



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 09:56 pm BST

PDB ID : 5TBP
Title : Crystal Structure of RXR-alpha ligand binding domain complexed with synthetic modulator K8003
Authors : Aleshin, A.E.; Liddington, R.C.; Su, Y.; Zhang, X.
Deposited on : 2016-09-12
Resolution : 2.60 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

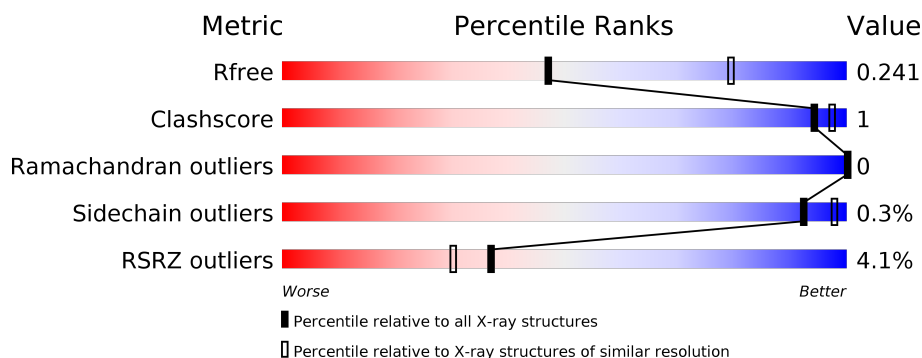
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 76%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 5% 19% </div> </div>
1	B	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 1%, green 84%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 84% • 13% </div> </div>
1	C	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 1%, green 84%, grey 13%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 84% • 13% </div> </div>
1	D	244	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 80%, grey 19%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 80% • 19% </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13844 atoms, of which 6898 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.

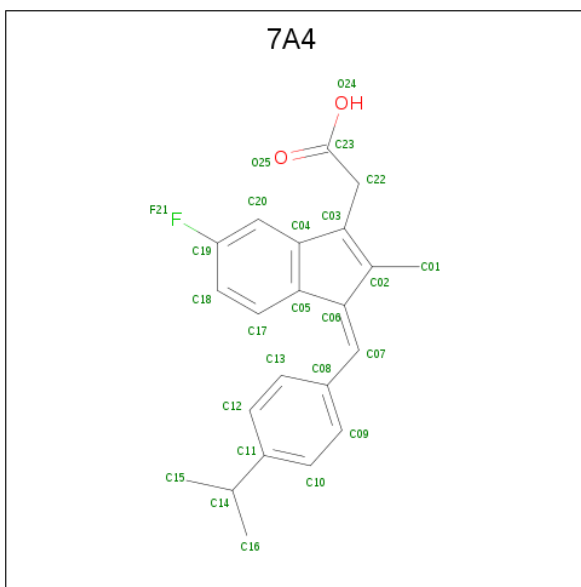
- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	H	N	O	S	0	4	0
			3208	1019	1621	279	280	9			
1	B	213	Total	C	H	N	O	S	0	9	0
			3463	1097	1745	296	315	10			
1	C	213	Total	C	H	N	O	S	0	6	0
			3438	1091	1735	292	310	10			
1	D	198	Total	C	H	N	O	S	0	9	0
			3244	1031	1634	281	289	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	expression tag	UNP P19793
A	220	SER	-	expression tag	UNP P19793
A	221	HIS	-	expression tag	UNP P19793
A	222	MET	-	expression tag	UNP P19793
B	219	GLY	-	expression tag	UNP P19793
B	220	SER	-	expression tag	UNP P19793
B	221	HIS	-	expression tag	UNP P19793
B	222	MET	-	expression tag	UNP P19793
C	219	GLY	-	expression tag	UNP P19793
C	220	SER	-	expression tag	UNP P19793
C	221	HIS	-	expression tag	UNP P19793
C	222	MET	-	expression tag	UNP P19793
D	219	GLY	-	expression tag	UNP P19793
D	220	SER	-	expression tag	UNP P19793
D	221	HIS	-	expression tag	UNP P19793
D	222	MET	-	expression tag	UNP P19793

- Molecule 2 is [(1Z)-5-fluoro-2-methyl-1-{[4-(propan-2-yl)phenyl]methylidene}-1H-inden-3-yl]acetic acid (three-letter code: 7A4) (formula: C₂₂H₂₁FO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	H	O	0	0
			45	22	1	20	2		
2	A	1	Total	C	F	H	O	0	0
			45	22	1	20	2		
2	A	1	Total	C	F	H	O	0	0
			45	22	1	20	2		
2	B	1	Total	C	F	H	O	0	0
			45	22	1	20	2		
2	D	1	Total	C	F	H	O	0	0
			45	22	1	20	2		
2	D	1	Total	C	F	H	O	0	0
			45	22	1	20	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	B	1	Total	C	H	O	0	0
			7	2	3	2		
3	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

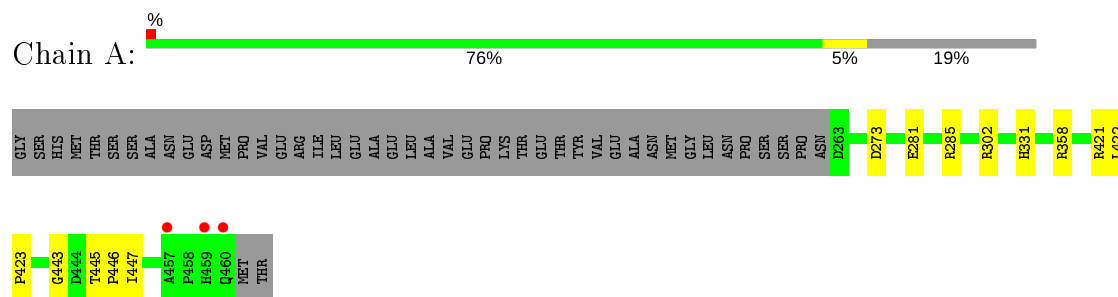
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	50	Total 50	O 50	0	2
6	B	39	Total 39	O 39	0	3
6	C	21	Total 21	O 21	0	1
6	D	24	Total 24	O 24	0	0

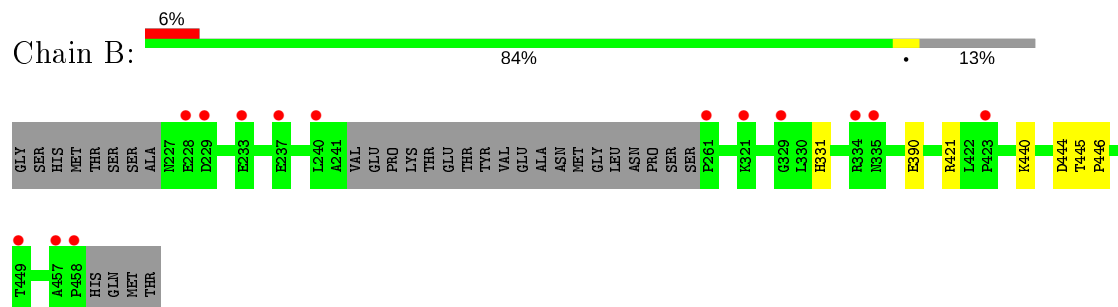
3 Residue-property plots [i](#)

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.

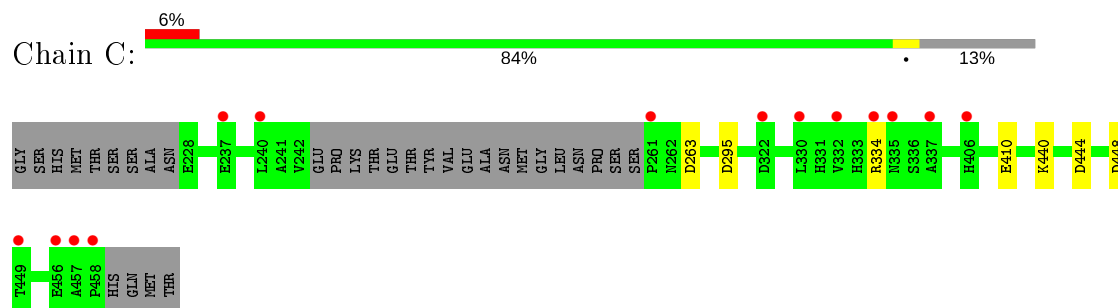
• Molecule 1: Retinoic acid receptor RXR-alpha



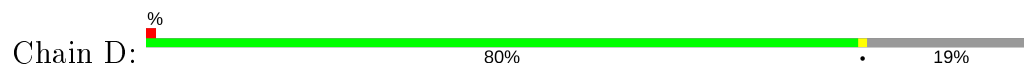
• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 1: Retinoic acid receptor RXR-alpha



GLY	SER	HIS	MET	THR	SER	SER	ALA	ASN	GLU	ASP	MET	PRO	VAL	GLU	ARG	ILE	LEU	GLU	ALA	GLU	LEU	ALA	VAL	GLU	PRO	LYS	THR	GLU	THR	TYR	VAL	GLU	ALA	ASN	MET	GLY	LEU	ASN	PRO	SER	SER	PRO	ASN	D263	F277	R302	L441	Q460	MET	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.64Å 99.38Å 109.86Å 90.00° 99.15° 90.00°	Depositor
Resolution (Å)	36.15 – 2.60 33.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.15-2.60) 98.9 (33.98-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.61Å)	Xtriage
Refinement program	PHENIX (DEV_2645: ???)	Depositor
R, R_{free}	0.196 , 0.242 0.196 , 0.241	Depositor DCC
R_{free} test set	1501 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13844	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: GOL, DMS, 7A4, ACT

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	0.24	0/1637	0.39	0/2215
1	B	0.24	0/1775	0.38	0/2401
1	C	0.23	0/1755	0.38	0/2374
1	D	0.23	0/1674	0.38	0/2267
All	All	0.24	0/6841	0.38	0/9257

There are no bond length outliers.

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	1587	1621	1599	8	0
1	B	1718	1745	1714	5	0
1	C	1703	1735	1711	4	1
1	D	1610	1634	1604	3	0
2	A	75	60	0	0	0
2	B	25	20	0	0	0
2	D	50	40	0	0	0
3	A	16	12	12	1	0
3	B	8	6	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	3	3	0	0
4	A	4	6	6	0	0
5	B	6	8	8	0	0
5	C	6	8	8	0	0
6	A	50	0	0	2	0
6	B	39	0	0	1	0
6	C	21	0	0	0	0
6	D	24	0	0	0	0
All	All	6946	6898	6671	17	1

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 1.

All (17) 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:331[B]:HIS:NE2	6:A:601:HOH:O	2.24	0.70
1:C:440:LYS:O	1:C:444:ASP:N	2.30	0.63
1:A:302:ARG:NH2	1:C:448:ASP:OD1	2.32	0.62
1:B:440:LYS:O	1:B:444:ASP:N	2.40	0.53
1:A:358:ARG:NH1	6:A:608:HOH:O	2.41	0.47
1:C:410:GLU:OE1	1:C:410:GLU:N	2.36	0.47
1:B:445:THR:HB	1:B:446:PRO:HD3	1.98	0.45
1:B:390[B]:GLU:OE1	6:B:601[B]:HOH:O	2.21	0.45
1:B:444:ASP:OD1	1:D:302:ARG:NH1	2.50	0.45
3:A:507:ACT:O	1:B:421:ARG:NH2	2.50	0.44
3:B:503:ACT:H1	1:D:460:GLN:N	2.34	0.42
1:A:281:GLU:O	1:A:285[B]:ARG:HG3	2.20	0.41
1:A:443:GLY:O	1:A:447:ILE:HG12	2.20	0.41
1:A:445:THR:HB	1:A:446:PRO:HD3	2.02	0.41
1:A:273:ASP:CG	1:C:263:ASP:HB3	2.42	0.40
1:A:422:LEU:N	1:A:423:PRO:CD	2.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ASP:OD2	1:C:334:ARG:NH1[1_455]	2.19	0.01

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	200/244 (82%)	193 (96%)	7 (4%)	0	100	100
1	B	218/244 (89%)	211 (97%)	7 (3%)	0	100	100
1	C	215/244 (88%)	209 (97%)	6 (3%)	0	100	100
1	D	205/244 (84%)	197 (96%)	8 (4%)	0	100	100
All	All	838/976 (86%)	810 (97%)	28 (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	174/210 (83%)	173 (99%)	1 (1%)	86	95
1	B	189/210 (90%)	188 (100%)	1 (0%)	88	96
1	C	187/210 (89%)	187 (100%)	0	100	100
1	D	178/210 (85%)	178 (100%)	0	100	100
All	All	728/840 (87%)	726 (100%)	2 (0%)	92	98

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

Mol	Chain	Res	Type
1	A	421	ARG
1	B	331	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	ACT	A	505	-	1,3,3	6.40	1 (100%)	0,3,3	0.00	-
3	ACT	B	504	-	1,3,3	6.51	1 (100%)	0,3,3	0.00	-
2	7A4	A	502	-	24,27,27	2.72	5 (20%)	32,39,39	1.46	5 (15%)
5	GOL	C	501	-	5,5,5	0.97	0	5,5,5	0.98	0
2	7A4	D	501	-	24,27,27	2.71	5 (20%)	32,39,39	1.45	4 (12%)
4	DMS	A	506	-	3,3,3	0.66	0	3,3,3	0.51	0
2	7A4	A	503	-	24,27,27	2.73	5 (20%)	32,39,39	1.49	5 (15%)
2	7A4	B	501	-	24,27,27	2.73	5 (20%)	32,39,39	1.49	4 (12%)
3	ACT	A	508	-	1,3,3	6.30	1 (100%)	0,3,3	0.00	-
2	7A4	A	501	-	24,27,27	2.70	5 (20%)	32,39,39	1.54	4 (12%)
3	ACT	A	507	-	1,3,3	6.17	1 (100%)	0,3,3	0.00	-
3	ACT	D	503	-	1,3,3	6.46	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	B	503	-	1,3,3	6.25	1 (100%)	0,3,3	0.00	-
3	ACT	A	504	-	1,3,3	6.43	1 (100%)	0,3,3	0.00	-
5	GOL	B	502	-	5,5,5	1.02	0	5,5,5	0.94	0
2	7A4	D	502	-	24,27,27	2.71	5 (20%)	32,39,39	1.45	5 (15%)

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	7A4	A	502	-	-	3/10/28/28	0/3/3/3
5	GOL	C	501	-	-	2/4/4/4	-
2	7A4	D	501	-	-	2/10/28/28	0/3/3/3
2	7A4	A	503	-	-	2/10/28/28	0/3/3/3
2	7A4	B	501	-	-	0/10/28/28	0/3/3/3
2	7A4	A	501	-	-	2/10/28/28	0/3/3/3
5	GOL	B	502	-	-	2/4/4/4	-
2	7A4	D	502	-	-	2/10/28/28	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	7A4	C04-C03	10.77	1.64	1.44
2	B	501	7A4	C04-C03	10.76	1.64	1.44
2	A	502	7A4	C04-C03	10.75	1.63	1.44
2	A	501	7A4	C04-C03	10.74	1.63	1.44
2	D	501	7A4	C04-C03	10.74	1.63	1.44
2	D	502	7A4	C04-C03	10.71	1.63	1.44
3	B	504	ACT	CH3-C	6.51	1.57	1.48
3	D	503	ACT	CH3-C	6.46	1.57	1.48
3	A	504	ACT	CH3-C	6.43	1.56	1.48
3	A	505	ACT	CH3-C	6.40	1.56	1.48
3	A	508	ACT	CH3-C	6.30	1.56	1.48
3	B	503	ACT	CH3-C	6.25	1.56	1.48
3	A	507	ACT	CH3-C	6.17	1.56	1.48
2	B	501	7A4	C03-C02	5.88	1.49	1.36
2	A	503	7A4	C03-C02	5.88	1.49	1.36
2	A	502	7A4	C03-C02	5.79	1.49	1.36
2	D	501	7A4	C03-C02	5.77	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	7A4	C03-C02	5.71	1.48	1.36
2	A	501	7A4	C03-C02	5.69	1.48	1.36
2	D	502	7A4	C08-C07	2.82	1.52	1.46
2	A	502	7A4	C08-C07	2.79	1.52	1.46
2	A	503	7A4	C08-C07	2.71	1.52	1.46
2	B	501	7A4	C08-C07	2.69	1.52	1.46
2	D	501	7A4	C08-C07	2.63	1.51	1.46
2	A	501	7A4	C08-C07	2.61	1.51	1.46
2	A	502	7A4	C05-C04	2.60	1.45	1.39
2	B	501	7A4	C05-C04	2.52	1.44	1.39
2	D	502	7A4	C18-C19	2.52	1.42	1.37
2	D	502	7A4	C05-C04	2.51	1.44	1.39
2	A	502	7A4	C18-C19	2.50	1.42	1.37
2	A	503	7A4	C05-C04	2.49	1.44	1.39
2	B	501	7A4	C18-C19	2.48	1.42	1.37
2	A	503	7A4	C18-C19	2.47	1.41	1.37
2	A	501	7A4	C05-C04	2.46	1.44	1.39
2	D	501	7A4	C18-C19	2.44	1.41	1.37
2	D	501	7A4	C05-C04	2.43	1.44	1.39
2	A	501	7A4	C18-C19	2.40	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	503	7A4	C05-C04-C03	-4.97	105.24	109.16
2	A	501	7A4	C05-C04-C03	-4.81	105.37	109.16
2	B	501	7A4	C05-C04-C03	-4.81	105.37	109.16
2	A	502	7A4	C05-C04-C03	-4.79	105.38	109.16
2	D	501	7A4	C05-C04-C03	-4.77	105.40	109.16
2	D	502	7A4	C05-C04-C03	-4.57	105.56	109.16
2	B	501	7A4	C23-C22-C03	-3.62	111.23	116.07
2	A	503	7A4	C23-C22-C03	-3.42	111.49	116.07
2	A	501	7A4	C18-C19-C20	-2.96	119.45	123.29
2	A	501	7A4	C23-C22-C03	-2.95	112.13	116.07
2	D	501	7A4	C23-C22-C03	-2.87	112.22	116.07
2	A	501	7A4	C17-C05-C04	-2.85	117.87	121.07
2	A	503	7A4	C18-C19-C20	-2.74	119.72	123.29
2	B	501	7A4	C18-C19-C20	-2.73	119.75	123.29
2	A	502	7A4	C18-C19-C20	-2.72	119.76	123.29
2	D	502	7A4	C23-C22-C03	-2.69	112.47	116.07
2	D	501	7A4	C18-C19-C20	-2.69	119.79	123.29
2	D	502	7A4	C18-C19-C20	-2.65	119.85	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	7A4	C23-C22-C03	-2.58	112.62	116.07
2	B	501	7A4	C17-C05-C04	-2.52	118.24	121.07
2	A	502	7A4	C17-C05-C04	-2.37	118.41	121.07
2	A	503	7A4	C17-C05-C04	-2.37	118.41	121.07
2	D	501	7A4	C17-C05-C04	-2.31	118.47	121.07
2	D	502	7A4	C22-C03-C04	2.11	127.43	124.74
2	D	502	7A4	C17-C05-C04	-2.10	118.71	121.07
2	A	503	7A4	C17-C18-C19	2.07	120.50	118.36
2	A	502	7A4	C17-C18-C19	2.06	120.49	118.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	7A4	C04-C03-C22-C23
2	D	502	7A4	C06-C07-C08-C13
2	D	502	7A4	C06-C07-C08-C09
5	C	501	GOL	O1-C1-C2-C3
5	B	502	GOL	O1-C1-C2-C3
2	A	502	7A4	C06-C07-C08-C13
2	A	502	7A4	C06-C07-C08-C09
2	A	501	7A4	C06-C07-C08-C13
2	A	501	7A4	C06-C07-C08-C09
2	D	501	7A4	C06-C07-C08-C09
2	D	501	7A4	C06-C07-C08-C13
5	C	501	GOL	O1-C1-C2-O2
5	B	502	GOL	O1-C1-C2-O2
2	A	503	7A4	C10-C11-C14-C15
2	A	503	7A4	C12-C11-C14-C15

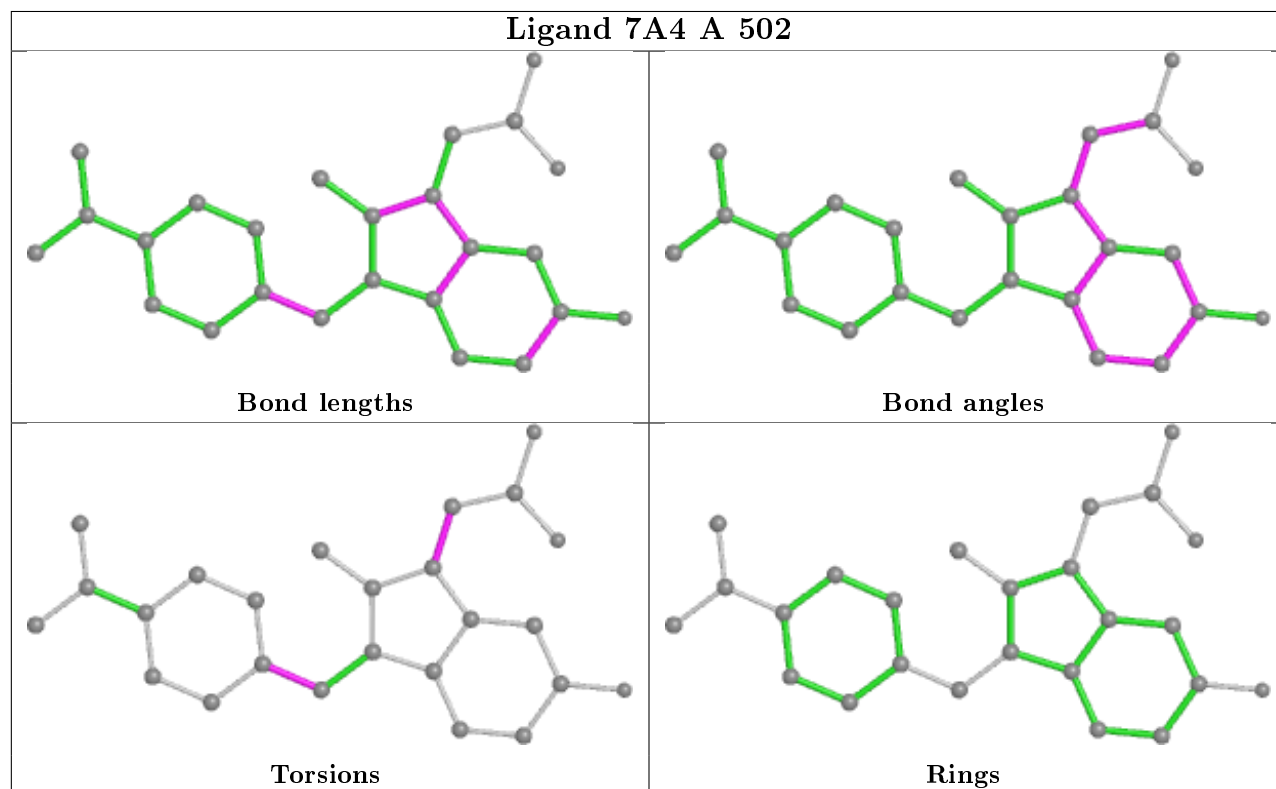
There are no ring outliers.

2 monomers are involved in 2 short contacts:

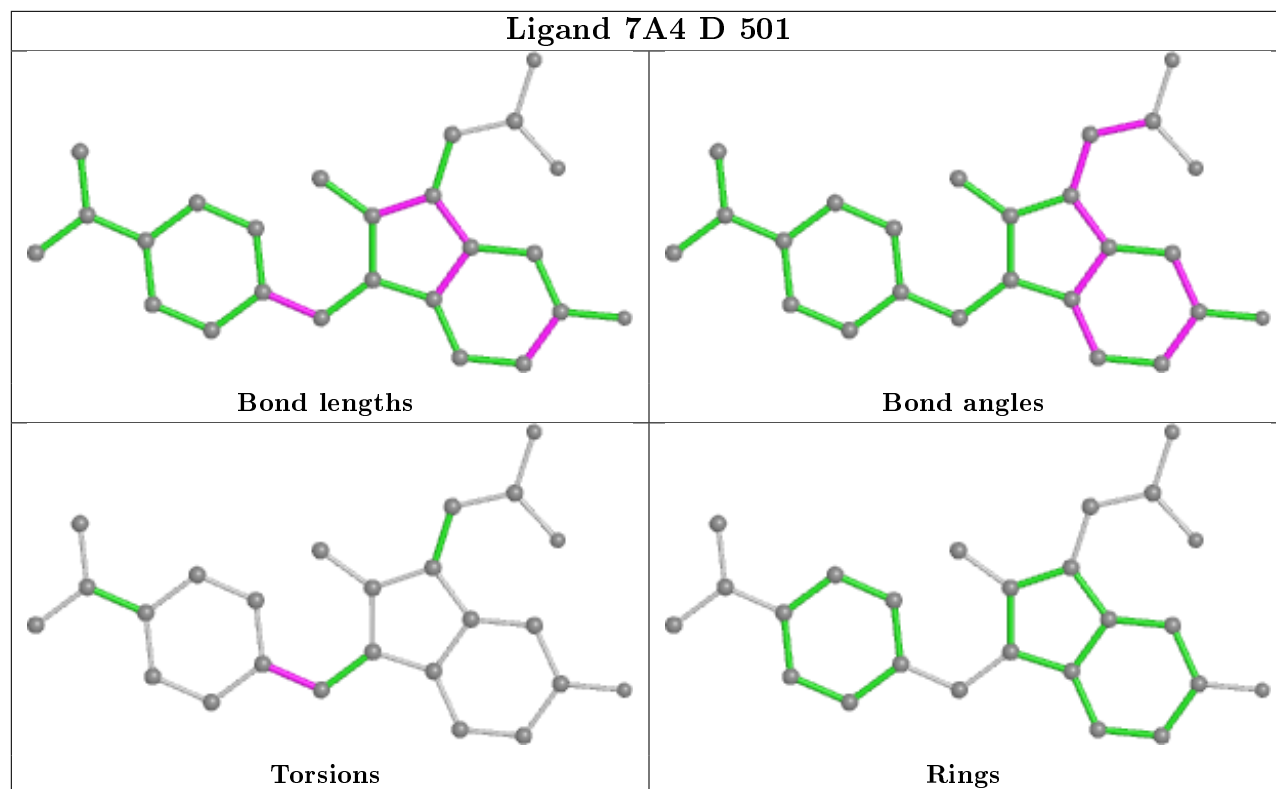
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	ACT	1	0
3	B	503	ACT	1	0

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.

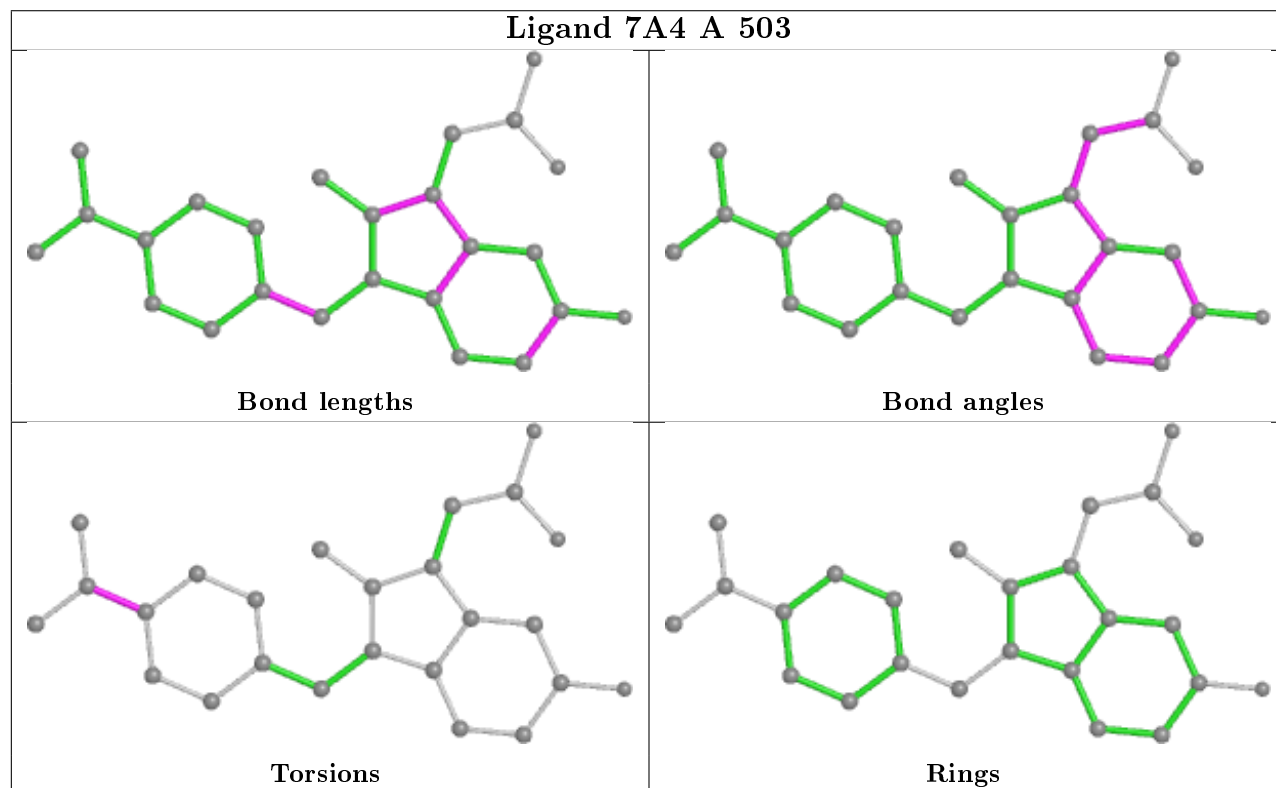
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



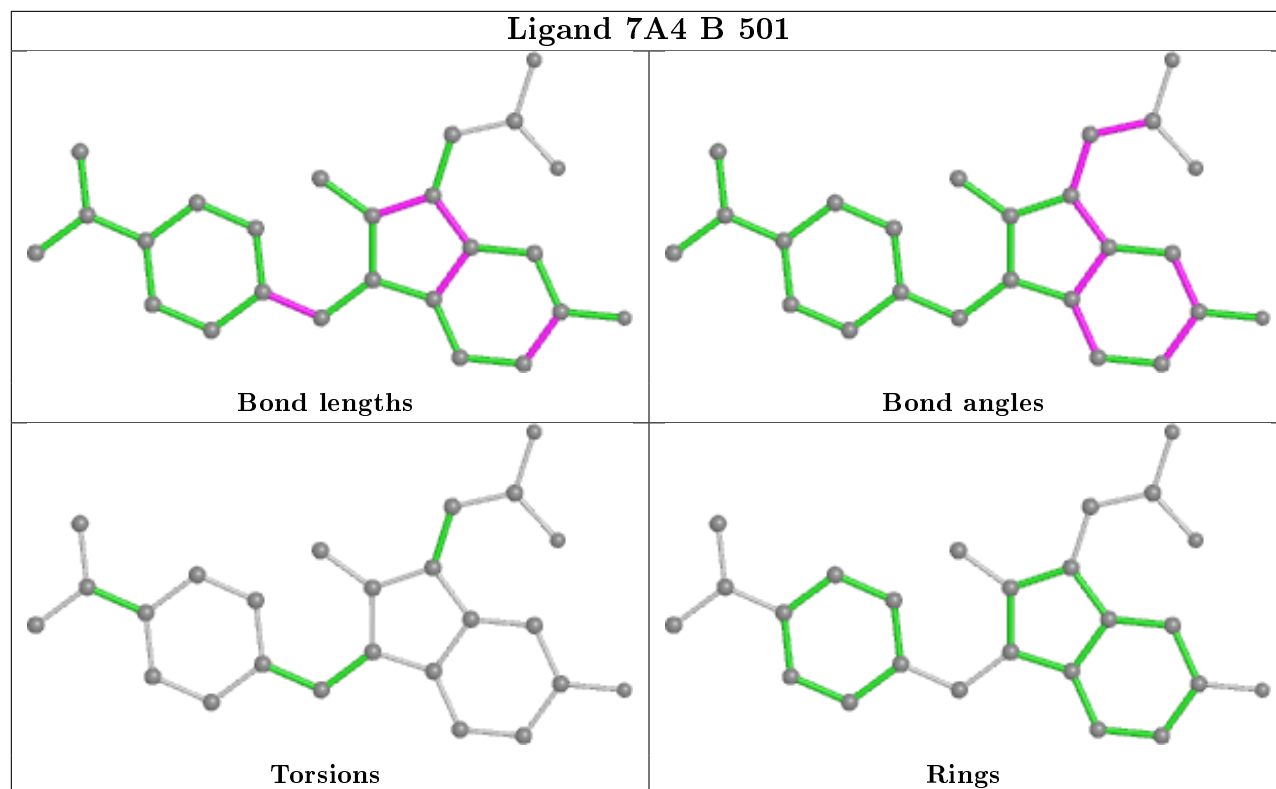
Ligand 7A4 D 501



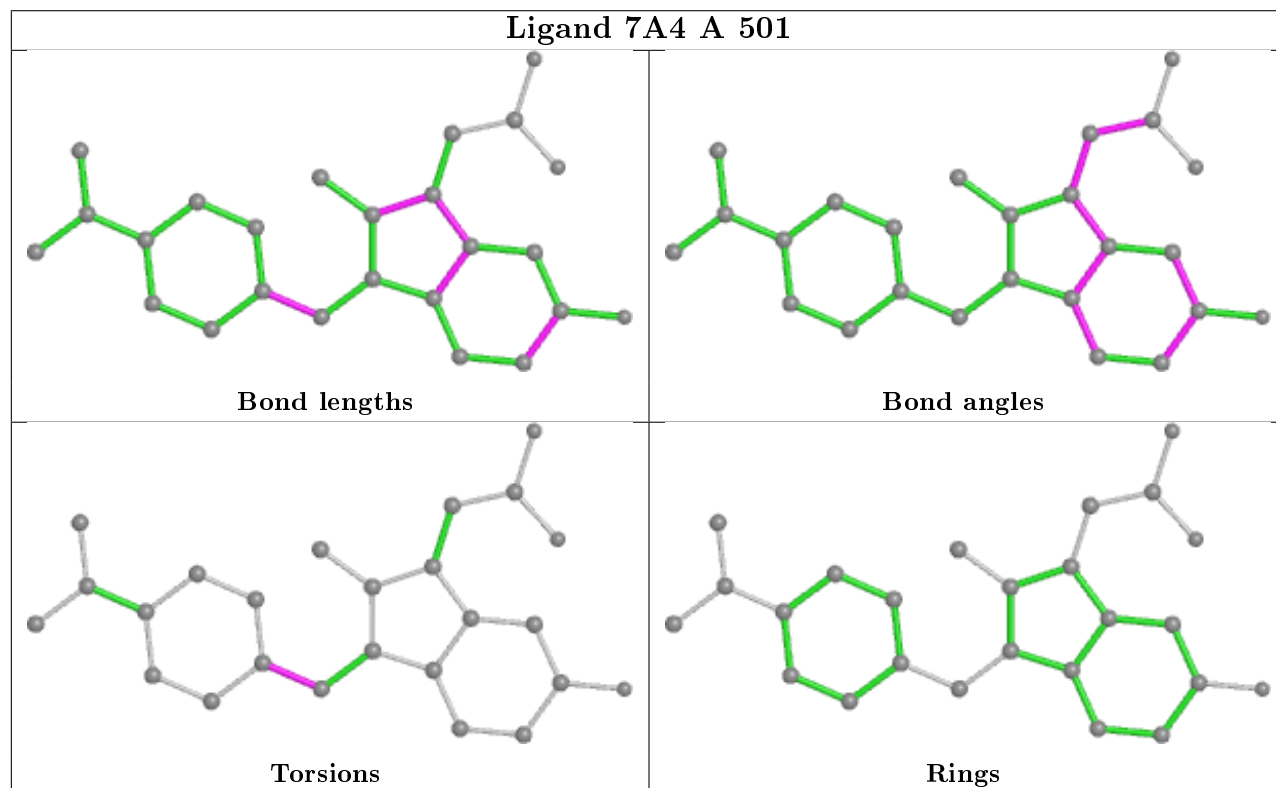
Ligand 7A4 A 503

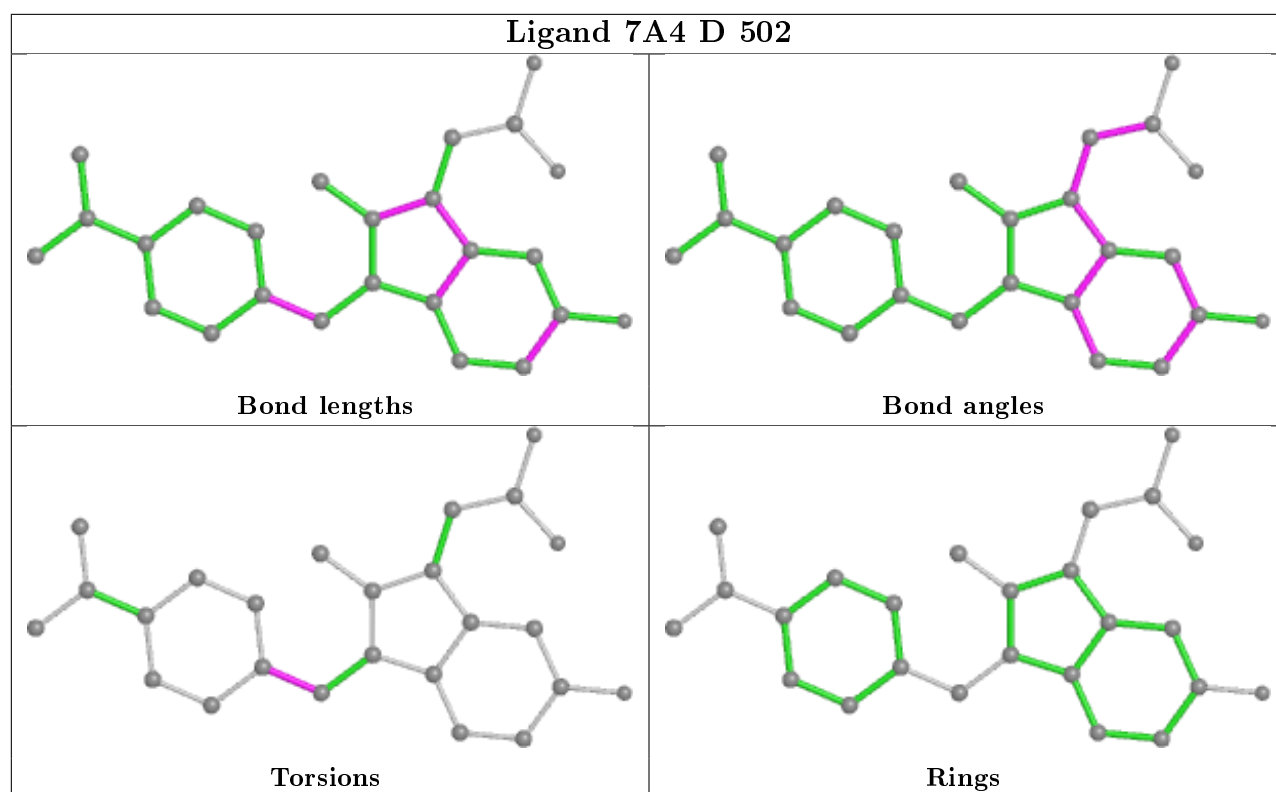


Ligand 7A4 B 501



Ligand 7A4 A 501





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	198/244 (81%)	-0.09	3 (1%) 73 70	31, 55, 90, 117	0
1	B	213/244 (87%)	0.20	14 (6%) 18 13	33, 58, 102, 120	0
1	C	213/244 (87%)	0.32	14 (6%) 18 13	43, 69, 102, 122	0
1	D	198/244 (81%)	-0.08	3 (1%) 73 70	43, 65, 93, 122	0
All	All	822/976 (84%)	0.09	34 (4%) 37 30	31, 63, 100, 122	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	228	GLU	4.0
1	C	457	ALA	4.0
1	A	459	HIS	3.3
1	C	240	LEU	3.3
1	C	261	PRO	3.2
1	B	321	LYS	3.1
1	A	457	ALA	3.1
1	C	237	GLU	3.0
1	C	334	ARG	2.9
1	C	406	HIS	2.9
1	B	334	ARG	2.9
1	D	263	ASP	2.8
1	C	458	PRO	2.7
1	C	332	VAL	2.7
1	B	229	ASP	2.7
1	D	441	LEU	2.7
1	C	335	ASN	2.6
1	C	456	GLU	2.6
1	C	337	ALA	2.6
1	A	460	GLN	2.5
1	B	261	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	233	GLU	2.5
1	C	322	ASP	2.4
1	B	458	PRO	2.4
1	D	277	PHE	2.4
1	B	240	LEU	2.3
1	B	457	ALA	2.3
1	B	335[A]	ASN	2.2
1	B	423	PRO	2.1
1	C	449	THR	2.1
1	C	330	LEU	2.1
1	B	237	GLU	2.1
1	B	329	GLY	2.0
1	B	449	THR	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 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
2	7A4	B	501	25/25	0.72	0.35	78,96,110,119	45
3	ACT	A	504	4/4	0.74	0.32	82,88,99,99	0
5	GOL	C	501	6/6	0.76	0.31	92,111,119,123	0
3	ACT	A	505	4/4	0.80	0.30	89,93,107,107	0
2	7A4	D	501	25/25	0.80	0.29	64,79,100,102	45
2	7A4	A	502	25/25	0.81	0.39	73,93,120,124	45
2	7A4	D	502	25/25	0.82	0.30	77,104,136,146	0
2	7A4	A	503	25/25	0.83	0.31	80,94,110,116	45
5	GOL	B	502	6/6	0.86	0.24	92,110,117,118	0
3	ACT	A	508	4/4	0.87	0.27	71,75,85,85	0

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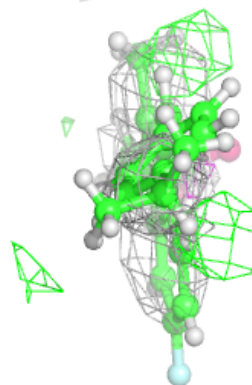
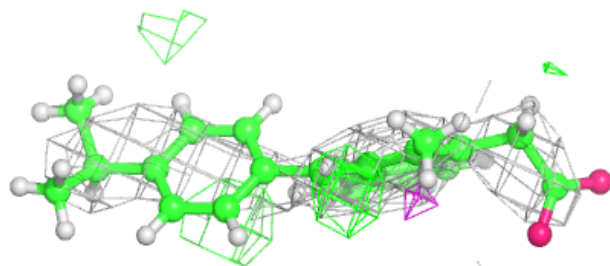
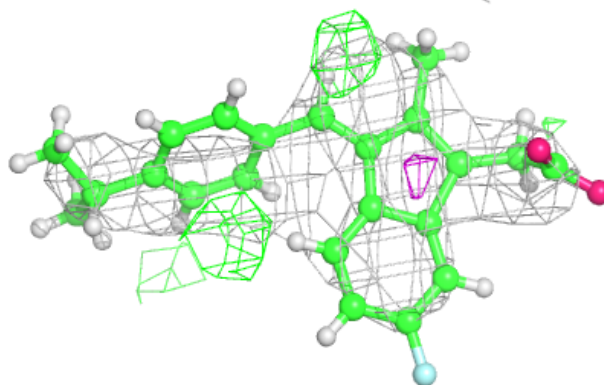
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMS	A	506	4/4	0.87	0.21	69,83,98,100	0
3	ACT	B	503	4/4	0.88	0.29	89,94,111,111	0
2	7A4	A	501	25/25	0.88	0.24	61,77,93,96	0
3	ACT	B	504	4/4	0.92	0.18	75,86,90,90	0
3	ACT	A	507	4/4	0.93	0.20	50,58,71,71	0
3	ACT	D	503	4/4	0.95	0.32	62,68,80,80	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.

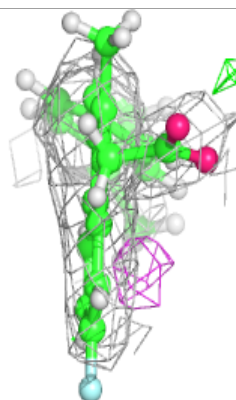
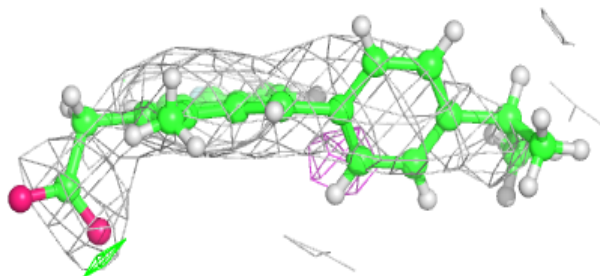
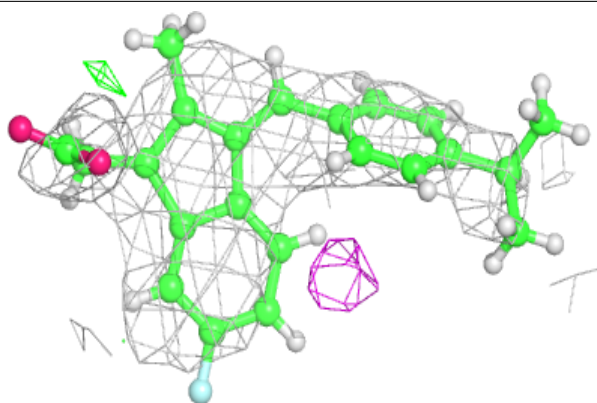
Electron density around 7A4 B 501:

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

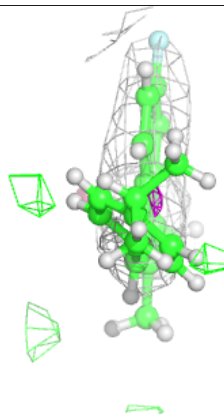
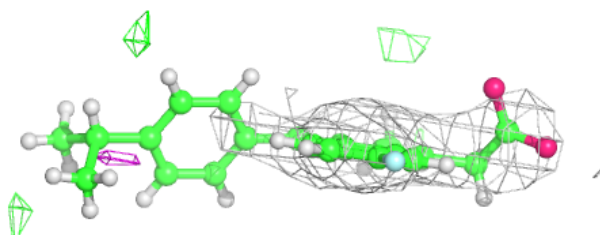
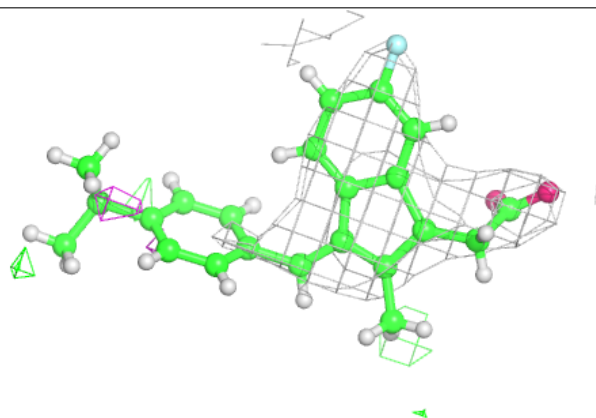


Electron density around 7A4 D 501:

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

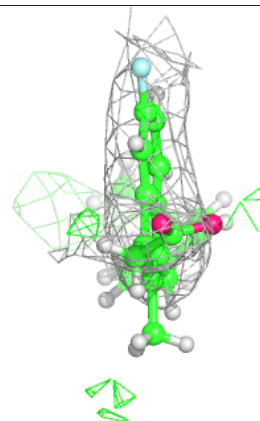
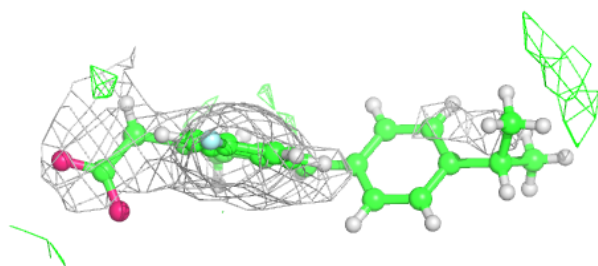
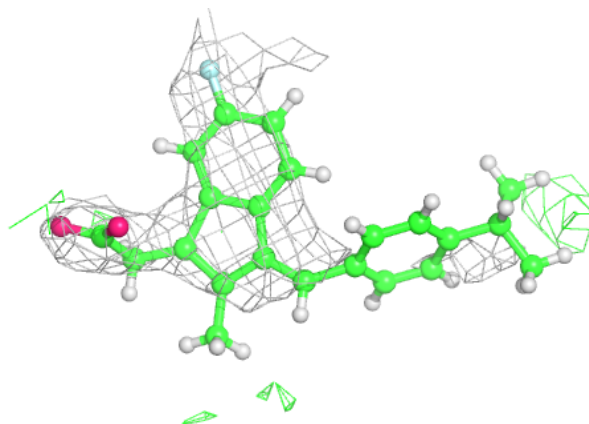
**Electron density around 7A4 A 502:**

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

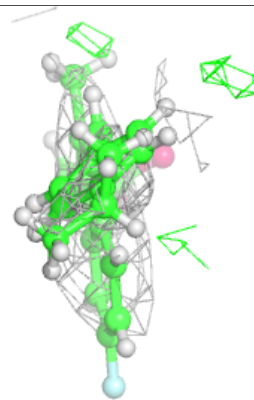
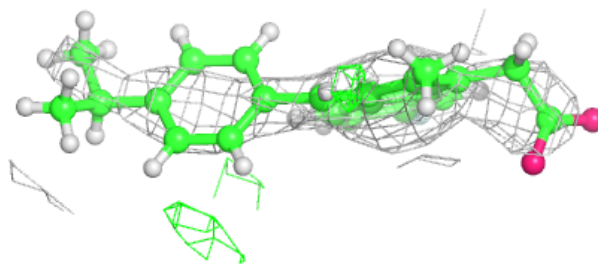
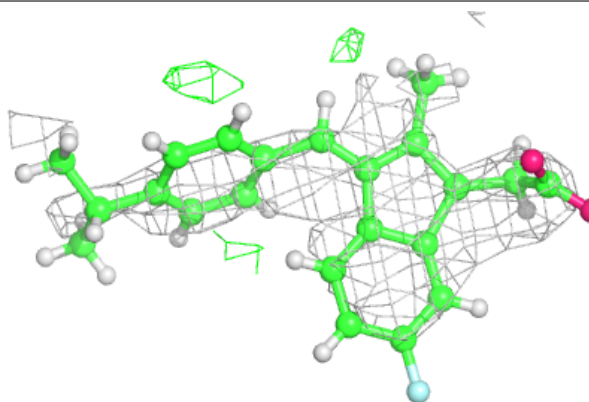


Electron density around 7A4 D 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

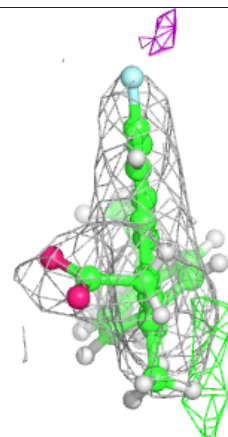
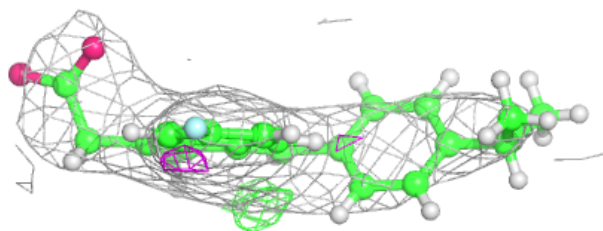
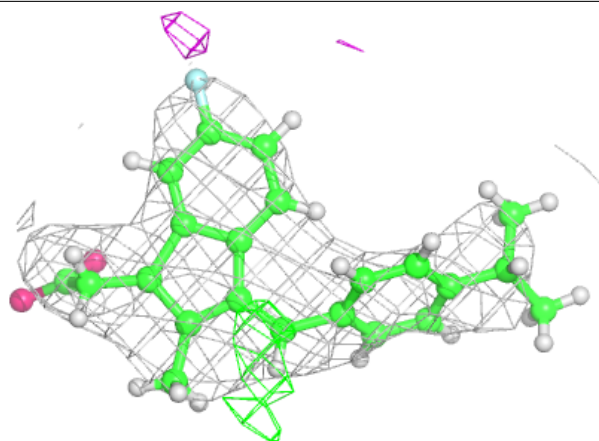
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7A4 A 501:

$2mF_o-DF_c$ (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.