



Full wwPDB X-ray Structure Validation Report

Dec 3, 2023 – 06:01 pm GMT


PDB ID : 2JED
Title : The crystal structure of the kinase domain of the protein kinase C theta in complex with NVP-XAA228 at 2.32Å resolution.
Authors : Stark, W.; Bitsch, F.; Berner, A.; Buelens, F.; Graff, P.; Depersin, H.; Geiser, M.; Knecht, R.; Rahuel, J.; Rummel, G.; Schlaeppli, J.M.; Schmitz, R.; Strauss, A.; Wagner, J.
Deposited on : 2007-01-16
Resolution : 2.32 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (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

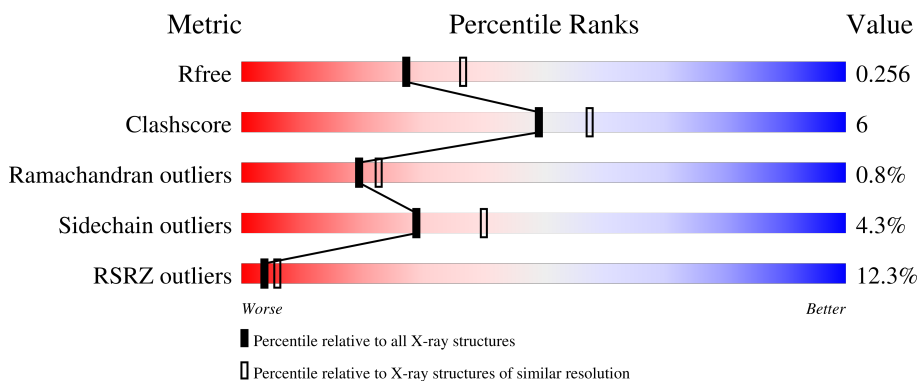
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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 ≥ 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	352	 11% 75% 15% • 7%
1	B	352	 12% 77% 13% • 9%

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
1	SEP	B	676	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5884 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.

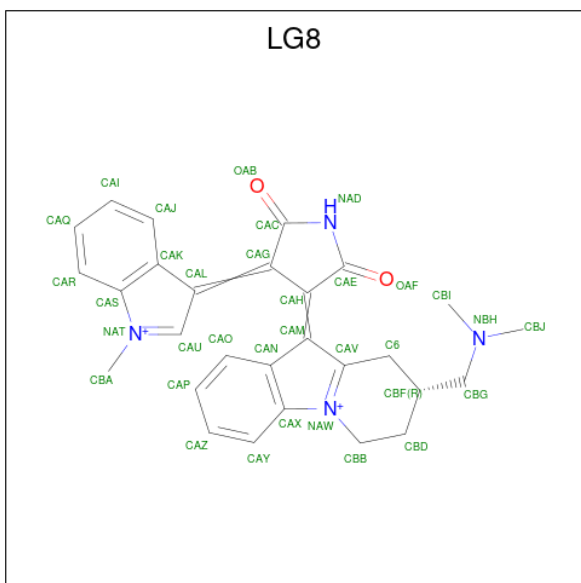
- Molecule 1 is a protein called PROTEIN KINASE C THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
1	A	326	Total	C	N	O	P	S	0	0	0
			2712	1753	450	488	2	19			
1	B	322	Total	C	N	O	P	S	0	0	0
			2684	1732	455	476	2	19			

There are 4 discrepancies between the modelled and reference sequences:

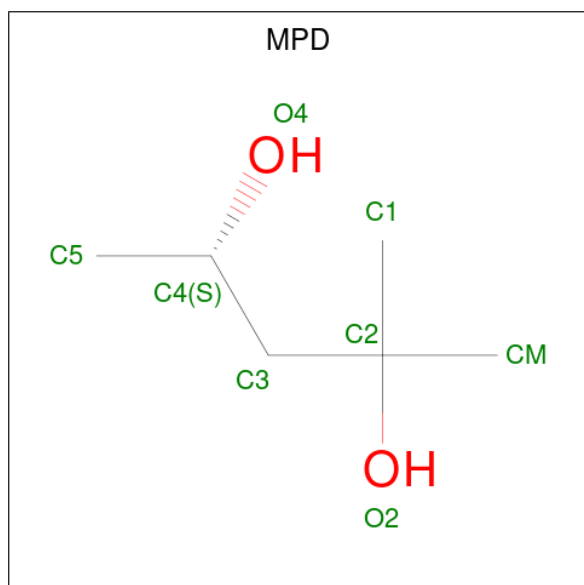
Chain	Residue	Modelled	Actual	Comment	Reference
A	381	GLU	ILE	engineered mutation	UNP Q04759
A	538	GLU	THR	engineered mutation	UNP Q04759
B	381	GLU	ILE	engineered mutation	UNP Q04759
B	538	GLU	THR	engineered mutation	UNP Q04759

- Molecule 2 is 3-(8-DIMETHYLAMINOMETHYL-6,7,8,9-TETRAHYDRO-PYRIDO[1,2-A]INDOL-10-YL)-4-(1-METHYL-1H-INDOL-3-YL)-PYRROLE-2,5-DIONE (three-letter code: LG8) (formula: C₂₈H₂₈N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	28	4	2		
2	B	1	Total	C	N	O	0	0
			34	28	4	2		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		

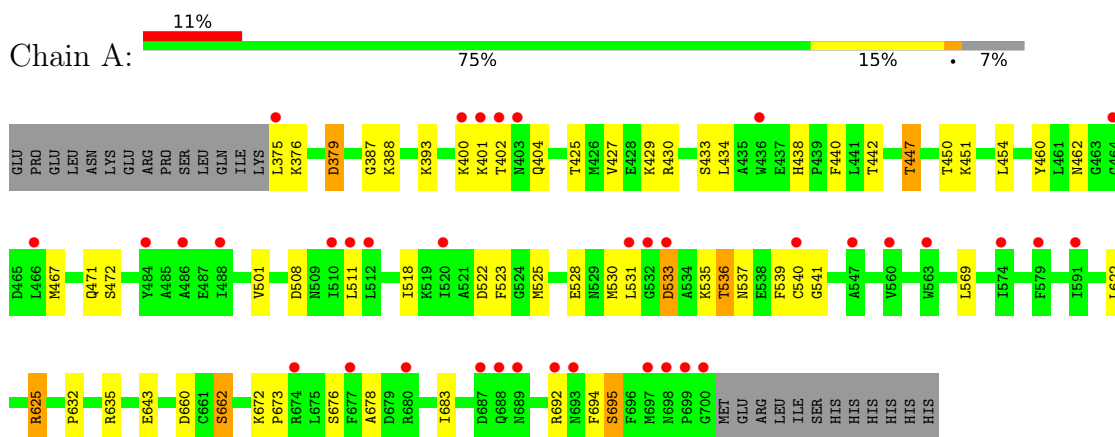
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	217	Total	O	0	0
			217	217		

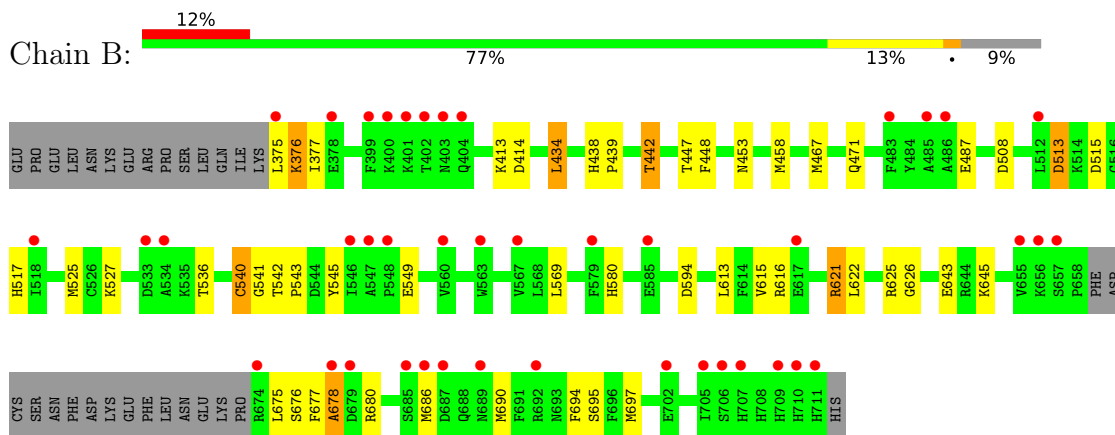
3 Residue-property plots [i](#)

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: PROTEIN KINASE C THETA



- Molecule 1: PROTEIN KINASE C THETA



4 Data and refinement statistics i

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	152.17Å 152.17Å 74.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 2.32 19.41 – 2.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.88-2.32) 100.0 (19.41-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.33Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.221 0.227 , 0.256	Depositor DCC
R_{free} test set	2131 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtrriage
Anisotropy	0.262	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5884	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: LG8, MPD, SEP

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	0.63	1/2762 (0.0%)	0.71	2/3711 (0.1%)
1	B	0.61	1/2734 (0.0%)	0.71	2/3672 (0.1%)
All	All	0.62	2/5496 (0.0%)	0.71	4/7383 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	CYS	C-N	-11.38	1.12	1.33
1	B	540	CYS	CB-SG	-7.83	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	539	PHE	O-C-N	-7.67	110.43	122.70
1	B	434	LEU	CA-CB-CG	7.28	132.04	115.30
1	A	539	PHE	C-N-CA	6.78	138.65	121.70
1	B	621	ARG	NE-CZ-NH2	-5.65	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	LYS	Peptide

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	2712	0	2653	34	0
1	B	2684	0	2630	30	0
2	A	34	0	28	2	0
2	B	34	0	28	0	0
3	B	8	0	14	3	0
4	A	195	0	0	2	0
4	B	217	0	0	5	0
All	All	5884	0	5353	64	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 (64) 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:447:THR:HG21	1:A:694:PHE:O	1.69	0.91
1:A:447:THR:CG2	1:A:694:PHE:O	2.27	0.83
1:B:613:LEU:O	1:B:621:ARG:HD2	1.84	0.76
1:B:442:THR:HG21	4:B:2098:HOH:O	1.84	0.76
1:A:536:THR:HG22	1:A:537:ASN:H	1.51	0.74
1:B:471:GLN:NE2	4:B:2057:HOH:O	2.22	0.71
1:A:442:THR:HG21	4:A:2068:HOH:O	1.93	0.68
1:B:414:ASP:HB2	4:B:2044:HOH:O	1.95	0.65
1:B:467:MET:HE1	3:B:1713:MPD:HM3	1.78	0.65
1:A:402:THR:HG21	1:A:404:GLN:OE1	1.99	0.62
1:B:487:GLU:OE2	1:B:517:HIS:HD2	1.82	0.62
1:A:376:LYS:HB3	1:A:379:ASP:OD1	2.01	0.61
1:A:447:THR:HG22	1:A:695:SEP:HA	1.81	0.61
1:A:438:HIS:HD2	1:A:440:PHE:H	1.49	0.59
1:A:442:THR:HG22	1:A:523:PHE:HE1	1.68	0.59
1:A:678:ALA:HB1	1:A:683:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:ALA:HB1	1:A:683:ILE:CD1	2.33	0.59
1:A:450:THR:HG22	1:A:451:LYS:N	2.18	0.59
1:B:549:GLU:OE2	1:B:621:ARG:NH2	2.32	0.59
1:A:429:LYS:HE3	1:A:694:PHE:O	2.03	0.58
1:B:375:LEU:O	1:B:376:LYS:HB2	2.04	0.57
1:A:438:HIS:CD2	1:A:440:PHE:H	2.24	0.56
1:B:453:ASN:HD21	1:B:678:ALA:HB2	1.72	0.54
1:A:660:ASP:OD1	1:A:662:SER:HB2	2.08	0.54
1:B:377:ILE:HB	1:B:448:PHE:HE1	1.73	0.52
1:B:375:LEU:O	1:B:376:LYS:CB	2.57	0.52
1:B:545:TYR:OH	4:B:2114:HOH:O	2.18	0.52
1:A:450:THR:CG2	1:A:451:LYS:N	2.74	0.51
1:A:632:PRO:O	1:A:635:ARG:HB2	2.11	0.50
1:A:501:VAL:HG23	1:A:530:MET:HG3	1.93	0.50
1:A:387:GLY:HA3	2:A:1701:LG8:HAQ	1.93	0.50
1:B:442:THR:HG23	1:B:458:MET:CE	2.42	0.50
1:B:594:ASP:O	1:B:616:ARG:NH2	2.45	0.49
1:A:625:ARG:NH2	4:A:2151:HOH:O	2.45	0.49
1:B:467:MET:HE1	3:B:1713:MPD:CM	2.44	0.48
1:A:525:MET:HE1	1:A:541:GLY:N	2.29	0.48
1:B:580:HIS:HD2	4:B:2143:HOH:O	1.97	0.47
1:A:438:HIS:HE1	1:A:643:GLU:OE2	1.98	0.46
1:B:413:LYS:HD3	1:B:686:MET:HE2	1.98	0.46
1:A:522:ASP:HB2	2:A:1701:LG8:HBB1	1.97	0.46
1:A:692:ARG:HD3	1:A:692:ARG:HA	1.44	0.45
1:A:425:THR:HG21	1:A:454:LEU:HD13	1.98	0.45
1:B:615:VAL:O	1:B:621:ARG:HD3	2.15	0.45
1:B:513:ASP:HB3	1:B:515:ASP:H	1.82	0.44
1:A:672:LYS:HA	1:A:673:PRO:HD3	1.76	0.44
1:A:678:ALA:CB	1:A:683:ILE:CD1	2.95	0.44
1:A:533:ASP:OD2	1:A:533:ASP:N	2.46	0.44
1:A:388:LYS:HG3	1:A:393:LYS:HG2	2.00	0.43
1:B:527:LYS:HG2	1:B:536:THR:HG21	2.00	0.43
1:A:427:VAL:HG13	1:A:528:GLU:HG3	2.01	0.42
1:B:525:MET:HE1	1:B:541:GLY:HA2	2.01	0.42
1:A:460:TYR:CZ	1:A:462:ASN:HB3	2.55	0.42
1:B:677:PHE:HB3	1:B:678:ALA:H	1.57	0.42
1:B:542:THR:HA	1:B:543:PRO:HD3	1.93	0.41
1:B:439:PRO:HB2	1:B:645:LYS:HE3	2.01	0.41
1:A:430:ARG:O	1:A:433:SER:HB2	2.19	0.41
1:B:375:LEU:HD12	1:B:376:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ILE:HB	1:B:448:PHE:CE1	2.54	0.41
1:B:625:ARG:HG2	1:B:626:GLY:N	2.35	0.41
1:B:438:HIS:HE1	1:B:643:GLU:OE2	2.04	0.40
1:B:467:MET:CE	3:B:1713:MPD:HM3	2.50	0.40
1:A:467:MET:O	1:A:471:GLN:HG2	2.21	0.40
1:B:447:THR:HB	1:B:694:PHE:CE2	2.57	0.40
1:A:450:THR:CG2	1:A:451:LYS:H	2.34	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	322/352 (92%)	308 (96%)	13 (4%)	1 (0%)	41	50
1	B	316/352 (90%)	296 (94%)	16 (5%)	4 (1%)	12	12
All	All	638/704 (91%)	604 (95%)	29 (4%)	5 (1%)	19	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	LYS
1	B	376	LYS
1	B	678	ALA
1	B	513	ASP
1	B	675	LEU

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	293/319 (92%)	277 (94%)	16 (6%)	21	29
1	B	289/319 (91%)	280 (97%)	9 (3%)	40	55
All	All	582/638 (91%)	557 (96%)	25 (4%)	29	40

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	375	LEU
1	A	379	ASP
1	A	434	LEU
1	A	447	THR
1	A	472	SER
1	A	508	ASP
1	A	511	LEU
1	A	518	ILE
1	A	531	LEU
1	A	533	ASP
1	A	535	LYS
1	A	536	THR
1	A	569	LEU
1	A	622	LEU
1	A	625	ARG
1	A	662	SER
1	B	434	LEU
1	B	442	THR
1	B	508	ASP
1	B	540	CYS
1	B	569	LEU
1	B	622	LEU
1	B	680	ARG
1	B	690	MET
1	B	697	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	438	HIS
1	A	558	HIS

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Mol	Chain	Res	Type
1	B	403	ASN
1	B	438	HIS
1	B	453	ASN
1	B	517	HIS
1	B	558	HIS
1	B	580	HIS
1	B	684	ASN
1	B	710	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	SEP	A	695	1	8,9,10	1.81	2 (25%)	8,12,14	1.41	1 (12%)
1	SEP	A	676	1	8,9,10	1.65	1 (12%)	8,12,14	3.09	2 (25%)
1	SEP	B	695	1	8,9,10	1.68	1 (12%)	8,12,14	1.89	3 (37%)
1	SEP	B	676	1	8,9,10	1.60	1 (12%)	8,12,14	1.87	2 (25%)

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
1	SEP	A	695	1	-	0/5/8/10	-
1	SEP	A	676	1	-	3/5/8/10	-
1	SEP	B	695	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	676	1	-	2/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	695	SEP	P-O1P	3.72	1.62	1.50
1	A	695	SEP	P-O1P	3.72	1.62	1.50
1	A	676	SEP	P-O1P	3.54	1.61	1.50
1	B	676	SEP	P-O1P	3.43	1.61	1.50
1	A	695	SEP	P-O3P	2.46	1.64	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	SEP	OG-CB-CA	6.74	114.70	108.14
1	A	676	SEP	P-OG-CB	-4.78	105.12	118.30
1	B	676	SEP	OG-CB-CA	4.25	112.28	108.14
1	A	695	SEP	P-OG-CB	-3.15	109.61	118.30
1	B	695	SEP	P-OG-CB	-3.04	109.91	118.30
1	B	695	SEP	O2P-P-OG	-2.55	99.95	106.73
1	B	676	SEP	P-OG-CB	-2.44	111.58	118.30
1	B	695	SEP	O3P-P-OG	2.10	112.31	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	676	SEP	CB-OG-P-O2P
1	B	695	SEP	N-CA-CB-OG
1	A	676	SEP	CB-OG-P-O1P
1	A	676	SEP	CB-OG-P-O3P
1	B	676	SEP	CA-CB-OG-P
1	B	676	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	695	SEP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	MPD	B	1713	-	7,7,7	0.36	0	9,10,10	0.68	0
2	LG8	A	1701	-	37,39,39	1.60	9 (24%)	42,59,59	2.06	11 (26%)
2	LG8	B	1712	-	37,39,39	1.60	8 (21%)	42,59,59	1.86	8 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	1713	-	-	3/5/5/5	-
2	LG8	A	1701	-	-	4/12/65/65	0/6/6/6
2	LG8	B	1712	-	-	5/12/65/65	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	LG8	CAL-CAG	3.62	1.48	1.39
2	B	1712	LG8	CAL-CAG	3.56	1.48	1.39
2	B	1712	LG8	CAM-CAH	3.39	1.49	1.36
2	A	1701	LG8	CAM-CAH	3.24	1.49	1.36
2	A	1701	LG8	CAK-CAL	3.14	1.51	1.45
2	B	1712	LG8	CAK-CAL	3.13	1.51	1.45
2	B	1712	LG8	CAX-NAW	-3.06	1.34	1.40
2	A	1701	LG8	CAS-NAT	-2.82	1.36	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1712	LG8	C6-CBF	2.80	1.57	1.53
2	A	1701	LG8	CAX-NAW	-2.70	1.35	1.40
2	B	1712	LG8	CAG-CAH	-2.54	1.36	1.45
2	B	1712	LG8	CAU-CAL	-2.45	1.36	1.42
2	A	1701	LG8	CAG-CAH	-2.44	1.36	1.45
2	A	1701	LG8	CAU-CAL	-2.30	1.36	1.42
2	A	1701	LG8	C6-CBF	2.24	1.56	1.53
2	B	1712	LG8	CAN-CAM	2.22	1.51	1.46
2	A	1701	LG8	CAN-CAM	2.08	1.51	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701	LG8	CAS-CAK-CAL	-7.76	102.45	106.87
2	B	1712	LG8	CAS-CAK-CAL	-7.33	102.69	106.87
2	A	1701	LG8	CAX-CAN-CAM	-4.64	103.58	107.57
2	B	1712	LG8	CAX-CAN-CAM	-4.28	103.89	107.57
2	A	1701	LG8	CAL-CAG-CAH	3.83	131.78	126.98
2	B	1712	LG8	CAL-CAG-CAH	3.61	131.50	126.98
2	A	1701	LG8	CAC-NAD-CAE	-3.40	107.70	111.29
2	B	1712	LG8	CAC-NAD-CAE	-3.22	107.89	111.29
2	A	1701	LG8	CBD-CBF-C6	2.73	112.18	109.10
2	A	1701	LG8	CBF-C6-CAV	2.58	116.07	110.71
2	A	1701	LG8	CBA-NAT-CAS	-2.56	123.19	125.71
2	B	1712	LG8	CBF-C6-CAV	2.54	115.99	110.71
2	A	1701	LG8	CAG-CAC-NAD	2.44	110.57	106.12
2	A	1701	LG8	CAS-NAT-CAU	2.36	110.90	108.57
2	B	1712	LG8	CAH-CAE-NAD	2.35	110.41	106.12
2	B	1712	LG8	CBD-CBF-C6	2.26	111.65	109.10
2	A	1701	LG8	CAH-CAE-NAD	2.14	110.02	106.12
2	A	1701	LG8	CAR-CAS-NAT	-2.08	128.44	131.16
2	B	1712	LG8	CBJ-NBH-CBG	2.06	116.41	111.01

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1701	LG8	CAE-CAH-CAM-CAV
2	A	1701	LG8	CAC-CAG-CAL-CAU
2	B	1712	LG8	CAE-CAH-CAM-CAV
2	B	1712	LG8	CAC-CAG-CAL-CAU
2	B	1712	LG8	CBF-CBG-NBH-CBJ

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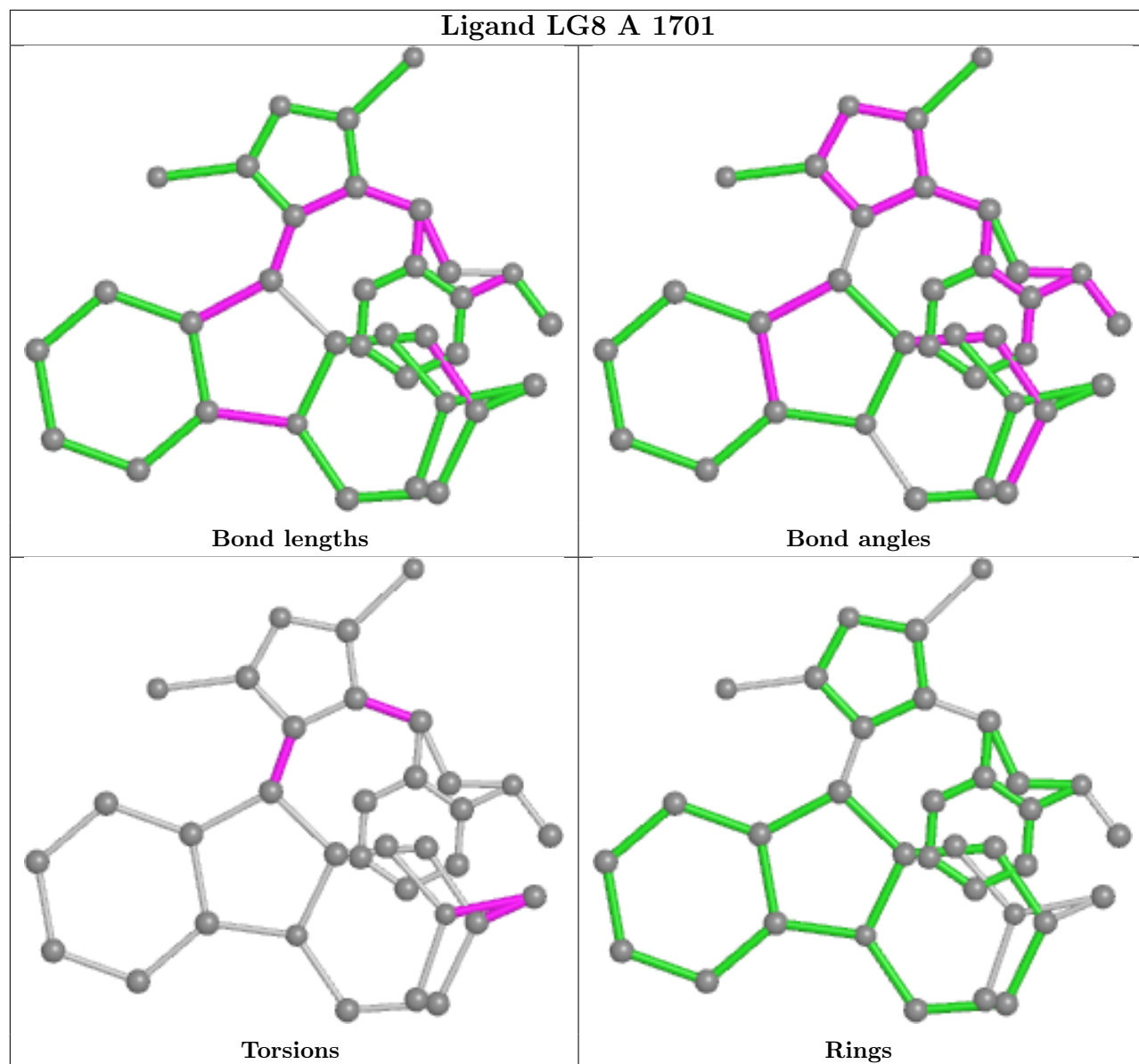
Mol	Chain	Res	Type	Atoms
3	B	1713	MPD	O2-C2-C3-C4
3	B	1713	MPD	C2-C3-C4-C5
2	A	1701	LG8	CBF-CBG-NBH-CBJ
2	B	1712	LG8	CBF-CBG-NBH-CBI
2	A	1701	LG8	CBD-CBF-CBG-NBH
2	B	1712	LG8	CBD-CBF-CBG-NBH
3	B	1713	MPD	C2-C3-C4-O4

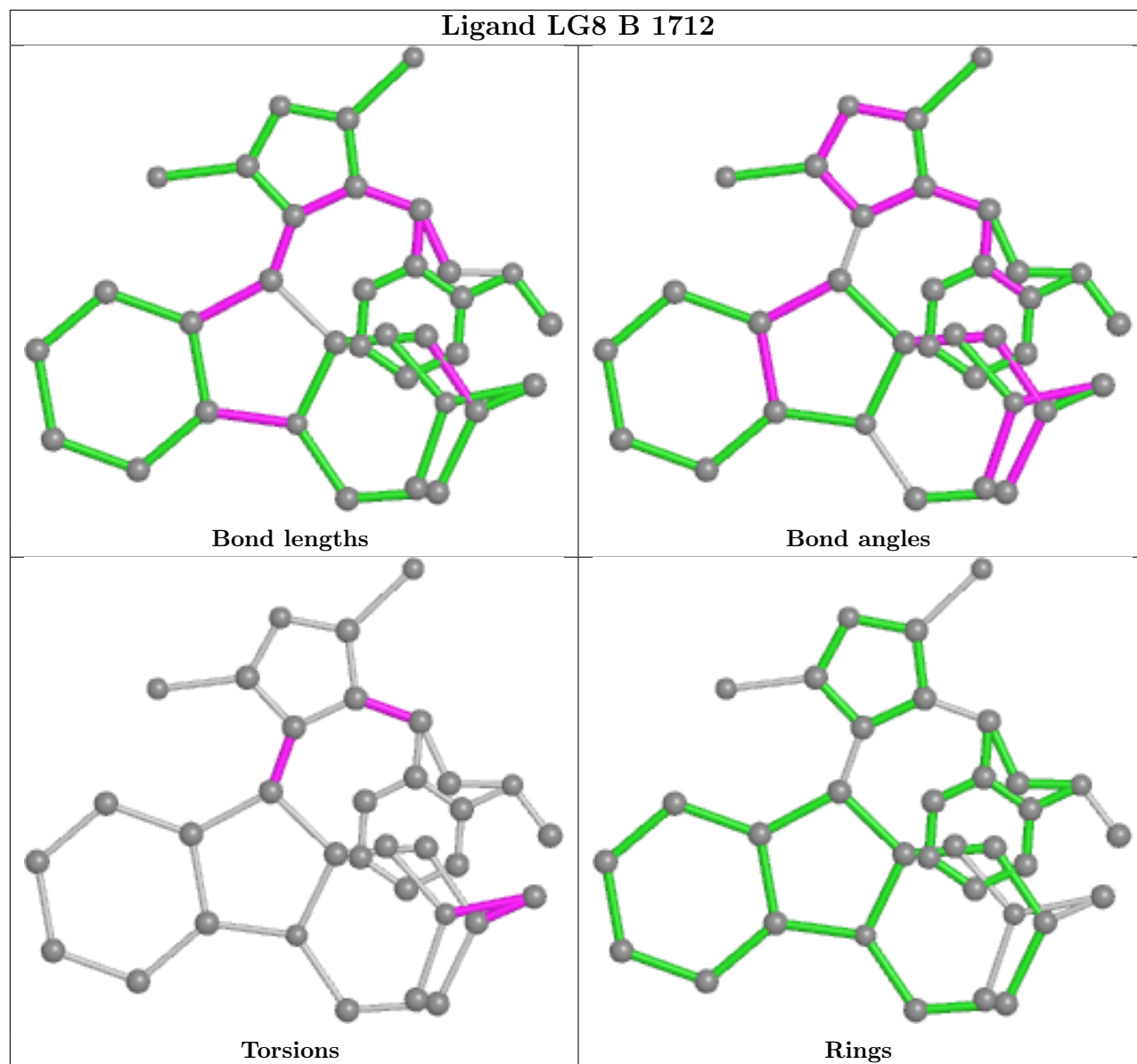
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1713	MPD	3	0
2	A	1701	LG8	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	540:CYS	C	541:GLY	N	1.12

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	324/352 (92%)	0.68	37 (11%) 5 7	26, 47, 59, 71	0
1	B	320/352 (90%)	0.80	42 (13%) 3 4	37, 47, 66, 92	0
All	All	644/704 (91%)	0.74	79 (12%) 4 6	26, 47, 62, 92	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	ALA	7.4
1	B	711	HIS	6.4
1	B	674	ARG	6.4
1	B	710	HIS	5.8
1	B	533	ASP	5.3
1	A	677	PHE	5.3
1	B	709	HIS	5.1
1	B	656	LYS	5.0
1	B	375	LEU	5.0
1	B	679	ASP	4.9
1	A	692	ARG	4.6
1	B	692	ARG	4.1
1	B	657	SER	3.9
1	A	693	ASN	3.8
1	B	685	SER	3.7
1	A	532	GLY	3.6
1	A	698	ASN	3.6
1	A	401	LYS	3.5
1	B	401	LYS	3.5
1	A	547	ALA	3.2
1	A	540	CYS	3.2
1	A	533	ASP	3.1
1	A	689	ASN	3.1
1	B	705	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	483	PHE	3.0
1	A	699	PRO	2.9
1	B	378	GLU	2.9
1	B	400	LYS	2.8
1	A	560	VAL	2.7
1	A	511	LEU	2.7
1	A	563	TRP	2.7
1	A	375	LEU	2.7
1	A	484	TYR	2.7
1	B	579	PHE	2.6
1	B	687	ASP	2.6
1	B	689	ASN	2.6
1	A	680	ARG	2.6
1	B	402	THR	2.5
1	B	707	HIS	2.5
1	B	399	PHE	2.5
1	B	486	ALA	2.5
1	B	686	MET	2.5
1	B	404	GLN	2.5
1	A	520	ILE	2.5
1	B	702	GLU	2.5
1	B	403	ASN	2.5
1	A	688	GLN	2.4
1	A	512	LEU	2.4
1	A	579	PHE	2.4
1	B	567	VAL	2.4
1	B	617	GLU	2.4
1	B	655	VAL	2.4
1	B	560	VAL	2.3
1	A	591	ILE	2.3
1	B	706	SER	2.3
1	A	400	LYS	2.3
1	A	574	ILE	2.3
1	A	488	ILE	2.3
1	A	510	ILE	2.3
1	B	547	ALA	2.3
1	A	486	ALA	2.2
1	B	534	ALA	2.2
1	A	464	GLY	2.2
1	A	700	GLY	2.2
1	B	563	TRP	2.2
1	B	585	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	687	ASP	2.2
1	A	531	LEU	2.1
1	B	485	ALA	2.1
1	A	674	ARG	2.1
1	A	697	MET	2.1
1	A	466	LEU	2.1
1	B	512	LEU	2.1
1	A	436	TRP	2.1
1	B	548	PRO	2.1
1	B	518	ILE	2.0
1	A	403	ASN	2.0
1	B	546	ILE	2.0
1	A	402	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	B	676	10/11	0.70	0.45	86,87,87,87	0
1	SEP	A	695	10/11	0.86	0.13	50,55,57,57	0
1	SEP	B	695	10/11	0.87	0.15	43,44,49,51	0
1	SEP	A	676	10/11	0.92	0.14	55,57,64,64	0

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.

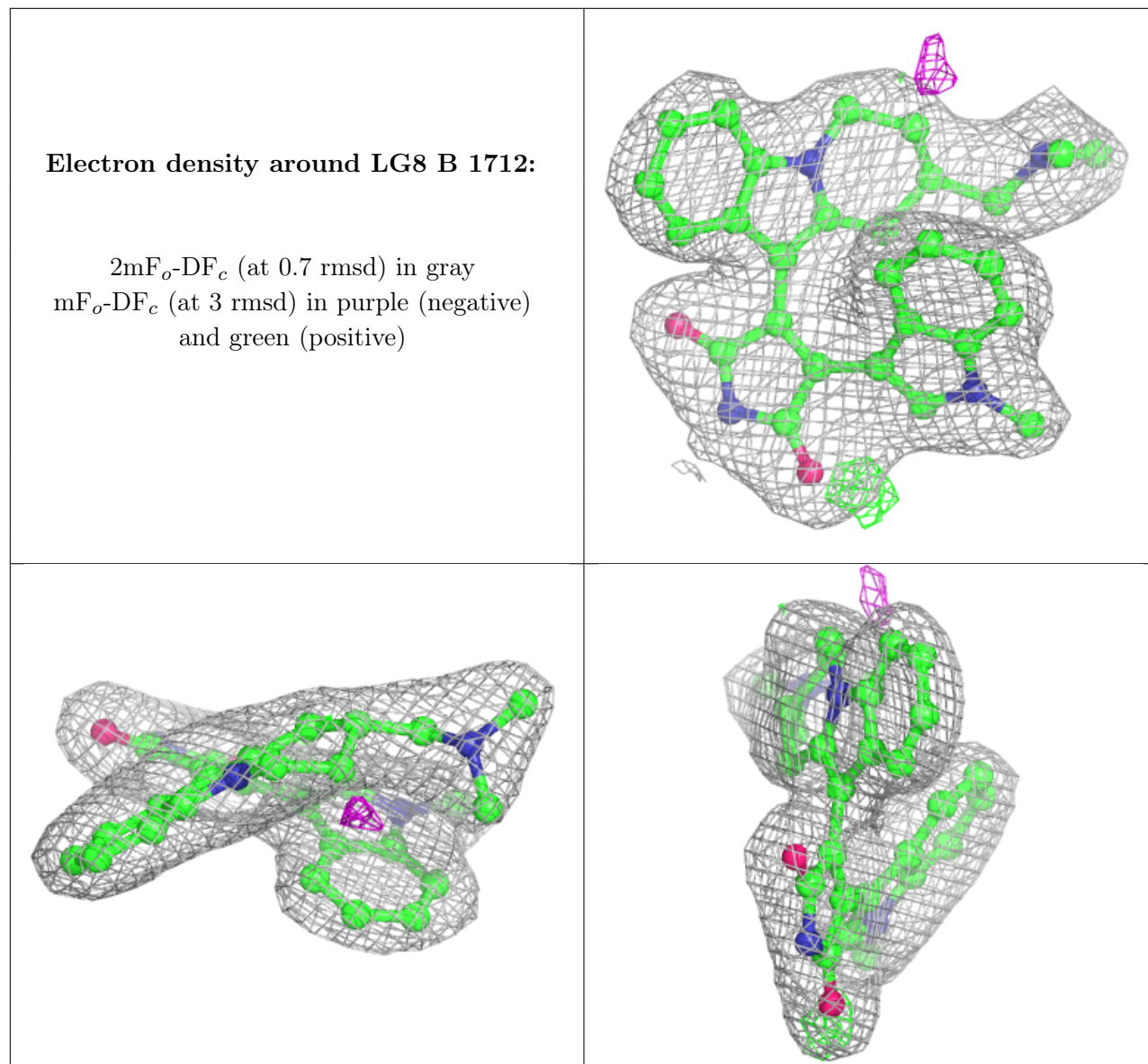
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MPD	B	1713	8/8	0.84	0.29	59,61,62,65	0

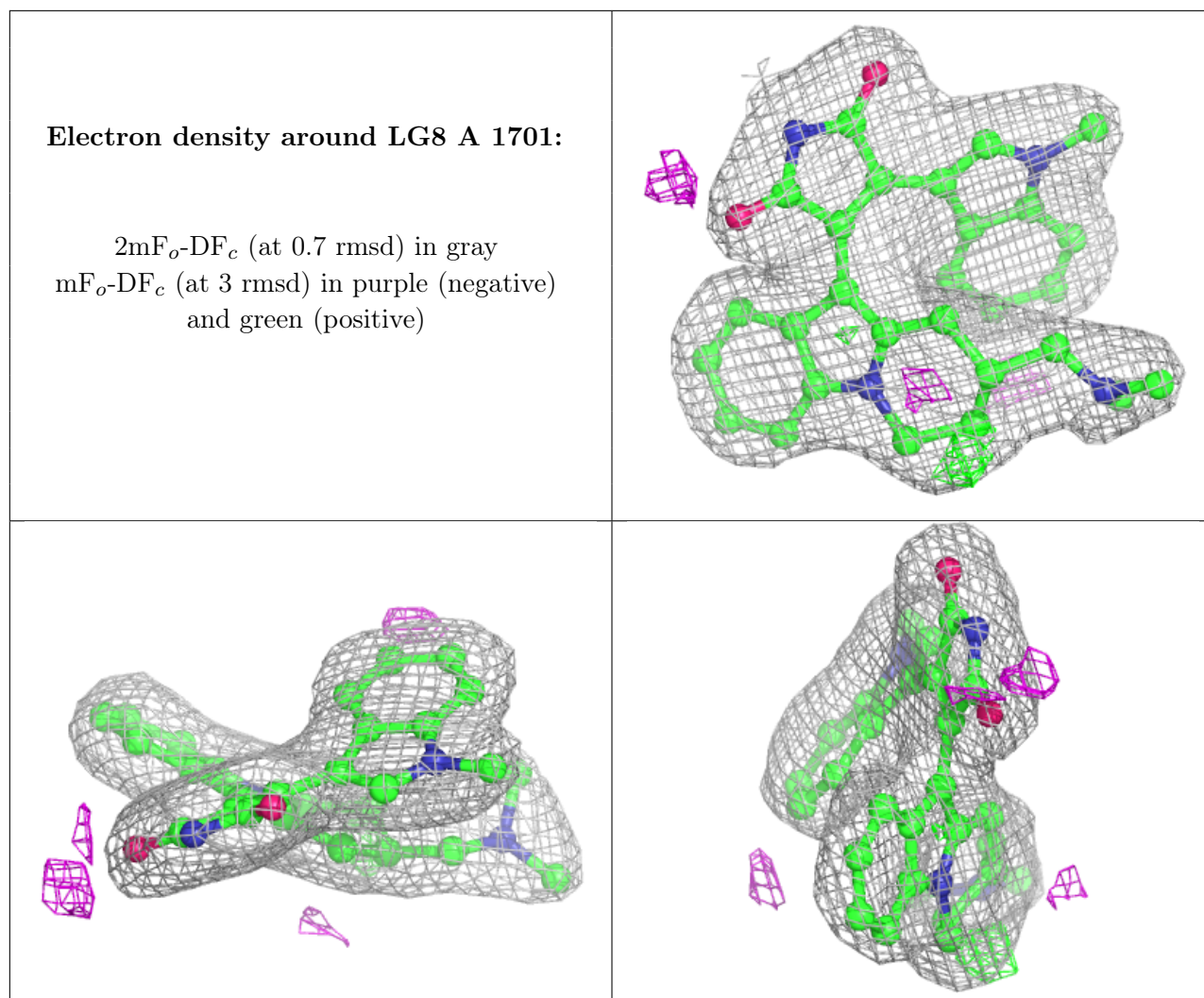
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LG8	B	1712	34/34	0.96	0.15	38,41,46,49	0
2	LG8	A	1701	34/34	0.96	0.20	35,39,42,45	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.