



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2024 – 05:53 PM EDT

PDB ID : 1J78  
Title : Crystallographic analysis of the human vitamin D binding protein  
Authors : Verboven, C.; Rabijns, A.; De Maeyer, M.; Van Baelen, H.; Bouillon, R.; De Ranter, C.  
Deposited on : 2001-05-16  
Resolution : 2.31 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

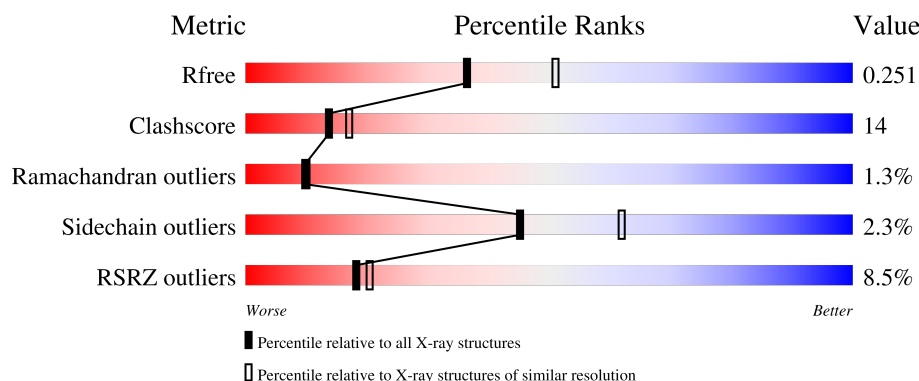
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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))
$R_{free}$	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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  $\geq 3$ , 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	458	<div> <div>8%</div> <div>70%</div> <div>23%</div> <div>5%</div> </div>
1	B	458	<div> <div>8%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7137 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.

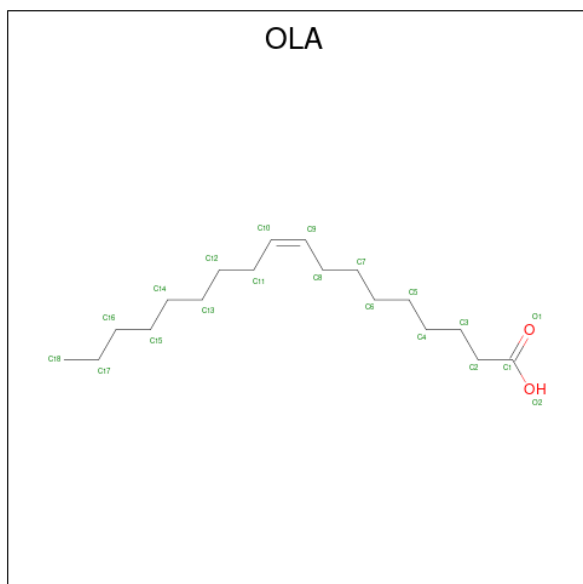
- Molecule 1 is a protein called vitamin D binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	0	0
			3334	2093	541	666	34			
1	B	447	Total	C	N	O	S	0	0	0
			3415	2140	552	688	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	THR	LYS	variant	UNP P02774
B	420	THR	LYS	variant	UNP P02774

- Molecule 2 is OLEIC ACID (three-letter code: OLA) (formula:  $C_{18}H_{34}O_2$ ).



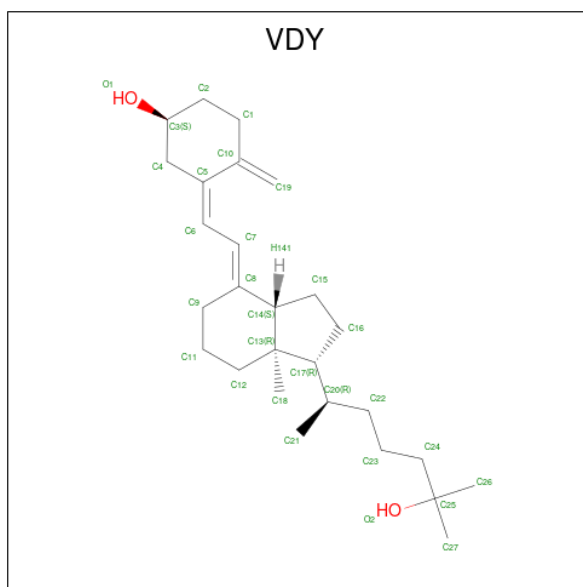
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	18	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	18	2		
2	B	1	Total	C	O	0	0
			20	18	2		

- Molecule 3 is 3-{2-[1-(5-HYDROXY-1,5-DIMETHYL-HEXYL)-7A-METHYL-OCTA HYDRO-INDEN-4-YLIDENE]-ETHYLIDENE}-4-METHYLENE-CYCLOHEXANOL (three-letter code: VDY) (formula: C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			29	27	2		

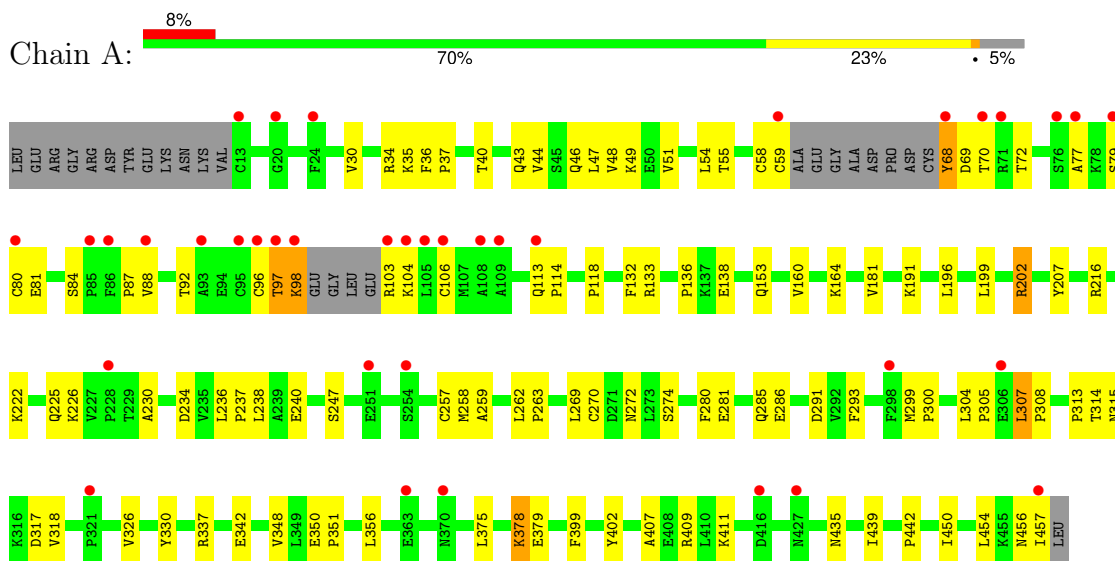
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	142	Total	O	0	0
			142	142		

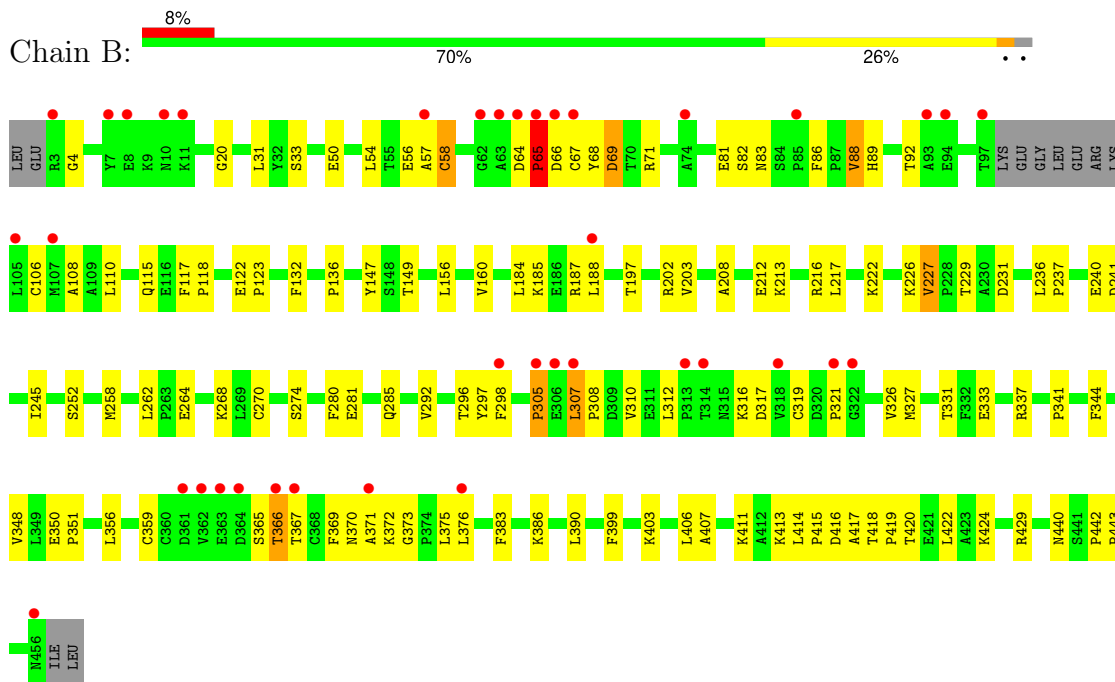
### 3 Residue-property plots [i](#)

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: vitamin D binding protein



#### • Molecule 1: vitamin D binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.25Å 132.25Å 73.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.38 – 2.31 29.38 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.38-2.31) 99.1 (29.38-2.31)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	0.03	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.29 (at 2.31Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.252 0.216 , 0.251	Depositor DCC
$R_{free}$ test set	2221 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7137	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OLA, VDY

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	0.34	0/3397	0.56	0/4601
1	B	0.33	0/3481	0.55	0/4723
All	All	0.33	0/6878	0.56	0/9324

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	3334	0	3233	91	0
1	B	3415	0	3271	102	0
2	A	20	0	34	1	0
2	B	40	0	68	1	0
3	B	29	0	44	3	0
4	A	157	0	0	8	0
4	B	142	0	0	9	0
All	All	7137	0	6650	193	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 14.

All (193) 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:98:LYS:HZ1	1:A:104:LYS:HB2	1.32	0.92
1:B:115:GLN:HE21	1:B:117:PHE:H	0.94	0.89
1:B:115:GLN:NE2	1:B:117:PHE:H	1.73	0.85
1:B:115:GLN:HE21	1:B:117:PHE:N	1.75	0.85
1:B:88:VAL:HG22	1:B:92:THR:HG21	1.61	0.81
1:A:326:VAL:HG13	4:A:606:HOH:O	1.81	0.81
1:B:216:ARG:NH1	1:B:240:GLU:HG2	1.97	0.80
1:B:372:LYS:HG2	1:B:376:LEU:HD22	1.63	0.80
1:A:317:ASP:HB3	1:A:326:VAL:HG21	1.62	0.80
1:A:315:ASN:ND2	1:A:317:ASP:HB2	1.97	0.79
1:A:315:ASN:HD21	1:A:317:ASP:HB2	1.50	0.77
1:B:227:VAL:HG22	1:B:280:PHE:CE1	2.21	0.75
1:B:67:CYS:SG	1:B:68:TYR:N	2.60	0.74
1:B:316:LYS:HE3	1:B:365:SER:HB2	1.70	0.74
1:A:103:ARG:HG3	1:A:104:LYS:H	1.51	0.74
1:A:88:VAL:HG13	1:A:92:THR:HB	1.73	0.70
1:A:350:GLU:HB3	1:A:351:PRO:HD3	1.73	0.70
1:B:216:ARG:HH12	1:B:240:GLU:HG2	1.56	0.69
1:B:50:GLU:HG3	1:B:86:PHE:HZ	1.56	0.69
1:B:208:ALA:HA	2:B:460:OLA:H32	1.75	0.69
1:A:133:ARG:HD3	4:A:572:HOH:O	1.94	0.67
1:A:118:PRO:HG3	4:A:467:HOH:O	1.94	0.67
1:B:217:LEU:HD11	1:B:331:THR:HG21	1.76	0.67
1:B:217:LEU:HD23	4:B:539:HOH:O	1.94	0.67
1:B:118:PRO:HG3	4:B:502:HOH:O	1.96	0.65
1:B:307:LEU:HB3	1:B:308:PRO:CD	2.25	0.65
1:B:341:PRO:HG2	1:B:344:PHE:HD1	1.62	0.65
1:B:440:ASN:HB2	4:B:575:HOH:O	1.97	0.65
1:A:281:GLU:O	1:A:285:GLN:HG2	1.97	0.65
1:B:371:ALA:O	1:B:375:LEU:HD23	1.96	0.65
1:A:103:ARG:HG3	1:A:104:LYS:N	2.12	0.65
1:A:58:CYS:SG	1:A:68:TYR:HB2	2.38	0.64
1:A:202:ARG:NH2	4:A:555:HOH:O	2.31	0.64
1:B:50:GLU:HG3	1:B:86:PHE:CZ	2.33	0.64
1:A:114:PRO:HG3	1:A:153:GLN:NE2	2.13	0.63
1:A:181:VAL:HG23	4:A:476:HOH:O	1.97	0.63
1:B:319:CYS:O	1:B:321:PRO:HD3	1.98	0.63
1:A:98:LYS:NZ	1:A:104:LYS:HB2	2.11	0.62
1:A:307:LEU:HD12	1:A:307:LEU:H	1.64	0.62
1:B:281:GLU:O	1:B:285:GLN:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:HG21	1:B:333:GLU:HB3	1.82	0.61
3:B:500:VDY:H271	4:B:597:HOH:O	2.00	0.61
1:A:103:ARG:CG	1:A:104:LYS:H	2.11	0.60
1:A:47:LEU:O	1:A:51:VAL:HG23	2.00	0.60
1:A:378:LYS:HD2	1:A:378:LYS:N	2.16	0.60
1:A:337:ARG:O	1:A:337:ARG:HD2	2.02	0.59
1:B:359:CYS:HB3	1:B:369:PHE:CE1	2.38	0.59
1:B:316:LYS:NZ	1:B:366:THR:HB	2.17	0.59
1:B:399:PHE:CE2	1:B:403:LYS:HE3	2.38	0.58
1:A:226:LYS:HE2	1:A:299:MET:O	2.03	0.58
1:B:341:PRO:HG2	1:B:344:PHE:CD1	2.37	0.58
1:B:236:LEU:HB3	1:B:237:PRO:HD3	1.85	0.58
1:B:307:LEU:HB3	1:B:308:PRO:HD2	1.85	0.57
1:B:407:ALA:O	1:B:411:LYS:HG3	2.04	0.57
1:A:69:ASP:HA	1:A:72:THR:HB	1.86	0.57
1:A:342:GLU:HG3	4:A:462:HOH:O	2.04	0.56
1:B:420:THR:HG22	1:B:424:LYS:HE3	1.87	0.56
1:B:54:LEU:C	1:B:54:LEU:HD23	2.26	0.56
1:B:156:LEU:O	1:B:160:VAL:HG23	2.06	0.56
1:A:375:LEU:O	1:A:379:GLU:HG3	2.06	0.56
1:B:317:ASP:HB3	1:B:326:VAL:HG21	1.87	0.56
1:B:54:LEU:HA	1:B:71:ARG:NH1	2.21	0.56
1:B:327:MET:O	1:B:331:THR:HG23	2.06	0.55
1:A:286:GLU:OE2	1:A:291:ASP:HB3	2.06	0.55
1:B:58:CYS:SG	1:B:68:TYR:HB2	2.47	0.55
1:B:227:VAL:HG22	1:B:280:PHE:HE1	1.70	0.55
1:B:147:TYR:HE2	1:B:197:THR:HG21	1.72	0.54
1:B:64:ASP:CB	1:B:65:PRO:HD2	2.38	0.54
1:B:213:LYS:HB3	4:B:504:HOH:O	2.08	0.54
1:B:270:CYS:O	1:B:274:SER:HB2	2.08	0.54
1:B:367:THR:HA	1:B:370:ASN:HD22	1.73	0.54
1:A:272:ASN:HD22	1:A:272:ASN:N	2.05	0.54
1:B:64:ASP:O	1:B:65:PRO:C	2.46	0.54
1:A:307:LEU:HD12	1:A:307:LEU:N	2.23	0.53
1:A:207:TYR:OH	1:A:247:SER:HB3	2.08	0.53
1:B:31:LEU:C	1:B:31:LEU:HD23	2.27	0.53
3:B:500:VDY:C27	4:B:597:HOH:O	2.54	0.53
1:B:264:GLU:HG2	1:B:268:LYS:NZ	2.24	0.53
1:A:160:VAL:O	1:A:164:LYS:HG2	2.09	0.52
1:A:307:LEU:HB3	1:A:308:PRO:CD	2.39	0.52
1:A:315:ASN:HD22	1:A:317:ASP:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:HIS:O	1:B:92:THR:HG23	2.10	0.51
1:B:81:GLU:C	1:B:83:ASN:H	2.13	0.51
1:A:409:ARG:HH11	1:A:409:ARG:HG2	1.76	0.51
1:B:350:GLU:HB3	1:B:351:PRO:CD	2.40	0.51
1:A:132:PHE:O	1:A:136:PRO:HG3	2.10	0.51
1:A:281:GLU:OE2	1:A:285:GLN:NE2	2.44	0.51
1:A:35:LYS:O	1:A:37:PRO:HD3	2.11	0.50
1:A:40:THR:OG1	1:A:43:GLN:HG3	2.11	0.50
1:A:270:CYS:O	1:A:274:SER:HB2	2.12	0.50
1:B:292:VAL:O	1:B:296:THR:HG23	2.11	0.50
1:B:222:LYS:O	1:B:226:LYS:HG3	2.11	0.50
1:B:414:LEU:HD22	1:B:414:LEU:N	2.27	0.50
1:A:348:VAL:HG23	2:A:459:OLA:H152	1.94	0.50
1:B:64:ASP:O	1:B:66:ASP:N	2.45	0.49
1:B:92:THR:HA	1:B:110:LEU:HD11	1.94	0.49
1:A:30:VAL:O	1:A:34:ARG:HG3	2.12	0.49
1:B:92:THR:HG22	1:B:110:LEU:HD12	1.94	0.49
1:A:258:MET:HE3	1:A:262:LEU:HD11	1.95	0.49
1:A:43:GLN:HB3	1:A:87:PRO:HG3	1.94	0.49
1:A:315:ASN:O	1:A:318:VAL:HG22	2.13	0.49
1:B:356:LEU:HD21	1:B:376:LEU:HD11	1.95	0.49
1:A:55:THR:O	1:A:59:CYS:SG	2.71	0.48
1:B:252:SER:HA	4:B:635:HOH:O	2.12	0.48
1:A:97:THR:HG23	1:A:97:THR:O	2.12	0.48
1:A:196:LEU:HD21	1:A:259:ALA:HB2	1.95	0.48
1:B:376:LEU:H	1:B:376:LEU:HD23	1.77	0.48
1:A:225:GLN:HG2	4:A:533:HOH:O	2.13	0.48
1:B:57:ALA:O	1:B:58:CYS:HB2	2.13	0.48
1:B:216:ARG:HH12	1:B:240:GLU:CG	2.26	0.48
1:B:372:LYS:O	1:B:375:LEU:HB2	2.14	0.48
1:B:414:LEU:HB3	1:B:417:ALA:HB2	1.96	0.48
1:A:77:ALA:C	1:A:79:SER:H	2.18	0.47
1:B:316:LYS:HZ2	1:B:366:THR:HB	1.77	0.47
1:A:230:ALA:HB1	1:A:234:ASP:HB2	1.96	0.47
1:B:71:ARG:HH11	1:B:71:ARG:HG2	1.80	0.47
1:A:450:ILE:O	1:A:454:LEU:HG	2.14	0.47
1:B:350:GLU:HB3	1:B:351:PRO:HD3	1.96	0.47
1:B:365:SER:C	1:B:367:THR:H	2.18	0.46
1:A:46:GLN:O	1:A:49:LYS:HB3	2.16	0.46
1:A:313:PRO:HB2	1:A:318:VAL:HG11	1.97	0.46
1:B:132:PHE:O	1:B:136:PRO:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:LYS:HE3	1:B:365:SER:CB	2.44	0.46
1:A:81:GLU:O	1:A:84:SER:HB3	2.16	0.46
1:B:88:VAL:HG22	1:B:92:THR:CG2	2.39	0.46
1:A:113:GLN:HB2	1:B:419:PRO:HD2	1.98	0.46
1:A:43:GLN:CB	1:A:87:PRO:HG3	2.46	0.45
1:A:238:LEU:HD13	1:A:269:LEU:HD23	1.99	0.45
1:A:44:VAL:O	1:A:48:VAL:HG23	2.16	0.45
1:A:202:ARG:NE	1:A:202:ARG:HA	2.31	0.45
1:A:199:LEU:HD11	1:A:293:PHE:CE1	2.51	0.45
1:A:313:PRO:HG3	1:A:330:TYR:HB2	1.97	0.45
1:A:313:PRO:HD2	1:A:356:LEU:CD1	2.47	0.45
1:A:222:LYS:HE2	1:A:439:ILE:O	2.17	0.45
1:B:310:VAL:CG2	1:B:333:GLU:HB3	2.46	0.45
1:B:406:LEU:HD11	1:B:429:ARG:HG2	1.99	0.45
1:A:96:CYS:O	1:A:98:LYS:N	2.50	0.44
1:B:33:SER:HB3	1:B:149:THR:HG23	1.99	0.44
1:A:216:ARG:HH21	1:A:240:GLU:CD	2.20	0.44
1:B:118:PRO:HG3	1:B:202:ARG:HH22	1.83	0.44
1:A:88:VAL:CG1	1:A:92:THR:HB	2.45	0.44
1:A:262:LEU:N	1:A:263:PRO:HD2	2.33	0.44
1:A:153:GLN:HA	1:A:153:GLN:OE1	2.18	0.44
1:A:36:PHE:CD2	1:A:87:PRO:HB2	2.53	0.44
1:B:92:THR:HG22	1:B:110:LEU:CD1	2.48	0.43
1:B:241:ASP:O	1:B:245:ILE:HG13	2.17	0.43
1:A:236:LEU:HB3	1:A:237:PRO:HD3	2.01	0.43
1:B:184:LEU:O	1:B:188:LEU:HG	2.19	0.43
1:A:222:LYS:CE	1:A:342:GLU:HG2	2.49	0.43
1:B:203:VAL:HG12	1:B:297:TYR:CE2	2.53	0.43
1:A:258:MET:CE	1:A:262:LEU:HD11	2.47	0.43
1:B:258:MET:O	1:B:262:LEU:HG	2.19	0.43
1:A:98:LYS:HG3	1:A:103:ARG:HG3	2.01	0.42
1:A:257:CYS:HA	4:A:573:HOH:O	2.19	0.42
1:B:122:GLU:CD	1:B:187:ARG:HH12	2.22	0.42
1:B:297:TYR:HD2	1:B:298:PHE:CE1	2.37	0.42
1:A:348:VAL:O	1:A:351:PRO:HD2	2.19	0.42
1:A:399:PHE:O	1:A:402:TYR:HB3	2.20	0.42
1:A:409:ARG:HG2	1:A:409:ARG:NH1	2.35	0.42
1:B:312:LEU:HD13	1:B:376:LEU:HG	2.01	0.42
1:B:31:LEU:HD23	1:B:31:LEU:O	2.19	0.42
1:B:81:GLU:HG2	1:B:83:ASN:H	1.84	0.42
1:B:413:LYS:HB2	1:B:414:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:THR:CG2	1:B:424:LYS:HE3	2.49	0.42
1:A:35:LYS:C	1:A:37:PRO:HD3	2.40	0.42
1:B:258:MET:HB2	4:B:524:HOH:O	2.18	0.42
1:B:312:LEU:CD1	1:B:376:LEU:HG	2.50	0.42
1:B:365:SER:O	1:B:369:PHE:HD1	2.01	0.42
1:A:407:ALA:O	1:A:411:LYS:HG3	2.19	0.41
1:A:435:ASN:O	1:A:442:PRO:HD2	2.20	0.41
1:A:88:VAL:HG13	1:A:92:THR:CB	2.44	0.41
1:A:314:THR:HG22	1:A:356:LEU:CD2	2.50	0.41
1:A:68:TYR:C	1:A:70:THR:H	2.23	0.41
1:A:191:LYS:HA	1:A:191:LYS:HD3	1.76	0.41
1:B:122:GLU:HA	1:B:123:PRO:HD3	1.86	0.41
1:A:54:LEU:HD11	1:A:68:TYR:CD2	2.55	0.41
1:A:80:CYS:O	1:A:81:GLU:C	2.59	0.41
1:B:64:ASP:CB	1:B:65:PRO:CD	2.99	0.41
1:B:106:CYS:C	1:B:108:ALA:H	2.23	0.41
1:B:185:LYS:HB2	1:B:185:LYS:HE3	1.88	0.41
1:B:348:VAL:HB	1:B:383:PHE:CE1	2.56	0.41
1:B:413:LYS:C	1:B:415:PRO:HD3	2.41	0.41
1:A:113:GLN:NE2	1:B:418:THR:HG22	2.36	0.41
1:B:20:GLY:HA3	4:B:616:HOH:O	2.21	0.41
1:B:442:PRO:HA	1:B:443:PRO:HD2	1.91	0.41
1:A:299:MET:HA	1:A:300:PRO:HD3	1.88	0.40
1:B:305:PRO:HB2	1:B:307:LEU:HG	2.02	0.40
1:A:317:ASP:CB	1:A:326:VAL:HG21	2.44	0.40
1:B:31:LEU:HD13	3:B:500:VDY:H273	2.03	0.40
1:B:386:LYS:O	1:B:390:LEU:HG	2.21	0.40
1:A:304:LEU:HA	1:A:305:PRO:HD3	1.91	0.40
1:A:456:ASN:OD1	1:A:457:ILE:N	2.55	0.40
1:B:376:LEU:H	1:B:376:LEU:CD2	2.35	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	427/458 (93%)	403 (94%)	23 (5%)	1 (0%)	44	54
1	B	443/458 (97%)	409 (92%)	24 (5%)	10 (2%)	5	4
All	All	870/916 (95%)	812 (93%)	47 (5%)	11 (1%)	10	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	THR
1	B	58	CYS
1	B	65	PRO
1	B	69	ASP
1	B	366	THR
1	B	56	GLU
1	B	82	SER
1	B	307	LEU
1	B	305	PRO
1	B	373	GLY
1	B	4	GLY

### 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	384/415 (92%)	376 (98%)	8 (2%)	48	65
1	B	389/415 (94%)	379 (97%)	10 (3%)	41	57
All	All	773/830 (93%)	755 (98%)	18 (2%)	45	62

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	TYR
1	A	98	LYS

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Mol	Chain	Res	Type
1	A	106	CYS
1	A	138	GLU
1	A	202	ARG
1	A	280	PHE
1	A	307	LEU
1	A	378	LYS
1	B	65	PRO
1	B	69	ASP
1	B	88	VAL
1	B	212	GLU
1	B	227	VAL
1	B	229	THR
1	B	231	ASP
1	B	337	ARG
1	B	416	ASP
1	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	89	HIS
1	A	244	ASN
1	A	272	ASN
1	A	285	GLN
1	A	315	ASN
1	A	427	ASN
1	B	83	ASN
1	B	89	HIS
1	B	115	GLN
1	B	125	ASN
1	B	370	ASN
1	B	388	GLN
1	B	435	ASN
1	B	440	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	OLA	A	459	-	19,19,19	0.72	1 (5%)	19,19,19	0.40	0
2	OLA	B	459	-	19,19,19	0.73	1 (5%)	19,19,19	0.40	0
3	VDY	B	500	-	31,31,31	1.24	4 (12%)	46,46,46	1.40	5 (10%)
2	OLA	B	460	-	19,19,19	0.81	1 (5%)	19,19,19	0.40	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
2	OLA	A	459	-	-	10/17/17/17	-
2	OLA	B	459	-	-	12/17/17/17	-
3	VDY	B	500	-	-	8/16/57/57	0/3/3/3
2	OLA	B	460	-	-	12/17/17/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	VDY	C13-C17	2.95	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	VDY	C10-C5	2.93	1.52	1.48
2	B	460	OLA	O2-C1	2.28	1.38	1.30
3	B	500	VDY	C20-C17	2.22	1.58	1.54
3	B	500	VDY	C18-C13	2.08	1.57	1.54
2	A	459	OLA	O2-C1	2.03	1.37	1.30
2	B	459	OLA	O2-C1	2.00	1.37	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	VDY	C14-C13-C17	-5.15	94.34	99.72
3	B	500	VDY	C21-C20-C17	3.94	118.79	112.88
3	B	500	VDY	C13-C17-C20	2.77	123.77	119.50
3	B	500	VDY	C6-C7-C8	2.47	129.78	126.13
3	B	500	VDY	C12-C13-C17	2.17	119.80	116.60

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	500	VDY	C4-C5-C6-C7
3	B	500	VDY	C16-C17-C20-C22
2	B	459	OLA	C1-C2-C3-C4
2	A	459	OLA	C1-C2-C3-C4
3	B	500	VDY	C16-C17-C20-C21
3	B	500	VDY	C13-C17-C20-C22
2	B	460	OLA	C1-C2-C3-C4
3	B	500	VDY	C22-C23-C24-C25
2	B	460	OLA	C12-C13-C14-C15
2	A	459	OLA	C3-C4-C5-C6
2	B	459	OLA	C5-C6-C7-C8
2	A	459	OLA	C2-C3-C4-C5
2	B	459	OLA	C12-C13-C14-C15
2	B	459	OLA	C6-C7-C8-C9
2	B	459	OLA	C3-C4-C5-C6
2	B	460	OLA	C6-C7-C8-C9
3	B	500	VDY	C20-C22-C23-C24
2	B	460	OLA	C5-C6-C7-C8
3	B	500	VDY	C21-C20-C22-C23
2	A	459	OLA	C12-C13-C14-C15
2	A	459	OLA	C6-C7-C8-C9
2	B	459	OLA	C4-C5-C6-C7

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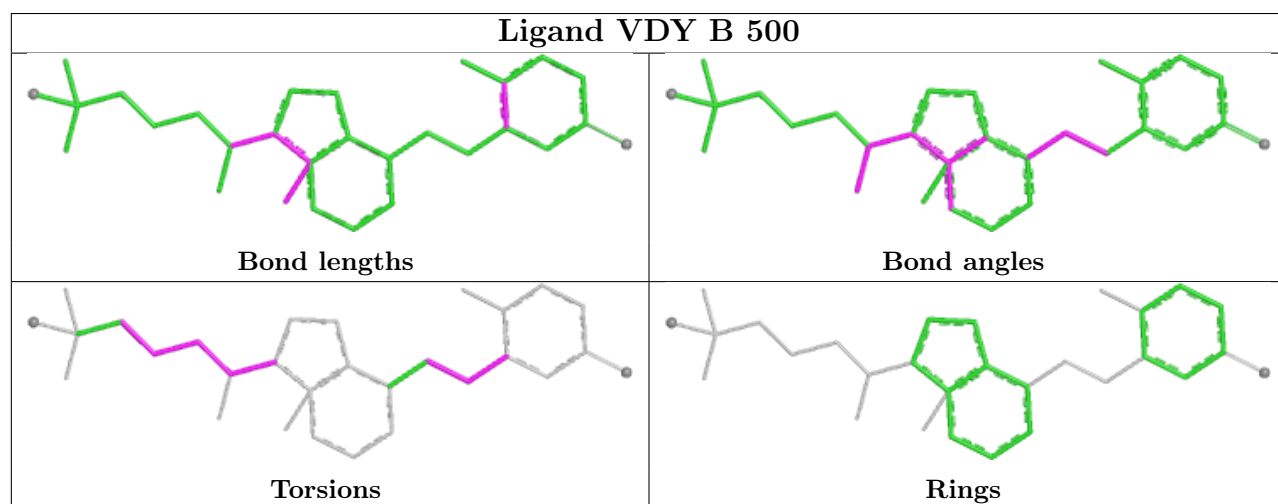
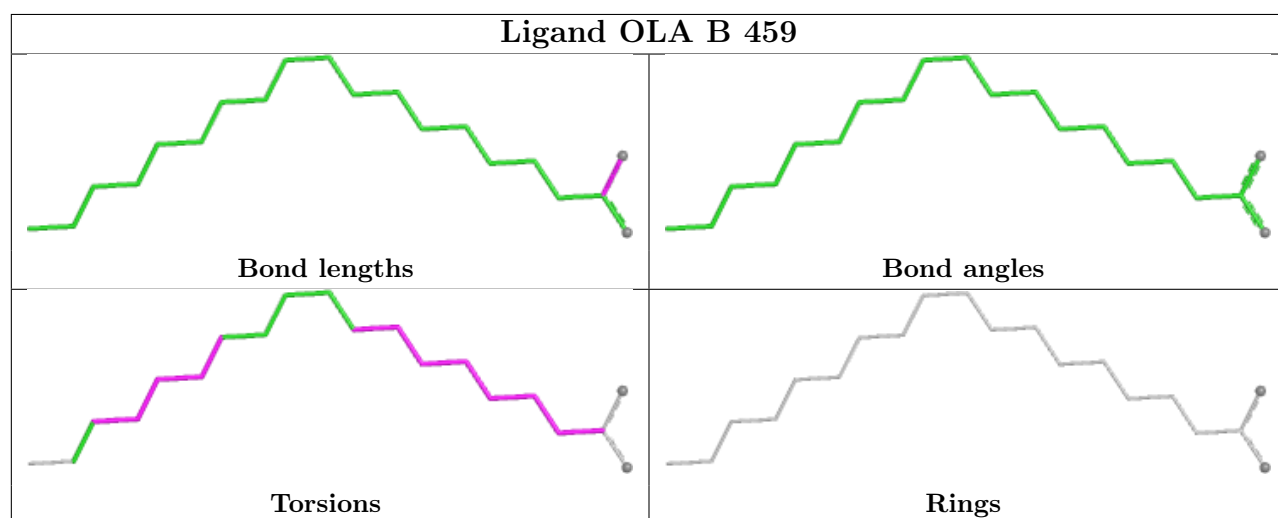
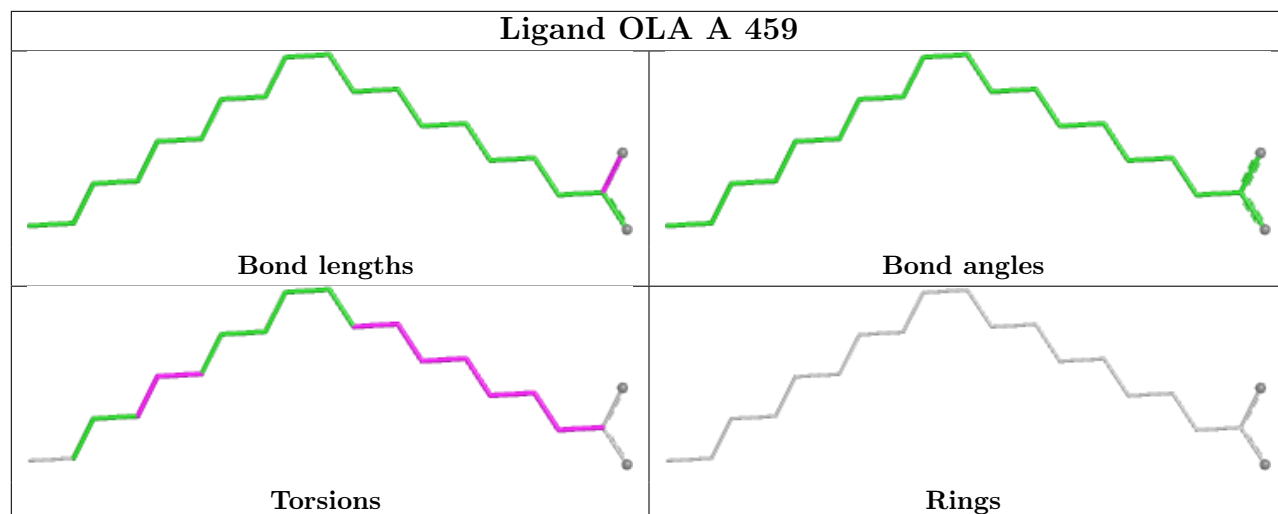
Mol	Chain	Res	Type	Atoms
2	B	460	OLA	C4-C5-C6-C7
2	A	459	OLA	C13-C14-C15-C16
2	B	460	OLA	C14-C15-C16-C17
2	B	459	OLA	C2-C3-C4-C5
2	A	459	OLA	C5-C6-C7-C8
2	B	460	OLA	C15-C16-C17-C18
2	B	459	OLA	C11-C12-C13-C14
2	B	460	OLA	C10-C11-C12-C13
2	B	460	OLA	C11-C12-C13-C14
3	B	500	VDY	C5-C6-C7-C8
2	B	459	OLA	C14-C15-C16-C17
2	B	459	OLA	C13-C14-C15-C16
2	B	459	OLA	O1-C1-C2-C3
2	A	459	OLA	O1-C1-C2-C3
2	B	459	OLA	O2-C1-C2-C3
2	A	459	OLA	C4-C5-C6-C7
2	A	459	OLA	O2-C1-C2-C3
2	B	460	OLA	O2-C1-C2-C3
2	B	460	OLA	O1-C1-C2-C3
2	B	460	OLA	C9-C10-C11-C12

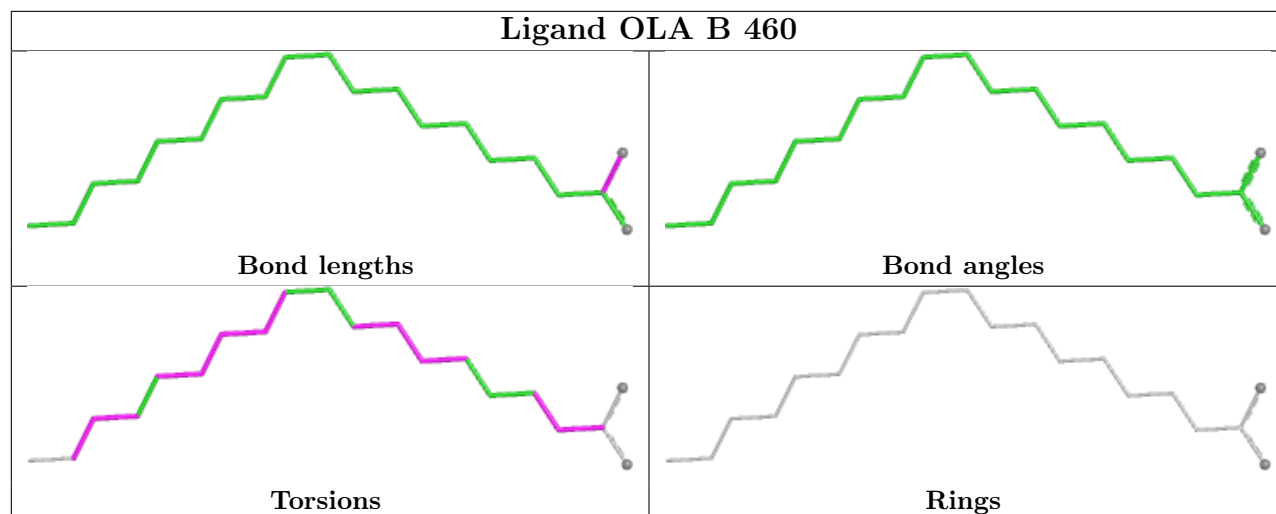
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	459	OLA	1	0
3	B	500	VDY	3	0
2	B	460	OLA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	433/458 (94%)	0.29	37 (8%) 18 20	30, 51, 122, 154	0
1	B	447/458 (97%)	0.44	38 (8%) 18 20	30, 54, 118, 150	0
All	All	880/916 (96%)	0.37	75 (8%) 18 20	30, 52, 121, 154	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	63	ALA	8.6
1	A	105	LEU	5.6
1	A	457	ILE	5.5
1	B	306	GLU	5.0
1	B	57	ALA	4.8
1	B	62	GLY	4.6
1	B	65	PRO	4.2
1	A	97	THR	4.2
1	B	10	ASN	4.1
1	B	367	THR	4.1
1	B	361	ASP	3.9
1	A	96	CYS	3.6
1	B	366	THR	3.4
1	B	105	LEU	3.4
1	B	64	ASP	3.4
1	B	305	PRO	3.3
1	A	108	ALA	3.2
1	A	76	SER	3.2
1	B	322	GLY	3.2
1	A	95	CYS	3.1
1	B	7	TYR	3.1
1	A	71	ARG	3.0
1	B	362	VAL	3.0
1	A	59	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	94	GLU	2.9
1	A	98	LYS	2.9
1	B	298	PHE	2.9
1	A	24	PHE	2.8
1	A	427	ASN	2.8
1	B	307	LEU	2.8
1	B	363	GLU	2.7
1	B	66	ASP	2.6
1	A	88	VAL	2.6
1	A	80	CYS	2.6
1	A	104	LYS	2.5
1	B	8	GLU	2.5
1	A	416	ASP	2.5
1	A	103	ARG	2.5
1	B	3	ARG	2.5
1	B	85	PRO	2.5
1	B	321	PRO	2.5
1	A	251	GLU	2.5
1	B	74	ALA	2.5
1	B	313	PRO	2.5
1	A	254	SER	2.4
1	B	188	LEU	2.4
1	A	306	GLU	2.4
1	B	93	ALA	2.4
1	A	68	TYR	2.4
1	B	318	VAL	2.4
1	B	364	ASP	2.4
1	A	86	PHE	2.3
1	A	109	ALA	2.3
1	B	11	LYS	2.3
1	A	321	PRO	2.3
1	B	67	CYS	2.3
1	B	314	THR	2.3
1	A	298	PHE	2.3
1	B	376	LEU	2.2
1	A	106	CYS	2.2
1	A	20	GLY	2.2
1	B	97	THR	2.2
1	A	113	GLN	2.2
1	A	77	ALA	2.2
1	A	85	PRO	2.2
1	A	363	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	13	CYS	2.1
1	A	93	ALA	2.1
1	B	371	ALA	2.1
1	A	228	PRO	2.1
1	B	107	MET	2.1
1	B	456	ASN	2.1
1	A	70	THR	2.0
1	A	79	SER	2.0
1	A	370	ASN	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

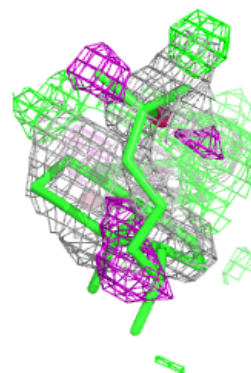
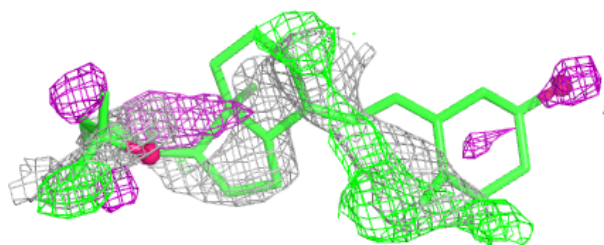
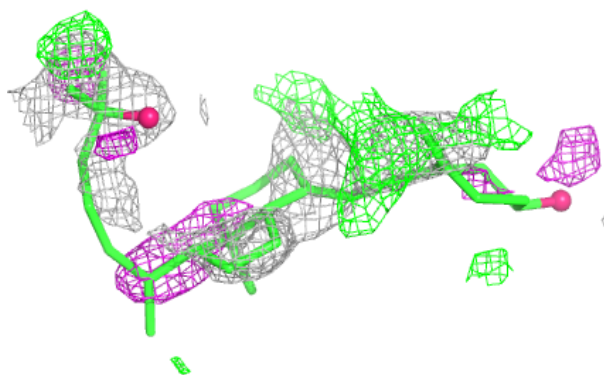
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	VDY	B	500	29/29	0.67	0.37	109,137,147,151	0
2	OLA	B	460	20/20	0.83	0.17	49,66,98,98	0
2	OLA	A	459	20/20	0.84	0.15	45,66,127,129	0
2	OLA	B	459	20/20	0.84	0.17	65,85,133,133	0

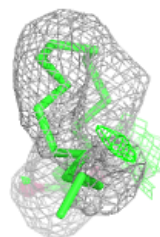
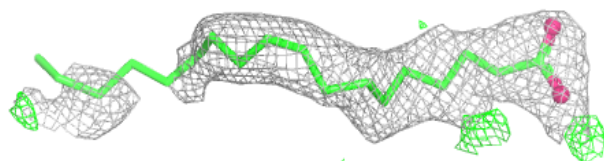
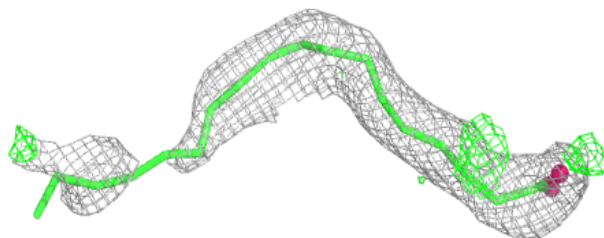
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around VDY B 500:**

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

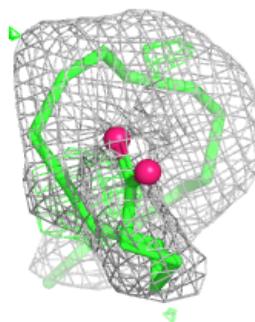
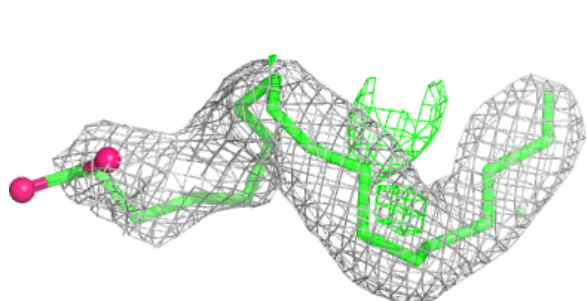
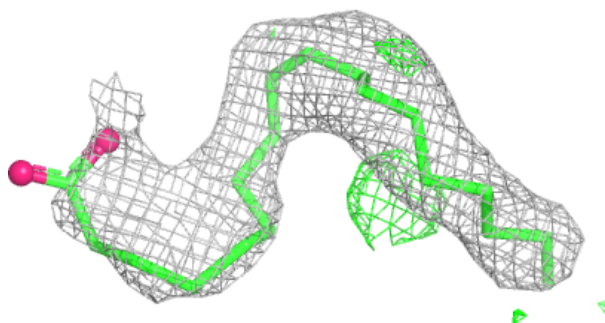
**Electron density around OLA B 460:**

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

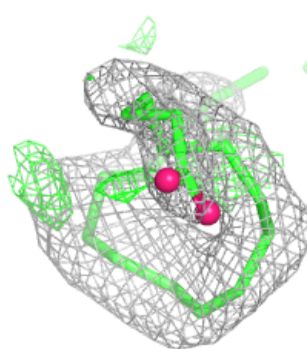
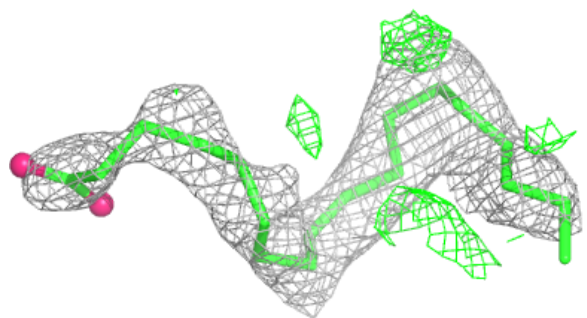
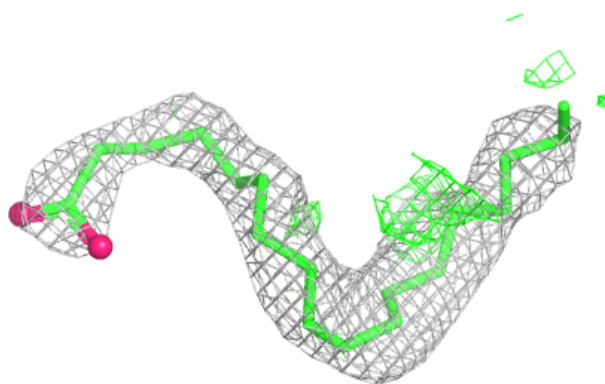


**Electron density around OLA A 459:**

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

**Electron density around OLA B 459:**

$2mF_o-DF_c$  (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.