



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:13 am BST

PDB ID : 6QAS
Title : Crystal structure of ULK1 in complexed with PF-03814735
Authors : Chaikuad, A.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Knapp, S.;
Structural Genomics Consortium; Structural Genomics Consortium (SGC)
Deposited on : 2018-12-19
Resolution : 1.75 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 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 : 2.11
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) : 2.11

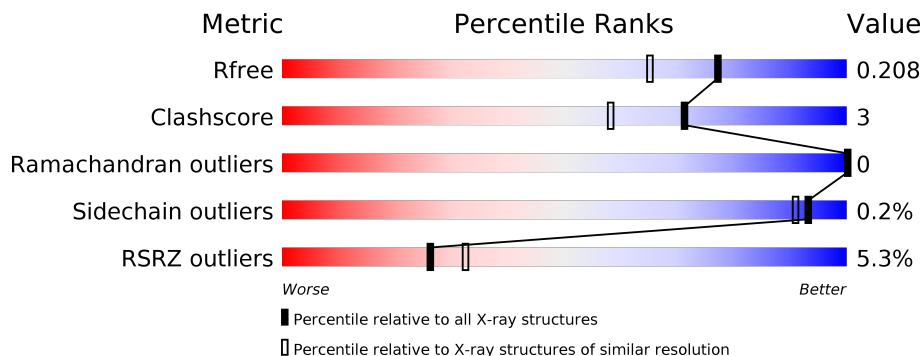
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 on 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	287	
1	B	287	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5104 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 ULK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	274	Total	C	N	O	P	S	0	6	0
			2218	1415	389	396	2	16			
1	B	273	Total	C	N	O	P	S	0	8	0
			2229	1421	391	398	2	17			

There are 12 discrepancies between the modelled and reference sequences:

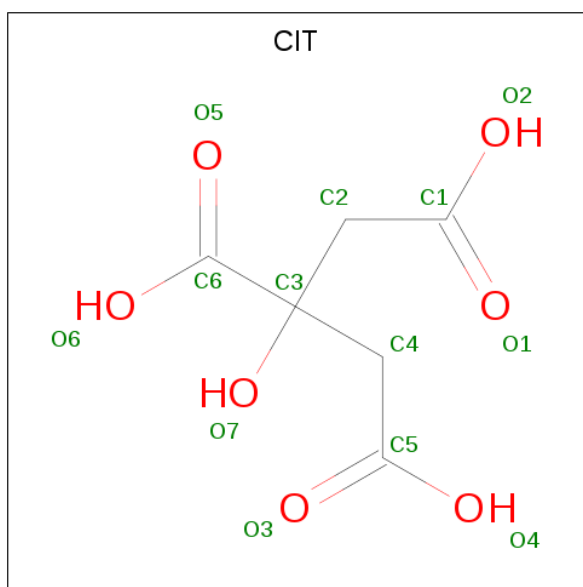
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O75385
A	-2	GLY	-	expression tag	UNP O75385
A	-1	GLY	-	expression tag	UNP O75385
A	0	SER	-	expression tag	UNP O75385
A	37	ALA	GLU	conflict	UNP O75385
A	38	ALA	LYS	conflict	UNP O75385
B	-3	GLY	-	expression tag	UNP O75385
B	-2	GLY	-	expression tag	UNP O75385
B	-1	GLY	-	expression tag	UNP O75385
B	0	SER	-	expression tag	UNP O75385
B	37	ALA	GLU	conflict	UNP O75385
B	38	ALA	LYS	conflict	UNP O75385

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



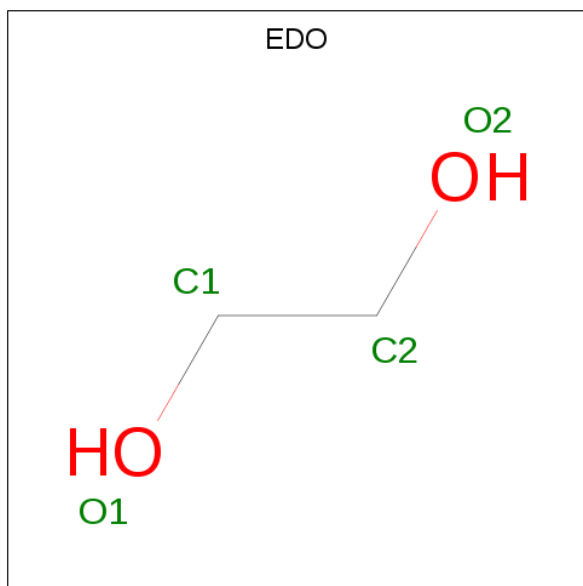
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



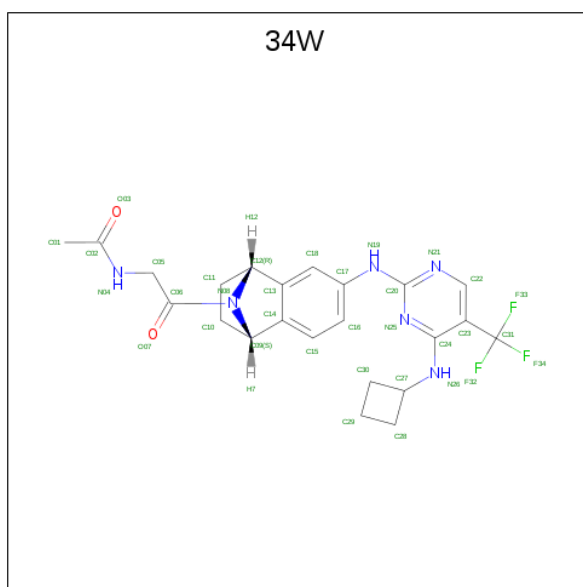
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is N-{2-[(1S,4R)-6-[[4-(cyclobutylamino)-5-(trifluoromethyl)pyrimidin-2-yl]amino]o}-1,2,3,4-tetrahydro-1,4-epiminonaphthalen-9-yl]-2-oxoethyl}acetamide (three-letter code: 34W) (formula: C₂₃H₂₅F₃N₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			34	23	3	6	2		
6	B	1	Total	C	F	N	O	0	0
			34	23	3	6	2		
6	B	1	Total	C	F	N	O	0	0
			34	23	3	6	2		

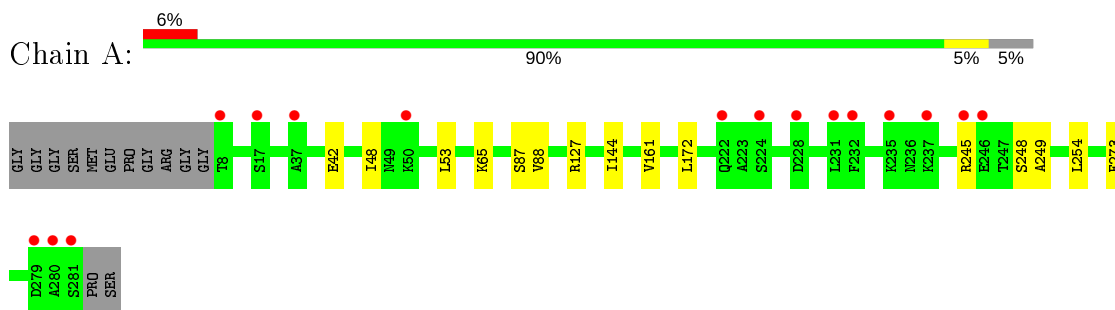
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	205	Total	O	0	0
			205	205		
7	B	180	Total	O	0	0
			180	180		

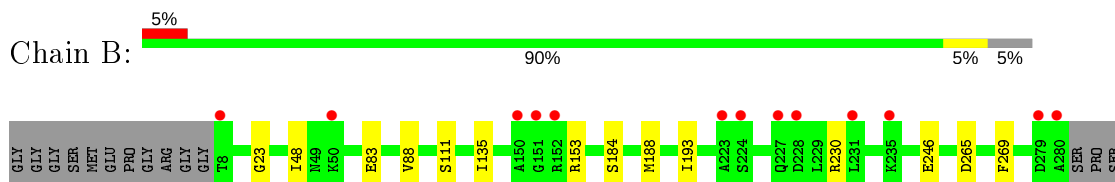
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Serine/threonine-protein kinase ULK1



- Molecule 1: Serine/threonine-protein kinase ULK1



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.24Å 74.24Å 222.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.47 – 1.75 47.47 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.47-1.75) 100.0 (47.47-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.170 , 0.197 0.181 , 0.208	Depositor DCC
R_{free} test set	3177 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtrriage
Anisotropy	0.140	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5104	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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, SEP, TPO, EDO, 34W, SO4, CIT

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	0.77	1/2259 (0.0%)	0.78	0/3040
1	B	0.79	0/2267	0.77	0/3049
All	All	0.78	1/4526 (0.0%)	0.77	0/6089

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	GLU	CD-OE2	-5.12	1.20	1.25

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	2218	0	2255	10	0
1	B	2229	0	2266	15	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	13	0	5	0	0
3	B	13	0	5	0	0
4	A	36	0	48	3	0
4	B	30	0	40	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	28	0	41	4	0
5	B	20	0	30	4	0
6	A	34	0	25	2	0
6	B	68	0	50	6	0
7	A	205	0	0	3	0
7	B	180	0	0	4	0
All	All	5104	0	4765	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 3.

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)
4:A:309:GOL:H2	7:A:537:HOH:O	1.95	0.67
6:B:316:34W:H15	6:B:316:34W:N25	2.12	0.65
1:B:23:GLY:HA3	6:B:315:34W:C29	2.30	0.61
5:A:314:EDO:H11	7:A:447:HOH:O	2.00	0.61
1:A:248:SER:HA	4:A:310:GOL:H11	1.82	0.61
1:A:48:ILE:HD11	1:A:88[B]:VAL:HG12	1.86	0.58
6:A:318:34W:H14	6:A:318:34W:N25	2.22	0.55
1:B:111:SER:CB	5:B:311:EDO:H21	2.37	0.55
1:B:111:SER:OG	5:B:311:EDO:H21	2.09	0.52
6:B:315:34W:H14	6:B:315:34W:N25	2.25	0.51
1:A:245:ARG:NH1	7:A:408:HOH:O	2.44	0.50
1:B:230:ARG:NE	7:B:406:HOH:O	2.43	0.49
1:B:188[A]:MET:HE2	1:B:193:ILE:HB	1.94	0.49
6:B:316:34W:C18	6:B:316:34W:N25	2.75	0.48
1:A:65:LYS:HE2	5:A:317:EDO:O2	2.13	0.47
1:A:53:LEU:HB3	5:A:311:EDO:H11	1.96	0.47
1:B:184:SER:O	1:B:188[A]:MET:HG3	2.15	0.47
1:A:249:ALA:H	4:A:310:GOL:H11	1.80	0.46
1:B:265:ASP:OD1	7:B:401:HOH:O	2.20	0.46
1:B:153:ARG:HB3	6:B:316:34W:H5	1.97	0.45
1:B:111:SER:HB3	5:B:311:EDO:H21	1.98	0.45
1:A:48:ILE:HD12	1:A:87:SEP:HA	2.01	0.43
1:B:88:VAL:HG21	7:B:552:HOH:O	2.18	0.43
6:A:318:34W:C16	6:A:318:34W:N25	2.82	0.42
1:A:127:ARG:HA	1:A:273:PHE:CZ	2.55	0.42
1:A:144:ILE:HG23	1:A:161:VAL:HG13	2.00	0.42
1:B:269:PHE:HB2	4:B:309:GOL:H2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD23	5:A:315:EDO:H12	2.01	0.41
6:B:315:34W:C16	6:B:315:34W:N25	2.83	0.41
1:B:83:GLU:HG2	1:B:88:VAL:HG13	2.03	0.41
1:B:246[A]:GLU:OE1	5:B:314:EDO:O1	2.37	0.41
1:B:48:ILE:HG12	7:B:434:HOH:O	2.19	0.41
1:B:135:ILE:HG22	4:B:307:GOL:H11	2.02	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	276/287 (96%)	267 (97%)	9 (3%)	0	100	100
1	B	277/287 (96%)	268 (97%)	9 (3%)	0	100	100
All	All	553/574 (96%)	535 (97%)	18 (3%)	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	237/239 (99%)	236 (100%)	1 (0%)	91	87
1	B	238/239 (100%)	238 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	475/478 (99%)	474 (100%)	1 (0%)	93 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 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	B	87	1	8,9,10	1.10	1 (12%)	8,12,14	1.05	1 (12%)
1	TPO	B	180	1	8,10,11	0.63	0	10,14,16	0.96	0
1	SEP	A	87	1	8,9,10	1.18	1 (12%)	8,12,14	1.12	1 (12%)
1	TPO	A	180	1	8,10,11	0.92	0	10,14,16	0.72	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
1	SEP	B	87	1	-	0/5/8/10	-
1	TPO	B	180	1	-	0/9/11/13	-
1	SEP	A	87	1	-	1/5/8/10	-
1	TPO	A	180	1	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	SEP	P-OG	2.65	1.68	1.60
1	B	87	SEP	P-OG	2.14	1.67	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	SEP	OG-CB-CA	2.30	110.38	108.14
1	B	87	SEP	O3P-P-O2P	2.04	115.43	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	87	SEP	CB-OG-P-O2P
1	A	180	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	87	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

34 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
5	EDO	B	310	-	3,3,3	0.18	0	2,2,2	0.05	0
5	EDO	A	315	-	3,3,3	0.20	0	2,2,2	0.27	0
2	SO4	A	301	-	4,4,4	0.28	0	6,6,6	0.12	0
4	GOL	B	307	-	5,5,5	0.09	0	5,5,5	0.33	0
3	CIT	A	304	-	3,12,12	0.75	0	3,17,17	0.46	0
5	EDO	A	314	-	3,3,3	0.37	0	2,2,2	0.01	0
5	EDO	A	317	-	3,3,3	0.98	0	2,2,2	0.25	0
6	34W	B	315	-	38,38,38	0.70	1 (2%)	47,57,57	1.25	7 (14%)
5	EDO	B	313	-	3,3,3	0.19	0	2,2,2	0.03	0
2	SO4	B	302	-	4,4,4	0.48	0	6,6,6	0.07	0
3	CIT	B	304	-	3,12,12	0.88	0	3,17,17	0.51	0
4	GOL	A	310	-	5,5,5	0.20	0	5,5,5	0.31	0
2	SO4	B	301	-	4,4,4	0.54	0	6,6,6	0.11	0
5	EDO	B	311	-	3,3,3	0.27	0	2,2,2	0.29	0
4	GOL	A	307	-	5,5,5	0.14	0	5,5,5	0.36	0
6	34W	A	318	-	38,38,38	0.55	0	47,57,57	1.24	7 (14%)
2	SO4	A	302	-	4,4,4	0.34	0	6,6,6	0.07	0
5	EDO	A	312	-	3,3,3	0.10	0	2,2,2	0.05	0
2	SO4	B	303	-	4,4,4	0.40	0	6,6,6	0.07	0
4	GOL	A	305	-	5,5,5	0.26	0	5,5,5	0.65	0
5	EDO	B	314	-	3,3,3	0.30	0	2,2,2	0.07	0
4	GOL	A	309	-	5,5,5	0.14	0	5,5,5	0.32	0
5	EDO	A	311	-	3,3,3	0.27	0	2,2,2	0.09	0
5	EDO	B	312	-	3,3,3	0.07	0	2,2,2	0.17	0
4	GOL	B	309	-	5,5,5	0.09	0	5,5,5	0.33	0
4	GOL	B	306	-	5,5,5	0.31	0	5,5,5	0.36	0
5	EDO	A	316	-	3,3,3	0.15	0	2,2,2	0.04	0
5	EDO	A	313	-	3,3,3	0.30	0	2,2,2	0.14	0
4	GOL	A	306	-	5,5,5	0.29	0	5,5,5	0.59	0
6	34W	B	316	-	38,38,38	0.87	2 (5%)	47,57,57	1.21	5 (10%)
2	SO4	A	303	-	4,4,4	0.42	0	6,6,6	0.07	0
4	GOL	A	308	-	5,5,5	0.14	0	5,5,5	0.29	0
4	GOL	B	308	-	5,5,5	0.13	0	5,5,5	0.32	0
4	GOL	B	305	-	5,5,5	0.10	0	5,5,5	0.32	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
5	EDO	B	310	-	-	1/1/1/1	-
5	EDO	A	315	-	-	1/1/1/1	-
5	EDO	B	311	-	-	1/1/1/1	-
4	GOL	B	307	-	-	2/4/4/4	-
3	CIT	A	304	-	-	0/6/16/16	-
5	EDO	A	314	-	-	1/1/1/1	-
5	EDO	A	317	-	-	0/1/1/1	-
6	34W	B	315	-	-	4/23/50/50	0/6/5/5
5	EDO	B	313	-	-	1/1/1/1	-
5	EDO	A	312	-	-	0/1/1/1	-
4	GOL	A	310	-	-	2/4/4/4	-
4	GOL	A	307	-	-	0/4/4/4	-
6	34W	A	318	-	-	3/23/50/50	0/6/5/5
3	CIT	B	304	-	-	0/6/16/16	-
6	34W	B	316	-	-	8/23/50/50	0/6/5/5
4	GOL	A	305	-	-	2/4/4/4	-
5	EDO	B	314	-	-	0/1/1/1	-
4	GOL	A	309	-	-	3/4/4/4	-
5	EDO	A	311	-	-	0/1/1/1	-
5	EDO	B	312	-	-	1/1/1/1	-
4	GOL	B	309	-	-	4/4/4/4	-
4	GOL	B	306	-	-	0/4/4/4	-
5	EDO	A	316	-	-	0/1/1/1	-
5	EDO	A	313	-	-	1/1/1/1	-
4	GOL	A	306	-	-	2/4/4/4	-
4	GOL	A	308	-	-	2/4/4/4	-
4	GOL	B	308	-	-	2/4/4/4	-
4	GOL	B	305	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	316	34W	C05-C06	2.86	1.64	1.52
6	B	316	34W	C11-C10	2.71	1.61	1.54
6	B	315	34W	C05-C06	2.11	1.61	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	316	34W	C11-C12-N08	-4.05	99.27	101.97
6	B	316	34W	C10-C09-N08	-3.92	99.36	101.97
6	B	315	34W	C11-C12-N08	-3.47	99.66	101.97
6	B	315	34W	C10-C09-N08	-3.44	99.68	101.97
6	A	318	34W	C11-C12-N08	-3.36	99.74	101.97
6	A	318	34W	C10-C09-N08	-3.02	99.96	101.97
6	A	318	34W	C24-N26-C27	-2.77	119.09	124.26
6	A	318	34W	C13-C14-C09	-2.77	105.81	110.49
6	B	315	34W	C29-C28-C27	2.55	90.58	88.37
6	B	315	34W	C13-C14-C09	-2.54	106.21	110.49
6	B	316	34W	C29-C28-C27	-2.45	86.24	88.37
6	A	318	34W	C15-C14-C09	2.44	133.16	129.06
6	B	315	34W	C29-C30-C27	2.42	90.47	88.37
6	B	316	34W	C14-C13-C12	-2.41	106.43	110.49
6	B	316	34W	C13-C14-C09	-2.39	106.46	110.49
6	A	318	34W	C14-C13-C12	-2.39	106.46	110.49
6	A	318	34W	C29-C28-C27	-2.33	86.34	88.37
6	B	315	34W	C15-C14-C09	2.28	132.89	129.06
6	B	315	34W	C14-C13-C12	-2.20	106.78	110.49

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	307	GOL	C1-C2-C3-O3
4	A	310	GOL	C1-C2-C3-O3
4	A	305	GOL	O1-C1-C2-O2
4	A	305	GOL	O1-C1-C2-C3
4	A	309	GOL	C1-C2-C3-O3
4	B	309	GOL	C1-C2-C3-O3
4	A	306	GOL	C1-C2-C3-O3
6	B	316	34W	C01-C02-N04-C05
6	B	316	34W	O03-C02-N04-C05
6	B	316	34W	N04-C05-C06-O07
6	B	316	34W	C05-C06-N08-C09
6	B	316	34W	C05-C06-N08-C12
6	B	316	34W	O07-C06-N08-C09
6	B	316	34W	O07-C06-N08-C12
4	A	308	GOL	O1-C1-C2-C3
4	B	308	GOL	O1-C1-C2-C3
6	A	318	34W	O07-C06-N08-C12
4	B	309	GOL	O1-C1-C2-C3
4	A	310	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	309	GOL	O1-C1-C2-O2
4	B	309	GOL	O2-C2-C3-O3
4	A	306	GOL	O2-C2-C3-O3
4	A	308	GOL	O1-C1-C2-O2
4	B	308	GOL	O1-C1-C2-O2
5	A	315	EDO	O1-C1-C2-O2
5	B	312	EDO	O1-C1-C2-O2
6	B	316	34W	N04-C05-C06-N08
4	B	307	GOL	O2-C2-C3-O3
4	A	309	GOL	O2-C2-C3-O3
5	A	314	EDO	O1-C1-C2-O2
5	B	311	EDO	O1-C1-C2-O2
6	B	315	34W	O07-C06-N08-C12
6	A	318	34W	C05-C06-N08-C12
6	B	315	34W	N04-C05-C06-N08
5	B	313	EDO	O1-C1-C2-O2
5	A	313	EDO	O1-C1-C2-O2
4	A	309	GOL	O1-C1-C2-C3
6	B	315	34W	N04-C05-C06-O07
6	B	315	34W	C30-C27-N26-C24
6	A	318	34W	C28-C27-N26-C24
5	B	310	EDO	O1-C1-C2-O2

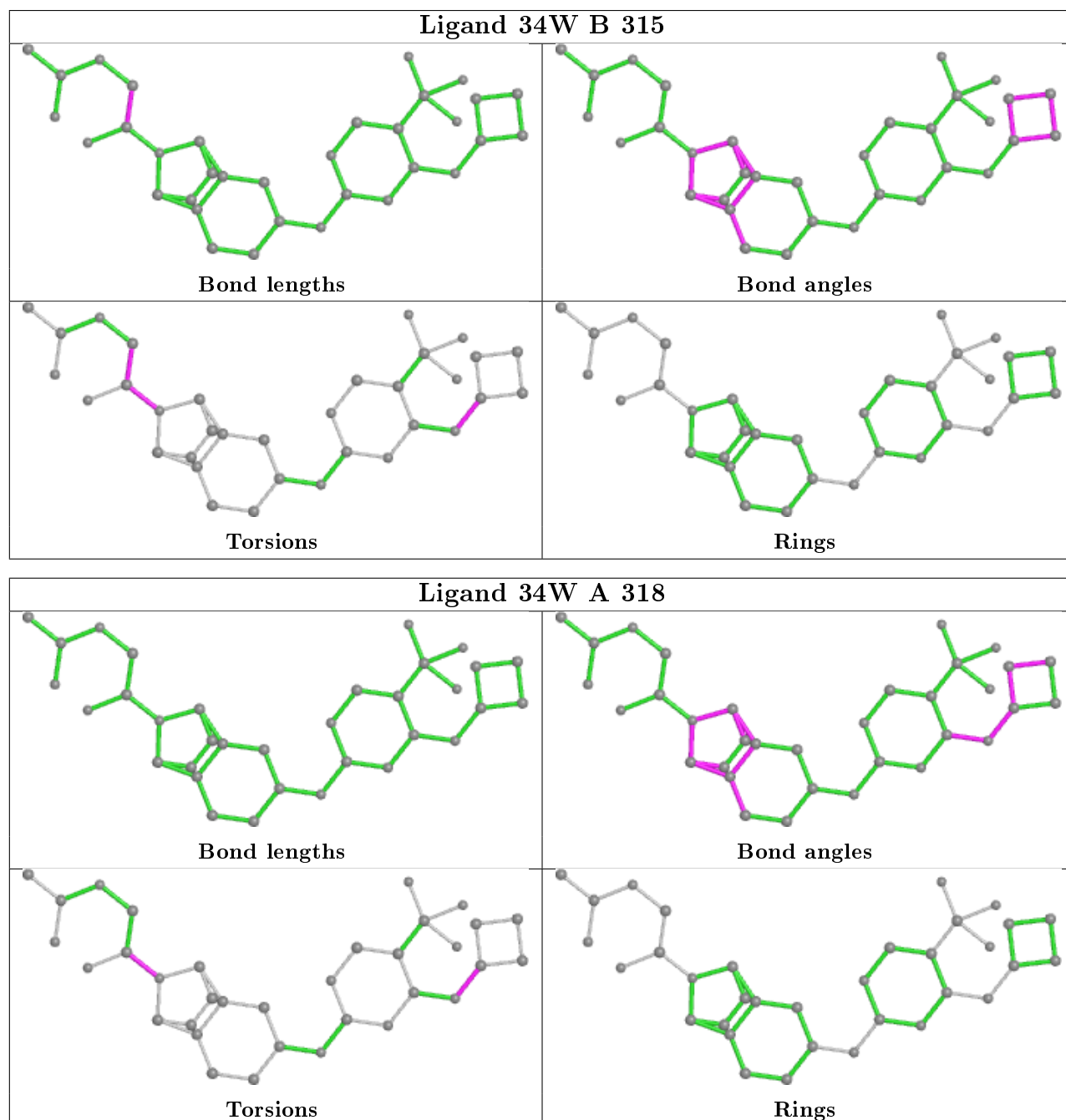
There are no ring outliers.

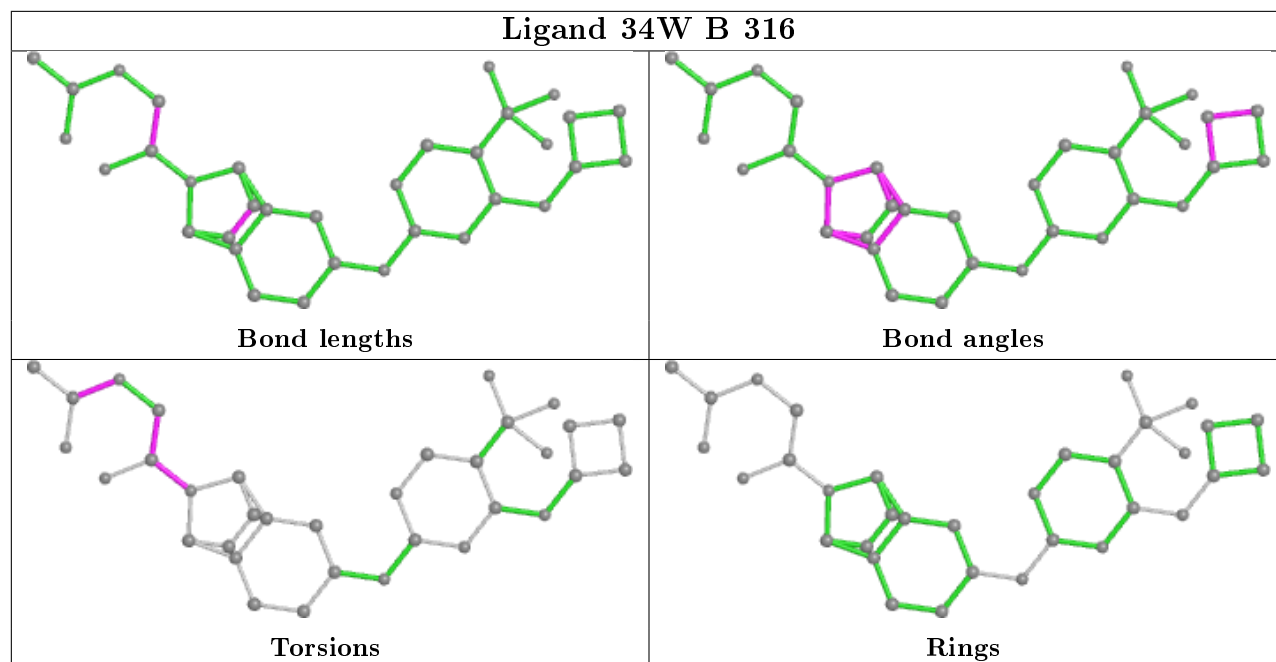
13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	315	EDO	1	0
4	B	307	GOL	1	0
5	A	314	EDO	1	0
5	A	317	EDO	1	0
6	B	315	34W	3	0
4	A	310	GOL	2	0
5	B	311	EDO	3	0
6	A	318	34W	2	0
5	B	314	EDO	1	0
4	A	309	GOL	1	0
5	A	311	EDO	1	0
4	B	309	GOL	1	0
6	B	316	34W	3	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

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	272/287 (94%)	0.33	16 (5%) 22 27	18, 26, 50, 66	0
1	B	271/287 (94%)	0.28	13 (4%) 30 36	17, 26, 48, 81	0
All	All	543/574 (94%)	0.31	29 (5%) 26 32	17, 26, 50, 81	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ALA	7.8
1	B	150	ALA	5.6
1	A	37	ALA	5.1
1	B	224	SER	4.9
1	B	151	GLY	4.7
1	A	8	THR	4.6
1	B	280	ALA	4.6
1	B	231	LEU	4.2
1	A	224	SER	3.6
1	A	231	LEU	3.6
1	B	152	ARG	3.4
1	B	228	ASP	3.2
1	A	245	ARG	3.1
1	A	246	GLU	2.9
1	A	228	ASP	2.7
1	A	237	LYS	2.6
1	A	50	LYS	2.6
1	B	279	ASP	2.5
1	A	235	LYS	2.4
1	A	17	SER	2.2
1	B	8	THR	2.2
1	A	232	PHE	2.2
1	B	223	ALA	2.2
1	A	222	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	227	GLN	2.1
1	A	281	SER	2.1
1	B	235	LYS	2.0
1	A	279	ASP	2.0
1	B	50	LYS	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	SEP	B	87	10/11	0.81	0.14	25,35,50,52	0
1	SEP	A	87	10/11	0.82	0.17	26,39,56,58	0
1	TPO	B	180	11/12	0.98	0.09	20,20,21,22	0
1	TPO	A	180	11/12	0.98	0.10	19,20,21,21	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	B	308	6/6	0.65	0.18	58,59,61,63	0
5	EDO	B	310	4/4	0.72	0.18	40,44,47,54	0
6	34W	B	316	34/34	0.75	0.27	38,46,73,80	0
5	EDO	A	312	4/4	0.75	0.24	54,56,56,58	0
4	GOL	B	305	6/6	0.78	0.17	36,52,54,64	0
5	EDO	B	313	4/4	0.80	0.21	48,51,52,55	0
4	GOL	B	309	6/6	0.81	0.20	48,52,57,57	0
4	GOL	A	309	6/6	0.81	0.17	43,54,58,59	0
4	GOL	B	306	6/6	0.82	0.16	33,36,39,40	0

Continued on next page...

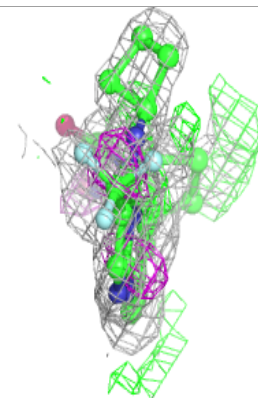
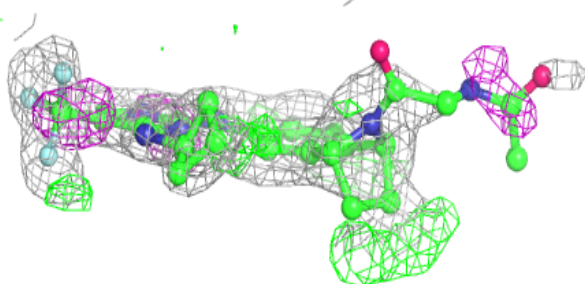
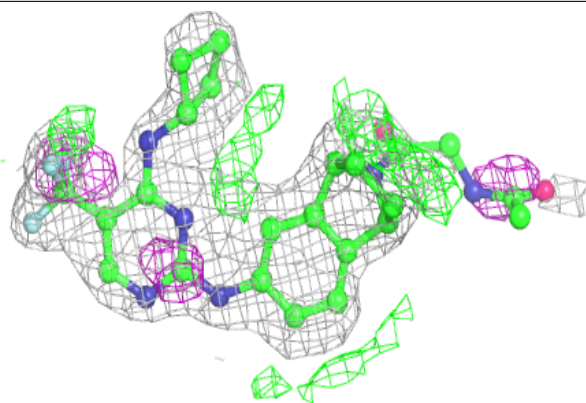
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	308	6/6	0.82	0.12	53,58,60,68	0
4	GOL	A	305	6/6	0.83	0.17	35,43,45,45	0
4	GOL	A	310	6/6	0.83	0.23	41,48,52,53	0
5	EDO	A	316	4/4	0.84	0.14	63,63,65,68	0
5	EDO	A	313	4/4	0.84	0.16	47,51,58,61	0
3	CIT	B	304	13/13	0.85	0.17	31,35,42,45	0
5	EDO	A	311	4/4	0.85	0.15	48,51,51,54	0
5	EDO	B	311	4/4	0.86	0.17	45,51,52,57	0
5	EDO	A	315	4/4	0.86	0.14	42,44,44,45	0
4	GOL	B	307	6/6	0.89	0.22	44,48,49,50	0
5	EDO	A	314	4/4	0.89	0.13	37,39,41,44	0
5	EDO	B	312	4/4	0.91	0.17	42,54,56,63	0
4	GOL	A	307	6/6	0.91	0.18	30,34,36,36	0
6	34W	B	315	34/34	0.91	0.13	21,31,73,74	0
3	CIT	A	304	13/13	0.93	0.14	29,35,41,43	0
2	SO4	A	303	5/5	0.93	0.17	71,72,76,77	0
6	34W	A	318	34/34	0.94	0.09	20,27,46,49	0
2	SO4	A	302	5/5	0.94	0.21	48,52,55,56	0
5	EDO	A	317	4/4	0.94	0.18	22,36,39,52	0
5	EDO	B	314	4/4	0.95	0.12	39,48,51,52	0
4	GOL	A	306	6/6	0.95	0.10	24,31,33,35	0
2	SO4	B	303	5/5	0.96	0.10	45,45,51,54	0
2	SO4	A	301	5/5	0.97	0.14	44,45,48,49	0
2	SO4	B	301	5/5	0.97	0.10	39,43,52,53	0
2	SO4	B	302	5/5	0.98	0.08	43,47,50,52	0

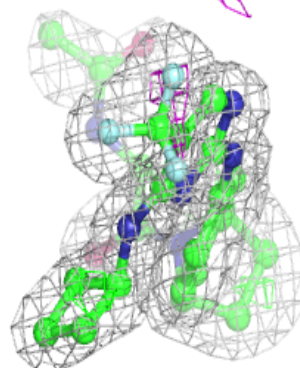
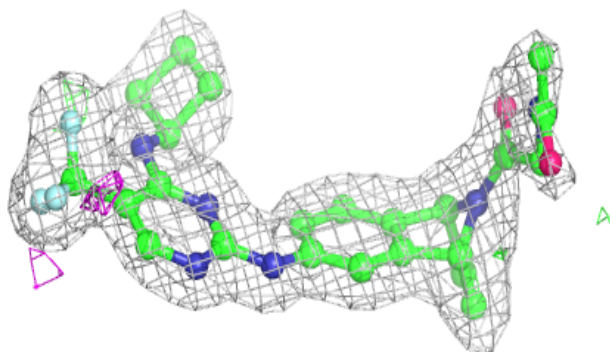
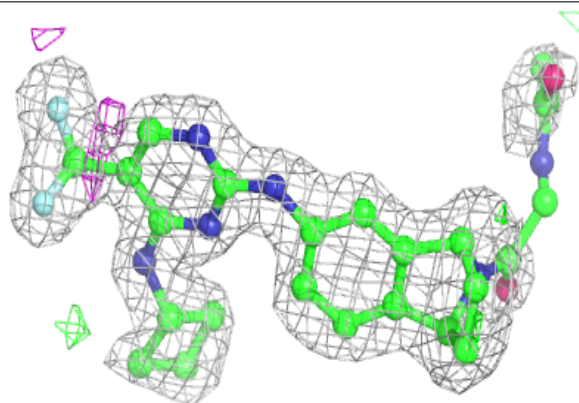
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

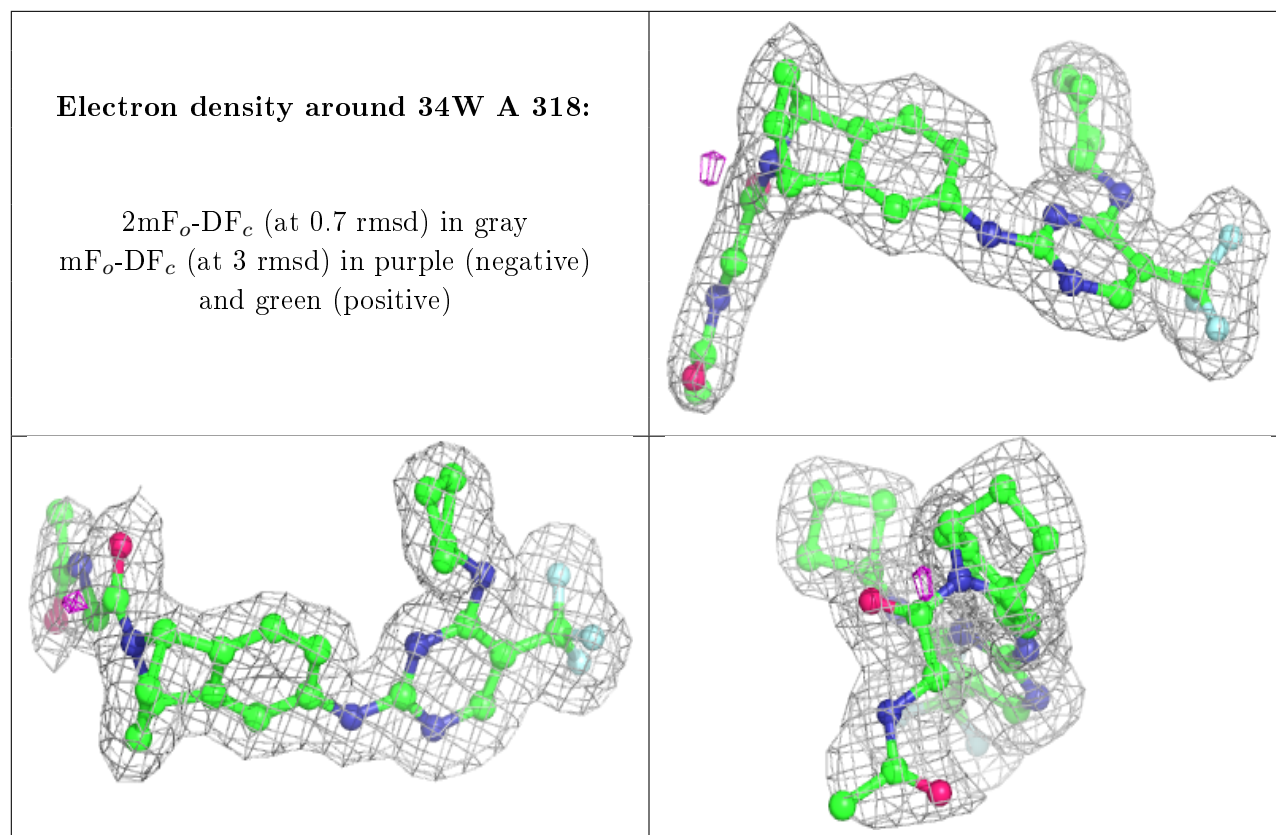
Electron density around 34W B 316:

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

**Electron density around 34W B 315:**

$2mF_o-DF_c$ (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.