



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2026 – 01:45 AM UTC

PDB ID : 4AL4 / pdb_00004al4
Title : rat LDHA in complex with 2-((4-(2-((3-((2-methyl-1,3-benzothiazol-6-yl)amino)3-oxo-propyl)carbamoylamino)ethoxy)phenyl)methylpropanedioic acid
Authors : Tucker, J.A.; Brassington, C.; Hassall, G.; Ward, R.; Tart, J.; Davies, G.; Hohson, M.; Pearson, S.
Deposited on : 2012-03-01
Resolution : 1.78 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

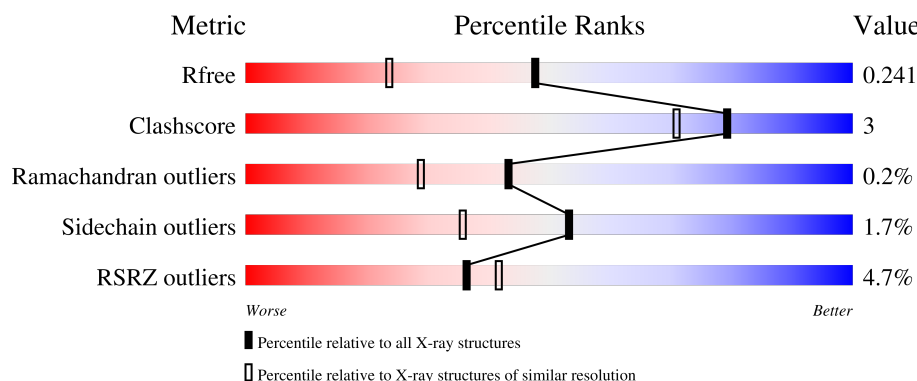
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	331	6% 91% 8%
1	B	331	3% 89% 11%
1	C	331	4% 90% 10%
1	D	331	6% 90% 10%

2 Entry composition [i](#)

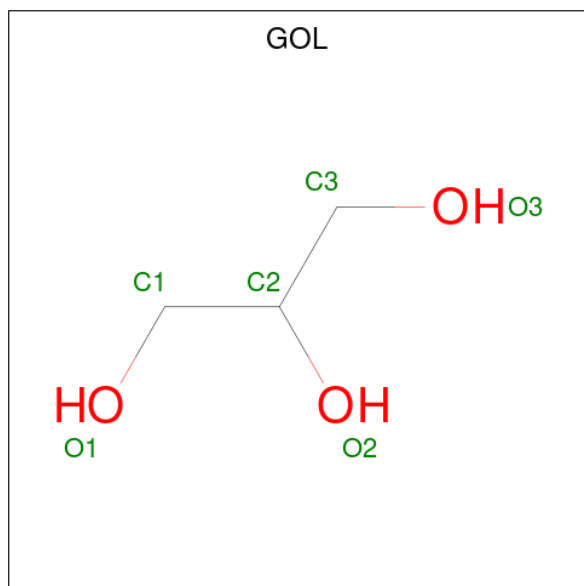
There are 4 unique types of molecules in this entry. The entry contains 11520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-LACTATE DEHYDROGENASE A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	5	0
			2540	1624	427	476	13			
1	B	330	Total	C	N	O	S	0	6	0
			2557	1633	431	480	13			
1	C	331	Total	C	N	O	S	0	2	1
			2514	1606	427	468	13			
1	D	331	Total	C	N	O	S	0	5	1
			2544	1624	425	482	13			

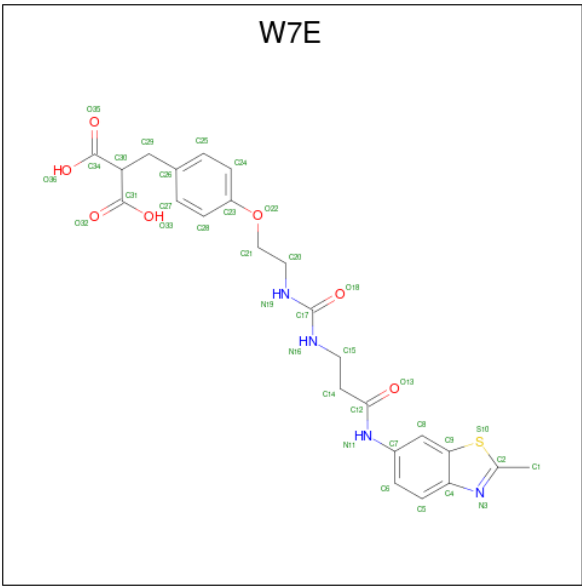
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is 2-[[4-[2-[[3-[(2-methyl-1,3-benzothiazol-6-yl)amino]-3-oxidanylidene-propyl]carbamoylamino]ethoxy]phenyl]methyl]propanedioic acid (CCD ID: W7E) (formula:

C₂₄H₂₆N₄O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			36	24	4	7	1		
3	A	1	Total	C	N	O	S	0	1
			72	48	8	14	2		
3	B	1	Total	C	N	O	S	0	0
			36	24	4	7	1		
3	B	1	Total	C	N	O	S	0	1
			72	48	8	14	2		
3	C	1	Total	C	N	O	S	0	0
			36	24	4	7	1		
3	C	1	Total	C	N	O	S	0	1
			72	48	8	14	2		
3	D	1	Total	C	N	O	S	0	0
			36	24	4	7	1		

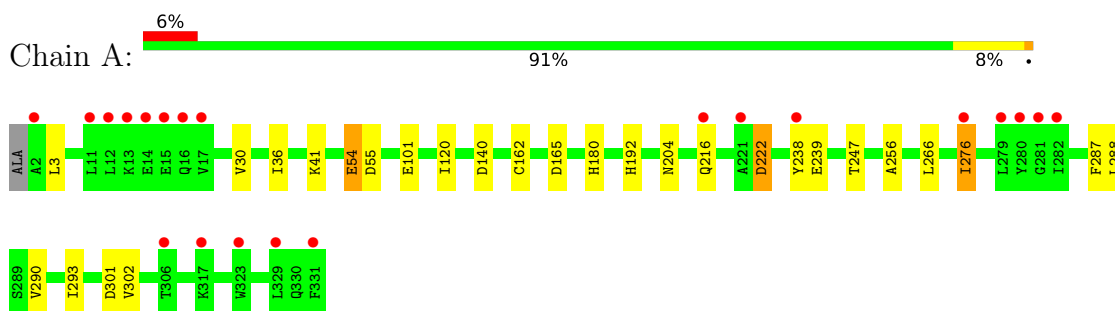
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	2
			270	270		
4	B	272	Total	O	0	1
			272	272		
4	C	224	Total	O	0	0
			224	224		
4	D	233	Total	O	0	1
			233	233		

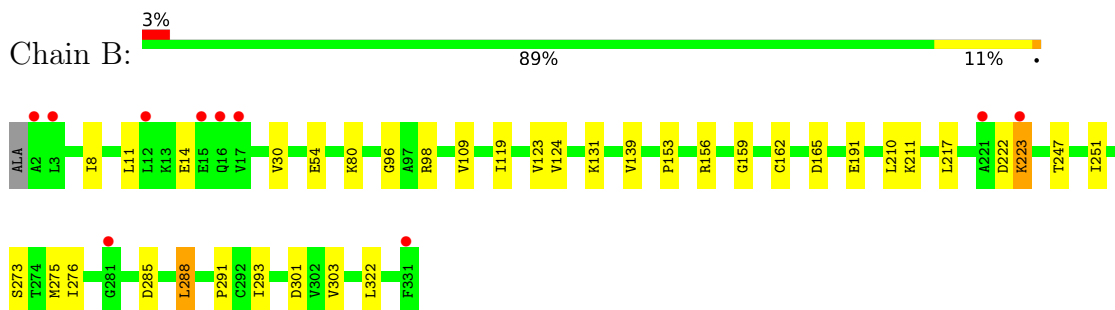
3 Residue-property plots [i](#)

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.

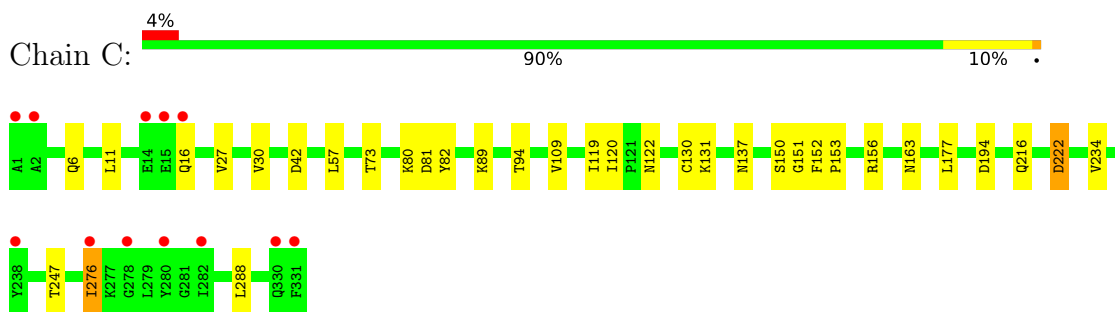
- Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN



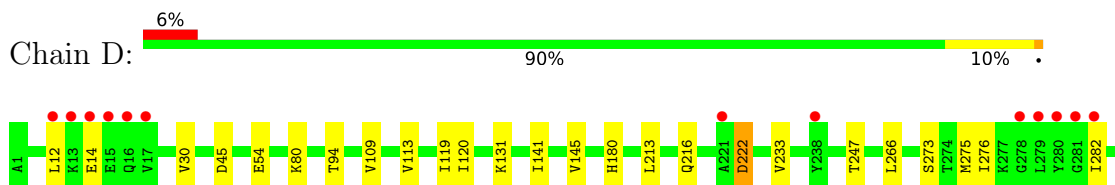
- Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN

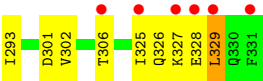


- Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN



- Molecule 1: L-LACTATE DEHYDROGENASE A CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.36Å 82.70Å 129.67Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	64.42 – 1.78 64.42 – 1.78	Depositor EDS
% Data completeness (in resolution range)	89.7 (64.42-1.78) 89.6 (64.42-1.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.78Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2	Depositor
R, R_{free}	0.188 , 0.229 0.196 , 0.241	Depositor DCC
R_{free} test set	5671 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11520	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 4.67% 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: W7E, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.01	0/2584	1.31	7/3510 (0.2%)
1	B	1.01	1/2601 (0.0%)	1.28	11/3531 (0.3%)
1	C	0.97	1/2557 (0.0%)	1.33	16/3472 (0.5%)
1	D	0.99	1/2588 (0.0%)	1.34	11/3516 (0.3%)
All	All	0.99	3/10330 (0.0%)	1.31	45/14029 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	120	ILE	CA-CB	7.19	1.57	1.54
1	D	120	ILE	CA-CB	5.80	1.57	1.54
1	B	251	ILE	CG1-CD1	5.06	1.71	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	GLU	N-CA-C	8.01	121.23	109.69
1	D	329	LEU	N-CA-C	7.74	121.86	109.24
1	D	109	VAL	N-CA-C	7.64	118.18	110.23
1	C	137	ASN	N-CA-C	7.50	120.13	110.39
1	C	119	ILE	N-CA-C	7.37	117.45	110.30
1	C	109	VAL	N-CA-C	7.01	117.72	110.36
1	A	54	GLU	N-CA-C	6.90	118.45	111.07
1	C	42	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	109	VAL	N-CA-C	6.59	117.08	110.23
1	C	73	THR	CB-CA-C	6.57	118.88	110.34
1	B	124	VAL	CA-C-N	6.51	129.30	120.38
1	B	124	VAL	C-N-CA	6.51	129.30	120.38
1	A	222	ASP	CA-CB-CG	6.41	119.01	112.60
1	D	222	ASP	CA-CB-CG	6.23	118.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	LYS	N-CA-C	-6.17	105.24	112.89
1	C	177	LEU	N-CA-C	6.03	120.70	113.23
1	D	119	ILE	N-CA-C	5.83	115.90	110.42
1	D	54	GLU	N-CA-C	5.80	117.61	111.28
1	C	131	LYS	N-CA-C	-5.77	100.29	109.76
1	D	233	VAL	N-CA-C	-5.75	104.91	110.42
1	C	120	ILE	N-CA-CB	5.56	114.25	110.52
1	B	131	LYS	N-CA-C	-5.53	101.16	109.95
1	C	130	CYS	N-CA-C	5.46	117.73	110.53
1	A	204	ASN	N-CA-C	5.38	117.25	109.07
1	C	222	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	150	SER	N-CA-C	5.24	116.99	111.28
1	C	81	ASP	CA-CB-CG	5.23	117.83	112.60
1	B	54	GLU	N-CA-C	5.23	117.38	111.11
1	D	12	LEU	N-CA-CB	-5.23	102.71	110.71
1	B	139	VAL	N-CA-C	5.21	116.56	110.62
1	B	119	ILE	N-CA-C	5.20	115.34	110.30
1	C	163	ASN	N-CA-C	-5.18	105.63	111.28
1	B	222	ASP	CA-CB-CG	5.18	117.78	112.60
1	C	151	GLY	N-CA-C	-5.16	108.49	115.36
1	A	36	ILE	N-CA-CB	5.16	116.59	110.55
1	B	96	GLY	N-CA-C	5.16	117.29	112.08
1	D	45	ASP	N-CA-C	-5.14	107.05	113.38
1	C	89	LYS	N-CA-C	-5.12	106.20	112.90
1	A	120	ILE	N-CA-CB	5.11	113.94	110.52
1	B	285	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	192	HIS	N-CA-C	-5.07	99.70	108.52
1	A	290	VAL	N-CA-C	-5.05	103.30	109.01
1	D	80	LYS	N-CA-C	-5.05	106.63	112.89
1	D	131	LYS	N-CA-C	-5.02	101.53	109.96
1	B	80	LYS	N-CA-C	-5.01	106.43	112.54

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	2540	0	2557	15	0
1	B	2557	0	2584	15	0
1	C	2514	0	2545	12	0
1	D	2544	0	2543	16	0
2	A	6	0	8	0	0
3	A	108	0	72	3	0
3	B	108	0	72	5	0
3	C	108	0	72	3	0
3	D	36	0	24	2	0
4	A	270	0	0	4	0
4	B	272	0	0	0	0
4	C	224	0	0	3	0
4	D	233	0	0	1	0
All	All	11520	0	10477	57	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 (57) 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:238[A]:TYR:CD1	4:A:2108:HOH:O	1.98	1.15
1:C:153:PRO:HD2	4:C:2128:HOH:O	1.62	0.99
1:A:101[A]:GLU:O	4:A:2108:HOH:O	1.98	0.80
1:B:223:LYS:HZ2	1:B:223:LYS:H	1.30	0.77
1:A:238[A]:TYR:HD1	4:A:2108:HOH:O	1.44	0.76
3:B:1332:W7E:N16	3:B:1333[A]:W7E:H27	2.09	0.68
1:C:276:ILE:HG12	1:C:288:LEU:HG	1.85	0.58
1:A:216:GLN:O	1:A:222:ASP:HB2	2.04	0.57
1:A:3:LEU:HD21	1:B:210:LEU:HD23	1.86	0.56
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.86	0.56
1:D:327:LYS:HA	4:D:2217:HOH:O	2.08	0.54
1:C:94:THR:O	3:C:1332:W7E:H202	2.08	0.54
1:D:113:VAL:HG21	1:D:329:LEU:HD22	1.91	0.53
1:A:276:ILE:HG12	1:A:288:LEU:HG	1.92	0.52
3:A:1333:W7E:N16	3:A:1334[A]:W7E:H25	2.25	0.51
1:D:30:VAL:HG21	3:D:1332:W7E:C28	2.42	0.50
1:D:216:GLN:O	1:D:222:ASP:HB2	2.11	0.49
1:D:293:ILE:HD12	1:D:301:ASP:HB2	1.93	0.49
1:A:30:VAL:HG21	3:A:1333:W7E:C28	2.43	0.49
1:D:94:THR:O	3:D:1332:W7E:H202	2.13	0.48
1:A:302:VAL:HG23	1:C:11:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:VAL:HG22	1:D:145:VAL:HG21	1.96	0.48
1:B:11:LEU:HD11	1:D:302:VAL:HG23	1.95	0.48
1:D:325:ILE:O	1:D:328:GLU:HB3	2.14	0.48
1:A:266:LEU:O	1:D:180:HIS:HB2	2.14	0.47
1:B:98:ARG:HG2	3:B:1332:W7E:H211	1.96	0.47
1:B:293:ILE:HD12	1:B:301:ASP:HB2	1.98	0.46
1:C:6:GLN:HB3	1:D:213:LEU:HD22	1.97	0.46
1:C:156:ARG:CZ	4:C:2128:HOH:O	2.63	0.46
1:B:162:CYS:HA	1:B:165:ASP:OD1	2.17	0.45
3:B:1332:W7E:C15	3:B:1333[A]:W7E:H27	2.46	0.45
1:A:180:HIS:HB2	1:D:266:LEU:O	2.16	0.45
1:B:288:LEU:HD12	1:B:288:LEU:C	2.42	0.45
1:B:153:PRO:HG2	1:B:156:ARG:HG3	1.98	0.45
1:C:30:VAL:HG21	3:C:1332:W7E:C28	2.47	0.45
1:B:30:VAL:HG21	3:B:1332:W7E:C28	2.46	0.44
3:C:1333[A]:W7E:H8	3:C:1333[A]:W7E:O13	2.17	0.44
1:A:55:ASP:HB2	4:A:2058:HOH:O	2.17	0.44
3:B:1333[A]:W7E:O13	3:B:1333[A]:W7E:H8	2.18	0.43
1:A:293:ILE:HD12	1:A:301:ASP:HB2	2.00	0.42
1:C:194:ASP:HA	1:C:234:VAL:HG13	2.01	0.42
1:B:223:LYS:H	1:B:223:LYS:NZ	2.09	0.42
1:B:159:GLY:HA3	1:B:273:SER:HB2	2.01	0.42
1:B:211:LYS:HG3	1:B:217:LEU:HB3	2.00	0.41
1:C:152:PHE:HB3	4:C:2128:HOH:O	2.20	0.41
1:C:216:GLN:O	1:C:222:ASP:HB2	2.20	0.41
1:D:141:ILE:HD12	1:D:326:GLN:HG3	2.03	0.41
1:C:27:VAL:HG21	1:C:57:LEU:HA	2.03	0.41
1:B:8:ILE:CG2	1:D:301:ASP:HB3	2.50	0.41
1:B:191:GLU:HG3	1:B:322:LEU:HD21	2.01	0.41
1:D:325:ILE:O	1:D:328:GLU:N	2.44	0.41
1:D:325:ILE:C	1:D:327:LYS:N	2.78	0.41
1:A:162:CYS:HA	1:A:165:ASP:OD1	2.21	0.41
1:A:41:LYS:HD3	1:A:256:ALA:HB1	2.03	0.41
3:A:1334[B]:W7E:H24	3:A:1334[B]:W7E:H212	1.76	0.41
1:C:82:TYR:CG	1:C:122:ASN:HB3	2.56	0.41
1:A:140:ASP:HB3	1:A:287:PHE:O	2.21	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	333/331 (101%)	319 (96%)	14 (4%)	0	100	100
1	B	334/331 (101%)	324 (97%)	9 (3%)	1 (0%)	36	22
1	C	331/331 (100%)	319 (96%)	11 (3%)	1 (0%)	36	22
1	D	334/331 (101%)	321 (96%)	13 (4%)	0	100	100
All	All	1332/1324 (101%)	1283 (96%)	47 (4%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	GLU
1	C	16	GLN

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	276/286 (96%)	272 (99%)	4 (1%)	59	44
1	B	281/286 (98%)	275 (98%)	6 (2%)	47	27
1	C	274/286 (96%)	272 (99%)	2 (1%)	76	66
1	D	276/286 (96%)	270 (98%)	6 (2%)	45	26
All	All	1107/1144 (97%)	1089 (98%)	18 (2%)	53	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	239	GLU
1	A	247	THR
1	A	276	ILE
1	B	123	VAL
1	B	223	LYS
1	B	247	THR
1	B	275	MET
1	B	276	ILE
1	B	288	LEU
1	C	247	THR
1	C	276	ILE
1	D	247	THR
1	D	273	SER
1	D	275	MET
1	D	276	ILE
1	D	282	ILE
1	D	306	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	20	ASN
1	A	65	GLN
1	B	10	ASN
1	B	129	GLN
1	B	216	GLN
1	C	6	GLN
1	C	10	ASN
1	C	20	ASN
1	C	129	GLN
1	D	10	ASN
1	D	129	GLN

5.3.3 RNA ⓘ

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	$\# Z > 2$
3	W7E	C	1333[A]	-	38,38,38	0.42	0	50,51,51	0.66	2 (4%)
3	W7E	D	1332	-	38,38,38	0.42	0	50,51,51	0.74	2 (4%)
3	W7E	A	1334[A]	-	38,38,38	0.41	0	50,51,51	0.74	2 (4%)
3	W7E	B	1333[B]	-	38,38,38	0.43	1 (2%)	50,51,51	0.72	2 (4%)
2	GOL	A	1332[B]	-	5,5,5	0.08	0	5,5,5	0.13	0
3	W7E	B	1332	-	38,38,38	0.41	0	50,51,51	0.73	1 (2%)
3	W7E	C	1333[B]	-	38,38,38	0.42	1 (2%)	50,51,51	0.68	2 (4%)
3	W7E	A	1334[B]	-	38,38,38	0.43	1 (2%)	50,51,51	0.68	2 (4%)
3	W7E	C	1332	-	38,38,38	0.40	0	50,51,51	0.73	2 (4%)
3	W7E	A	1333	-	38,38,38	0.45	1 (2%)	50,51,51	0.50	1 (2%)
3	W7E	B	1333[A]	-	38,38,38	0.43	1 (2%)	50,51,51	0.67	1 (2%)

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	W7E	C	1333[A]	-	-	2/29/29/29	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	W7E	D	1332	-	-	7/29/29/29	0/3/3/3
3	W7E	A	1334[A]	-	-	7/29/29/29	0/3/3/3
3	W7E	B	1333[B]	-	-	13/29/29/29	0/3/3/3
2	GOL	A	1332[B]	-	-	0/4/4/4	-
3	W7E	B	1332	-	-	3/29/29/29	0/3/3/3
3	W7E	C	1333[B]	-	-	5/29/29/29	0/3/3/3
3	W7E	A	1334[B]	-	-	4/29/29/29	0/3/3/3
3	W7E	C	1332	-	-	7/29/29/29	0/3/3/3
3	W7E	A	1333	-	-	6/29/29/29	0/3/3/3
3	W7E	B	1333[A]	-	-	15/29/29/29	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1333	W7E	C2-N3	2.11	1.31	1.29
3	A	1334[B]	W7E	C2-N3	2.05	1.31	1.29
3	B	1333[B]	W7E	C2-N3	2.04	1.31	1.29
3	B	1333[A]	W7E	C2-N3	2.03	1.31	1.29
3	C	1333[B]	W7E	C2-N3	2.00	1.31	1.29

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1334[A]	W7E	C1-C2-S10	3.86	121.95	120.08
3	D	1332	W7E	C1-C2-S10	3.82	121.93	120.08
3	C	1332	W7E	C1-C2-S10	3.80	121.92	120.08
3	B	1333[B]	W7E	C1-C2-S10	3.73	121.89	120.08
3	A	1334[B]	W7E	C1-C2-S10	3.64	121.84	120.08
3	B	1332	W7E	C1-C2-S10	3.63	121.84	120.08
3	C	1333[B]	W7E	C1-C2-S10	3.58	121.82	120.08
3	C	1333[A]	W7E	C1-C2-S10	3.48	121.77	120.08
3	B	1333[A]	W7E	C1-C2-S10	3.37	121.71	120.08
3	C	1332	W7E	C1-C2-N3	-2.37	122.37	124.01
3	A	1334[A]	W7E	C1-C2-N3	-2.32	122.40	124.01
3	A	1334[B]	W7E	C1-C2-N3	-2.26	122.44	124.01
3	D	1332	W7E	C1-C2-N3	-2.22	122.47	124.01
3	A	1333	W7E	C1-C2-S10	2.21	121.15	120.08
3	B	1333[B]	W7E	C1-C2-N3	-2.19	122.50	124.01
3	C	1333[A]	W7E	C1-C2-N3	-2.13	122.54	124.01
3	C	1333[B]	W7E	C1-C2-N3	-2.12	122.54	124.01

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1333	W7E	C29-C30-C34-O35
3	A	1333	W7E	C31-C30-C34-O36
3	A	1333	W7E	C29-C30-C34-O36
3	A	1334[B]	W7E	N16-C17-N19-C20
3	A	1334[B]	W7E	O18-C17-N19-C20
3	B	1333[B]	W7E	N16-C17-N19-C20
3	B	1333[B]	W7E	O18-C17-N19-C20
3	B	1333[B]	W7E	N19-C17-N16-C15
3	B	1333[B]	W7E	O18-C17-N16-C15
3	B	1333[B]	W7E	C26-C29-C30-C31
3	B	1333[B]	W7E	C26-C29-C30-C34
3	B	1333[B]	W7E	C12-C14-C15-N16
3	C	1332	W7E	C29-C30-C34-O35
3	C	1332	W7E	C29-C30-C34-O36
3	D	1332	W7E	C31-C30-C34-O36
3	D	1332	W7E	C29-C30-C34-O36
3	A	1334[A]	W7E	C14-C12-N11-C7
3	A	1334[A]	W7E	N19-C17-N16-C15
3	A	1334[A]	W7E	O18-C17-N16-C15
3	C	1333[B]	W7E	N16-C17-N19-C20
3	C	1332	W7E	N16-C17-N19-C20
3	C	1333[B]	W7E	O18-C17-N19-C20
3	C	1332	W7E	O18-C17-N19-C20
3	B	1333[A]	W7E	N19-C20-C21-O22
3	C	1333[B]	W7E	C28-C23-O22-C21
3	C	1333[B]	W7E	C24-C23-O22-C21
3	A	1334[A]	W7E	O13-C12-N11-C7
3	B	1333[A]	W7E	C28-C23-O22-C21
3	B	1333[A]	W7E	C24-C23-O22-C21
3	B	1333[B]	W7E	C28-C23-O22-C21
3	B	1333[B]	W7E	C24-C23-O22-C21
3	B	1333[B]	W7E	C14-C15-N16-C17
3	A	1334[B]	W7E	C20-C21-O22-C23
3	B	1333[B]	W7E	C6-C7-N11-C12
3	B	1333[B]	W7E	C8-C7-N11-C12
3	A	1333	W7E	O18-C17-N19-C20
3	B	1333[A]	W7E	C14-C12-N11-C7
3	D	1332	W7E	O18-C17-N19-C20
3	D	1332	W7E	N16-C17-N19-C20
3	B	1333[A]	W7E	O13-C12-N11-C7

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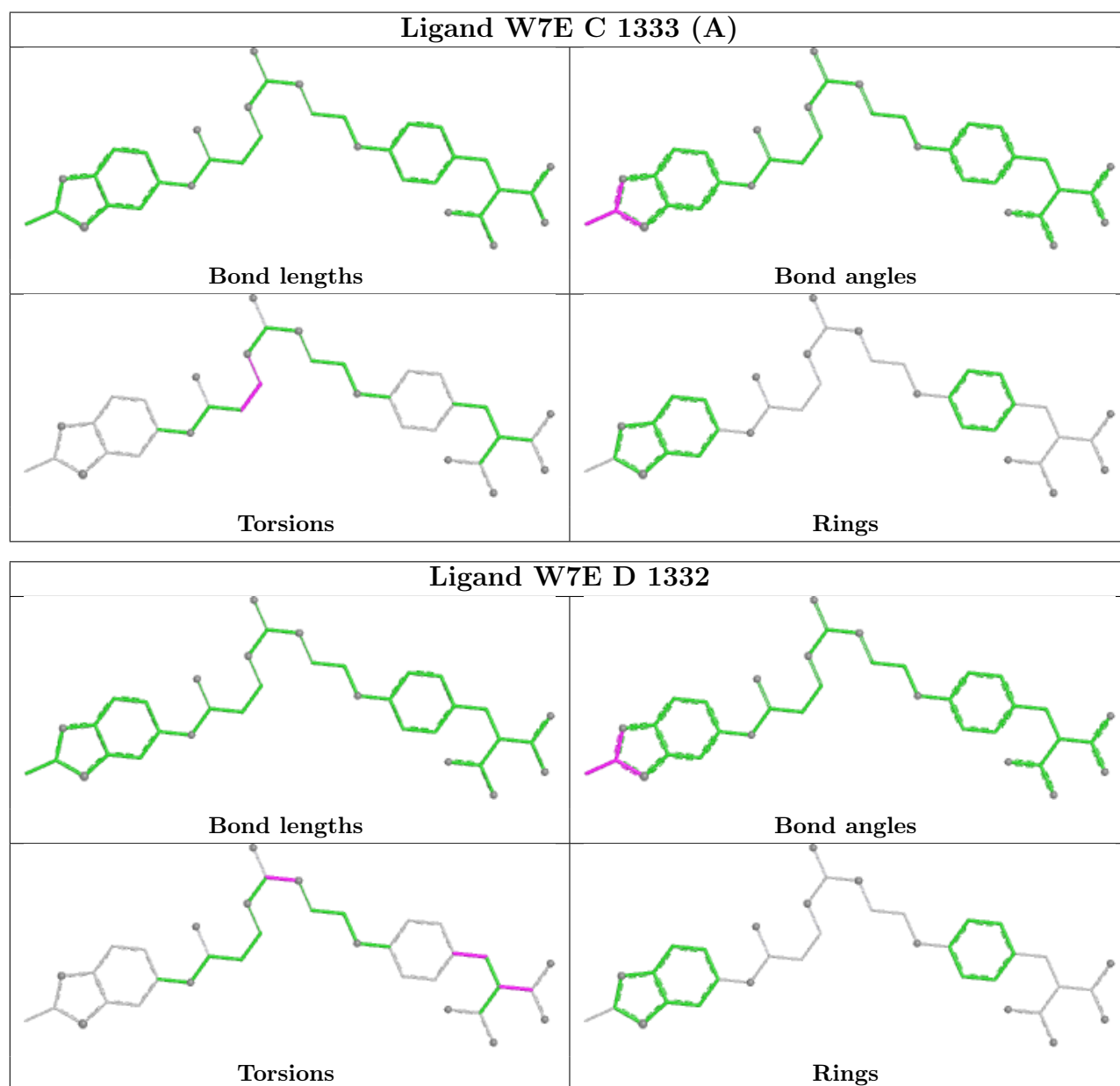
Mol	Chain	Res	Type	Atoms
3	A	1333	W7E	N16-C17-N19-C20
3	B	1332	W7E	C29-C30-C34-O35
3	B	1332	W7E	C29-C30-C34-O36
3	B	1333[A]	W7E	C29-C30-C34-O35
3	B	1333[A]	W7E	C29-C30-C34-O36
3	D	1332	W7E	C29-C30-C34-O35
3	A	1333	W7E	C31-C30-C34-O35
3	A	1334[A]	W7E	C31-C30-C34-O35
3	B	1332	W7E	C31-C30-C34-O36
3	C	1332	W7E	C31-C30-C34-O35
3	C	1332	W7E	C31-C30-C34-O36
3	D	1332	W7E	C31-C30-C34-O35
3	C	1333[B]	W7E	C20-C21-O22-C23
3	B	1333[A]	W7E	C27-C26-C29-C30
3	B	1333[B]	W7E	N19-C20-C21-O22
3	A	1334[A]	W7E	C26-C29-C30-C31
3	A	1334[A]	W7E	C26-C29-C30-C34
3	B	1333[A]	W7E	C26-C29-C30-C31
3	B	1333[A]	W7E	C26-C29-C30-C34
3	B	1333[A]	W7E	C25-C26-C29-C30
3	C	1333[A]	W7E	C12-C14-C15-N16
3	B	1333[A]	W7E	C20-C21-O22-C23
3	C	1332	W7E	C27-C26-C29-C30
3	D	1332	W7E	C27-C26-C29-C30
3	A	1334[B]	W7E	C21-C20-N19-C17
3	B	1333[A]	W7E	C21-C20-N19-C17
3	B	1333[A]	W7E	O18-C17-N16-C15
3	B	1333[A]	W7E	C14-C15-N16-C17
3	C	1333[A]	W7E	C14-C15-N16-C17

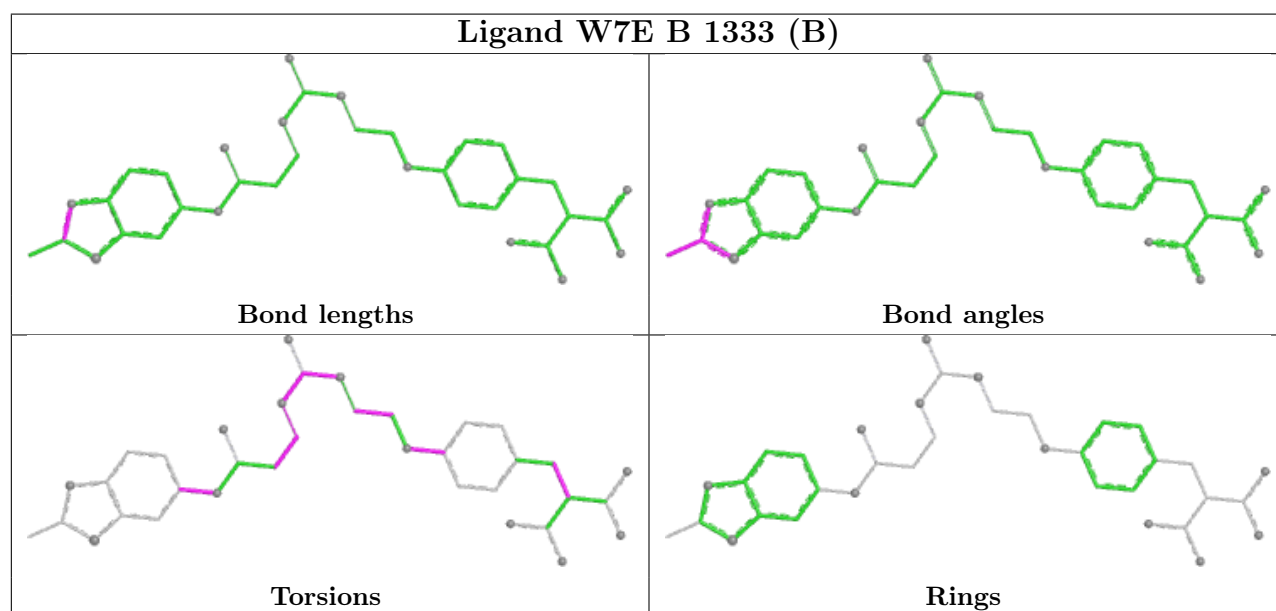
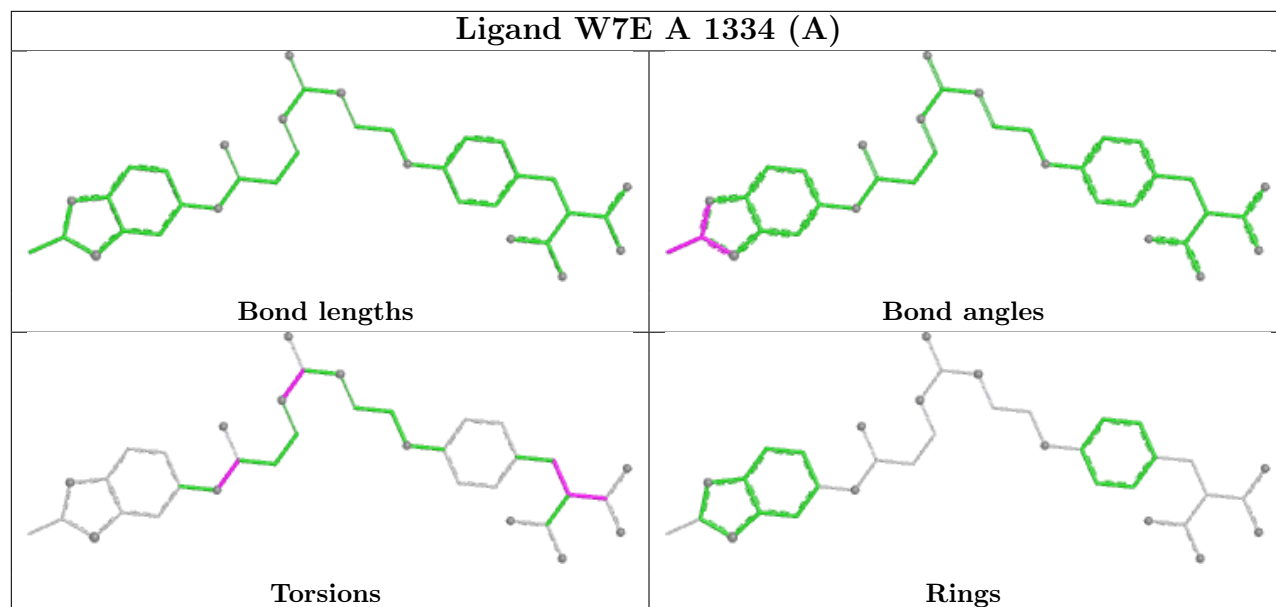
There are no ring outliers.

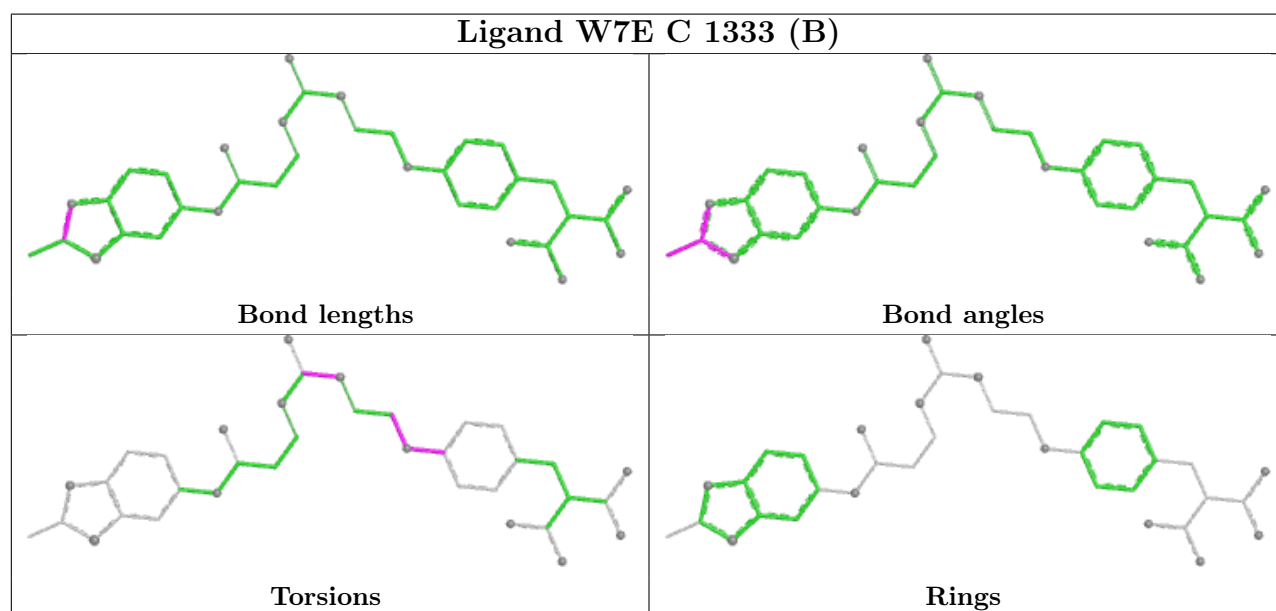
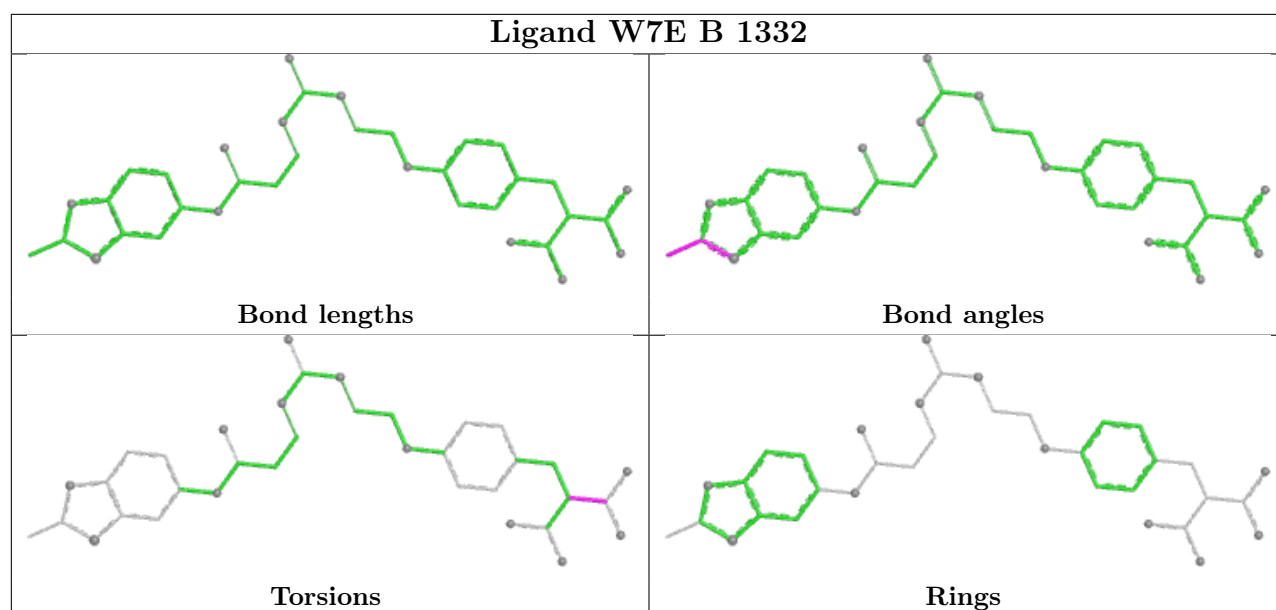
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1333[A]	W7E	1	0
3	D	1332	W7E	2	0
3	A	1334[A]	W7E	1	0
3	B	1332	W7E	4	0
3	A	1334[B]	W7E	1	0
3	C	1332	W7E	2	0
3	A	1333	W7E	2	0
3	B	1333[A]	W7E	3	0

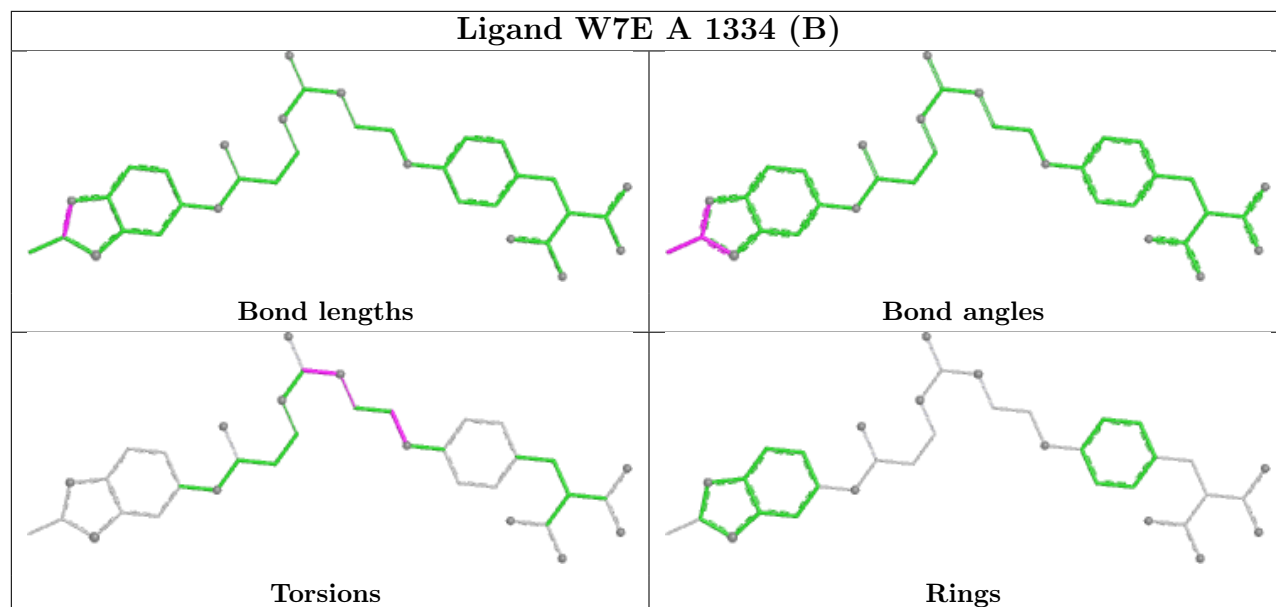
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



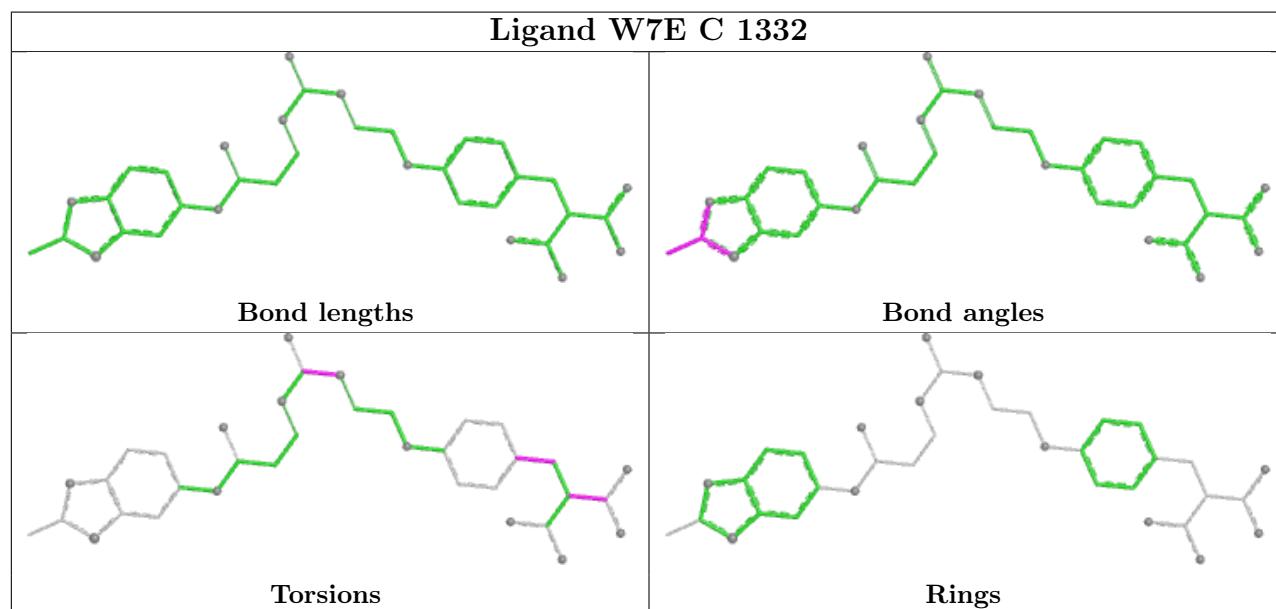


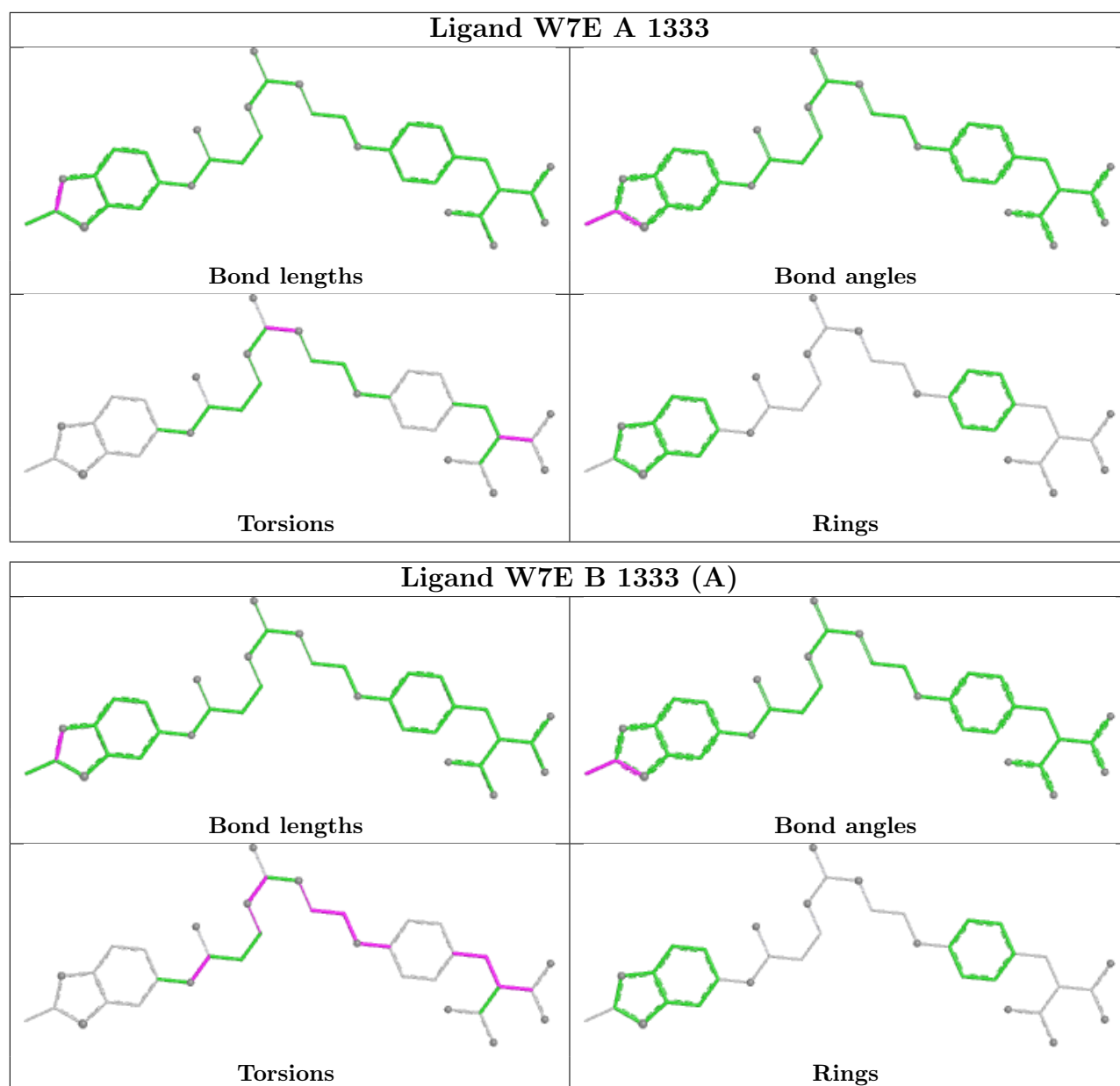


Ligand W7E A 1334 (B)



Ligand W7E C 1332





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	330/331 (99%)	0.26	21 (6%)	25 30	8, 24, 55, 76	5 (1%)
1	B	330/331 (99%)	-0.00	10 (3%)	52 60	9, 20, 45, 62	6 (1%)
1	C	331/331 (100%)	0.16	12 (3%)	46 52	9, 24, 49, 92	2 (0%)
1	D	331/331 (100%)	0.23	19 (5%)	29 35	9, 25, 51, 68	5 (1%)
All	All	1322/1324 (99%)	0.16	62 (4%)	36 42	8, 24, 51, 92	18 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	331	PHE	7.4
1	A	331	PHE	5.2
1	D	238[A]	TYR	5.0
1	A	279	LEU	4.5
1	D	327	LYS	4.3
1	D	329	LEU	4.0
1	D	280	TYR	4.0
1	A	238[A]	TYR	3.7
1	C	1	ALA	3.6
1	B	331	PHE	3.5
1	B	281	GLY	3.5
1	D	281	GLY	3.3
1	D	279	LEU	3.3
1	C	330	GLN	3.3
1	B	2	ALA	3.3
1	A	282	ILE	3.3
1	C	14	GLU	3.2
1	A	323	TRP	3.2
1	A	221	ALA	3.2
1	A	15	GLU	3.2
1	D	12	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	12	LEU	3.0
1	D	331	PHE	3.0
1	D	13	LYS	3.0
1	D	14	GLU	2.9
1	A	17	VAL	2.8
1	C	280	TYR	2.8
1	A	276	ILE	2.7
1	B	15	GLU	2.7
1	D	306	THR	2.7
1	A	14	GLU	2.7
1	A	329	LEU	2.7
1	A	280	TYR	2.7
1	A	11	LEU	2.6
1	C	282	ILE	2.6
1	D	282	ILE	2.6
1	D	325	ILE	2.6
1	C	2	ALA	2.6
1	D	278	GLY	2.6
1	B	223	LYS	2.5
1	A	2	ALA	2.5
1	A	16	GLN	2.5
1	A	281	GLY	2.5
1	B	16	GLN	2.5
1	D	15	GLU	2.5
1	A	317	LYS	2.4
1	B	17	VAL	2.4
1	D	17	VAL	2.4
1	D	221	ALA	2.4
1	C	16	GLN	2.4
1	C	278	GLY	2.4
1	C	238	TYR	2.3
1	B	3	LEU	2.3
1	D	328	GLU	2.3
1	C	276	ILE	2.3
1	D	16	GLN	2.2
1	B	221	ALA	2.2
1	B	12	LEU	2.2
1	A	306	THR	2.1
1	C	15	GLU	2.1
1	A	216	GLN	2.1
1	A	13	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](#)

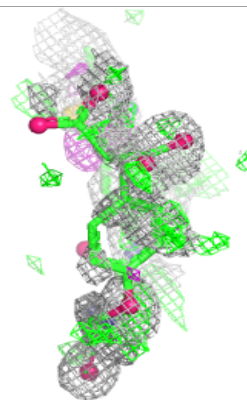
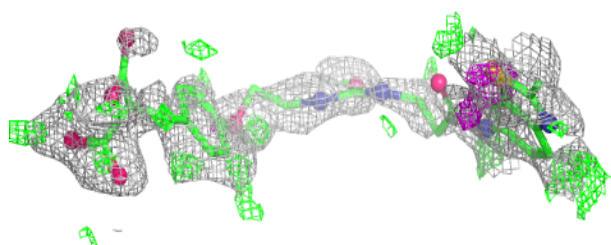
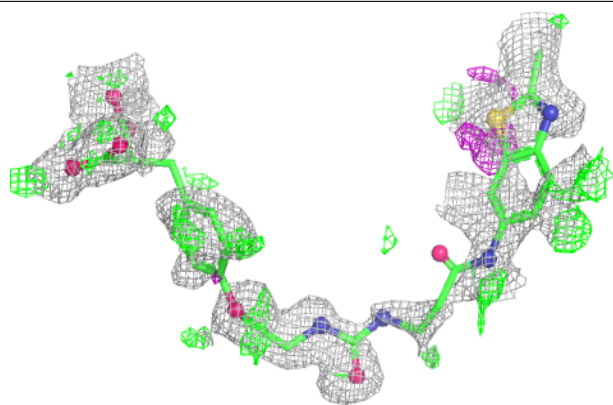
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	W7E	B	1333[A]	36/36	0.68	0.25	20,35,56,57	36
3	W7E	B	1333[B]	36/36	0.68	0.25	27,45,57,58	36
2	GOL	A	1332[B]	6/6	0.72	0.22	46,49,50,51	6
3	W7E	A	1334[A]	36/36	0.76	0.25	18,27,58,59	36
3	W7E	A	1334[B]	36/36	0.76	0.25	18,27,51,53	36
3	W7E	C	1333[A]	36/36	0.79	0.23	23,28,50,50	36
3	W7E	C	1333[B]	36/36	0.79	0.23	22,31,57,57	36
3	W7E	A	1333	36/36	0.96	0.06	17,20,27,28	0
3	W7E	B	1332	36/36	0.96	0.06	16,20,23,24	0
3	W7E	D	1332	36/36	0.96	0.06	20,25,29,30	0
3	W7E	C	1332	36/36	0.97	0.05	18,22,25,27	0

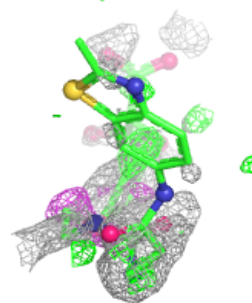
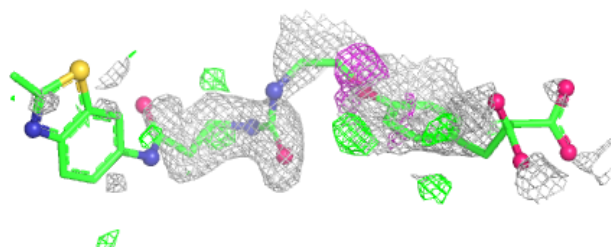
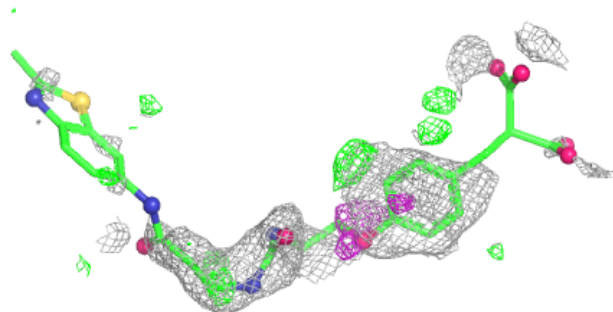
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W7E B 1333 (A):

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

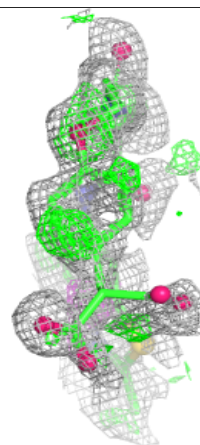
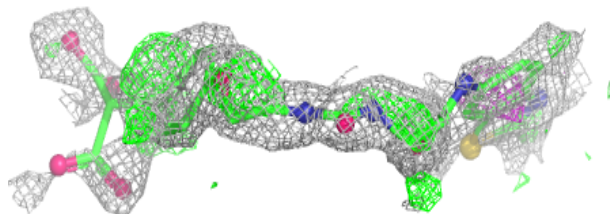
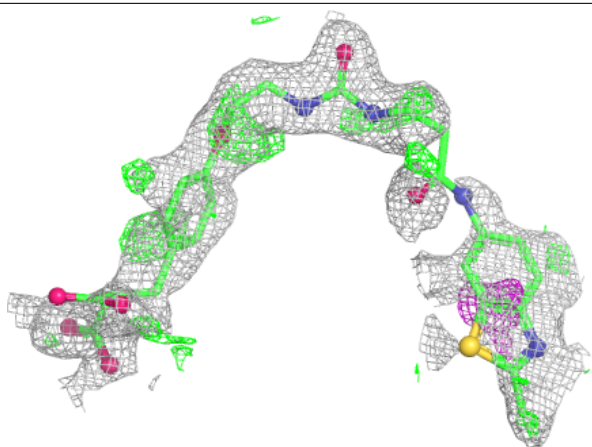
**Electron density around W7E B 1333 (B):**

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

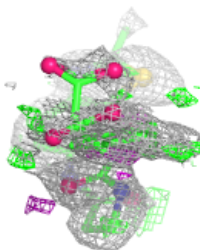
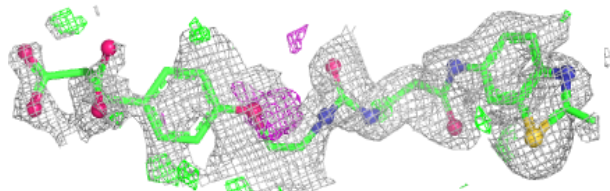
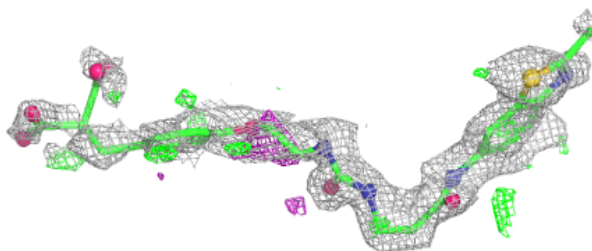


Electron density around W7E A 1334 (A):

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

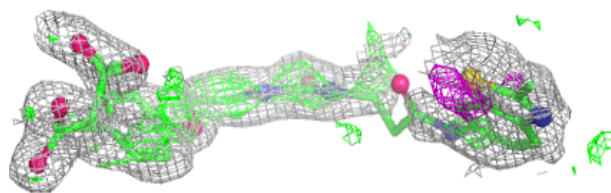
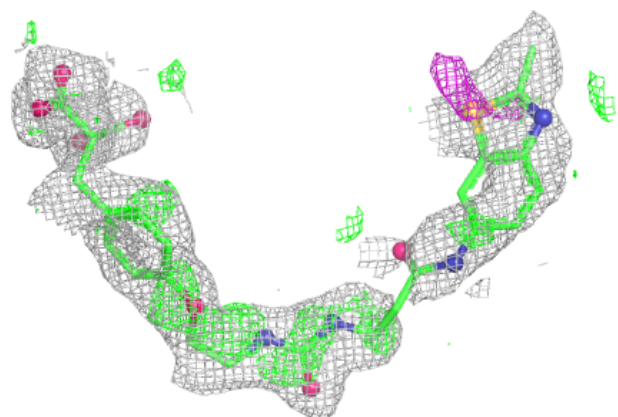
**Electron density around W7E A 1334 (B):**

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

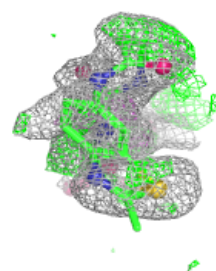
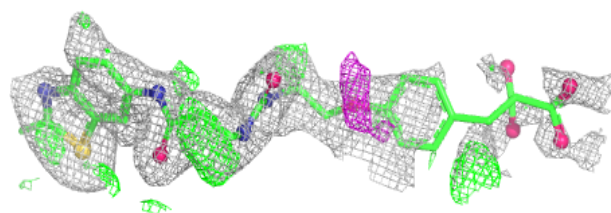
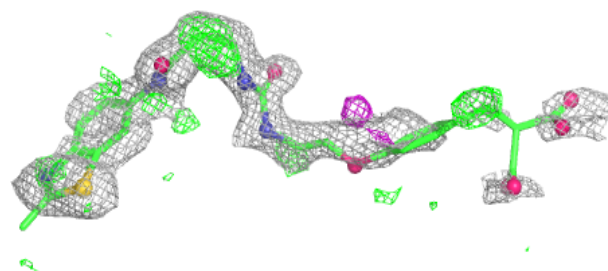


Electron density around W7E C 1333 (A):

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

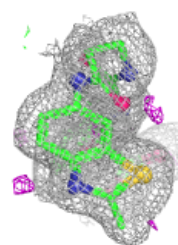
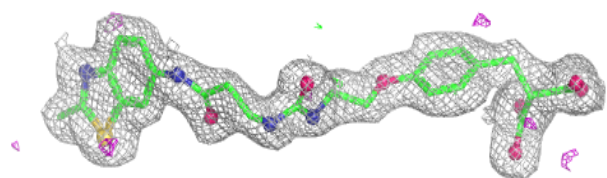
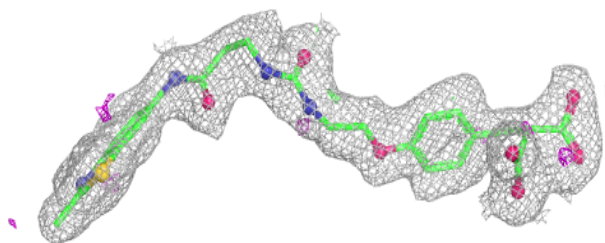
**Electron density around W7E C 1333 (B):**

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

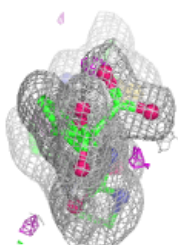
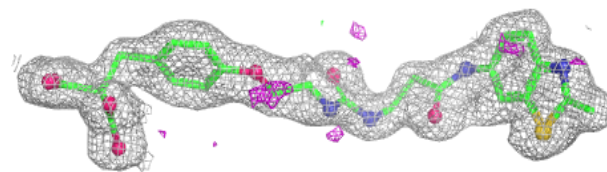
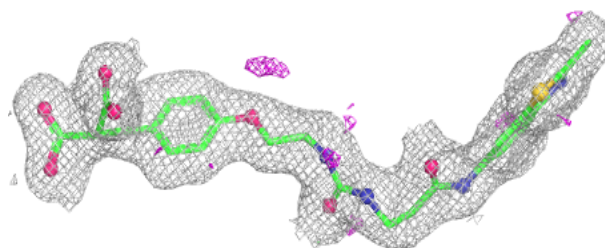


Electron density around W7E A 1333:

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

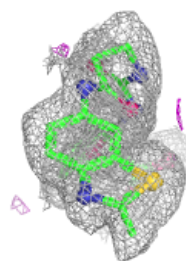
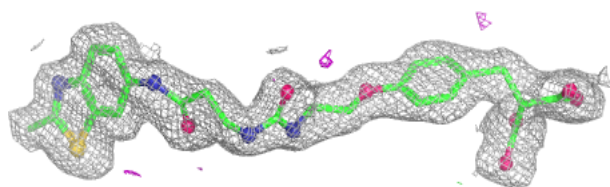
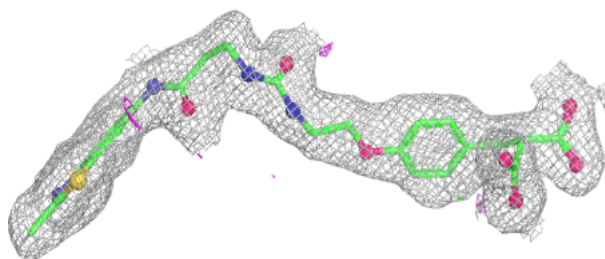
**Electron density around W7E B 1332:**

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

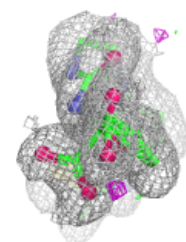
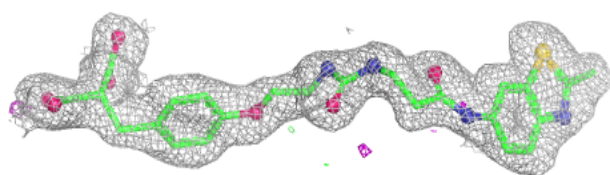
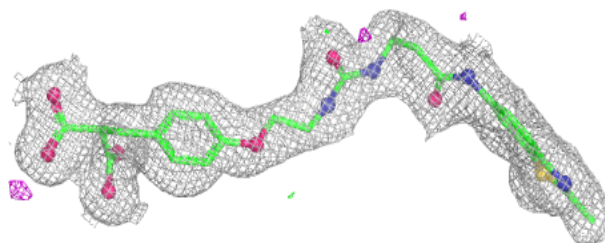


Electron density around W7E D 1332:

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

**Electron density around W7E C 1332:**

$2mF_o-DF_c$ (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.