



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:09 AM UTC

PDB ID : 7Y4G / pdb_00007y4g
Title : sit-bound btDPP4
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Deposited on : 2022-06-14
Resolution : 1.97 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

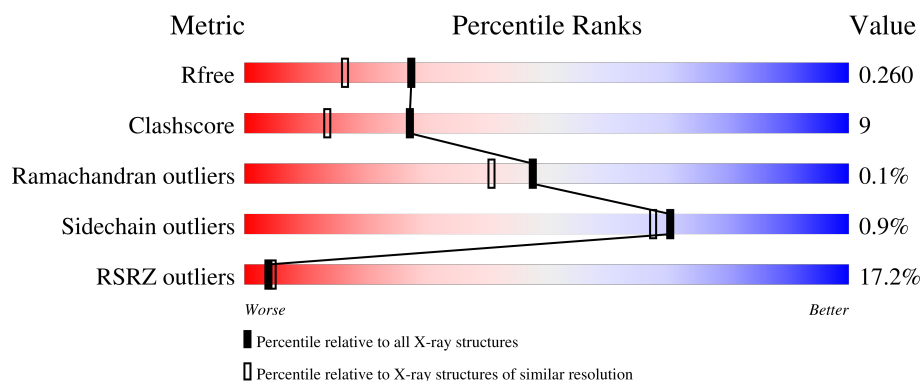
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	715	14% 80% 18% .
1	B	715	18% 82% 16% .
1	C	715	20% 80% 17% .

2 Entry composition [i](#)

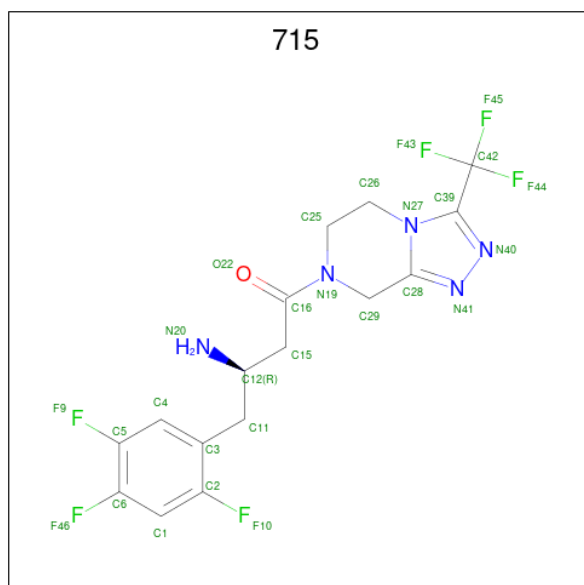
There are 3 unique types of molecules in this entry. The entry contains 18622 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 btDPP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	0	0	0
			5779	3693	962	1098	26			
1	B	715	Total	C	N	O	S	0	0	0
			5779	3693	962	1098	26			
1	C	715	Total	C	N	O	S	0	0	0
			5779	3693	962	1098	26			

- Molecule 2 is (2R)-4-oxo-4-[3-(trifluoromethyl)-5,6-dihydro[1,2,4]triazol-4,3-a]pyrazin-7(8H)-yl-1-(2,4,5-trifluorophenyl)butan-2-amine (CCD ID: 715) (formula: C₁₆H₁₅F₆N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	16	6	5	1		
2	B	1	Total	C	F	N	O	0	0
			28	16	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			28	16	6	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	504	Total	O	0	0
			504	504		
3	B	353	Total	O	0	0
			353	353		
3	C	344	Total	O	0	0
			344	344		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.30Å 110.99Å 134.39Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	44.79 – 1.97 44.79 – 1.98	Depositor EDS
% Data completeness (in resolution range)	84.6 (44.79-1.97) 84.6 (44.79-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.223 , 0.263 0.223 , 0.260	Depositor DCC
R_{free} test set	1992 reflections (1.17%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18622	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 84.42 % 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 1.6741e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
715

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	1.21	6/5927 (0.1%)	1.41	52/8020 (0.6%)
1	B	1.12	9/5927 (0.2%)	1.32	53/8020 (0.7%)
1	C	1.09	9/5927 (0.2%)	1.26	51/8020 (0.6%)
All	All	1.14	24/17781 (0.1%)	1.33	156/24060 (0.6%)

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	3
1	B	0	4
1	C	0	4
All	All	0	11

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	LYS	CB-CG	-11.84	1.17	1.52
1	B	44	ILE	CB-CG2	11.18	1.89	1.52
1	C	187	GLN	CB-CG	-10.44	1.21	1.52
1	B	465	LYS	CB-CG	-9.31	1.24	1.52
1	B	477	LYS	CG-CD	-8.97	1.25	1.52
1	C	23	LYS	CG-CD	-8.45	1.27	1.52
1	B	44	ILE	CA-CB	-7.83	1.44	1.54
1	C	187	GLN	CD-NE2	7.57	1.49	1.33
1	B	477	LYS	N-CA	-6.15	1.38	1.46
1	C	315	ARG	CZ-NH1	6.14	1.41	1.32
1	A	266	LYS	CD-CE	6.12	1.70	1.52
1	C	736	LEU	CG-CD2	-5.97	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	GLY	C-N	-5.93	1.24	1.33
1	A	611	MET	CG-SD	5.90	1.95	1.80
1	A	667	ASP	CB-CG	5.71	1.66	1.52
1	B	214	ASP	CB-CG	-5.70	1.37	1.52
1	C	183	GLU	CD-OE2	5.46	1.35	1.25
1	A	336	SER	CA-C	5.43	1.57	1.52
1	B	477	LYS	CD-CE	5.22	1.68	1.52
1	A	372	MET	CB-CG	-5.16	1.36	1.52
1	C	243	ILE	CG1-CD1	-5.13	1.31	1.51
1	C	283	LYS	CA-C	-5.10	1.47	1.53
1	B	44	ILE	C-N	-5.02	1.27	1.33
1	B	465	LYS	CD-CE	-5.02	1.37	1.52

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	475	GLN	N-CA-CB	23.63	145.13	110.16
1	A	428	GLN	CG-CD-NE2	-23.35	81.37	116.40
1	C	183	GLU	CG-CD-OE1	19.57	163.42	118.40
1	B	475	GLN	CA-CB-CG	19.53	153.16	114.10
1	A	252	GLU	CG-CD-OE1	19.31	162.81	118.40
1	A	489	GLU	CG-CD-OE1	18.77	161.56	118.40
1	B	489	GLU	CG-CD-OE1	18.41	160.74	118.40
1	A	64	LYS	CG-CD-CE	-18.33	69.14	111.30
1	C	327	LEU	CB-CG-CD2	18.17	165.21	110.70
1	B	475	GLN	CB-CG-CD	18.13	143.42	112.60
1	A	252	GLU	OE1-CD-OE2	-17.80	80.19	122.90
1	C	183	GLU	CG-CD-OE2	-17.20	78.83	118.40
1	A	428	GLN	CA-CB-CG	-16.68	80.74	114.10
1	A	428	GLN	CG-CD-OE1	16.59	153.97	120.80
1	A	375	ASN	CB-CG-ND2	-16.44	91.75	116.40
1	B	489	GLU	CG-CD-OE2	-16.00	81.60	118.40
1	A	64	LYS	N-CA-CB	15.63	135.85	110.85
1	B	475	GLN	CB-CA-C	-15.55	84.42	110.85
1	A	427	SER	CA-C-N	15.47	141.01	120.28
1	A	427	SER	C-N-CA	15.47	141.01	120.28
1	A	252	GLU	CG-CD-OE2	-15.46	82.83	118.40
1	A	489	GLU	CG-CD-OE2	-15.29	83.24	118.40
1	A	489	GLU	OE1-CD-OE2	-15.17	86.49	122.90
1	B	489	GLU	OE1-CD-OE2	-15.07	86.72	122.90
1	C	315	ARG	CG-CD-NE	14.66	144.26	112.00
1	B	477	LYS	CG-CD-CE	-13.99	79.12	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ASN	N-CA-CB	-13.62	88.23	110.42
1	C	183	GLU	OE1-CD-OE2	-13.19	91.24	122.90
1	A	456	LEU	CD1-CG-CD2	-13.16	81.85	110.80
1	C	187	GLN	CA-CB-CG	12.80	139.69	114.10
1	B	44	ILE	CB-CG1-CD1	12.72	140.52	113.80
1	C	327	LEU	CB-CG-CD1	-12.42	73.44	110.70
1	A	64	LYS	CB-CA-C	-12.32	86.83	109.37
1	C	315	ARG	CD-NE-CZ	-12.19	107.33	124.40
1	B	44	ILE	N-CA-C	-11.75	83.51	108.88
1	A	64	LYS	CD-CE-NZ	11.46	148.57	111.90
1	B	474	ASP	CA-C-N	-11.44	104.04	120.29
1	B	474	ASP	C-N-CA	-11.44	104.04	120.29
1	A	428	GLN	OE1-CD-NE2	-11.17	111.43	122.60
1	A	447	LYS	CA-CB-CG	10.60	135.31	114.10
1	C	183	GLU	CB-CA-C	10.54	129.12	110.35
1	C	187	GLN	N-CA-CB	10.20	125.22	109.83
1	B	44	ILE	CB-CA-C	-9.87	93.41	111.36
1	C	23	LYS	CG-CD-CE	-9.72	88.94	111.30
1	A	447	LYS	CB-CG-CD	-9.71	88.96	111.30
1	B	43	VAL	CA-C-N	-9.61	104.35	122.13
1	B	43	VAL	C-N-CA	-9.61	104.35	122.13
1	A	428	GLN	CB-CA-C	9.45	126.47	110.79
1	A	64	LYS	N-CA-C	-9.42	94.97	109.95
1	B	465	LYS	CG-CD-CE	9.25	132.58	111.30
1	A	375	ASN	CB-CA-C	9.18	125.07	110.19
1	B	44	ILE	CA-CB-CG2	-9.15	94.94	110.50
1	C	187	GLN	CB-CA-C	-9.09	94.63	109.72
1	C	326	THR	CA-C-N	-9.07	106.23	122.74
1	C	326	THR	C-N-CA	-9.07	106.23	122.74
1	C	315	ARG	CB-CG-CD	-8.97	90.67	111.30
1	C	23	LYS	CA-CB-CG	-8.88	96.35	114.10
1	B	465	LYS	CD-CE-NZ	8.78	139.99	111.90
1	A	456	LEU	CB-CG-CD2	-8.77	84.38	110.70
1	A	372	MET	CB-CA-C	8.47	126.80	109.95
1	B	44	ILE	CA-C-O	-8.38	108.73	119.95
1	A	374	GLY	CA-C-N	8.34	133.87	122.77
1	A	374	GLY	C-N-CA	8.34	133.87	122.77
1	C	182	THR	CA-C-N	-8.29	107.59	121.18
1	C	182	THR	C-N-CA	-8.29	107.59	121.18
1	A	181	VAL	N-CA-C	8.19	118.99	110.72
1	B	44	ILE	CA-CB-CG1	-8.09	96.65	110.40
1	C	375	ASN	CB-CG-ND2	-8.05	104.33	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	MET	N-CA-CB	-8.03	96.92	110.41
1	C	399	SER	N-CA-C	8.00	122.83	110.42
1	A	63	ILE	CA-C-N	-7.78	110.34	122.87
1	A	63	ILE	C-N-CA	-7.78	110.34	122.87
1	C	36	ARG	CA-C-N	-7.74	111.94	120.14
1	C	36	ARG	C-N-CA	-7.74	111.94	120.14
1	B	515	LYS	N-CA-C	7.73	122.62	110.32
1	C	392	GLY	N-CA-C	7.66	122.32	110.91
1	C	515	LYS	N-CA-C	7.24	121.83	110.32
1	A	428	GLN	N-CA-CB	-7.21	99.52	110.12
1	B	210	GLU	CA-CB-CG	7.18	128.45	114.10
1	C	183	GLU	N-CA-CB	-7.16	97.97	111.43
1	A	375	ASN	CB-CG-OD1	7.15	135.10	120.80
1	A	46	MET	CA-CB-CG	-7.07	99.96	114.10
1	B	399	SER	N-CA-C	7.04	120.05	110.55
1	A	375	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	B	126	LYS	CB-CG-CD	-6.82	95.63	111.30
1	C	137	ILE	N-CA-C	6.79	119.19	108.87
1	A	511	PHE	N-CA-C	6.79	120.22	110.24
1	C	376	LEU	CD1-CG-CD2	-6.74	95.97	110.80
1	C	134	THR	N-CA-C	6.71	119.43	111.71
1	B	68	ARG	N-CA-C	6.70	118.67	111.36
1	C	79	VAL	N-CA-C	6.58	116.73	110.42
1	C	315	ARG	N-CA-C	6.53	119.10	107.80
1	B	388	LYS	N-CA-C	6.45	118.11	111.14
1	B	274	ILE	CA-CB-CG1	6.35	121.19	110.40
1	B	74	GLU	N-CA-C	6.33	117.76	108.14
1	B	354	THR	N-CA-C	6.31	118.37	108.96
1	C	374	GLY	CA-C-N	-6.24	113.36	122.65
1	C	374	GLY	C-N-CA	-6.24	113.36	122.65
1	C	376	LEU	CB-CG-CD2	-6.17	92.20	110.70
1	C	375	ASN	N-CA-CB	6.11	120.60	110.52
1	C	75	VAL	CB-CA-C	-6.07	103.54	111.25
1	B	44	ILE	CA-C-N	-6.03	113.57	119.90
1	B	44	ILE	C-N-CA	-6.03	113.57	119.90
1	B	274	ILE	CG1-CB-CG2	-6.00	92.69	110.70
1	B	361	ARG	CB-CG-CD	-6.00	97.51	111.30
1	C	172	LEU	N-CA-C	5.96	117.85	111.36
1	A	456	LEU	CB-CA-C	5.91	119.60	110.14
1	C	186	LYS	CA-C-N	-5.91	112.31	120.71
1	C	186	LYS	C-N-CA	-5.91	112.31	120.71
1	A	329	LYS	CB-CG-CD	5.91	124.88	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	GLN	OE1-CD-NE2	-5.85	116.75	122.60
1	C	276	SER	N-CA-C	5.80	117.68	111.36
1	C	76	ILE	N-CA-C	5.79	118.33	111.09
1	B	477	LYS	CD-CE-NZ	5.78	130.40	111.90
1	B	328	CYS	N-CA-C	5.73	118.24	108.90
1	A	517	TYR	N-CA-C	5.72	118.90	109.58
1	B	341	LYS	CA-C-N	5.65	128.17	120.54
1	B	341	LYS	C-N-CA	5.65	128.17	120.54
1	A	100	ASP	N-CA-C	5.57	120.08	113.28
1	A	341	LYS	CA-C-N	5.53	127.69	120.28
1	A	341	LYS	C-N-CA	5.53	127.69	120.28
1	A	449	SER	N-CA-CB	5.49	120.83	111.66
1	B	87	PHE	N-CA-C	5.47	118.58	110.48
1	B	437	PHE	N-CA-C	5.47	117.93	110.55
1	B	477	LYS	CB-CG-CD	-5.45	98.78	111.30
1	C	284	LEU	CA-C-N	-5.44	113.71	120.79
1	C	284	LEU	C-N-CA	-5.44	113.71	120.79
1	C	327	LEU	CD1-CG-CD2	-5.39	98.93	110.80
1	A	465	LYS	CB-CG-CD	-5.39	98.90	111.30
1	B	41	GLN	N-CA-C	5.36	118.48	109.95
1	A	259	LYS	CA-CB-CG	-5.36	103.38	114.10
1	A	455	MET	CA-C-N	-5.28	115.33	122.77
1	A	455	MET	C-N-CA	-5.28	115.33	122.77
1	C	327	LEU	CA-CB-CG	-5.28	97.82	116.30
1	A	399	SER	CB-CA-C	5.25	118.97	109.37
1	C	479	THR	N-CA-C	-5.21	105.60	111.28
1	C	437	PHE	N-CA-C	5.21	117.84	110.50
1	B	411	ARG	CA-CB-CG	-5.20	103.70	114.10
1	B	36	ARG	CA-CB-CG	-5.19	103.72	114.10
1	B	213	ALA	CA-C-N	5.19	127.75	120.28
1	B	213	ALA	C-N-CA	5.19	127.75	120.28
1	C	212	SER	N-CA-C	5.19	117.38	110.53
1	B	476	LEU	CA-C-N	-5.17	111.90	120.68
1	B	476	LEU	C-N-CA	-5.17	111.90	120.68
1	C	46	MET	CG-SD-CE	-5.14	89.59	100.90
1	B	635	TRP	CA-C-N	-5.13	112.15	120.72
1	B	635	TRP	C-N-CA	-5.13	112.15	120.72
1	A	428	GLN	CB-CG-CD	-5.11	103.91	112.60
1	B	327	LEU	N-CA-C	5.11	117.82	109.59
1	C	68	ARG	N-CA-C	5.10	116.92	111.36
1	B	465	LYS	N-CA-CB	-5.09	101.47	109.51
1	A	507	LYS	CA-CB-CG	-5.08	103.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	TYR	N-CA-C	5.08	116.56	108.79
1	C	375	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	B	55	MET	CA-CB-CG	5.06	124.21	114.10
1	A	411	ARG	CG-CD-NE	-5.00	100.99	112.00

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	ASN	Sidechain
1	A	428	GLN	Sidechain
1	A	489	GLU	Sidechain
1	B	36	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	411	ARG	Sidechain
1	B	489	GLU	Sidechain
1	C	187	GLN	Sidechain
1	C	315	ARG	Sidechain
1	C	361	ARG	Sidechain
1	C	375	ASN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5779	0	5607	120	2
1	B	5779	0	5607	97	2
1	C	5779	0	5607	98	3
2	A	28	0	15	0	0
2	B	28	0	15	0	0
2	C	28	0	15	2	0
3	A	504	0	0	35	0
3	B	353	0	0	19	1
3	C	344	0	0	15	2
All	All	18622	0	16866	312	7

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 9.

All (312) 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:44:ILE:CG2	1:B:44:ILE:CB	1.89	1.49
1:C:284:LEU:CD2	1:C:286:ILE:HD11	1.48	1.42
1:C:284:LEU:HD23	1:C:286:ILE:CD1	1.49	1.41
1:A:51:HIS:HB3	1:A:64:LYS:NZ	1.54	1.21
1:B:47:PRO:HA	1:B:439:GLN:OE1	1.57	1.03
1:C:284:LEU:HD21	1:C:286:ILE:HD11	1.44	0.99
1:A:247:LYS:NZ	3:A:902:HOH:O	1.95	0.99
1:C:284:LEU:HD23	1:C:286:ILE:HD11	0.99	0.96
1:C:457:VAL:HG12	1:C:471:ILE:HB	1.47	0.96
1:B:108:THR:O	3:B:901:HOH:O	1.84	0.94
1:C:284:LEU:HD23	1:C:286:ILE:HD12	1.49	0.94
1:A:51:HIS:HB3	1:A:64:LYS:HZ3	1.31	0.92
1:B:44:ILE:CG2	1:B:44:ILE:CA	2.47	0.92
1:B:47:PRO:HA	1:B:439:GLN:CD	1.95	0.90
1:B:117:THR:OG1	3:B:903:HOH:O	1.90	0.89
1:A:51:HIS:HB3	1:A:64:LYS:HZ2	1.31	0.89
1:B:588:TYR:OH	3:B:902:HOH:O	1.90	0.89
1:C:475:GLN:OE1	1:C:475:GLN:N	2.06	0.87
1:A:428:GLN:NE2	3:A:908:HOH:O	2.07	0.86
1:A:82:ALA:N	3:A:909:HOH:O	2.07	0.86
1:A:81:GLN:C	3:A:909:HOH:O	2.18	0.85
1:A:317:ASP:OD2	3:A:901:HOH:O	1.94	0.84
1:B:164:ASP:OD2	3:B:904:HOH:O	2.00	0.79
1:A:494:GLN:O	3:A:903:HOH:O	1.99	0.79
1:C:652:GLU:OE2	3:C:901:HOH:O	2.00	0.79
1:A:445:MET:HE2	1:A:447:LYS:HE3	1.65	0.78
1:C:227:GLU:OE2	1:C:227:GLU:HA	1.84	0.78
1:C:475:GLN:H	1:C:475:GLN:CD	1.92	0.78
1:C:472:ASN:ND2	1:C:474:ASP:CG	2.43	0.77
1:B:286:ILE:HA	3:B:905:HOH:O	1.85	0.77
1:B:47:PRO:CA	1:B:439:GLN:OE1	2.32	0.75
1:A:22:GLN:N	3:A:915:HOH:O	2.18	0.75
1:A:47:PRO:HA	1:A:439:GLN:HG3	1.68	0.75
1:C:295:ILE:O	3:C:902:HOH:O	2.05	0.75
1:B:140:ARG:NH1	3:B:907:HOH:O	2.12	0.74
1:A:439:GLN:O	3:A:904:HOH:O	2.03	0.74
1:A:88:LYS:HD2	1:A:88:LYS:N	2.03	0.74
1:A:394:ASP:OD2	3:A:907:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:OE1	3:A:905:HOH:O	2.06	0.73
1:B:44:ILE:CG2	1:B:44:ILE:CG1	2.68	0.72
1:C:187:GLN:NE2	3:C:905:HOH:O	2.09	0.72
1:B:285:PRO:O	3:B:905:HOH:O	2.07	0.71
1:C:290:GLY:O	3:C:903:HOH:O	2.07	0.71
1:A:324:ARG:NH1	3:A:913:HOH:O	2.22	0.71
1:A:557:ARG:HD3	1:A:581:ASP:OD2	1.91	0.71
1:B:704:ASP:OD1	1:C:704:ASP:OD1	2.09	0.71
1:C:567:GLU:OE2	3:C:904:HOH:O	2.08	0.71
1:B:475:GLN:O	1:B:476:LEU:C	2.34	0.70
1:A:430:GLU:OE2	3:A:910:HOH:O	2.08	0.70
1:A:88:LYS:HD2	1:A:88:LYS:H	1.56	0.70
1:A:315:ARG:NE	3:A:901:HOH:O	2.24	0.70
1:B:475:GLN:O	1:B:478:GLN:N	2.24	0.69
1:A:507:LYS:HE2	3:A:1306:HOH:O	1.91	0.69
1:B:272:TYR:OH	3:B:906:HOH:O	2.11	0.69
1:C:284:LEU:CD2	1:C:286:ILE:CD1	2.29	0.69
1:A:81:GLN:O	1:A:134:THR:O	2.11	0.68
1:A:214:ASP:OD2	1:A:301:ALA:HB1	1.94	0.68
1:A:333:ARG:NH2	3:A:901:HOH:O	2.27	0.68
1:C:567:GLU:OE1	3:C:906:HOH:O	2.12	0.68
1:B:283:LYS:N	3:B:914:HOH:O	2.26	0.67
1:A:590:GLY:O	3:A:911:HOH:O	2.13	0.67
1:A:46:MET:HE1	1:A:64:LYS:HD2	1.76	0.67
1:A:332:LEU:HD12	1:A:333:ARG:N	2.10	0.66
1:B:408:SER:HB3	1:B:411:ARG:HD2	1.76	0.66
1:C:326:THR:OG1	3:C:907:HOH:O	2.13	0.66
1:B:47:PRO:O	1:B:439:GLN:OE1	2.13	0.66
1:B:45:PRO:HD3	1:B:436:LEU:HD21	1.78	0.66
1:B:347:ASN:OD1	3:B:908:HOH:O	2.14	0.66
1:B:569:CYS:O	1:B:577:LYS:NZ	2.25	0.65
1:C:736:LEU:O	3:C:908:HOH:O	2.15	0.65
1:A:441:MET:HG2	3:A:904:HOH:O	1.96	0.65
1:C:46:MET:HE3	1:C:53:THR:HG23	1.79	0.64
1:A:51:HIS:HB3	1:A:64:LYS:CE	2.25	0.64
1:A:51:HIS:CB	1:A:64:LYS:NZ	2.47	0.64
1:A:332:LEU:HD21	1:A:357:LEU:HD22	1.79	0.64
1:A:360:GLU:OE2	3:A:912:HOH:O	2.15	0.64
1:C:29:ASP:OD2	3:C:909:HOH:O	2.15	0.64
1:A:203:PHE:HA	1:A:342:GLU:HG3	1.79	0.64
1:A:569:CYS:O	1:A:577:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LYS:HG2	1:B:457:VAL:HG22	1.80	0.64
1:C:302:SER:HB2	1:C:322:ASP:OD1	1.98	0.64
1:C:375:ASN:N	1:C:375:ASN:HD22	1.94	0.63
1:A:224:ASP:OD2	1:A:266:LYS:HE2	1.98	0.63
1:A:275:LYS:NZ	3:A:921:HOH:O	2.30	0.63
1:C:297:PHE:CE1	1:C:304:LEU:HB2	2.33	0.63
1:C:46:MET:HE3	1:C:53:THR:CG2	2.28	0.62
1:B:701:LYS:NZ	3:B:916:HOH:O	2.32	0.61
1:A:271:THR:HG23	1:A:282:MET:HE3	1.81	0.61
1:B:46:MET:CE	1:B:53:THR:HG23	2.30	0.61
1:A:309:LEU:HD11	1:A:345:PHE:HZ	1.65	0.61
1:A:489:GLU:HG2	3:A:1306:HOH:O	2.01	0.61
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.66	0.61
1:B:468:LYS:HD3	1:B:469:THR:N	2.16	0.60
1:A:445:MET:HE2	1:A:447:LYS:CE	2.30	0.60
1:B:210:GLU:OE2	3:B:909:HOH:O	2.17	0.60
1:B:276:SER:OG	1:B:278:VAL:HG23	2.02	0.60
1:C:332:LEU:HD23	1:C:333:ARG:N	2.16	0.60
1:C:273:ASP:HB3	1:C:276:SER:HB3	1.82	0.60
1:B:665:ARG:HB2	1:B:668:LYS:HZ3	1.67	0.59
1:A:397:ASP:OD1	1:A:399:SER:HB3	2.02	0.59
1:B:459:LEU:HD12	1:B:470:LEU:HD21	1.85	0.59
1:B:455:MET:HE3	1:B:456:LEU:H	1.68	0.58
1:B:459:LEU:HG	1:B:470:LEU:HD11	1.84	0.58
1:B:460:ASN:HA	1:B:465:LYS:O	2.03	0.58
1:C:315:ARG:HB2	1:C:335:GLU:HG2	1.84	0.58
1:B:247:LYS:HG2	3:C:1175:HOH:O	2.02	0.58
1:A:44:ILE:HD12	1:A:93:TYR:CE2	2.39	0.58
1:B:567:GLU:OE2	3:B:910:HOH:O	2.17	0.58
1:B:282:MET:HA	1:B:282:MET:HE2	1.85	0.57
1:C:455:MET:HA	1:C:455:MET:HE2	1.85	0.57
1:A:121:TYR:CE1	1:A:140:ARG:HG3	2.39	0.57
1:A:123:TYR:N	3:A:923:HOH:O	2.32	0.57
1:A:214:ASP:OD2	3:A:913:HOH:O	2.17	0.57
1:B:129:ASP:OD1	1:B:129:ASP:N	2.36	0.57
1:B:273:ASP:CG	1:B:276:SER:HB3	2.30	0.57
1:B:564:GLU:HG3	1:B:568:LYS:HE3	1.87	0.57
1:B:445:MET:HE2	1:B:470:LEU:HD12	1.87	0.57
3:B:967:HOH:O	1:C:727:ARG:HD3	2.04	0.56
1:A:51:HIS:CB	1:A:64:LYS:HZ3	2.11	0.56
1:A:300:ASP:HB3	1:A:303:LYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ARG:HB2	1:B:668:LYS:NZ	2.20	0.56
1:A:51:HIS:CB	1:A:64:LYS:HZ2	2.13	0.56
1:A:273:ASP:CG	1:A:276:SER:HB3	2.31	0.56
1:A:88:LYS:H	1:A:88:LYS:CD	2.18	0.56
1:A:445:MET:HE3	1:A:457:VAL:CG1	2.36	0.56
1:B:135:ASN:HB3	3:B:1065:HOH:O	2.05	0.55
1:A:273:ASP:HB3	1:A:276:SER:HB3	1.88	0.55
1:C:457:VAL:HG12	1:C:471:ILE:CB	2.29	0.55
1:B:44:ILE:CG2	1:B:44:ILE:HA	2.36	0.55
1:B:214:ASP:HB2	1:B:301:ALA:HB1	1.89	0.55
1:B:486:PRO:HB2	1:B:506:MET:HE2	1.88	0.55
1:A:459:LEU:HD21	1:A:470:LEU:HD11	1.88	0.55
1:C:447:LYS:NZ	3:C:923:HOH:O	2.40	0.55
1:A:52:TYR:HB3	1:A:67:PHE:CZ	2.42	0.55
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.73	0.54
1:B:410:LEU:C	1:B:411:ARG:HG3	2.32	0.54
1:A:88:LYS:N	1:A:88:LYS:CD	2.71	0.54
1:C:736:LEU:O	3:C:910:HOH:O	2.18	0.54
1:B:475:GLN:C	1:B:477:LYS:N	2.64	0.53
1:C:472:ASN:HD21	1:C:474:ASP:CG	2.13	0.53
1:A:329:LYS:NZ	3:A:928:HOH:O	2.37	0.53
1:A:451:LEU:O	1:A:536:TRP:HD1	1.93	0.52
1:B:321:ALA:HB2	1:B:328:CYS:SG	2.48	0.52
1:A:439:GLN:HA	1:A:439:GLN:NE2	2.24	0.52
1:B:46:MET:HE2	1:B:53:THR:HG23	1.91	0.52
1:C:320:PHE:CD2	1:C:331:VAL:HG21	2.45	0.52
1:A:610:TYR:HB2	1:A:632:PRO:HD2	1.91	0.52
1:C:375:ASN:N	1:C:375:ASN:ND2	2.58	0.52
1:A:590:GLY:C	3:A:911:HOH:O	2.53	0.52
1:A:214:ASP:HB3	1:A:216:THR:HG23	1.92	0.52
1:B:46:MET:HE3	1:B:53:THR:HG23	1.91	0.52
1:B:450:ASN:HB2	1:B:534:ASP:OD1	2.10	0.52
1:A:53:THR:HG21	1:A:95:PHE:CE1	2.44	0.52
1:B:658:LYS:HG3	3:B:1243:HOH:O	2.10	0.52
1:B:127:ARG:HG2	1:B:127:ARG:NH1	2.20	0.52
1:C:302:SER:HA	1:C:323:PRO:HD2	1.92	0.52
1:A:191:LEU:HD11	3:A:1137:HOH:O	2.10	0.51
1:A:333:ARG:CZ	3:A:901:HOH:O	2.57	0.51
1:A:438:SER:O	1:A:441:MET:HE2	2.10	0.51
1:C:564:GLU:HG3	1:C:568:LYS:HE3	1.91	0.51
1:A:121:TYR:HB3	1:A:138:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LYS:HB3	1:A:455:MET:SD	2.50	0.51
1:C:456:LEU:HD21	1:C:458:THR:HG23	1.93	0.51
1:B:322:ASP:HB3	1:B:325:SER:OG	2.10	0.51
1:B:475:GLN:HB3	1:B:478:GLN:HB3	1.94	0.50
1:A:46:MET:CE	1:A:64:LYS:HD2	2.42	0.50
1:A:122:ILE:HG23	3:A:923:HOH:O	2.12	0.50
1:A:150:PRO:HD2	3:A:1188:HOH:O	2.11	0.50
1:B:507:LYS:HE2	3:B:1197:HOH:O	2.12	0.50
1:B:538:ILE:HG23	1:B:542:THR:HG21	1.92	0.50
1:A:322:ASP:HB3	1:A:325:SER:OG	2.11	0.50
1:C:242:GLN:OE1	1:C:244:THR:HG22	2.11	0.50
1:C:327:LEU:HG	1:C:328:CYS:N	2.25	0.50
1:A:536:TRP:CH2	1:A:538:ILE:HD12	2.47	0.50
1:B:358:LEU:HD23	1:B:367:LEU:HA	1.94	0.50
1:A:95:PHE:N	3:A:934:HOH:O	2.42	0.50
1:A:529:SER:O	1:A:559:THR:HB	2.11	0.50
1:C:332:LEU:HD23	1:C:332:LEU:C	2.37	0.50
1:B:63:ILE:HG12	1:B:75:VAL:HG22	1.94	0.49
1:B:573:LYS:HD3	1:B:659:GLU:OE1	2.12	0.49
2:C:801:715:C2	2:C:801:715:H201	2.23	0.49
1:A:445:MET:HE3	1:A:457:VAL:HG11	1.95	0.49
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.10	0.49
1:C:472:ASN:ND2	1:C:474:ASP:OD2	2.45	0.49
1:C:456:LEU:CD2	1:C:458:THR:HG23	2.43	0.49
1:C:358:LEU:HD23	1:C:367:LEU:HA	1.95	0.49
1:C:327:LEU:CG	1:C:328:CYS:H	2.26	0.48
1:A:459:LEU:HD23	1:A:470:LEU:HG	1.96	0.48
1:A:52:TYR:N	1:A:64:LYS:NZ	2.60	0.48
1:A:486:PRO:HB3	1:A:507:LYS:O	2.13	0.48
1:B:43:VAL:HA	1:B:53:THR:O	2.14	0.48
1:B:47:PRO:C	1:B:439:GLN:OE1	2.56	0.48
1:A:429:ARG:HD2	3:A:1218:HOH:O	2.13	0.48
1:A:42:GLY:N	3:A:942:HOH:O	2.47	0.48
1:A:232:SER:HA	1:A:253:TYR:O	2.14	0.48
1:C:456:LEU:O	1:C:456:LEU:HD23	2.14	0.48
1:C:452:ASP:OD1	1:C:452:ASP:N	2.45	0.47
1:B:455:MET:HE3	1:B:456:LEU:N	2.29	0.47
1:A:214:ASP:OD1	3:A:916:HOH:O	2.20	0.47
1:C:368:TYR:HD2	1:C:376:LEU:HD11	1.80	0.47
1:A:61:GLN:HA	1:A:77:PHE:O	2.15	0.47
1:C:457:VAL:HG13	1:C:470:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:VAL:HG11	1:C:206:ASN:O	2.15	0.47
1:C:184:ASP:OD2	1:C:222:ARG:NH2	2.39	0.47
1:B:127:ARG:O	3:B:911:HOH:O	2.21	0.47
1:C:309:LEU:HD11	1:C:345:PHE:HZ	1.80	0.47
1:C:325:SER:O	1:C:326:THR:OG1	2.31	0.47
1:B:280:ARG:HG3	1:B:280:ARG:NH1	2.30	0.47
1:C:327:LEU:CG	1:C:328:CYS:N	2.77	0.47
1:B:341:LYS:O	1:B:344:VAL:HG22	2.14	0.46
1:C:56:SER:HB3	1:C:61:GLN:HB2	1.97	0.46
1:A:53:THR:HG21	1:A:95:PHE:HE1	1.81	0.46
1:C:454:PRO:HA	1:C:536:TRP:CG	2.51	0.46
1:A:564:GLU:HG3	1:A:568:LYS:HE3	1.97	0.46
1:C:610:TYR:HB2	1:C:632:PRO:HD2	1.98	0.46
1:B:309:LEU:HD11	1:B:345:PHE:HZ	1.80	0.46
1:A:315:ARG:CD	3:A:901:HOH:O	2.63	0.45
1:B:58:ASP:HB3	1:B:60:THR:HG23	1.97	0.45
1:C:187:GLN:NE2	1:C:188:ASN:H	2.14	0.45
1:C:472:ASN:HD22	1:C:474:ASP:CG	2.19	0.45
1:B:28:LYS:HE2	1:B:28:LYS:HB3	1.66	0.45
1:B:121:TYR:HB3	1:B:138:ILE:HG12	1.97	0.45
1:C:327:LEU:HG	1:C:328:CYS:H	1.80	0.45
1:B:414:VAL:HG22	1:B:435:PRO:HG3	1.99	0.45
1:B:504:TRP:CE2	1:B:553:CYS:HB3	2.52	0.45
1:B:727:ARG:HD2	3:B:1047:HOH:O	2.16	0.45
1:A:150:PRO:HA	1:A:160:ALA:O	2.17	0.45
1:A:273:ASP:CB	1:A:276:SER:HB3	2.47	0.45
1:C:286:ILE:HG22	1:C:287:ASP:O	2.17	0.45
1:C:456:LEU:HD23	1:C:456:LEU:C	2.42	0.44
1:B:468:LYS:HD3	1:B:469:THR:H	1.80	0.44
1:A:83:ARG:HD3	1:A:135:ASN:O	2.17	0.44
1:B:445:MET:HE2	1:B:470:LEU:CD1	2.47	0.44
1:B:459:LEU:CD1	1:B:470:LEU:HD21	2.47	0.44
1:B:697:VAL:HG22	1:C:723:HIS:CE1	2.53	0.44
1:B:45:PRO:HD3	1:B:436:LEU:CD2	2.47	0.44
1:B:214:ASP:O	1:B:215:ASN:HB2	2.17	0.44
1:B:265:SER:HB3	1:B:267:VAL:HG12	2.00	0.44
1:B:324:ARG:HG2	1:B:324:ARG:HH11	1.83	0.44
1:B:610:TYR:HB2	1:B:632:PRO:HD2	2.00	0.44
1:B:282:MET:CE	1:B:326:THR:HA	2.48	0.44
1:A:55:MET:HE3	1:A:90:PHE:CE2	2.53	0.43
1:B:486:PRO:HB3	1:B:507:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:HA	1:A:225:GLU:OE2	2.19	0.43
1:C:475:GLN:N	1:C:475:GLN:CD	2.70	0.43
1:A:165:ASN:ND2	1:A:191:LEU:HD12	2.34	0.43
1:C:137:ILE:HA	1:C:137:ILE:HD12	1.84	0.43
1:A:457:VAL:HB	1:A:471:ILE:HB	2.01	0.43
1:C:420:LYS:HA	1:C:420:LYS:HD2	1.74	0.43
1:A:271:THR:CG2	1:A:282:MET:HE3	2.47	0.43
1:A:332:LEU:HD12	1:A:333:ARG:H	1.81	0.42
1:C:104:ILE:O	1:C:120:HIS:HA	2.19	0.42
1:C:283:LYS:HB2	3:C:924:HOH:O	2.19	0.42
1:A:237:ALA:CB	1:A:247:LYS:HD2	2.49	0.42
1:A:320:PHE:CG	1:A:331:VAL:HG21	2.54	0.42
1:A:439:GLN:HA	1:A:439:GLN:HE21	1.84	0.42
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.77	0.42
1:C:22:GLN:N	1:C:482:GLY:O	2.53	0.42
1:A:190:VAL:C	1:A:191:LEU:HD12	2.44	0.42
1:A:369:TRP:CD2	1:A:400:PHE:HE2	2.37	0.42
1:A:284:LEU:HA	1:A:285:PRO:HD3	1.88	0.42
1:C:158:MET:HB3	1:C:169:LEU:HD11	2.02	0.42
1:C:286:ILE:HG22	1:C:287:ASP:N	2.35	0.42
1:A:227:GLU:H	1:A:266:LYS:NZ	2.18	0.42
1:B:476:LEU:O	1:B:480:LEU:HG	2.20	0.42
1:B:723:HIS:CE1	1:C:697:VAL:HG22	2.55	0.42
1:A:655:GLU:HG2	1:B:338:TYR:CE1	2.54	0.42
1:A:333:ARG:HE	1:A:333:ARG:HB2	1.68	0.42
1:A:388:LYS:HD3	1:A:388:LYS:HA	1.83	0.41
1:C:216:THR:CB	1:C:324:ARG:HH22	2.33	0.41
1:C:250:PRO:O	3:C:912:HOH:O	2.22	0.41
1:C:23:LYS:N	1:C:23:LYS:HD2	2.35	0.41
1:C:569:CYS:O	1:C:577:LYS:NZ	2.49	0.41
1:A:191:LEU:CD1	1:A:191:LEU:N	2.83	0.41
1:B:40:ILE:HD12	1:B:445:MET:HE1	2.02	0.41
1:A:315:ARG:HD2	3:A:901:HOH:O	2.21	0.41
1:A:455:MET:HB3	1:A:473:ASN:ND2	2.36	0.41
1:C:100:ASP:OD1	1:C:100:ASP:C	2.63	0.41
1:C:414:VAL:HG22	1:C:435:PRO:HG3	2.02	0.41
1:C:620:THR:HG22	1:C:622:VAL:HG13	2.02	0.41
1:A:104:ILE:O	1:A:120:HIS:HA	2.21	0.41
1:C:362:ASP:OD1	1:C:362:ASP:N	2.36	0.41
1:C:575:GLY:HA2	1:C:611:MET:HE1	2.03	0.41
1:A:324:ARG:HH11	1:A:324:ARG:HD2	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:THR:C	1:A:459:LEU:HD22	2.46	0.41
1:C:154:PRO:HD3	1:C:211:PHE:HB3	2.03	0.41
1:C:284:LEU:HG	1:C:286:ILE:HG13	2.01	0.41
1:B:309:LEU:HD23	1:B:316:PHE:HA	2.03	0.41
1:C:342:GLU:OE1	2:C:801:715:N41	2.53	0.41
1:C:459:LEU:HG	1:C:470:LEU:HD11	2.02	0.41
1:C:517:TYR:HB2	1:C:550:ILE:HD12	2.03	0.41
1:C:627:VAL:HG22	1:C:674:LEU:HB3	2.03	0.41
1:A:55:MET:HG3	1:A:93:TYR:HE1	1.86	0.41
1:A:465:LYS:HB2	1:A:465:LYS:HE2	1.29	0.41
1:B:410:LEU:C	1:B:411:ARG:CG	2.94	0.41
1:B:447:LYS:CA	1:B:455:MET:HE1	2.50	0.41
1:B:475:GLN:C	1:B:478:GLN:H	2.29	0.41
1:C:202:GLU:OE2	1:C:639:ASP:OD2	2.38	0.41
1:A:247:LYS:HD2	1:A:247:LYS:HA	1.62	0.41
1:C:203:PHE:CE2	1:C:641:ILE:HD13	2.56	0.41
1:C:480:LEU:HD23	1:C:480:LEU:HA	1.75	0.41
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.77	0.40
1:C:391:LEU:C	3:C:967:HOH:O	2.64	0.40
1:A:53:THR:HG23	1:A:93:TYR:OH	2.20	0.40
1:C:468:LYS:HG2	1:C:469:THR:N	2.36	0.40
1:A:41:GLN:NE2	3:A:954:HOH:O	2.53	0.40
1:B:202:GLU:OE2	1:B:639:ASP:OD2	2.39	0.40
1:B:259:LYS:O	1:B:260:ALA:C	2.63	0.40
1:C:162:VAL:HA	1:C:166:ASN:O	2.22	0.40
1:C:408:SER:HB3	1:C:411:ARG:HD2	2.04	0.40
1:C:412:LYS:HB3	1:C:412:LYS:HE3	1.76	0.40
1:A:108:THR:HG23	1:A:116:TYR:CD2	2.57	0.40

All (7) 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)
3:C:1106:HOH:O	3:C:1106:HOH:O[2_554]	1.63	0.57
1:A:515:LYS:NZ	1:C:129:ASP:OD1[3_555]	1.77	0.43
1:C:83:ARG:NH1	1:C:83:ARG:NH1[2_555]	1.90	0.30
3:B:958:HOH:O	3:C:1207:HOH:O[3_545]	1.98	0.22
1:A:704:ASP:OD1	1:A:704:ASP:OD1[2_655]	1.99	0.21
1:B:353:GLU:OE2	1:C:593:PRO:CG[3_545]	2.07	0.13
1:B:465:LYS:NZ	1:B:465:LYS:NZ[2_654]	2.08	0.12

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	713/715 (100%)	688 (96%)	24 (3%)	1 (0%)	48	41
1	B	713/715 (100%)	688 (96%)	24 (3%)	1 (0%)	48	41
1	C	713/715 (100%)	684 (96%)	28 (4%)	1 (0%)	48	41
All	All	2139/2145 (100%)	2060 (96%)	76 (4%)	3 (0%)	48	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	715	ILE
1	A	715	ILE
1	B	715	ILE

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	627/627 (100%)	624 (100%)	3 (0%)	81	79
1	B	627/627 (100%)	622 (99%)	5 (1%)	73	71
1	C	627/627 (100%)	619 (99%)	8 (1%)	61	57
All	All	1881/1881 (100%)	1865 (99%)	16 (1%)	70	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	286	ILE
1	A	424	LEU
1	B	40	ILE
1	B	79	VAL
1	B	267	VAL
1	B	286	ILE
1	B	331	VAL
1	C	40	ILE
1	C	44	ILE
1	C	84	GLU
1	C	122	ILE
1	C	214	ASP
1	C	278	VAL
1	C	412	LYS
1	C	456	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	187	GLN
1	A	188	ASN
1	A	192	ASN
1	A	242	GLN
1	A	439	GLN
1	A	487	GLN
1	A	531	GLN
1	A	670	HIS
1	B	81	GLN
1	B	136	ASN
1	B	187	GLN
1	B	188	ASN
1	B	446	ASN
1	B	460	ASN
1	B	494	GLN
1	B	502	ASN
1	C	187	GLN
1	C	375	ASN
1	C	428	GLN
1	C	446	ASN
1	C	472	ASN
1	C	478	GLN

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Mol	Chain	Res	Type
1	C	530	GLN
1	C	735	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	715	A	801	-	30,30,30	3.56	12 (40%)	36,45,45	2.19	14 (38%)
2	715	B	801	-	30,30,30	3.14	12 (40%)	36,45,45	2.14	13 (36%)
2	715	C	801	-	30,30,30	3.38	11 (36%)	36,45,45	2.05	15 (41%)

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	715	A	801	-	-	1/18/27/27	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	715	B	801	-	-	1/18/27/27	0/3/3/3
2	715	C	801	-	-	0/18/27/27	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	715	C4-C5	8.95	1.53	1.37
2	C	801	715	C4-C5	8.43	1.52	1.37
2	B	801	715	C1-C2	7.07	1.49	1.37
2	A	801	715	C3-C2	6.97	1.50	1.38
2	B	801	715	C4-C3	6.79	1.50	1.39
2	C	801	715	C1-C2	6.68	1.49	1.37
2	A	801	715	C1-C2	6.67	1.49	1.37
2	C	801	715	C4-C3	6.56	1.49	1.39
2	A	801	715	C1-C6	6.46	1.48	1.37
2	C	801	715	C16-N19	6.37	1.47	1.35
2	A	801	715	C16-N19	6.27	1.47	1.35
2	B	801	715	C4-C5	6.25	1.48	1.37
2	B	801	715	C16-N19	6.16	1.47	1.35
2	C	801	715	C3-C2	5.71	1.48	1.38
2	A	801	715	C4-C3	5.35	1.47	1.39
2	B	801	715	C3-C2	5.23	1.47	1.38
2	C	801	715	C1-C6	5.18	1.46	1.37
2	B	801	715	C1-C6	4.96	1.46	1.37
2	A	801	715	C29-C28	4.85	1.58	1.50
2	C	801	715	C39-N40	4.47	1.37	1.31
2	C	801	715	C29-C28	4.29	1.57	1.50
2	A	801	715	C39-N40	4.14	1.37	1.31
2	A	801	715	C6-C5	3.69	1.50	1.38
2	B	801	715	O22-C16	-3.57	1.15	1.23
2	B	801	715	C6-C5	3.55	1.49	1.38
2	A	801	715	C28-N41	3.55	1.36	1.31
2	B	801	715	C29-C28	3.23	1.55	1.50
2	C	801	715	C28-N41	3.15	1.36	1.31
2	B	801	715	C39-N40	2.86	1.35	1.31
2	C	801	715	C6-C5	2.82	1.47	1.38
2	C	801	715	C11-C12	-2.44	1.49	1.53
2	A	801	715	C15-C16	2.35	1.55	1.51
2	B	801	715	C25-N19	-2.31	1.42	1.47
2	A	801	715	C26-N27	2.20	1.51	1.47
2	B	801	715	C28-N41	2.15	1.34	1.31

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	715	F43-C42-C39	-5.77	104.00	111.95
2	A	801	715	C25-C26-N27	5.61	117.74	109.06
2	C	801	715	C25-C26-N27	5.10	116.95	109.06
2	B	801	715	C25-C26-N27	5.06	116.89	109.06
2	A	801	715	C4-C3-C2	4.50	121.49	116.54
2	C	801	715	F43-C42-C39	-4.21	106.16	111.95
2	A	801	715	C26-N27-C28	-4.11	118.73	125.08
2	C	801	715	C26-N27-C28	-3.74	119.31	125.08
2	A	801	715	N27-C28-N41	-3.58	105.62	110.42
2	B	801	715	F44-C42-C39	-3.52	107.11	111.95
2	B	801	715	C26-N27-C28	-3.41	119.82	125.08
2	B	801	715	C15-C16-N19	3.31	124.46	118.37
2	A	801	715	F10-C2-C3	2.96	122.88	117.96
2	B	801	715	O22-C16-C15	-2.89	116.68	122.07
2	B	801	715	N27-C28-N41	-2.88	106.57	110.42
2	A	801	715	C28-N41-N40	2.83	110.70	107.59
2	C	801	715	F10-C2-C3	2.83	122.67	117.96
2	C	801	715	F10-C2-C1	-2.78	113.08	118.64
2	C	801	715	C12-C15-C16	-2.74	108.14	112.67
2	A	801	715	F10-C2-C1	-2.72	113.19	118.64
2	A	801	715	C39-N40-N41	-2.66	104.55	107.40
2	C	801	715	C29-N19-C16	2.64	127.76	121.03
2	C	801	715	N27-C28-N41	-2.62	106.92	110.42
2	B	801	715	F45-C42-F43	2.59	117.38	106.20
2	C	801	715	C1-C6-C5	-2.56	117.07	121.24
2	A	801	715	O22-C16-C15	-2.54	117.32	122.07
2	A	801	715	F9-C5-C4	2.47	123.57	118.64
2	C	801	715	O22-C16-C15	-2.40	117.59	122.07
2	B	801	715	F46-C6-C1	2.38	123.39	118.64
2	C	801	715	F44-C42-C39	-2.37	108.69	111.95
2	A	801	715	F45-C42-C39	-2.35	108.71	111.95
2	A	801	715	F43-C42-C39	-2.33	108.75	111.95
2	B	801	715	C29-N19-C16	2.32	126.96	121.03
2	B	801	715	C28-N41-N40	2.26	110.07	107.59
2	B	801	715	C39-N40-N41	-2.26	104.98	107.40
2	C	801	715	F45-C42-F43	2.26	115.92	106.20
2	C	801	715	C39-N40-N41	-2.22	105.02	107.40
2	C	801	715	C28-N41-N40	2.21	110.02	107.59
2	C	801	715	F46-C6-C1	2.17	122.98	118.64
2	A	801	715	C29-N19-C16	2.09	126.36	121.03
2	B	801	715	F9-C5-C4	2.07	122.78	118.64
2	A	801	715	C3-C4-C5	-2.05	116.03	119.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

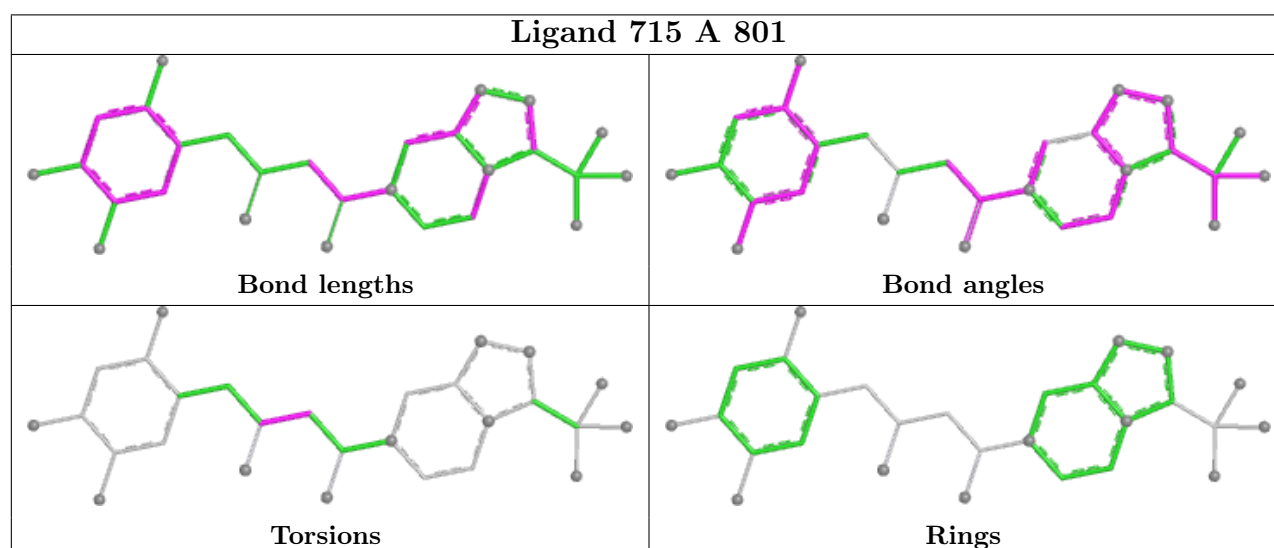
Mol	Chain	Res	Type	Atoms
2	B	801	715	N20-C12-C15-C16
2	A	801	715	N20-C12-C15-C16

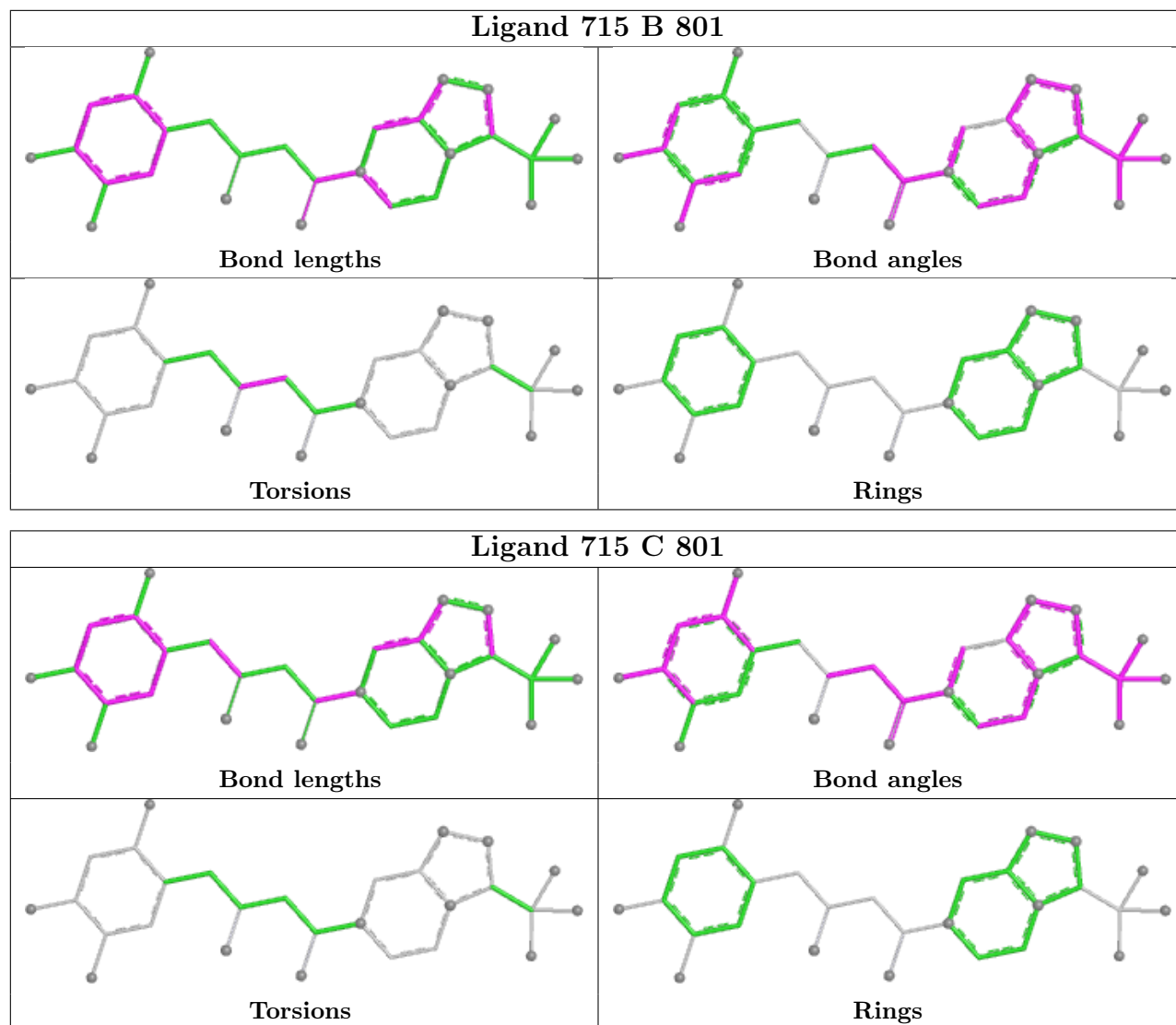
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	715	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](#)

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	715/715 (100%)	0.77	100 (13%) 6 9	12, 33, 56, 74	0
1	B	715/715 (100%)	0.89	127 (17%) 4 4	14, 38, 67, 83	0
1	C	715/715 (100%)	0.88	141 (19%) 3 3	15, 42, 77, 114	0
All	All	2145/2145 (100%)	0.85	368 (17%) 4 5	12, 36, 70, 114	0

All (368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	132	VAL	7.2
1	C	327	LEU	7.2
1	C	79	VAL	6.9
1	C	353	GLU	6.7
1	B	79	VAL	6.1
1	C	85	CYS	5.7
1	A	64	LYS	5.6
1	C	129	ASP	5.4
1	A	459	LEU	5.4
1	B	86	ASP	5.3
1	C	133	THR	5.3
1	C	137	ILE	5.2
1	B	327	LEU	5.2
1	B	400	PHE	5.1
1	A	418	ASP	5.1
1	A	132	VAL	5.1
1	C	214	ASP	5.0
1	B	396	ALA	4.9
1	C	98	ASP	4.9
1	C	86	ASP	4.6
1	B	44	ILE	4.5
1	C	284	LEU	4.4
1	C	301	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	4.4
1	A	417	ILE	4.3
1	C	397	ASP	4.3
1	C	134	THR	4.3
1	C	213	ALA	4.3
1	B	98	ASP	4.3
1	B	47	PRO	4.2
1	B	476	LEU	4.2
1	C	463	THR	4.2
1	B	439	GLN	4.2
1	B	464	GLY	4.1
1	B	417	ILE	4.1
1	C	352	PRO	4.1
1	C	286	ILE	4.1
1	A	367	LEU	4.1
1	B	328	CYS	4.1
1	A	102	LEU	4.0
1	B	395	GLU	4.0
1	B	353	GLU	3.9
1	B	331	VAL	3.9
1	A	285	PRO	3.9
1	C	441	MET	3.9
1	A	474	ASP	3.9
1	B	274	ILE	3.9
1	B	457	VAL	3.9
1	C	396	ALA	3.8
1	B	444	TYR	3.8
1	A	286	ILE	3.8
1	C	315	ARG	3.8
1	B	401	TYR	3.8
1	B	402	TYR	3.8
1	A	301	ALA	3.8
1	B	351	TYR	3.7
1	C	382	ASN	3.7
1	A	137	ILE	3.7
1	C	128	ASN	3.7
1	B	463	THR	3.7
1	A	76	ILE	3.7
1	A	382	ASN	3.7
1	C	400	PHE	3.6
1	C	514	SER	3.6
1	A	396	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	ASP	3.6
1	B	479	THR	3.5
1	A	376	LEU	3.5
1	C	174	TYR	3.5
1	C	135	ASN	3.5
1	A	426	LEU	3.5
1	C	68	ARG	3.5
1	C	83	ARG	3.5
1	B	394	ASP	3.5
1	A	513	THR	3.5
1	C	471	ILE	3.5
1	C	372	MET	3.5
1	B	382	ASN	3.4
1	C	393	TYR	3.4
1	A	372	MET	3.4
1	C	82	ALA	3.4
1	B	52	TYR	3.4
1	C	402	TYR	3.4
1	A	129	ASP	3.4
1	C	474	ASP	3.4
1	B	441	MET	3.4
1	A	47	PRO	3.3
1	B	393	TYR	3.3
1	C	136	ASN	3.3
1	C	175	GLY	3.3
1	C	332	LEU	3.2
1	C	354	THR	3.2
1	A	95	PHE	3.2
1	B	390	PHE	3.2
1	B	420	LYS	3.2
1	C	274	ILE	3.2
1	A	57	ALA	3.2
1	A	298	THR	3.2
1	A	428	GLN	3.2
1	B	443	TYR	3.2
1	C	87	PHE	3.2
1	C	95	PHE	3.2
1	A	45	PRO	3.1
1	C	41	GLN	3.1
1	A	49	GLY	3.1
1	B	385	TYR	3.1
1	C	374	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	457	VAL	3.1
1	A	447	LYS	3.1
1	B	45	PRO	3.1
1	B	514	SER	3.1
1	A	44	ILE	3.1
1	B	65	TYR	3.1
1	B	460	ASN	3.1
1	B	411	ARG	3.1
1	B	500	THR	3.1
1	B	419	LYS	3.0
1	B	133	THR	3.0
1	C	392	GLY	3.0
1	C	54	GLN	3.0
1	C	81	GLN	3.0
1	C	104	ILE	3.0
1	B	438	SER	3.0
1	B	275	LYS	3.0
1	B	36	ARG	3.0
1	C	417	ILE	3.0
1	B	426	LEU	3.0
1	C	304	LEU	3.0
1	C	443	TYR	3.0
1	C	300	ASP	3.0
1	B	85	CYS	3.0
1	B	286	ILE	3.0
1	C	138	ILE	3.0
1	A	477	LYS	2.9
1	B	53	THR	2.9
1	C	36	ARG	2.9
1	B	59	GLY	2.9
1	C	77	PHE	2.9
1	B	326	THR	2.9
1	A	154	PRO	2.9
1	A	334	ASP	2.9
1	A	452	ASP	2.9
1	C	302	SER	2.9
1	A	133	THR	2.9
1	A	204	GLY	2.9
1	A	479	THR	2.9
1	C	401	TYR	2.9
1	B	352	PRO	2.9
1	C	90	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	515	LYS	2.9
1	A	214	ASP	2.9
1	C	84	GLU	2.9
1	A	377	ILE	2.9
1	C	173	LEU	2.9
1	B	69	THR	2.8
1	C	298	THR	2.8
1	C	331	VAL	2.8
1	B	388	LYS	2.8
1	B	477	LYS	2.8
1	A	46	MET	2.8
1	C	46	MET	2.8
1	C	52	TYR	2.8
1	B	214	ASP	2.8
1	C	394	ASP	2.8
1	B	46	MET	2.8
1	A	464	GLY	2.8
1	A	330	LEU	2.8
1	A	456	LEU	2.8
1	A	515	LYS	2.8
1	B	442	LYS	2.8
1	B	513	THR	2.8
1	C	303	LYS	2.8
1	A	457	VAL	2.8
1	A	399	SER	2.8
1	A	413	ALA	2.8
1	C	67	PHE	2.8
1	C	131	GLY	2.8
1	B	380	VAL	2.8
1	A	440	SER	2.7
1	C	179	SER	2.7
1	A	385	TYR	2.7
1	C	351	TYR	2.7
1	A	375	ASN	2.7
1	B	472	ASN	2.7
1	C	215	ASN	2.7
1	C	466	THR	2.7
1	B	284	LEU	2.7
1	C	76	ILE	2.7
1	A	323	PRO	2.7
1	C	399	SER	2.7
1	B	132	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	444	TYR	2.7
1	B	49	GLY	2.7
1	B	459	LEU	2.7
1	C	62	ILE	2.7
1	A	331	VAL	2.7
1	C	398	GLY	2.7
1	B	95	PHE	2.7
1	B	297	PHE	2.7
1	C	355	PHE	2.7
1	B	134	THR	2.7
1	A	284	LEU	2.7
1	A	332	LEU	2.7
1	A	476	LEU	2.7
1	A	380	VAL	2.7
1	C	369	TRP	2.6
1	A	266	LYS	2.6
1	A	79	VAL	2.6
1	A	60	THR	2.6
1	A	86	ASP	2.6
1	B	418	ASP	2.6
1	B	301	ALA	2.6
1	B	344	VAL	2.6
1	C	416	LYS	2.6
1	B	39	ASN	2.6
1	A	357	LEU	2.6
1	A	391	LEU	2.6
1	C	44	ILE	2.6
1	C	122	ILE	2.6
1	C	395	GLU	2.6
1	B	70	GLY	2.6
1	A	416	LYS	2.6
1	B	213	ALA	2.6
1	A	37	PRO	2.5
1	B	67	PHE	2.5
1	C	187	GLN	2.5
1	B	63	ILE	2.5
1	B	343	ASN	2.5
1	A	151	VAL	2.5
1	A	443	TYR	2.5
1	A	66	SER	2.5
1	C	276	SER	2.5
1	C	500	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	415	TYR	2.5
1	A	374	GLY	2.5
1	B	304	LEU	2.5
1	B	511	PHE	2.5
1	C	297	PHE	2.5
1	B	84	GLU	2.5
1	B	321	ALA	2.5
1	C	326	THR	2.5
1	A	43	VAL	2.5
1	B	129	ASP	2.5
1	C	419	LYS	2.5
1	A	454	PRO	2.5
1	C	65	TYR	2.4
1	A	480	LEU	2.4
1	B	364	PHE	2.4
1	C	476	LEU	2.4
1	B	475	GLN	2.4
1	C	273	ASP	2.4
1	A	97	PRO	2.4
1	B	71	GLU	2.4
1	A	467	LEU	2.4
1	B	468	LYS	2.4
1	B	389	ASP	2.4
1	C	40	ILE	2.4
1	C	281	THR	2.4
1	C	57	ALA	2.4
1	C	411	ARG	2.4
1	A	73	VAL	2.4
1	A	536	TRP	2.4
1	B	50	GLU	2.4
1	B	462	ASN	2.4
1	C	343	ASN	2.4
1	A	59	GLY	2.4
1	A	175	GLY	2.4
1	A	475	GLN	2.4
1	B	22	GLN	2.4
1	C	99	GLY	2.4
1	C	170	VAL	2.4
1	C	278	VAL	2.4
1	C	23	LYS	2.4
1	C	123	TYR	2.3
1	A	511	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	458	THR	2.3
1	C	50	GLU	2.3
1	C	60	THR	2.3
1	B	62	ILE	2.3
1	B	137	ILE	2.3
1	C	285	PRO	2.3
1	A	373	GLY	2.3
1	A	75	VAL	2.3
1	B	512	SER	2.3
1	C	100	ASP	2.3
1	A	368	TYR	2.3
1	B	60	THR	2.3
1	B	80	ASN	2.3
1	B	446	ASN	2.3
1	B	416	LYS	2.3
1	C	127	ARG	2.3
1	C	318	LEU	2.3
1	C	211	PHE	2.3
1	B	82	ALA	2.3
1	B	454	PRO	2.3
1	C	475	GLN	2.3
1	C	75	VAL	2.3
1	A	370	TYR	2.2
1	B	355	PHE	2.2
1	B	56	SER	2.2
1	B	399	SER	2.2
1	A	63	ILE	2.2
1	C	496	THR	2.2
1	A	50	GLU	2.2
1	A	131	GLY	2.2
1	C	97	PRO	2.2
1	C	472	ASN	2.2
1	C	73	VAL	2.2
1	A	53	THR	2.2
1	A	436	LEU	2.2
1	C	125	LEU	2.2
1	B	42	GLY	2.2
1	B	58	ASP	2.2
1	B	474	ASP	2.2
1	C	70	GLY	2.2
1	A	444	TYR	2.2
1	B	77	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	510	ASN	2.2
1	C	139	GLU	2.2
1	B	403	THR	2.2
1	B	440	SER	2.2
1	A	383	GLY	2.2
1	C	421	GLY	2.2
1	C	321	ALA	2.2
1	A	390	PHE	2.1
1	B	90	PHE	2.1
1	C	460	ASN	2.1
1	C	462	ASN	2.1
1	A	485	ILE	2.1
1	B	397	ASP	2.1
1	B	452	ASP	2.1
1	B	466	THR	2.1
1	B	325	SER	2.1
1	B	40	ILE	2.1
1	C	370	TYR	2.1
1	A	300	ASP	2.1
1	B	287	ASP	2.1
1	B	66	SER	2.1
1	B	354	THR	2.1
1	B	356	SER	2.1
1	C	53	THR	2.1
1	C	177	SER	2.1
1	C	375	ASN	2.1
1	C	446	ASN	2.1
1	A	514	SER	2.1
1	C	66	SER	2.1
1	B	453	THR	2.1
1	B	277	HIS	2.1
1	B	414	VAL	2.1
1	C	80	ASN	2.1
1	C	456	LEU	2.1
1	C	78	ASP	2.1
1	C	452	ASP	2.1
1	C	324	ARG	2.1
1	B	76	ILE	2.0
1	B	448	PHE	2.0
1	C	325	SER	2.0
1	C	438	SER	2.0
1	B	99	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	464	GLY	2.0
1	B	81	GLN	2.0
1	B	128	ASN	2.0
1	C	323	PRO	2.0
1	A	71	GLU	2.0
1	A	96	SER	2.0
1	A	35	PHE	2.0
1	C	277	HIS	2.0
1	B	499	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

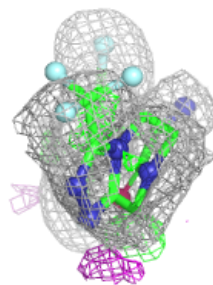
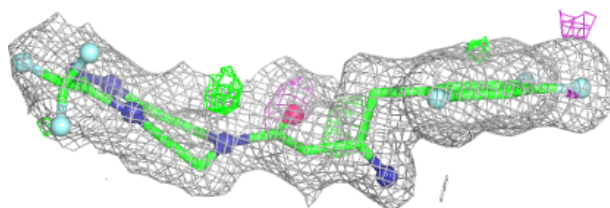
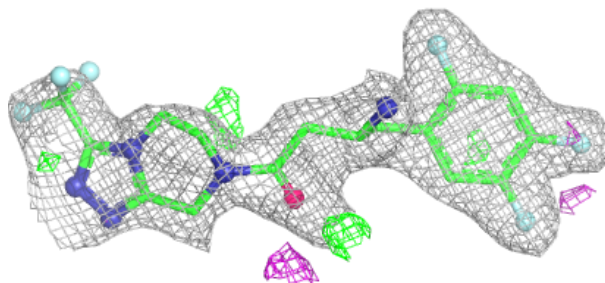
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	715	B	801	28/28	0.92	0.11	19,35,53,55	7
2	715	A	801	28/28	0.95	0.09	17,27,43,44	9
2	715	C	801	28/28	0.96	0.08	18,29,49,50	7

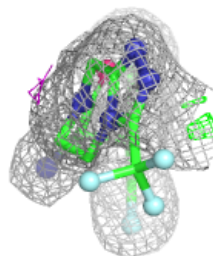
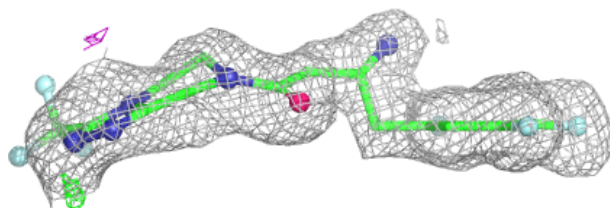
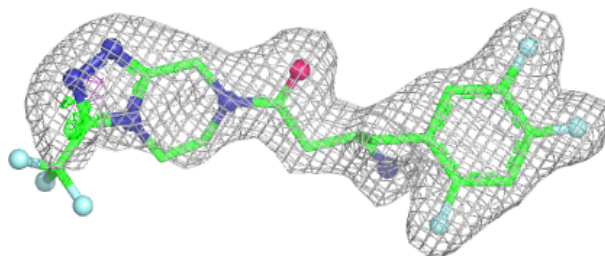
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

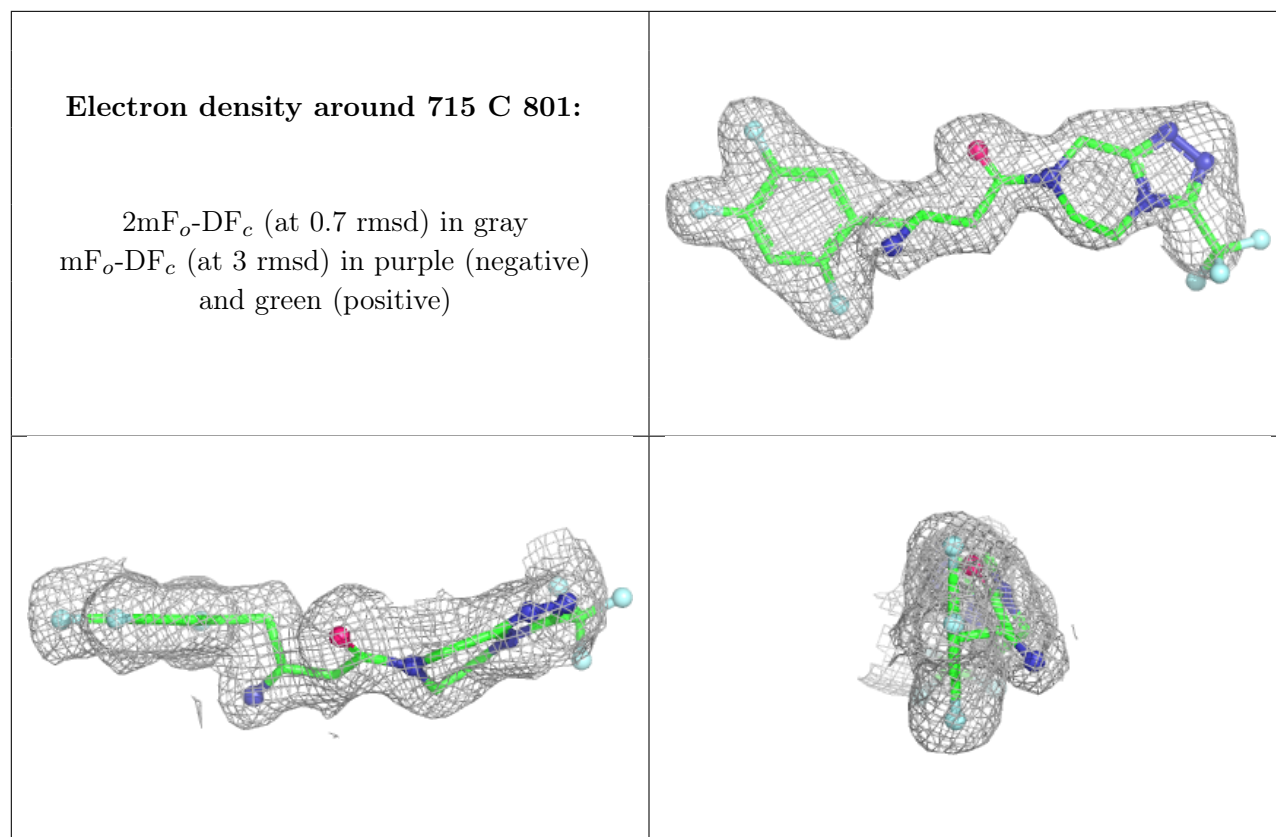
Electron density around 715 B 801:

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

**Electron density around 715 A 801:**

$2mF_o-DF_c$ (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.