



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 03:27 PM EDT

PDB ID : 1ZKY
Title : Human Estrogen Receptor Alpha Ligand-Binding Domain In Complex With
OBCP-3M and A Glucocorticoid Receptor Interacting Protein 1 Nr Box II
Peptide
Authors : Rajan, S.S.; Hsieh, R.W.; Sharma, S.K.; Hahm, J.B.; Nettles, K.W.; Greene,
G.L.
Deposited on : 2005-05-04
Resolution : 2.25 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 : 2.23.2
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) : 2.23.2

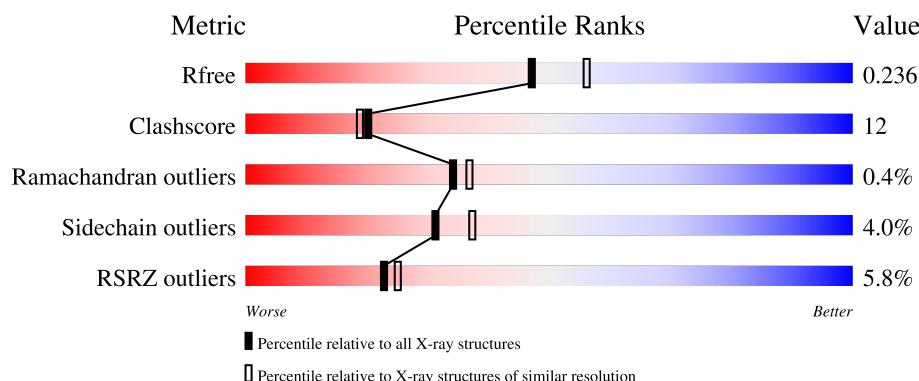
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	257	 6% 74% 17% • 7%
1	B	257	 5% 72% 19% • 5%
2	C	13	 15% 54% 23% 23%
2	D	13	 62% 8% 31%

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
3	689	A	700	X	-	-	-
3	689	B	801	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4277 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	9	0
			1943	1241	329	349	24			
1	B	245	Total	C	N	O	S	0	4	0
			1980	1265	335	355	25			

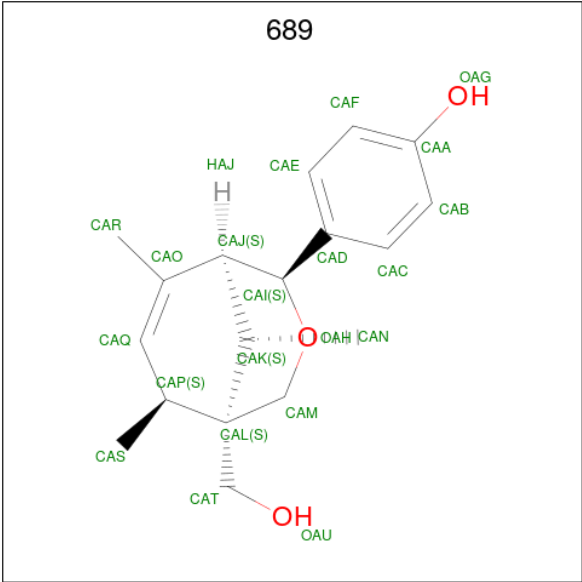
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	CME	CYS	modified residue	UNP P03372
A	417	CME	CYS	modified residue	UNP P03372
A	530	CME	CYS	modified residue	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372
B	381	CME	CYS	modified residue	UNP P03372
B	417	CME	CYS	modified residue	UNP P03372
B	530	CME	CYS	modified residue	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	10	Total	C	N	O	0	0	0
			89	57	19	13			
2	D	9	Total	C	N	O	0	0	0
			79	51	16	12			

- Molecule 3 is 4-[(1S,2S,5S)-5-(HYDROXYMETHYL)-6,8,9-TRIMETHYL-3-OXABICYCLO[3.3.1]NON-7-EN-2-YL]PHENOL (three-letter code: 689) (formula: C₁₈H₂₄O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	18	3		
3	B	1	Total	C	O	0	0
			21	18	3		

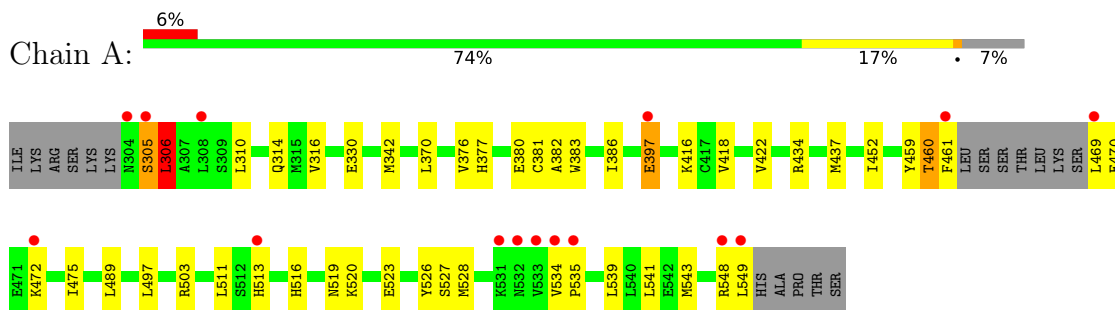
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	78	Total	O	0	0
			78	78		
4	C	1	Total	O	0	0
			1	1		

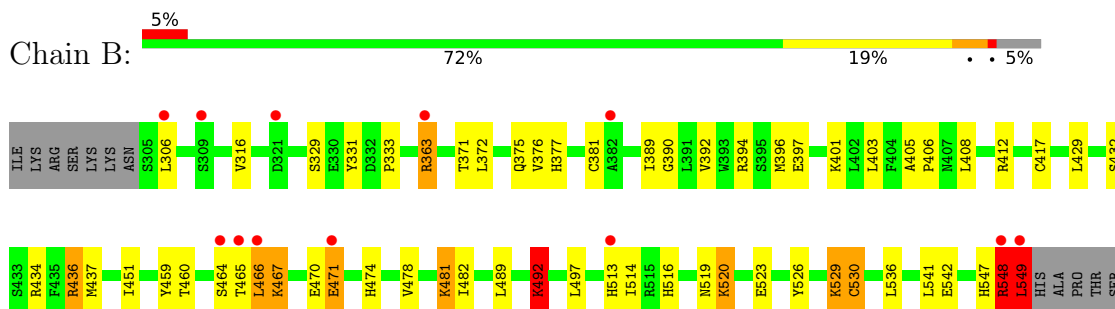
3 Residue-property plots [i](#)

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.

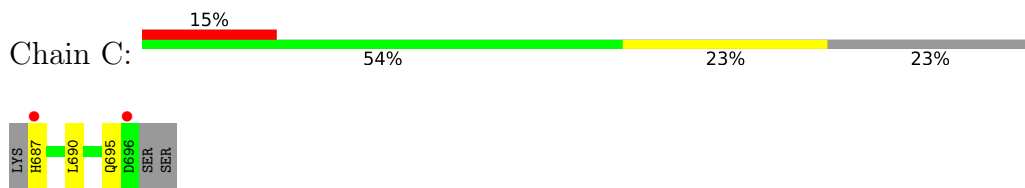
- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor



- Molecule 2: Nuclear receptor coactivator 2



- Molecule 2: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.93Å 84.13Å 58.22Å 90.00° 109.06° 90.00°	Depositor
Resolution (Å)	27.01 – 2.25 27.01 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.01-2.25) 99.6 (27.01-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.2.0005, XTALVIEW	Depositor
R, R_{free}	0.185 , 0.231 0.193 , 0.236	Depositor DCC
R_{free} test set	1233 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4277	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% 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: CME, 689

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	0.45	0/1976	0.58	2/2664 (0.1%)
1	B	0.44	0/1990	0.65	9/2684 (0.3%)
2	C	0.40	0/90	0.43	0/119
2	D	0.41	0/79	0.50	0/104
All	All	0.44	0/4135	0.61	11/5571 (0.2%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	ARG	CD-NE-CZ	10.86	138.80	123.60
1	B	548	ARG	CB-CA-C	9.28	128.96	110.40
1	B	549	LEU	CB-CA-C	-6.68	97.50	110.20
1	B	492	LYS	CB-CA-C	-6.19	98.02	110.40
1	B	481	LYS	CB-CA-C	-6.04	98.31	110.40
1	B	437	MET	CB-CA-C	5.86	122.13	110.40
1	B	471	GLU	CB-CA-C	5.83	122.05	110.40
1	B	513[A]	HIS	CB-CA-C	5.58	121.56	110.40
1	B	513[B]	HIS	CB-CA-C	5.58	121.56	110.40
1	A	397	GLU	CB-CA-C	5.33	121.06	110.40
1	B	467	LYS	CB-CA-C	5.15	120.69	110.40

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	1943	0	1983	43	0
1	B	1980	0	2038	68	0
2	C	89	0	95	1	0
2	D	79	0	88	1	0
3	A	21	0	23	4	0
3	B	21	0	23	3	0
4	A	65	0	0	1	0
4	B	78	0	0	2	0
4	C	1	0	0	0	0
All	All	4277	0	4250	105	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 12.

All (105) 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:B:396:MET:O	1:B:436:ARG:HD3	1.39	1.22
1:B:549:LEU:HD22	1:B:549:LEU:N	1.61	1.16
1:B:526:TYR:OH	1:B:530:CME:HZ3	1.51	1.08
1:A:519:ASN:ND2	1:B:519:ASN:HD22	1.63	0.97
1:A:519:ASN:HD22	1:B:519:ASN:ND2	1.65	0.93
1:B:549:LEU:N	1:B:549:LEU:CD2	2.30	0.91
1:B:377:HIS:NE2	1:B:460:THR:HG23	1.86	0.91
1:B:523:GLU:OE1	1:B:549:LEU:HB3	1.75	0.86
1:A:381[B]:CME:HB3	1:A:381[B]:CME:HZ2	1.56	0.86
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.60	0.84
1:A:377:HIS:CE1	1:A:381[A]:CME:SD	2.71	0.84
1:B:549:LEU:HD22	1:B:549:LEU:H	1.49	0.77
1:B:481:LYS:NZ	1:B:481:LYS:HB3	1.99	0.77
1:A:377:HIS:O	1:A:381[A]:CME:SG	2.43	0.76
1:A:516:HIS:CE1	1:B:381[A]:CME:HZ2	2.22	0.75
1:B:523:GLU:OE1	1:B:549:LEU:CB	2.35	0.74
1:A:434:ARG:HH11	1:A:437:MET:HE2	1.53	0.74
1:B:526:TYR:OH	1:B:530:CME:CZ	2.35	0.74
1:B:363:ARG:HH21	1:B:363:ARG:CG	2.01	0.74
1:B:396:MET:O	1:B:436:ARG:CD	2.29	0.73
1:B:363:ARG:NH2	1:B:363:ARG:HG2	2.04	0.72
1:B:481:LYS:HB3	1:B:481:LYS:HZ2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381[A]:CME:SD	1:B:460:THR:HG21	2.32	0.68
1:A:381[A]:CME:OH	1:A:460:THR:HG21	1.93	0.68
3:A:700:689:CAP	3:A:700:689:HAI	2.23	0.67
1:B:363:ARG:HH21	1:B:363:ARG:HG2	1.57	0.67
1:B:548:ARG:C	1:B:549:LEU:HD22	2.15	0.66
1:B:306:LEU:HD12	1:B:306:LEU:H	1.61	0.65
1:B:381[A]:CME:OH	1:B:547:HIS:CE1	2.50	0.64
1:A:381[B]:CME:HZ2	1:A:381[B]:CME:CB	2.28	0.64
1:B:516:HIS:O	1:B:520:LYS:HG2	1.98	0.63
1:A:513[B]:HIS:CD2	1:B:459:TYR:HD1	2.18	0.61
1:B:401:LYS:HE3	4:B:95:HOH:O	1.99	0.61
1:B:331:TYR:CZ	1:B:333:PRO:HA	2.36	0.61
1:A:377:HIS:NE2	1:A:460:THR:HB	2.16	0.60
1:A:519:ASN:HD22	1:B:519:ASN:HD22	0.81	0.59
1:A:548:ARG:O	1:A:549:LEU:HB2	2.02	0.59
1:B:465:THR:O	1:B:466:LEU:HB2	2.03	0.59
1:A:382:ALA:O	1:A:386[B]:ILE:HG12	2.04	0.58
1:B:492:LYS:HE3	1:B:492:LYS:CA	2.34	0.58
1:A:516:HIS:NE2	1:B:381[A]:CME:HZ2	2.18	0.57
1:B:329[B]:SER:OG	1:B:405:ALA:HB3	2.06	0.56
1:B:371:THR:O	1:B:375:GLN:HG3	2.06	0.56
1:B:329[B]:SER:OG	1:B:405:ALA:CB	2.55	0.55
1:A:516:HIS:CE1	1:B:381[A]:CME:CZ	2.90	0.54
1:B:381[B]:CME:HE3	1:B:460:THR:HG21	1.89	0.54
3:A:700:689:CAP	3:A:700:689:CAI	2.83	0.54
1:A:534:VAL:HG22	1:A:535:PRO:HD2	1.90	0.54
1:A:469:LEU:CB	1:A:472:LYS:HD3	2.38	0.54
1:B:389:ILE:HD12	1:B:514:ILE:CD1	2.38	0.53
1:A:370:LEU:CD1	1:A:475:ILE:HD11	2.36	0.53
3:B:801:689:CAO	3:B:801:689:CAM	2.43	0.52
1:B:492:LYS:HE3	1:B:492:LYS:HA	1.91	0.52
1:A:526:TYR:CD1	1:A:548:ARG:HD2	2.45	0.52
1:B:460:THR:HG22	4:B:67:HOH:O	2.10	0.52
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.91	0.52
3:A:700:689:HAI	3:A:700:689:HAP	1.92	0.51
1:A:539:LEU:O	1:A:543:MET:HG2	2.12	0.50
1:B:474:HIS:O	1:B:478:VAL:HG23	2.11	0.50
1:A:497:LEU:HD11	1:B:497:LEU:HD11	1.94	0.50
1:A:380:GLU:O	1:A:383:TRP:HD1	1.95	0.50
1:B:331:TYR:CE2	1:B:333:PRO:HA	2.47	0.49
1:B:529:LYS:HG3	1:B:530:CME:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:THR:O	1:B:466:LEU:CB	2.61	0.49
1:A:434:ARG:HD3	1:B:459:TYR:CE2	2.48	0.49
1:A:520:LYS:O	1:A:523:GLU:HG2	2.13	0.49
1:A:370:LEU:HD21	1:A:475:ILE:HD11	1.95	0.48
1:B:403:LEU:HD11	1:B:406:PRO:HA	1.96	0.47
1:B:542:GLU:OE1	2:D:689:ILE:HD13	2.14	0.47
1:A:434:ARG:NE	1:B:459:TYR:OH	2.47	0.47
1:A:513[B]:HIS:CD2	1:B:459:TYR:CD1	3.01	0.47
1:B:390:GLY:O	1:B:394:ARG:HG3	2.15	0.47
1:A:416:LYS:HA	4:A:79:HOH:O	2.15	0.47
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.98	0.46
1:B:549:LEU:O	1:B:549:LEU:HD23	2.16	0.45
1:A:416:LYS:HG3	1:A:422:VAL:HB	1.98	0.45
1:B:492:LYS:HE3	1:B:492:LYS:N	2.32	0.44
1:B:412:ARG:HB2	1:B:429:LEU:CD1	2.47	0.44
1:A:459:TYR:CZ	1:B:434:ARG:HG2	2.52	0.44
1:A:461:PHE:HD2	1:A:472:LYS:HG2	1.82	0.44
1:A:534:VAL:CG2	1:A:535:PRO:HD2	2.48	0.43
1:B:392:VAL:HG13	1:B:432:SER:HA	1.99	0.43
1:B:451:ILE:HG13	1:B:482:ILE:HG21	2.00	0.43
3:B:801:689:HAC	3:B:801:689:HAJ	1.78	0.43
1:B:464:SER:O	1:B:467:LYS:HE3	2.18	0.43
1:B:397:GLU:OE2	1:B:397:GLU:HA	2.17	0.43
1:A:452:ILE:HD11	1:A:511:LEU:HD22	2.01	0.42
3:A:700:689:HAS1	3:A:700:689:HAT2	1.52	0.42
1:A:376:VAL:HG13	2:C:690:LEU:HD23	2.00	0.42
1:A:310:LEU:HD22	1:A:314:GLN:HB3	2.01	0.42
1:B:536:LEU:HB2	1:B:541:LEU:CD2	2.49	0.42
1:B:377:HIS:CE1	1:B:460:THR:HG23	2.51	0.42
1:B:481:LYS:NZ	1:B:481:LYS:CB	2.76	0.42
1:B:536:LEU:HB2	1:B:541:LEU:HD21	2.00	0.42
1:A:528:MET:HA	1:A:528:MET:HE2	2.01	0.42
1:A:513[B]:HIS:NE2	1:B:459:TYR:CD1	2.88	0.41
1:B:372:LEU:O	1:B:376:VAL:HG23	2.21	0.41
1:A:305:SER:OG	1:A:306:LEU:N	2.54	0.41
1:B:549:LEU:CD2	1:B:549:LEU:H	2.15	0.41
1:B:520:LYS:HB3	1:B:520:LYS:NZ	2.36	0.41
1:B:526:TYR:CZ	1:B:530:CME:HZ3	2.47	0.41
3:B:801:689:HAI	3:B:801:689:HAN2	1.57	0.41
1:B:405:ALA:HB3	1:B:408:LEU:HB3	2.02	0.41
1:A:342[B]:MET:HG2	1:A:418:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLU:OE2	1:A:330:GLU:N	2.48	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	240/257 (93%)	236 (98%)	2 (1%)	2 (1%)	19	17
1	B	243/257 (95%)	239 (98%)	4 (2%)	0	100	100
2	C	8/13 (62%)	8 (100%)	0	0	100	100
2	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	498/540 (92%)	490 (98%)	6 (1%)	2 (0%)	34	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	SER
1	A	306	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	219/229 (96%)	212 (97%)	7 (3%)	39	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	221/229 (96%)	211 (96%)	10 (4%)	27	31
2	C	10/13 (77%)	8 (80%)	2 (20%)	1	0
2	D	9/13 (69%)	9 (100%)	0	100	100
All	All	459/484 (95%)	440 (96%)	19 (4%)	31	36

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	LEU
1	A	397	GLU
1	A	460	THR
1	A	470	GLU
1	A	527[A]	SER
1	A	527[B]	SER
1	A	541	LEU
1	B	363	ARG
1	B	436	ARG
1	B	466	LEU
1	B	470	GLU
1	B	471	GLU
1	B	492	LYS
1	B	520	LYS
1	B	529	LYS
1	B	548	ARG
1	B	549	LEU
2	C	687	HIS
2	C	695	GLN

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	373	HIS
1	A	488	HIS
1	A	498	GLN
1	A	519	ASN
1	A	532	ASN
1	B	359	ASN
1	B	455	ASN
1	B	547	HIS
2	C	691	HIS

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Mol	Chain	Res	Type
2	C	695	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 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	CME	B	530	1	8,9,10	1.35	2 (25%)	5,9,11	1.88	2 (40%)
1	CME	A	417	1	8,9,10	0.76	0	5,9,11	0.64	0
1	CME	B	381[A]	-	8,9,10	0.80	0	5,9,11	0.51	0
1	CME	B	381[B]	-	8,9,10	0.80	0	5,9,11	0.51	0
1	CME	A	381[A]	-	8,9,10	0.65	0	5,9,11	0.97	0
1	CME	A	381[B]	-	8,9,10	0.66	0	5,9,11	0.97	0
1	CME	A	530	1	4,5,10	0.51	0	1,5,11	0.08	0
1	CME	B	417	1	8,9,10	2.26	1 (12%)	5,9,11	1.09	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
1	CME	B	530	1	-	1/5/8/10	-
1	CME	A	417	1	-	3/5/8/10	-
1	CME	B	381[A]	-	-	2/5/8/10	-
1	CME	B	381[B]	-	-	2/5/8/10	-
1	CME	A	381[A]	-	-	2/5/8/10	-
1	CME	A	381[B]	-	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CME	A	530	1	-	0/1/4/10	-
1	CME	B	417	1	-	2/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	417	CME	O-C	5.82	1.43	1.19
1	B	530	CME	OH-CZ	2.43	1.54	1.42
1	B	530	CME	CE-CZ	2.00	1.63	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	CME	OH-CZ-CE	-2.97	99.12	110.83
1	B	530	CME	CZ-CE-SD	-2.61	104.30	113.37

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	417	CME	CA-CB-SG-SD
1	A	417	CME	CZ-CE-SD-SG
1	B	381[A]	CME	CE-SD-SG-CB
1	B	381[A]	CME	SD-CE-CZ-OH
1	A	381[B]	CME	CE-SD-SG-CB
1	A	417	CME	CE-SD-SG-CB
1	B	417	CME	CE-SD-SG-CB
1	A	381[A]	CME	CE-SD-SG-CB
1	B	381[B]	CME	SD-CE-CZ-OH
1	B	381[B]	CME	CZ-CE-SD-SG
1	A	381[A]	CME	CA-CB-SG-SD
1	B	417	CME	CZ-CE-SD-SG
1	B	530	CME	CZ-CE-SD-SG

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	530	CME	4	0
1	B	381[A]	CME	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	381[B]	CME	1	0
1	A	381[A]	CME	3	0
1	A	381[B]	CME	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	689	A	700	-	22,23,23	2.05	6 (27%)	26,35,35	2.53	8 (30%)
3	689	B	801	-	22,23,23	2.09	6 (27%)	26,35,35	3.41	11 (42%)

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	689	A	700	-	3/3/6/7	0/7/41/41	1/3/3/3
3	689	B	801	-	2/2/6/7	1/7/41/41	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	689	OAH-CAI	-5.20	1.38	1.43
3	B	801	689	CAJ-CAO	5.12	1.58	1.51
3	A	700	689	CAP-CAQ	4.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	700	689	CAQ-CAO	4.13	1.38	1.33
3	B	801	689	CAQ-CAO	3.76	1.37	1.33
3	B	801	689	CAL-CAP	-3.52	1.50	1.55
3	B	801	689	OAH-CAM	3.47	1.48	1.43
3	B	801	689	CAJ-CAI	-3.13	1.48	1.54
3	B	801	689	CAL-CAK	-3.10	1.50	1.55
3	A	700	689	CAJ-CAO	-2.82	1.47	1.51
3	A	700	689	CAL-CAK	-2.56	1.51	1.55
3	A	700	689	CAS-CAP	-2.04	1.50	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	689	OAH-CAM-CAL	9.52	121.98	110.52
3	B	801	689	CAD-CAI-CAJ	-7.31	103.12	114.93
3	A	700	689	OAH-CAI-CAD	6.68	118.84	107.84
3	B	801	689	OAH-CAI-CAD	6.57	118.67	107.84
3	A	700	689	CAM-OAH-CAI	-6.41	104.61	112.01
3	B	801	689	CAM-OAH-CAI	5.91	118.85	112.01
3	A	700	689	OAH-CAM-CAL	4.53	115.97	110.52
3	A	700	689	CAS-CAP-CAL	-4.34	106.73	115.71
3	B	801	689	CAR-CAO-CAJ	4.21	122.75	117.02
3	B	801	689	CAR-CAO-CAQ	-3.88	115.25	123.56
3	A	700	689	CAL-CAK-CAJ	-3.28	105.37	109.86
3	B	801	689	CAS-CAP-CAQ	-3.07	105.50	111.41
3	B	801	689	CAP-CAL-CAK	-2.99	104.61	111.25
3	A	700	689	CAR-CAO-CAJ	2.92	121.01	117.02
3	A	700	689	CAM-CAL-CAT	-2.62	106.91	110.84
3	B	801	689	CAL-CAK-CAJ	-2.57	106.34	109.86
3	B	801	689	CAN-CAK-CAL	-2.38	111.59	114.54
3	B	801	689	CAS-CAP-CAL	-2.26	111.03	115.71
3	A	700	689	CAJ-CAO-CAQ	-2.04	114.46	120.28

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	700	689	CAP
3	A	700	689	CAK
3	A	700	689	CAI
3	B	801	689	CAP
3	B	801	689	CAK

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	801	689	CAC-CAD-CAI-CAJ

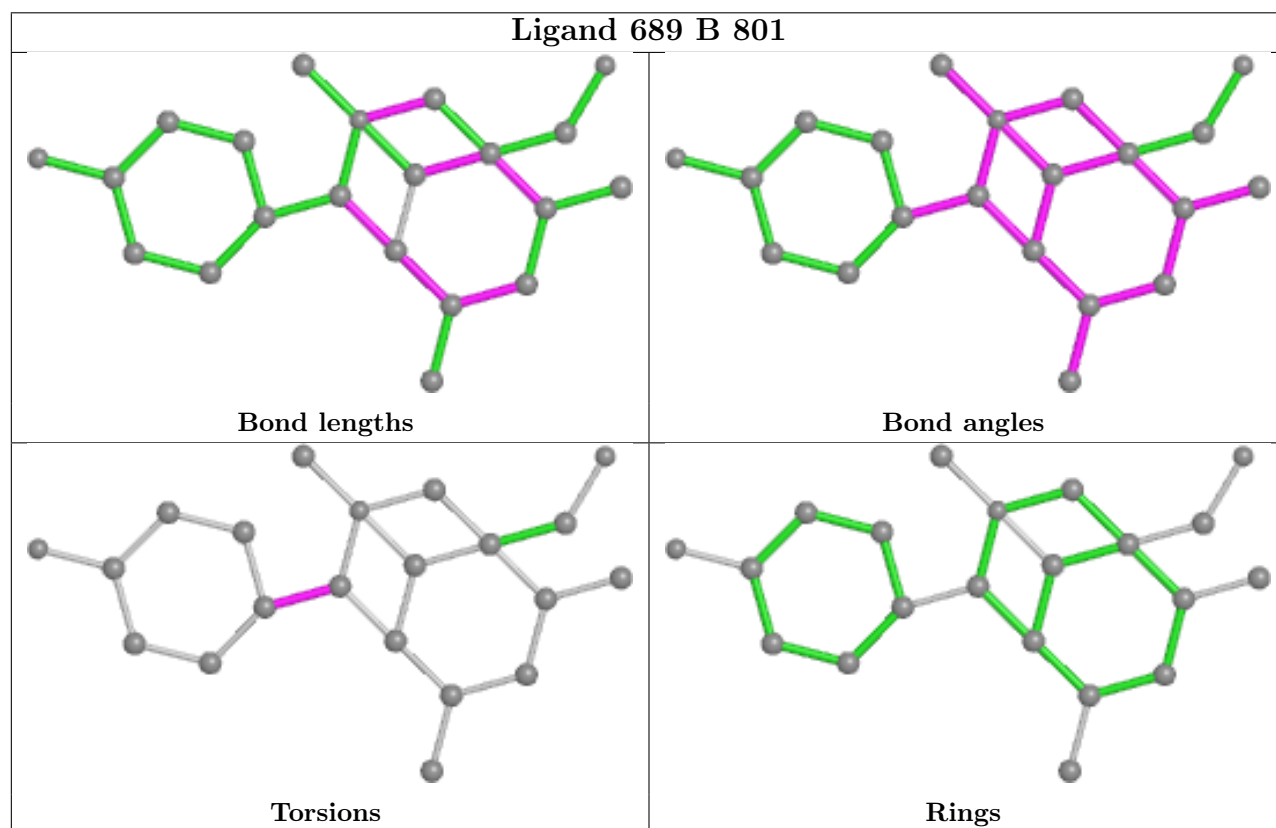
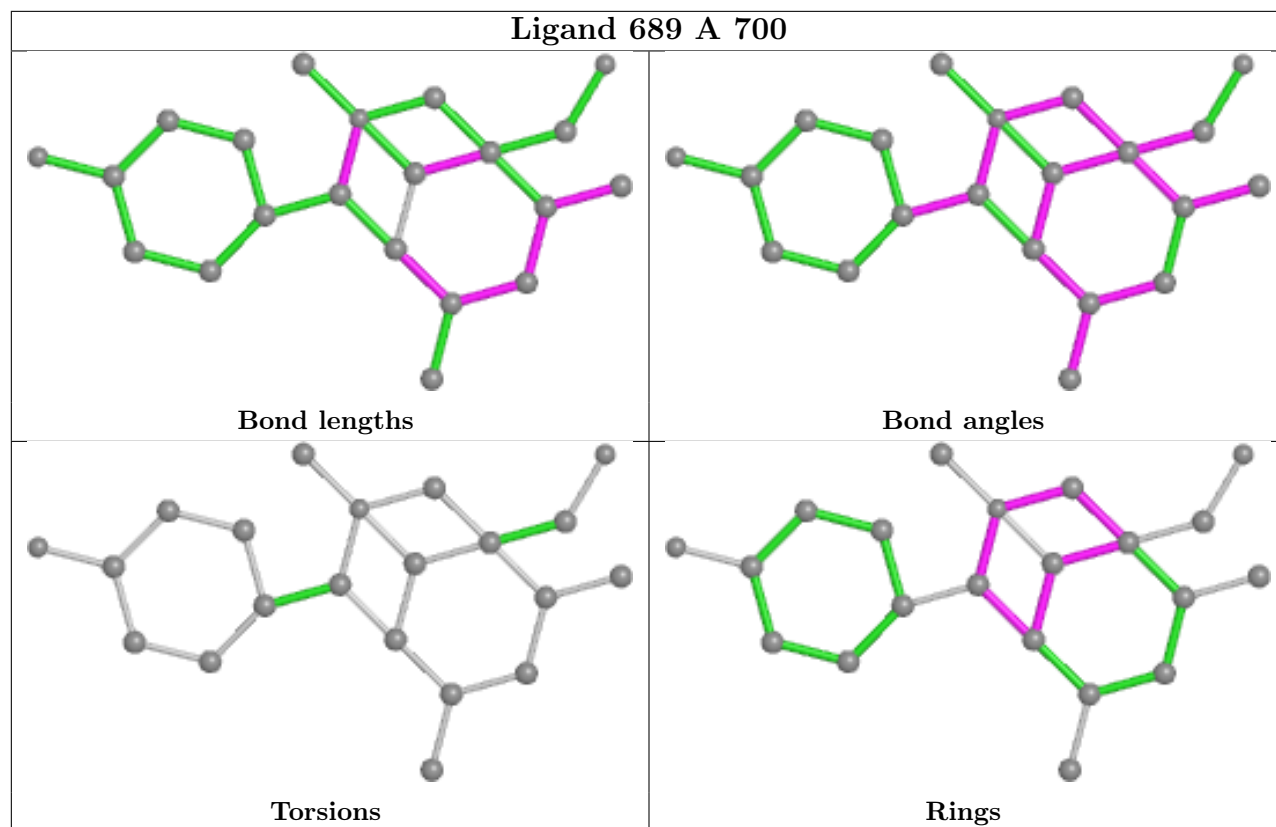
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	689	CAI-CAJ-CAK-CAL-CAM-OAH

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	689	4	0
3	B	801	689	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	236/257 (91%)	0.18	15 (6%) 19 21	15, 26, 51, 71	0
1	B	242/257 (94%)	0.09	12 (4%) 28 31	15, 25, 44, 58	0
2	C	10/13 (76%)	0.44	2 (20%) 1 1	30, 38, 52, 66	0
2	D	9/13 (69%)	0.08	0 100 100	27, 32, 45, 47	0
All	All	497/540 (92%)	0.14	29 (5%) 23 25	15, 26, 50, 71	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	549	LEU	8.8
1	A	304	ASN	8.0
1	B	466	LEU	5.5
1	B	549	LEU	5.2
1	A	533	VAL	4.5
1	B	548	ARG	4.4
1	A	472	LYS	3.6
1	B	465	THR	3.6
1	B	306	LEU	3.2
1	B	471	GLU	3.2
1	A	305	SER	3.1
1	A	534	VAL	2.6
1	B	363	ARG	2.5
1	A	513[A]	HIS	2.5
1	A	531	LYS	2.5
2	C	687	HIS	2.4
1	A	469	LEU	2.3
1	A	532	ASN	2.3
1	A	308	LEU	2.3
1	A	397	GLU	2.2
1	A	461	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	696	ASP	2.2
1	A	535	PRO	2.2
1	B	382	ALA	2.2
1	B	321	ASP	2.2
1	B	513[A]	HIS	2.0
1	A	548	ARG	2.0
1	B	309	SER	2.0
1	B	464	SER	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	CME	A	417	10/11	0.76	0.27	46,53,67,70	0
1	CME	B	417	10/11	0.83	0.26	52,54,81,92	0
1	CME	A	381[A]	10/11	0.84	0.28	28,33,52,60	6
1	CME	B	381[A]	10/11	0.84	0.27	21,27,41,48	6
1	CME	B	381[B]	10/11	0.84	0.27	21,27,41,48	6
1	CME	A	381[B]	10/11	0.84	0.28	28,33,52,60	6
1	CME	B	530	10/11	0.86	0.18	37,40,57,58	0
1	CME	A	530	6/11	0.91	0.20	43,44,47,48	0

6.3 Carbohydrates [i](#)

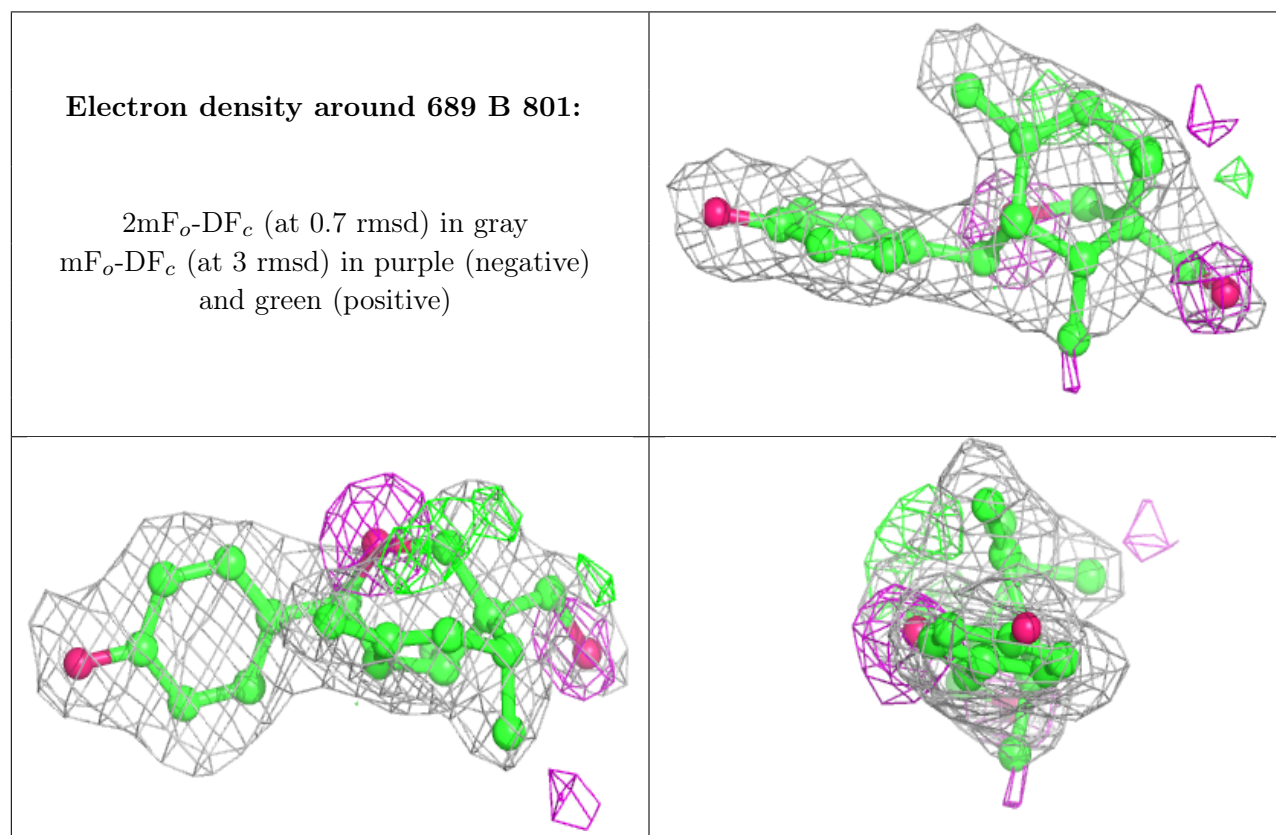
There are no monosaccharides in this entry.

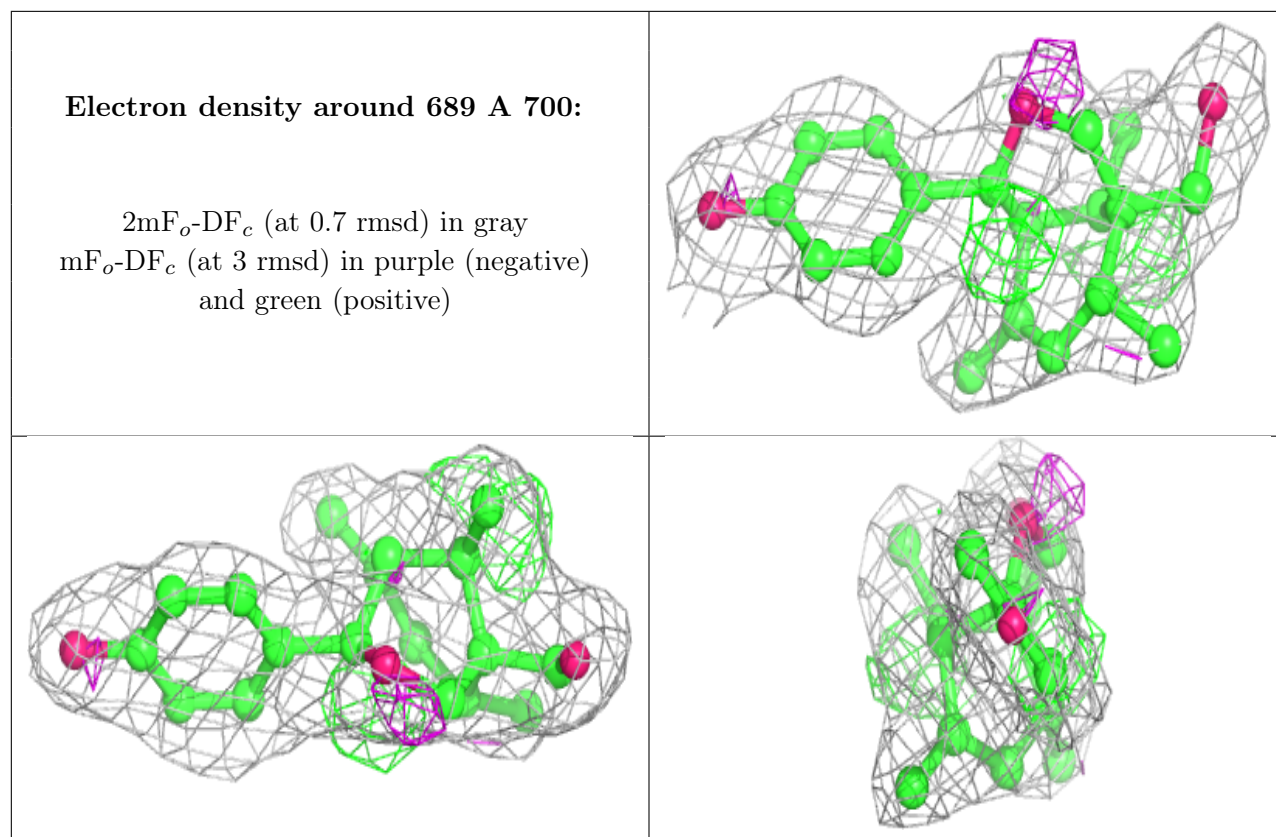
6.4 Ligands [i](#)

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	689	B	801	21/21	0.87	0.18	15,21,25,28	0
3	689	A	700	21/21	0.89	0.14	17,22,24,26	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.