



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:19 AM UTC

PDB ID : 2X7O / pdb_00002x7o
Title : Crystal structure of TGFbRI complexed with an indolinone inhibitor
Authors : Roth, G.J.; Heckel, A.; Brandl, T.; Grauert, M.; Hoerer, S.; Kley, J.T.; Schnapp, G.; Baum, P.; Mennerich, D.; Schnapp, A.; Park, J.E.
Deposited on : 2010-03-03
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

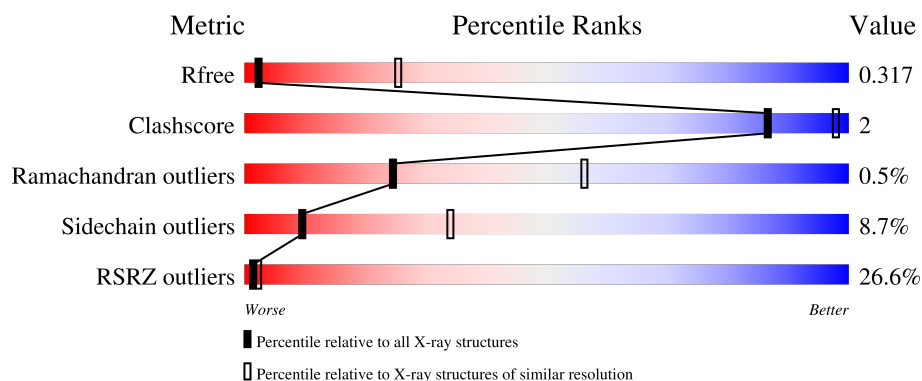
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	342	18% 82% 14% ••
1	B	342	30% 82% 14% •
1	C	342	36% 84% 12% •
1	D	342	25% 85% 11% •
1	E	342	21% 84% 13% •

2 Entry composition [i](#)

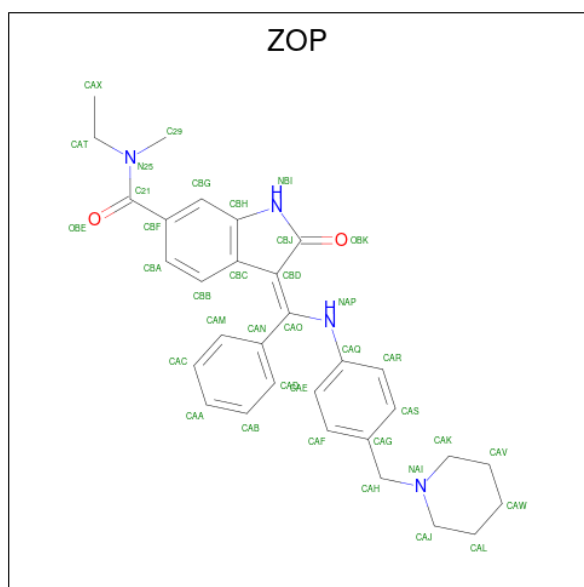
There are 2 unique types of molecules in this entry. The entry contains 13330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TGF-BETA RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	B	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	C	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	D	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			
1	E	330	Total	C	N	O	S	0	0	0
			2629	1658	471	484	16			

- Molecule 2 is (3Z)-N-ETHYL-N-METHYL-2-OXO-3-(PHENYL{[4-(PIPERIDIN-1-YLMETHYL)PHENYL]AMINO}METHYLIDENE)-2,3-DIHYDRO-1H-INDOLE-6-CARBOXAMIDE (CCD ID: ZOP) (formula: C₃₁H₃₄N₄O₂).

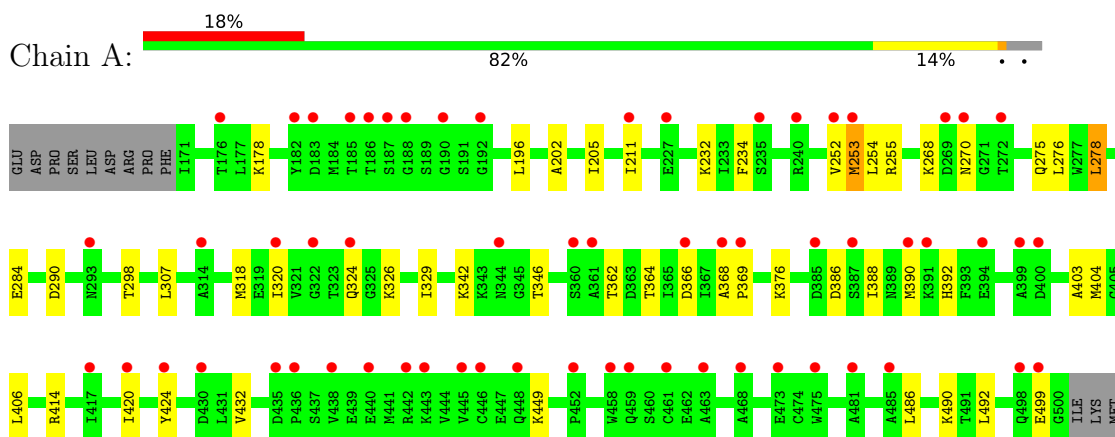


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	31	4	2		
2	B	1	Total	C	N	O	0	0
			37	31	4	2		
2	C	1	Total	C	N	O	0	0
			37	31	4	2		
2	D	1	Total	C	N	O	0	0
			37	31	4	2		
2	E	1	Total	C	N	O	0	0
			37	31	4	2		

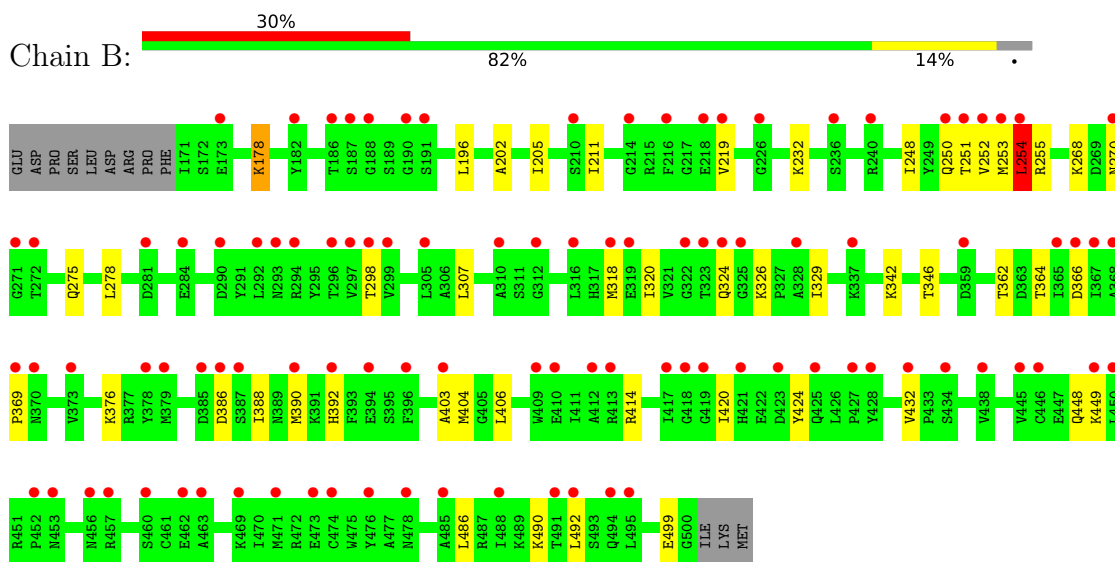
3 Residue-property plots [i](#)

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.

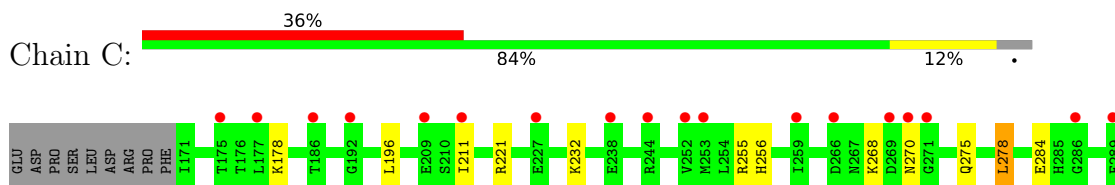
• Molecule 1: TGF-BETA RECEPTOR TYPE I

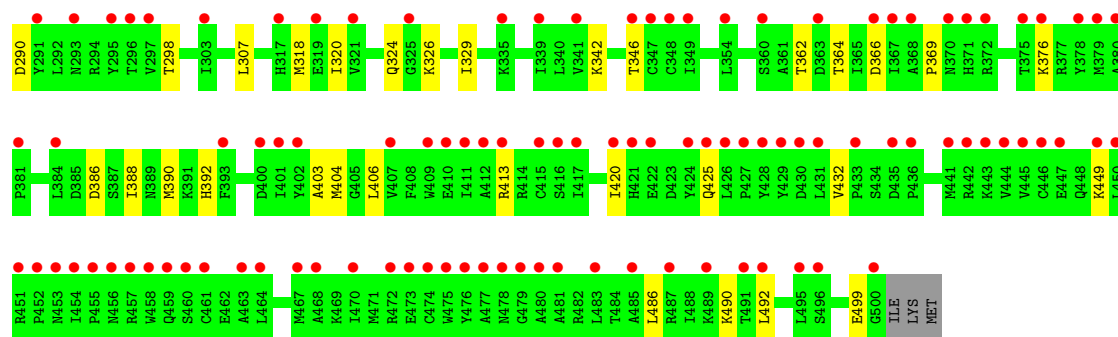


• Molecule 1: TGF-BETA RECEPTOR TYPE I

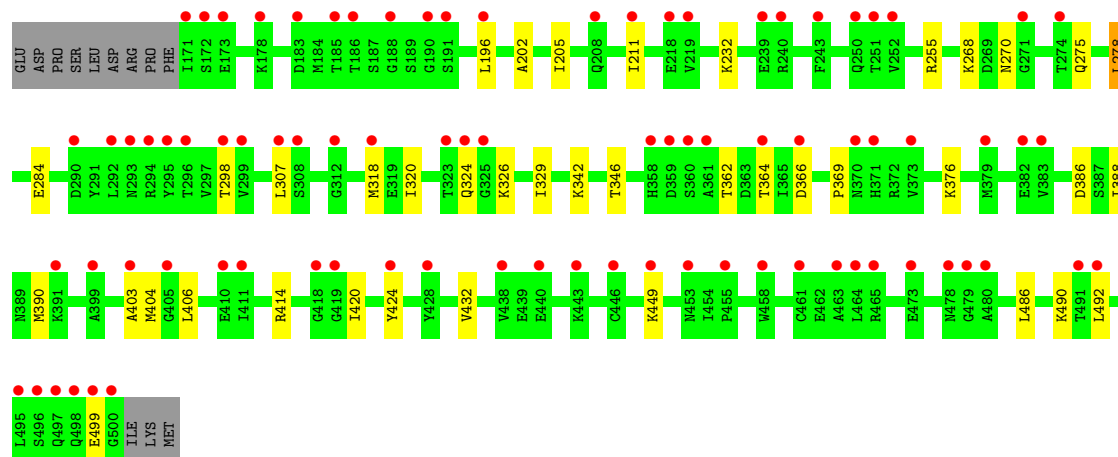
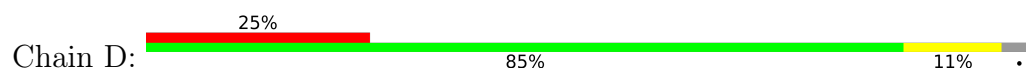


• Molecule 1: TGF-BETA RECEPTOR TYPE I

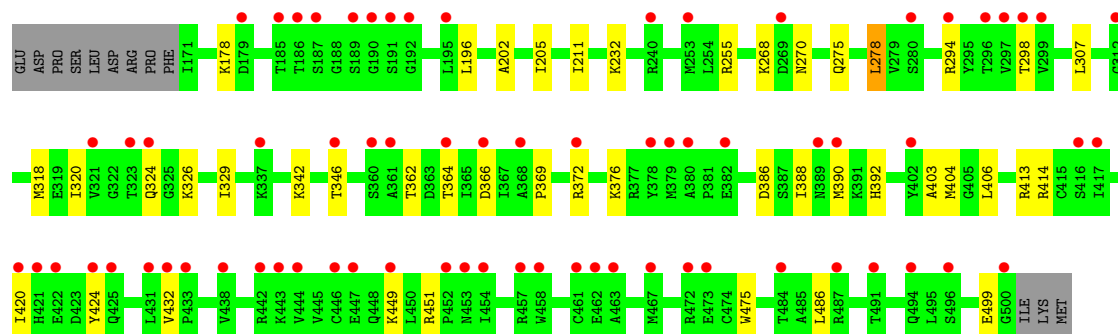
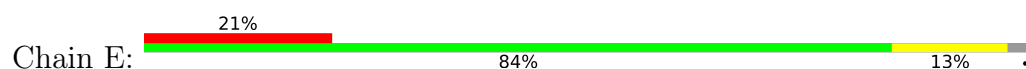




● Molecule 1: TGF-BETA RECEPTOR TYPE I



● Molecule 1: TGF-BETA RECEPTOR TYPE I



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	179.93Å 246.56Å 131.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.72 – 3.70 22.72 – 3.70	Depositor EDS
% Data completeness (in resolution range)	78.6 (22.72-3.70) 76.1 (22.72-3.70)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.06 (at 3.73Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.267 , 0.273 0.318 , 0.317	Depositor DCC
R_{free} test set	1260 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	13330	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: ZOP

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	0.72	0/2682	1.29	1/3622 (0.0%)
1	B	0.72	0/2682	1.31	4/3622 (0.1%)
1	C	0.73	0/2682	1.30	3/3622 (0.1%)
1	D	0.72	0/2682	1.29	1/3622 (0.0%)
1	E	0.72	0/2682	1.29	1/3622 (0.0%)
All	All	0.72	0/13410	1.30	10/18110 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	251	THR	N-CA-C	6.20	118.83	111.33
1	E	366	ASP	N-CA-C	5.77	117.57	111.28
1	A	366	ASP	N-CA-C	5.74	117.54	111.28
1	B	366	ASP	N-CA-C	5.74	117.53	111.28
1	C	366	ASP	N-CA-C	5.73	117.53	111.28
1	D	366	ASP	N-CA-C	5.64	117.43	111.28
1	B	250	GLN	CA-C-N	5.32	127.67	120.38
1	B	250	GLN	C-N-CA	5.32	127.67	120.38
1	C	256	HIS	CA-C-N	5.15	127.18	120.28
1	C	256	HIS	C-N-CA	5.15	127.18	120.28

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	2629	0	2631	14	0
1	B	2629	0	2631	12	0
1	C	2629	0	2631	9	0
1	D	2629	0	2631	10	0
1	E	2629	0	2631	12	0
2	A	37	0	34	4	0
2	B	37	0	34	1	0
2	C	37	0	34	3	0
2	D	37	0	34	3	0
2	E	37	0	34	4	0
All	All	13330	0	13325	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HB2	2:B:600:ZOP:H293	1.58	0.84
1:D:232:LYS:HB2	2:D:600:ZOP:H293	1.59	0.84
1:A:232:LYS:HB2	2:A:600:ZOP:H293	1.62	0.82
1:E:232:LYS:HB2	2:E:600:ZOP:H293	1.65	0.78
1:C:232:LYS:HB2	2:C:600:ZOP:H293	1.64	0.77
1:A:290:ASP:HB3	2:A:600:ZOP:HAL2	1.80	0.62
1:E:369:PRO:HB2	1:E:390:MET:HB3	1.84	0.60
1:B:252:VAL:HG23	1:B:254:LEU:HD23	1.82	0.60
1:C:369:PRO:HB2	1:C:390:MET:HB3	1.84	0.60
1:A:369:PRO:HB2	1:A:390:MET:HB3	1.83	0.59
1:B:369:PRO:HB2	1:B:390:MET:HB3	1.84	0.59
1:D:369:PRO:HB2	1:D:390:MET:HB3	1.84	0.58
1:C:278:LEU:HD23	2:C:600:ZOP:HAT1	1.85	0.57
1:C:413:ARG:HH22	1:C:425:GLN:HB2	1.75	0.51
1:E:268:LYS:HB2	1:E:275:GLN:HB2	1.94	0.50
1:B:268:LYS:HB2	1:B:275:GLN:HB2	1.94	0.49
1:D:268:LYS:HB2	1:D:275:GLN:HB2	1.93	0.49
1:A:268:LYS:HB2	1:A:275:GLN:HB2	1.94	0.49
1:C:268:LYS:HB2	1:C:275:GLN:HB2	1.93	0.48
1:A:414:ARG:HH21	1:A:424:TYR:H	1.61	0.48
1:A:368:ALA:HB2	1:B:178:LYS:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ALA:HA	1:C:406:LEU:HD12	1.96	0.48
1:A:403:ALA:HA	1:A:406:LEU:HD12	1.96	0.48
1:A:320:ILE:HD12	1:A:326:LYS:HG2	1.96	0.48
1:D:320:ILE:HD12	1:D:326:LYS:HG2	1.96	0.47
1:C:320:ILE:HD12	1:C:326:LYS:HG2	1.96	0.47
1:D:403:ALA:HA	1:D:406:LEU:HD12	1.96	0.47
1:B:403:ALA:HA	1:B:406:LEU:HD12	1.96	0.47
1:B:414:ARG:HD2	1:B:424:TYR:HB2	1.96	0.47
1:E:320:ILE:HD12	1:E:326:LYS:HG2	1.96	0.47
1:B:320:ILE:HD12	1:B:326:LYS:HG2	1.97	0.47
1:E:414:ARG:HH21	1:E:424:TYR:H	1.63	0.46
1:E:403:ALA:HA	1:E:406:LEU:HD12	1.96	0.46
1:D:342:LYS:HD3	1:D:346:THR:HB	1.99	0.44
1:B:342:LYS:HD3	1:B:346:THR:HB	1.99	0.44
1:E:294:ARG:HH11	2:E:600:ZOP:HAW1	1.82	0.44
1:E:342:LYS:HD3	1:E:346:THR:HB	1.99	0.44
1:A:211:ILE:HG23	2:A:600:ZOP:HAD	1.99	0.43
1:C:342:LYS:HD3	1:C:346:THR:HB	2.00	0.43
1:A:253:MET:O	1:A:253:MET:HG3	2.19	0.43
1:D:414:ARG:HH21	1:D:424:TYR:H	1.67	0.43
1:B:211:ILE:HD12	1:B:219:VAL:HG12	1.99	0.43
1:A:278:LEU:HD23	2:A:600:ZOP:HAT1	2.00	0.42
1:A:342:LYS:HD3	1:A:346:THR:HB	2.01	0.42
1:E:211:ILE:HG23	2:E:600:ZOP:HAD	2.01	0.42
1:D:211:ILE:HG23	2:D:600:ZOP:HAD	2.00	0.42
1:A:234:PHE:HB2	1:A:276:LEU:HB2	2.02	0.42
1:C:290:ASP:HB3	2:C:600:ZOP:HAL2	2.01	0.42
1:B:202:ALA:HA	1:B:205:ILE:HD12	2.02	0.41
1:E:202:ALA:HA	1:E:205:ILE:HD12	2.03	0.41
1:B:248:ILE:O	1:B:252:VAL:HG22	2.20	0.41
1:D:202:ALA:HA	1:D:205:ILE:HD12	2.02	0.40
1:D:278:LEU:HD23	2:D:600:ZOP:HAT1	2.02	0.40
1:A:202:ALA:HA	1:A:205:ILE:HD12	2.02	0.40
1:E:278:LEU:HD23	2:E:600:ZOP:HAT1	2.03	0.40
1:E:451:ARG:HG2	1:E:475:TRP:HB3	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	328/342 (96%)	306 (93%)	20 (6%)	2 (1%)	21	52
1	B	328/342 (96%)	306 (93%)	19 (6%)	3 (1%)	14	45
1	C	328/342 (96%)	305 (93%)	22 (7%)	1 (0%)	36	65
1	D	328/342 (96%)	305 (93%)	22 (7%)	1 (0%)	36	65
1	E	328/342 (96%)	306 (93%)	21 (6%)	1 (0%)	36	65
All	All	1640/1710 (96%)	1528 (93%)	104 (6%)	8 (0%)	24	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	ARG
1	B	254	LEU
1	B	255	ARG
1	C	255	ARG
1	D	255	ARG
1	E	255	ARG
1	B	253	MET
1	A	252	VAL

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	282/294 (96%)	256 (91%)	26 (9%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	282/294 (96%)	257 (91%)	25 (9%)	9	33
1	C	282/294 (96%)	256 (91%)	26 (9%)	8	32
1	D	282/294 (96%)	260 (92%)	22 (8%)	11	37
1	E	282/294 (96%)	259 (92%)	23 (8%)	10	36
All	All	1410/1470 (96%)	1288 (91%)	122 (9%)	9	34

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	LYS
1	A	196	LEU
1	A	253	MET
1	A	254	LEU
1	A	270	ASN
1	A	278	LEU
1	A	284	GLU
1	A	298	THR
1	A	307	LEU
1	A	318	MET
1	A	324	GLN
1	A	329	ILE
1	A	362	THR
1	A	364	THR
1	A	376	LYS
1	A	386	ASP
1	A	388	ILE
1	A	392	HIS
1	A	404	MET
1	A	420	ILE
1	A	432	VAL
1	A	449	LYS
1	A	486	LEU
1	A	490	LYS
1	A	492	LEU
1	A	499	GLU
1	B	178	LYS
1	B	196	LEU
1	B	254	LEU
1	B	270	ASN
1	B	278	LEU
1	B	298	THR

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Mol	Chain	Res	Type
1	B	307	LEU
1	B	318	MET
1	B	324	GLN
1	B	329	ILE
1	B	362	THR
1	B	364	THR
1	B	376	LYS
1	B	386	ASP
1	B	388	ILE
1	B	392	HIS
1	B	404	MET
1	B	420	ILE
1	B	432	VAL
1	B	448	GLN
1	B	449	LYS
1	B	486	LEU
1	B	490	LYS
1	B	492	LEU
1	B	499	GLU
1	C	178	LYS
1	C	196	LEU
1	C	211	ILE
1	C	221	ARG
1	C	270	ASN
1	C	278	LEU
1	C	284	GLU
1	C	298	THR
1	C	307	LEU
1	C	318	MET
1	C	324	GLN
1	C	329	ILE
1	C	362	THR
1	C	364	THR
1	C	376	LYS
1	C	386	ASP
1	C	388	ILE
1	C	392	HIS
1	C	404	MET
1	C	420	ILE
1	C	432	VAL
1	C	449	LYS
1	C	486	LEU

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Mol	Chain	Res	Type
1	C	490	LYS
1	C	492	LEU
1	C	499	GLU
1	D	196	LEU
1	D	270	ASN
1	D	278	LEU
1	D	284	GLU
1	D	298	THR
1	D	307	LEU
1	D	318	MET
1	D	324	GLN
1	D	329	ILE
1	D	362	THR
1	D	364	THR
1	D	376	LYS
1	D	386	ASP
1	D	388	ILE
1	D	404	MET
1	D	420	ILE
1	D	432	VAL
1	D	449	LYS
1	D	486	LEU
1	D	490	LYS
1	D	492	LEU
1	D	499	GLU
1	E	178	LYS
1	E	196	LEU
1	E	270	ASN
1	E	278	LEU
1	E	298	THR
1	E	307	LEU
1	E	318	MET
1	E	324	GLN
1	E	329	ILE
1	E	362	THR
1	E	364	THR
1	E	372	ARG
1	E	376	LYS
1	E	386	ASP
1	E	388	ILE
1	E	392	HIS
1	E	404	MET

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Mol	Chain	Res	Type
1	E	413	ARG
1	E	420	ILE
1	E	432	VAL
1	E	449	LYS
1	E	486	LEU
1	E	499	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	283	HIS
1	A	285	HIS
1	A	315	HIS
1	A	425	GLN
1	A	478	ASN
1	A	494	GLN
1	B	267	ASN
1	B	283	HIS
1	B	285	HIS
1	B	425	GLN
1	B	478	ASN
1	B	494	GLN
1	C	267	ASN
1	C	478	ASN
1	C	494	GLN
1	D	425	GLN
1	D	478	ASN
1	D	494	GLN
1	E	267	ASN
1	E	283	HIS
1	E	425	GLN
1	E	478	ASN
1	E	494	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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ZOP	A	600	-	40,41,41	1.24	3 (7%)	52,57,57	1.29	4 (7%)
2	ZOP	C	600	-	40,41,41	1.25	5 (12%)	52,57,57	1.34	7 (13%)
2	ZOP	B	600	-	40,41,41	1.29	5 (12%)	52,57,57	1.36	7 (13%)
2	ZOP	E	600	-	40,41,41	1.28	4 (10%)	52,57,57	1.43	5 (9%)
2	ZOP	D	600	-	40,41,41	1.23	2 (5%)	52,57,57	1.39	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZOP	A	600	-	-	2/26/46/46	0/5/5/5
2	ZOP	C	600	-	-	2/26/46/46	0/5/5/5
2	ZOP	B	600	-	-	2/26/46/46	0/5/5/5
2	ZOP	E	600	-	-	2/26/46/46	0/5/5/5
2	ZOP	D	600	-	-	2/26/46/46	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ZOP	CBD-CBJ	-2.45	1.43	1.49
2	E	600	ZOP	CBD-CBJ	-2.42	1.43	1.49
2	C	600	ZOP	CBJ-NBI	-2.34	1.33	1.36
2	D	600	ZOP	CBD-CBJ	-2.33	1.44	1.49
2	A	600	ZOP	CBD-CBJ	-2.27	1.44	1.49
2	C	600	ZOP	CBD-CBJ	-2.26	1.44	1.49
2	D	600	ZOP	C21-N25	2.22	1.38	1.34
2	B	600	ZOP	C21-N25	2.21	1.38	1.34
2	E	600	ZOP	C21-N25	2.20	1.38	1.34
2	A	600	ZOP	CBJ-NBI	-2.16	1.33	1.36
2	C	600	ZOP	CAM-CAN	2.12	1.42	1.39
2	B	600	ZOP	CBG-CBF	2.10	1.42	1.39
2	B	600	ZOP	CAD-CAN	2.09	1.42	1.39
2	E	600	ZOP	CBJ-NBI	-2.08	1.33	1.36
2	C	600	ZOP	C21-N25	2.07	1.38	1.34
2	E	600	ZOP	CAM-CAN	2.03	1.42	1.39
2	A	600	ZOP	CAM-CAN	2.03	1.42	1.39
2	B	600	ZOP	CAM-CAN	2.01	1.42	1.39
2	C	600	ZOP	CBA-CBF	2.01	1.42	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	ZOP	CBD-CBJ-NBI	4.80	110.27	107.01
2	A	600	ZOP	CBD-CBJ-NBI	4.70	110.20	107.01
2	D	600	ZOP	CBD-CBJ-NBI	4.65	110.17	107.01
2	B	600	ZOP	CBD-CBJ-NBI	4.59	110.12	107.01
2	E	600	ZOP	CBD-CBJ-NBI	4.54	110.09	107.01
2	E	600	ZOP	CAG-CAH-NAI	-3.63	105.73	113.15
2	D	600	ZOP	CAG-CAH-NAI	-3.54	105.89	113.15
2	A	600	ZOP	CBG-CBH-CBC	-3.52	119.72	122.52
2	B	600	ZOP	CAG-CAH-NAI	-3.40	106.18	113.15
2	C	600	ZOP	CAN-CAO-NAP	3.39	123.58	119.03
2	B	600	ZOP	CBG-CBH-CBC	-3.19	119.98	122.52
2	D	600	ZOP	CBG-CBH-CBC	-3.07	120.07	122.52
2	A	600	ZOP	CAN-CAO-NAP	2.98	123.02	119.03
2	E	600	ZOP	CBG-CBH-CBC	-2.96	120.16	122.52
2	E	600	ZOP	CAN-CAO-NAP	2.95	122.99	119.03
2	B	600	ZOP	CAN-CAO-NAP	2.93	122.96	119.03
2	D	600	ZOP	CAN-CAO-NAP	2.79	122.77	119.03
2	C	600	ZOP	CBG-CBH-CBC	-2.77	120.31	122.52
2	E	600	ZOP	CBF-C21-N25	2.38	122.94	118.92
2	C	600	ZOP	CAQ-NAP-CAO	2.28	134.81	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ZOP	CAN-CAO-CBD	-2.25	119.01	121.67
2	B	600	ZOP	CBF-C21-N25	2.14	122.53	118.92
2	B	600	ZOP	CAK-NAI-CAJ	2.11	113.39	108.84
2	C	600	ZOP	CAK-NAI-CAJ	2.06	113.28	108.84
2	C	600	ZOP	CAM-CAN-CAO	-2.06	118.32	120.76
2	A	600	ZOP	CAN-CAO-CBD	-2.06	119.24	121.67
2	C	600	ZOP	CAG-CAH-NAI	-2.05	108.95	113.15
2	D	600	ZOP	CBF-C21-N25	2.01	122.31	118.92
2	D	600	ZOP	CAQ-NAP-CAO	2.01	133.93	127.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	ZOP	CAG-CAH-NAI-CAJ
2	E	600	ZOP	CAG-CAH-NAI-CAK
2	B	600	ZOP	CAG-CAH-NAI-CAK
2	E	600	ZOP	CAG-CAH-NAI-CAJ
2	A	600	ZOP	CAG-CAH-NAI-CAJ
2	D	600	ZOP	CAG-CAH-NAI-CAK
2	A	600	ZOP	CAG-CAH-NAI-CAK
2	D	600	ZOP	CAG-CAH-NAI-CAJ
2	C	600	ZOP	CAG-CAH-NAI-CAK
2	C	600	ZOP	CAG-CAH-NAI-CAJ

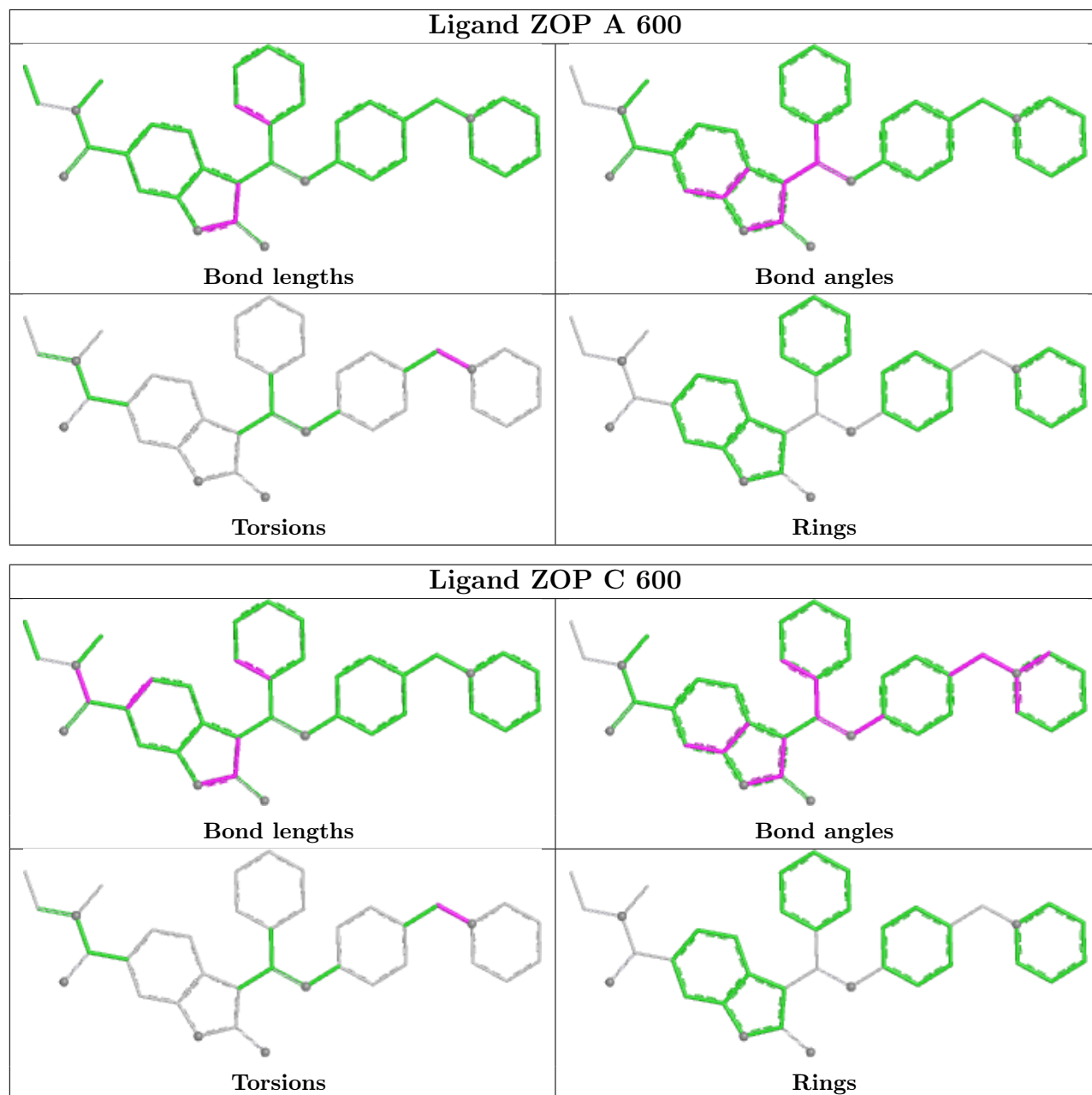
There are no ring outliers.

5 monomers are involved in 15 short contacts:

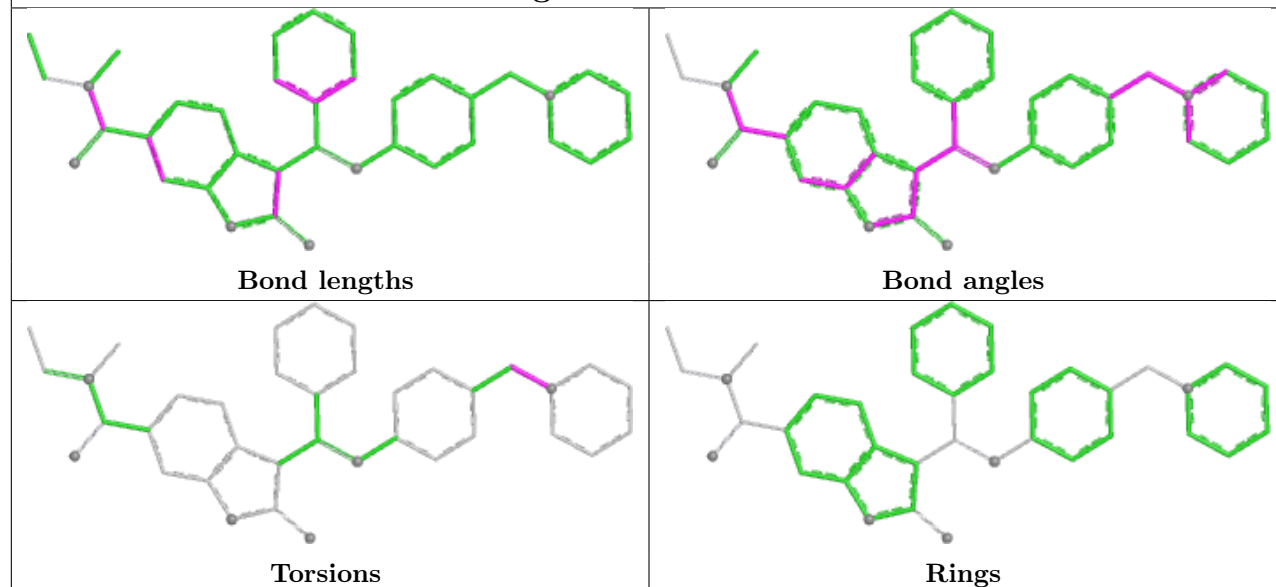
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	ZOP	4	0
2	C	600	ZOP	3	0
2	B	600	ZOP	1	0
2	E	600	ZOP	4	0
2	D	600	ZOP	3	0

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

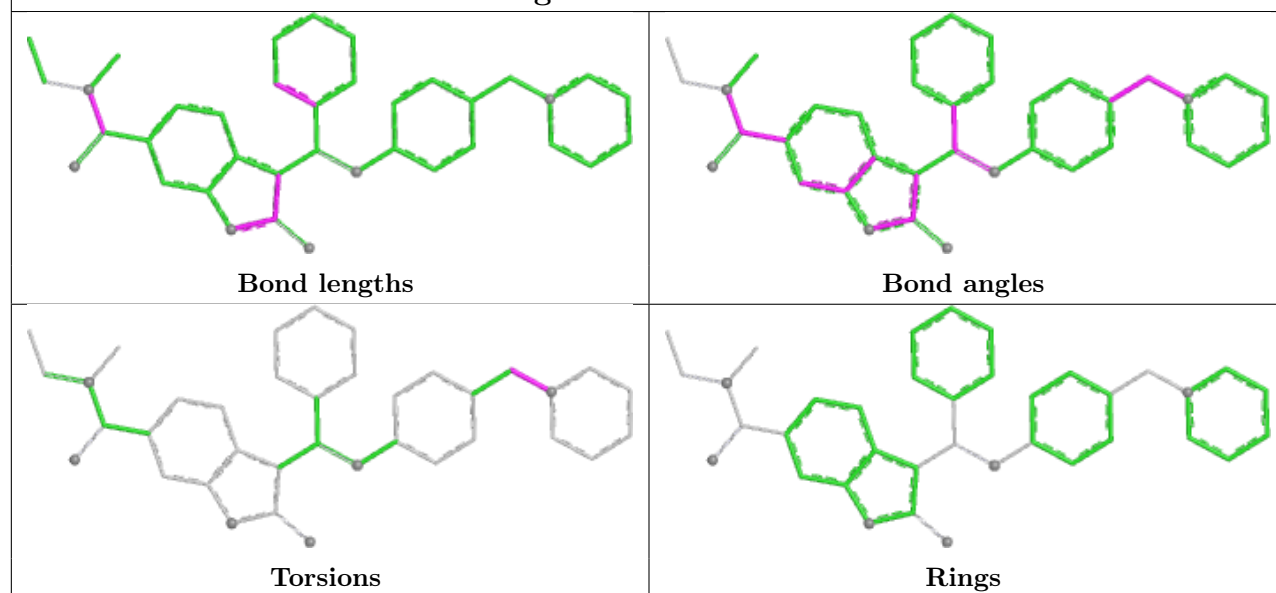
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

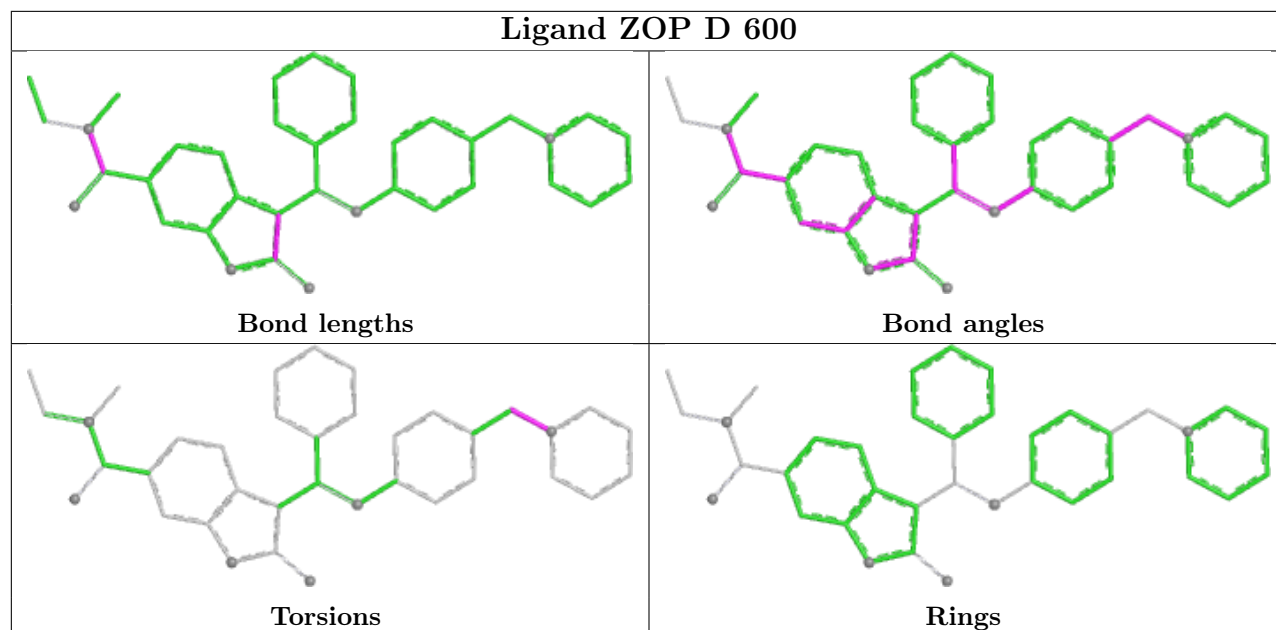


Ligand ZOP B 600



Ligand ZOP E 600





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	330/342 (96%)	1.33	61 (18%) 3 4	19, 52, 81, 91	0
1	B	330/342 (96%)	1.60	101 (30%) 1 1	19, 51, 81, 92	0
1	C	330/342 (96%)	1.80	122 (36%) 1 1	20, 53, 82, 92	0
1	D	330/342 (96%)	1.50	84 (25%) 1 2	18, 52, 82, 91	0
1	E	330/342 (96%)	1.30	71 (21%) 2 3	19, 52, 82, 92	0
All	All	1650/1710 (96%)	1.51	439 (26%) 1 2	18, 52, 82, 92	0

All (439) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	441	MET	6.6
1	A	446	CYS	6.4
1	C	477	ALA	6.4
1	C	455	PRO	6.3
1	C	458	TRP	6.2
1	C	416	SER	5.7
1	C	454	ILE	5.5
1	D	183	ASP	5.3
1	B	186	THR	5.2
1	B	410	GLU	5.2
1	C	407	VAL	5.2
1	D	438	VAL	5.1
1	C	400	ASP	5.1
1	C	368	ALA	5.0
1	E	368	ALA	4.9
1	C	491	THR	4.9
1	C	451	ARG	4.9
1	B	394	GLU	4.8
1	C	427	PRO	4.8
1	A	390	MET	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	424	TYR	4.7
1	B	251	THR	4.7
1	D	498	GLN	4.6
1	C	421	HIS	4.6
1	B	312	GLY	4.6
1	C	483	LEU	4.5
1	C	485	ALA	4.5
1	C	450	LEU	4.4
1	C	380	ALA	4.3
1	D	473	GLU	4.3
1	D	299	VAL	4.3
1	D	446	CYS	4.2
1	D	252	VAL	4.2
1	D	323	THR	4.2
1	C	409	TRP	4.2
1	E	496	SER	4.2
1	B	323	THR	4.2
1	C	452	PRO	4.2
1	D	361	ALA	4.2
1	A	481	ALA	4.1
1	B	290	ASP	4.0
1	E	190	GLY	4.0
1	A	435	ASP	3.9
1	D	496	SER	3.9
1	B	368	ALA	3.9
1	C	367	ILE	3.9
1	C	467	MET	3.8
1	C	474	CYS	3.8
1	B	182	TYR	3.8
1	B	324	GLN	3.8
1	B	187	SER	3.8
1	C	286	GLY	3.8
1	C	375	THR	3.7
1	E	433	PRO	3.7
1	C	496	SER	3.7
1	C	464	LEU	3.7
1	C	433	PRO	3.6
1	A	183	ASP	3.6
1	B	390	MET	3.6
1	A	369	PRO	3.6
1	B	296	THR	3.6
1	C	463	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	176	THR	3.6
1	A	368	ALA	3.5
1	C	500	GLY	3.5
1	B	432	VAL	3.5
1	C	411	ILE	3.5
1	C	456	ASN	3.5
1	D	290	ASP	3.5
1	C	445	VAL	3.5
1	D	211	ILE	3.5
1	C	443	LYS	3.5
1	A	186	THR	3.5
1	E	444	VAL	3.5
1	C	266	ASP	3.5
1	E	297	VAL	3.4
1	D	418	GLY	3.4
1	C	429	TYR	3.4
1	B	403	ALA	3.4
1	A	188	GLY	3.4
1	B	421	HIS	3.4
1	D	366	ASP	3.3
1	C	461	CYS	3.3
1	D	478	ASN	3.3
1	B	366	ASP	3.3
1	D	465	ARG	3.3
1	D	497	GLN	3.3
1	C	381	PRO	3.2
1	B	379	MET	3.2
1	C	415	CYS	3.2
1	B	473	GLU	3.2
1	B	281	ASP	3.2
1	E	324	GLN	3.2
1	E	299	VAL	3.2
1	B	396	PHE	3.2
1	C	384	LEU	3.2
1	B	386	ASP	3.1
1	B	214	GLY	3.1
1	C	475	TRP	3.1
1	B	438	VAL	3.1
1	D	495	LEU	3.1
1	B	460	SER	3.1
1	B	452	PRO	3.1
1	E	294	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	226	GLY	3.1
1	D	325	GLY	3.1
1	A	475	TRP	3.1
1	C	472	ARG	3.1
1	A	417	ILE	3.0
1	C	420	ILE	3.0
1	D	383	VAL	3.0
1	D	458	TRP	3.0
1	A	227	GLU	3.0
1	B	318	MET	3.0
1	D	294	ARG	3.0
1	C	446	CYS	3.0
1	D	461	CYS	3.0
1	B	252	VAL	3.0
1	A	458	TRP	3.0
1	A	420	ILE	3.0
1	B	270	ASN	3.0
1	C	417	ILE	3.0
1	C	449	LYS	3.0
1	B	219	VAL	3.0
1	B	417	ILE	3.0
1	C	431	LEU	3.0
1	E	189	SER	3.0
1	B	453	ASN	3.0
1	E	458	TRP	3.0
1	D	172	SER	3.0
1	C	422	GLU	2.9
1	E	420	ILE	2.9
1	D	364	THR	2.9
1	D	296	THR	2.9
1	C	468	ALA	2.9
1	C	489	LYS	2.9
1	C	303	ILE	2.9
1	D	358	HIS	2.9
1	B	190	GLY	2.9
1	C	341	VAL	2.9
1	D	419	GLY	2.9
1	B	469	LYS	2.9
1	C	426	LEU	2.9
1	E	453	ASN	2.9
1	B	367	ILE	2.9
1	D	382	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	500	GLY	2.9
1	C	360	SER	2.8
1	C	430	ASP	2.8
1	D	500	GLY	2.8
1	C	253	MET	2.8
1	A	424	TYR	2.8
1	A	360	SER	2.8
1	B	173	GLU	2.8
1	D	218	GLU	2.8
1	A	385	ASP	2.8
1	B	250	GLN	2.8
1	E	366	ASP	2.8
1	D	188	GLY	2.8
1	D	440	GLU	2.8
1	A	463	ALA	2.8
1	C	366	ASP	2.8
1	C	349	ILE	2.8
1	C	478	ASN	2.8
1	B	310	ALA	2.8
1	B	191	SER	2.8
1	B	299	VAL	2.8
1	B	434	SER	2.8
1	C	436	PRO	2.8
1	C	295	TYR	2.8
1	B	328	ALA	2.8
1	E	185	THR	2.8
1	E	296	THR	2.8
1	A	400	ASP	2.7
1	E	461	CYS	2.7
1	C	459	GLN	2.7
1	D	479	GLY	2.7
1	E	462	GLU	2.7
1	C	413	ARG	2.7
1	E	457	ARG	2.7
1	B	423	ASP	2.7
1	B	322	GLY	2.7
1	C	378	TYR	2.7
1	B	463	ALA	2.7
1	B	456	ASN	2.7
1	E	191	SER	2.7
1	B	325	GLY	2.7
1	D	307	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	478	ASN	2.7
1	B	488	ILE	2.7
1	B	319	GLU	2.7
1	A	445	VAL	2.7
1	C	442	ARG	2.7
1	C	447	GLU	2.7
1	C	297	VAL	2.6
1	C	371	HIS	2.6
1	C	325	GLY	2.6
1	B	370	ASN	2.6
1	C	372	ARG	2.6
1	A	293	ASN	2.6
1	A	344	ASN	2.6
1	D	243	PHE	2.6
1	E	454	ILE	2.6
1	D	403	ALA	2.6
1	E	494	GLN	2.6
1	A	366	ASP	2.6
1	B	365	ILE	2.6
1	E	431	LEU	2.6
1	E	186	THR	2.6
1	C	269	ASP	2.6
1	B	387	SER	2.6
1	A	436	PRO	2.6
1	A	498	GLN	2.6
1	A	461	CYS	2.6
1	A	185	THR	2.6
1	B	491	THR	2.6
1	B	236	SER	2.6
1	B	385	ASP	2.6
1	C	321	VAL	2.6
1	E	467	MET	2.6
1	A	361	ALA	2.6
1	A	448	GLN	2.6
1	C	291	TYR	2.5
1	D	171	ILE	2.5
1	A	394	GLU	2.5
1	E	425	GLN	2.5
1	E	424	TYR	2.5
1	D	191	SER	2.5
1	E	446	CYS	2.5
1	B	254	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	316	LEU	2.5
1	A	452	PRO	2.5
1	C	481	ALA	2.5
1	A	192	GLY	2.5
1	B	418	GLY	2.5
1	E	312	GLY	2.5
1	C	492	LEU	2.5
1	C	293	ASN	2.5
1	C	393	PHE	2.5
1	E	192	GLY	2.5
1	E	487	ARG	2.5
1	E	491	THR	2.5
1	B	428	TYR	2.5
1	C	177	LEU	2.5
1	D	371	HIS	2.5
1	E	187	SER	2.5
1	A	438	VAL	2.5
1	B	471	MET	2.5
1	B	271	GLY	2.5
1	B	413	ARG	2.5
1	A	187	SER	2.5
1	A	252	VAL	2.5
1	C	428	TYR	2.5
1	D	411	ILE	2.5
1	D	271	GLY	2.5
1	E	364	THR	2.5
1	C	444	VAL	2.5
1	A	182	TYR	2.5
1	E	372	ARG	2.4
1	C	348	CYS	2.4
1	E	378	TYR	2.4
1	D	379	MET	2.4
1	D	298	THR	2.4
1	E	179	ASP	2.4
1	C	252	VAL	2.4
1	B	474	CYS	2.4
1	A	440	GLU	2.4
1	D	239	GLU	2.4
1	C	412	ALA	2.4
1	D	240	ARG	2.4
1	B	427	PRO	2.4
1	D	190	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	335	LYS	2.4
1	C	460	SER	2.4
1	E	443	LYS	2.4
1	D	373	VAL	2.4
1	E	432	VAL	2.4
1	C	339	ILE	2.4
1	E	402	TYR	2.4
1	C	487	ARG	2.4
1	E	380	ALA	2.4
1	B	409	TRP	2.4
1	B	188	GLY	2.4
1	B	369	PRO	2.4
1	D	312	GLY	2.4
1	D	186	THR	2.4
1	E	321	VAL	2.4
1	E	422	GLU	2.4
1	C	480	ALA	2.4
1	E	361	ALA	2.4
1	A	235	SER	2.4
1	A	387	SER	2.4
1	B	305	LEU	2.4
1	B	240	ARG	2.4
1	C	244	ARG	2.4
1	C	402	TYR	2.4
1	C	238	GLU	2.4
1	B	449	LYS	2.4
1	B	419	GLY	2.3
1	E	438	VAL	2.3
1	C	379	MET	2.3
1	D	449	LYS	2.3
1	A	468	ALA	2.3
1	D	410	GLU	2.3
1	C	211	ILE	2.3
1	D	292	LEU	2.3
1	E	416	SER	2.3
1	E	390	MET	2.3
1	A	443	LYS	2.3
1	D	250	GLN	2.3
1	C	495	LEU	2.3
1	B	297	VAL	2.3
1	B	253	MET	2.3
1	B	446	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	376	LYS	2.3
1	A	499	GLU	2.3
1	C	470	ILE	2.3
1	D	359	ASP	2.3
1	B	298	THR	2.3
1	C	296	THR	2.3
1	D	274	THR	2.3
1	E	463	ALA	2.3
1	B	492	LEU	2.3
1	A	314	ALA	2.3
1	B	378	TYR	2.3
1	E	449	LYS	2.3
1	A	430	ASP	2.3
1	C	346	THR	2.2
1	D	370	ASN	2.2
1	C	401	ILE	2.2
1	E	452	PRO	2.2
1	E	472	ARG	2.2
1	A	269	ASP	2.2
1	C	363	ASP	2.2
1	B	392	HIS	2.2
1	A	459	GLN	2.2
1	C	476	TYR	2.2
1	D	499	GLU	2.2
1	C	453	ASN	2.2
1	E	421	HIS	2.2
1	D	463	ALA	2.2
1	B	494	GLN	2.2
1	A	190	GLY	2.2
1	B	462	GLU	2.2
1	C	227	GLU	2.2
1	C	271	GLY	2.2
1	E	447	GLU	2.2
1	C	259	ILE	2.2
1	B	293	ASN	2.2
1	B	425	GLN	2.2
1	E	379	MET	2.2
1	D	360	SER	2.2
1	A	442	ARG	2.2
1	B	218	GLU	2.2
1	B	284	GLU	2.2
1	C	209	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	382	GLU	2.2
1	E	417	ILE	2.2
1	D	251	THR	2.2
1	E	484	THR	2.2
1	C	370	ASN	2.2
1	E	269	ASP	2.2
1	B	457	ARG	2.2
1	B	373	VAL	2.2
1	C	473	GLU	2.2
1	E	473	GLU	2.2
1	E	346	THR	2.2
1	A	253	MET	2.2
1	C	270	ASN	2.2
1	D	318	MET	2.2
1	A	399	ALA	2.1
1	A	485	ALA	2.1
1	C	317	HIS	2.1
1	D	208	GLN	2.1
1	A	211	ILE	2.1
1	D	219	VAL	2.1
1	A	473	GLU	2.1
1	D	491	THR	2.1
1	E	389	ASN	2.1
1	A	324	GLN	2.1
1	B	210	SER	2.1
1	D	295	TYR	2.1
1	D	405	GLY	2.1
1	B	272	THR	2.1
1	D	185	THR	2.1
1	B	294	ARG	2.1
1	C	457	ARG	2.1
1	E	240	ARG	2.1
1	A	320	ILE	2.1
1	D	324	GLN	2.1
1	D	443	LYS	2.1
1	D	455	PRO	2.1
1	C	354	LEU	2.1
1	E	323	THR	2.1
1	A	240	ARG	2.1
1	B	450	LEU	2.1
1	B	476	TYR	2.1
1	D	492	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	253	MET	2.1
1	A	272	THR	2.1
1	C	186	THR	2.1
1	D	178	LYS	2.1
1	A	270	ASN	2.1
1	B	216	PHE	2.1
1	C	289	PHE	2.1
1	C	425	GLN	2.1
1	D	196	LEU	2.1
1	B	359	ASP	2.1
1	C	175	THR	2.1
1	E	442	ARG	2.1
1	D	480	ALA	2.1
1	E	280	SER	2.1
1	D	453	ASN	2.1
1	C	192	GLY	2.0
1	A	391	LYS	2.0
1	C	319	GLU	2.0
1	D	173	GLU	2.0
1	D	391	LYS	2.0
1	E	337	LYS	2.0
1	B	412	ALA	2.0
1	D	308	SER	2.0
1	E	360	SER	2.0
1	D	464	LEU	2.0
1	B	445	VAL	2.0
1	A	322	GLY	2.0
1	B	337	LYS	2.0
1	C	435	ASP	2.0
1	B	485	ALA	2.0
1	B	495	LEU	2.0
1	D	399	ALA	2.0
1	C	347	CYS	2.0
1	D	293	ASN	2.0
1	C	479	GLY	2.0
1	D	424	TYR	2.0
1	D	428	TYR	2.0
1	E	298	THR	2.0
1	B	292	LEU	2.0
1	C	410	GLU	2.0
1	E	195	LEU	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](#)

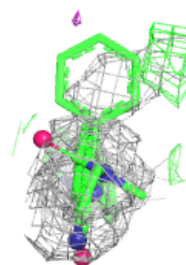
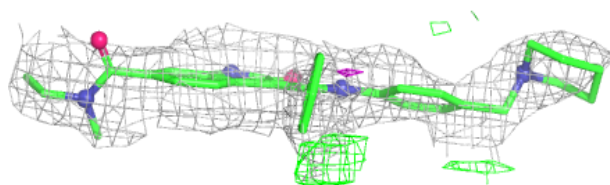
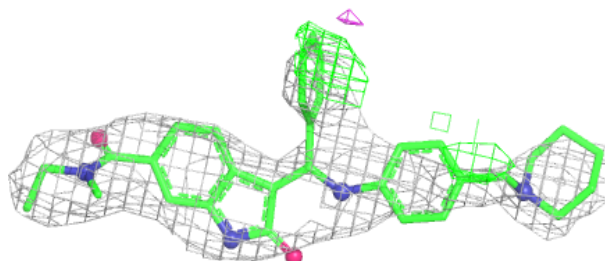
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZOP	C	600	37/37	0.81	0.27	76,79,81,81	0
2	ZOP	B	600	37/37	0.89	0.17	25,29,48,49	0
2	ZOP	E	600	37/37	0.89	0.19	34,40,51,52	0
2	ZOP	D	600	37/37	0.92	0.17	31,33,51,52	0
2	ZOP	A	600	37/37	0.93	0.17	30,33,44,44	0

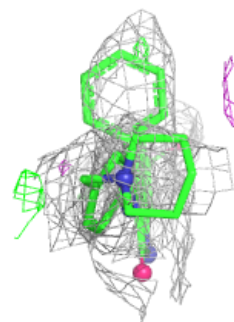
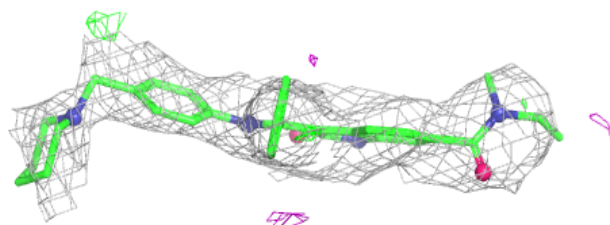
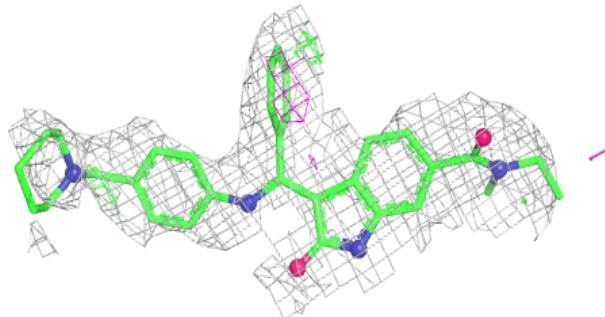
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ZOP C 600:

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

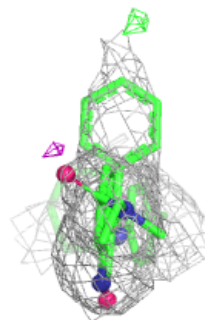
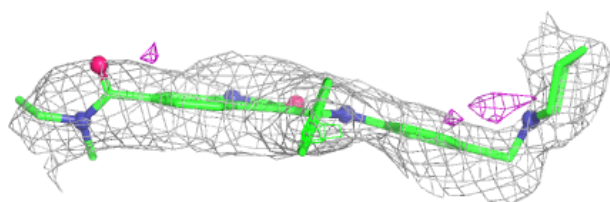
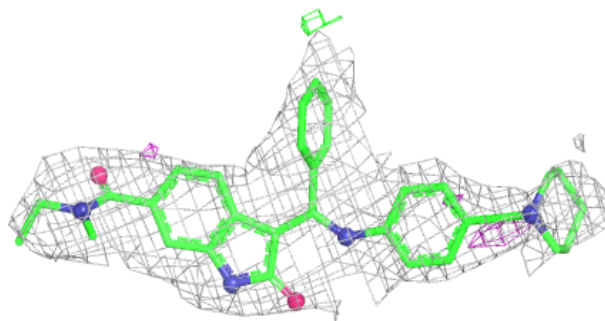
**Electron density around ZOP B 600:**

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

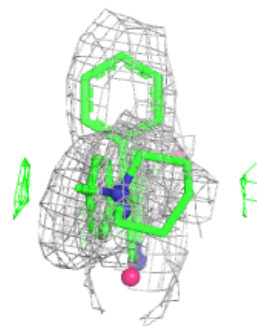
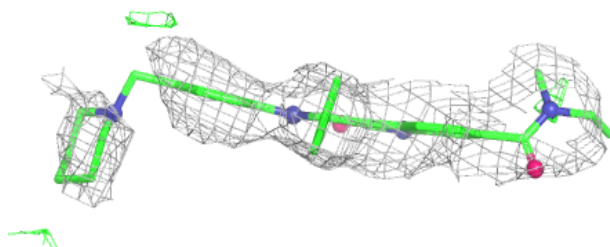
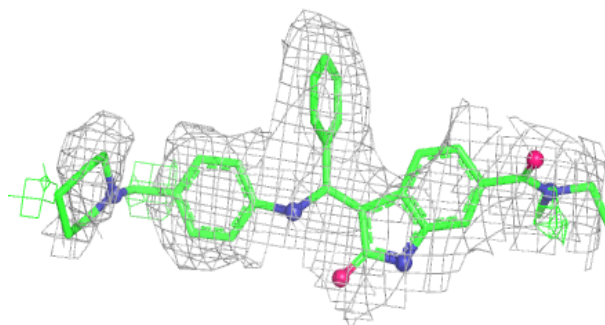


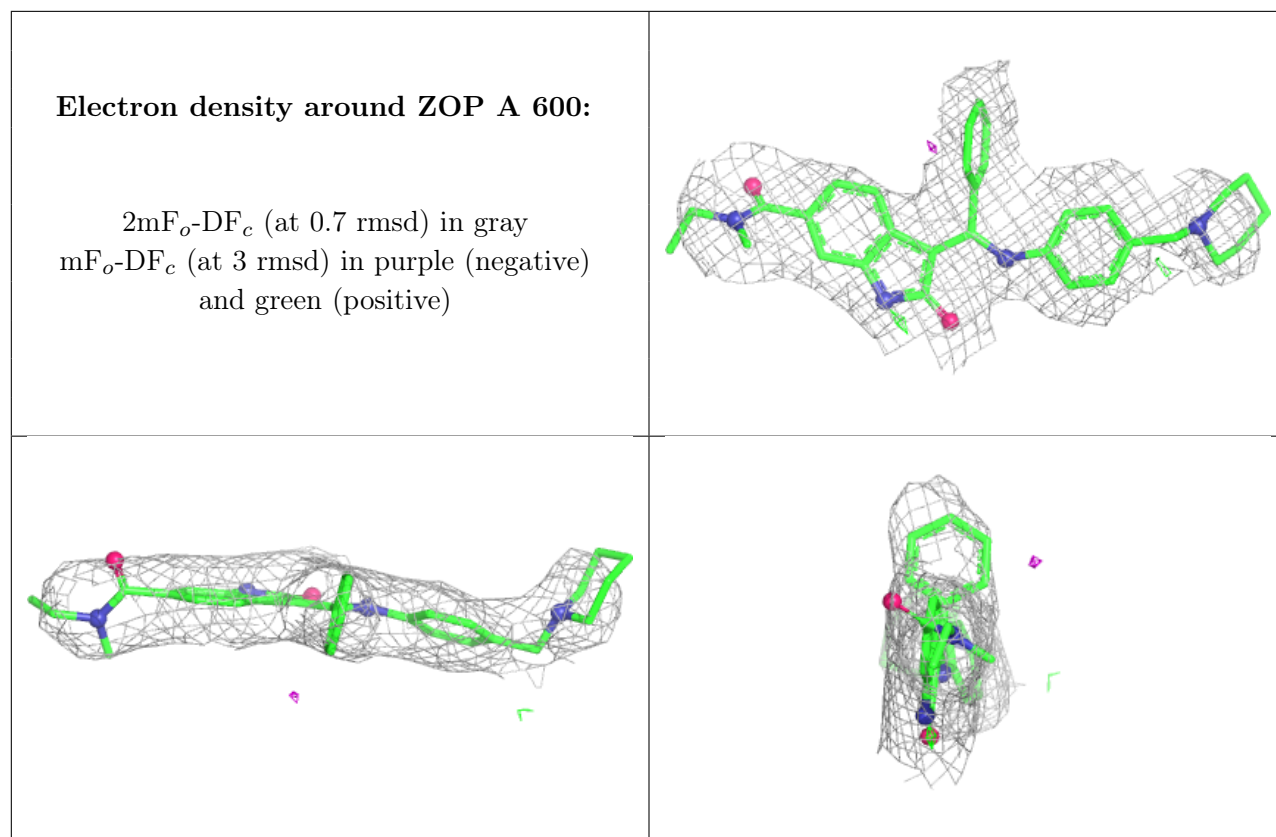
Electron density around ZOP E 600:

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

**Electron density around ZOP D 600:**

$2mF_o-DF_c$ (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.