MET:HG3	4:B:1872:HOH:O	2.17	0.43
1:A:309:ILE:HG22	1:A:351:ILE:HG22	2.01	0.43
1:B:264:HIS:O	1:B:268:GLN:HG2	2.19	0.43
1:B:149:GLU:HG3	1:B:399:PHE:CD1	2.54	0.42
1:B:54:TYR:HE2	1:B:394:LEU:HD11	1.84	0.42
1:A:253:TRP:CG	1:A:261:ALA:HB2	2.54	0.42
1:A:112:LEU:O	1:A:464:ASN:HA	2.20	0.42
1:A:226:LEU:C	1:A:226:LEU:HD23	2.45	0.42
1:B:179:THR:HB	1:B:374:SER:HA	2.02	0.41
1:A:309:ILE:HD11	3:A:1302:QCT:H262	2.01	0.41
1:A:398:SER:OG	2:B:1501:A12:O1B	2.28	0.41
1:A:37:PHE:HA	1:A:398:SER:O	2.21	0.41
1:A:242:VAL:HG22	3:A:1302:QCT:C6	2.50	0.41
1:A:18:TYR:HD1	1:B:219:ASP:OD2	2.03	0.41
1:A:264:HIS:O	1:A:268:GLN:HG2	2.21	0.41
1:B:226:LEU:C	1:B:226:LEU:HD23	2.46	0.41
1:B:31:SER:O	1:B:139:PRO:HA	2.21	0.40
1:A:282:ASP:HA	1:B:418:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	468/499 (94%)	459 (98%)	9 (2%)	0	100	100
1	B	470/499 (94%)	459 (98%)	11 (2%)	0	100	100
All	All	938/998 (94%)	918 (98%)	20 (2%)	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	411/438 (94%)	409 (100%)	2 (0%)	81	90
1	B	415/438 (95%)	415 (100%)	0	100	100
All	All	826/876 (94%)	824 (100%)	2 (0%)	87	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	418	VAL

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	201	GLN

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Mol	Chain	Res	Type
1	A	214	ASN
1	A	247	HIS
1	A	359	ASN
1	A	396	ASN
1	B	29	ASN
1	B	154	GLN
1	B	168	GLN
1	B	214	ASN
1	B	268	GLN
1	B	407	ASN
1	B	412	ASN
1	B	439	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](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	QCT	B	1502	-	35,35,35	2.34	14 (40%)	53,53,53	2.66	22 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A12	B	1501	-	26,29,29	1.95	8 (30%)	40,45,45	1.84	10 (25%)
2	A12	A	1301	-	26,29,29	2.12	10 (38%)	40,45,45	1.97	11 (27%)
3	QCT	A	1302	-	35,35,35	2.15	11 (31%)	53,53,53	2.92	23 (43%)

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
3	QCT	B	1502	-	-	1/8/28/28	0/4/4/4
2	A12	B	1501	-	-	2/16/32/32	0/3/3/3
2	A12	A	1301	-	-	2/16/32/32	0/3/3/3
3	QCT	A	1302	-	-	1/8/28/28	0/4/4/4

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1502	QCT	C11-C2	8.80	1.60	1.47
3	A	1302	QCT	O1-C2	5.97	1.44	1.37
2	B	1501	A12	PB-O1B	5.06	1.60	1.50
2	A	1301	A12	PB-O1B	4.83	1.60	1.50
2	A	1301	A12	C5-C4	4.45	1.47	1.39
2	B	1501	A12	C5-C4	4.44	1.47	1.39
3	A	1302	QCT	C14-C13	4.37	1.47	1.40
3	A	1302	QCT	C11-C2	4.16	1.53	1.47
3	A	1302	QCT	C22-C23	3.96	1.62	1.52
2	A	1301	A12	PA-O1A	3.83	1.60	1.51
2	A	1301	A12	PA-O2A	-3.68	1.47	1.56
2	B	1501	A12	PB-O2B	-3.64	1.46	1.55
3	A	1302	QCT	O8-C21	-3.62	1.32	1.41
2	A	1301	A12	PB-O2B	-3.36	1.47	1.55
3	B	1502	QCT	O8-C25	-3.25	1.37	1.44
3	B	1502	QCT	C14-C13	3.18	1.45	1.40
3	A	1302	QCT	C6-C7	2.98	1.43	1.39
3	B	1502	QCT	O1-C2	2.97	1.41	1.37
3	B	1502	QCT	O9-C22	-2.64	1.36	1.43
3	A	1302	QCT	C6-C5	2.60	1.42	1.38
2	B	1501	A12	C5-N7	-2.60	1.34	1.39
2	A	1301	A12	C5-N7	-2.59	1.34	1.39
2	A	1301	A12	C5-C6	2.55	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	A12	C5-C6	2.40	1.47	1.41
3	B	1502	QCT	C3-C4	2.39	1.54	1.47
2	B	1501	A12	C4-N9	-2.37	1.32	1.37
2	A	1301	A12	C4-N9	-2.35	1.32	1.37
3	B	1502	QCT	O6-C14	-2.33	1.31	1.36
2	A	1301	A12	PB-O3B	2.31	1.60	1.55
3	B	1502	QCT	O5-C13	-2.29	1.31	1.36
3	B	1502	QCT	C22-C23	2.26	1.58	1.52
3	A	1302	QCT	C26-C25	-2.25	1.46	1.51
2	B	1501	A12	PB-O3B	2.25	1.60	1.55
3	B	1502	QCT	C12-C13	2.24	1.42	1.38
3	A	1302	QCT	O9-C22	-2.22	1.37	1.43
3	A	1302	QCT	O5-C13	-2.20	1.31	1.36
3	B	1502	QCT	O2-C4	-2.20	1.18	1.23
3	B	1502	QCT	O10-C23	-2.20	1.37	1.43
3	B	1502	QCT	C10-C5	2.15	1.44	1.41
2	A	1301	A12	C8-N7	2.02	1.35	1.31
3	A	1302	QCT	C12-C13	2.02	1.41	1.38
3	B	1502	QCT	O11-C24	-2.01	1.38	1.43
2	B	1501	A12	C8-N7	2.01	1.35	1.31

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1302	QCT	O7-C3-C4	-7.49	111.38	118.24
3	B	1502	QCT	C11-C12-C13	7.16	126.33	120.09
3	A	1302	QCT	C23-C24-C25	-6.71	99.61	109.81
3	B	1502	QCT	C16-C11-C12	-6.27	112.00	119.25
3	A	1302	QCT	O7-C3-C2	5.95	127.40	119.80
3	A	1302	QCT	C11-C12-C13	5.68	125.04	120.09
2	A	1301	A12	C5-C4-N3	-5.54	119.08	126.72
3	A	1302	QCT	O8-C25-C24	5.47	119.39	109.55
2	B	1501	A12	C5-C4-N3	-5.33	119.38	126.72
3	A	1302	QCT	C21-O7-C3	5.32	127.63	115.60
3	B	1502	QCT	O1-C9-C8	5.12	123.08	115.83
3	A	1302	QCT	O1-C9-C8	5.00	122.92	115.83
3	B	1502	QCT	C12-C11-C2	4.87	127.53	120.65
3	A	1302	QCT	C15-C14-C13	-4.78	114.55	119.66
3	B	1502	QCT	C21-O7-C3	4.78	126.42	115.60
3	B	1502	QCT	C15-C14-C13	-4.76	114.58	119.66
3	A	1302	QCT	C16-C11-C12	-4.65	113.87	119.25
2	A	1301	A12	N3-C4-N9	4.59	134.97	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	A12	N3-C4-N9	4.36	134.58	127.17
3	B	1502	QCT	O7-C3-C4	-4.24	114.35	118.24
3	B	1502	QCT	O7-C3-C2	4.19	125.16	119.80
3	A	1302	QCT	C12-C11-C2	4.17	126.55	120.65
2	A	1301	A12	C2'-C1'-N9	-4.16	102.98	113.30
3	A	1302	QCT	C5-C10-C9	4.14	121.36	117.41
3	B	1502	QCT	C5-C10-C9	4.06	121.29	117.41
3	B	1502	QCT	C9-O1-C2	4.03	126.84	120.67
3	B	1502	QCT	C15-C16-C11	3.75	124.81	120.80
2	B	1501	A12	C2'-C1'-N9	-3.67	104.17	113.30
2	B	1501	A12	C2-N3-C4	3.48	120.34	111.83
2	A	1301	A12	C2-N3-C4	3.46	120.28	111.83
2	A	1301	A12	C4-C5-N7	-3.42	106.67	110.58
2	B	1501	A12	N3-C2-N1	-3.42	123.41	128.58
3	B	1502	QCT	O1-C2-C11	3.41	115.64	110.87
2	B	1501	A12	C4-C5-N7	-3.27	106.84	110.58
3	A	1302	QCT	C21-O8-C25	3.27	119.21	113.63
3	A	1302	QCT	C15-C16-C11	3.26	124.29	120.80
3	B	1502	QCT	C21-O8-C25	3.25	119.17	113.63
2	A	1301	A12	C4-N9-C8	3.21	109.11	105.74
2	A	1301	A12	N3-C2-N1	-3.09	123.91	128.58
3	B	1502	QCT	C16-C15-C14	2.99	123.48	120.50
2	B	1501	A12	C4-N9-C8	2.94	108.82	105.74
3	A	1302	QCT	O3-C5-C10	-2.93	115.71	121.14
3	B	1502	QCT	O8-C25-C26	2.88	113.14	106.74
3	B	1502	QCT	O7-C21-C22	2.87	115.83	107.49
3	A	1302	QCT	O1-C9-C10	-2.84	118.40	121.19
2	A	1301	A12	C5-N7-C8	2.56	107.47	103.45
3	B	1502	QCT	O1-C2-C3	-2.49	117.30	120.44
3	A	1302	QCT	O8-C25-C26	-2.49	101.21	106.74
3	A	1302	QCT	O7-C21-C22	2.49	114.71	107.49
3	A	1302	QCT	C5-C10-C4	-2.38	117.93	121.45
2	B	1501	A12	C5-N7-C8	2.37	107.18	103.45
3	A	1302	QCT	C9-O1-C2	2.33	124.25	120.67
2	B	1501	A12	C2-N1-C6	2.33	122.56	118.73
3	B	1502	QCT	O6-C14-C15	2.29	125.52	119.36
3	B	1502	QCT	C26-C25-C24	-2.26	108.94	113.08
3	B	1502	QCT	C8-C9-C10	-2.26	117.85	121.79
3	A	1302	QCT	O3-C5-C6	2.23	125.47	119.45
2	A	1301	A12	N9-C8-N7	-2.21	110.79	113.94
3	A	1302	QCT	O6-C14-C15	2.20	125.28	119.36
3	A	1302	QCT	C16-C15-C14	2.19	122.69	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	QCT	O1-C9-C10	-2.17	119.06	121.19
2	B	1501	A12	C6-C5-N7	2.14	136.22	132.09
3	B	1502	QCT	C9-C8-C7	2.14	122.35	118.98
3	A	1302	QCT	C9-C8-C7	2.10	122.29	118.98
2	A	1301	A12	C6-C5-N7	2.06	136.06	132.09
2	A	1301	A12	C2-N1-C6	2.04	122.07	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

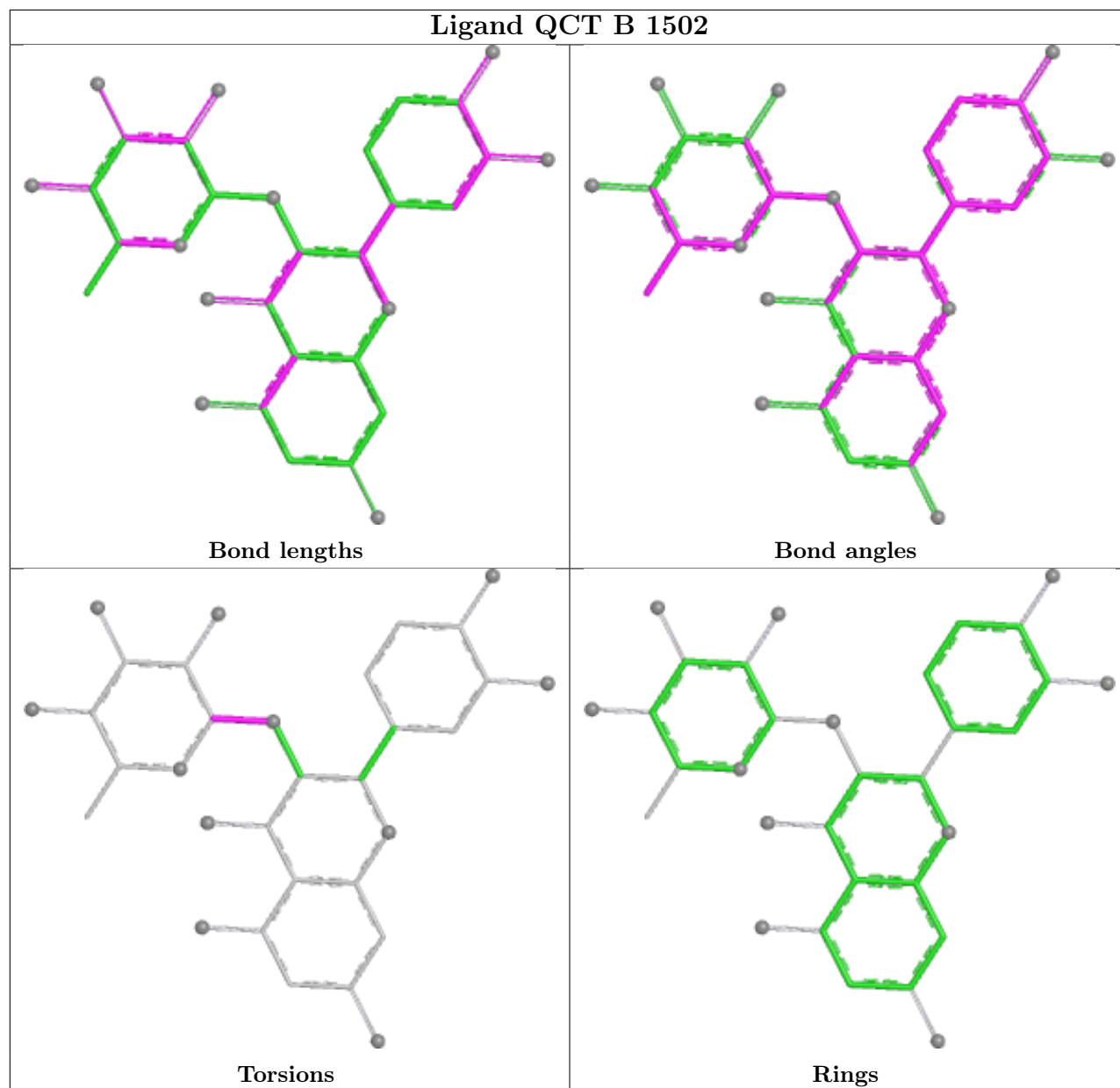
Mol	Chain	Res	Type	Atoms
2	B	1501	A12	PA-C3A-PB-O1B
3	A	1302	QCT	O8-C21-O7-C3
3	B	1502	QCT	O8-C21-O7-C3
2	A	1301	A12	PB-C3A-PA-O2A
2	B	1501	A12	PA-C3A-PB-O2B
2	A	1301	A12	PB-C3A-PA-O1A

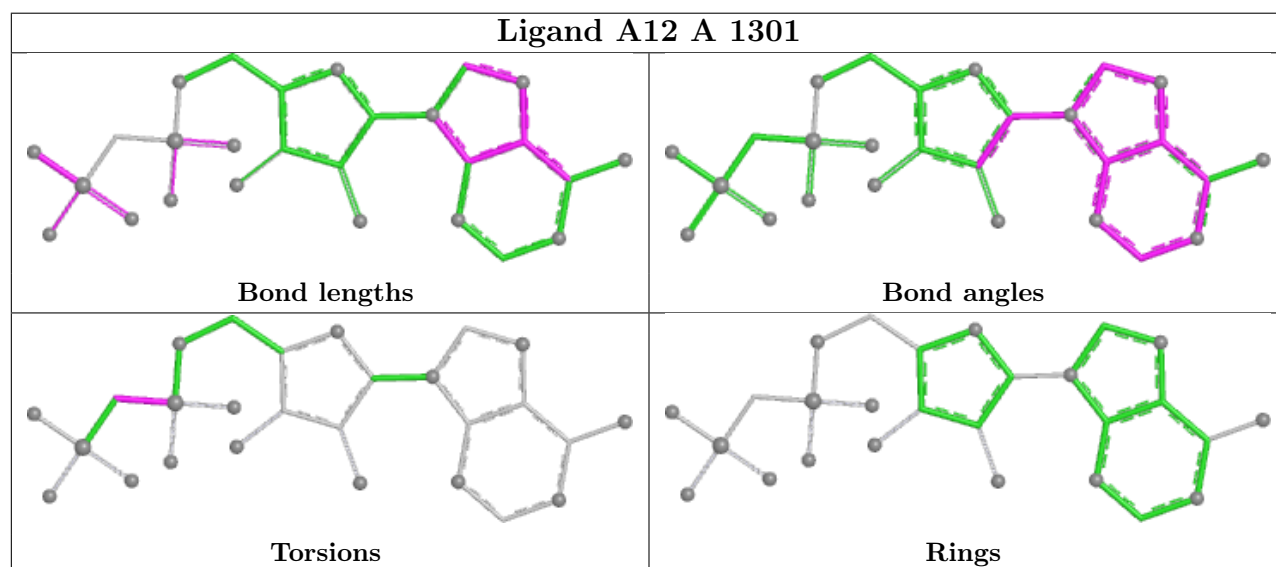
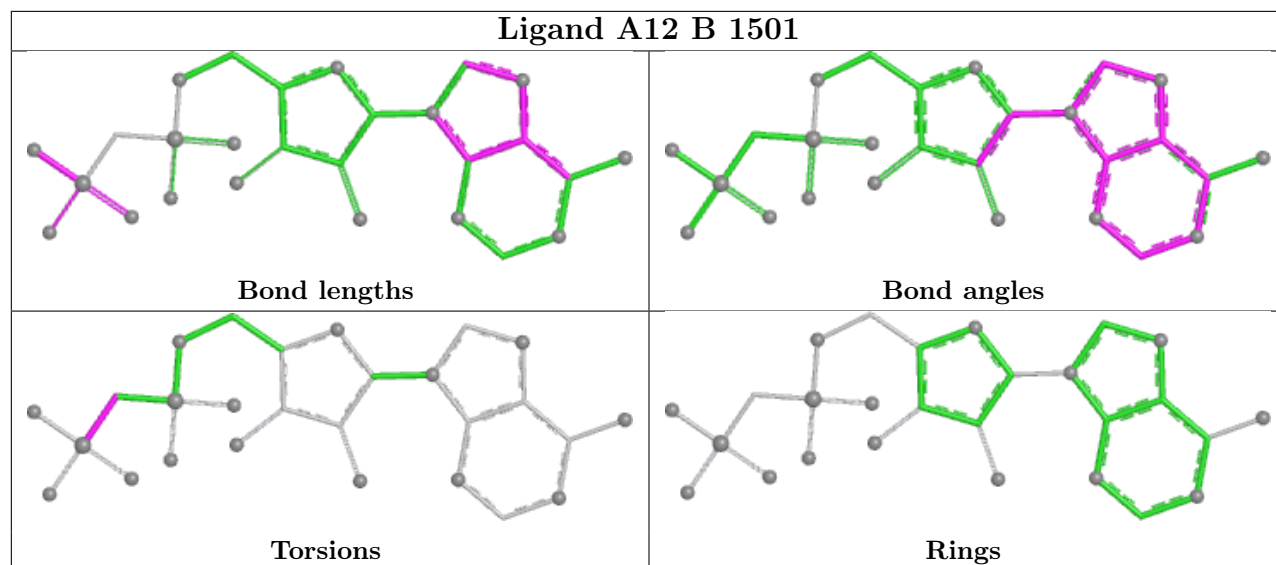
There are no ring outliers.

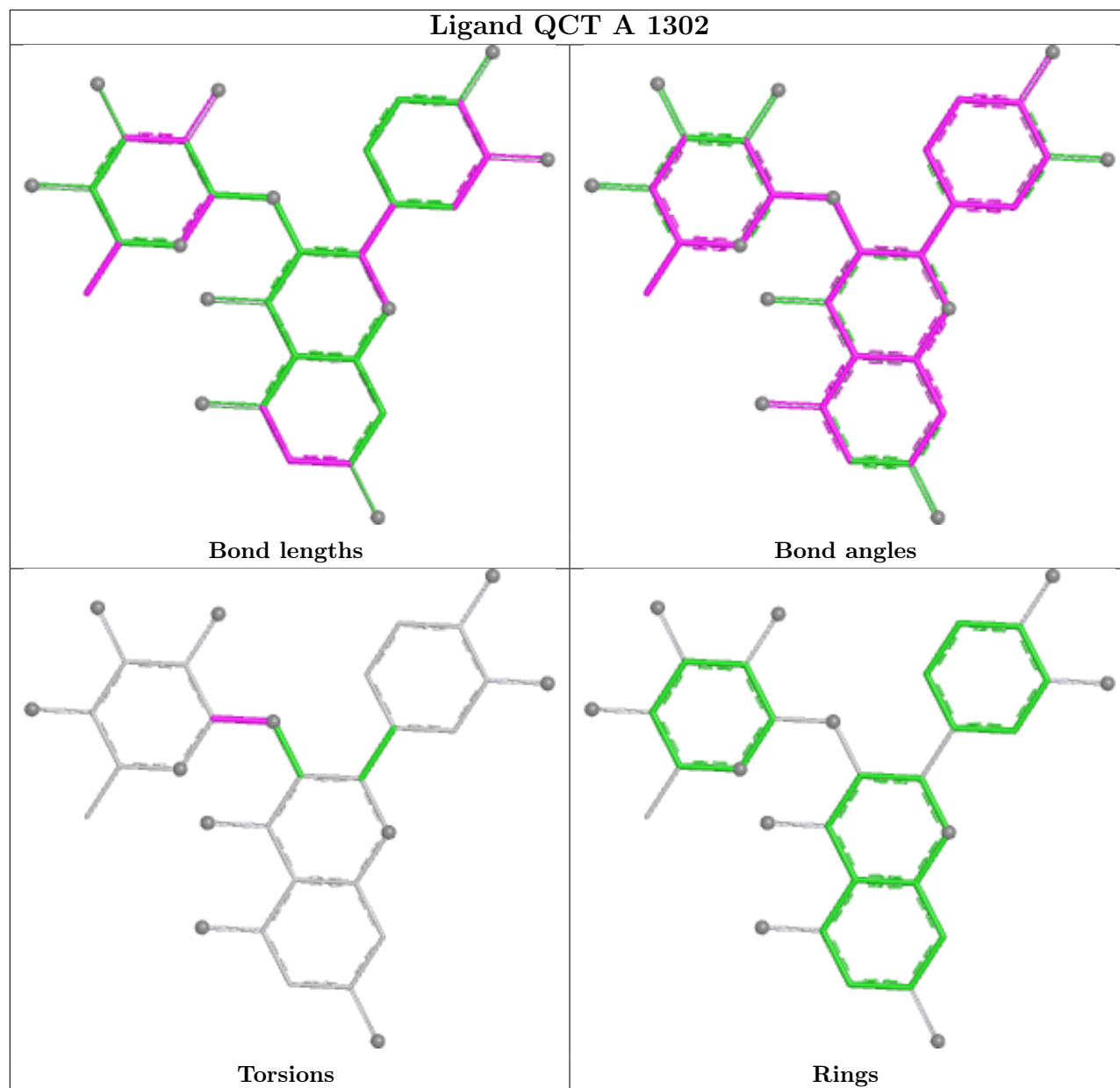
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1502	QCT	1	0
2	B	1501	A12	2	0
2	A	1301	A12	3	0
3	A	1302	QCT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	470/499 (94%)	-0.39	6 (1%) 75 73	16, 26, 41, 60	2 (0%)
1	B	473/499 (94%)	-0.41	2 (0%) 88 87	16, 26, 42, 74	1 (0%)
All	All	943/998 (94%)	-0.40	8 (0%) 82 80	16, 26, 41, 74	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	ALA	4.2
1	A	421	PRO	4.2
1	A	419	ALA	2.7
1	A	422	ASN	2.7
1	A	484	ILE	2.2
1	A	487	GLU	2.0
1	B	393	ASP	2.0
1	A	42	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.

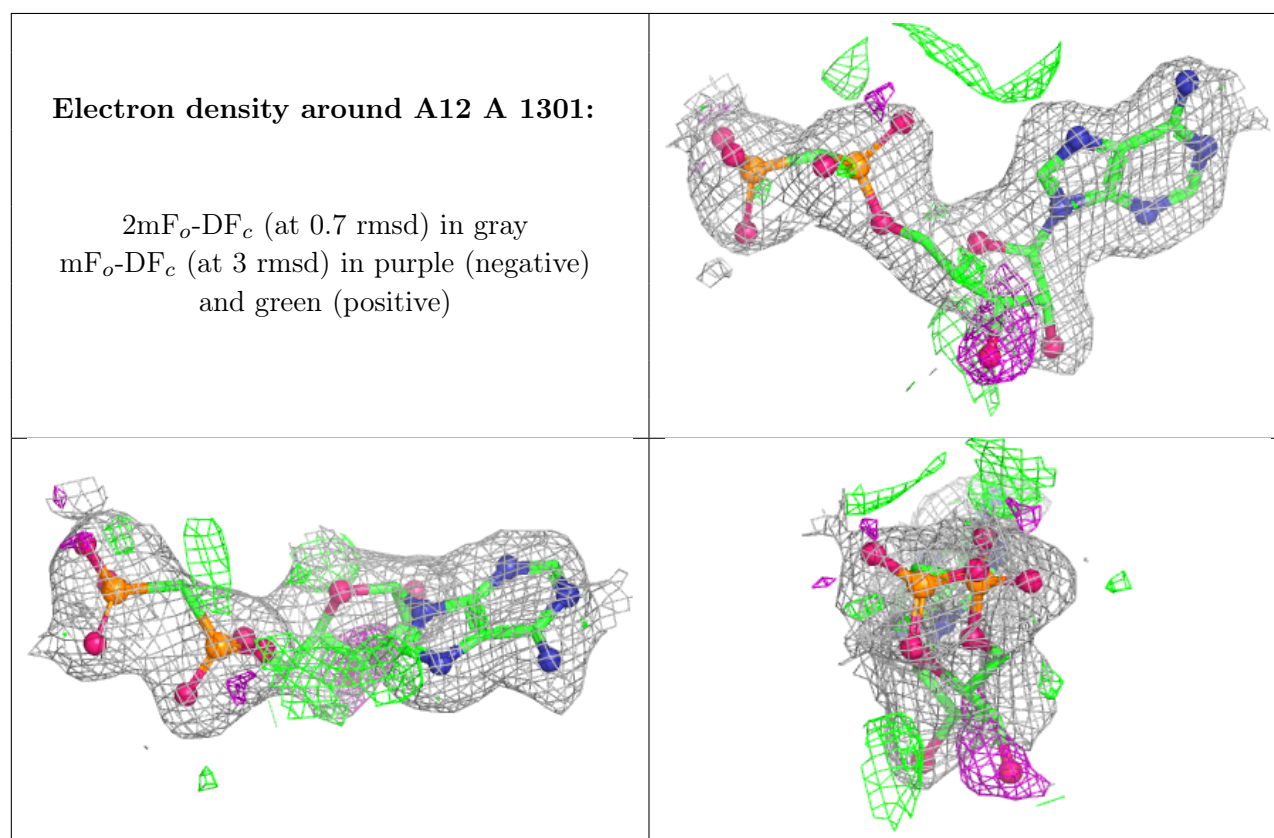
6.4 Ligands [i](#)

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.

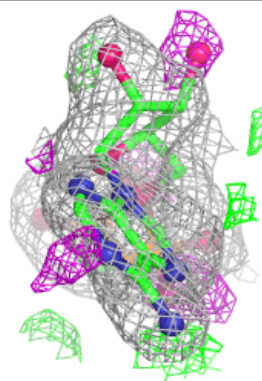
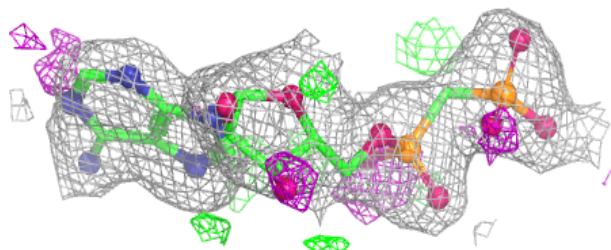
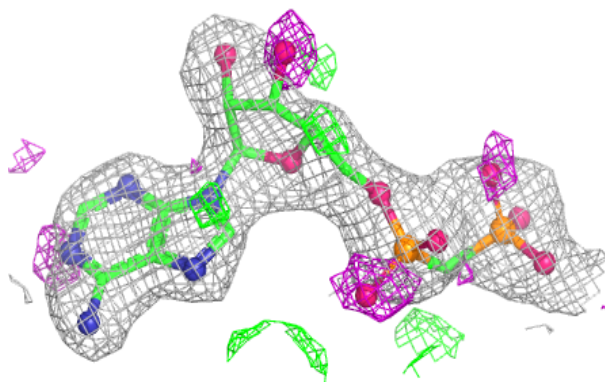
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A12	A	1301	27/27	0.89	0.11	27,39,49,51	0
2	A12	B	1501	27/27	0.89	0.12	28,39,52,57	0
3	QCT	B	1502	32/32	0.91	0.08	26,36,54,67	0
3	QCT	A	1302	32/32	0.92	0.07	24,35,55,60	0

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.



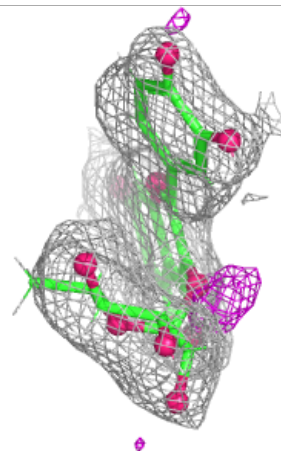
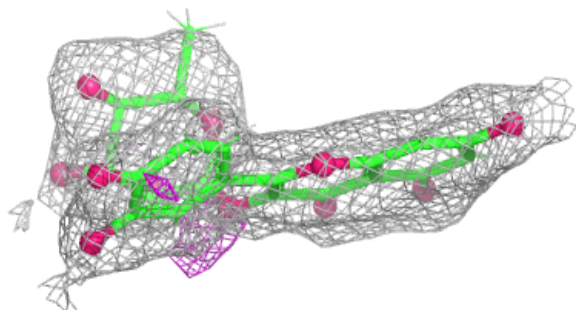
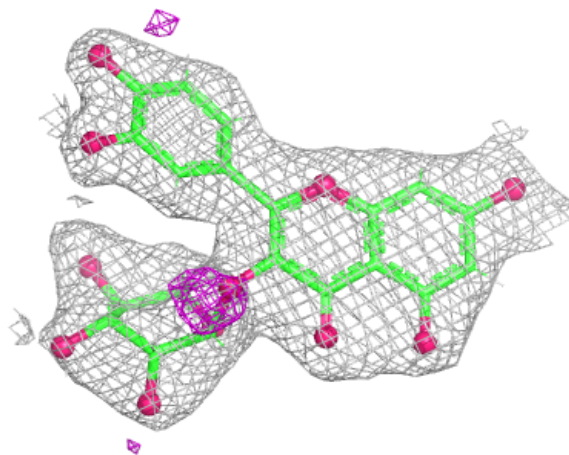
Electron density around A12 B 1501:

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



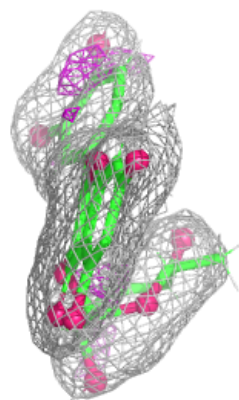
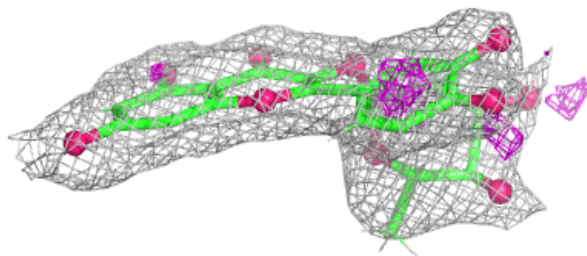
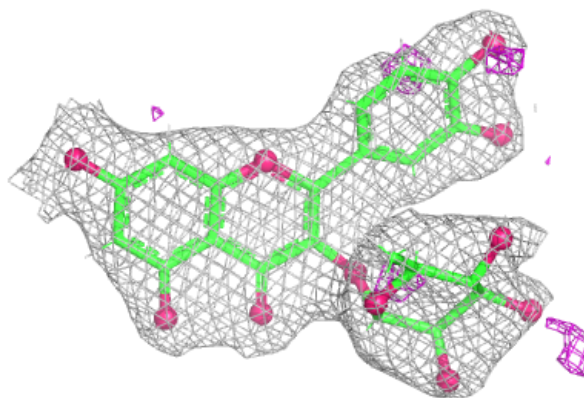
Electron density around QCT B 1502:

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



Electron density around QCT A 1302:

$2mF_o-DF_c$ (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.