W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2025 – 12:10 PM JST

PDB ID	:	8XQ0
Title	:	Crystal structure of spleen tyrosine kinase(SYK)in complex with SKI-G-1653
Authors	:	Bong, S.M.; Lee, B.I.
Deposited on	:	2024-01-04
Resolution	:	1.95 Å(reported)

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

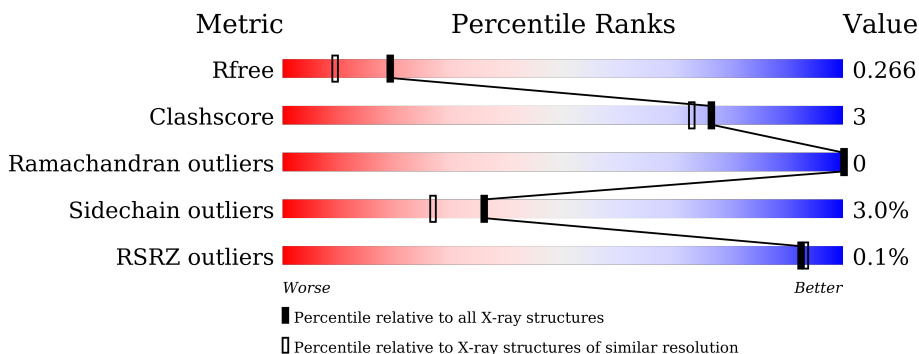|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.95 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	Percentile Ranks	Value
Rfree		0.266
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		3.0%
RSRZ outliers		0.1%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

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 <=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	290	86% ... 5% 9%
1	B	290	77% ... 10% 13%
1	C	290	81% ... 9% • 9%
1	D	290	80% ... 8% • 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8818 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 Tyrosine-protein kinase SYK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2145	1377	358	391	19			
1	B	253	Total	C	N	O	S	0	0	0
			2070	1333	345	374	18			
1	C	263	Total	C	N	O	S	0	0	0
			2141	1373	358	391	19			
1	D	258	Total	C	N	O	S	0	0	0
			2109	1357	353	380	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	636	LEU	-	expression tag	UNP P43405
A	637	GLU	-	expression tag	UNP P43405
A	638	HIS	-	expression tag	UNP P43405
A	639	HIS	-	expression tag	UNP P43405
A	640	HIS	-	expression tag	UNP P43405
A	641	HIS	-	expression tag	UNP P43405
A	642	HIS	-	expression tag	UNP P43405
A	643	HIS	-	expression tag	UNP P43405
A	644	HIS	-	expression tag	UNP P43405
A	645	HIS	-	expression tag	UNP P43405
B	636	LEU	-	expression tag	UNP P43405
B	637	GLU	-	expression tag	UNP P43405
B	638	HIS	-	expression tag	UNP P43405
B	639	HIS	-	expression tag	UNP P43405
B	640	HIS	-	expression tag	UNP P43405
B	641	HIS	-	expression tag	UNP P43405
B	642	HIS	-	expression tag	UNP P43405
B	643	HIS	-	expression tag	UNP P43405
B	644	HIS	-	expression tag	UNP P43405
B	645	HIS	-	expression tag	UNP P43405
C	636	LEU	-	expression tag	UNP P43405

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Chain	Residue	Modelled	Actual	Comment	Reference
C	637	GLU	-	expression tag	UNP P43405
C	638	HIS	-	expression tag	UNP P43405
C	639	HIS	-	expression tag	UNP P43405
C	640	HIS	-	expression tag	UNP P43405
C	641	HIS	-	expression tag	UNP P43405
C	642	HIS	-	expression tag	UNP P43405
C	643	HIS	-	expression tag	UNP P43405
C	644	HIS	-	expression tag	UNP P43405
C	645	HIS	-	expression tag	UNP P43405
D	636	LEU	-	expression tag	UNP P43405
D	637	GLU	-	expression tag	UNP P43405
D	638	HIS	-	expression tag	UNP P43405
D	639	HIS	-	expression tag	UNP P43405
D	640	HIS	-	expression tag	UNP P43405
D	641	HIS	-	expression tag	UNP P43405
D	642	HIS	-	expression tag	UNP P43405
D	643	HIS	-	expression tag	UNP P43405
D	644	HIS	-	expression tag	UNP P43405
D	645	HIS	-	expression tag	UNP P43405

- Molecule 2 is cyclopropyl-[5-[[4-[4-[[(3 {S},4 {S})-3-methoxy-4-oxidanyl-pyrrolidin-1-yl]methyl]-3-methyl-pyrazol-1-yl]pyrimidin-2-yl]amino]-1-methyl-indol-3-yl]methanone (three-letter code: A1LV4) (formula: $C_{27}H_{31}N_7O_3$) (labeled as "Ligand of Interest" by depositor).
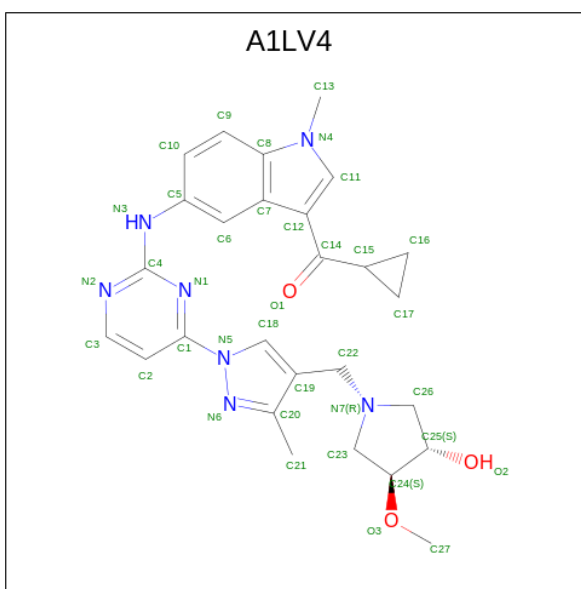
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	37	27	7	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 37	C 27	N 7	O 3	0	0
2	C	1	Total 37	C 27	N 7	O 3	0	0
2	D	1	Total 37	C 27	N 7	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	57	Total 57	O 57	0	0
3	B	54	Total 54	O 54	0	0
3	C	42	Total 42	O 42	0	0
3	D	52	Total 52	O 52	0	0

3 Residue-property plots ⓘ

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.
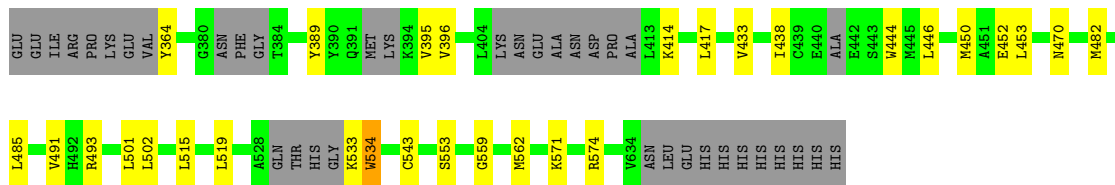
- Molecule 1: Tyrosine-protein kinase SYK

Chain A:
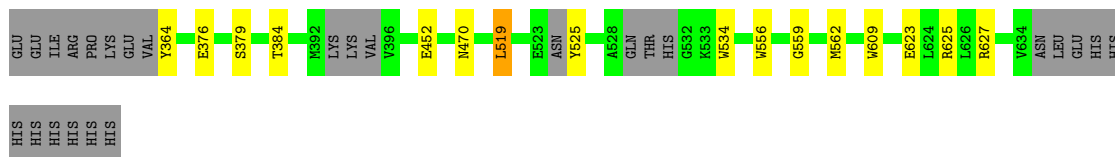
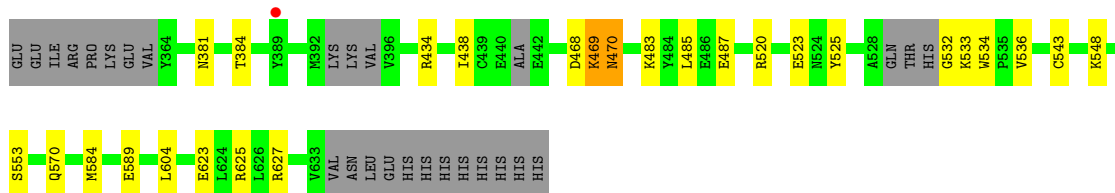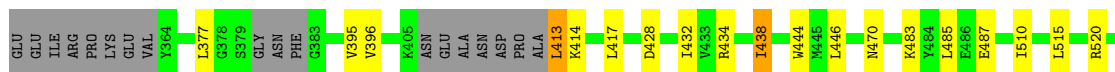- Molecule 1: Tyrosine-protein kinase SYK

Chain B:

- Molecule 1: Tyrosine-protein kinase SYK

Chain C:

- Molecule 1: Tyrosine-protein kinase SYK

Chain D:

E523 N524 A528 GLN THR HIS GLY K533 W534 M584 E589 V634 N635 LEU GLU HIS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.76Å 85.26Å 79.57Å 90.00° 85.19° 90.03°	Depositor
Resolution (Å)	39.65 – 1.95 39.65 – 1.95	Depositor EDS
% Data completeness (in resolution range)	91.3 (39.65-1.95) 91.4 (39.65-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.219 , 0.265 0.219 , 0.266	Depositor DCC
R_{free} test set	3585 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.8	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.397 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8818	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7941e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: A1LV4

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	0.31	0/2192	0.51	0/2952
1	B	0.32	0/2113	0.52	0/2842
1	C	0.32	0/2188	0.50	0/2946
1	D	0.33	0/2154	0.53	0/2898
All	All	0.32	0/8647	0.51	0/11638

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 ⓘ

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	2145	0	2122	7	0
1	B	2070	0	2061	15	0
1	C	2141	0	2114	14	0
1	D	2109	0	2109	12	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
2	C	37	0	0	0	0
2	D	37	0	0	0	0
3	A	57	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	0	0	0
3	C	42	0	0	2	0
3	D	52	0	0	0	0
All	All	8818	0	8406	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (47) 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:C:381:ASN:HB3	1:D:634:VAL:HG11	1.78	0.65
1:C:532:GLY:N	3:C:802:HOH:O	2.30	0.63
1:B:364:TYR:N	1:B:438:ILE:O	2.32	0.63
1:B:389:TYR:HB3	1:B:396:VAL:HG11	1.82	0.61
1:D:584:MET:HG3	1:D:589:GLU:HB2	1.82	0.60
1:D:428:ASP:OD1	1:D:434:ARG:NH2	2.37	0.57
1:C:534:TRP:CD1	1:C:536:VAL:HG22	2.40	0.57
1:D:413:LEU:HD13	1:D:414:LYS:HG2	1.86	0.57
1:B:417:LEU:HD21	1:B:446:LEU:HB2	1.86	0.57
1:D:438:ILE:HD11	1:D:444:TRP:HE3	1.69	0.57
1:C:483:LYS:NZ	1:C:487:GLU:OE2	2.36	0.56
1:C:604:LEU:HD13	1:C:625:ARG:HD3	1.88	0.54
1:A:559:GLY:HA2	1:A:562:MET:HE2	1.90	0.54
1:B:453:LEU:HB2	1:B:502:LEU:HB2	1.91	0.54
1:B:515:LEU:HD21	1:B:533:LYS:HD2	1.91	0.53
1:C:584:MET:HG3	1:C:589:GLU:HB2	1.91	0.52
1:B:389:TYR:HB3	1:B:396:VAL:CG1	2.42	0.50
1:A:364:TYR:N	3:A:801:HOH:O	2.46	0.49
1:B:559:GLY:HA2	1:B:562:MET:HE2	1.96	0.47
1:D:483:LYS:NZ	1:D:487:GLU:OE2	2.45	0.47
1:B:533:LYS:O	1:B:534:TRP:HD1	1.98	0.46
1:D:520:ARG:HB2	1:D:523:GLU:HG2	1.97	0.46
1:A:452:GLU:HG3	3:A:833:HOH:O	2.14	0.46
1:A:519:LEU:HD11	1:A:525:TYR:N	2.31	0.46
1:C:520:ARG:HB2	1:C:523:GLU:HG2	1.98	0.46
1:B:450:MET:HG3	1:B:452:GLU:HG2	1.96	0.45
1:D:515:LEU:HD21	1:D:533:LYS:HE3	1.97	0.45
1:B:414:LYS:HD2	1:B:444:TRP:CZ2	2.51	0.45
1:D:438:ILE:HD11	1:D:444:TRP:CE3	2.51	0.44
1:C:543:CYS:SG	1:C:553:SER:OG	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ILE:HD13	1:D:510:ILE:HB	2.00	0.44
1:B:482:MET:SD	1:B:485:LEU:HD12	2.57	0.43
1:B:543:CYS:SG	1:B:553:SER:HB3	2.58	0.43
1:C:469:LYS:HG3	1:C:470:ASN:N	2.34	0.43
1:C:623:GLU:OE1	1:C:627:ARG:NH2	2.53	0.42
1:D:417:LEU:HD11	1:D:446:LEU:HB2	2.02	0.42
1:C:434:ARG:HD3	3:C:819:HOH:O	2.19	0.41
1:B:493:ARG:HD3	1:B:515:LEU:O	2.20	0.41
1:D:413:LEU:HD22	1:D:413:LEU:HA	1.90	0.41
1:A:376:GLU:OE2	1:A:379:SER:HB2	2.20	0.41
1:A:623:GLU:OE1	1:A:627:ARG:NH2	2.43	0.41
1:B:433:VAL:HG21	1:B:501:LEU:HD12	2.03	0.41
1:C:534:TRP:HD1	1:C:536:VAL:HG22	1.86	0.41
1:A:556:TRP:CE3	1:A:609:TRP:HA	2.56	0.40
1:C:485:LEU:HD12	1:C:485:LEU:HA	1.95	0.40
1:C:525:TYR:CE2	1:C:548:LYS:HE3	2.56	0.40
1:B:491:VAL:HG12	1:B:493:ARG:HG3	2.03	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	256/290 (88%)	249 (97%)	7 (3%)	0	100	100
1	B	241/290 (83%)	235 (98%)	6 (2%)	0	100	100
1	C	255/290 (88%)	250 (98%)	5 (2%)	0	100	100
1	D	250/290 (86%)	243 (97%)	7 (3%)	0	100	100
All	All	1002/1160 (86%)	977 (98%)	25 (2%)	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	228/254 (90%)	223 (98%)	5 (2%)	47	41
1	B	222/254 (87%)	216 (97%)	6 (3%)	40	31
1	C	228/254 (90%)	221 (97%)	7 (3%)	35	25
1	D	226/254 (89%)	217 (96%)	9 (4%)	27	16
All	All	904/1016 (89%)	877 (97%)	27 (3%)	36	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	THR
1	A	470	ASN
1	A	519	LEU
1	A	534	TRP
1	A	625	ARG
1	B	395	VAL
1	B	470	ASN
1	B	519	LEU
1	B	534	TRP
1	B	571	LYS
1	B	574	ARG
1	C	384	THR
1	C	438	ILE
1	C	468	ASP
1	C	469	LYS
1	C	470	ASN
1	C	533	LYS
1	C	570	GLN
1	D	377	LEU
1	D	395	VAL
1	D	396	VAL
1	D	413	LEU
1	D	438	ILE
1	D	470	ASN

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Mol	Chain	Res	Type
1	D	485	LEU
1	D	524	ASN
1	D	534	TRP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	A1LV4	D	701	-	37,42,42	3.53	9 (24%)	47,62,62	2.08	10 (21%)
2	A1LV4	B	701	-	37,42,42	3.48	10 (27%)	47,62,62	2.13	10 (21%)
2	A1LV4	C	701	-	37,42,42	3.46	9 (24%)	47,62,62	2.07	10 (21%)
2	A1LV4	A	701	-	37,42,42	3.42	9 (24%)	47,62,62	1.97	11 (23%)

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	A1LV4	D	701	-	-	2/15/36/36	0/6/6/6
2	A1LV4	B	701	-	-	1/15/36/36	0/6/6/6
2	A1LV4	C	701	-	-	2/15/36/36	0/6/6/6
2	A1LV4	A	701	-	-	1/15/36/36	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	A1LV4	C22-N7	-14.59	1.19	1.47
2	C	701	A1LV4	C22-N7	-14.25	1.20	1.47
2	B	701	A1LV4	C22-N7	-14.15	1.20	1.47
2	A	701	A1LV4	C22-N7	-14.04	1.20	1.47
2	B	701	A1LV4	C11-N4	-9.40	1.24	1.38
2	D	701	A1LV4	C11-N4	-9.34	1.24	1.38
2	C	701	A1LV4	C11-N4	-9.02	1.25	1.38
2	A	701	A1LV4	C11-N4	-9.01	1.25	1.38
2	D	701	A1LV4	C12-C7	7.60	1.49	1.42
2	C	701	A1LV4	C12-C7	7.46	1.48	1.42
2	A	701	A1LV4	C12-C7	7.06	1.48	1.42
2	B	701	A1LV4	C12-C7	6.88	1.48	1.42
2	C	701	A1LV4	C4-N3	5.12	1.47	1.36
2	B	701	A1LV4	C4-N3	5.07	1.46	1.36
2	A	701	A1LV4	C4-N3	5.02	1.46	1.36
2	C	701	A1LV4	C25-C24	-4.91	1.39	1.53
2	D	701	A1LV4	C4-N3	4.87	1.46	1.36
2	D	701	A1LV4	C25-C24	-4.80	1.39	1.53
2	B	701	A1LV4	C25-C24	-4.74	1.40	1.53
2	A	701	A1LV4	C25-C24	-4.68	1.40	1.53
2	B	701	A1LV4	C5-N3	3.34	1.48	1.40
2	D	701	A1LV4	C5-N3	3.32	1.48	1.40
2	A	701	A1LV4	C22-C19	3.18	1.56	1.51
2	B	701	A1LV4	C22-C19	2.98	1.56	1.51
2	C	701	A1LV4	C22-C19	2.95	1.56	1.51
2	A	701	A1LV4	C5-N3	2.85	1.47	1.40
2	C	701	A1LV4	C5-N3	2.83	1.47	1.40
2	D	701	A1LV4	C22-C19	2.82	1.56	1.51
2	A	701	A1LV4	O2-C25	2.74	1.49	1.43
2	B	701	A1LV4	C21-C20	2.64	1.54	1.50
2	D	701	A1LV4	C21-C20	2.45	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	A1LV4	O2-C25	2.25	1.48	1.43
2	B	701	A1LV4	O2-C25	2.24	1.48	1.43
2	A	701	A1LV4	C6-C5	2.23	1.42	1.37
2	B	701	A1LV4	C6-C5	2.18	1.42	1.37
2	D	701	A1LV4	C6-C5	2.13	1.42	1.37
2	C	701	A1LV4	C6-C5	2.10	1.42	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	A1LV4	N2-C4-N1	-7.26	119.67	126.55
2	C	701	A1LV4	N2-C4-N1	-6.98	119.93	126.55
2	D	701	A1LV4	N2-C4-N1	-6.69	120.21	126.55
2	A	701	A1LV4	N2-C4-N1	-6.64	120.26	126.55
2	C	701	A1LV4	C3-N2-C4	5.98	120.76	115.45
2	D	701	A1LV4	C3-N2-C4	5.84	120.62	115.45
2	A	701	A1LV4	C3-N2-C4	5.65	120.46	115.45
2	B	701	A1LV4	C3-N2-C4	5.50	120.33	115.45
2	B	701	A1LV4	C18-N5-N6	-4.53	108.10	112.72
2	D	701	A1LV4	C18-N5-N6	-4.10	108.54	112.72
2	B	701	A1LV4	C9-C8-N4	3.98	135.55	132.14
2	B	701	A1LV4	C26-C25-C24	-3.88	100.45	104.18
2	D	701	A1LV4	C26-C25-C24	-3.86	100.47	104.18
2	C	701	A1LV4	C18-N5-N6	-3.81	108.84	112.72
2	D	701	A1LV4	C9-C8-N4	3.74	135.35	132.14
2	A	701	A1LV4	C18-N5-N6	-3.74	108.91	112.72
2	A	701	A1LV4	C2-C3-N2	-3.72	119.33	123.96
2	C	701	A1LV4	C26-C25-C24	-3.67	100.65	104.18
2	D	701	A1LV4	C2-C3-N2	-3.65	119.43	123.96
2	C	701	A1LV4	C2-C3-N2	-3.64	119.44	123.96
2	D	701	A1LV4	C13-N4-C11	-3.33	118.64	124.90
2	B	701	A1LV4	C13-N4-C11	-3.30	118.69	124.90
2	C	701	A1LV4	C9-C8-N4	3.26	134.93	132.14
2	A	701	A1LV4	C26-C25-C24	-3.25	101.06	104.18
2	B	701	A1LV4	C2-C3-N2	-3.13	120.07	123.96
2	D	701	A1LV4	C18-C19-C20	2.80	107.82	104.71
2	C	701	A1LV4	C13-N4-C11	-2.63	119.95	124.90
2	C	701	A1LV4	C23-N7-C26	2.62	108.08	104.19
2	D	701	A1LV4	C23-N7-C26	2.57	108.01	104.19
2	C	701	A1LV4	C16-C15-C14	-2.51	114.59	117.43
2	B	701	A1LV4	C18-C19-C20	2.49	107.47	104.71
2	B	701	A1LV4	C16-C15-C14	-2.49	114.61	117.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	A1LV4	C16-C15-C14	-2.45	114.66	117.43
2	A	701	A1LV4	C23-N7-C26	2.33	107.65	104.19
2	A	701	A1LV4	C17-C15-C14	-2.27	114.86	117.43
2	B	701	A1LV4	C21-C20-N6	2.27	124.67	119.78
2	A	701	A1LV4	C9-C8-N4	2.14	133.98	132.14
2	C	701	A1LV4	C18-C19-C20	2.12	107.06	104.71
2	A	701	A1LV4	C18-C19-C20	2.09	107.03	104.71
2	A	701	A1LV4	C13-N4-C11	-2.03	121.08	124.90
2	D	701	A1LV4	C21-C20-N6	2.02	124.14	119.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	A1LV4	C23-C24-O3-C27
2	C	701	A1LV4	C25-C24-O3-C27
2	D	701	A1LV4	C25-C24-O3-C27
2	A	701	A1LV4	C23-C24-O3-C27
2	C	701	A1LV4	C23-C24-O3-C27
2	D	701	A1LV4	C23-C24-O3-C27

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 then 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 A1LV4 D 701

Bond lengths

Bond angles

Torsions

Rings

Ligand A1LV4 B 701

Bond lengths

Bond angles

Torsions

Rings

Ligand A1LV4 C 701	
Bond lengths	Bond angles
Torsions	Rings

Ligand A1LV4 A 701	
Bond lengths	Bond angles
Torsions	Rings
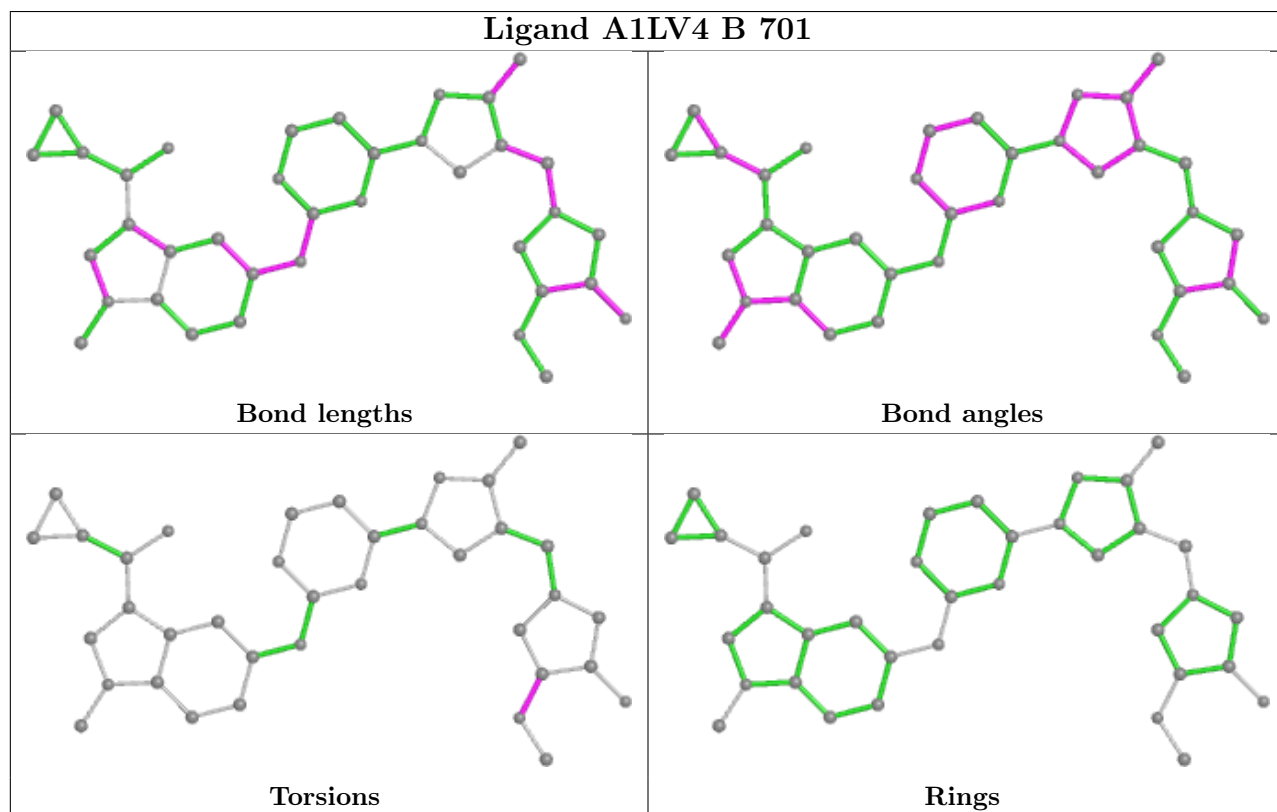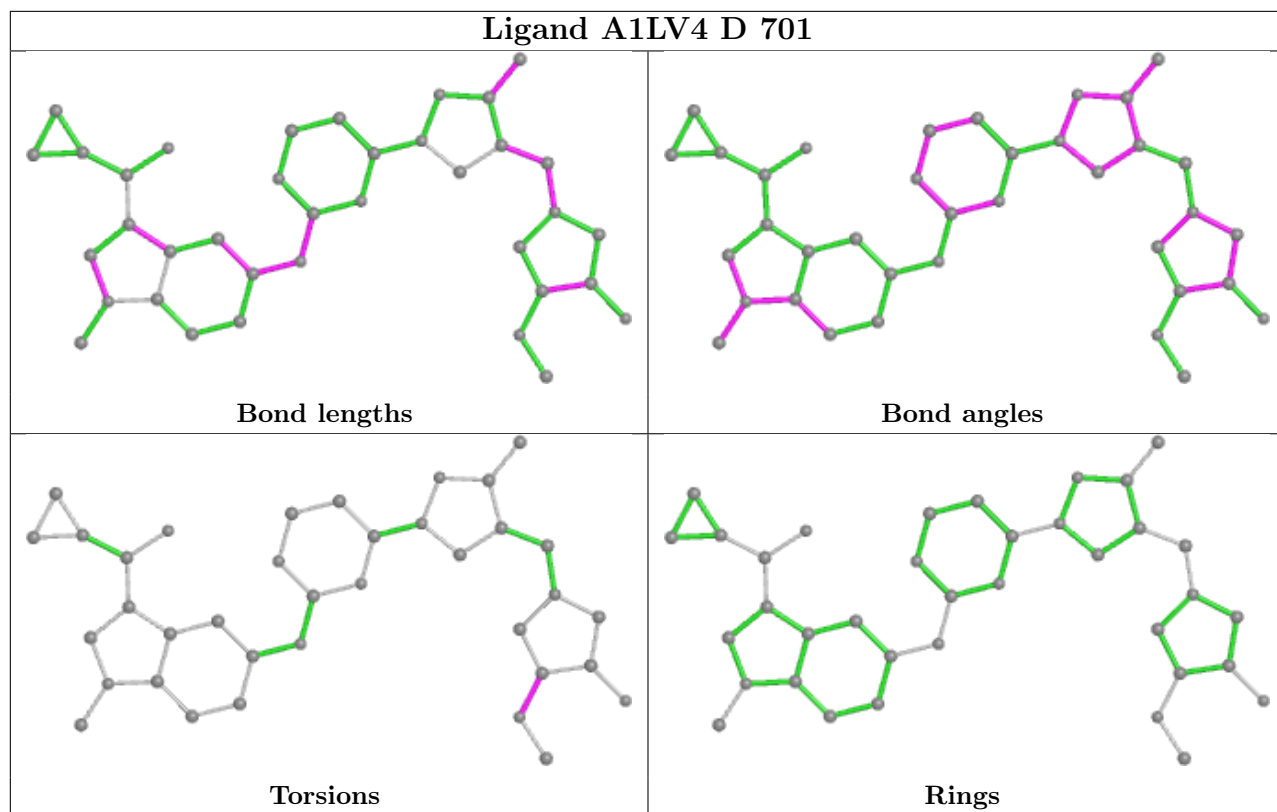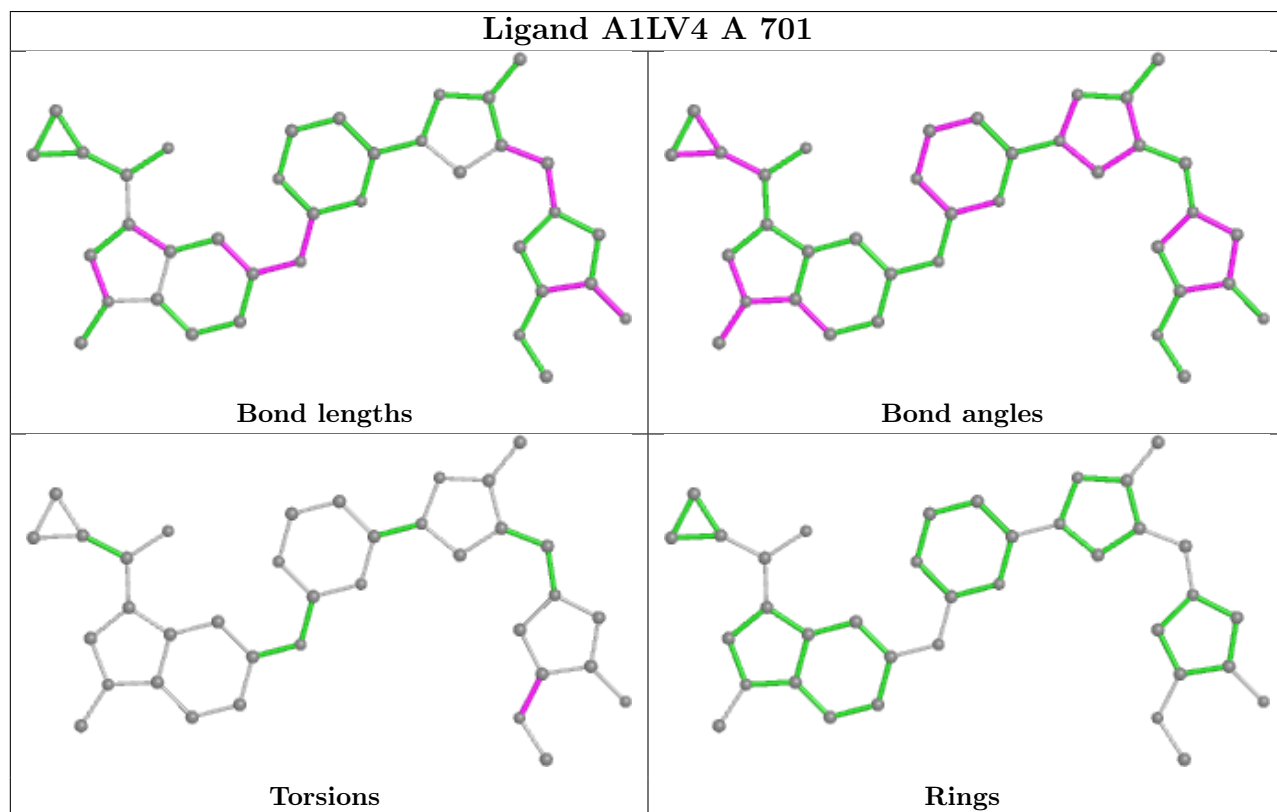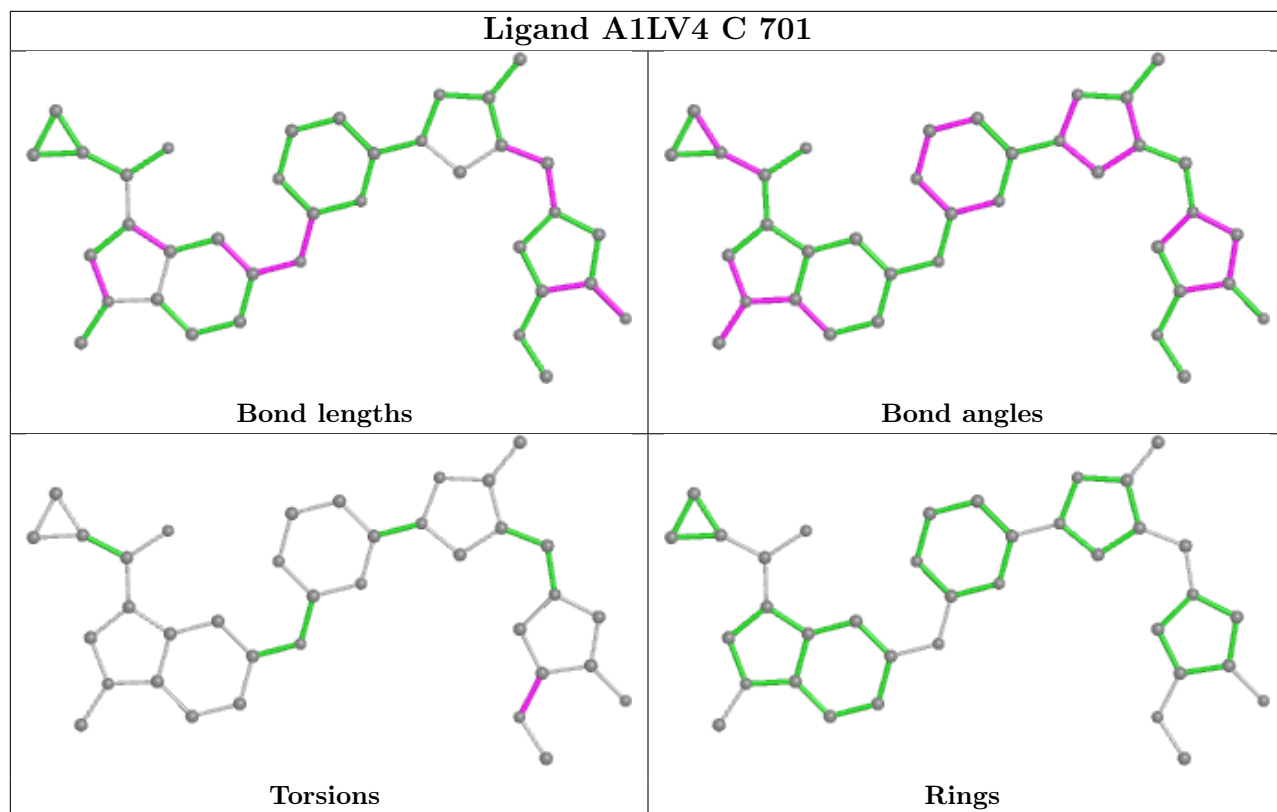
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	264/290 (91%)	-0.65	0	100	100	19, 28, 42, 58	0
1	B	253/290 (87%)	-0.69	0	100	100	18, 27, 44, 52	0
1	C	263/290 (90%)	-0.65	1 (0%)	89	91	20, 28, 42, 56	0
1	D	258/290 (88%)	-0.64	0	100	100	18, 27, 46, 54	0
All	All	1038/1160 (89%)	-0.66	1 (0%)	92	93	18, 28, 44, 58	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	389	TYR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
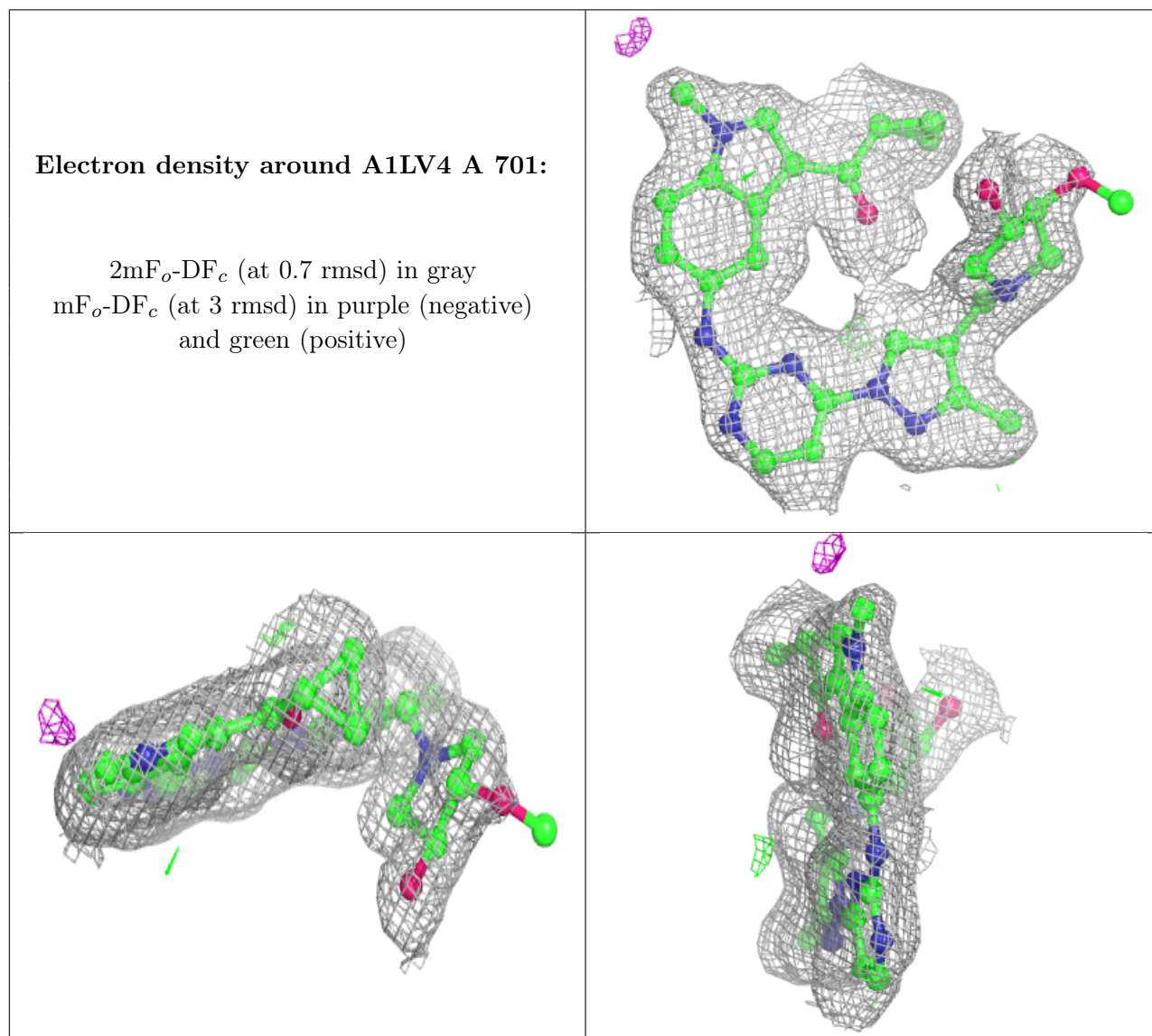
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1LV4	A	701	37/37	0.98	0.05	20,24,31,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	A1LV4	B	701	37/37	0.98	0.05	20,25,33,43	0
2	A1LV4	C	701	37/37	0.98	0.05	19,24,34,44	0
2	A1LV4	D	701	37/37	0.99	0.04	20,24,33,45	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 A1LV4 A 701:

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

Electron density around A1LV4 B 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
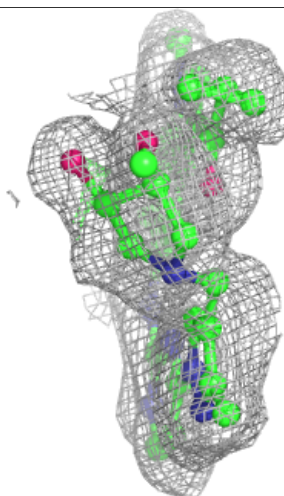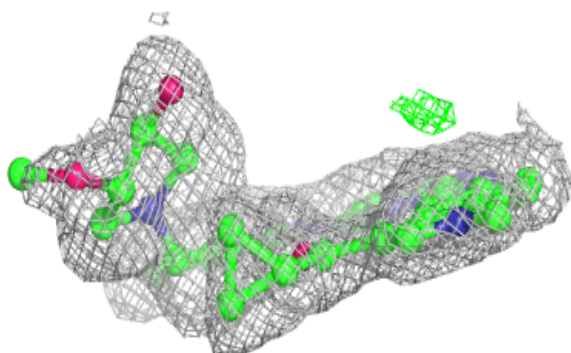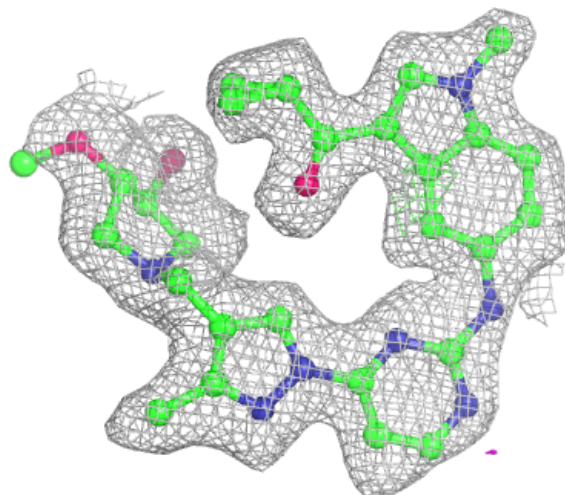
Electron density around A1LV4 C 701:

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

Electron density around A1LV4 D 701:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
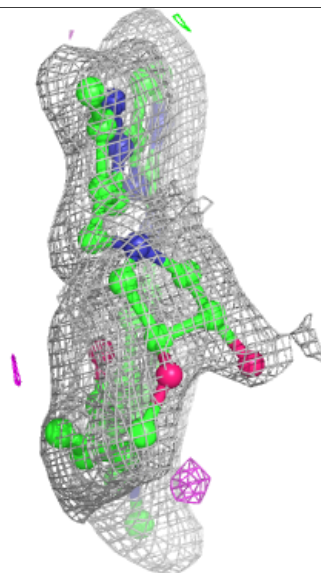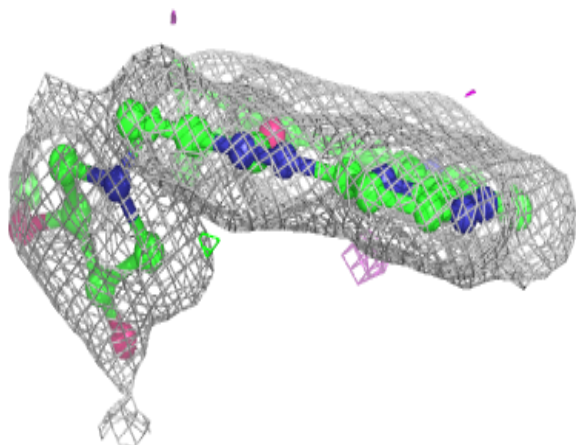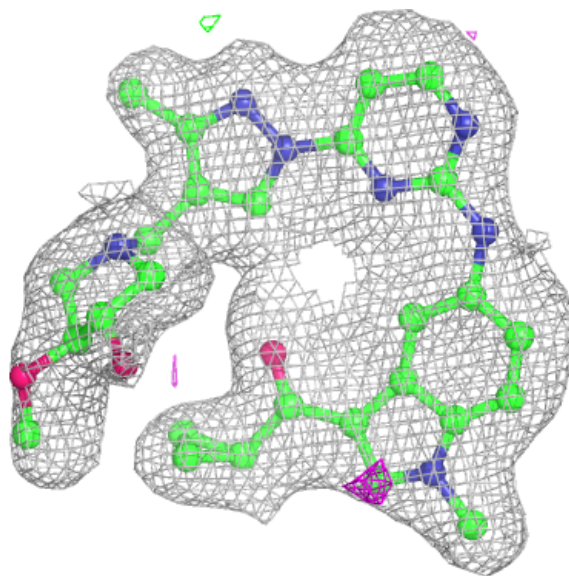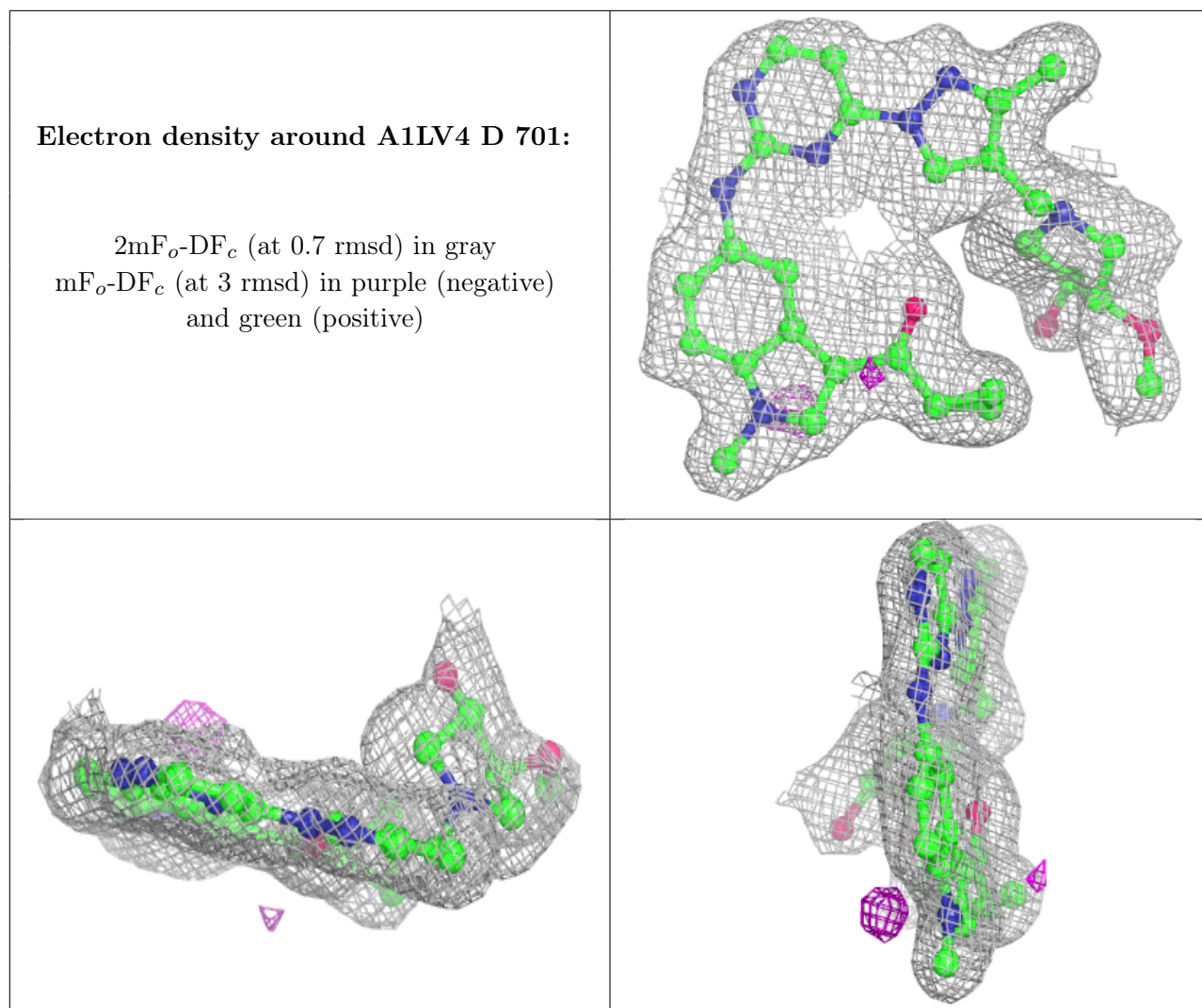
6.5 Other polymers (i)

There are no such residues in this entry.