



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:42 AM UTC

PDB ID : 6O95 / pdb_00006o95
Title : Structure of the IRAK4 kinase domain with compound 41
Authors : Yu, C.; Drobnick, J.; Bryan, M.C.; Kiefer, J.; Lupardus, P.J.
Deposited on : 2019-03-13
Resolution : 1.77 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:

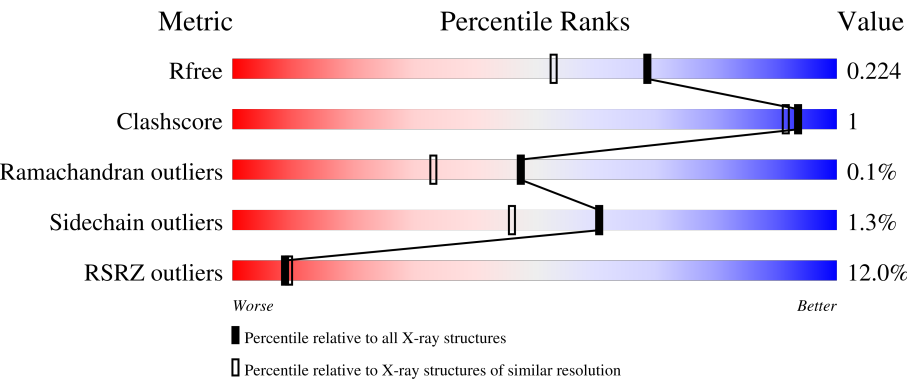
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	320	12% 85% 6% 9%
1	B	320	11% 84% • 13%
1	C	320	13% 84% 6% 11%
1	D	320	7% 87% • • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10033 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	P	S	0	2	0
			2302	1444	385	454	3	16			
1	B	279	Total	C	N	O	P	S	0	0	0
			2201	1382	367	435	3	14			
1	C	286	Total	C	N	O	P	S	0	0	0
			2253	1415	376	444	3	15			
1	D	292	Total	C	N	O	P	S	0	2	0
			2306	1446	386	457	2	15			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	MET	-	initiating methionine	UNP Q9NWZ3
A	145	HIS	-	expression tag	UNP Q9NWZ3
A	146	HIS	-	expression tag	UNP Q9NWZ3
A	147	HIS	-	expression tag	UNP Q9NWZ3
A	148	HIS	-	expression tag	UNP Q9NWZ3
A	149	HIS	-	expression tag	UNP Q9NWZ3
A	150	HIS	-	expression tag	UNP Q9NWZ3
A	151	GLY	-	expression tag	UNP Q9NWZ3
A	152	GLU	-	expression tag	UNP Q9NWZ3
A	153	ASN	-	expression tag	UNP Q9NWZ3
A	154	LEU	-	expression tag	UNP Q9NWZ3
A	155	TYR	-	expression tag	UNP Q9NWZ3
A	156	PHE	-	expression tag	UNP Q9NWZ3
A	157	GLN	-	expression tag	UNP Q9NWZ3
A	158	GLY	-	expression tag	UNP Q9NWZ3
A	159	SER	-	expression tag	UNP Q9NWZ3
A	461	GLY	-	expression tag	UNP Q9NWZ3
A	462	ASN	-	expression tag	UNP Q9NWZ3
A	463	SER	-	expression tag	UNP Q9NWZ3
B	144	MET	-	initiating methionine	UNP Q9NWZ3
B	145	HIS	-	expression tag	UNP Q9NWZ3

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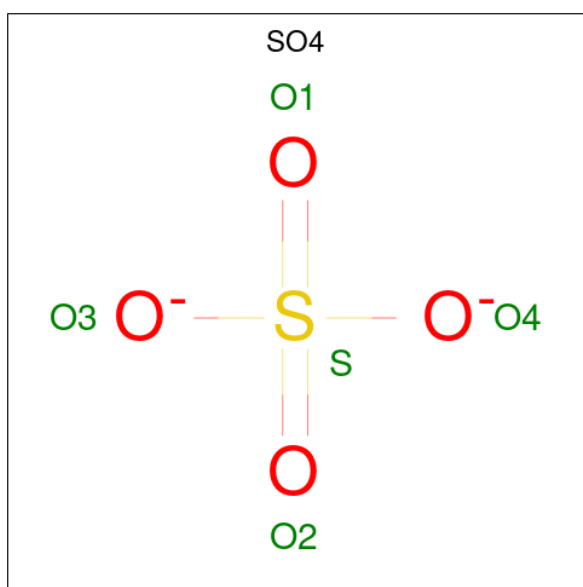
Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	HIS	-	expression tag	UNP Q9NWZ3
B	148	HIS	-	expression tag	UNP Q9NWZ3
B	149	HIS	-	expression tag	UNP Q9NWZ3
B	150	HIS	-	expression tag	UNP Q9NWZ3
B	151	GLY	-	expression tag	UNP Q9NWZ3
B	152	GLU	-	expression tag	UNP Q9NWZ3
B	153	ASN	-	expression tag	UNP Q9NWZ3
B	154	LEU	-	expression tag	UNP Q9NWZ3
B	155	TYR	-	expression tag	UNP Q9NWZ3
B	156	PHE	-	expression tag	UNP Q9NWZ3
B	157	GLN	-	expression tag	UNP Q9NWZ3
B	158	GLY	-	expression tag	UNP Q9NWZ3
B	159	SER	-	expression tag	UNP Q9NWZ3
B	461	GLY	-	expression tag	UNP Q9NWZ3
B	462	ASN	-	expression tag	UNP Q9NWZ3
B	463	SER	-	expression tag	UNP Q9NWZ3
C	144	MET	-	initiating methionine	UNP Q9NWZ3
C	145	HIS	-	expression tag	UNP Q9NWZ3
C	146	HIS	-	expression tag	UNP Q9NWZ3
C	147	HIS	-	expression tag	UNP Q9NWZ3
C	148	HIS	-	expression tag	UNP Q9NWZ3
C	149	HIS	-	expression tag	UNP Q9NWZ3
C	150	HIS	-	expression tag	UNP Q9NWZ3
C	151	GLY	-	expression tag	UNP Q9NWZ3
C	152	GLU	-	expression tag	UNP Q9NWZ3
C	153	ASN	-	expression tag	UNP Q9NWZ3
C	154	LEU	-	expression tag	UNP Q9NWZ3
C	155	TYR	-	expression tag	UNP Q9NWZ3
C	156	PHE	-	expression tag	UNP Q9NWZ3
C	157	GLN	-	expression tag	UNP Q9NWZ3
C	158	GLY	-	expression tag	UNP Q9NWZ3
C	159	SER	-	expression tag	UNP Q9NWZ3
C	461	GLY	-	expression tag	UNP Q9NWZ3
C	462	ASN	-	expression tag	UNP Q9NWZ3
C	463	SER	-	expression tag	UNP Q9NWZ3
D	144	MET	-	initiating methionine	UNP Q9NWZ3
D	145	HIS	-	expression tag	UNP Q9NWZ3
D	146	HIS	-	expression tag	UNP Q9NWZ3
D	147	HIS	-	expression tag	UNP Q9NWZ3
D	148	HIS	-	expression tag	UNP Q9NWZ3
D	149	HIS	-	expression tag	UNP Q9NWZ3

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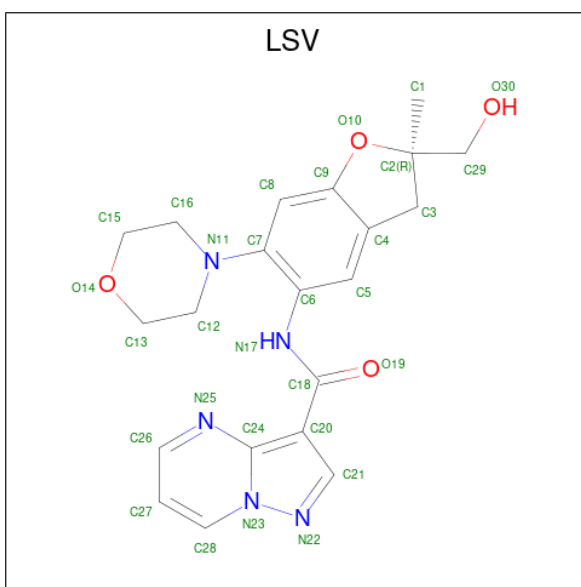
Chain	Residue	Modelled	Actual	Comment	Reference
D	150	HIS	-	expression tag	UNP Q9NWZ3
D	151	GLY	-	expression tag	UNP Q9NWZ3
D	152	GLU	-	expression tag	UNP Q9NWZ3
D	153	ASN	-	expression tag	UNP Q9NWZ3
D	154	LEU	-	expression tag	UNP Q9NWZ3
D	155	TYR	-	expression tag	UNP Q9NWZ3
D	156	PHE	-	expression tag	UNP Q9NWZ3
D	157	GLN	-	expression tag	UNP Q9NWZ3
D	158	GLY	-	expression tag	UNP Q9NWZ3
D	159	SER	-	expression tag	UNP Q9NWZ3
D	461	GLY	-	expression tag	UNP Q9NWZ3
D	462	ASN	-	expression tag	UNP Q9NWZ3
D	463	SER	-	expression tag	UNP Q9NWZ3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is N-[(2R)-2-(hydroxymethyl)-2-methyl-6-(morpholin-4-yl)-2,3-dihydro-1-benzofuran-5-yl]pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: LSV) (formula: C₂₁H₂₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	21	5	4		
3	B	1	Total	C	N	O	0	0
			30	21	5	4		
3	C	1	Total	C	N	O	0	0
			30	21	5	4		
3	D	1	Total	C	N	O	0	0
			30	21	5	4		

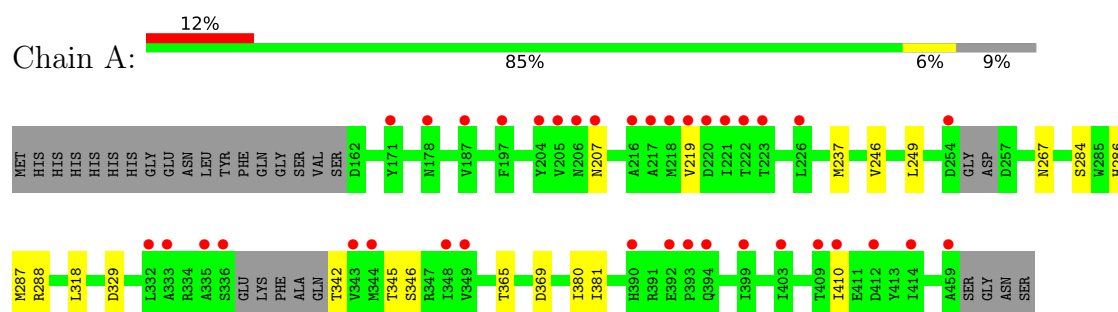
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	212	Total	O	0	0
			212	212		
4	B	201	Total	O	0	0
			201	201		
4	C	203	Total	O	0	0
			203	203		
4	D	220	Total	O	0	0
			220	220		

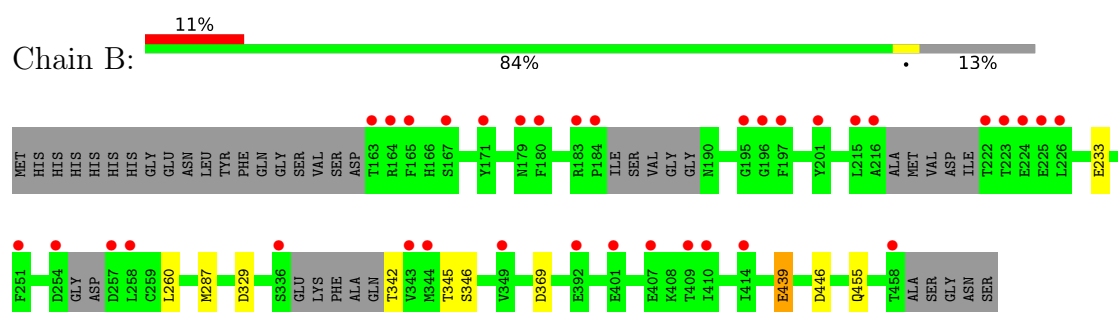
3 Residue-property plots [i](#)

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.

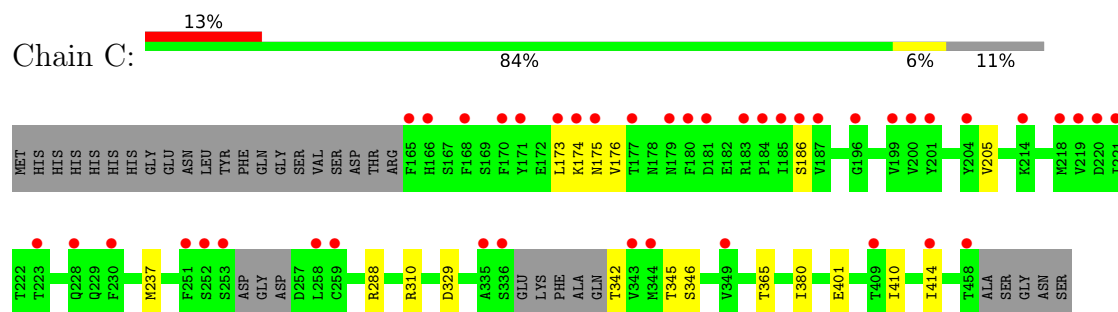
- Molecule 1: Interleukin-1 receptor-associated kinase 4



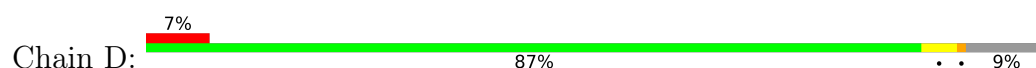
- Molecule 1: Interleukin-1 receptor-associated kinase 4

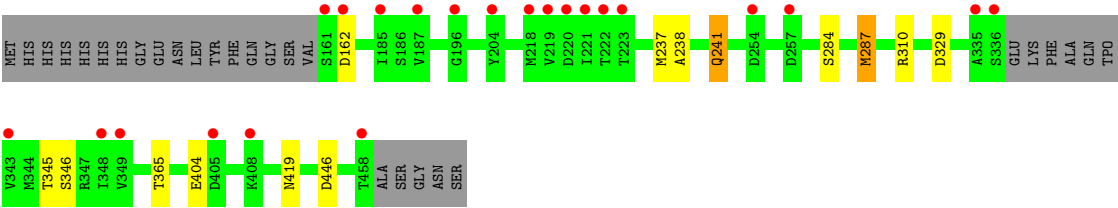


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.84Å 140.62Å 87.56Å 90.00° 123.71° 90.00°	Depositor
Resolution (Å)	72.84 – 1.77 72.84 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.5 (72.84-1.77) 99.5 (72.84-1.77)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.77Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.188 , 0.217 0.194 , 0.224	Depositor DCC
R_{free} test set	6866 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.1	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	0.96	EDS
Total number of atoms	10033	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LSV, SEP, TPO

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	0.83	0/2312	1.17	3/3115 (0.1%)
1	B	0.83	0/2203	1.14	2/2967 (0.1%)
1	C	0.85	0/2257	1.13	1/3042 (0.0%)
1	D	0.86	2/2328 (0.1%)	1.13	1/3138 (0.0%)
All	All	0.84	2/9100 (0.0%)	1.14	7/12262 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	287	MET	SD-CE	-7.92	1.59	1.79
1	D	241	GLN	CD-OE1	5.11	1.33	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ASN	CA-CB-CG	-6.17	106.43	112.60
1	C	175	ASN	CA-CB-CG	6.14	118.74	112.60
1	D	446	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	369	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	207	ASN	N-CA-C	-5.42	105.30	112.24
1	B	369	ASP	CA-CB-CG	5.30	117.90	112.60
1	B	446	ASP	CA-CB-CG	5.07	117.67	112.60

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	2302	0	2271	8	0
1	B	2201	0	2155	4	0
1	C	2253	0	2218	8	0
1	D	2306	0	2272	6	0
2	A	5	0	0	0	0
2	D	10	0	0	0	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
4	A	212	0	0	1	0
4	B	201	0	0	2	0
4	C	203	0	0	2	0
4	D	220	0	0	2	0
All	All	10033	0	8916	25	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 1.

All (25) 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:284:SER:H	1:A:287[A]:MET:HE3	1.27	0.97
1:D:284:SER:H	1:D:287:MET:HE3	1.32	0.93
1:D:237:MET:HA	1:D:237:MET:HE2	1.77	0.65
1:A:284:SER:N	1:A:287[A]:MET:HE3	2.10	0.57
1:C:186:SER:HB2	1:D:419:ASN:HB2	1.90	0.54
1:C:173:LEU:HA	1:C:176:VAL:HG22	1.90	0.53
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.91	0.51
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.93	0.50
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.93	0.50
1:A:286:HIS:HD2	4:C:602:HOH:O	1.95	0.49
1:D:162:ASP:HB3	1:D:238:ALA:HB1	1.95	0.48
1:A:287[A]:MET:HE1	4:A:763:HOH:O	2.13	0.47
1:B:439:GLU:CD	1:B:439:GLU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:MET:HE2	1:C:237:MET:HA	1.98	0.46
1:C:176:VAL:HG21	1:C:205:VAL:CG1	2.46	0.45
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.98	0.45
1:B:455:GLN:HG3	4:B:704:HOH:O	2.17	0.44
1:D:310:ARG:HD2	4:D:770:HOH:O	2.18	0.43
1:D:287:MET:HE1	4:D:706:HOH:O	2.19	0.43
1:A:288:ARG:HB3	1:A:380:ILE:HG23	2.02	0.42
1:C:310:ARG:HD2	4:C:753:HOH:O	2.19	0.42
1:C:176:VAL:HG11	1:C:205:VAL:HG12	2.01	0.42
1:C:410:ILE:O	1:C:414:ILE:HG13	2.20	0.42
1:A:381:ILE:HG21	1:A:410:ILE:HD11	2.03	0.41
1:B:287:MET:HG2	4:B:799:HOH:O	2.20	0.41

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	285/320 (89%)	277 (97%)	7 (2%)	1 (0%)	30	16
1	B	267/320 (83%)	261 (98%)	6 (2%)	0	100	100
1	C	278/320 (87%)	272 (98%)	6 (2%)	0	100	100
1	D	288/320 (90%)	283 (98%)	5 (2%)	0	100	100
All	All	1118/1280 (87%)	1093 (98%)	24 (2%)	1 (0%)	48	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	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	251/275 (91%)	248 (99%)	3 (1%)	63	49
1	B	239/275 (87%)	237 (99%)	2 (1%)	73	63
1	C	245/275 (89%)	241 (98%)	4 (2%)	55	38
1	D	254/275 (92%)	250 (98%)	4 (2%)	55	38
All	All	989/1100 (90%)	976 (99%)	13 (1%)	61	46

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	249	LEU
1	A	329	ASP
1	A	365	THR
1	B	329	ASP
1	B	439	GLU
1	C	174	LYS
1	C	329	ASP
1	C	365	THR
1	C	401	GLU
1	D	241	GLN
1	D	329	ASP
1	D	365	THR
1	D	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	HIS
1	A	451	GLN
1	B	178	ASN
1	B	229	GLN
1	B	390	HIS
1	C	175	ASN

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Mol	Chain	Res	Type
1	C	435	GLN
1	D	229	GLN
1	D	241	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	C	345	1	8,10,11	1.03	0	10,14,16	1.35	3 (30%)
1	SEP	D	346	1	8,9,10	1.00	0	7,12,14	2.45	2 (28%)
1	TPO	B	345	1	8,10,11	1.28	2 (25%)	10,14,16	1.03	0
1	TPO	D	345	1	8,10,11	1.15	0	10,14,16	1.35	1 (10%)
1	TPO	A	345	1	8,10,11	1.22	2 (25%)	10,14,16	1.20	1 (10%)
1	TPO	B	342	1	8,10,11	1.03	0	10,14,16	1.34	2 (20%)
1	SEP	A	346	1	8,9,10	0.79	0	7,12,14	1.43	1 (14%)
1	SEP	C	346	1	8,9,10	0.86	0	7,12,14	1.39	1 (14%)
1	TPO	A	342	1	8,10,11	1.34	1 (12%)	10,14,16	1.17	2 (20%)
1	SEP	B	346	1	8,9,10	0.89	0	7,12,14	2.00	2 (28%)
1	TPO	C	342	1	8,10,11	1.16	1 (12%)	10,14,16	1.44	2 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	2/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	A	345	1	-	5/9/11/13	-
1	TPO	B	342	1	-	0/9/11/13	-
1	SEP	A	346	1	-	3/6/8/10	-
1	SEP	C	346	1	-	4/6/8/10	-
1	TPO	A	342	1	-	2/9/11/13	-
1	SEP	B	346	1	-	2/6/8/10	-
1	TPO	C	342	1	-	3/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TPO	P-OG1	-2.81	1.54	1.59
1	C	342	TPO	P-OG1	-2.38	1.55	1.59
1	B	345	TPO	CB-CA	2.28	1.58	1.53
1	B	345	TPO	CG2-CB	2.21	1.56	1.51
1	A	345	TPO	CB-CA	2.16	1.58	1.53
1	A	345	TPO	CG2-CB	2.13	1.56	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	5.70	113.69	108.14
1	B	346	SEP	OG-CB-CA	4.29	112.31	108.14
1	C	346	SEP	OG-P-O1P	3.35	115.50	106.44
1	A	346	SEP	O3P-P-OG	3.04	114.59	106.67
1	C	345	TPO	O2P-P-OG1	2.92	117.23	105.85
1	D	346	SEP	O3P-P-OG	2.79	113.94	106.67
1	C	342	TPO	P-OG1-CB	-2.77	115.79	123.33
1	D	345	TPO	O3P-P-OG1	2.75	116.56	105.85
1	B	346	SEP	O3P-P-OG	2.71	113.73	106.67
1	B	342	TPO	O3P-P-OG1	2.54	115.74	105.85
1	B	342	TPO	P-OG1-CB	-2.54	116.43	123.33
1	A	345	TPO	O2P-P-OG1	2.46	115.43	105.85
1	C	342	TPO	O2P-P-OG1	2.35	115.00	105.85
1	A	342	TPO	O2P-P-OG1	2.17	114.31	105.85
1	C	345	TPO	O-C-CA	-2.02	119.58	124.77
1	A	342	TPO	P-OG1-CB	-2.01	117.86	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	345	TPO	P-OG1-CB	-2.01	117.87	123.33

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	CB-OG-P-O2P
1	A	346	SEP	CB-OG-P-O3P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
1	C	345	TPO	N-CA-CB-OG1
1	C	346	SEP	CB-OG-P-O1P
1	C	346	SEP	CB-OG-P-O2P
1	C	346	SEP	CB-OG-P-O3P
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	C-CA-CB-OG
1	A	346	SEP	CB-OG-P-O1P
1	A	342	TPO	C-CA-CB-CG2
1	C	345	TPO	CB-OG1-P-O1P
1	C	342	TPO	CB-OG1-P-O3P
1	D	345	TPO	CA-CB-OG1-P
1	A	345	TPO	CB-OG1-P-O1P
1	A	342	TPO	CB-OG1-P-O3P
1	A	345	TPO	CB-OG1-P-O2P
1	B	345	TPO	CB-OG1-P-O2P
1	C	342	TPO	C-CA-CB-CG2
1	C	345	TPO	O-C-CA-CB
1	C	346	SEP	C-CA-CB-OG
1	C	342	TPO	CB-OG1-P-O1P
1	A	345	TPO	CG2-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	LSV	A	502	-	34,34,34	1.71	5 (14%)	42,50,50	2.45	10 (23%)
2	SO4	D	502	-	4,4,4	0.30	0	6,6,6	0.11	0
3	LSV	D	503	-	34,34,34	1.58	8 (23%)	42,50,50	2.12	10 (23%)
2	SO4	D	501	-	4,4,4	0.21	0	6,6,6	0.10	0
3	LSV	B	501	-	34,34,34	1.56	6 (17%)	42,50,50	2.22	8 (19%)
2	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.15	0
3	LSV	C	501	-	34,34,34	1.69	6 (17%)	42,50,50	2.31	11 (26%)

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	LSV	D	503	-	-	4/15/33/33	0/5/5/5
3	LSV	C	501	-	-	4/15/33/33	0/5/5/5
3	LSV	B	501	-	-	7/15/33/33	0/5/5/5
3	LSV	A	502	-	-	4/15/33/33	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	LSV	O10-C2	-4.24	1.39	1.47
3	A	502	LSV	C21-N22	-4.20	1.26	1.32
3	D	503	LSV	O10-C2	-4.06	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	LSV	C21-N22	-3.99	1.27	1.32
3	A	502	LSV	O19-C18	-3.98	1.16	1.23
3	B	501	LSV	C21-N22	-3.89	1.27	1.32
3	A	502	LSV	O10-C2	-3.78	1.40	1.47
3	A	502	LSV	O10-C9	-3.69	1.32	1.38
3	D	503	LSV	C21-N22	-3.42	1.27	1.32
3	B	501	LSV	O19-C18	-3.41	1.17	1.23
3	C	501	LSV	O19-C18	-3.27	1.17	1.23
3	B	501	LSV	O10-C2	-3.21	1.41	1.47
3	B	501	LSV	O10-C9	-3.15	1.33	1.38
3	C	501	LSV	O10-C9	-2.94	1.33	1.38
3	C	501	LSV	C20-C24	-2.88	1.37	1.45
3	D	503	LSV	O19-C18	-2.79	1.18	1.23
3	A	502	LSV	C20-C24	-2.49	1.38	1.45
3	D	503	LSV	C6-C7	-2.45	1.37	1.40
3	D	503	LSV	O10-C9	-2.38	1.34	1.38
3	D	503	LSV	C20-C24	-2.27	1.39	1.45
3	B	501	LSV	C24-N23	-2.22	1.33	1.38
3	D	503	LSV	C8-C7	-2.20	1.36	1.39
3	D	503	LSV	C3-C4	-2.15	1.48	1.50
3	B	501	LSV	C20-C24	-2.11	1.39	1.45
3	C	501	LSV	C8-C9	-2.10	1.35	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	LSV	C26-N25-C24	7.80	121.61	115.55
3	B	501	LSV	C26-N25-C24	7.34	121.25	115.55
3	D	503	LSV	C26-N25-C24	7.29	121.21	115.55
3	A	502	LSV	C21-N22-N23	7.24	110.90	103.81
3	C	501	LSV	C26-N25-C24	6.72	120.78	115.55
3	A	502	LSV	C2-O10-C9	6.50	111.89	107.17
3	B	501	LSV	C21-N22-N23	6.22	109.89	103.81
3	B	501	LSV	C2-O10-C9	5.60	111.24	107.17
3	C	501	LSV	C8-C9-C4	-5.51	116.91	123.19
3	D	503	LSV	C8-C9-C4	-5.07	117.41	123.19
3	C	501	LSV	C2-O10-C9	5.01	110.81	107.17
3	D	503	LSV	C21-N22-N23	4.68	108.39	103.81
3	B	501	LSV	C8-C9-C4	-4.37	118.22	123.19
3	A	502	LSV	C8-C9-C4	-4.05	118.58	123.19
3	C	501	LSV	C21-N22-N23	3.95	107.68	103.81
3	C	501	LSV	C20-C18-N17	3.68	120.80	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	LSV	C28-N23-N22	3.65	132.43	127.01
3	C	501	LSV	C5-C6-C7	-3.62	115.84	119.80
3	B	501	LSV	C27-C26-N25	-3.40	119.89	124.25
3	D	503	LSV	C27-C26-N25	-3.17	120.19	124.25
3	A	502	LSV	C27-C26-N25	-3.17	120.19	124.25
3	D	503	LSV	C28-N23-N22	3.01	131.48	127.01
3	C	501	LSV	C27-C26-N25	-2.98	120.44	124.25
3	B	501	LSV	C28-N23-N22	2.92	131.34	127.01
3	D	503	LSV	C5-C4-C9	2.78	121.75	119.59
3	C	501	LSV	C28-N23-N22	2.78	131.14	127.01
3	A	502	LSV	C20-C21-N22	-2.63	109.19	112.45
3	A	502	LSV	C1-C2-C3	-2.61	107.92	112.12
3	C	501	LSV	C3-C4-C9	-2.59	105.40	108.42
3	D	503	LSV	C8-C7-N11	-2.57	118.84	122.59
3	D	503	LSV	C2-O10-C9	2.49	108.98	107.17
3	C	501	LSV	C3-C4-C5	2.46	133.11	128.94
3	C	501	LSV	C5-C4-C9	2.43	121.48	119.59
3	B	501	LSV	C3-C4-C5	2.38	132.97	128.94
3	A	502	LSV	C3-C4-C5	2.29	132.81	128.94
3	D	503	LSV	C1-C2-C3	-2.20	108.58	112.12
3	D	503	LSV	C3-C4-C9	-2.10	105.97	108.42
3	B	501	LSV	C16-N11-C7	-2.09	111.21	116.19
3	A	502	LSV	C5-C6-C7	-2.02	117.59	119.80

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	LSV	C3-C2-C29-O30
3	C	501	LSV	C8-C7-N11-C12
3	D	503	LSV	C8-C7-N11-C16
3	B	501	LSV	C8-C7-N11-C16
3	A	502	LSV	C8-C7-N11-C12
3	B	501	LSV	O10-C2-C29-O30
3	C	501	LSV	C8-C7-N11-C16
3	D	503	LSV	C8-C7-N11-C12
3	A	502	LSV	C8-C7-N11-C16
3	B	501	LSV	C8-C7-N11-C12
3	B	501	LSV	C1-C2-C29-O30
3	B	501	LSV	C6-C7-N11-C16
3	C	501	LSV	C6-C7-N11-C16
3	A	502	LSV	C6-C7-N11-C16

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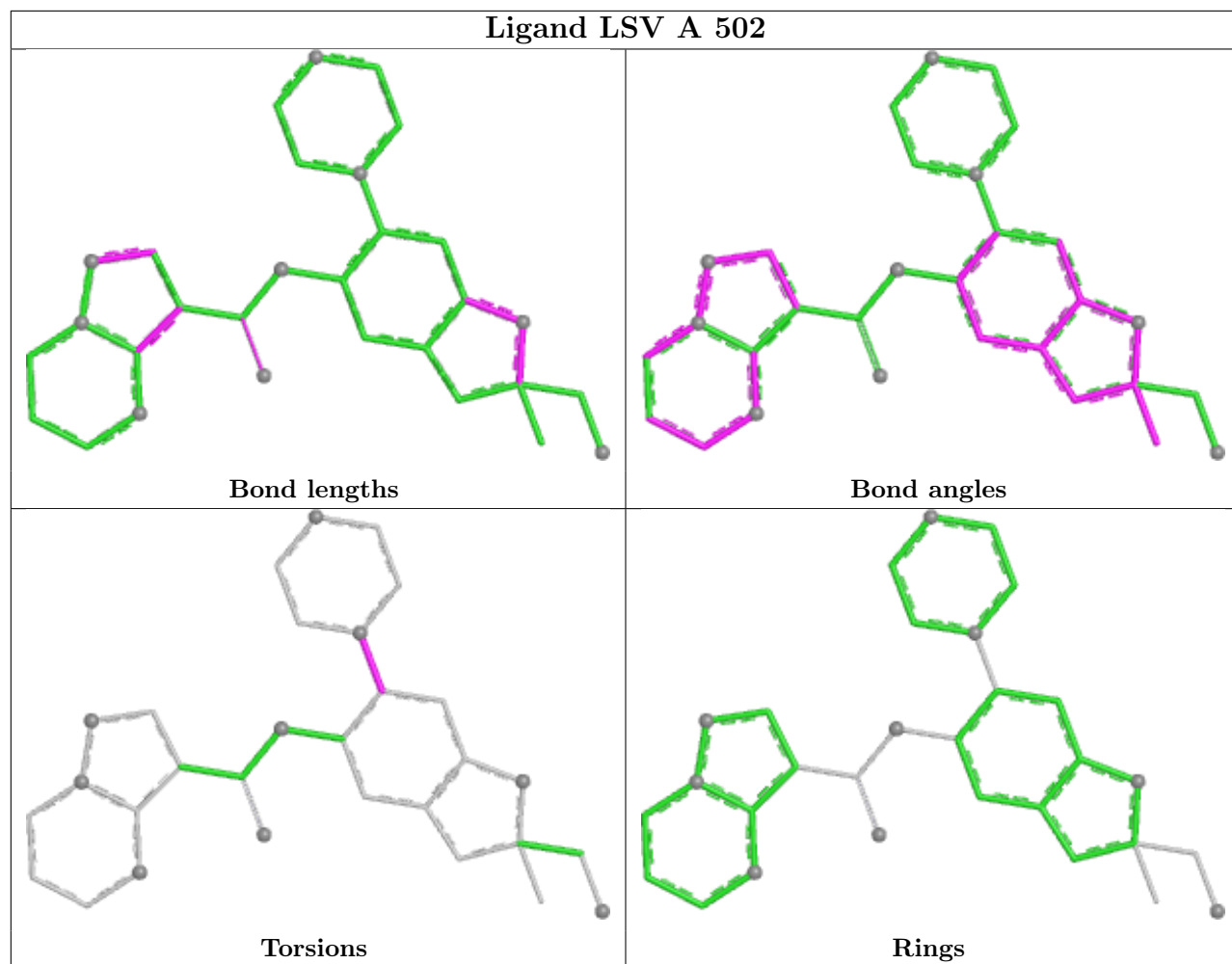
Mol	Chain	Res	Type	Atoms
3	B	501	LSV	C6-C7-N11-C12
3	C	501	LSV	C6-C7-N11-C12
3	D	503	LSV	C6-C7-N11-C12
3	A	502	LSV	C6-C7-N11-C12
3	D	503	LSV	C6-C7-N11-C16

There are no ring outliers.

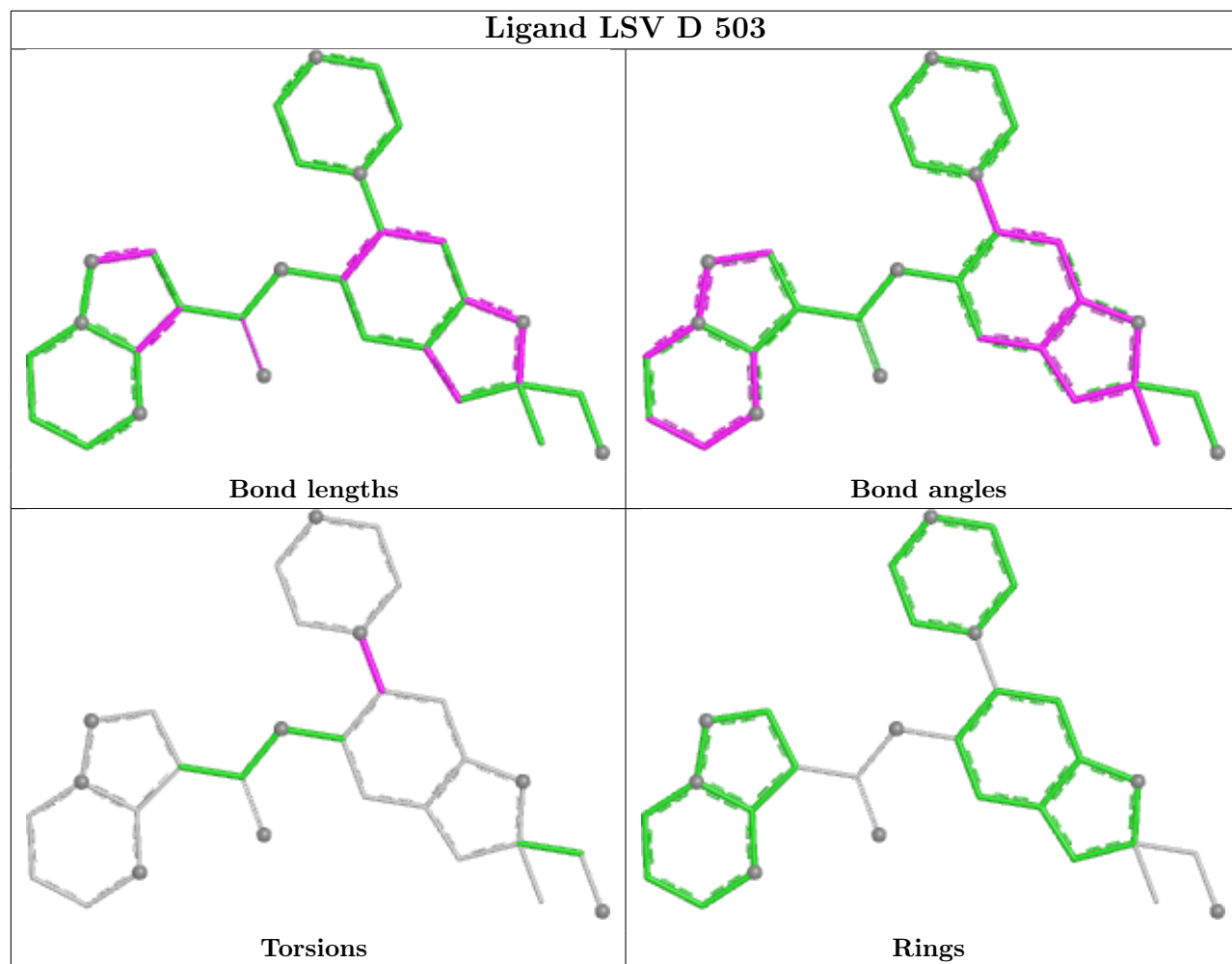
No monomer is involved in short contacts.

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.

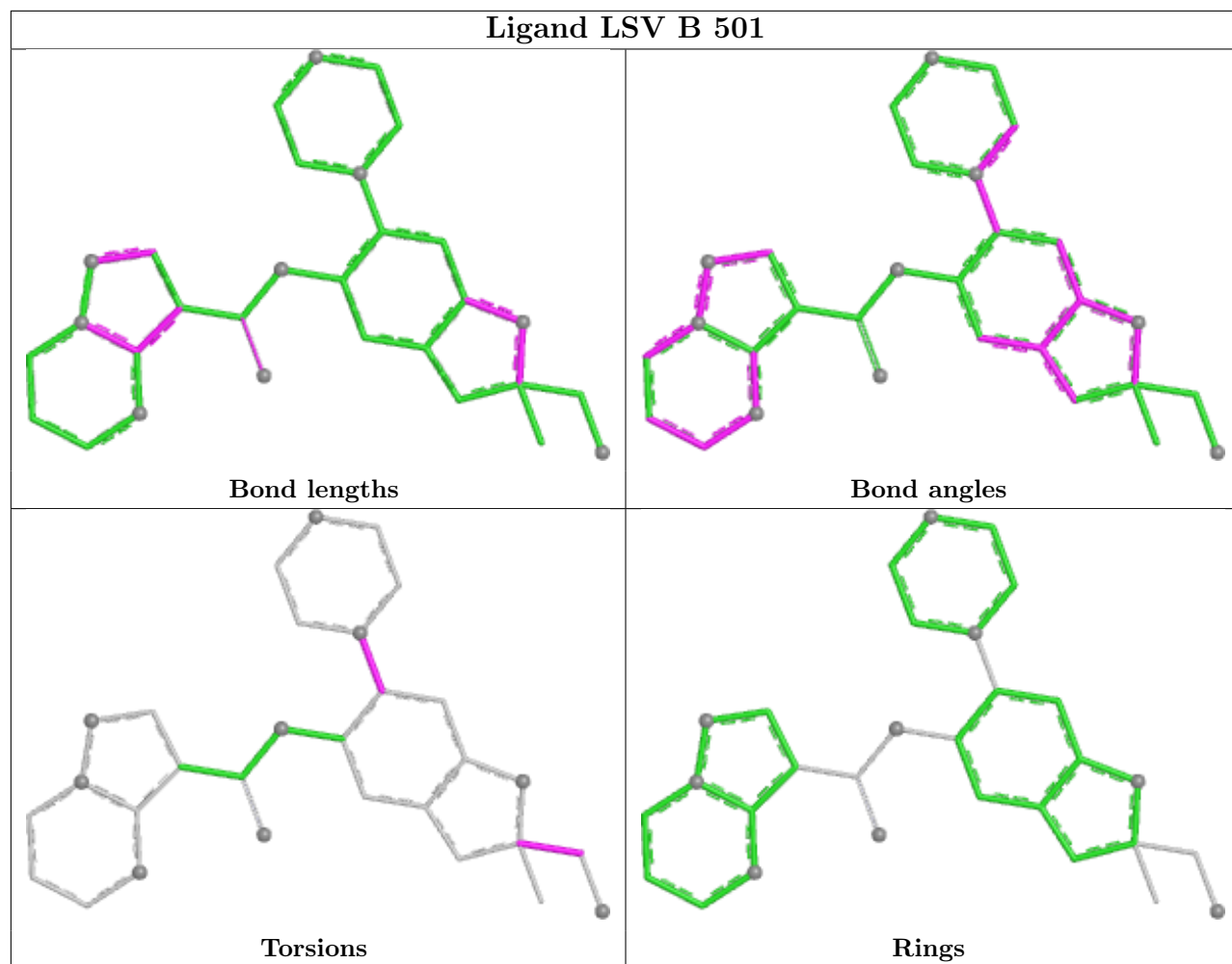
Ligand LSV A 502

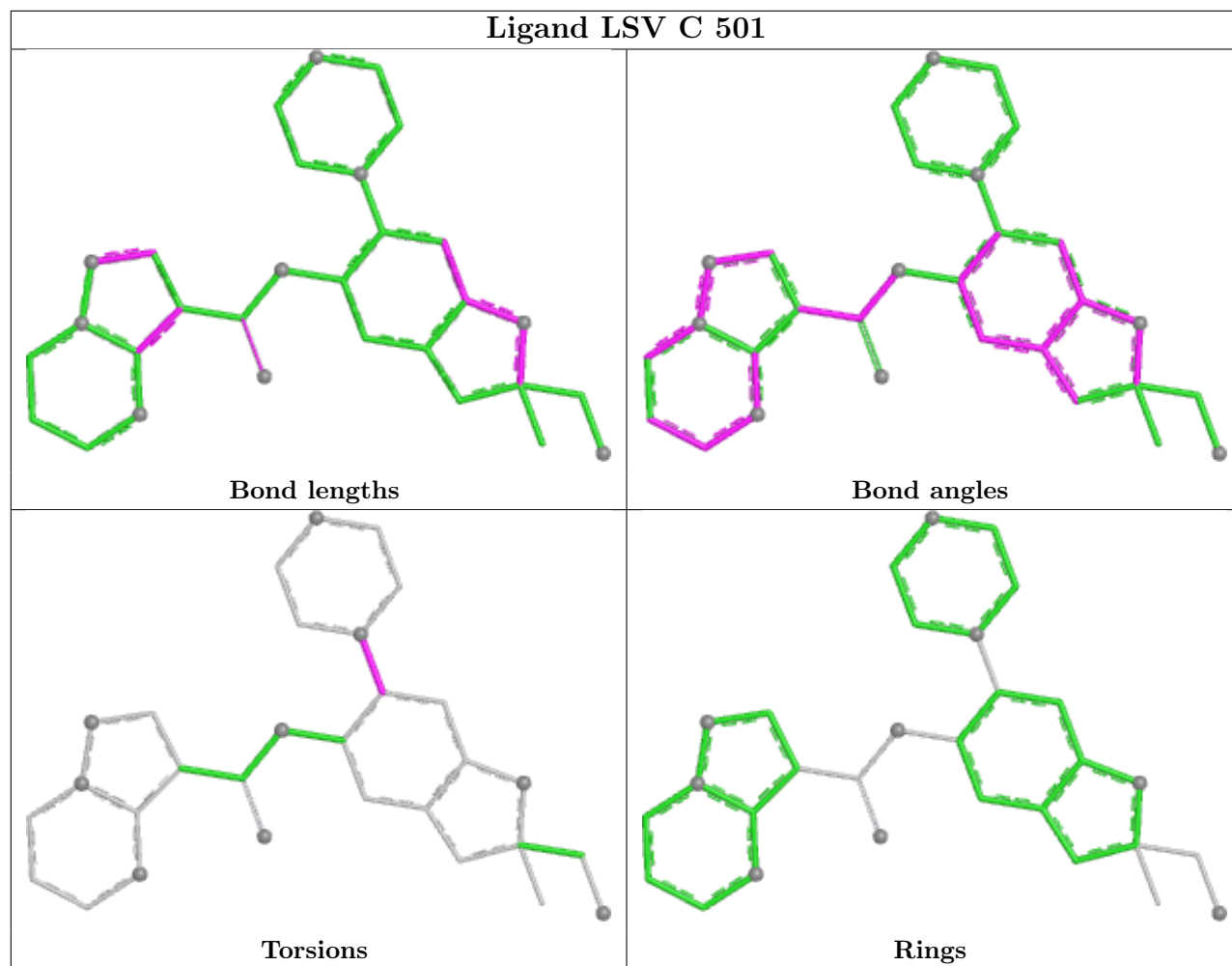


Ligand LSV D 503



Ligand LSV B 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	288/320 (90%)	0.68	37 (12%) 7 8	13, 30, 64, 83	2 (0%)
1	B	276/320 (86%)	0.71	35 (12%) 8 8	18, 31, 62, 80	0
1	C	283/320 (88%)	0.66	43 (15%) 5 5	17, 30, 53, 65	0
1	D	290/320 (90%)	0.37	22 (7%) 20 23	14, 29, 53, 70	2 (0%)
All	All	1137/1280 (88%)	0.60	137 (12%) 9 9	13, 30, 58, 83	4 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	VAL	6.1
1	B	184	PRO	6.1
1	B	216	ALA	5.5
1	A	459	ALA	5.1
1	A	335	ALA	5.0
1	C	253	SER	5.0
1	B	458	THR	4.9
1	B	222	THR	4.9
1	C	170	PHE	4.9
1	A	336	SER	4.6
1	A	204	TYR	4.4
1	B	197	PHE	4.4
1	A	344	MET	4.3
1	C	258	LEU	4.3
1	A	254	ASP	4.2
1	B	196	GLY	4.2
1	B	163	THR	4.2
1	D	187	VAL	4.2
1	A	343	VAL	4.1
1	D	335	ALA	4.0
1	A	217	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	195	GLY	4.0
1	D	343	VAL	4.0
1	A	205	VAL	3.9
1	C	221	ILE	3.9
1	A	206	ASN	3.9
1	A	409	THR	3.8
1	C	458	THR	3.7
1	B	254	ASP	3.6
1	D	257	ASP	3.6
1	B	171	TYR	3.5
1	B	410	ILE	3.5
1	C	185	ILE	3.4
1	D	336	SER	3.4
1	A	220	ASP	3.4
1	A	393	PRO	3.4
1	A	410	ILE	3.3
1	A	226	LEU	3.3
1	A	187	VAL	3.3
1	C	219	VAL	3.3
1	C	180	PHE	3.3
1	B	349	VAL	3.3
1	C	414	ILE	3.2
1	B	179	ASN	3.2
1	A	219	VAL	3.2
1	A	221	ILE	3.2
1	B	226	LEU	3.1
1	B	225	GLU	3.1
1	C	230	PHE	3.1
1	C	336	SER	3.1
1	A	333	ALA	3.1
1	A	403	ILE	3.0
1	A	222	THR	3.0
1	B	164	ARG	3.0
1	B	165	PHE	3.0
1	D	221	ILE	2.9
1	D	220	ASP	2.9
1	A	349	VAL	2.9
1	C	343	VAL	2.9
1	B	336	SER	2.8
1	D	161	SER	2.8
1	C	199	VAL	2.8
1	A	348	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	186	SER	2.8
1	B	215	LEU	2.7
1	D	162	ASP	2.7
1	C	187	VAL	2.7
1	C	171	TYR	2.7
1	C	201	TYR	2.7
1	C	173	LEU	2.7
1	C	220	ASP	2.7
1	B	180	PHE	2.6
1	C	165	PHE	2.6
1	B	223	THR	2.6
1	C	200	VAL	2.6
1	B	167	SER	2.6
1	D	349	VAL	2.6
1	A	390	HIS	2.6
1	C	218	MET	2.6
1	C	183	ARG	2.6
1	B	258	LEU	2.5
1	C	174	LYS	2.5
1	B	224	GLU	2.5
1	D	204	TYR	2.5
1	A	207	ASN	2.5
1	D	218	MET	2.5
1	C	184	PRO	2.4
1	B	201	TYR	2.4
1	C	259	CYS	2.4
1	C	228	GLN	2.4
1	C	204	TYR	2.4
1	C	349	VAL	2.4
1	A	392	GLU	2.4
1	A	414	ILE	2.4
1	A	197	PHE	2.3
1	D	196	GLY	2.3
1	C	177	THR	2.3
1	B	392	GLU	2.3
1	B	407	GLU	2.3
1	C	252	SER	2.3
1	A	178	ASN	2.3
1	C	179	ASN	2.3
1	A	412	ASP	2.3
1	A	218	MET	2.3
1	B	409	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	458	THR	2.2
1	B	414	ILE	2.2
1	C	166	HIS	2.2
1	D	223	THR	2.2
1	C	335	ALA	2.2
1	B	257	ASP	2.2
1	B	251	PHE	2.2
1	A	171	TYR	2.2
1	D	348	ILE	2.2
1	A	399	ILE	2.2
1	D	185	ILE	2.2
1	C	409	THR	2.2
1	D	222	THR	2.2
1	D	219	VAL	2.1
1	A	216	ALA	2.1
1	C	196	GLY	2.1
1	A	332	LEU	2.1
1	A	223	THR	2.1
1	A	394	GLN	2.1
1	B	183	ARG	2.1
1	B	344	MET	2.1
1	B	401	GLU	2.1
1	D	254	ASP	2.1
1	D	405	ASP	2.1
1	C	223	THR	2.1
1	C	214	LYS	2.0
1	D	408	LYS	2.0
1	C	175	ASN	2.0
1	C	344	MET	2.0
1	C	168	PHE	2.0
1	C	251	PHE	2.0
1	C	181	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	D	346	10/11	0.64	0.14	56,58,61,61	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPO	B	342	11/12	0.73	0.16	62,64,67,67	4
1	TPO	C	342	11/12	0.74	0.15	54,56,58,58	4
1	SEP	A	346	10/11	0.76	0.13	52,54,56,56	4
1	TPO	A	342	11/12	0.77	0.16	71,71,73,73	4
1	SEP	B	346	10/11	0.79	0.12	51,56,57,57	4
1	SEP	C	346	10/11	0.81	0.12	44,47,48,48	4
1	TPO	D	345	11/12	0.92	0.10	52,54,57,58	0
1	TPO	C	345	11/12	0.93	0.10	43,45,50,51	0
1	TPO	A	345	11/12	0.93	0.11	52,53,55,55	0
1	TPO	B	345	11/12	0.94	0.11	46,49,51,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

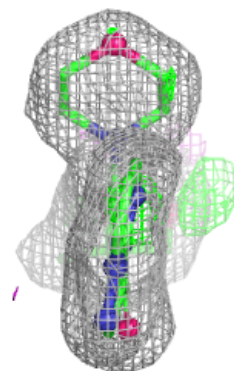
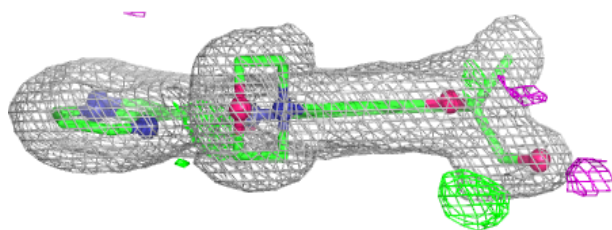
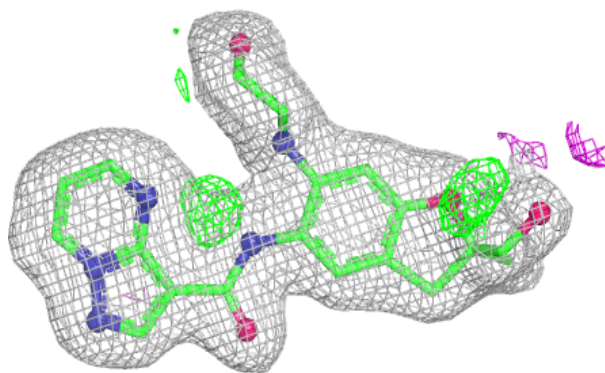
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	D	502	5/5	0.74	0.13	89,89,89,90	0
2	SO4	D	501	5/5	0.81	0.12	78,79,80,80	0
2	SO4	A	501	5/5	0.94	0.07	47,51,52,54	0
3	LSV	C	501	30/30	0.95	0.08	21,25,40,42	0
3	LSV	B	501	30/30	0.96	0.07	21,25,42,47	0
3	LSV	A	502	30/30	0.97	0.06	17,21,32,33	0
3	LSV	D	503	30/30	0.97	0.06	19,22,37,39	0

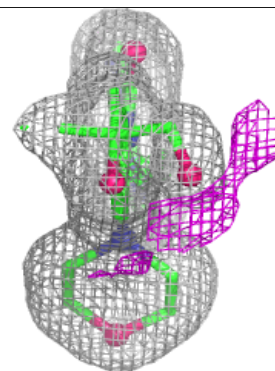
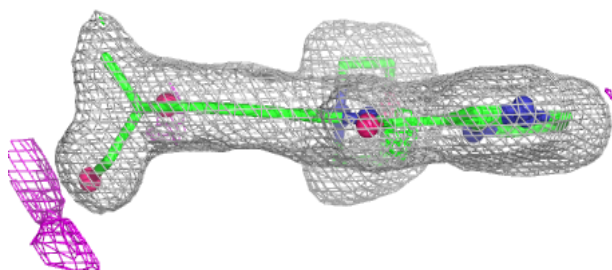
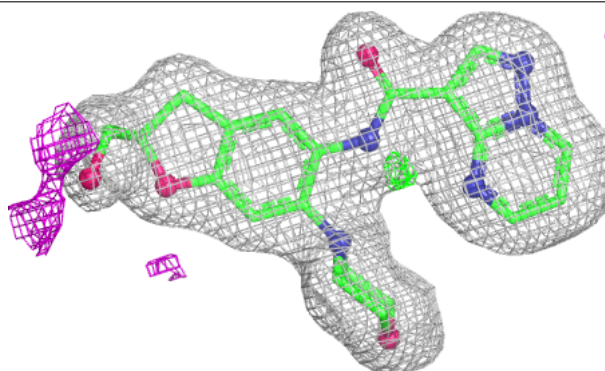
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LSV C 501:

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

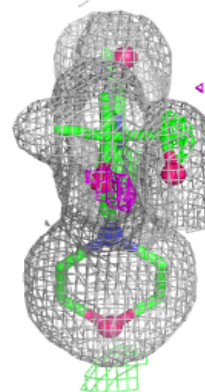
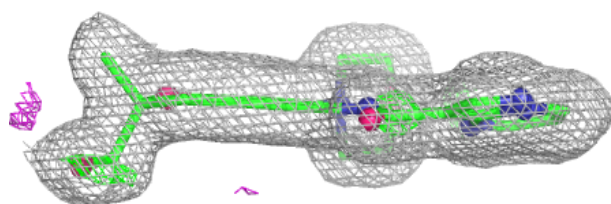
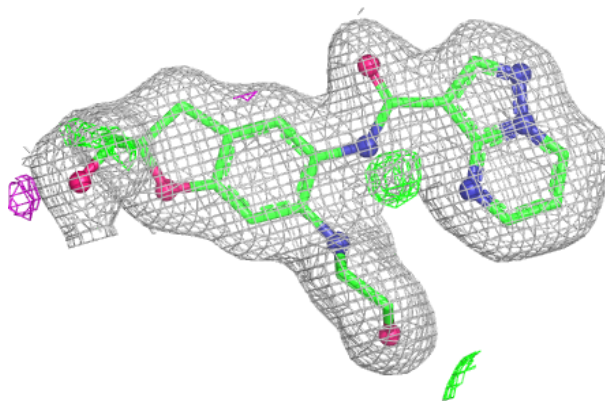
**Electron density around LSV B 501:**

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

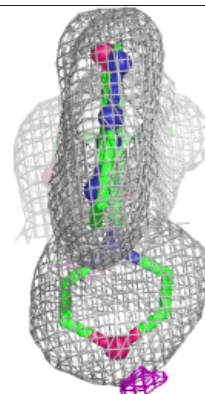
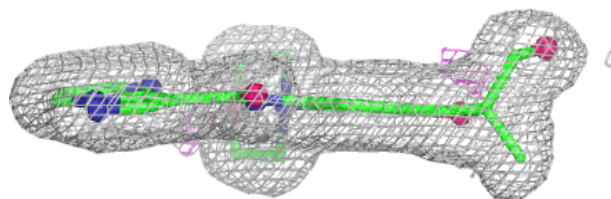
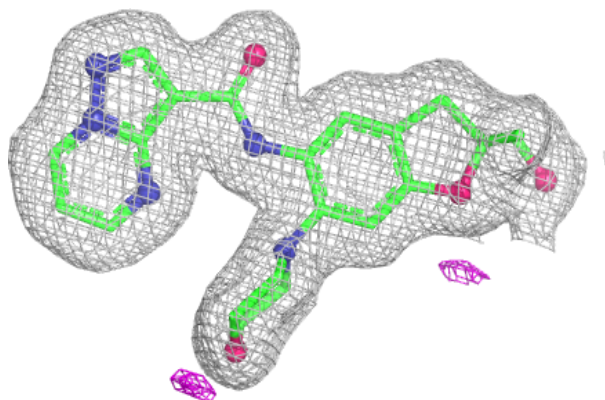


Electron density around LSV A 502:

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

**Electron density around LSV D 503:**

$2mF_o-DF_c$ (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.