



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 07:55 pm GMT

PDB ID : 8QJR
Title : BRG1 bromodomain in complex with VBC via compound 17
Authors : Kerry, P.S.; Hole, A.J.; Perez-Dorado, J.I.
Deposited on : 2023-09-13
Resolution : 3.17 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

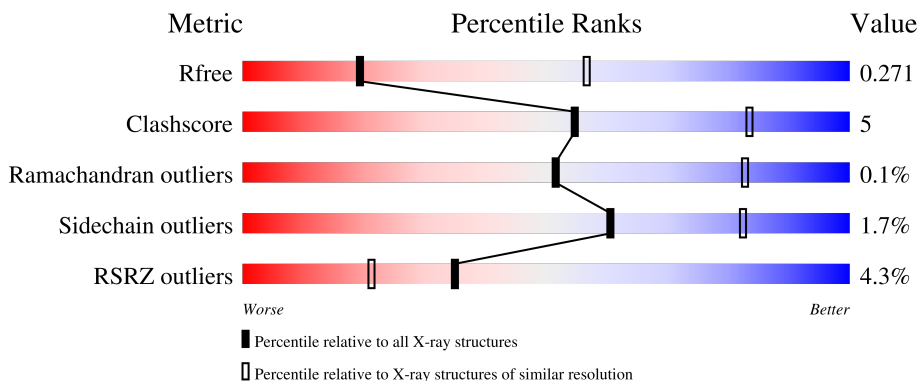
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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	104	 3% (red), 84% (green), 15% (yellow), 0% (orange), 0% (grey)
1	D	104	 5% (red), 83% (green), 16% (yellow), 0% (orange), 0% (grey)
2	B	97	 4% (red), 68% (green), 22% (yellow), 10% (grey)
2	E	97	 6% (red), 70% (green), 20% (yellow), 10% (grey)
3	C	162	 0% (red), 81% (green), 13% (yellow), 6% (grey)

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Mol	Chain	Length	Quality of chain
3	F	162	<p>%</p> <p>82% 12% 5%</p>
4	G	121	<p>83% 7% 9%</p>
4	H	121	<p>15% 74% 9% 17%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	F	301	-	-	X	-
5	PO4	F	302	-	-	X	-
5	PO4	G	1601	-	-	X	-
6	GOL	C	304	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7553 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	103	813	514	136	158	5	0	0	0
1	D	103	813	514	136	158	5	0	0	0

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	87	695	448	111	129	7	0	0	0
2	E	87	696	449	111	129	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	initiating methionine	UNP Q15369
E	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	153	1262	798	235	226	3	0	1	0
3	F	154	1263	798	236	226	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	GLY	-	expression tag	UNP P40337
C	53	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337

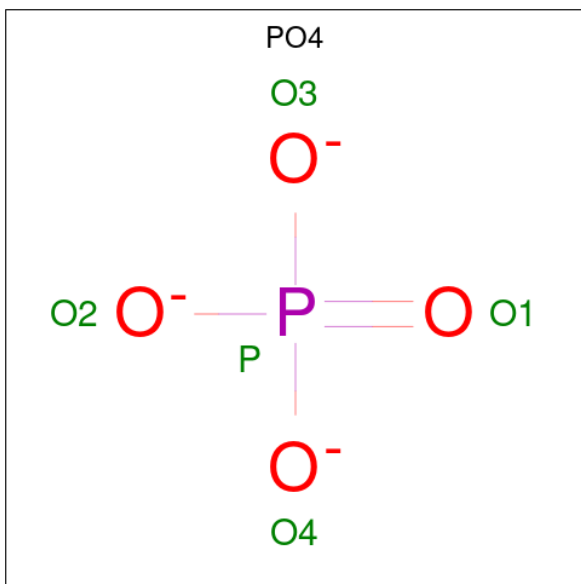
- Molecule 4 is a protein called Transcription activator BRG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	110	Total	C	N	O	S	0	0	0
			915	584	159	169	3			
4	H	101	Total	C	N	O	S	0	0	0
			843	540	144	156	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1449	SER	-	expression tag	UNP P51532
G	1450	MET	-	expression tag	UNP P51532
H	1449	SER	-	expression tag	UNP P51532
H	1450	MET	-	expression tag	UNP P51532

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



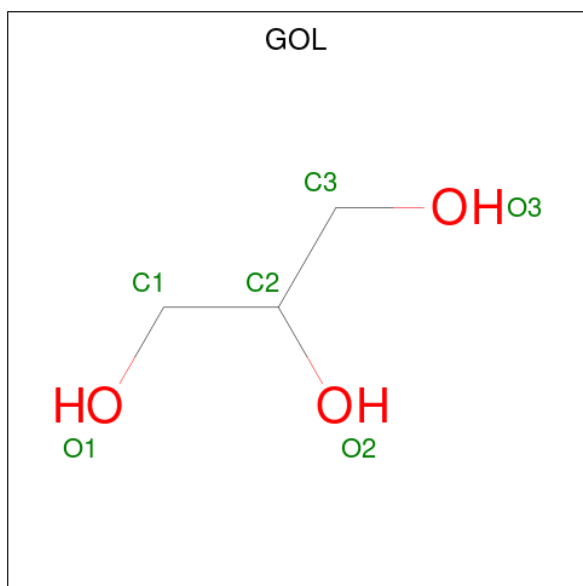
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

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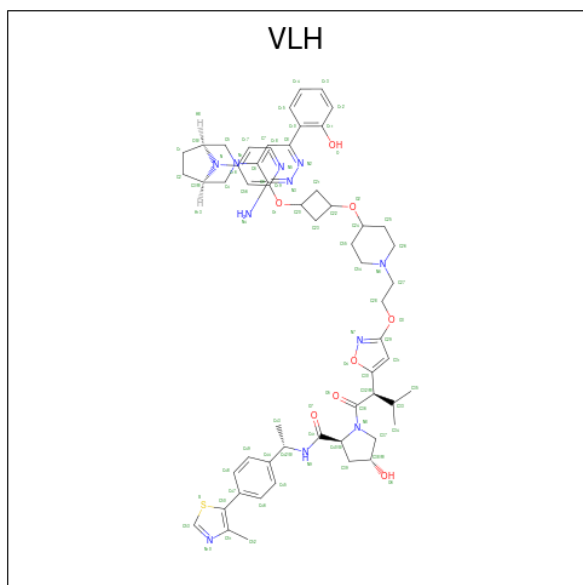
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	F	1	Total	O	P	0	0
			5	4	1		
5	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is (2S,4R)-1-[(2R)-2-[3-[2-[4-[3-[4-[(1R,5S)-3-[3-azanyl-6-(2-hydroxyphenyl)pyridazin-4-yl]-3,8-diazabicyclo[3.2.1]octan-8-yl]pyridin-2-yl]oxycyclobutyl]oxypiperidin-1-yl]ethoxy]-1,2-oxazol-5-yl]-3-methyl-butanoyl]-N-[(1S)-1-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]ethyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: VLH) (formula: C₅₇H₆₉N₁₁O₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	S	0	0
			77	57	11	8	1		
7	F	1	Total	C	N	O	S	0	0
			77	57	11	8	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	7	Total	O	0	0
			7	7		
9	B	8	Total	O	0	0
			8	8		
9	C	13	Total	O	0	0
			13	13		
9	D	2	Total	O	0	0
			2	2		
9	E	8	Total	O	0	0
			8	8		
9	F	9	Total	O	0	0
			9	9		

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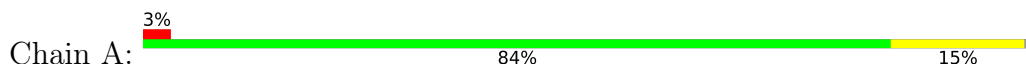
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	G	7	Total O 7 7	0	0
9	H	3	Total O 3 3	0	0

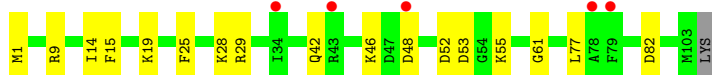
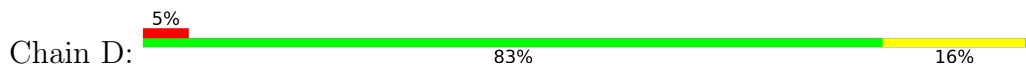
3 Residue-property plots [i](#)

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.

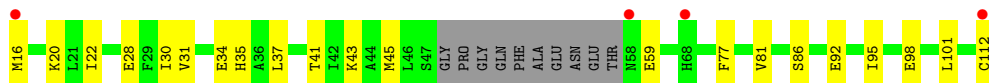
- Molecule 1: Elongin-B



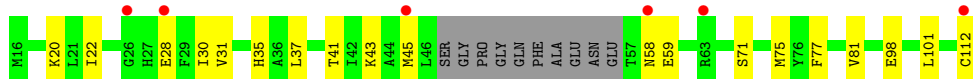
- Molecule 1: Elongin-B



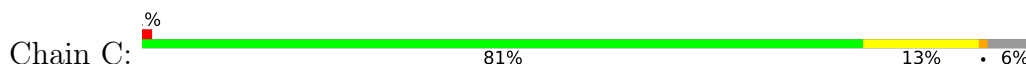
- Molecule 2: Elongin-C




- Molecule 2: Elongin-C



- Molecule 3: von Hippel-Lindau disease tumor suppressor




- Molecule 3: von Hippel-Lindau disease tumor suppressor

Chain F:  82% 12% 5%




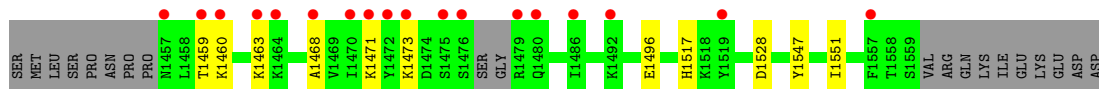
• Molecule 4: Transcription activator BRG1

Chain G:  83% 7% 9%



• Molecule 4: Transcription activator BRG1

Chain H:  15% 74% 9% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.68Å 88.04Å 84.98Å 90.00° 105.89° 90.00°	Depositor
Resolution (Å)	80.64 – 3.17 80.64 – 3.17	Depositor EDS
% Data completeness (in resolution range)	98.8 (80.64-3.17) 98.8 (80.64-3.17)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.19Å)	Xtrriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.262 , 0.278 0.249 , 0.271	Depositor DCC
R_{free} test set	1020 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	62.7	Xtrriage
Anisotropy	0.141	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7553	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, VLH, CL

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	0.25	0/829	0.47	0/1121
1	D	0.24	0/829	0.47	0/1121
2	B	0.23	0/709	0.45	0/955
2	E	0.23	0/710	0.45	0/957
3	C	0.26	0/1295	0.48	0/1765
3	F	0.26	0/1295	0.47	0/1764
4	G	0.23	0/927	0.44	0/1239
4	H	0.22	0/854	0.42	0/1142
All	All	0.24	0/7448	0.46	0/10064

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	813	0	811	9	0
1	D	813	0	811	13	0
2	B	695	0	697	14	0
2	E	696	0	699	11	0
3	C	1262	0	1256	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1263	0	1261	15	0
4	G	915	0	963	6	1
4	H	843	0	881	6	1
5	B	5	0	0	1	0
5	C	15	0	0	2	0
5	F	10	0	0	4	0
5	G	5	0	0	2	0
6	C	6	0	8	0	0
7	C	77	0	0	1	0
7	F	77	0	0	2	0
8	E	1	0	0	0	0
9	A	7	0	0	0	0
9	B	8	0	0	0	0
9	C	13	0	0	0	0
9	D	2	0	0	0	0
9	E	8	0	0	0	0
9	F	9	0	0	0	0
9	G	7	0	0	0	0
9	H	3	0	0	0	0
All	All	7553	0	7387	78	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (78) 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)
4:G:1457:ASN:HB3	5:G:1601:PO4:O2	1.89	0.72
2:B:86:SER:HA	5:B:201:PO4:O4	1.93	0.68
2:B:20:LYS:HB3	2:B:59:GLU:HG2	1.78	0.65
3:C:194:VAL:N	5:C:301:PO4:O3	2.30	0.65
2:E:20:LYS:HB3	2:E:59:GLU:HG2	1.78	0.64
4:H:1459:THR:HG21	4:H:1517:HIS:CE1	2.33	0.64
1:A:14:ILE:HG12	2:B:30:ILE:HB	1.81	0.62
4:H:1459:THR:HG21	4:H:1517:HIS:NE2	2.16	0.61
1:D:25:PHE:HB2	1:D:53:ASP:HB3	1.83	0.60
1:D:25:PHE:HE2	1:D:29:ARG:NH2	1.98	0.60
1:D:9:ARG:HB2	1:D:77:LEU:HB3	1.85	0.59
1:A:25:PHE:HB2	1:A:53:ASP:HB3	1.86	0.57
1:A:9:ARG:HB2	1:A:77:LEU:HB3	1.85	0.57
1:D:25:PHE:HE2	1:D:29:ARG:HH21	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:THR:O	2:B:45:MET:HG3	2.05	0.56
2:E:41:THR:O	2:E:45:MET:HG3	2.05	0.56
3:F:98:TYR:HB3	7:F:303:VLH:S	2.47	0.55
4:H:1468:ALA:HA	4:H:1471:LYS:HE2	1.89	0.54
4:H:1468:ALA:HA	4:H:1471:LYS:HG2	1.89	0.54
3:C:87:VAL:HB	3:C:118:LEU:HG	1.90	0.54
3:F:105:THR:HB	5:F:301:PO4:P	2.48	0.54
2:B:22:ILE:HG12	2:B:28:GLU:HG2	1.90	0.54
3:F:87:VAL:HB	3:F:118:LEU:HG	1.90	0.53
2:E:22:ILE:HG12	2:E:28:GLU:HG2	1.90	0.53
3:F:193:ASN:HA	5:F:302:PO4:O1	2.09	0.53
3:F:105:THR:HB	5:F:301:PO4:O3	2.09	0.51
2:B:101:LEU:HD11	3:C:178:LEU:HD22	1.93	0.51
3:F:64:ARG:HD2	3:F:91:PHE:O	2.11	0.51
2:E:37:LEU:HD22	2:E:43:LYS:HG3	1.92	0.50
2:B:37:LEU:HD22	2:B:43:LYS:HG3	1.93	0.50
4:G:1468:ALA:HA	4:G:1471:LYS:HG2	1.93	0.50
3:C:105:THR:HB	5:C:303:PO4:O3	2.12	0.50
4:G:1460:LYS:HA	4:G:1463:LYS:HD2	1.94	0.49
3:F:181:VAL:HG12	3:F:183:SER:H	1.78	0.48
4:H:1547:TYR:CE1	4:H:1551:ILE:HD11	2.48	0.48
4:H:1460:LYS:HA	4:H:1463:LYS:HD2	1.95	0.48
3:C:181:VAL:HG12	3:C:183:SER:H	1.79	0.48
4:G:1468:ALA:HA	4:G:1471:LYS:HE2	1.96	0.48
1:D:52:ASP:HB3	1:D:55:LYS:HG3	1.96	0.48
4:G:1547:TYR:CE1	4:G:1551:ILE:HD11	2.49	0.47
3:F:193:ASN:HB3	3:F:196:LYS:HB2	1.96	0.47
3:C:193:ASN:HB3	3:C:196:LYS:HB2	1.95	0.47
1:A:34:ILE:HG21	2:B:30:ILE:HG21	1.96	0.47
1:D:14:ILE:HG12	2:E:30:ILE:HB	1.97	0.47
2:E:98:GLU:H	2:E:98:GLU:CD	2.18	0.46
2:B:98:GLU:H	2:B:98:GLU:CD	2.18	0.46
1:D:46:LYS:NZ	1:D:61:GLY:HA3	2.31	0.46
4:G:1457:ASN:HB3	5:G:1601:PO4:P	2.55	0.46
1:D:1:MET:HG2	1:D:19:LYS:HD2	1.98	0.46
1:D:25:PHE:HE2	1:D:29:ARG:CZ	2.29	0.46
2:B:92:GLU:HB2	3:C:81:PRO:HG3	1.96	0.46
1:D:25:PHE:CE2	1:D:29:ARG:NE	2.83	0.46
1:A:1:MET:HG2	1:A:19:LYS:HD2	1.97	0.46
1:A:52:ASP:HB3	1:A:55:LYS:HG3	1.96	0.46
1:A:46:LYS:NZ	1:A:61:GLY:HA3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PHE:HB2	2:B:31:VAL:HG12	1.98	0.45
2:B:95:ILE:HB	3:C:165:VAL:HG21	1.99	0.45
3:C:107:ARG:NH1	7:C:305:VLH:N10	2.62	0.44
3:F:102:PRO:HD2	3:F:105:THR:OG1	2.18	0.44
3:C:102:PRO:HD2	3:C:105:THR:OG1	2.18	0.44
2:B:35:HIS:CD2	2:B:81:VAL:HG21	2.53	0.44
1:D:28:LYS:HE2	1:D:42:GLN:O	2.18	0.43
2:E:101:LEU:HD11	3:F:178:LEU:HD22	1.98	0.43
1:D:15:PHE:HB2	2:E:31:VAL:HG12	2.00	0.43
1:D:25:PHE:HE2	1:D:29:ARG:NE	2.17	0.43
3:F:74:VAL:HG12	3:F:75:ILE:N	2.34	0.43
1:A:28:LYS:HE2	1:A:42:GLN:O	2.18	0.43
2:E:35:HIS:CD2	2:E:81:VAL:HG21	2.54	0.43
3:F:99:PRO:HD2	7:F:303:VLH:S	2.59	0.42
2:B:77:PHE:HE1	2:B:112:CYS:SG	2.43	0.41
3:C:83:VAL:HG22	3:C:103:PRO:HD3	2.03	0.41
3:C:74:VAL:HG12	3:C:75:ILE:N	2.35	0.41
3:C:120:ARG:HD3	3:C:127:GLY:HA2	2.03	0.41
3:F:120:ARG:HD3	3:F:127:GLY:HA2	2.02	0.41
2:E:71:SER:O	2:E:75:MET:HG3	2.21	0.41
2:E:77:PHE:HE1	2:E:112:CYS:SG	2.44	0.40
3:F:194:VAL:N	5:F:302:PO4:O1	2.40	0.40
3:C:160:GLU:OE1	3:F:210:ARG:HG2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1483:GLU:CA	4:H:1473:LYS:NZ[1_545]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
1	D	101/104 (97%)	96 (95%)	4 (4%)	1 (1%)	15	52
2	B	83/97 (86%)	82 (99%)	1 (1%)	0	100	100
2	E	83/97 (86%)	82 (99%)	1 (1%)	0	100	100
3	C	152/162 (94%)	142 (93%)	10 (7%)	0	100	100
3	F	152/162 (94%)	142 (93%)	10 (7%)	0	100	100
4	G	108/121 (89%)	107 (99%)	1 (1%)	0	100	100
4	H	97/121 (80%)	97 (100%)	0	0	100	100
All	All	877/968 (91%)	845 (96%)	31 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	82	ASP

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	91/92 (99%)	90 (99%)	1 (1%)	73	88
1	D	91/92 (99%)	90 (99%)	1 (1%)	73	88
2	B	79/86 (92%)	77 (98%)	2 (2%)	47	76
2	E	79/86 (92%)	78 (99%)	1 (1%)	69	86
3	C	143/148 (97%)	140 (98%)	3 (2%)	53	79
3	F	143/148 (97%)	140 (98%)	3 (2%)	53	79
4	G	106/117 (91%)	105 (99%)	1 (1%)	78	91
4	H	98/117 (84%)	96 (98%)	2 (2%)	55	79
All	All	830/886 (94%)	816 (98%)	14 (2%)	60	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
2	B	16	MET
2	B	34	GLU
3	C	118	LEU
3	C	148	PHE
3	C	195	GLN
1	D	48	ASP
2	E	58	ASN
3	F	118	LEU
3	F	148	PHE
3	F	209	GLN
4	G	1528	ASP
4	H	1496	GLU
4	H	1528	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	191	HIS
4	G	1516	ASN
4	G	1537	GLN
4	H	1516	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is 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
5	PO4	C	302	-	4,4,4	0.21	0	6,6,6	0.27	0
5	PO4	G	1601	-	4,4,4	0.16	0	6,6,6	0.24	0
7	VLH	F	303	-	77,87,87	1.08	7 (9%)	83,126,126	1.32	10 (12%)
5	PO4	B	201	-	4,4,4	0.17	0	6,6,6	0.25	0
5	PO4	F	302	-	4,4,4	0.17	0	6,6,6	0.26	0
7	VLH	C	305	-	77,87,87	1.10	7 (9%)	83,126,126	1.33	9 (10%)
6	GOL	C	304	-	5,5,5	0.04	0	5,5,5	0.23	0
5	PO4	C	303	-	4,4,4	0.22	0	6,6,6	0.22	0
5	PO4	F	301	-	4,4,4	0.25	0	6,6,6	0.22	0
5	PO4	C	301	-	4,4,4	0.21	0	6,6,6	0.24	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
6	GOL	C	304	-	-	0/4/4/4	-
7	VLH	F	303	-	-	12/50/109/109	0/11/11/11
7	VLH	C	305	-	-	8/50/109/109	0/11/11/11

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	305	VLH	C31-C30	-3.95	1.34	1.39
7	F	303	VLH	C31-C30	-3.80	1.34	1.39
7	C	305	VLH	C3-N	3.74	1.51	1.47
7	F	303	VLH	C3-N	3.64	1.51	1.47
7	C	305	VLH	C6-N1	3.61	1.49	1.41
7	C	305	VLH	C16-N	3.60	1.48	1.40
7	F	303	VLH	C6-N1	3.56	1.49	1.41
7	F	303	VLH	C16-N	3.54	1.48	1.40
7	F	303	VLH	C-N	3.48	1.50	1.47
7	C	305	VLH	C-N	3.37	1.50	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	305	VLH	C5-N1	3.05	1.52	1.46
7	F	303	VLH	C5-N1	2.93	1.52	1.46
7	C	305	VLH	C4-N1	2.93	1.52	1.46
7	F	303	VLH	C4-N1	2.90	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	303	VLH	C16-N-C	-5.61	115.00	121.18
7	F	303	VLH	C-C5-N1	4.85	115.89	109.57
7	C	305	VLH	C-C5-N1	4.81	115.84	109.57
7	F	303	VLH	C3-C4-N1	4.77	115.78	109.57
7	C	305	VLH	C16-N-C3	4.70	126.36	121.18
7	C	305	VLH	C3-C4-N1	4.58	115.54	109.57
7	C	305	VLH	C16-N-C	-4.42	116.30	121.18
7	C	305	VLH	C7-C6-N1	-3.39	117.50	122.52
7	F	303	VLH	C7-C6-N1	-3.13	117.89	122.52
7	F	303	VLH	C16-N-C3	2.87	124.34	121.18
7	F	303	VLH	C1-C-C5	2.80	114.19	111.63
7	C	305	VLH	C1-C-C5	2.69	114.09	111.63
7	F	303	VLH	C30-C32-C33	-2.28	108.24	114.51
7	F	303	VLH	C2-C3-C4	2.24	113.68	111.63
7	C	305	VLH	C2-C3-C4	2.17	113.61	111.63
7	C	305	VLH	C2-C3-N	-2.15	100.68	102.11
7	F	303	VLH	C2-C3-N	-2.10	100.71	102.11
7	C	305	VLH	C7-C6-C9	-2.08	115.35	118.94
7	F	303	VLH	C7-C6-C9	-2.03	115.43	118.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	305	VLH	N5-C19-O1-C20
7	C	305	VLH	C56-C19-O1-C20
7	F	303	VLH	N5-C19-O1-C20
7	F	303	VLH	C56-C19-O1-C20
7	C	305	VLH	C7-C6-N1-C4
7	F	303	VLH	C7-C6-N1-C4
7	F	303	VLH	C7-C6-N1-C5
7	F	303	VLH	C9-C6-N1-C5
7	C	305	VLH	C9-C6-N1-C5
7	C	305	VLH	C7-C6-N1-C5

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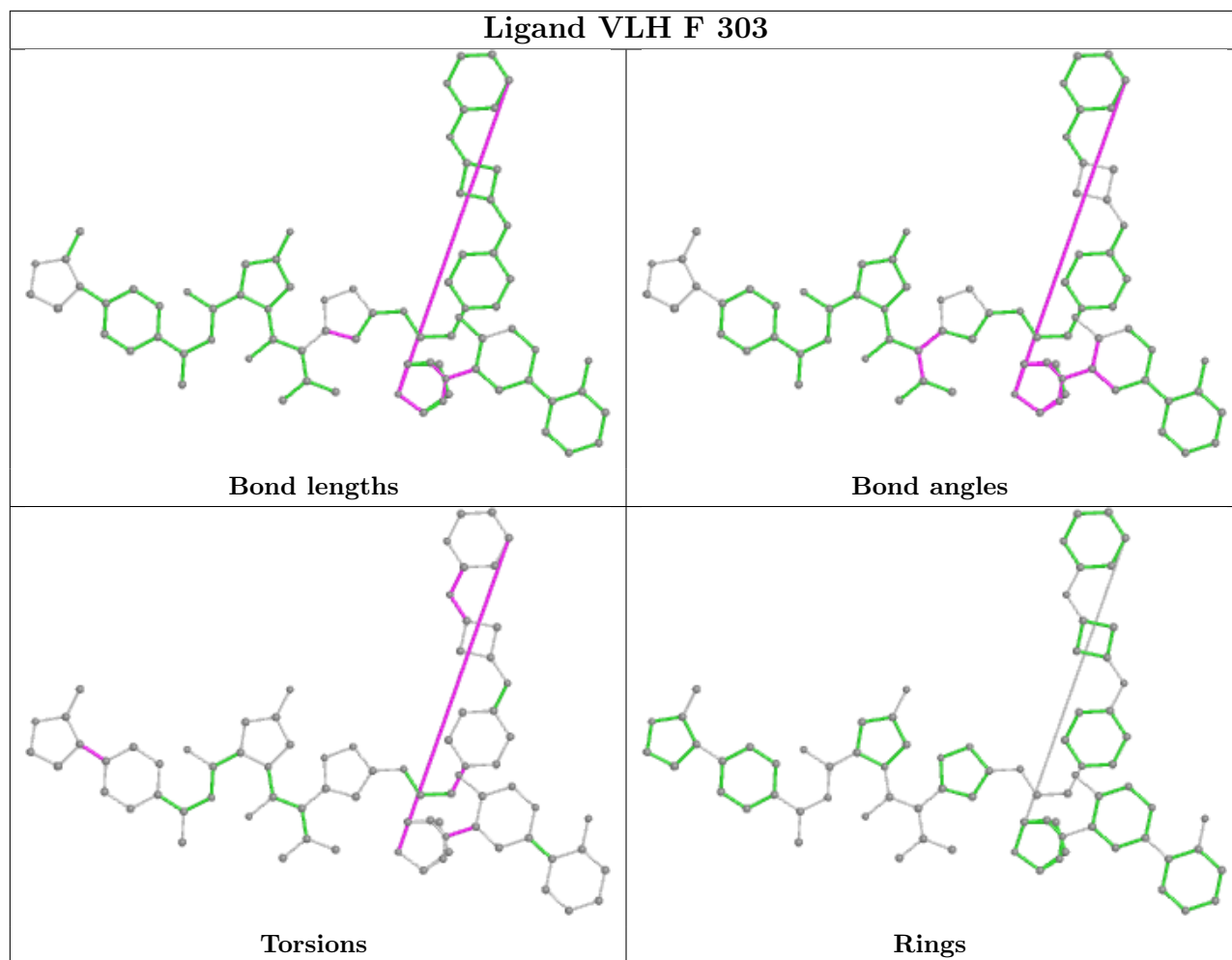
Mol	Chain	Res	Type	Atoms
7	F	303	VLH	C23-C20-O1-C19
7	F	303	VLH	C48-C47-C50-S
7	F	303	VLH	C46-C47-C50-S
7	C	305	VLH	C17-C16-N-C
7	F	303	VLH	C17-C16-N-C
7	C	305	VLH	C9-C6-N1-C4
7	F	303	VLH	C9-C6-N1-C4
7	C	305	VLH	C56-C16-N-C
7	F	303	VLH	C28-C27-N6-C26
7	F	303	VLH	C28-C27-N6-C54

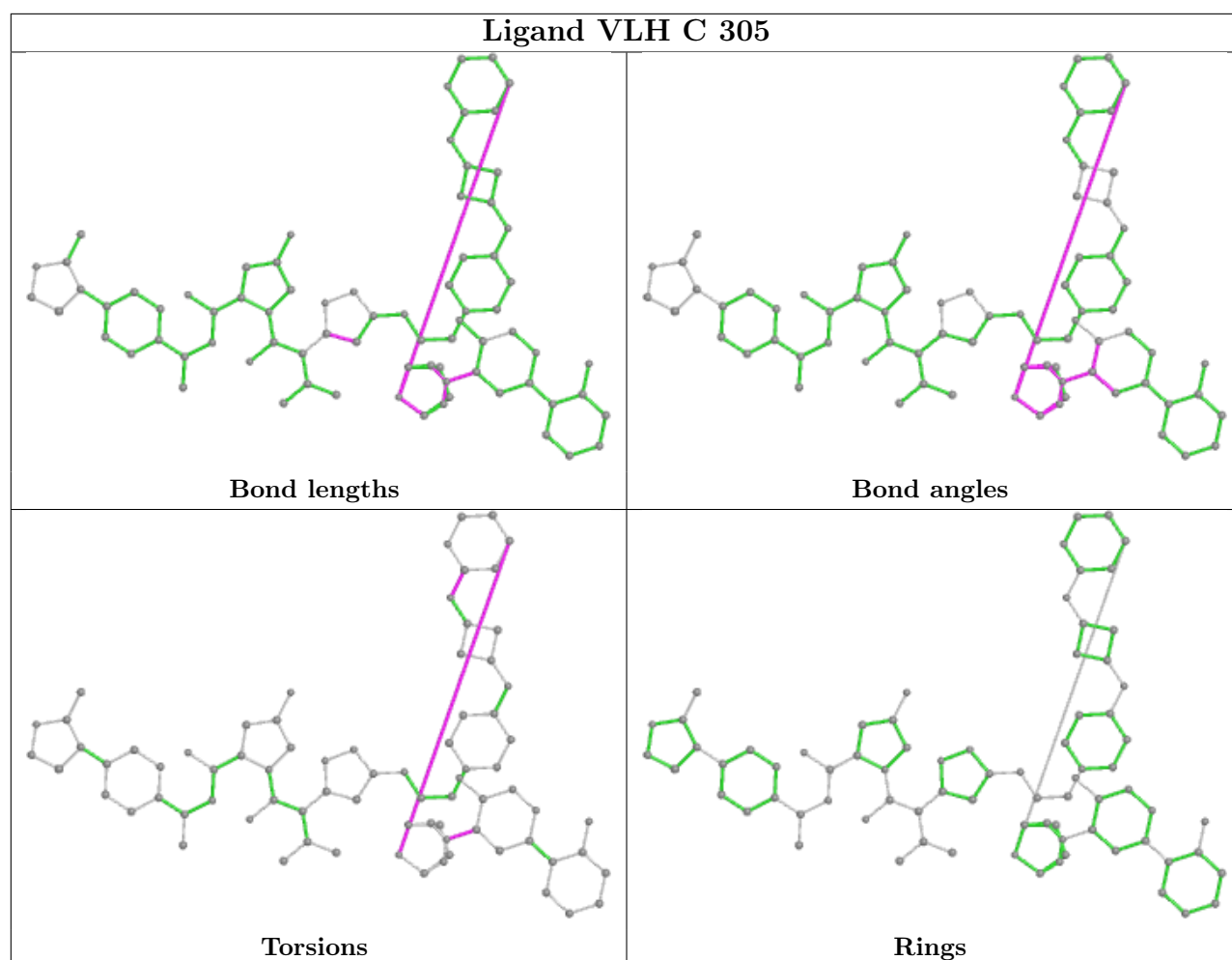
There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1601	PO4	2	0
7	F	303	VLH	2	0
5	B	201	PO4	1	0
5	F	302	PO4	2	0
7	C	305	VLH	1	0
5	C	303	PO4	1	0
5	F	301	PO4	2	0
5	C	301	PO4	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, 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	103/104 (99%)	0.52	3 (2%) 51 35	47, 64, 84, 90	0
1	D	103/104 (99%)	0.75	5 (4%) 29 16	58, 71, 98, 102	0
2	B	87/97 (89%)	0.45	4 (4%) 32 19	45, 61, 73, 77	0
2	E	87/97 (89%)	0.73	6 (6%) 16 9	50, 71, 83, 88	0
3	C	153/162 (94%)	0.22	2 (1%) 77 65	41, 55, 69, 75	0
3	F	154/162 (95%)	0.32	1 (0%) 89 83	44, 56, 82, 88	0
4	G	110/121 (90%)	0.33	0 100 100	55, 72, 79, 82	0
4	H	101/121 (83%)	0.95	18 (17%) 1 1	54, 80, 155, 164	0
All	All	898/968 (92%)	0.50	39 (4%) 35 21	41, 65, 94, 164	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	1480	GLN	4.8
2	E	26	GLY	4.4
2	E	112	CYS	4.1
4	H	1486	ILE	3.7
4	H	1471	LYS	3.7
4	H	1459	THR	3.2
2	B	68	HIS	3.1
4	H	1470	ILE	3.0
4	H	1492	LYS	3.0
1	A	101	ASP	2.9
3	F	213	ASP	2.8
4	H	1476	SER	2.8
1	D	78	ALA	2.8
4	H	1457	ASN	2.7
4	H	1472	TYR	2.7
2	B	112	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
4	H	1468	ALA	2.6
1	D	43	ARG	2.5
3	C	213	ASP	2.4
2	E	45	MET	2.4
4	H	1460	LYS	2.4
2	E	58	ASN	2.4
2	E	28	GLU	2.4
1	D	34	ILE	2.4
4	H	1475	SER	2.4
2	B	16	MET	2.4
2	B	58	ASN	2.4
1	D	48	ASP	2.3
4	H	1519	TYR	2.2
1	A	91	GLU	2.2
3	C	208	HIS	2.2
4	H	1479	ARG	2.2
4	H	1557	PHE	2.1
1	D	79	PHE	2.1
2	E	63	ARG	2.1
4	H	1463	LYS	2.1
4	H	1464	LYS	2.0
4	H	1473	LYS	2.0
1	A	66	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

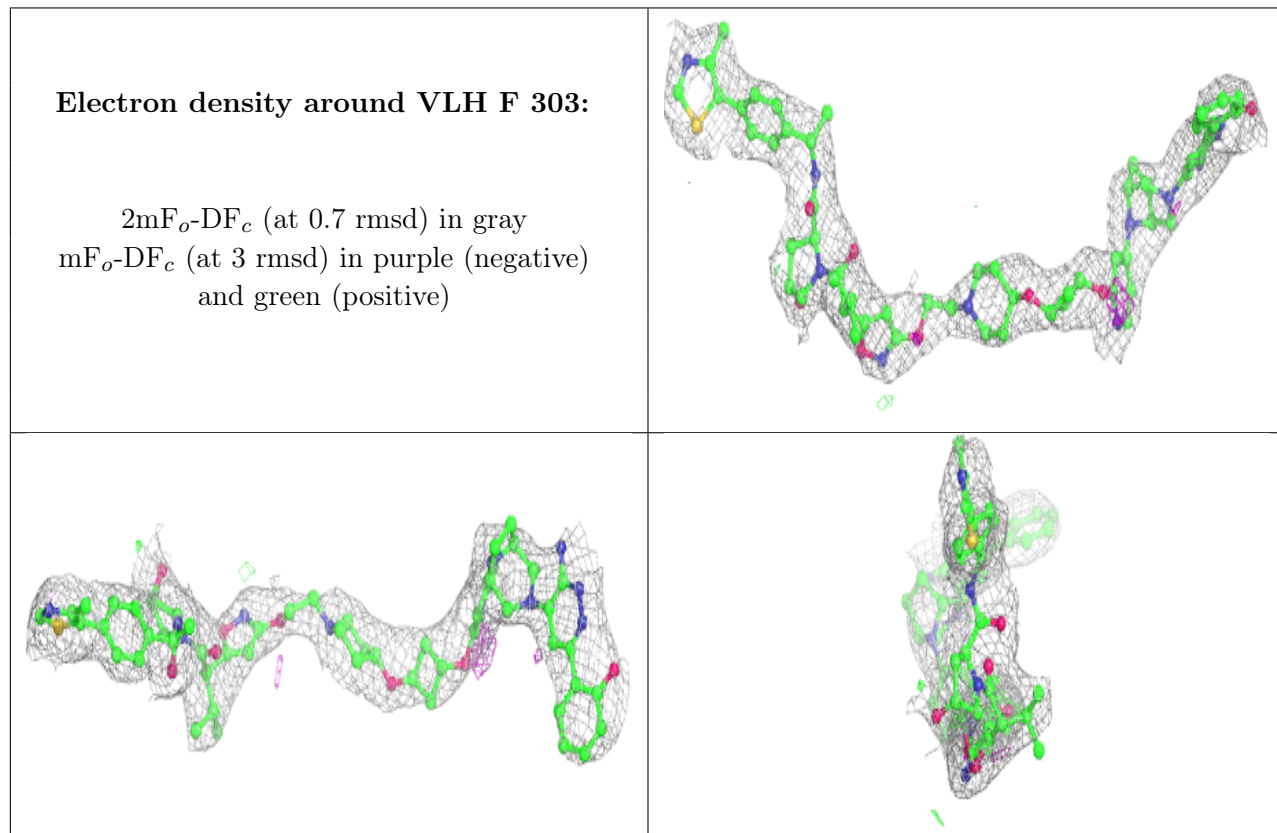
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

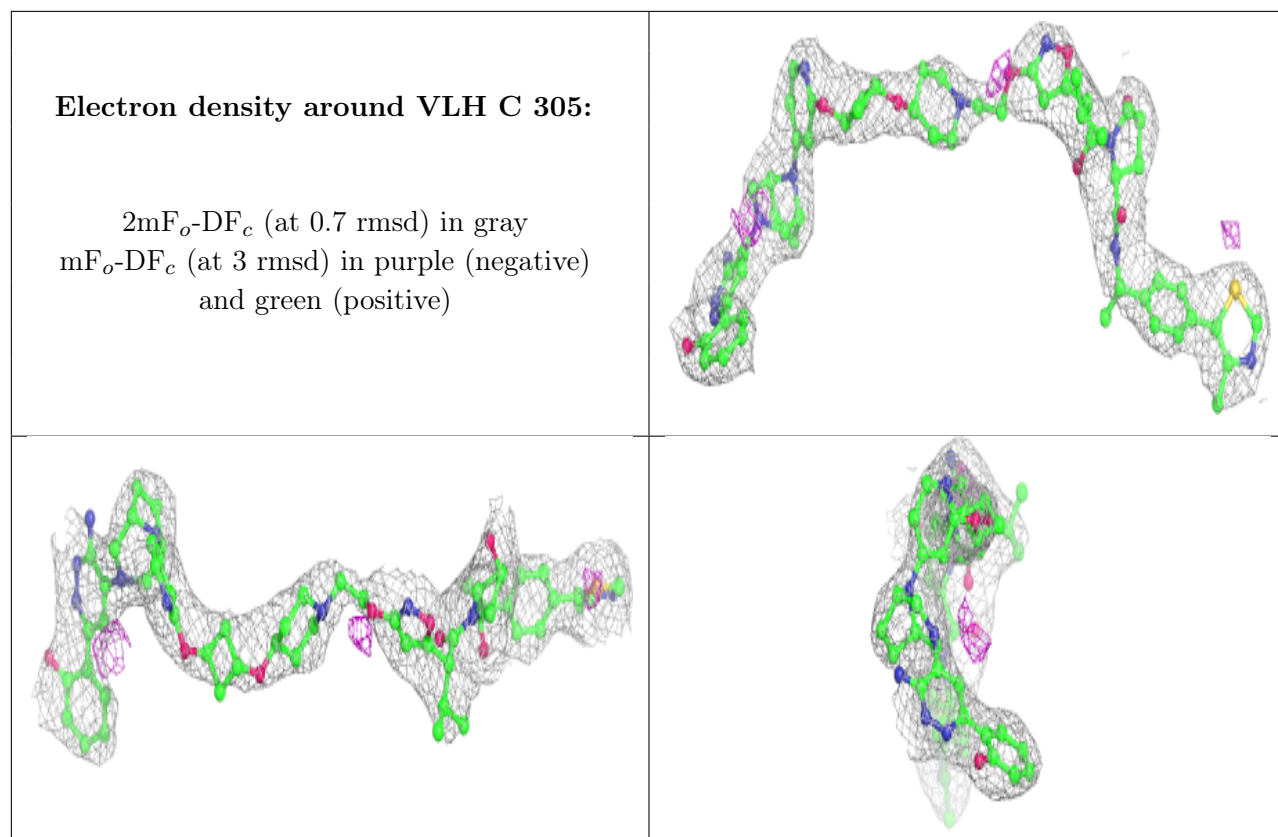
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	C	304	6/6	0.76	0.79	92,92,92,92	0
5	PO4	B	201	5/5	0.81	0.23	104,104,104,104	0
5	PO4	C	302	5/5	0.86	0.25	72,72,72,72	0
8	CL	E	201	1/1	0.89	0.20	54,54,54,54	0
5	PO4	C	301	5/5	0.90	0.17	85,85,86,86	0
5	PO4	G	1601	5/5	0.90	0.15	90,90,90,90	0
7	VLH	F	303	77/77	0.92	0.30	51,56,57,57	0
5	PO4	C	303	5/5	0.92	0.19	80,80,80,80	0
5	PO4	F	301	5/5	0.93	0.22	77,77,77,77	0
7	VLH	C	305	77/77	0.93	0.30	53,58,59,59	0
5	PO4	F	302	5/5	0.95	0.18	84,84,84,84	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.