



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:52 AM UTC

PDB ID : 5HK7 / pdb_00005hk7
Title : Bacterial sodium channel pore, 2.95 Angstrom resolution
Authors : Shaya, D.; Findeisen, F.; Rohaim, A.; Minor, D.L.
Deposited on : 2016-01-14
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

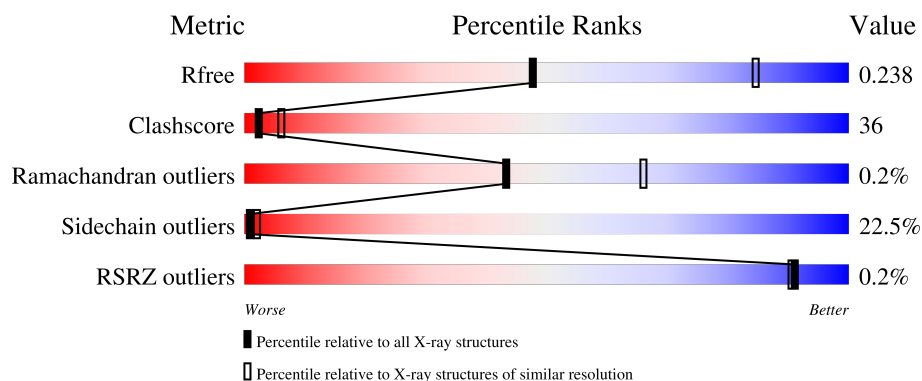
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	152	
1	B	152	
1	C	152	
1	D	152	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4667 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	1	0
			1132	750	181	195	6			
1	B	138	Total	C	N	O	S	0	1	0
			1126	745	180	195	6			
1	C	138	Total	C	N	O	S	0	0	0
			1122	742	178	196	6			
1	D	138	Total	C	N	O	S	0	0	0
			1128	745	181	196	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP Q0ABW0
A	138	PRO	-	expression tag	UNP Q0ABW0
A	139	SER	-	expression tag	UNP Q0ABW0
A	140	SER	-	expression tag	UNP Q0ABW0
A	141	PRO	-	expression tag	UNP Q0ABW0
A	142	SER	-	expression tag	UNP Q0ABW0
B	137	GLY	-	expression tag	UNP Q0ABW0
B	138	PRO	-	expression tag	UNP Q0ABW0
B	139	SER	-	expression tag	UNP Q0ABW0
B	140	SER	-	expression tag	UNP Q0ABW0
B	141	PRO	-	expression tag	UNP Q0ABW0
B	142	SER	-	expression tag	UNP Q0ABW0
C	137	GLY	-	expression tag	UNP Q0ABW0
C	138	PRO	-	expression tag	UNP Q0ABW0
C	139	SER	-	expression tag	UNP Q0ABW0
C	140	SER	-	expression tag	UNP Q0ABW0
C	141	PRO	-	expression tag	UNP Q0ABW0
C	142	SER	-	expression tag	UNP Q0ABW0
D	137	GLY	-	expression tag	UNP Q0ABW0
D	138	PRO	-	expression tag	UNP Q0ABW0
D	139	SER	-	expression tag	UNP Q0ABW0

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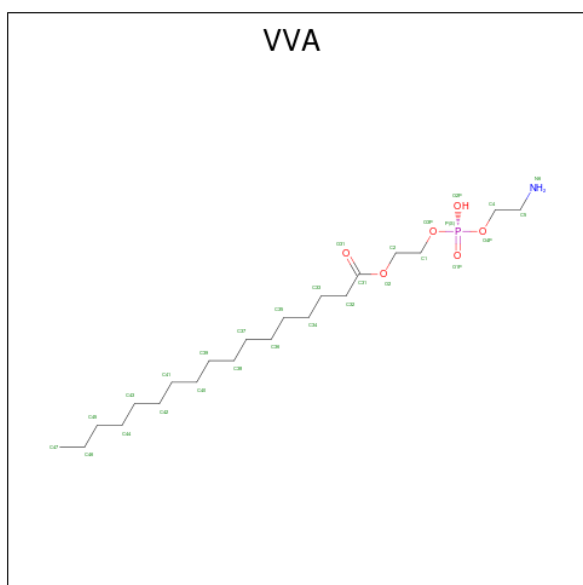
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Chain	Residue	Modelled	Actual	Comment	Reference
D	140	SER	-	expression tag	UNP Q0ABW0
D	141	PRO	-	expression tag	UNP Q0ABW0
D	142	SER	-	expression tag	UNP Q0ABW0

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0

- Molecule 3 is 2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}ethyl heptadecanoate (CCD ID: VVA) (formula: C₂₁H₄₄NO₆P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 21 13 1 6 1	0	0
3	A	1	Total C 13 13	0	0
3	B	1	Total C N O P 21 13 1 6 1	0	0
3	B	1	Total C N O P 21 13 1 6 1	0	0
3	B	1	Total C 17 17	0	0
3	C	1	Total C N O P 21 13 1 6 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C 10 10	0	0
3	C	1	Total C 6 6	0	0
3	C	1	Total C 11 11	0	0
3	D	1	Total C 10 10	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	C	1	Total Na 1 1	0	0

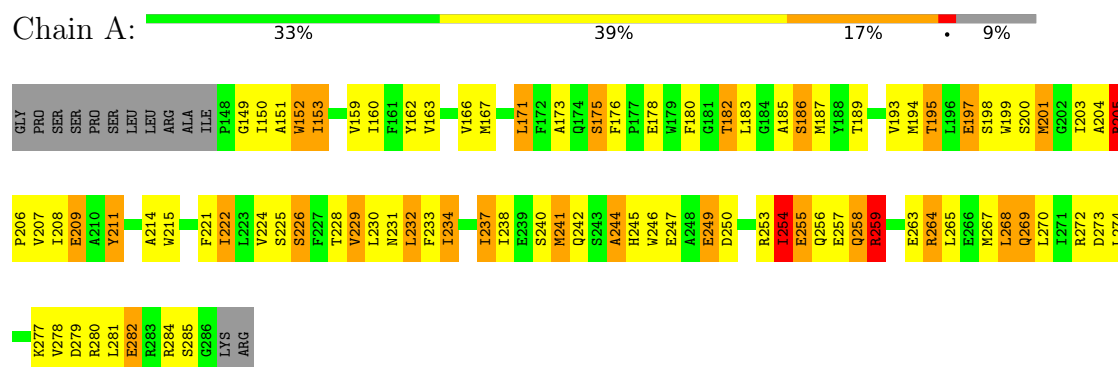
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 1 1	0	0
5	B	1	Total O 1 1	0	0
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0

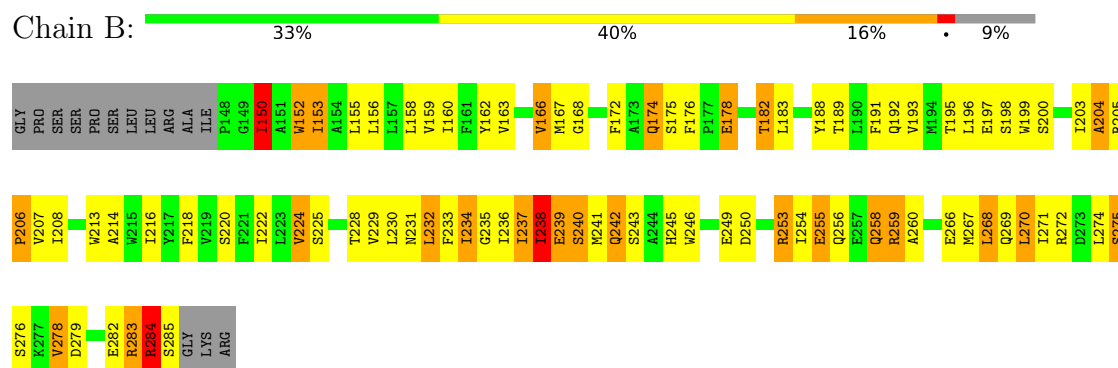
3 Residue-property plots

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.

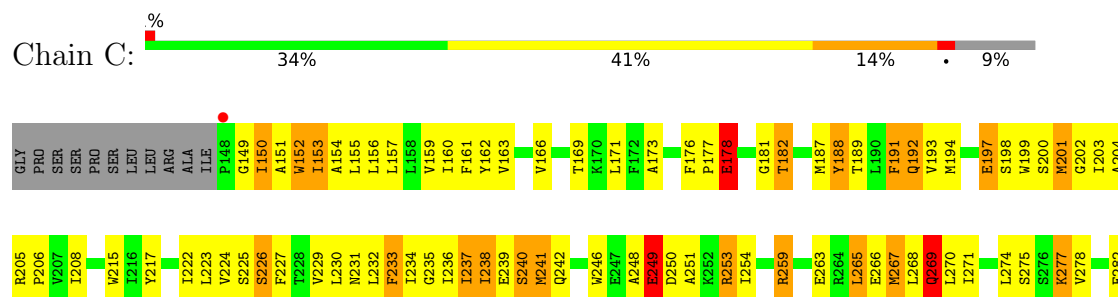
• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



• Molecule 1: Ion transport protein



R283
R284
S285
GLY
LYS
ARG

● Molecule 1: Ion transport protein



GLY	PRO	SER	SER	PRO	SER	LEU	LEU	ARG	ALA	ILE	P148	G149	I150	W152	I153	A154	L155	L156	L157	L158	V159	Y162	V163	L171	F172	A173	Q174	S175	F176	G181	T182	L183	S186	M187	Y188	Q192	V193	M194	T195	L196	E197	S198	W199	S200	M201	Q202	I203	A204	R205	P206	V207	I208	E209
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A210	T211	F212	W213	A214	W215	T216	T217	F218	V219	I222	L223	V224	S225	S226	F227	T228	V229	L230	I231	L232	F233	I234	G235	I236	I237	S240	N241	Q242	D250	A251	K252	R253	I254	E255	Q256	E257	Q258	H261	Q262	E263	R264	L265	E266	N267	L268	Q269	L270	I271	L274	S275	S276	K277	V278	D279
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R280
L281
E282
R283
R284
S285
GLY
LYS
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.51Å 160.52Å 166.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.95 15.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (15.00-2.95) 97.9 (15.00-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.205 , 0.236 0.205 , 0.238	Depositor DCC
R_{free} test set	2185 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4667	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: CL, VVA, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	0/1167	1.45	17/1585 (1.1%)
1	B	1.09	1/1160 (0.1%)	1.34	10/1575 (0.6%)
1	C	1.14	0/1153	1.44	15/1566 (1.0%)
1	D	1.22	1/1159 (0.1%)	1.38	7/1573 (0.4%)
All	All	1.14	2/4639 (0.0%)	1.40	49/6299 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	204	ALA	C-O	-6.13	1.17	1.24
1	B	204	ALA	CA-C	-5.20	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	150	ILE	N-CA-C	9.35	120.16	110.62
1	A	285	SER	N-CA-C	9.32	124.20	113.02
1	B	284	ARG	N-CA-C	9.14	122.17	111.02
1	C	201	MET	N-CA-C	-9.03	101.52	111.36
1	C	188	TYR	N-CA-C	-8.67	101.91	111.36
1	A	203	ILE	CB-CA-C	-8.30	103.56	111.44
1	C	249	GLU	N-CA-C	-8.24	102.30	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ALA	N-CA-C	-7.82	102.72	111.71
1	C	182	THR	N-CA-C	-7.61	97.14	108.79
1	D	284	ARG	N-CA-C	-7.49	104.55	112.93
1	D	216	ILE	CB-CA-C	-7.26	102.33	112.14
1	D	210	ALA	N-CA-C	-7.18	104.14	113.12
1	D	203	ILE	CB-CA-C	-7.14	104.66	111.44
1	A	229	VAL	N-CA-C	-7.08	104.51	113.22
1	A	264	ARG	N-CA-C	-6.53	104.16	111.28
1	A	211	TYR	CA-C-N	6.44	126.13	119.82
1	A	211	TYR	C-N-CA	6.44	126.13	119.82
1	C	191	PHE	N-CA-C	-6.39	104.40	111.36
1	B	278	VAL	N-CA-C	-6.17	104.49	110.72
1	C	176	PHE	CA-C-N	6.00	125.55	119.19
1	C	176	PHE	C-N-CA	6.00	125.55	119.19
1	D	201	MET	N-CA-C	-5.99	104.87	111.82
1	C	284	ARG	N-CA-C	-5.99	105.08	112.38
1	C	251	ALA	N-CA-C	5.85	117.65	111.28
1	A	209	GLU	N-CA-C	-5.83	105.01	111.36
1	B	237	ILE	CB-CA-C	-5.82	104.53	111.81
1	A	205	ARG	CA-C-N	5.81	125.94	119.32
1	A	205	ARG	C-N-CA	5.81	125.94	119.32
1	A	171	LEU	N-CA-C	5.80	117.68	111.36
1	A	214	ALA	N-CA-C	-5.78	105.81	112.92
1	B	150	ILE	CB-CA-C	-5.73	104.63	111.97
1	A	254	ILE	N-CA-C	-5.66	104.41	110.36
1	C	269	GLN	N-CA-C	5.52	117.75	111.02
1	B	166	VAL	CB-CA-C	-5.45	104.71	112.22
1	B	283	ARG	N-CA-C	5.44	116.89	111.07
1	C	171	LEU	N-CA-C	5.35	116.80	111.07
1	B	174	GLN	N-CA-C	-5.35	104.87	111.40
1	B	188	TYR	N-CA-C	5.34	117.52	111.11
1	B	237	ILE	N-CA-C	-5.33	105.13	110.30
1	A	195	THR	N-CA-C	-5.27	106.82	113.20
1	A	259	ARG	CA-C-O	-5.25	115.28	120.90
1	D	252	LYS	N-CA-C	-5.24	106.58	113.12
1	C	278	VAL	N-CA-C	-5.19	104.49	111.44
1	D	277	LYS	N-CA-C	-5.18	105.32	111.69
1	B	182	THR	N-CA-C	-5.15	101.47	109.14
1	C	178	GLU	N-CA-C	-5.08	105.82	111.36
1	A	259	ARG	N-CA-CB	5.08	117.51	109.94
1	C	259	ARG	N-CA-C	-5.07	105.44	110.97
1	A	201	MET	N-CA-C	-5.06	105.76	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ALA	Peptide

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	1132	0	1120	121	0
1	B	1126	0	1119	103	0
1	C	1122	0	1112	93	0
1	D	1128	0	1123	87	0
2	A	2	0	0	0	0
3	A	34	0	0	3	0
3	B	59	0	0	0	0
3	C	48	0	0	0	0
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	4667	0	4474	325	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 36.

All (325) 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:229:VAL:HG12	1:A:233[A]:PHE:CE2	1.62	1.35
1:B:241:MET:SD	1:C:241:MET:HE1	1.73	1.26
1:A:221:PHE:O	1:A:225:SER:HB3	1.50	1.12
1:A:229:VAL:CG1	1:A:233[A]:PHE:HE2	1.68	1.06
1:A:153:ILE:CG2	1:A:232:LEU:HD12	1.87	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PHE:HE1	1:C:194:MET:CE	1.71	1.04
1:A:267:MET:HG2	1:B:268:LEU:HD23	1.41	1.01
1:C:241:MET:SD	1:D:241:MET:HE1	2.00	1.01
1:A:229:VAL:CG1	1:A:233[A]:PHE:CE2	2.42	1.00
1:A:229:VAL:O	1:A:233[A]:PHE:CD2	2.14	1.00
1:A:229:VAL:HG12	1:A:233[A]:PHE:HE2	0.90	1.00
1:C:222:ILE:O	1:C:226:SER:OG	1.79	0.97
1:A:268:LEU:HD23	1:D:267:MET:HG2	1.47	0.97
1:B:200:SER:O	1:B:205:ARG:HB2	1.67	0.93
1:A:233[B]:PHE:CE1	1:B:230:LEU:HD11	2.04	0.93
1:C:156:LEU:HD11	1:C:160:ILE:HD11	1.53	0.90
1:C:161:PHE:CE1	1:C:194:MET:CE	2.56	0.88
1:D:150:ILE:HD12	1:D:151:ALA:H	1.39	0.87
1:A:233[B]:PHE:CE2	1:D:233:PHE:HZ	1.92	0.87
1:C:177:PRO:HD2	1:C:178:GLU:OE1	1.74	0.86
1:B:178[A]:GLU:H	1:B:178[A]:GLU:CD	1.84	0.86
1:A:180:PHE:HD1	1:A:186:SER:HG	1.23	0.86
1:C:150:ILE:HD12	1:C:151:ALA:N	1.92	0.85
1:C:161:PHE:HE1	1:C:194:MET:HE3	1.41	0.83
1:A:267:MET:HG2	1:B:268:LEU:CD2	2.08	0.82
1:A:229:VAL:O	1:A:233[A]:PHE:HD2	1.63	0.82
1:B:162:TYR:O	1:B:166:VAL:HG23	1.79	0.82
1:A:241:MET:SD	1:B:241:MET:HE1	2.20	0.82
1:B:233:PHE:O	1:B:237:ILE:HG12	1.81	0.81
1:A:153:ILE:HG23	1:A:232:LEU:HD12	1.61	0.81
1:B:225:SER:O	1:B:229:VAL:HG23	1.82	0.79
1:B:249:GLU:O	1:B:253:ARG:HG3	1.83	0.79
1:A:233[B]:PHE:CD1	1:B:230:LEU:HD11	2.19	0.78
1:A:222:ILE:O	1:A:226:SER:HB2	1.83	0.77
1:B:272:ARG:HG2	1:B:272:ARG:HH21	1.50	0.75
1:A:233[B]:PHE:HZ	1:B:233:PHE:HE2	1.33	0.75
1:A:233[B]:PHE:HE2	1:D:233:PHE:HZ	1.35	0.75
1:C:208:ILE:HD12	1:C:215:TRP:HB3	1.69	0.74
1:A:241:MET:HE1	1:D:241:MET:SD	2.27	0.74
1:A:268:LEU:HD23	1:D:267:MET:CG	2.19	0.73
1:A:167:MET:O	1:A:171:LEU:HD12	1.88	0.73
1:A:204:ALA:O	1:A:208:ILE:HG13	1.89	0.73
1:A:268:LEU:HD11	1:A:272:ARG:NH2	2.04	0.73
1:C:156:LEU:CD1	1:C:160:ILE:HD11	2.18	0.73
1:A:233[B]:PHE:HE1	1:B:230:LEU:HD11	1.54	0.73
1:A:153:ILE:HG23	1:A:232:LEU:CD1	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:HG3	1:A:250:ASP:N	2.04	0.73
1:A:233[B]:PHE:HE1	1:B:230:LEU:CD1	2.02	0.72
1:A:233[B]:PHE:CE1	1:B:230:LEU:CD1	2.73	0.72
1:D:218:PHE:O	1:D:222:ILE:HG13	1.89	0.72
1:A:153:ILE:CG2	1:A:232:LEU:CD1	2.66	0.72
1:C:267:MET:HB3	1:D:268:LEU:HD21	1.70	0.72
1:B:284:ARG:O	1:B:285:SER:O	2.08	0.72
1:C:204:ALA:O	1:C:208:ILE:HG12	1.89	0.72
1:D:159:VAL:O	1:D:163:VAL:HG23	1.91	0.71
1:B:191:PHE:O	1:B:195:THR:HG23	1.90	0.70
1:B:218:PHE:O	1:B:222:ILE:HG12	1.91	0.70
1:B:241:MET:SD	1:C:241:MET:CE	2.67	0.70
1:C:161:PHE:HE1	1:C:194:MET:HE2	1.56	0.70
1:A:149:GLY:O	1:A:152:TRP:HB2	1.91	0.70
1:A:244:ALA:HB2	1:B:238:ILE:HD13	1.74	0.69
1:D:171:LEU:HD13	1:D:213:TRP:HH2	1.57	0.69
1:D:250:ASP:HA	1:D:253:ARG:HD3	1.75	0.69
1:C:161:PHE:CE1	1:C:194:MET:HE3	2.25	0.69
1:A:233[B]:PHE:HZ	1:B:233:PHE:CE2	2.10	0.68
1:C:241:MET:SD	1:D:241:MET:CE	2.80	0.68
1:C:197:GLU:HG3	1:D:199:TRP:CD1	2.28	0.68
1:D:171:LEU:HD13	1:D:213:TRP:CH2	2.29	0.68
1:A:189:THR:O	1:A:193:VAL:HG23	1.93	0.68
1:A:241:MET:O	1:A:242:GLN:C	2.37	0.67
1:C:151:ALA:HA	1:C:154:ALA:HB3	1.76	0.66
1:B:258:GLN:OE1	1:B:258:GLN:HA	1.95	0.66
1:A:180:PHE:HD1	1:A:186:SER:OG	1.78	0.66
1:B:231:ASN:O	1:B:235:GLY:N	2.24	0.66
1:A:233[B]:PHE:CE2	1:D:233:PHE:CZ	2.82	0.65
1:B:271:ILE:O	1:B:275:SER:HB2	1.97	0.65
1:C:274:LEU:HD21	1:D:274:LEU:HD23	1.79	0.64
1:D:150:ILE:CD1	1:D:151:ALA:H	2.09	0.64
1:A:150:ILE:O	1:A:153:ILE:HG22	1.98	0.64
1:A:153:ILE:HG21	1:A:232:LEU:HD12	1.79	0.64
1:B:239:GLU:HG3	1:B:239:GLU:O	1.96	0.64
1:B:152:TRP:HA	1:B:152:TRP:CE3	2.32	0.64
1:C:162:TYR:O	1:C:166:VAL:HG23	1.98	0.63
1:A:221:PHE:O	1:A:225:SER:CB	2.39	0.63
1:D:153:ILE:O	1:D:156:LEU:N	2.32	0.63
1:B:276:SER:HA	1:B:279:ASP:HB2	1.81	0.63
1:D:252:LYS:O	1:D:256:GLN:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ILE:HG13	1:C:201:MET:CE	2.30	0.62
1:C:160:ILE:HG21	1:C:224:VAL:HG12	1.81	0.62
1:D:152:TRP:HA	1:D:152:TRP:CE3	2.34	0.62
1:A:159:VAL:O	1:A:163:VAL:HG23	2.00	0.61
1:D:253:ARG:HH11	1:D:253:ARG:HG3	1.64	0.61
1:B:241:MET:CG	1:C:241:MET:HE1	2.30	0.61
1:C:267:MET:HE1	1:D:267:MET:HE3	1.82	0.61
1:D:253:ARG:HH11	1:D:253:ARG:CG	2.14	0.61
1:A:264:ARG:NH2	1:D:263:GLU:OE1	2.32	0.60
1:B:152:TRP:HA	1:B:152:TRP:HE3	1.66	0.59
1:C:225:SER:O	1:C:229:VAL:HG23	2.02	0.59
1:C:237:ILE:HD12	1:D:234:ILE:HG12	1.84	0.59
1:A:149:GLY:O	1:A:152:TRP:CB	2.50	0.59
1:A:250:ASP:O	1:A:253:ARG:HG3	2.02	0.59
1:B:189:THR:O	1:B:193:VAL:HG23	2.02	0.59
1:C:233:PHE:CD2	1:D:230:LEU:HD11	2.38	0.59
1:A:234:ILE:CD1	1:D:236:ILE:HG22	2.33	0.58
1:A:200:SER:O	1:A:205:ARG:HB2	2.03	0.58
1:C:236:ILE:O	1:C:240:SER:HB2	2.04	0.58
1:A:176:PHE:CZ	1:A:207:VAL:HA	2.38	0.57
1:A:193:VAL:HG13	1:A:199:TRP:HB2	1.86	0.57
1:C:169:THR:O	1:C:173:ALA:HB2	2.04	0.57
1:C:156:LEU:CD1	1:C:160:ILE:CD1	2.83	0.57
1:A:233[B]:PHE:HE2	1:D:233:PHE:CZ	2.18	0.57
1:C:156:LEU:HD11	1:C:160:ILE:CD1	2.32	0.57
1:B:270:LEU:N	1:B:270:LEU:HD23	2.20	0.57
1:B:197:GLU:OE1	1:B:198:SER:HB2	2.05	0.57
1:C:267:MET:HB3	1:D:268:LEU:CD2	2.35	0.57
1:C:208:ILE:CD1	1:C:215:TRP:HB3	2.35	0.56
1:A:195:THR:HB	1:B:196:LEU:HD13	1.87	0.56
1:C:263:GLU:OE2	1:D:261:HIS:ND1	2.39	0.56
1:B:238:ILE:HG22	1:B:239:GLU:N	2.21	0.56
1:B:241:MET:HE3	1:B:246:TRP:CH2	2.41	0.56
1:D:205:ARG:HB2	1:D:206:PRO:HD2	1.88	0.56
1:A:194:MET:HG3	1:A:225:SER:OG	2.06	0.55
1:D:176:PHE:CZ	1:D:207:VAL:HA	2.41	0.55
1:A:256:GLN:CD	1:B:253:ARG:NH2	2.63	0.55
1:C:248:ALA:O	1:C:249:GLU:C	2.49	0.55
1:A:280:ARG:O	1:A:281:LEU:C	2.47	0.55
1:C:200:SER:O	1:C:205:ARG:HG3	2.06	0.55
1:D:162:TYR:CD1	1:D:162:TYR:C	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:PHE:CE1	1:C:194:MET:HE2	2.35	0.55
1:C:233:PHE:CD1	1:C:233:PHE:C	2.85	0.55
1:B:160:ILE:HD13	1:B:224:VAL:HG13	1.89	0.55
1:A:268:LEU:CD1	1:A:272:ARG:NH2	2.70	0.55
1:A:284:ARG:HH21	1:A:284:ARG:HB3	1.73	0.54
1:C:237:ILE:HD11	1:D:237:ILE:HD12	1.88	0.54
1:A:167:MET:O	1:A:171:LEU:CD1	2.53	0.54
1:A:269:GLN:OE1	1:A:269:GLN:HA	2.07	0.54
1:C:189:THR:O	1:C:193:VAL:HG23	2.06	0.54
1:A:233[B]:PHE:CZ	1:B:233:PHE:HE2	2.21	0.54
1:B:204:ALA:O	1:B:208:ILE:HG13	2.08	0.54
1:A:152:TRP:HA	1:A:152:TRP:CE3	2.43	0.54
1:A:205:ARG:NH1	1:D:192:GLN:OE1	2.41	0.54
1:A:267:MET:HE1	1:B:267:MET:HE3	1.90	0.54
1:C:270:LEU:HB2	1:D:271:ILE:HG21	1.91	0.53
1:C:274:LEU:HD13	1:D:275:SER:HA	1.91	0.53
1:A:197:GLU:HG3	1:B:199:TRP:CD1	2.43	0.53
1:A:162:TYR:O	1:A:166:VAL:HG23	2.08	0.53
1:C:227:PHE:O	1:C:230:LEU:HB3	2.09	0.53
1:D:200:SER:HA	1:D:204:ALA:HB3	1.91	0.53
1:D:154:ALA:O	1:D:158:LEU:HD12	2.08	0.52
1:D:283:ARG:C	1:D:285:SER:H	2.16	0.52
1:A:182:THR:HG23	1:A:185:ALA:HB2	1.90	0.52
1:B:192:GLN:NE2	1:B:197:GLU:O	2.41	0.52
1:B:155:LEU:O	1:B:159:VAL:HG23	2.10	0.52
1:C:249:GLU:HG3	1:C:250:ASP:N	2.24	0.52
1:A:256:GLN:NE2	1:B:253:ARG:NH2	2.57	0.52
1:A:256:GLN:OE1	1:B:253:ARG:NH2	2.41	0.52
1:B:250:ASP:O	1:B:253:ARG:HD3	2.09	0.52
1:D:242:GLN:O	1:D:242:GLN:HG3	2.09	0.52
1:A:246:TRP:O	1:A:250:ASP:HB2	2.10	0.52
1:C:197:GLU:OE2	1:C:198:SER:CB	2.57	0.52
1:C:271:ILE:HG13	1:D:271:ILE:HD13	1.91	0.52
1:A:183:LEU:O	1:A:187:MET:HG3	2.10	0.51
1:B:241:MET:HG2	1:C:241:MET:CE	2.40	0.51
1:D:195:THR:O	1:D:196:LEU:HB2	2.10	0.51
1:C:149:GLY:O	1:C:152:TRP:HB2	2.11	0.51
1:B:234:ILE:O	1:B:237:ILE:N	2.42	0.51
1:C:191:PHE:CD2	1:D:219:VAL:HG22	2.45	0.51
1:D:278:VAL:HG12	1:D:278:VAL:O	2.10	0.51
1:D:253:ARG:CG	1:D:253:ARG:NH1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:O	1:D:233:PHE:HB3	2.11	0.51
1:A:279:ASP:O	1:A:282:GLU:HB3	2.11	0.50
1:B:197:GLU:HG3	1:C:199:TRP:CD1	2.46	0.50
1:B:272:ARG:HG2	1:B:272:ARG:NH2	2.22	0.50
1:D:205:ARG:HB2	1:D:206:PRO:CD	2.40	0.50
1:B:189:THR:HG23	1:B:203:ILE:HD13	1.92	0.50
1:A:194:MET:HE1	3:A:303:VVA:C36	2.42	0.50
1:A:233[B]:PHE:CZ	1:A:237:ILE:HD11	2.46	0.50
1:A:167:MET:O	1:A:171:LEU:CG	2.60	0.49
1:A:160:ILE:HD13	1:A:224:VAL:HG12	1.93	0.49
1:A:268:LEU:HD13	1:A:272:ARG:NH1	2.27	0.49
1:D:152:TRP:HA	1:D:152:TRP:HE3	1.75	0.49
1:C:239:GLU:O	1:C:239:GLU:HG3	2.12	0.49
1:B:205:ARG:N	1:B:206:PRO:HD2	2.27	0.49
1:A:198:SER:HA	1:D:197:GLU:OE2	2.11	0.49
1:A:233[B]:PHE:CE2	1:A:237:ILE:CD1	2.96	0.49
1:A:228:THR:O	1:A:228:THR:HG22	2.12	0.49
1:A:258:GLN:O	1:A:259:ARG:C	2.54	0.49
1:C:223:LEU:HD23	1:C:223:LEU:HA	1.64	0.49
1:C:157:LEU:C	1:C:157:LEU:HD13	2.37	0.48
1:C:197:GLU:OE2	1:C:198:SER:HB2	2.12	0.48
1:C:230:LEU:O	1:C:233:PHE:HB3	2.12	0.48
1:D:150:ILE:HD12	1:D:151:ALA:N	2.20	0.48
1:A:175:SER:OG	1:A:211:TYR:OH	2.20	0.48
1:C:159:VAL:O	1:C:163:VAL:HG23	2.13	0.48
1:C:253:ARG:O	1:C:254:ILE:C	2.57	0.48
1:A:200:SER:HA	1:A:204:ALA:HB3	1.96	0.48
1:B:245:HIS:CE1	1:C:246:TRP:HB3	2.49	0.48
1:A:256:GLN:CD	1:B:253:ARG:HH21	2.21	0.47
1:D:213:TRP:CE3	1:D:214:ALA:HA	2.50	0.47
1:A:199:TRP:CD1	1:D:197:GLU:HG3	2.48	0.47
1:B:213:TRP:CE3	1:B:214:ALA:HA	2.49	0.47
1:A:208:ILE:HG22	1:A:208:ILE:O	2.14	0.47
1:A:194:MET:CE	3:A:303:VVA:C36	2.93	0.47
1:A:274:LEU:HD11	1:B:278:VAL:HG21	1.96	0.47
1:D:151:ALA:HA	1:D:154:ALA:HB3	1.97	0.47
1:A:167:MET:HG3	1:A:171:LEU:HD11	1.96	0.47
1:B:236:ILE:HG22	1:C:234:ILE:CD1	2.45	0.47
1:C:160:ILE:HG21	1:C:224:VAL:CG1	2.45	0.47
1:A:258:GLN:OE1	1:A:258:GLN:HA	2.13	0.47
1:B:259:ARG:O	1:B:260:ALA:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD23	1:B:270:LEU:H	1.79	0.47
1:C:188:TYR:HH	1:D:200:SER:HG	1.63	0.46
1:B:240:SER:HB3	1:C:238:ILE:HD11	1.97	0.46
1:C:153:ILE:HD13	1:C:231:ASN:CB	2.45	0.46
1:C:178:GLU:CD	1:C:178:GLU:H	2.24	0.46
1:D:153:ILE:O	1:D:154:ALA:C	2.57	0.46
1:D:278:VAL:O	1:D:278:VAL:CG1	2.63	0.46
1:A:206:PRO:O	1:A:209:GLU:HB2	2.16	0.46
1:A:245:HIS:CE1	1:B:246:TRP:HB3	2.51	0.46
1:D:155:LEU:O	1:D:155:LEU:HG	2.14	0.46
1:A:284:ARG:HH11	1:B:282:GLU:CG	2.28	0.46
1:D:150:ILE:CD1	1:D:151:ALA:N	2.77	0.46
1:D:208:ILE:O	1:D:212:PRO:HA	2.16	0.46
1:D:150:ILE:C	1:D:152:TRP:N	2.74	0.45
1:A:270:LEU:O	1:A:273:ASP:HB2	2.16	0.45
1:A:274:LEU:HD13	1:B:275:SER:HA	1.97	0.45
1:C:177:PRO:O	1:C:181:GLY:HA3	2.15	0.45
1:B:242:GLN:HA	1:B:246:TRP:HB2	1.98	0.45
1:B:272:ARG:HH21	1:B:272:ARG:CG	2.24	0.45
1:A:259:ARG:O	1:A:263:GLU:HG3	2.17	0.45
1:B:205:ARG:H	1:B:206:PRO:HD2	1.80	0.45
1:D:236:ILE:O	1:D:240:SER:HB2	2.17	0.45
1:A:234:ILE:HD11	1:D:236:ILE:HG22	1.99	0.45
1:C:192:GLN:HG3	1:D:200:SER:CB	2.47	0.45
1:A:230:LEU:HD11	1:D:233:PHE:CE1	2.52	0.45
1:B:203:ILE:O	1:B:207:VAL:HG23	2.16	0.45
1:D:188:TYR:CD1	1:D:188:TYR:C	2.95	0.45
1:B:241:MET:CG	1:C:241:MET:CE	2.95	0.45
1:C:153:ILE:HD13	1:C:231:ASN:HB2	1.99	0.45
1:A:233[B]:PHE:CE2	1:A:237:ILE:HD12	2.52	0.44
1:A:268:LEU:CD1	1:A:272:ARG:CZ	2.94	0.44
1:B:272:ARG:NH2	1:B:272:ARG:CG	2.79	0.44
1:C:205:ARG:HB2	1:C:206:PRO:CD	2.47	0.44
1:C:277:LYS:HD3	1:D:279:ASP:HB3	1.98	0.44
1:B:153:ILE:HG22	1:B:228:THR:HG23	2.00	0.44
1:B:159:VAL:O	1:B:163:VAL:HG23	2.17	0.44
1:A:173:ALA:HB2	1:A:180:PHE:O	2.17	0.44
1:A:257:GLU:O	1:A:257:GLU:HG3	2.16	0.44
1:C:274:LEU:HD21	1:D:274:LEU:CD2	2.47	0.44
1:C:152:TRP:HA	1:C:152:TRP:CE3	2.52	0.44
1:A:265:LEU:HD12	1:A:265:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PHE:HD2	1:D:230:LEU:HD11	1.82	0.44
1:C:217:TYR:CD1	1:C:217:TYR:C	2.96	0.44
1:C:269:GLN:O	1:C:270:LEU:C	2.61	0.44
1:A:284:ARG:NH1	1:B:282:GLU:CG	2.82	0.43
1:B:203:ILE:HG13	1:C:201:MET:HE3	2.00	0.43
1:D:155:LEU:O	1:D:159:VAL:HG23	2.17	0.43
1:A:253:ARG:O	1:A:254:ILE:C	2.61	0.43
1:A:246:TRP:O	1:A:250:ASP:CB	2.66	0.43
1:B:153:ILE:O	1:B:156:LEU:HB3	2.18	0.43
1:C:270:LEU:N	1:C:270:LEU:HD23	2.33	0.43
1:D:153:ILE:HD11	1:D:232:LEU:HA	2.00	0.43
1:B:176:PHE:CZ	1:B:207:VAL:HA	2.54	0.43
1:B:205:ARG:N	1:B:206:PRO:CD	2.80	0.43
1:D:197:GLU:O	1:D:198:SER:HB2	2.17	0.43
1:B:150:ILE:O	1:B:153:ILE:N	2.46	0.43
1:B:231:ASN:O	1:B:232:LEU:C	2.62	0.43
1:B:233:PHE:HD1	1:C:230:LEU:CD1	2.32	0.43
1:B:253:ARG:HE	1:B:253:ARG:HB2	1.63	0.43
1:C:156:LEU:HD12	1:C:160:ILE:HG13	2.01	0.43
1:A:274:LEU:O	1:A:278:VAL:HG23	2.19	0.43
1:A:233[B]:PHE:CE2	1:A:237:ILE:HD11	2.53	0.43
1:A:284:ARG:HH11	1:B:282:GLU:HG2	1.84	0.43
1:B:284:ARG:HH21	1:C:282:GLU:HG2	1.84	0.43
1:D:173:ALA:HB1	1:D:181:GLY:HA2	2.01	0.42
1:A:234:ILE:O	1:A:237:ILE:N	2.52	0.42
1:A:241:MET:CE	1:D:241:MET:SD	3.02	0.42
1:C:156:LEU:CG	1:C:160:ILE:HD11	2.49	0.42
1:D:225:SER:O	1:D:229:VAL:HG23	2.19	0.42
1:B:234:ILE:HG22	1:B:235:GLY:N	2.34	0.42
1:B:213:TRP:HE3	1:B:213:TRP:O	2.02	0.42
1:B:269:GLN:O	1:B:272:ARG:N	2.52	0.42
1:D:203:ILE:O	1:D:207:VAL:HG23	2.19	0.42
1:B:150:ILE:HG21	1:B:236:ILE:HG13	2.02	0.42
1:C:234:ILE:O	1:C:235:GLY:C	2.61	0.42
1:D:208:ILE:O	1:D:208:ILE:HG22	2.19	0.42
1:D:258:GLN:OE1	1:D:258:GLN:HA	2.18	0.42
1:C:202:GLY:C	1:C:203:ILE:HD12	2.45	0.42
1:D:283:ARG:C	1:D:285:SER:N	2.78	0.42
1:A:268:LEU:HD13	1:A:272:ARG:CZ	2.50	0.42
1:A:233[B]:PHE:CD1	1:B:230:LEU:CD1	2.97	0.42
1:A:229:VAL:O	1:A:233[A]:PHE:CE2	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:VAL:HG12	1:A:233[A]:PHE:CD2	2.38	0.41
1:B:238:ILE:HA	1:B:241:MET:HE2	2.02	0.41
1:C:193:VAL:HG13	1:C:199:TRP:HB2	2.02	0.41
1:D:279:ASP:HA	1:D:282:GLU:HB2	2.01	0.41
1:B:266:GLU:O	1:B:267:MET:C	2.62	0.41
1:C:265:LEU:O	1:C:266:GLU:C	2.63	0.41
1:D:150:ILE:O	1:D:153:ILE:N	2.52	0.41
1:B:216:ILE:O	1:B:220:SER:HB3	2.20	0.41
1:B:258:GLN:O	1:B:259:ARG:C	2.61	0.41
1:B:230:LEU:O	1:B:233:PHE:HB3	2.20	0.41
1:A:233[B]:PHE:CZ	1:B:233:PHE:CE2	2.99	0.41
1:B:168:GLY:O	1:B:172:PHE:HB2	2.20	0.41
1:C:205:ARG:HB2	1:C:206:PRO:HD3	2.03	0.41
1:B:255:GLU:O	1:B:256:GLN:C	2.61	0.41
1:C:198:SER:OG	1:D:201:MET:HG3	2.21	0.41
1:C:277:LYS:CD	1:D:279:ASP:HB3	2.51	0.41
1:A:215:TRP:CD2	3:A:302:VVA:O31	2.74	0.40
1:A:231:ASN:N	1:A:231:ASN:HD22	2.19	0.40
1:A:242:GLN:HA	1:A:246:TRP:HB2	2.02	0.40
1:A:255:GLU:HG2	1:A:256:GLN:N	2.34	0.40
1:A:264:ARG:O	1:A:265:LEU:C	2.61	0.40
1:B:150:ILE:O	1:B:153:ILE:HG13	2.21	0.40
1:B:203:ILE:CG1	1:C:201:MET:CE	2.98	0.40
1:C:208:ILE:HD11	1:C:215:TRP:HA	2.02	0.40
1:C:197:GLU:OE2	1:C:198:SER:HB3	2.20	0.40
1:D:200:SER:O	1:D:205:ARG:HG3	2.21	0.40
1:D:268:LEU:HD23	1:D:268:LEU:HA	1.75	0.40
1:A:197:GLU:C	1:A:197:GLU:OE1	2.65	0.40
1:C:283:ARG:C	1:C:285:SER:N	2.79	0.40
1:A:274:LEU:HD21	1:B:274:LEU:HG	2.03	0.40
1:B:270:LEU:N	1:B:270:LEU:CD2	2.84	0.40
1:D:183:LEU:O	1:D:187:MET:HG3	2.21	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	138/152 (91%)	131 (95%)	7 (5%)	0	100	100
1	B	137/152 (90%)	130 (95%)	6 (4%)	1 (1%)	18	40
1	C	136/152 (90%)	130 (96%)	6 (4%)	0	100	100
1	D	136/152 (90%)	130 (96%)	6 (4%)	0	100	100
All	All	547/608 (90%)	521 (95%)	25 (5%)	1 (0%)	43	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ILE

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	118/131 (90%)	91 (77%)	27 (23%)	1	2
1	B	118/131 (90%)	88 (75%)	30 (25%)	0	1
1	C	118/131 (90%)	92 (78%)	26 (22%)	1	2
1	D	119/131 (91%)	95 (80%)	24 (20%)	1	3
All	All	473/524 (90%)	366 (77%)	107 (23%)	1	2

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	TRP
1	A	153	ILE
1	A	175	SER
1	A	178	GLU
1	A	182	THR

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Mol	Chain	Res	Type
1	A	186	SER
1	A	197	GLU
1	A	201	MET
1	A	205	ARG
1	A	222	ILE
1	A	226	SER
1	A	232	LEU
1	A	234	ILE
1	A	237	ILE
1	A	238	ILE
1	A	240	SER
1	A	241	MET
1	A	247	GLU
1	A	249	GLU
1	A	254	ILE
1	A	255	GLU
1	A	258	GLN
1	A	259	ARG
1	A	268	LEU
1	A	269	GLN
1	A	277	LYS
1	A	282	GLU
1	B	150	ILE
1	B	152	TRP
1	B	153	ILE
1	B	158	LEU
1	B	167	MET
1	B	174	GLN
1	B	175	SER
1	B	178[A]	GLU
1	B	178[B]	GLU
1	B	182	THR
1	B	183	LEU
1	B	206	PRO
1	B	224	VAL
1	B	232	LEU
1	B	234	ILE
1	B	238	ILE
1	B	239	GLU
1	B	240	SER
1	B	242	GLN
1	B	243	SER

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Mol	Chain	Res	Type
1	B	253	ARG
1	B	254	ILE
1	B	255	GLU
1	B	258	GLN
1	B	259	ARG
1	B	268	LEU
1	B	270	LEU
1	B	275	SER
1	B	283	ARG
1	B	284	ARG
1	C	152	TRP
1	C	153	ILE
1	C	155	LEU
1	C	178	GLU
1	C	182	THR
1	C	187	MET
1	C	192	GLN
1	C	197	GLU
1	C	226	SER
1	C	232	LEU
1	C	233	PHE
1	C	237	ILE
1	C	238	ILE
1	C	240	SER
1	C	241	MET
1	C	242	GLN
1	C	249	GLU
1	C	253	ARG
1	C	259	ARG
1	C	265	LEU
1	C	267	MET
1	C	268	LEU
1	C	269	GLN
1	C	275	SER
1	C	277	LYS
1	C	285	SER
1	D	150	ILE
1	D	152	TRP
1	D	153	ILE
1	D	155	LEU
1	D	158	LEU
1	D	162	TYR

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Mol	Chain	Res	Type
1	D	174	GLN
1	D	175	SER
1	D	182	THR
1	D	186	SER
1	D	194	MET
1	D	222	ILE
1	D	224	VAL
1	D	227	PHE
1	D	240	SER
1	D	252	LYS
1	D	253	ARG
1	D	254	ILE
1	D	256	GLN
1	D	265	LEU
1	D	270	LEU
1	D	275	SER
1	D	280	ARG
1	D	283	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	245	HIS
1	B	231	ASN
1	B	242	GLN
1	B	245	HIS
1	C	242	GLN
1	C	245	HIS
1	D	256	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	VVA	C	301	-	20,20,28	1.65	2 (10%)	22,23,31	2.23	5 (22%)
3	VVA	A	302	-	20,20,28	1.79	2 (10%)	22,23,31	1.68	3 (13%)
3	VVA	C	303	-	5,5,28	0.61	0	4,4,31	0.43	0
3	VVA	C	302	-	9,9,28	0.71	0	8,8,31	0.51	0
3	VVA	A	303	-	12,12,28	0.49	0	11,11,31	0.39	0
3	VVA	B	301	-	20,20,28	1.58	1 (5%)	22,23,31	1.78	5 (22%)
3	VVA	D	301	-	9,9,28	0.53	0	8,8,31	0.64	0
3	VVA	B	302	-	20,20,28	1.53	1 (5%)	22,23,31	1.60	3 (13%)
3	VVA	C	304	-	10,10,28	0.55	0	9,9,31	0.30	0
3	VVA	B	303	-	16,16,28	0.43	0	15,15,31	0.61	0

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	VVA	C	301	-	-	8/21/21/29	-
3	VVA	A	302	-	-	10/21/21/29	-
3	VVA	C	303	-	-	2/3/3/29	-
3	VVA	C	302	-	-	2/7/7/29	-
3	VVA	A	303	-	-	5/10/10/29	-
3	VVA	B	301	-	-	8/21/21/29	-
3	VVA	D	301	-	-	4/7/7/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VVA	B	302	-	-	6/21/21/29	-
3	VVA	C	304	-	-	7/8/8/29	-
3	VVA	B	303	-	-	11/14/14/29	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	VVA	O2-C31	6.43	1.52	1.33
3	B	301	VVA	O2-C31	6.10	1.51	1.33
3	C	301	VVA	O2-C31	5.92	1.50	1.33
3	B	302	VVA	O2-C31	5.66	1.49	1.33
3	A	302	VVA	C32-C31	2.60	1.58	1.50
3	C	301	VVA	C32-C31	2.16	1.57	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	VVA	O2-C31-C32	5.73	129.30	111.83
3	C	301	VVA	C2-O2-C31	5.01	132.56	116.90
3	A	302	VVA	O2-C31-C32	4.68	126.09	111.83
3	C	301	VVA	O2-C31-O31	-4.67	111.94	123.63
3	B	301	VVA	O2-C31-C32	4.59	125.82	111.83
3	B	301	VVA	C2-O2-C31	4.41	130.69	116.90
3	B	302	VVA	O2-C31-C32	4.15	124.47	111.83
3	B	302	VVA	C2-O2-C31	4.12	129.77	116.90
3	A	302	VVA	O2-C31-O31	-3.34	115.28	123.63
3	A	302	VVA	C2-O2-C31	2.86	125.84	116.90
3	B	301	VVA	O2-C31-O31	-2.55	117.25	123.63
3	B	301	VVA	O3P-C1-C2	2.54	118.45	109.45
3	B	302	VVA	O2-C31-O31	-2.54	117.28	123.63
3	C	301	VVA	O3P-C1-C2	2.47	118.20	109.45
3	B	301	VVA	O2-C2-C1	2.37	115.54	108.61
3	C	301	VVA	O2P-P-O1P	2.05	122.00	112.44

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	VVA	C4-O4P-P-O1P
3	A	302	VVA	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	A	302	VVA	C4-O4P-P-O3P
3	A	302	VVA	C1-O3P-P-O2P
3	A	302	VVA	C1-O3P-P-O4P
3	A	302	VVA	C2-C1-O3P-P
3	A	302	VVA	O3P-C1-C2-O2
3	B	301	VVA	O3P-C1-C2-O2
3	B	301	VVA	C1-C2-O2-C31
3	B	302	VVA	C1-O3P-P-O4P
3	B	302	VVA	O3P-C1-C2-O2
3	C	301	VVA	O3P-C1-C2-O2
3	C	301	VVA	C1-C2-O2-C31
3	C	301	VVA	C32-C31-O2-C2
3	C	301	VVA	O31-C31-O2-C2
3	D	301	VVA	C35-C36-C37-C38
3	B	301	VVA	C32-C31-O2-C2
3	C	304	VVA	C35-C36-C37-C38
3	A	303	VVA	C35-C36-C37-C38
3	B	303	VVA	C40-C41-C42-C43
3	A	303	VVA	C36-C37-C38-C39
3	B	301	VVA	O31-C31-O2-C2
3	B	303	VVA	C43-C44-C45-C46
3	A	302	VVA	C34-C35-C36-C37
3	C	303	VVA	C33-C34-C35-C36
3	B	302	VVA	C34-C35-C36-C37
3	B	303	VVA	C33-C34-C35-C36
3	B	303	VVA	C41-C42-C43-C44
3	C	301	VVA	C33-C34-C35-C36
3	C	304	VVA	C32-C33-C34-C35
3	A	302	VVA	C35-C36-C37-C38
3	B	303	VVA	C32-C33-C34-C35
3	C	304	VVA	C37-C38-C39-C40
3	D	301	VVA	C34-C35-C36-C37
3	C	302	VVA	C32-C33-C34-C35
3	B	303	VVA	C44-C45-C46-C47
3	A	302	VVA	C36-C37-C38-C39
3	B	303	VVA	C36-C37-C38-C39
3	D	301	VVA	C36-C37-C38-C39
3	C	304	VVA	C31-C32-C33-C34
3	B	302	VVA	C36-C37-C38-C39
3	C	303	VVA	C32-C33-C34-C35
3	C	301	VVA	C36-C37-C38-C39
3	C	304	VVA	C33-C34-C35-C36

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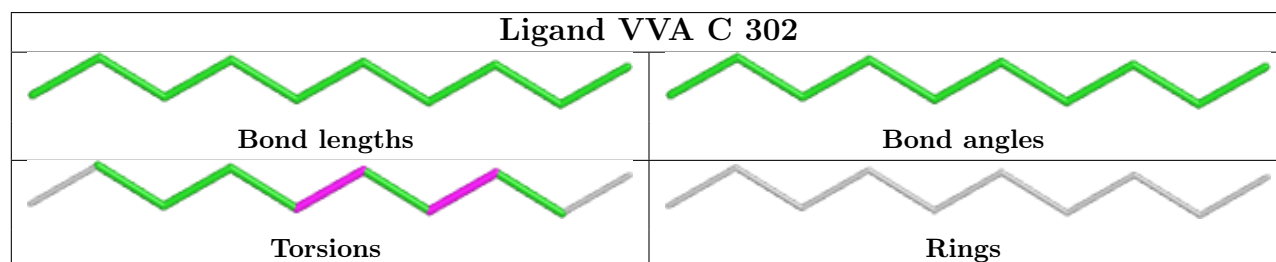
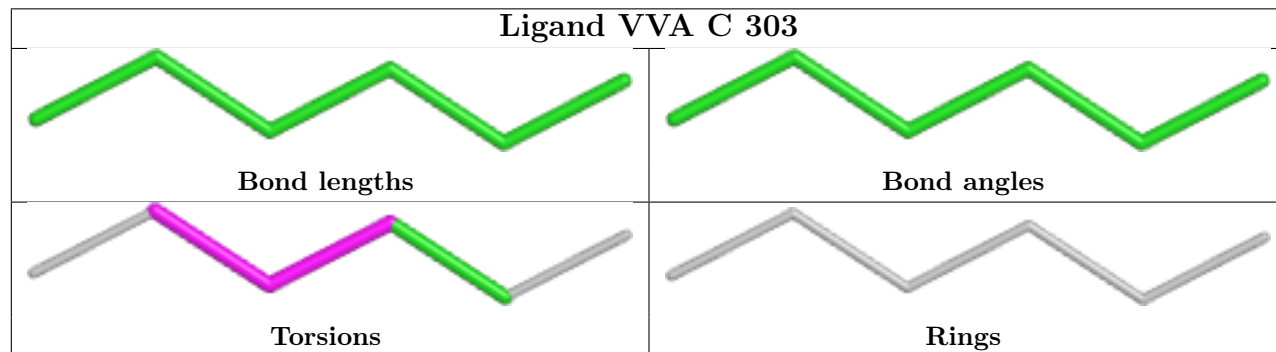
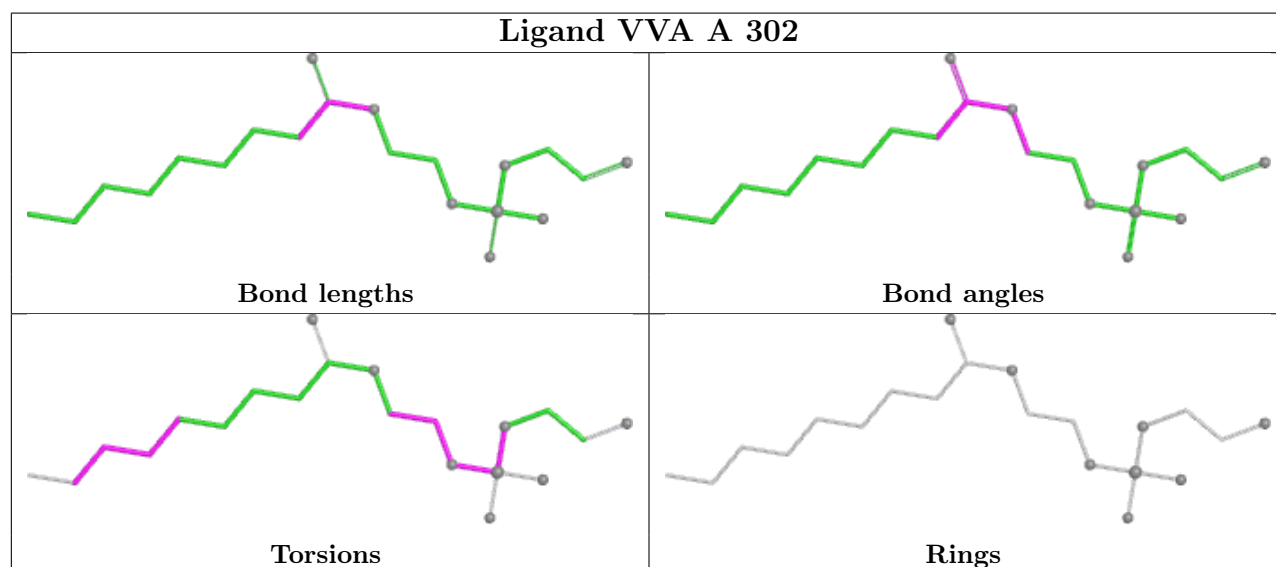
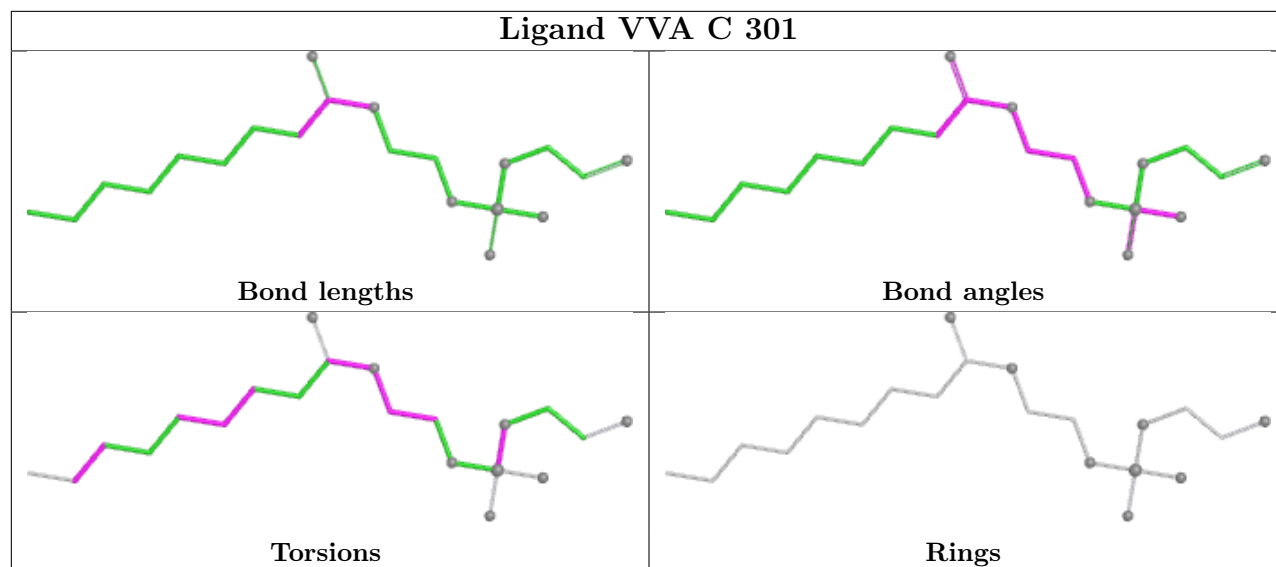
Mol	Chain	Res	Type	Atoms
3	A	303	VVA	C38-C39-C40-C41
3	C	304	VVA	C38-C39-C40-C41
3	C	304	VVA	C34-C35-C36-C37
3	B	301	VVA	C4-O4P-P-O1P
3	B	301	VVA	O4P-C4-C5-N6
3	B	302	VVA	C1-O3P-P-O1P
3	C	301	VVA	C4-O4P-P-O1P
3	B	303	VVA	C35-C36-C37-C38
3	B	302	VVA	C35-C36-C37-C38
3	B	303	VVA	C37-C38-C39-C40
3	A	303	VVA	C31-C32-C33-C34
3	D	301	VVA	C37-C38-C39-C40
3	B	301	VVA	C35-C36-C37-C38
3	A	303	VVA	C33-C34-C35-C36
3	C	301	VVA	C32-C33-C34-C35
3	B	303	VVA	C34-C35-C36-C37
3	C	302	VVA	C34-C35-C36-C37
3	B	303	VVA	C39-C40-C41-C42
3	B	301	VVA	C36-C37-C38-C39

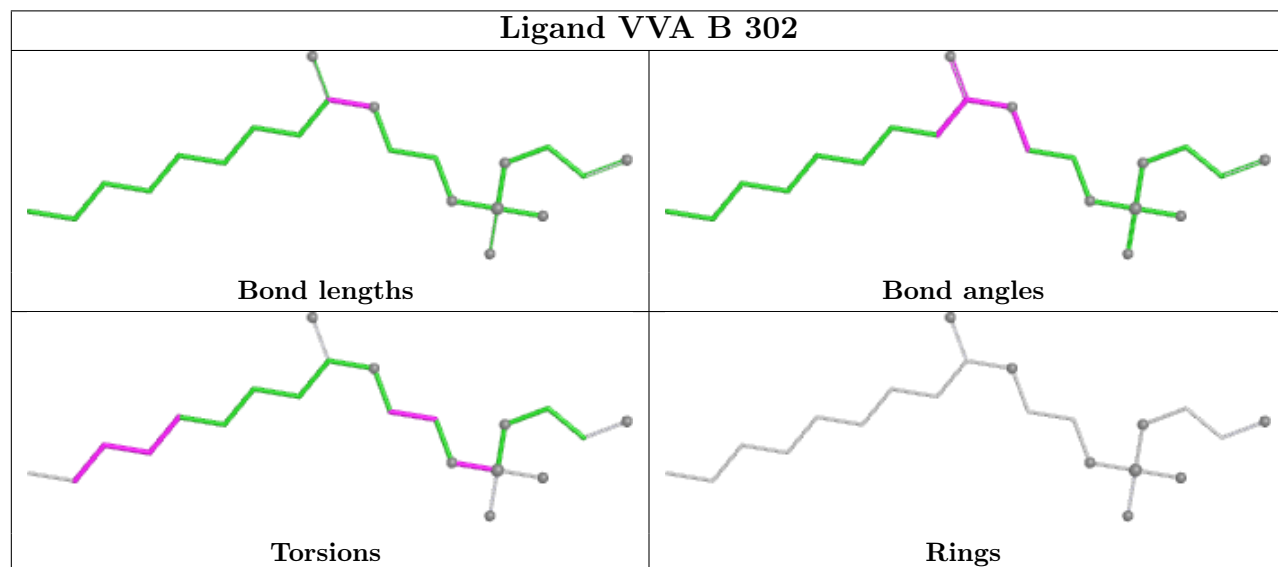
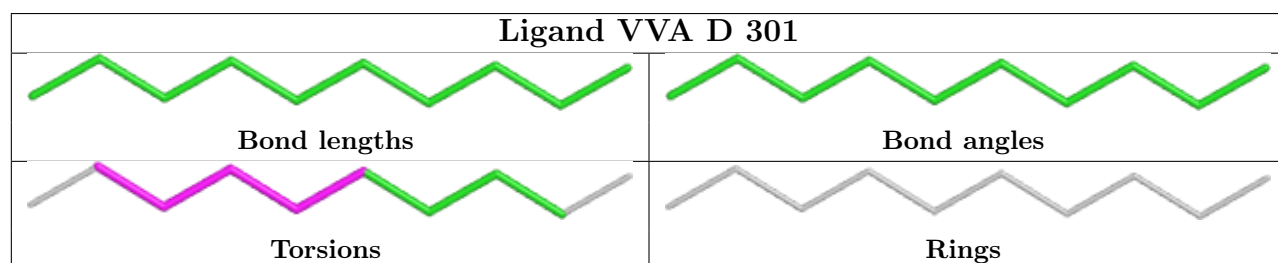
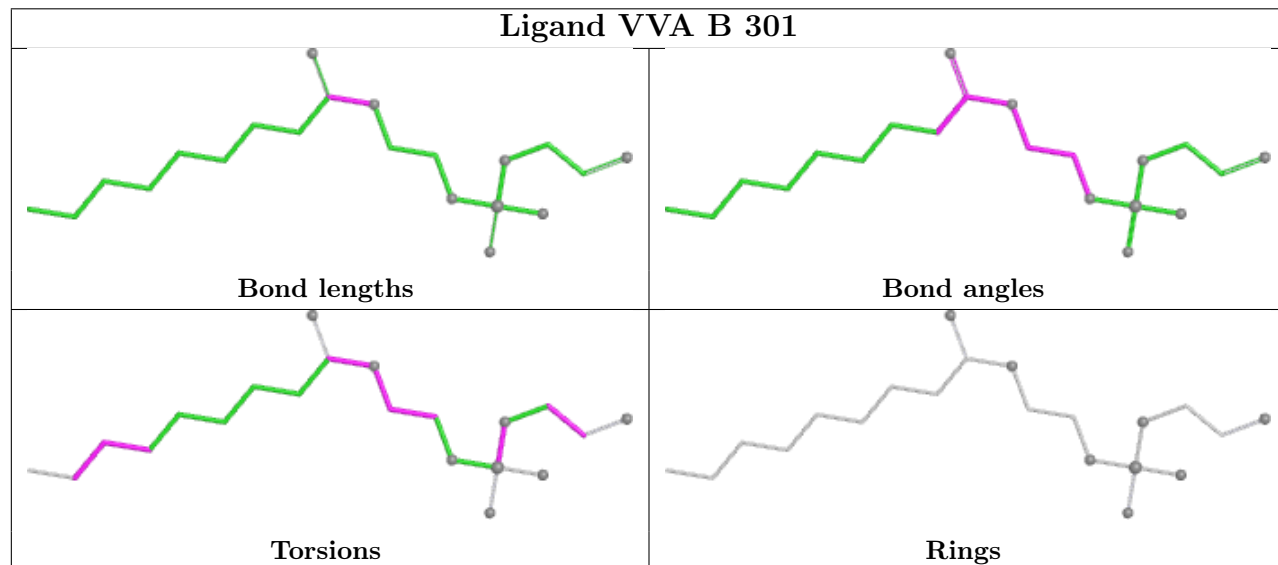
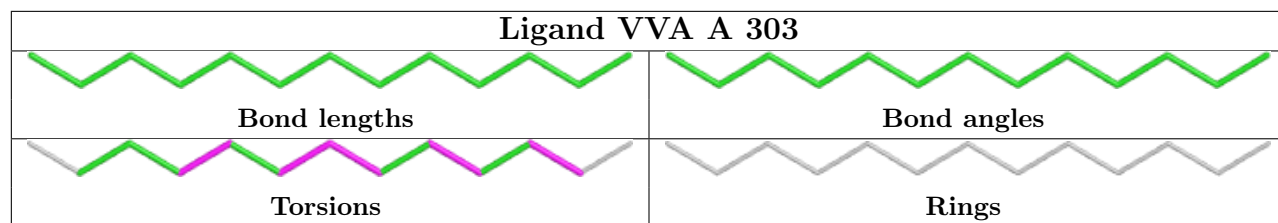
There are no ring outliers.

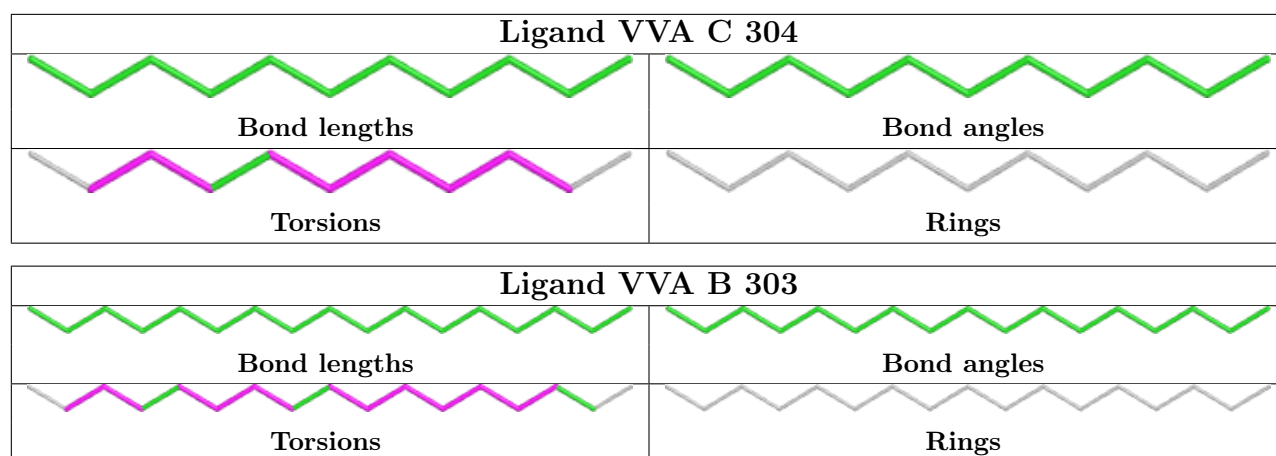
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	VVA	1	0
3	A	303	VVA	2	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.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	139/152 (91%)	-0.56	0 100 100	60, 87, 127, 165	1 (0%)
1	B	138/152 (90%)	-0.51	0 100 100	48, 93, 131, 168	2 (1%)
1	C	138/152 (90%)	-0.56	1 (0%) 84 80	56, 87, 135, 168	0
1	D	138/152 (90%)	-0.58	0 100 100	53, 82, 125, 145	1 (0%)
All	All	553/608 (90%)	-0.55	1 (0%) 91 90	48, 87, 131, 168	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

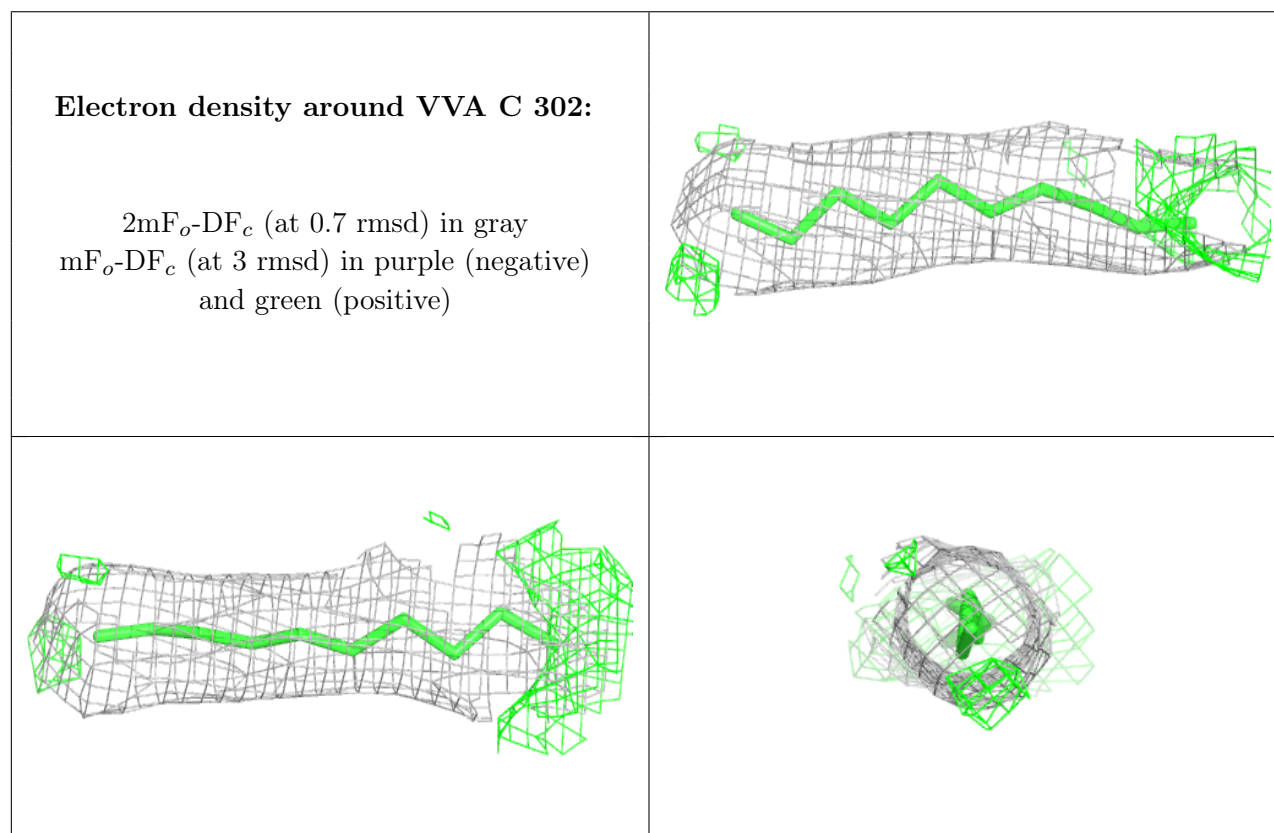
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	VVA	C	302	10/29	0.75	0.14	69,86,95,100	0

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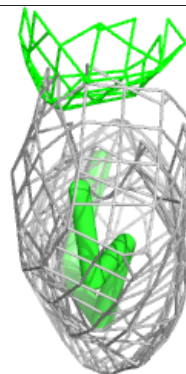
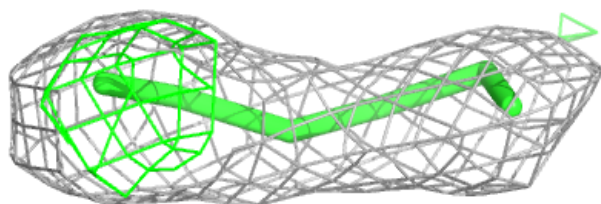
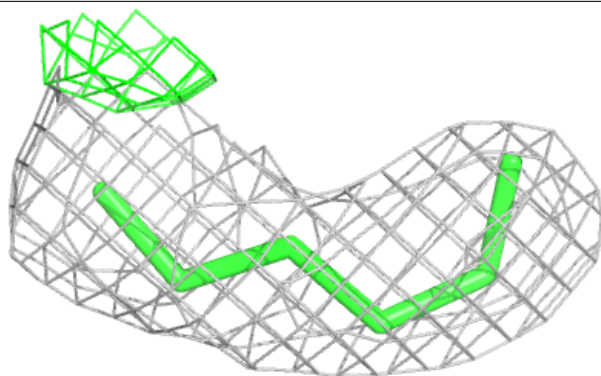
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	VVA	C	303	6/29	0.84	0.17	79,104,110,113	0
3	VVA	D	301	10/29	0.86	0.16	78,97,108,111	0
3	VVA	B	303	17/29	0.88	0.14	99,108,130,131	0
3	VVA	B	301	21/29	0.89	0.17	68,85,135,197	0
3	VVA	A	302	21/29	0.90	0.16	59,91,139,194	0
3	VVA	C	301	21/29	0.91	0.14	63,97,146,166	0
3	VVA	B	302	21/29	0.91	0.15	67,90,161,187	0
4	NA	C	305	1/1	0.92	0.78	105,105,105,105	0
3	VVA	A	303	13/29	0.93	0.13	94,108,143,150	0
3	VVA	C	304	11/29	0.93	0.15	77,112,125,131	0
4	NA	B	304	1/1	0.96	0.82	81,81,81,81	0
2	CL	A	304	1/1	0.97	0.23	108,108,108,108	0
2	CL	A	301	1/1	0.99	0.03	72,72,72,72	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.

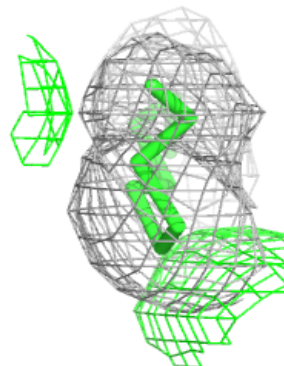
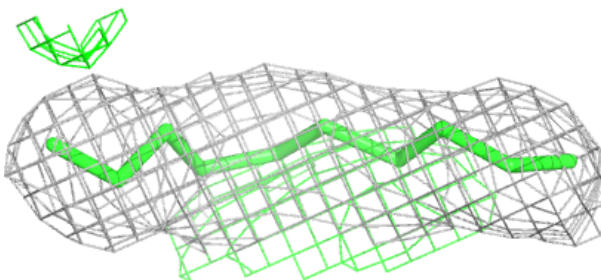
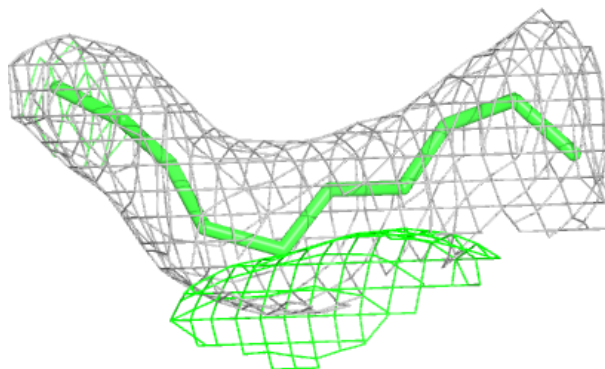


Electron density around VVA C 303:

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

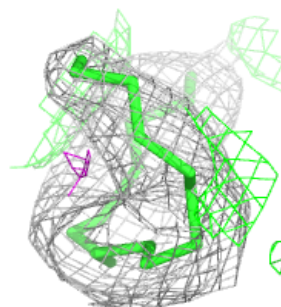
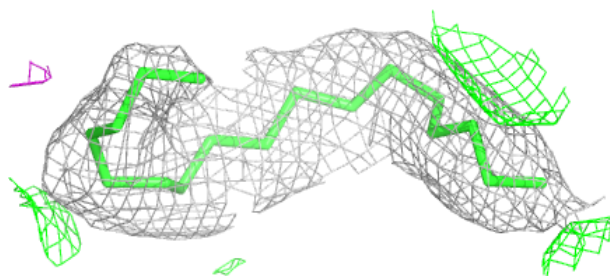
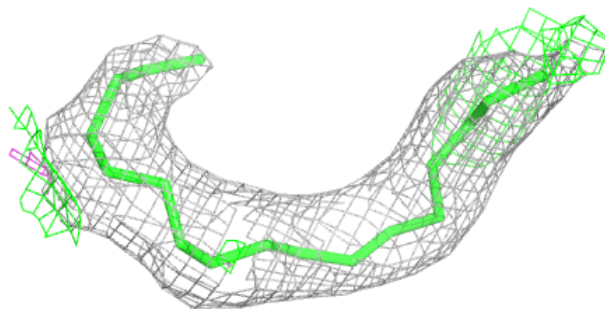
**Electron density around VVA D 301:**

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

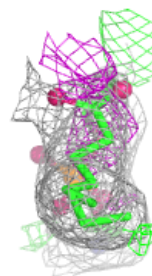
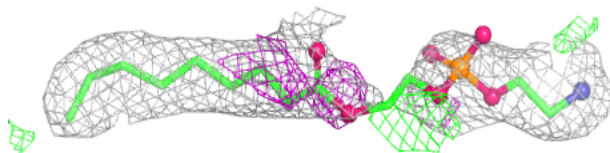
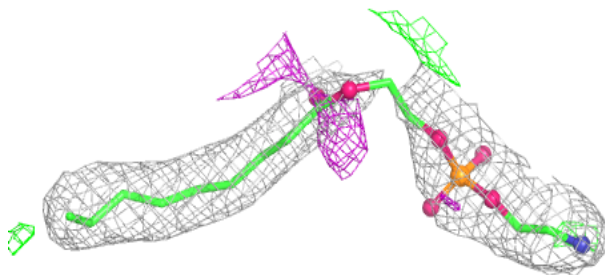


Electron density around VVA B 303:

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

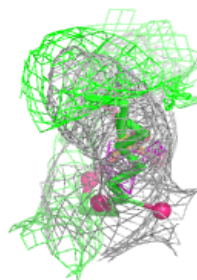
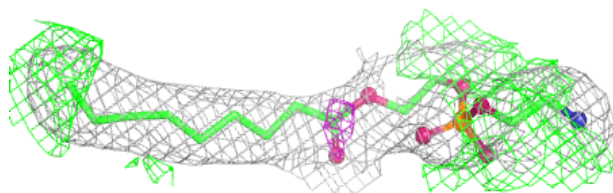
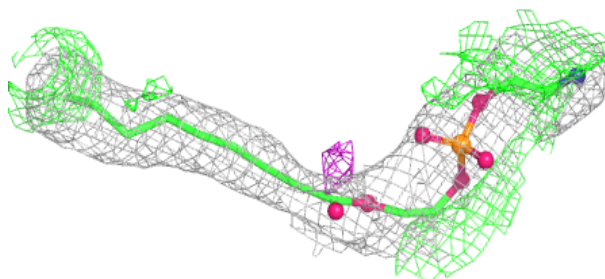
**Electron density around VVA B 301:**

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

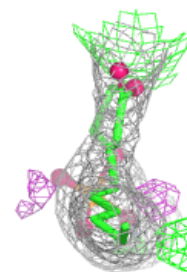
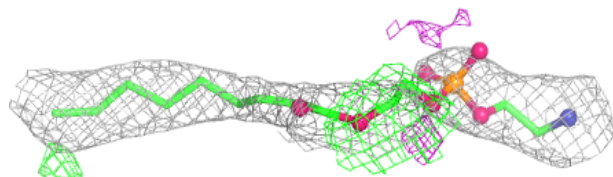
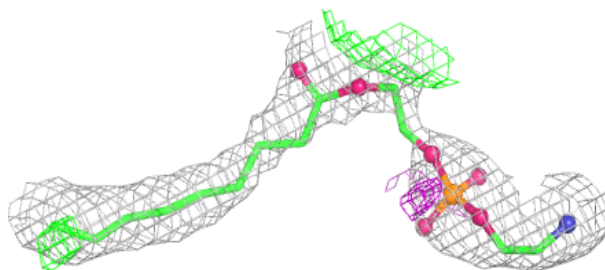


Electron density around VVA A 302:

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

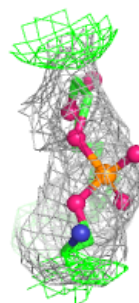
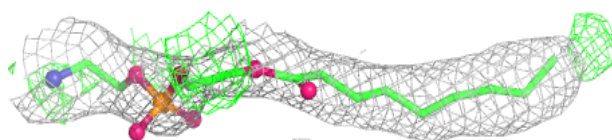
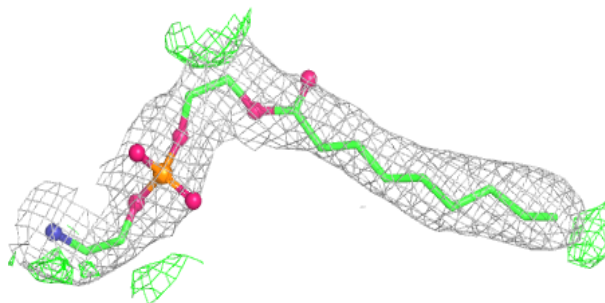
**Electron density around VVA C 301:**

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

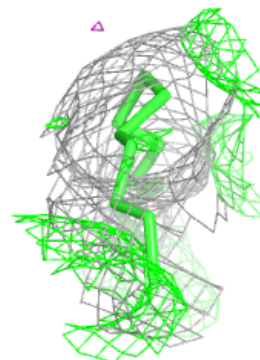
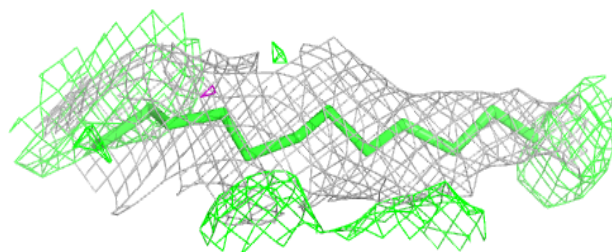
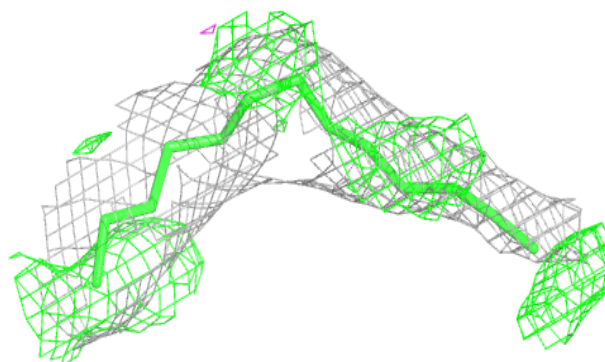


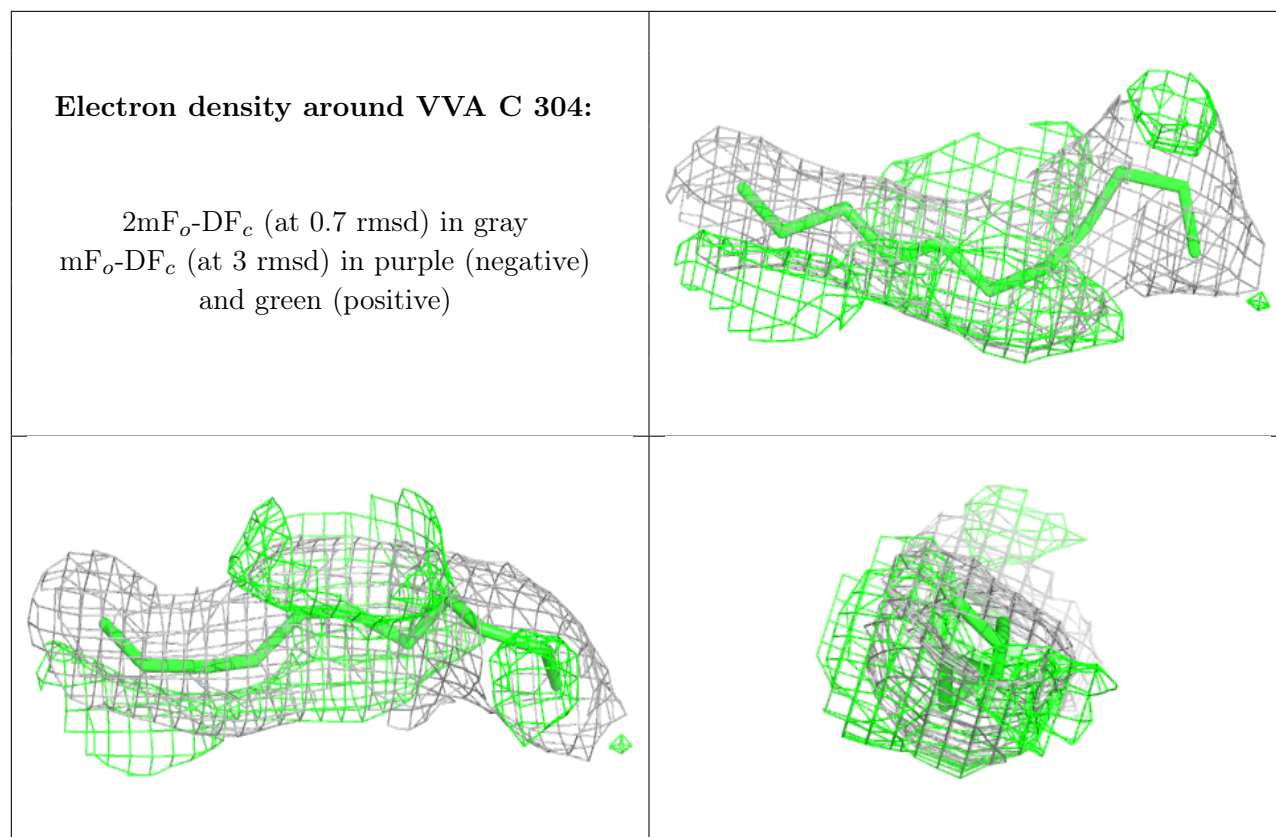
Electron density around VVA B 302:

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

**Electron density around VVA A 303:**

$2mF_o-DF_c$ (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.