



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:13 pm BST

PDB ID : 2JC0
Title : CRYSTAL STRUCTURE OF HEPATITIS C VIRUS POLYMERASE IN
COMPLEX WITH INHIBITOR SB655264
Authors : Wonacott, A.; Skarzynski, T.; Singh, O.M.
Deposited on : 2006-12-18
Resolution : 2.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

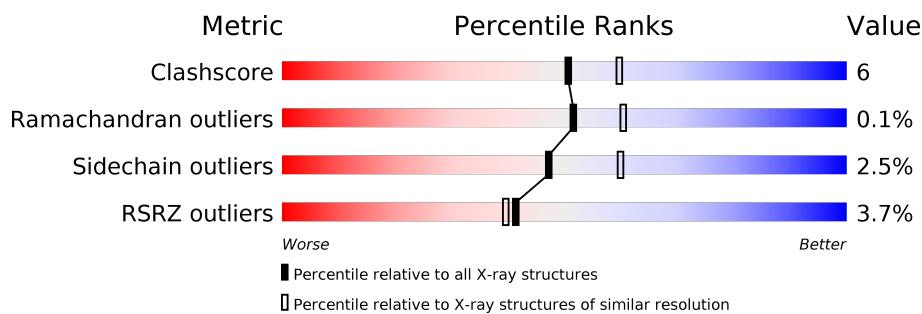
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	570	 4% 86% 11% ..
1	B	570	 4% 84% 13% ..

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
2	699	A	1564	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9423 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.

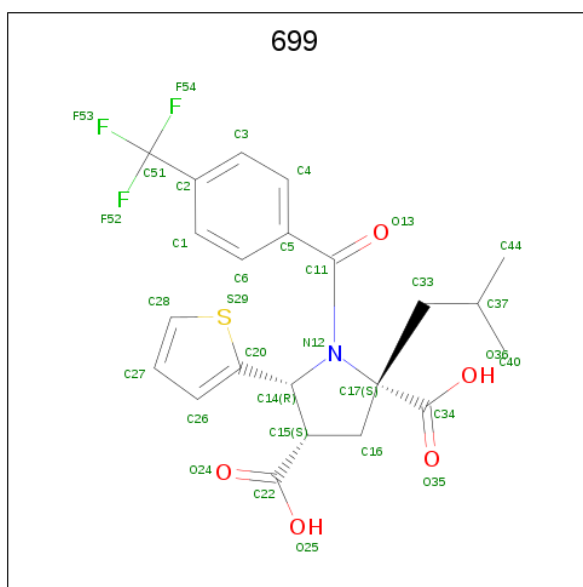
- Molecule 1 is a protein called RNA-DEPENDENT RNA-POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	Total	C	N	O	S	0	0	0
			4334	2736	764	803	31			
1	B	556	Total	C	N	O	S	0	0	0
			4322	2727	762	802	31			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	HIS	ARG	conflict	UNP O39930
A	131	VAL	GLU	conflict	UNP O39930
A	185	VAL	ALA	conflict	UNP O39930
A	213	ASN	CYS	conflict	UNP O39930
A	254	LYS	ARG	conflict	UNP O39930
A	316	ASN	CYS	conflict	UNP O39930
A	329	VAL	THR	conflict	UNP O39930
A	338	VAL	ALA	conflict	UNP O39930
A	464	GLU	GLN	conflict	UNP O39930
A	531	LYS	ARG	conflict	UNP O39930
B	120	HIS	ARG	conflict	UNP O39930
B	131	VAL	GLU	conflict	UNP O39930
B	185	VAL	ALA	conflict	UNP O39930
B	213	ASN	CYS	conflict	UNP O39930
B	254	LYS	ARG	conflict	UNP O39930
B	316	ASN	CYS	conflict	UNP O39930
B	329	VAL	THR	conflict	UNP O39930
B	338	VAL	ALA	conflict	UNP O39930
B	464	GLU	GLN	conflict	UNP O39930
B	531	LYS	ARG	conflict	UNP O39930

- Molecule 2 is (2S,4S,5R)-2-ISOBUTYL-5-(2-THIENYL)-1-[4-(TRIFLUOROMETHYL)B ENZOYL]PYRROLIDINE-2,4-DICARBOXYLIC ACID (three-letter code: 699) (formula: C₂₂H₂₂F₃N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf		
			Total	C	F	N	O			S	
2	A	1	Total	32	22	3	1	5	1	0	0
2	A	1	Total	32	22	3	1	5	1	0	0
2	B	1	Total	32	22	3	1	5	1	0	0
2	B	1	Total	32	22	3	1	5	1	0	0

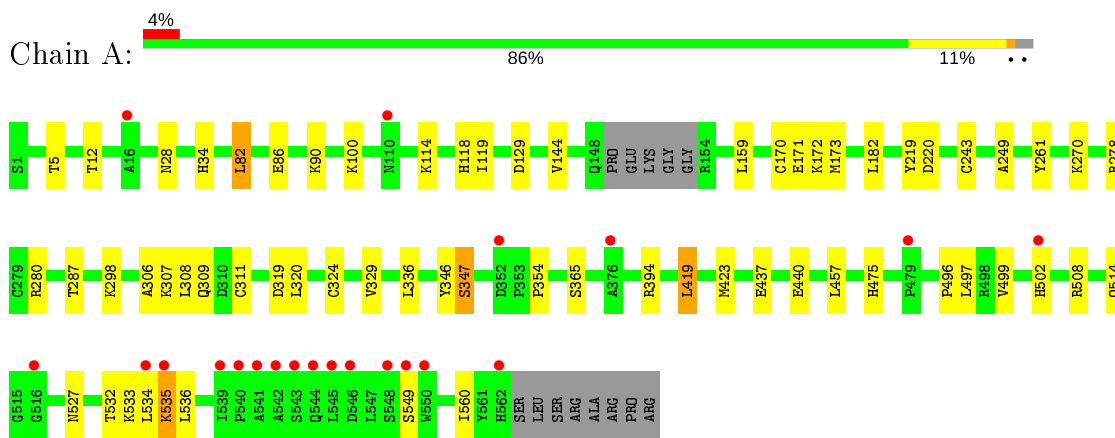
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	318	Total	O	0	0
			318	318		
3	B	321	Total	O	0	0
			321	321		

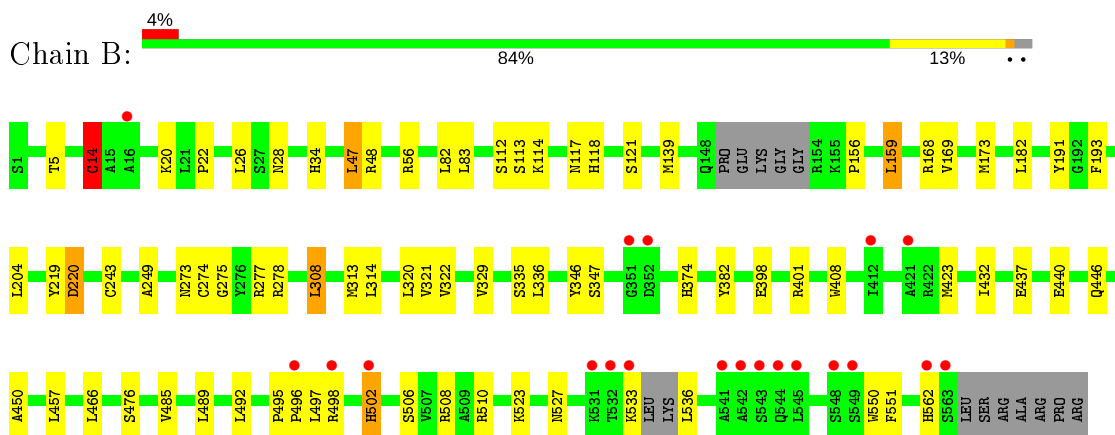
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: RNA-DEPENDENT RNA-POLYMERASE



- Molecule 1: RNA-DEPENDENT RNA-POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.74Å 105.89Å 126.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 27.25 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.20) 96.5 (27.25-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.99Å)	Xtrriage
Refinement program	REFMAC 5.3.0006	Depositor
R, R_{free}	0.181 , 0.248 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtrriage
Anisotropy	0.312	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9423	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9919e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 699

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	0.92	1/4428 (0.0%)	0.85	4/6009 (0.1%)
1	B	0.91	2/4415 (0.0%)	0.82	4/5990 (0.1%)
All	All	0.91	3/8843 (0.0%)	0.84	8/11999 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	CYS	CB-SG	-10.92	1.63	1.82
1	A	311	CYS	CB-SG	-6.45	1.71	1.82
1	B	274	CYS	CB-SG	-5.42	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	LEU	CB-CG-CD2	-7.21	98.75	111.00
1	A	82	LEU	CA-CB-CG	6.31	129.82	115.30
1	A	129	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	419	LEU	CA-CB-CG	5.78	128.59	115.30
1	B	277	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	277	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	336	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	168	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	4334	0	4352	44	0
1	B	4322	0	4332	50	0
2	A	64	0	40	10	0
2	B	64	0	40	6	0
3	A	318	0	0	6	0
3	B	321	0	0	5	0
All	All	9423	0	8764	100	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 6.

All (100) 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:423:MET:SD	2:A:1564:699:H1	2.00	1.02
1:A:508:ARG:NH1	3:A:2300:HOH:O	1.84	0.95
1:A:535:LYS:HE3	1:A:536:LEU:H	1.31	0.94
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.32	0.92
1:B:423:MET:SD	2:B:1565:699:H1	2.09	0.92
2:A:1564:699:O13	3:A:2318:HOH:O	1.96	0.84
1:B:5:THR:HG23	1:B:278:ARG:HH12	1.43	0.83
1:A:90:LYS:HD2	3:A:2075:HOH:O	1.79	0.82
1:A:346:TYR:O	1:A:347:SER:HB3	1.79	0.80
1:B:423:MET:CG	2:B:1565:699:F54	2.18	0.80
1:B:440:GLU:HG2	1:B:457:LEU:HD12	1.69	0.74
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.68	0.74
1:A:535:LYS:CE	1:A:536:LEU:H	2.01	0.72
1:B:440:GLU:HG2	1:B:457:LEU:CD1	2.21	0.71
1:A:440:GLU:HG2	1:A:457:LEU:HD12	1.73	0.70
1:B:220:ASP:HB2	3:B:2161:HOH:O	1.92	0.69
1:B:423:MET:SD	1:B:497:LEU:HD22	2.34	0.67
1:A:12:THR:HG21	1:A:270:LYS:HD2	1.76	0.66
1:B:423:MET:HG2	2:B:1565:699:F54	1.86	0.65
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.37	0.65
1:A:533:LYS:HE2	2:A:1564:699:H28	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:VAL:HG12	1:B:173:MET:CE	2.27	0.64
1:A:527:ASN:HD21	1:A:534:LEU:H	1.46	0.63
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.79	0.63
2:A:1564:699:O35	2:A:1564:699:H26	1.98	0.63
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.29	0.63
1:B:113:SER:O	1:B:117:ASN:HB2	1.97	0.63
1:B:423:MET:HG3	2:B:1565:699:F54	1.87	0.62
1:B:169:VAL:HG12	1:B:173:MET:HE3	1.81	0.61
1:B:314:LEU:HB3	1:B:321:VAL:HG12	1.84	0.60
1:A:100:LYS:HG3	3:A:2127:HOH:O	2.02	0.59
2:A:1564:699:O13	2:A:1564:699:H331	2.03	0.58
1:B:346:TYR:O	1:B:347:SER:HB3	2.02	0.58
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.85	0.57
1:B:308:LEU:HD11	1:B:335:SER:HB3	1.87	0.56
1:A:533:LYS:HE2	2:A:1564:699:C28	2.37	0.55
1:B:527:ASN:ND2	1:B:533:LYS:HB3	2.22	0.54
1:A:535:LYS:HE3	1:A:536:LEU:N	2.13	0.54
1:B:347:SER:OG	1:B:347:SER:O	2.16	0.53
1:B:508:ARG:NH1	3:B:2298:HOH:O	2.41	0.53
1:A:309:GLN:O	1:A:324:CYS:HB2	2.10	0.52
1:A:5:THR:HG23	1:A:278:ARG:NH1	2.14	0.51
1:A:86:GLU:O	1:A:90:LYS:HG3	2.10	0.51
1:B:5:THR:HG23	1:B:278:ARG:NH1	2.21	0.51
2:A:1564:699:C34	2:A:1564:699:H26	2.42	0.50
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.93	0.50
1:A:329:VAL:HG12	3:A:2211:HOH:O	2.11	0.49
1:B:47:LEU:HD13	1:B:156:PRO:HG3	1.95	0.49
1:A:475:HIS:HA	2:A:1564:699:H4	1.94	0.49
1:A:423:MET:CG	2:A:1564:699:F54	2.50	0.49
1:B:114:LYS:O	1:B:118:HIS:HD2	1.96	0.49
2:B:1565:699:O36	2:B:1565:699:H26	2.13	0.49
1:A:306:ALA:CB	1:A:308:LEU:HD13	2.43	0.48
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.94	0.48
1:B:374:HIS:CD2	1:B:476:SER:HB2	2.49	0.48
1:B:28:ASN:OD1	1:B:34:HIS:CE1	2.67	0.48
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.77	0.47
1:B:508:ARG:HH12	1:B:523:LYS:HA	1.79	0.47
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.96	0.47
1:A:170:CYS:HA	1:A:173:MET:HE2	1.96	0.47
1:B:273:ASN:ND2	1:B:275:GLY:H	2.12	0.47
1:A:114:LYS:O	1:A:118:HIS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:TRP:CD1	1:B:562:HIS:CE1	3.03	0.47
1:B:446:GLN:HA	1:B:450:ALA:O	2.16	0.46
1:A:423:MET:SD	1:A:497:LEU:HD22	2.55	0.46
1:A:298:LYS:HE2	1:A:346:TYR:O	2.16	0.46
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.57	0.45
1:A:496:PRO:HG2	1:A:499:VAL:HG23	1.99	0.45
1:B:191:TYR:CZ	1:B:193:PHE:HB2	2.52	0.45
1:A:535:LYS:HD2	1:A:535:LYS:HA	1.27	0.44
1:B:48:ARG:HG3	1:B:159:LEU:HD22	1.99	0.44
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.99	0.44
1:A:28:ASN:OD1	1:A:34:HIS:CE1	2.70	0.44
1:B:398:GLU:OE1	1:B:408:TRP:HD1	2.00	0.44
1:A:5:THR:HG21	1:A:278:ARG:HH22	1.83	0.44
1:A:119:ILE:CG2	1:A:173:MET:HE1	2.47	0.44
1:A:306:ALA:O	1:A:307:LYS:HB2	2.18	0.44
1:A:319:ASP:OD1	1:A:365:SER:HB2	2.17	0.43
1:A:306:ALA:HB3	1:A:308:LEU:HD13	2.00	0.43
2:B:1564:699:H37	2:B:1564:699:H15	2.00	0.43
1:A:423:MET:HG3	2:A:1564:699:F54	2.08	0.43
1:A:171:GLU:HG2	1:A:261:TYR:OH	2.18	0.43
1:A:336:LEU:HD13	1:A:354:PRO:HB2	2.01	0.43
1:B:28:ASN:OD1	1:B:34:HIS:NE2	2.50	0.43
1:A:298:LYS:HG2	1:A:346:TYR:HB3	2.01	0.43
1:B:495:PRO:HA	1:B:496:PRO:HD3	1.91	0.42
1:A:502:HIS:CD2	3:A:2298:HOH:O	2.73	0.42
1:B:22:PRO:HG2	1:B:401:ARG:HG3	2.01	0.42
1:B:26:LEU:HD13	1:B:432:ILE:HG12	2.00	0.42
1:B:506:SER:O	1:B:510:ARG:HG3	2.20	0.42
1:B:527:ASN:HD21	1:B:533:LYS:HB3	1.85	0.42
1:B:308:LEU:CD1	1:B:335:SER:HB3	2.50	0.42
1:B:502:HIS:CD2	3:B:2294:HOH:O	2.72	0.41
1:B:204:LEU:HA	1:B:204:LEU:HD23	1.89	0.41
1:B:382:TYR:OH	3:B:2239:HOH:O	2.17	0.41
1:A:280:ARG:HD2	1:A:287:THR:HA	2.02	0.41
1:B:14:CYS:HB3	1:B:139:MET:CE	2.52	0.40
1:B:423:MET:CE	1:B:497:LEU:HB3	2.51	0.40
1:B:485:VAL:O	1:B:489:LEU:HG	2.21	0.40
1:B:510:ARG:NH1	3:B:2299:HOH:O	2.54	0.40

There are no symmetry-related clashes.

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	553/570 (97%)	539 (98%)	13 (2%)	1 (0%)	47	55
1	B	550/570 (96%)	536 (98%)	14 (2%)	0	100	100
All	All	1103/1140 (97%)	1075 (98%)	27 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	549	SER

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	475/487 (98%)	467 (98%)	8 (2%)	60	74
1	B	474/487 (97%)	458 (97%)	16 (3%)	37	47
All	All	949/974 (97%)	925 (98%)	24 (2%)	47	60

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	LEU
1	A	220	ASP
1	A	347	SER
1	A	419	LEU
1	A	437	GLU

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Mol	Chain	Res	Type
1	A	514	GLN
1	A	532	THR
1	A	535	LYS
1	B	14	CYS
1	B	20	LYS
1	B	47	LEU
1	B	56	ARG
1	B	83	LEU
1	B	112	SER
1	B	121	SER
1	B	159	LEU
1	B	220	ASP
1	B	308	LEU
1	B	329	VAL
1	B	437	GLU
1	B	492	LEU
1	B	498	ARG
1	B	502	HIS
1	B	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	118	HIS
1	A	231	ASN
1	A	411	ASN
1	A	514	GLN
1	A	527	ASN
1	A	544	GLN
1	B	49	GLN
1	B	118	HIS
1	B	120	HIS
1	B	273	ASN
1	B	527	ASN
1	B	544	GLN

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 carbohydrates 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	699	A	1564	-	27,34,34	1.24	2 (7%)	29,52,52	1.90	7 (24%)
2	699	A	1563	-	27,34,34	1.52	7 (25%)	29,52,52	1.58	4 (13%)
2	699	B	1564	-	27,34,34	1.67	6 (22%)	29,52,52	1.69	6 (20%)
2	699	B	1565	-	27,34,34	1.44	4 (14%)	29,52,52	1.56	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	699	A	1564	-	-	3/19/52/52	0/3/3/3
2	699	A	1563	-	-	1/19/52/52	0/3/3/3
2	699	B	1564	-	-	1/19/52/52	0/3/3/3
2	699	B	1565	-	-	1/19/52/52	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1564	699	C33-C17	4.04	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1565	699	C17-N12	3.37	1.53	1.48
2	B	1565	699	C14-N12	3.34	1.51	1.47
2	A	1564	699	C17-N12	3.18	1.52	1.48
2	A	1563	699	C33-C17	2.95	1.57	1.54
2	B	1564	699	C6-C1	2.91	1.44	1.38
2	B	1565	699	C33-C17	2.69	1.57	1.54
2	A	1563	699	C17-N12	2.66	1.52	1.48
2	B	1564	699	C1-C2	2.59	1.43	1.39
2	A	1563	699	C1-C2	2.48	1.43	1.39
2	A	1563	699	O13-C11	2.40	1.27	1.22
2	A	1563	699	C15-C14	-2.35	1.51	1.55
2	A	1564	699	C6-C1	2.33	1.43	1.38
2	B	1564	699	C4-C5	2.27	1.43	1.39
2	A	1563	699	C4-C5	2.21	1.43	1.39
2	B	1564	699	C15-C14	-2.19	1.51	1.55
2	B	1564	699	C17-N12	2.18	1.51	1.48
2	A	1563	699	C3-C2	2.17	1.42	1.39
2	B	1565	699	C11-N12	2.09	1.41	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1564	699	C20-C14-C15	5.95	124.23	113.95
2	B	1565	699	F52-C51-C2	-4.96	102.05	112.93
2	A	1563	699	F52-C51-C2	-4.73	102.54	112.93
2	B	1564	699	F53-C51-C2	-4.30	103.49	112.93
2	A	1563	699	F53-C51-C2	-3.49	105.26	112.93
2	A	1564	699	F53-C51-C2	-3.48	105.29	112.93
2	B	1564	699	F52-C51-C2	-3.43	105.40	112.93
2	A	1564	699	C17-C33-C37	3.39	124.53	118.37
2	B	1564	699	F53-C51-F54	2.97	116.63	105.72
2	B	1564	699	C27-C28-S29	-2.96	110.58	112.98
2	A	1563	699	F53-C51-F54	2.96	116.56	105.72
2	A	1564	699	C5-C11-N12	2.70	122.68	117.86
2	B	1564	699	C5-C11-N12	2.58	122.45	117.86
2	A	1564	699	C1-C6-C5	-2.54	117.83	120.78
2	B	1564	699	C14-N12-C11	-2.52	121.82	125.76
2	B	1565	699	F53-C51-F54	2.40	114.54	105.72
2	B	1565	699	C20-C14-C15	2.23	117.80	113.95
2	B	1565	699	F53-C51-C2	-2.20	108.09	112.93
2	A	1564	699	F53-C51-F52	2.12	113.50	105.72
2	A	1564	699	C1-C2-C51	2.11	123.32	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1565	699	O13-C11-C5	-2.10	116.15	120.23
2	A	1563	699	C27-C28-S29	-2.03	111.33	112.98
2	B	1565	699	C5-C11-N12	2.02	121.46	117.86

There are no chirality outliers.

All (6) torsion outliers are listed below:

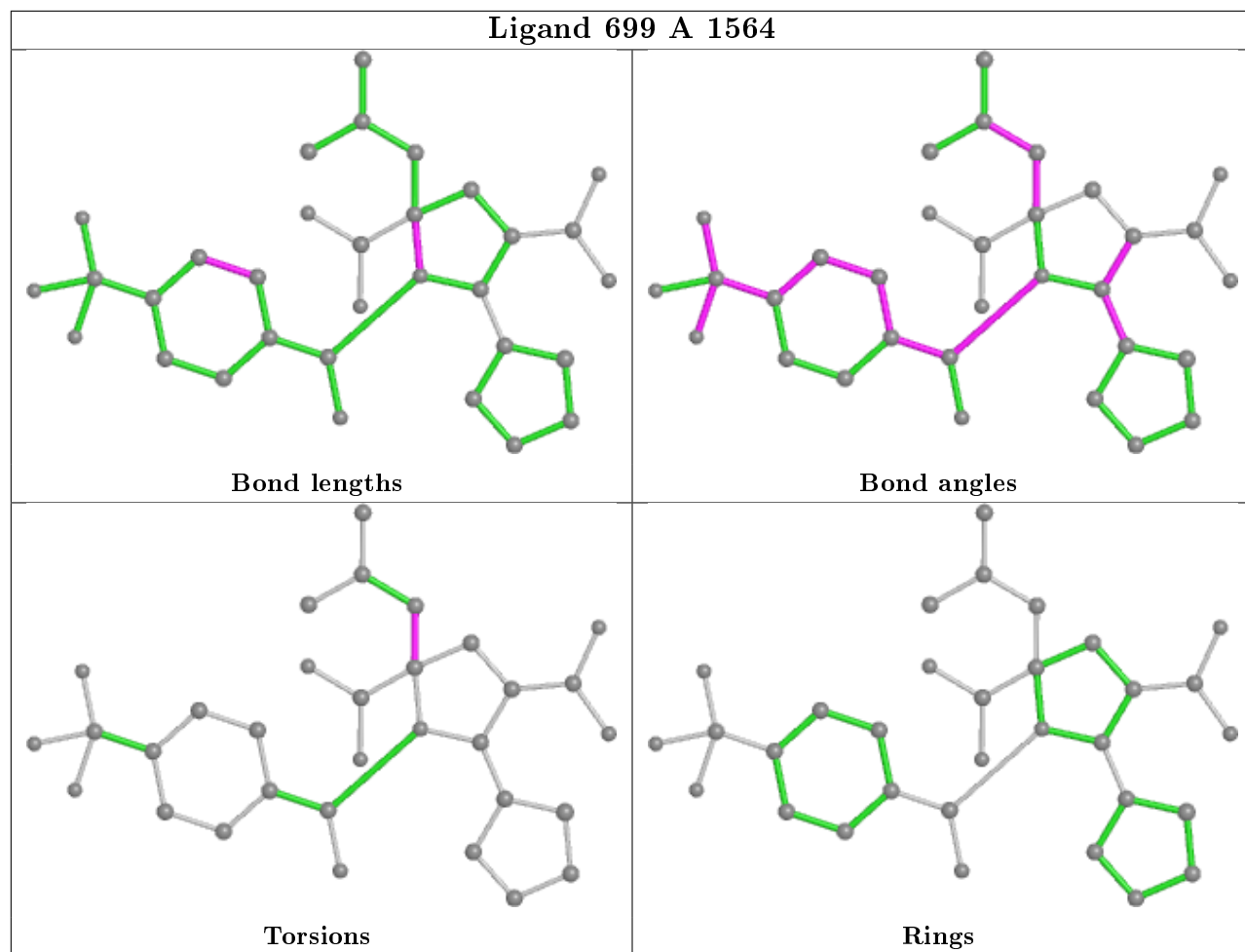
Mol	Chain	Res	Type	Atoms
2	A	1564	699	N12-C17-C33-C37
2	A	1564	699	C34-C17-C33-C37
2	A	1563	699	C34-C17-C33-C37
2	B	1564	699	C34-C17-C33-C37
2	B	1565	699	C34-C17-C33-C37
2	A	1564	699	C16-C17-C33-C37

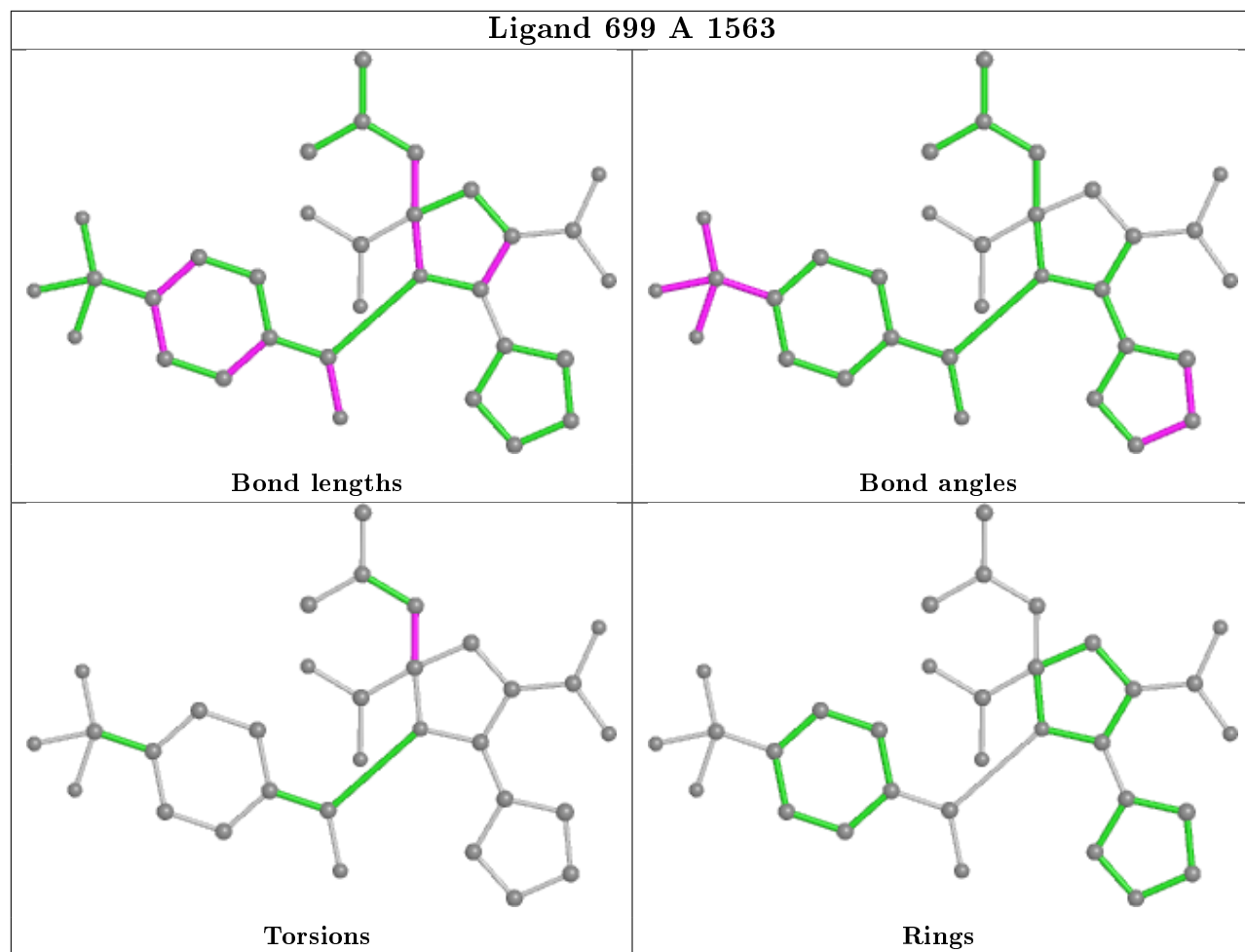
There are no ring outliers.

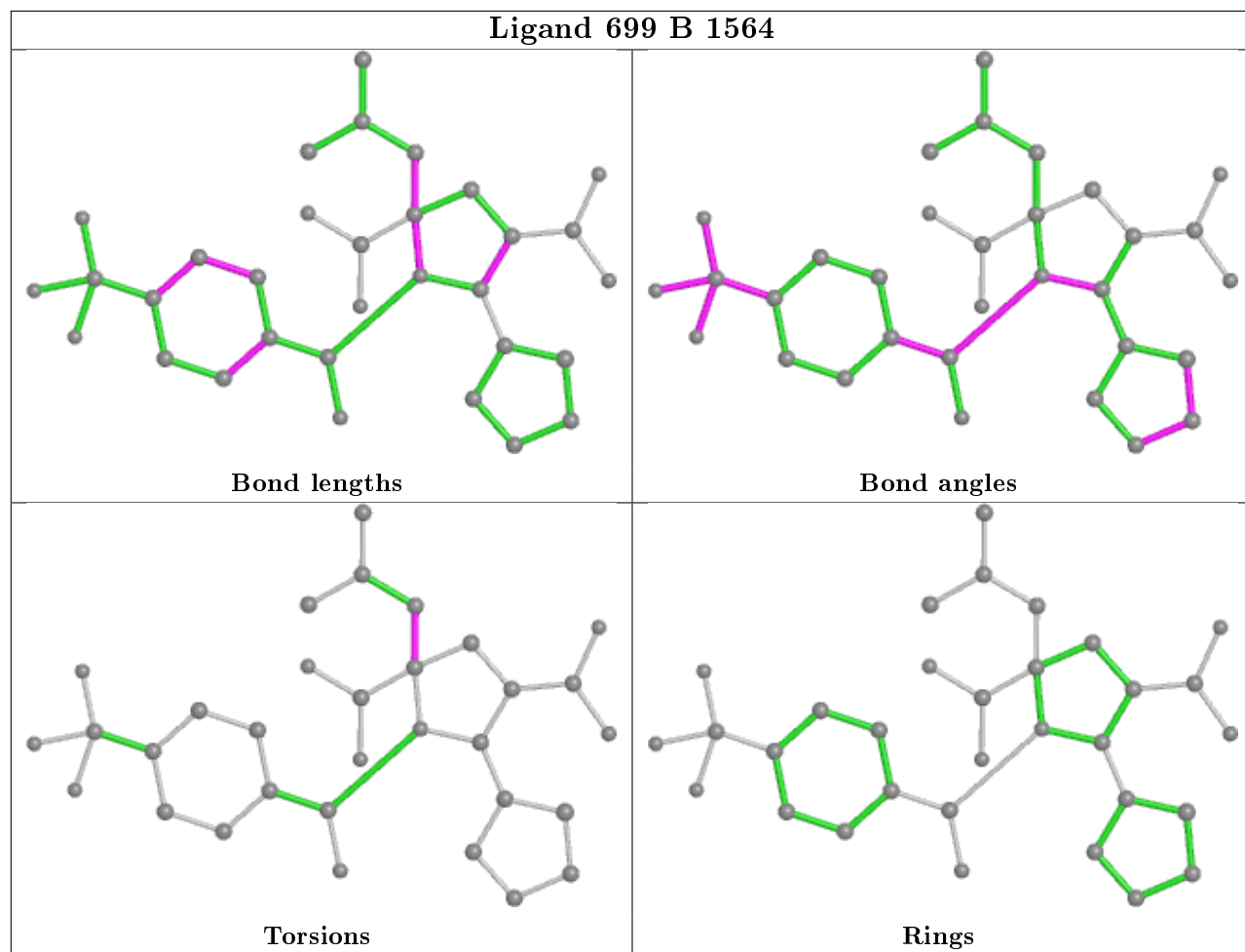
3 monomers are involved in 16 short contacts:

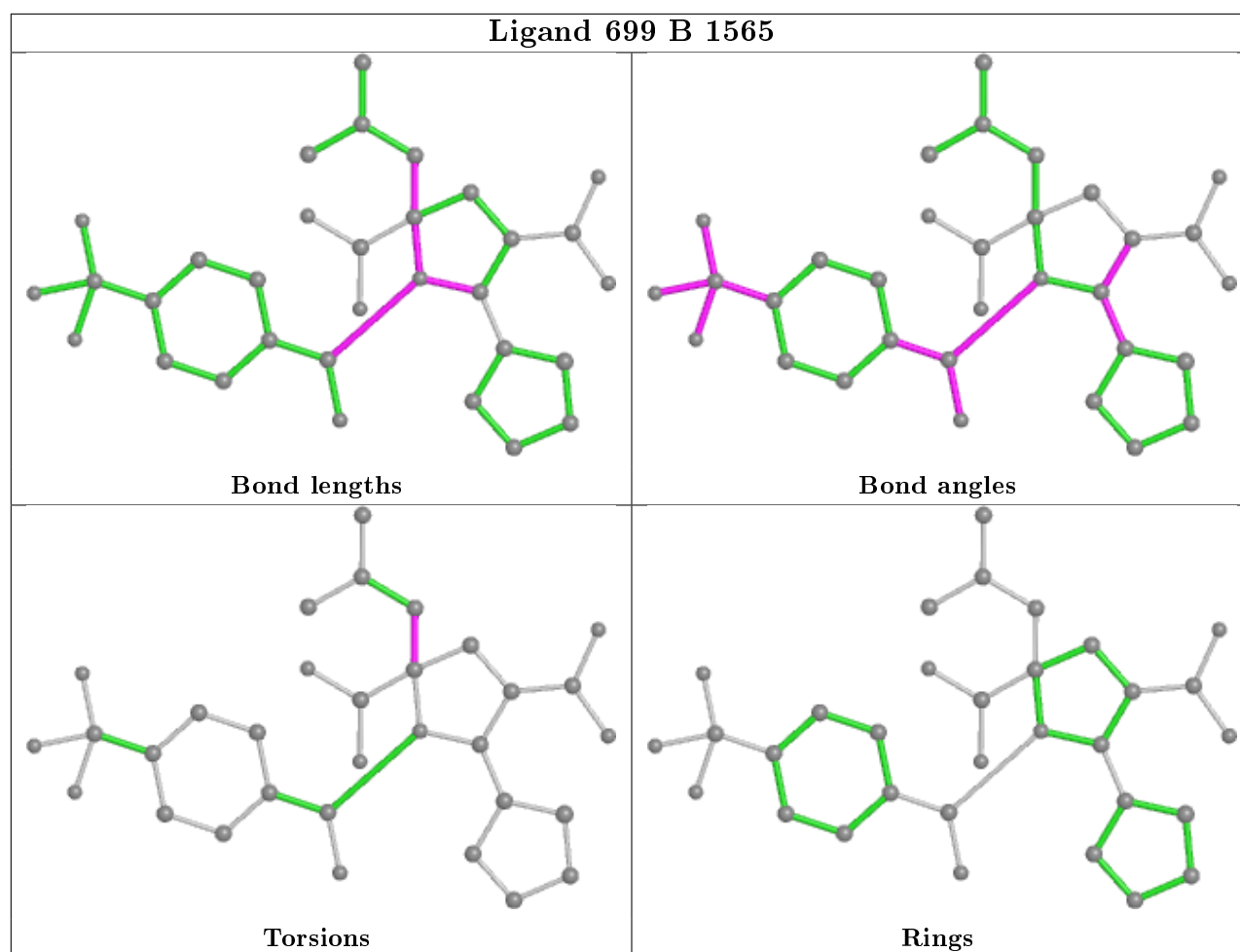
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1564	699	10	0
2	B	1564	699	1	0
2	B	1565	699	5	0

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	557/570 (97%)	-0.12	21 (3%) 40 38	19, 29, 47, 83	0
1	B	556/570 (97%)	-0.08	20 (3%) 42 41	20, 30, 46, 77	0
All	All	1113/1140 (97%)	-0.10	41 (3%) 41 39	19, 30, 47, 83	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	548	SER	7.8
1	A	545	LEU	6.6
1	B	543	SER	6.5
1	A	544	GLN	5.5
1	B	542	ALA	5.4
1	B	548	SER	5.1
1	B	545	LEU	5.1
1	B	562	HIS	4.5
1	A	534	LEU	4.1
1	A	543	SER	4.1
1	B	544	GLN	3.9
1	B	532	THR	3.8
1	B	563	SER	3.8
1	A	376	ALA	3.6
1	B	352	ASP	3.6
1	A	16	ALA	3.5
1	A	535	LYS	3.3
1	A	541	ALA	3.2
1	A	550	TRP	3.1
1	B	421	ALA	3.0
1	A	352	ASP	2.8
1	B	549	SER	2.7
1	B	16	ALA	2.6
1	B	498	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	351	GLY	2.4
1	A	549	SER	2.4
1	A	562	HIS	2.3
1	A	516	GLY	2.3
1	B	502	HIS	2.3
1	A	110	ASN	2.3
1	B	531	LYS	2.3
1	B	541	ALA	2.2
1	A	546	ASP	2.1
1	A	502	HIS	2.1
1	A	540	PRO	2.1
1	A	479	PRO	2.1
1	B	412	ILE	2.1
1	A	542	ALA	2.0
1	A	539	ILE	2.0
1	B	496	PRO	2.0
1	B	533	LYS	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 carbohydrates in this entry.

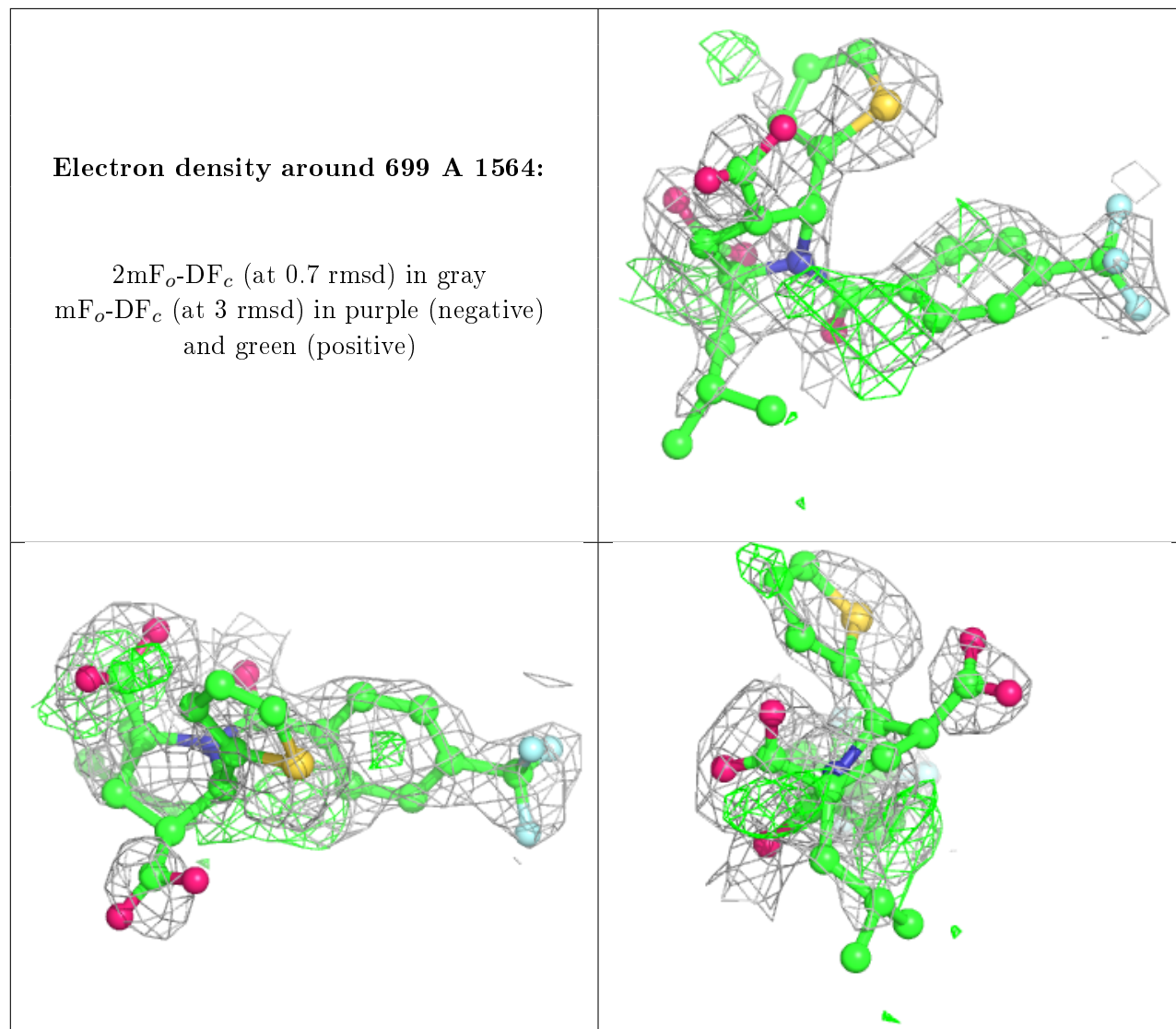
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	699	A	1564	32/32	0.74	0.26	35,41,45,46	32
2	699	B	1565	32/32	0.78	0.27	28,33,37,38	32
2	699	A	1563	32/32	0.88	0.15	31,38,46,51	0
2	699	B	1564	32/32	0.90	0.13	33,37,46,49	0

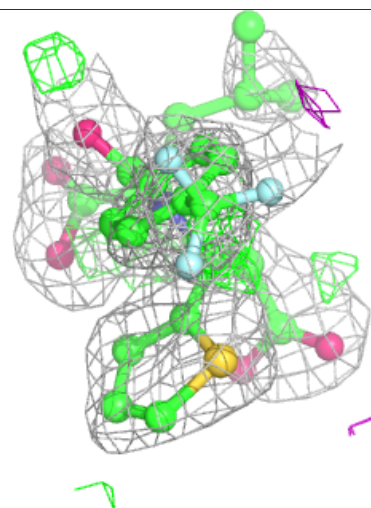
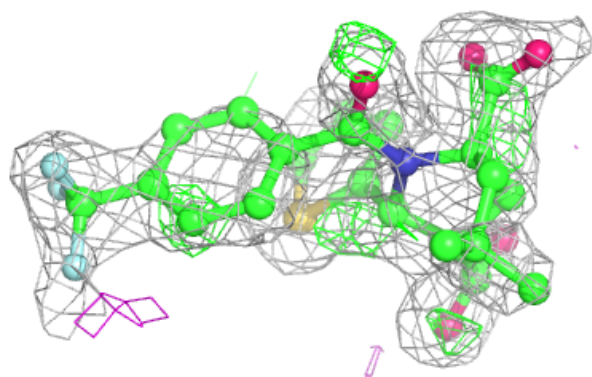
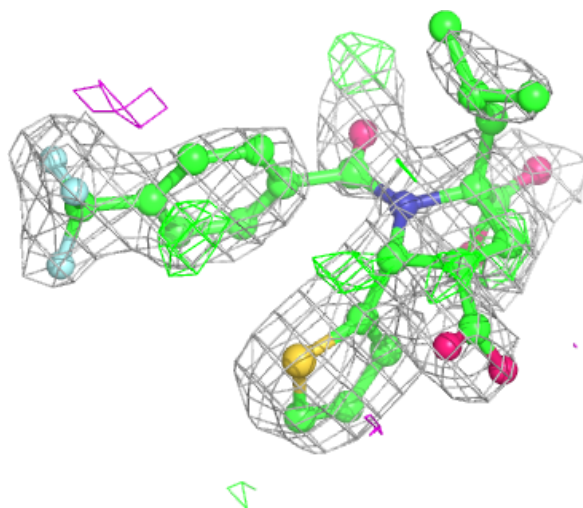
The following is a graphical depiction of the model fit to experimental electron density of all

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.



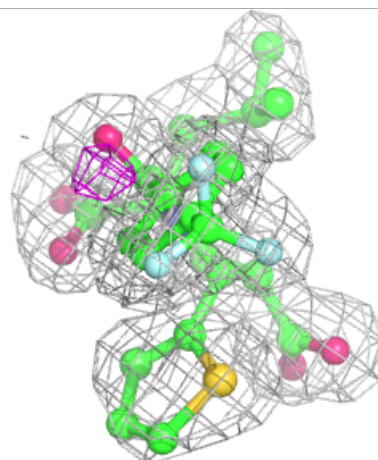
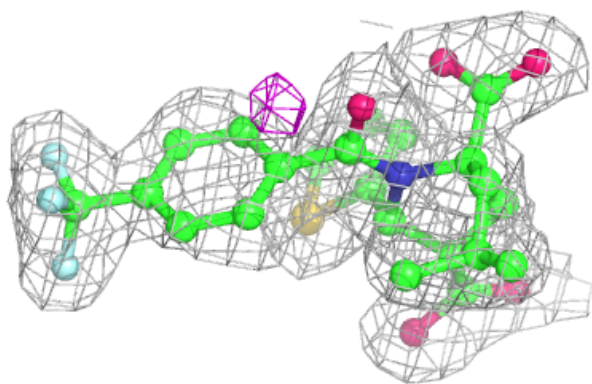
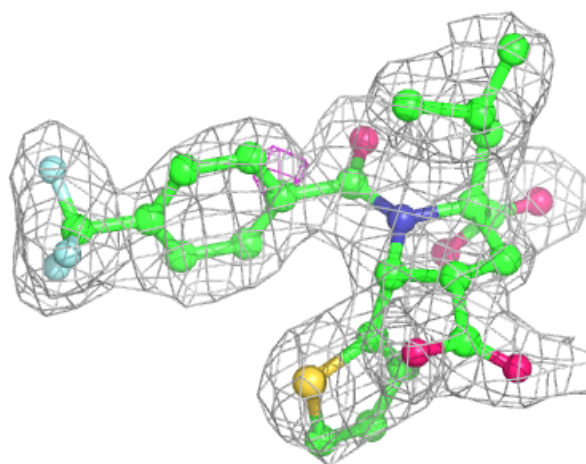
Electron density around 699 B 1565:

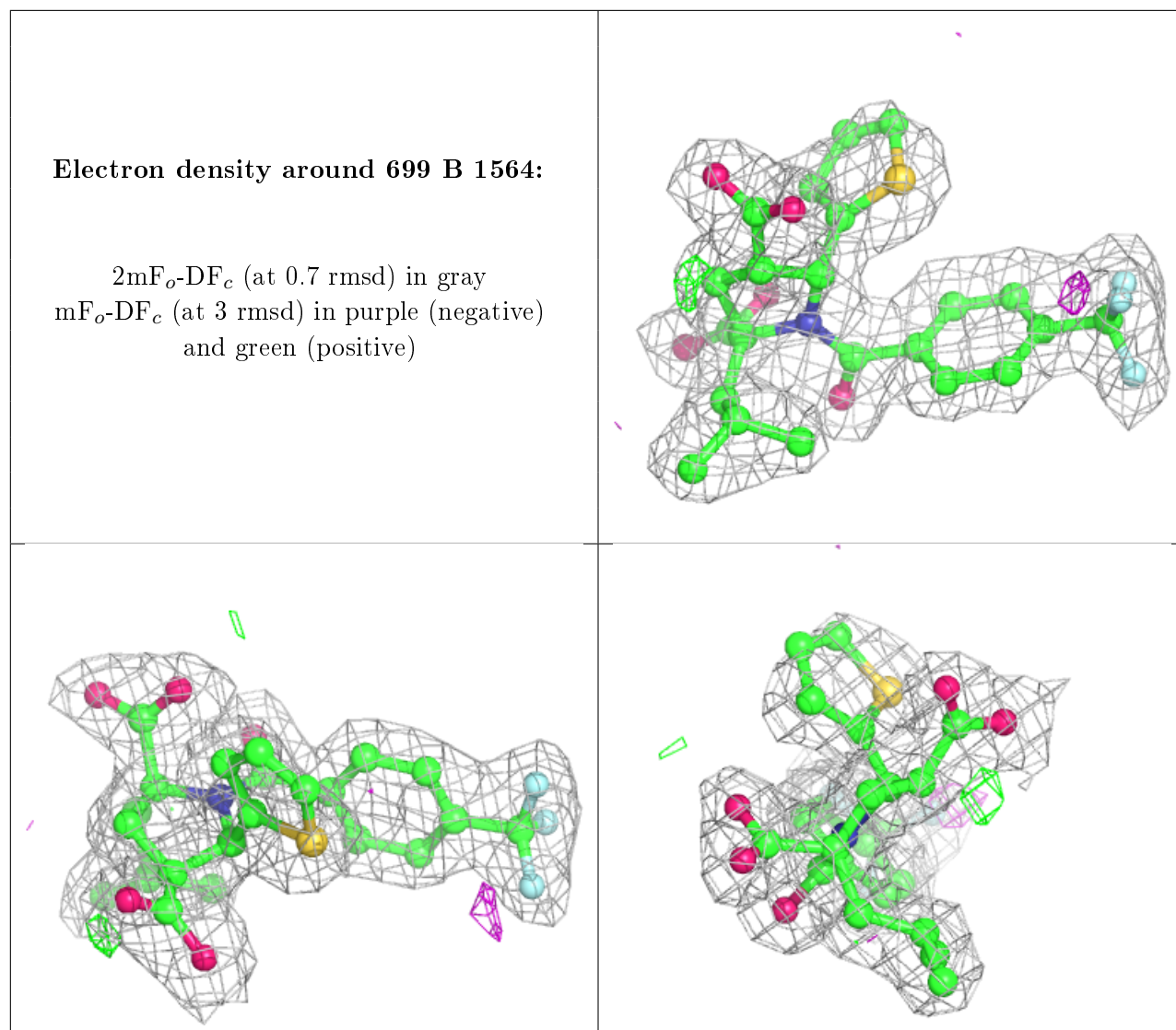
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 699 A 1563:

$2mF_o-DF_c$ (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.