Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2023 – 04:19 PM JST

PDB ID	:	7Y4G
Title	:	sit-bound btDPP4
Authors	:	Hang, J.; Jiang, C.; Wang, K.; Zhang, Z.; Guo, F.; Liu, J.; Wang, G.; Lei, X.; Gonzalez, F.; Qiao, J.
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:

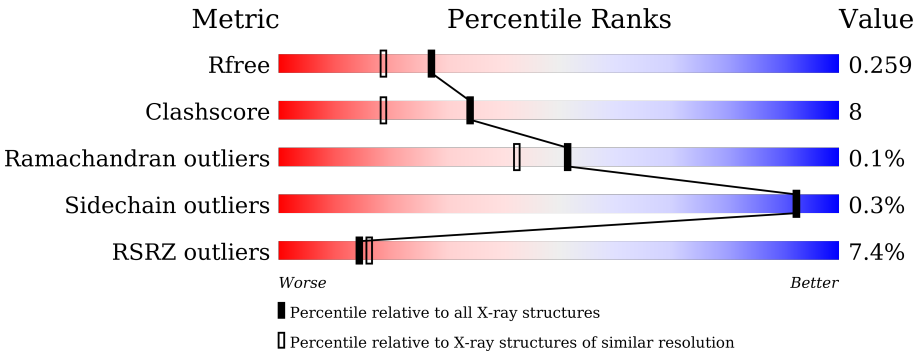
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	8% 79% 19%
1	B	715	6% 83% 15%
1	C	715	8% 82% 17%

2 Entry composition

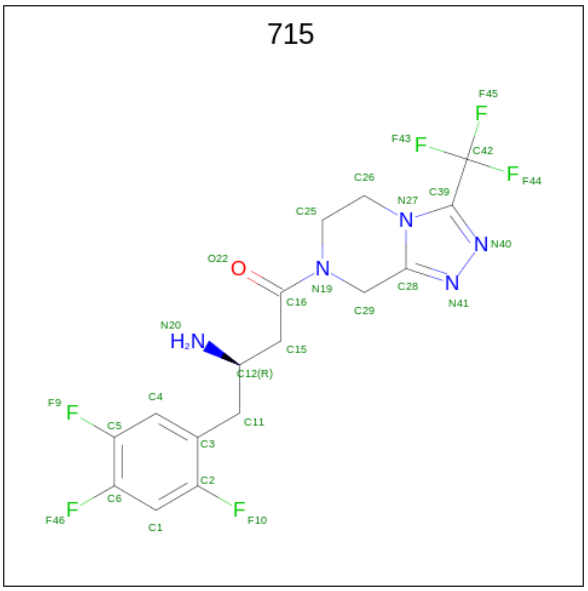
There are 3 unique types of molecules in this entry. The entry contains 18622 atoms, of which 0 are hydrogens and 0 are deuteriums.

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]TRIAZOLO[4,3-A]PYRAZIN-7(8H)-YL]-1-(2,4,5-TRIFLUOROPHENYL)BUTAN-2-AMINE (three-letter code: 715) (formula: $C_{16}H_{15}F_6N_5O$) (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		

Continued on next page...

Continued from previous page...

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.

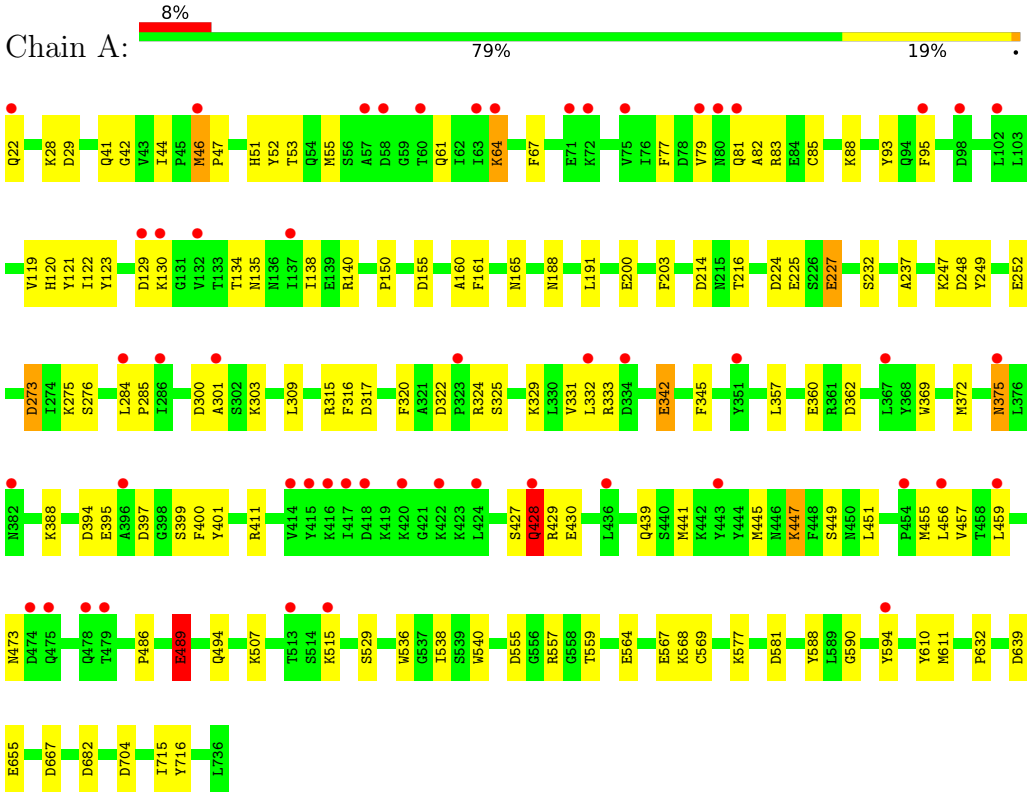
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	504	Total	O	0	0
			504	504		
3	B	353	Total	O	0	0
			353	353		
3	C	344	Total	O	0	0
			344	344		

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.

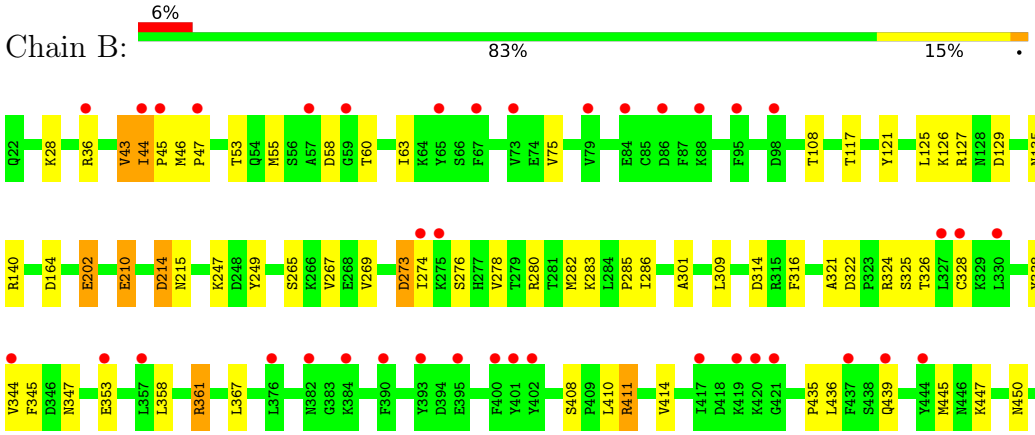
• Molecule 1: btDPP4

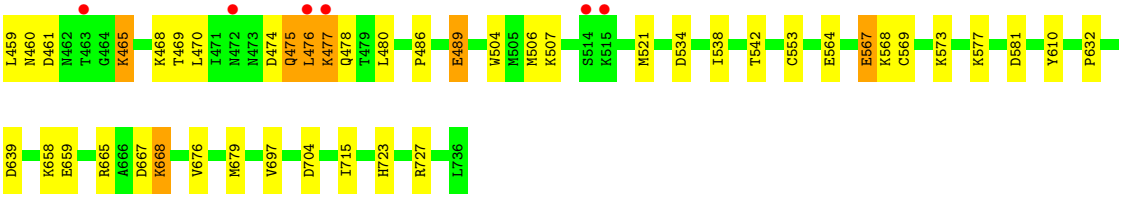
Chain A:



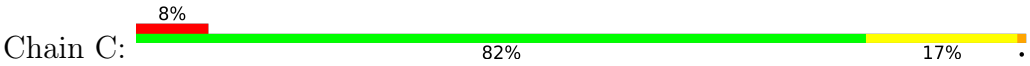
• Molecule 1: btDPP4

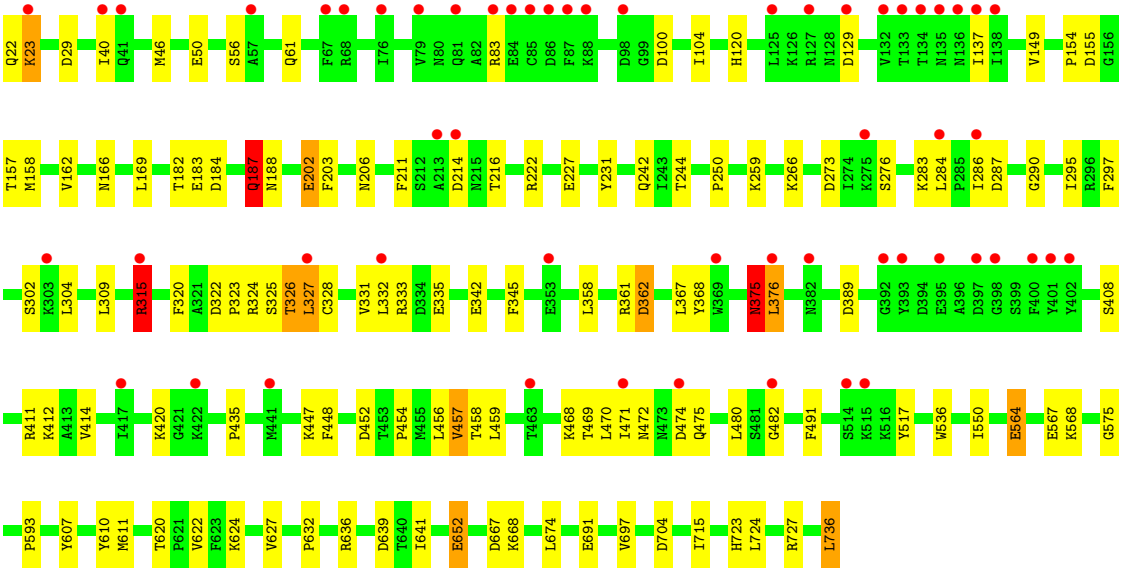
Chain B:





• Molecule 1: btDPP4





4 Data and refinement statistics (i)

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 – 1.97	Depositor EDS
% Data completeness (in resolution range)	84.6 (44.79-1.97) 84.6 (44.79-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.223 , 0.263 0.224 , 0.259	Depositor DCC
R_{free} test set	1984 reflections (1.38%)	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)	0.36 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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 $< |L| >$, $< L^2 >$ 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	1.23	28/5927 (0.5%)	1.41	46/8020 (0.6%)
1	B	1.08	13/5927 (0.2%)	1.23	40/8020 (0.5%)
1	C	1.06	24/5927 (0.4%)	1.23	30/8020 (0.4%)
All	All	1.13	65/17781 (0.4%)	1.29	116/24060 (0.5%)

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 (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	23	LYS	CB-CG	-13.19	1.17	1.52
1	B	44	ILE	CB-CG2	11.81	1.89	1.52
1	C	187	GLN	CB-CG	-11.64	1.21	1.52
1	B	465	LYS	CB-CG	-10.38	1.24	1.52
1	C	183	GLU	CD-OE2	9.16	1.35	1.25
1	A	249	TYR	CD2-CE2	7.96	1.51	1.39
1	B	477	LYS	CG-CD	-7.92	1.25	1.52
1	A	266	LYS	CD-CE	7.83	1.70	1.51
1	A	227	GLU	CD-OE1	7.62	1.34	1.25
1	C	23	LYS	CG-CD	-7.46	1.27	1.52
1	A	161	PHE	CE1-CZ	7.28	1.51	1.37
1	A	642	TYR	CG-CD2	6.99	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	TYR	CE1-CZ	6.97	1.47	1.38
1	A	667	ASP	CB-CG	6.93	1.66	1.51
1	A	227	GLU	CG-CD	6.75	1.62	1.51
1	B	477	LYS	CD-CE	6.74	1.68	1.51
1	B	214	ASP	CB-CG	-6.64	1.37	1.51
1	C	187	GLN	CD-NE2	6.51	1.49	1.32
1	C	607	TYR	CB-CG	6.46	1.61	1.51
1	C	315	ARG	CZ-NH1	6.38	1.41	1.33
1	A	79	VAL	CB-CG2	-6.36	1.39	1.52
1	A	401	TYR	CD2-CE2	6.36	1.48	1.39
1	A	716	TYR	CD1-CE1	6.35	1.48	1.39
1	A	652	GLU	CD-OE1	6.33	1.32	1.25
1	B	269	VAL	CB-CG1	6.29	1.66	1.52
1	C	491	PHE	CE1-CZ	6.14	1.49	1.37
1	B	210	GLU	CD-OE1	6.12	1.32	1.25
1	C	50	GLU	CB-CG	-6.11	1.40	1.52
1	B	342	GLU	CG-CD	6.00	1.60	1.51
1	A	594	TYR	CE2-CZ	5.95	1.46	1.38
1	A	395	GLU	CG-CD	5.79	1.60	1.51
1	C	636	ARG	CG-CD	5.77	1.66	1.51
1	B	249	TYR	CE2-CZ	5.77	1.46	1.38
1	C	202	GLU	CB-CG	5.75	1.63	1.52
1	C	457	VAL	CB-CG1	-5.70	1.40	1.52
1	A	316	PHE	CE1-CZ	5.68	1.48	1.37
1	B	676	VAL	CB-CG2	-5.61	1.41	1.52
1	B	202	GLU	CB-CG	5.59	1.62	1.52
1	B	465	LYS	CD-CE	-5.54	1.37	1.51
1	C	202	GLU	CG-CD	5.54	1.60	1.51
1	A	611	MET	CG-SD	5.52	1.95	1.81
1	A	268	GLU	CG-CD	5.51	1.60	1.51
1	C	668	LYS	CE-NZ	5.50	1.62	1.49
1	C	652	GLU	CD-OE1	5.42	1.31	1.25
1	A	200	GLU	CB-CG	5.39	1.62	1.52
1	A	252	GLU	CD-OE2	5.34	1.31	1.25
1	A	329	LYS	CE-NZ	5.33	1.62	1.49
1	C	624	LYS	CE-NZ	5.31	1.62	1.49
1	A	227	GLU	CB-CG	5.29	1.62	1.52
1	A	28	LYS	CD-CE	5.27	1.64	1.51
1	A	428	GLN	CG-CD	5.27	1.63	1.51
1	B	567	GLU	CG-CD	5.24	1.59	1.51
1	A	85	CYS	CB-SG	-5.19	1.73	1.81
1	C	667	ASP	CB-CG	5.19	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	266	LYS	CE-NZ	5.14	1.61	1.49
1	C	736	LEU	CG-CD2	-5.14	1.32	1.51
1	A	266	LYS	CE-NZ	5.14	1.61	1.49
1	A	540	TRP	CZ3-CH2	5.13	1.48	1.40
1	C	231	TYR	CD2-CE2	5.13	1.47	1.39
1	C	183	GLU	CB-CG	-5.13	1.42	1.52
1	C	448	PHE	CD1-CE1	5.12	1.49	1.39
1	A	588	TYR	CD1-CE1	5.09	1.47	1.39
1	A	119	VAL	CB-CG2	5.09	1.63	1.52
1	C	564	GLU	CB-CG	-5.08	1.42	1.52
1	C	259	LYS	CD-CE	5.01	1.63	1.51

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	GLU	OE1-CD-OE2	-35.92	80.19	123.30
1	C	327	LEU	CB-CG-CD2	31.89	165.21	111.00
1	A	489	GLU	OE1-CD-OE2	-30.67	86.49	123.30
1	B	489	GLU	OE1-CD-OE2	-30.48	86.72	123.30
1	C	183	GLU	OE1-CD-OE2	-26.72	91.24	123.30
1	C	183	GLU	CG-CD-OE1	22.56	163.42	118.30
1	A	252	GLU	CG-CD-OE1	22.25	162.81	118.30
1	C	327	LEU	CB-CG-CD1	-22.09	73.44	111.00
1	A	489	GLU	CG-CD-OE1	21.63	161.56	118.30
1	B	489	GLU	CG-CD-OE1	21.22	160.74	118.30
1	C	183	GLU	CG-CD-OE2	-19.73	78.83	118.30
1	B	475	GLN	N-CA-CB	19.19	145.13	110.60
1	B	489	GLU	CG-CD-OE2	-18.35	81.60	118.30
1	B	475	GLN	CA-CB-CG	18.07	153.16	113.40
1	A	252	GLU	CG-CD-OE2	-17.73	82.83	118.30
1	A	489	GLU	CG-CD-OE2	-17.53	83.24	118.30
1	A	428	GLN	CG-CD-OE1	16.19	153.97	121.60
1	A	64	LYS	CD-CE-NZ	16.03	148.57	111.70
1	A	456	LEU	CB-CG-CD2	-15.66	84.38	111.00
1	C	315	ARG	CG-CD-NE	15.46	144.26	111.80
1	A	428	GLN	CA-CB-CG	-14.85	80.74	113.40
1	A	428	GLN	CG-CD-NE2	-14.72	81.37	116.70
1	A	64	LYS	CG-CD-CE	-14.25	69.14	111.90
1	A	64	LYS	N-CA-CB	14.03	135.85	110.60
1	B	475	GLN	CB-CA-C	-12.99	84.42	110.40
1	A	375	ASN	N-CA-CB	-12.43	88.23	110.60
1	B	465	LYS	CD-CE-NZ	12.30	139.99	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	475	GLN	CB-CG-CD	12.24	143.42	111.60
1	A	667	ASP	CB-CG-OD1	12.16	129.25	118.30
1	C	187	GLN	CA-CB-CG	11.95	139.69	113.40
1	A	64	LYS	CB-CA-C	-11.79	86.83	110.40
1	C	315	ARG	CD-NE-CZ	-11.62	107.33	123.60
1	C	667	ASP	CB-CG-OD1	11.15	128.34	118.30
1	C	376	LEU	CB-CG-CD2	-11.06	92.20	111.00
1	B	477	LYS	CG-CD-CE	-10.93	79.12	111.90
1	A	375	ASN	CB-CG-ND2	-10.40	91.75	116.70
1	B	44	ILE	N-CA-C	-10.18	83.51	111.00
1	A	447	LYS	CA-CB-CG	9.96	135.31	113.40
1	A	456	LEU	CD1-CG-CD2	-9.55	81.85	110.50
1	B	44	ILE	CB-CG1-CD1	9.51	140.52	113.90
1	C	183	GLU	CB-CA-C	9.36	129.12	110.40
1	A	362	ASP	CB-CG-OD1	9.22	126.60	118.30
1	B	44	ILE	CB-CA-C	-9.10	93.41	111.60
1	B	273	ASP	CB-CG-OD2	-8.88	110.30	118.30
1	A	447	LYS	CB-CG-CD	-8.71	88.96	111.60
1	B	274	ILE	CG1-CB-CG2	-8.51	92.69	111.40
1	A	372	MET	CB-CA-C	8.20	126.80	110.40
1	B	477	LYS	CD-CE-NZ	8.13	130.40	111.70
1	C	187	GLN	N-CA-CB	8.12	125.22	110.60
1	C	315	ARG	CB-CG-CD	-8.05	90.67	111.60
1	A	428	GLN	CB-CA-C	8.04	126.47	110.40
1	B	44	ILE	CA-CB-CG2	-7.98	94.94	110.90
1	C	187	GLN	CB-CA-C	-7.89	94.63	110.40
1	A	46	MET	CA-CB-CG	-7.85	99.96	113.30
1	C	23	LYS	CA-CB-CG	-7.75	96.35	113.40
1	A	427	SER	C-N-CA	7.72	141.01	121.70
1	C	23	LYS	CG-CD-CE	-7.65	88.94	111.90
1	A	372	MET	N-CA-CB	-7.60	96.92	110.60
1	C	327	LEU	CA-CB-CG	-7.60	97.82	115.30
1	B	214	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	B	44	ILE	CA-CB-CG1	-7.55	96.65	111.00
1	A	375	ASN	CB-CA-C	7.33	125.07	110.40
1	B	474	ASP	C-N-CA	-7.06	104.04	121.70
1	C	183	GLU	N-CA-CB	-7.02	97.97	110.60
1	B	476	LEU	CB-CG-CD2	-6.99	99.12	111.00
1	B	43	VAL	C-N-CA	-6.94	104.35	121.70
1	A	555	ASP	CB-CG-OD1	6.93	124.54	118.30
1	B	465	LYS	CG-CD-CE	6.89	132.58	111.90
1	A	449	SER	N-CA-CB	6.89	120.83	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	210	GLU	CA-CB-CG	6.84	128.45	113.40
1	A	375	ASN	CB-CG-OD1	6.75	135.10	121.60
1	C	46	MET	CG-SD-CE	-6.63	89.59	100.20
1	B	55	MET	CA-CB-CG	6.42	124.21	113.30
1	C	326	THR	C-N-CA	-6.19	106.23	121.70
1	A	428	GLN	N-CA-CB	-6.16	99.52	110.60
1	B	126	LYS	CB-CG-CD	-6.14	95.63	111.60
1	B	445	MET	CG-SD-CE	-6.14	90.37	100.20
1	C	362	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	C	315	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	C	46	MET	CA-CB-CG	5.99	123.49	113.30
1	A	64	LYS	N-CA-C	-5.94	94.97	111.00
1	A	682	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	125	LEU	CB-CG-CD2	-5.89	100.99	111.00
1	B	668	LYS	CD-CE-NZ	5.85	125.16	111.70
1	B	581	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	667	ASP	OD1-CG-OD2	-5.81	112.26	123.30
1	B	314	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	470	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	B	667	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	182	THR	C-N-CA	-5.65	107.59	121.70
1	C	375	ASN	N-CA-CB	5.55	120.60	110.60
1	A	155	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	521	MET	CG-SD-CE	-5.48	91.42	100.20
1	A	449	SER	CB-CA-C	-5.44	99.77	110.10
1	B	361	ARG	CB-CG-CD	-5.42	97.51	111.60
1	B	44	ILE	CA-C-O	-5.42	108.73	120.10
1	B	461	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	B	274	ILE	CA-CB-CG1	5.37	121.19	111.00
1	B	679	MET	CA-CB-CG	-5.35	104.20	113.30
1	C	691	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	A	273	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	667	ASP	OD1-CG-OD2	-5.23	113.36	123.30
1	A	248	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	29	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	379	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	A	639	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	389	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	C	375	ASN	CB-CG-ND2	-5.16	104.33	116.70
1	A	372	MET	CG-SD-CE	-5.15	91.96	100.20
1	A	411	ARG	CG-CD-NE	-5.14	100.99	111.80
1	B	461	ASP	CB-CG-OD1	5.11	122.90	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	LYS	CB-CG-CD	5.11	124.88	111.60
1	C	724	LEU	CB-CG-CD2	5.08	119.63	111.00
1	B	465	LYS	N-CA-CB	-5.07	101.47	110.60
1	B	273	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	642	TYR	CZ-CE2-CD2	-5.07	115.24	119.80

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 (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	5779	0	5606	110	2
1	B	5779	0	5607	89	2
1	C	5779	0	5607	91	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	34	0
3	B	353	0	0	17	1
3	C	344	0	0	14	2
All	All	18622	0	16865	287	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 8.

All (287) 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: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: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:B:47:PRO:HA	1:B:439:GLN:CD	1.95	0.86
1:A:317:ASP:OD2	3:A:901:HOH:O	1.94	0.84
1:A:81:GLN:C	3:A:909:HOH:O	2.18	0.79
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:B:455:MET:HE3	1:B:456:LEU:N	1.99	0.78
1:C:227:GLU:OE2	1:C:227:GLU:HA	1.84	0.78
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
1:C:475:GLN:H	1:C:475:GLN:CD	1.92	0.73
1:A:567:GLU:OE1	3:A:905:HOH:O	2.06	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ASN:ND2	1:C:474:ASP:CG	2.43	0.72
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: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: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: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:475:GLN:O	1:B:476:LEU:C	2.34	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASP:OD2	1:A:266:LYS:HE2	1.98	0.63
1:C:297:PHE:CE1	1:C:304:LEU:HB2	2.33	0.63
1:B:455:MET:HE3	1:B:456:LEU:H	1.64	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: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: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: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:564:GLU:HG3	1:B:568:LYS:HE3	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
1:B:282:MET:HE2	1:B:326:THR:HA	1.88	0.56
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:88:LYS:H	1:A:88:LYS:CD	2.18	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.73	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: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:B:273:ASP:CG	1:B:276:SER:HB3	2.30	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:C:327:LEU:HG	1:C:328:CYS:N	2.25	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:273:ASP:CG	1:A:276:SER:HB3	2.31	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
1:A:227:GLU:OE1	1:A:227:GLU:HA	2.10	0.51
1:A:275:LYS:NZ	3:A:921:HOH:O	2.30	0.51
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:C:472:ASN:ND2	1:C:474:ASP:OD2	2.45	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: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:B:410:LEU:C	1:B:411:ARG:HG3	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:456:LEU:CD2	1:C:458:THR:HG23	2.43	0.49
1:B:475:GLN:C	1:B:477:LYS:N	2.64	0.49
1:C:358:LEU:HD23	1:C:367:LEU:HA	1.95	0.49
1:C:472:ASN:HD21	1:C:474:ASP:CG	2.13	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:C:452:ASP:N	1:C:452:ASP:OD1	2.45	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:447:LYS:HA	1:B:455:MET:HE2	1.95	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:B:506:MET:HE1	3:B:960:HOH:O	2.14	0.47
1:A:214:ASP:OD1	3:A:916:HOH:O	2.20	0.47
1:A:590:GLY:C	3:A:911:HOH:O	2.53	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:332:LEU:HD23	1:C:332:LEU:C	2.37	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: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: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:282:MET:HE2	1:B:282:MET:HA	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:486:PRO:HB3	1:B:507:LYS:O	2.18	0.43
1:C:155:ASP:OD1	1:C:157:THR:OG1	2.29	0.43
1:B:47:PRO:C	1:B:439:GLN:OE1	2.56	0.43
1:B:282:MET:CE	1:B:326:THR:HA	2.48	0.43
1:A:188:ASN:HA	1:A:225:GLU:OE2	2.19	0.43
1:A:165:ASN:ND2	1:A:191:LEU:HD12	2.34	0.43
1:A:445:MET:HE2	1:A:447:LYS:HE3	1.99	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: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:369:TRP:CD2	1:A:400:PHE:HE2	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:575:GLY:HA2	1:C:611:MET:HE1	2.02	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:A:191:LEU:CD1	1:A:191:LEU:N	2.83	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: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:A:324:ARG:HH11	1:A:324:ARG:HD2	1.73	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:A:489:GLU:O	1:A:489:GLU:HG3	2.21	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: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: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:C:162:VAL:HA	1:C:166:ASN:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:472:ASN:HD22	1:C:474:ASP:CG	2.19	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%)	51	42
1	B	713/715 (100%)	688 (96%)	24 (3%)	1 (0%)	51	42
1	C	713/715 (100%)	684 (96%)	28 (4%)	1 (0%)	51	42
All	All	2139/2145 (100%)	2060 (96%)	76 (4%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	625 (100%)	2 (0%)	92 92
1	B	627/627 (100%)	627 (100%)	0	100 100
1	C	627/627 (100%)	624 (100%)	3 (0%)	88 87
All	All	1881/1881 (100%)	1876 (100%)	5 (0%)	92 92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASP
1	A	342	GLU
1	C	40	ILE
1	C	100	ASP
1	C	214	ASP

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	136	ASN
1	A	187	GLN
1	A	188	ASN
1	A	439	GLN
1	B	136	ASN
1	C	187	GLN
1	C	277	HIS
1	C	375	ASN
1	C	472	ASN
1	C	478	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
2	715	A	801	-	27,30,30	3.54	11 (40%)	32,45,45	2.18	15 (46%)
2	715	B	801	-	27,30,30	3.13	10 (37%)	32,45,45	2.29	13 (40%)
2	715	C	801	-	27,30,30	3.32	9 (33%)	32,45,45	2.20	15 (46%)

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	0/2/3/3
2	715	B	801	-	-	1/18/27/27	0/2/3/3
2	715	C	801	-	-	0/18/27/27	0/2/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	715	C4-C5	9.01	1.53	1.37
2	C	801	715	C4-C5	8.49	1.52	1.37
2	B	801	715	C1-C2	7.12	1.49	1.37
2	A	801	715	C3-C2	6.85	1.50	1.38
2	C	801	715	C1-C2	6.72	1.49	1.37
2	A	801	715	C1-C2	6.72	1.49	1.37
2	A	801	715	C1-C6	6.51	1.48	1.37
2	B	801	715	C4-C5	6.30	1.48	1.37
2	B	801	715	C4-C3	6.24	1.50	1.39
2	C	801	715	C4-C3	6.02	1.49	1.39
2	C	801	715	C16-N19	6.02	1.47	1.35
2	A	801	715	C16-N19	5.93	1.47	1.35
2	B	801	715	C16-N19	5.83	1.47	1.35
2	C	801	715	C3-C2	5.61	1.48	1.38
2	C	801	715	C1-C6	5.23	1.46	1.37
2	B	801	715	C3-C2	5.15	1.47	1.38
2	B	801	715	C1-C6	5.00	1.46	1.37
2	A	801	715	C4-C3	4.91	1.47	1.39
2	A	801	715	C29-C28	3.92	1.58	1.51
2	B	801	715	O22-C16	-3.49	1.15	1.23
2	C	801	715	C29-C28	3.39	1.57	1.51
2	A	801	715	C6-C5	3.34	1.50	1.38
2	A	801	715	N41-N40	3.21	1.43	1.37
2	B	801	715	C6-C5	3.21	1.49	1.38
2	C	801	715	C11-C12	-2.64	1.49	1.53
2	C	801	715	C6-C5	2.55	1.47	1.38
2	A	801	715	C42-C39	2.49	1.53	1.51
2	B	801	715	C29-C28	2.39	1.55	1.51
2	B	801	715	C25-N19	-2.32	1.42	1.47
2	A	801	715	C15-C16	2.24	1.55	1.51

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	715	F43-C42-C39	-6.81	104.00	111.32
2	C	801	715	F43-C42-C39	-4.81	106.16	111.32
2	A	801	715	C25-C26-N27	4.26	117.74	109.07
2	A	801	715	C4-C3-C2	4.22	121.49	116.58
2	B	801	715	F44-C42-C39	-3.92	107.11	111.32
2	C	801	715	C25-C26-N27	3.87	116.95	109.07
2	B	801	715	C25-C26-N27	3.84	116.89	109.07
2	C	801	715	C26-N27-C39	3.65	132.80	125.38
2	C	801	715	C1-C6-C5	-3.48	117.07	121.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	715	C26-N27-C39	3.43	132.33	125.38
2	A	801	715	C26-N27-C39	3.28	132.03	125.38
2	A	801	715	C3-C4-C5	-3.20	116.03	119.91
2	B	801	715	F45-C42-F43	3.18	117.38	105.72
2	A	801	715	C42-C39-N40	3.16	125.43	122.36
2	B	801	715	C15-C16-N19	3.08	124.46	118.52
2	B	801	715	O22-C16-C15	-3.06	116.68	122.20
2	A	801	715	F10-C2-C3	3.02	122.88	117.96
2	C	801	715	C42-C39-N40	2.95	125.22	122.36
2	A	801	715	C28-C29-N19	2.94	118.06	111.49
2	C	801	715	F10-C2-C3	2.88	122.67	117.96
2	C	801	715	C28-C29-N19	2.86	117.87	111.49
2	C	801	715	C4-C5-C6	2.79	124.21	121.03
2	C	801	715	F45-C42-F43	2.78	115.92	105.72
2	C	801	715	F10-C2-C1	-2.78	113.08	118.61
2	A	801	715	F10-C2-C1	-2.72	113.19	118.61
2	A	801	715	O22-C16-C15	-2.70	117.32	122.20
2	C	801	715	C29-N19-C16	2.65	127.76	120.88
2	C	801	715	O22-C16-C15	-2.55	117.59	122.20
2	A	801	715	C28-N41-N40	2.52	110.70	105.96
2	A	801	715	F9-C5-C4	2.49	123.57	118.61
2	C	801	715	F44-C42-C39	-2.45	108.69	111.32
2	A	801	715	F45-C42-C39	-2.43	108.71	111.32
2	A	801	715	C1-C6-C5	2.42	123.79	121.03
2	B	801	715	F46-C6-C1	2.41	123.39	118.61
2	A	801	715	F43-C42-C39	-2.39	108.75	111.32
2	B	801	715	C29-N19-C16	2.34	126.96	120.88
2	C	801	715	F46-C6-C1	2.20	122.98	118.61
2	B	801	715	C28-N41-N40	2.19	110.07	105.96
2	C	801	715	C28-N41-N40	2.16	110.02	105.96
2	A	801	715	C29-N19-C16	2.11	126.36	120.88
2	B	801	715	C42-C39-N40	2.10	124.40	122.36
2	B	801	715	F9-C5-C4	2.09	122.78	118.61
2	B	801	715	C1-C6-C5	-2.07	118.67	121.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

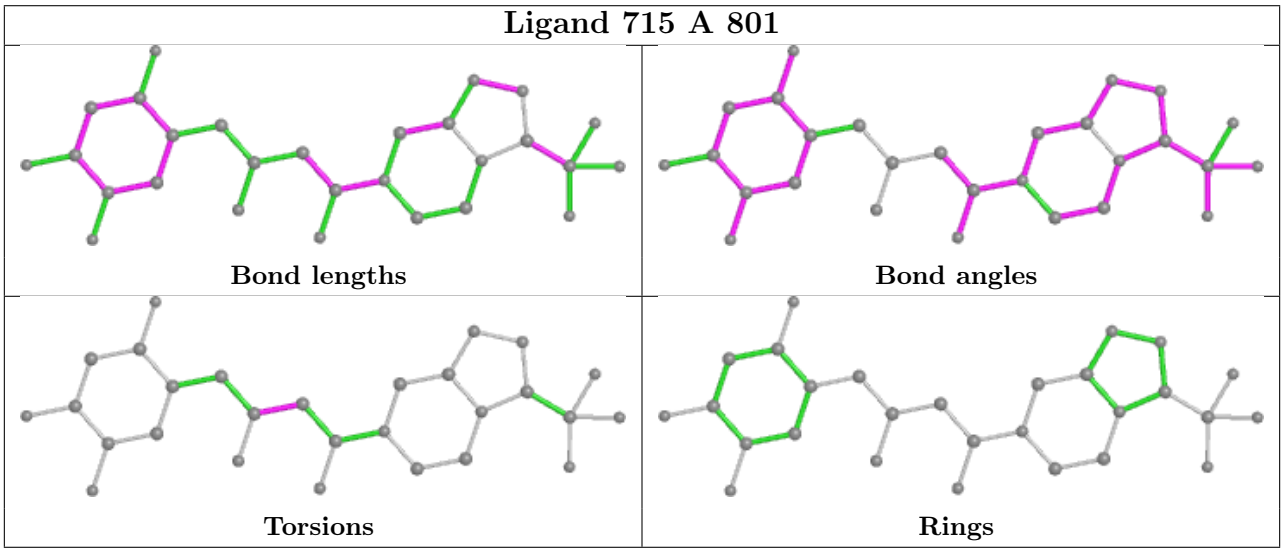
Mol	Chain	Res	Type	Atoms
2	B	801	715	N20-C12-C15-C16
2	A	801	715	N20-C12-C15-C16

There are no ring outliers.

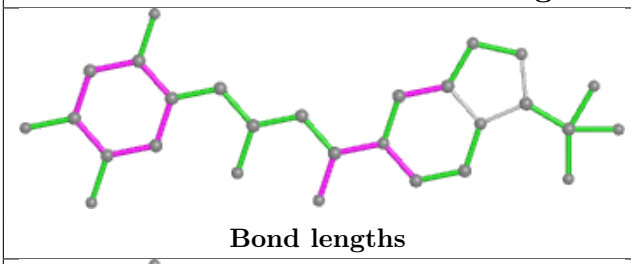
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	715	2	0

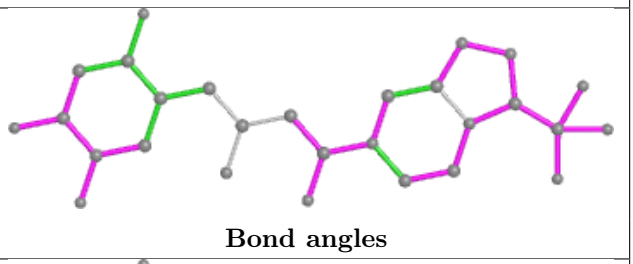
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



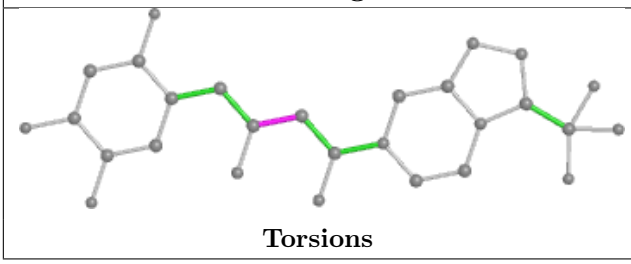
Ligand 715 B 801



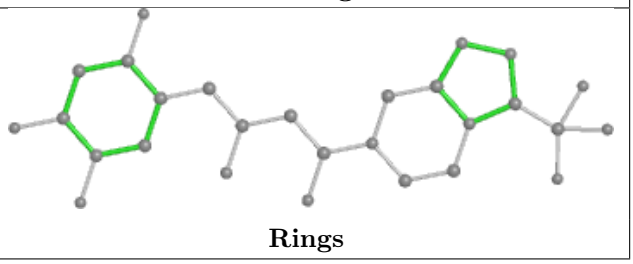
Bond lengths



Bond angles

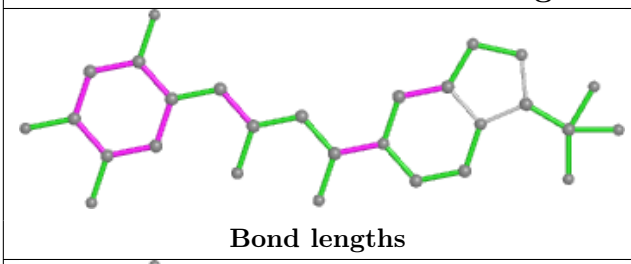


Torsions

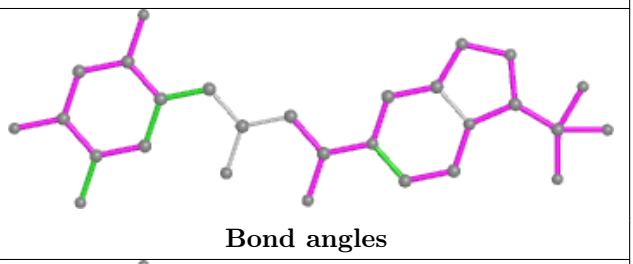


Rings

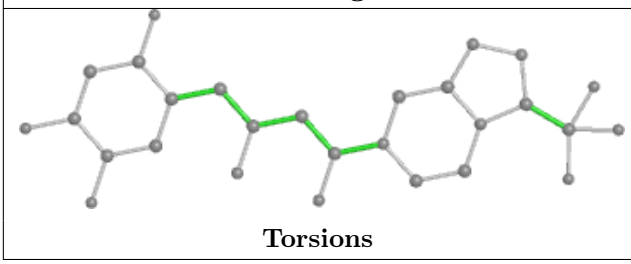
Ligand 715 C 801



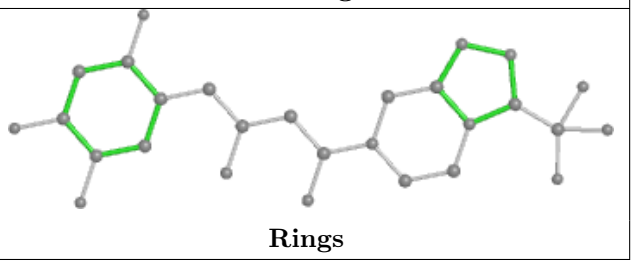
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.46	57 (7%)	12	14	12, 33, 56, 74	0
1	B	715/715 (100%)	0.47	46 (6%)	19	21	14, 38, 67, 83	0
1	C	715/715 (100%)	0.48	56 (7%)	13	14	15, 42, 77, 114	0
All	All	2145/2145 (100%)	0.47	159 (7%)	14	16	12, 36, 70, 114	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	132	VAL	6.5
1	C	327	LEU	6.3
1	C	79	VAL	5.6
1	C	129	ASP	5.6
1	A	418	ASP	5.5
1	B	476	LEU	5.4
1	A	377	ILE	5.2
1	B	327	LEU	5.2
1	A	64	LYS	5.1
1	C	137	ILE	4.9
1	A	132	VAL	4.7
1	B	419	LYS	4.7
1	B	79	VAL	4.7
1	C	84	GLU	4.7
1	A	515	LYS	4.5
1	A	513	THR	4.5
1	A	137	ILE	4.4
1	C	83	ARG	4.4
1	A	286	ILE	4.4
1	C	88	LYS	4.3
1	C	353	GLU	4.2
1	A	479	THR	4.2
1	A	129	ASP	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	135	ASN	4.1
1	C	284	LEU	4.1
1	B	86	ASP	4.1
1	C	87	PHE	4.1
1	B	395	GLU	4.0
1	C	85	CYS	4.0
1	A	475	GLN	3.9
1	A	459	LEU	3.9
1	B	420	LYS	3.9
1	B	463	THR	3.7
1	B	421	GLY	3.7
1	B	477	LYS	3.6
1	A	75	VAL	3.6
1	C	134	THR	3.5
1	C	98	ASP	3.5
1	B	382	ASN	3.5
1	C	86	ASP	3.3
1	B	439	GLN	3.3
1	A	102	LEU	3.3
1	A	95	PHE	3.3
1	A	478	GLN	3.3
1	C	286	ILE	3.2
1	B	353	GLU	3.2
1	A	424	LEU	3.2
1	C	393	TYR	3.2
1	A	396	ALA	3.2
1	A	375	ASN	3.2
1	A	382	ASN	3.1
1	B	98	ASP	3.1
1	B	417	ILE	3.1
1	C	138	ILE	3.1
1	A	454	PRO	3.1
1	C	81	GLN	3.1
1	C	382	ASN	3.1
1	C	214	ASP	3.0
1	C	474	ASP	3.0
1	A	428	GLN	3.0
1	A	420	LYS	3.0
1	B	328	CYS	3.0
1	A	130	LYS	3.0
1	B	402	TYR	2.9
1	A	63	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	133	THR	2.9
1	A	284	LEU	2.9
1	C	514	SER	2.9
1	C	402	TYR	2.9
1	A	98	ASP	2.9
1	A	81	GLN	2.9
1	A	332	LEU	2.9
1	A	367	LEU	2.9
1	C	41	GLN	2.9
1	B	400	PHE	2.9
1	C	463	THR	2.9
1	A	71	GLU	2.9
1	B	73	VAL	2.9
1	B	45	PRO	2.9
1	A	334	ASP	2.9
1	B	393	TYR	2.8
1	B	401	TYR	2.8
1	B	84	GLU	2.8
1	B	44	ILE	2.8
1	C	136	ASN	2.8
1	B	390	PHE	2.8
1	A	46	MET	2.7
1	B	514	SER	2.7
1	C	471	ILE	2.7
1	B	344	VAL	2.7
1	A	436	LEU	2.7
1	A	60	THR	2.7
1	B	384	LYS	2.7
1	A	474	ASP	2.7
1	A	79	VAL	2.7
1	B	444	TYR	2.7
1	B	65	TYR	2.6
1	C	515	LYS	2.6
1	B	57	ALA	2.6
1	A	470	LEU	2.6
1	A	422	LYS	2.6
1	C	397	ASP	2.6
1	A	414	VAL	2.6
1	C	400	PHE	2.5
1	B	36	ARG	2.5
1	A	417	ILE	2.5
1	A	351	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	137	ILE	2.5
1	B	47	PRO	2.5
1	C	67	PHE	2.4
1	A	22	GLN	2.4
1	C	40	ILE	2.4
1	A	301	ALA	2.4
1	B	515	LYS	2.4
1	C	392	GLY	2.4
1	C	401	TYR	2.4
1	C	315	ARG	2.4
1	C	68	ARG	2.3
1	A	415	TYR	2.3
1	B	330	LEU	2.3
1	C	57	ALA	2.3
1	A	594	TYR	2.3
1	C	398	GLY	2.3
1	C	369	TRP	2.3
1	C	422	LYS	2.3
1	C	332	LEU	2.3
1	A	416	LYS	2.3
1	C	23	LYS	2.3
1	B	274	ILE	2.2
1	C	275	LYS	2.2
1	A	380	VAL	2.2
1	A	471	ILE	2.2
1	C	376	LEU	2.2
1	C	213	ALA	2.2
1	B	275	LYS	2.2
1	A	80	ASN	2.2
1	B	376	LEU	2.2
1	B	95	PHE	2.2
1	B	472	ASN	2.2
1	A	381	THR	2.2
1	C	127	ARG	2.2
1	C	395	GLU	2.1
1	C	417	ILE	2.1
1	A	443	TYR	2.1
1	C	76	ILE	2.1
1	B	59	GLY	2.1
1	B	357	LEU	2.1
1	B	67	PHE	2.1
1	A	58	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	303	LYS	2.1
1	C	441	MET	2.0
1	B	88	LYS	2.0
1	A	57	ALA	2.0
1	A	323	PRO	2.0
1	B	437	PHE	2.0
1	C	482	GLY	2.0
1	A	456	LEU	2.0
1	C	125	LEU	2.0
1	A	72	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

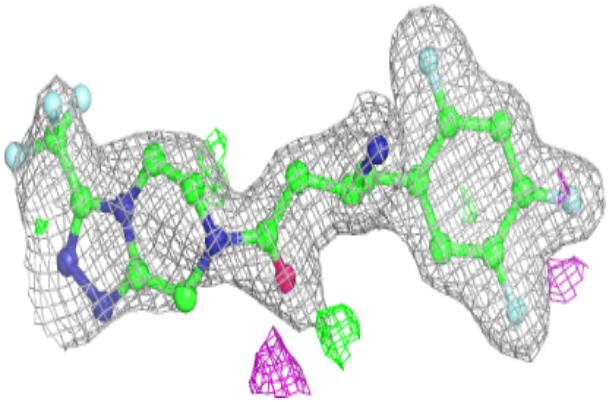
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

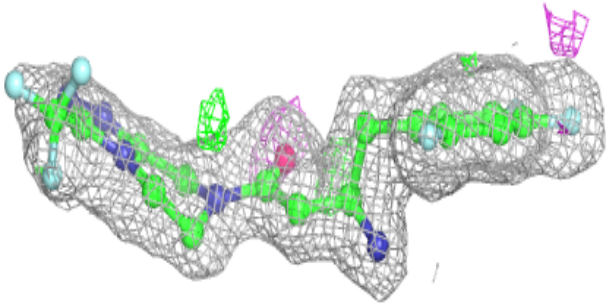
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	715	B	801	28/28	0.93	0.16	19,35,53,55	7
2	715	C	801	28/28	0.95	0.14	18,29,49,50	7
2	715	A	801	28/28	0.96	0.14	17,27,43,44	9

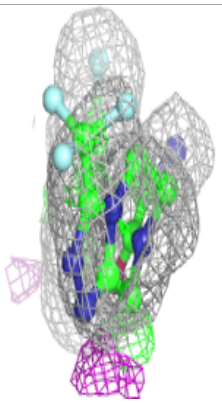
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

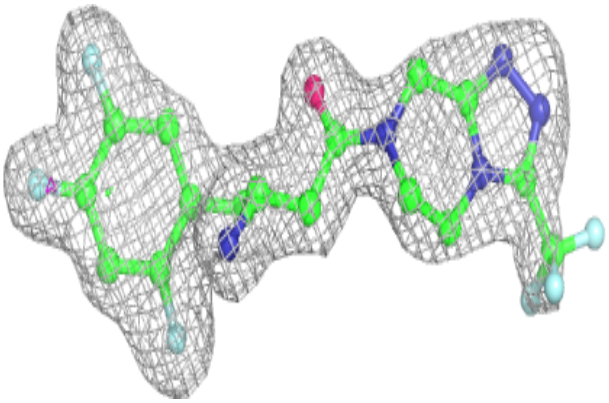


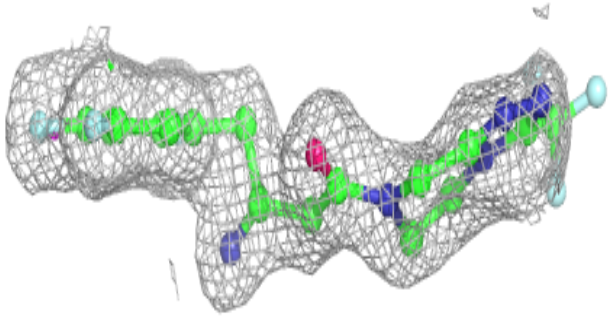


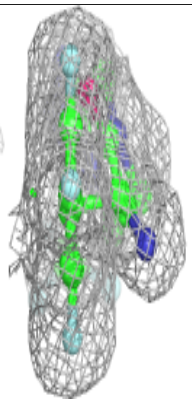


Electron density around 715 C 801:

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

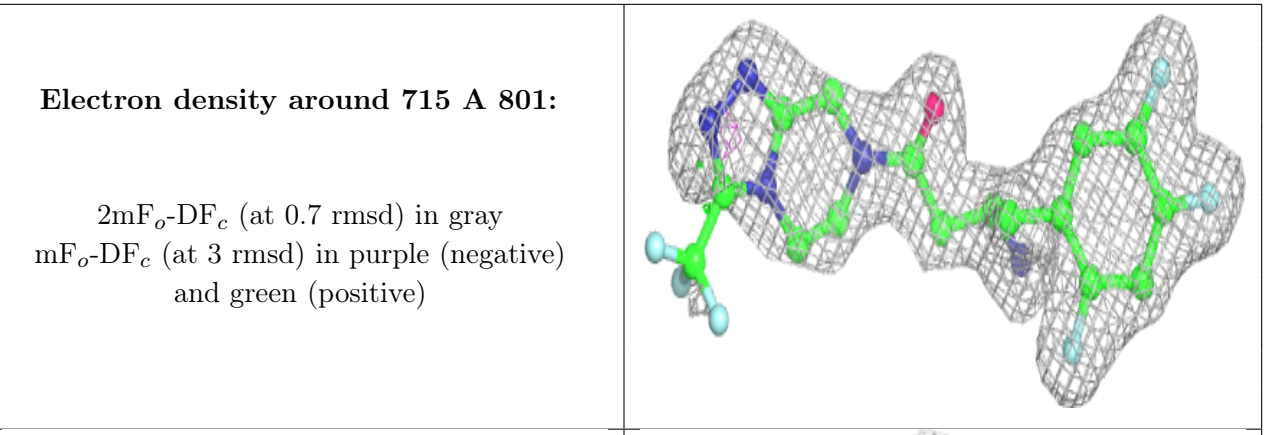


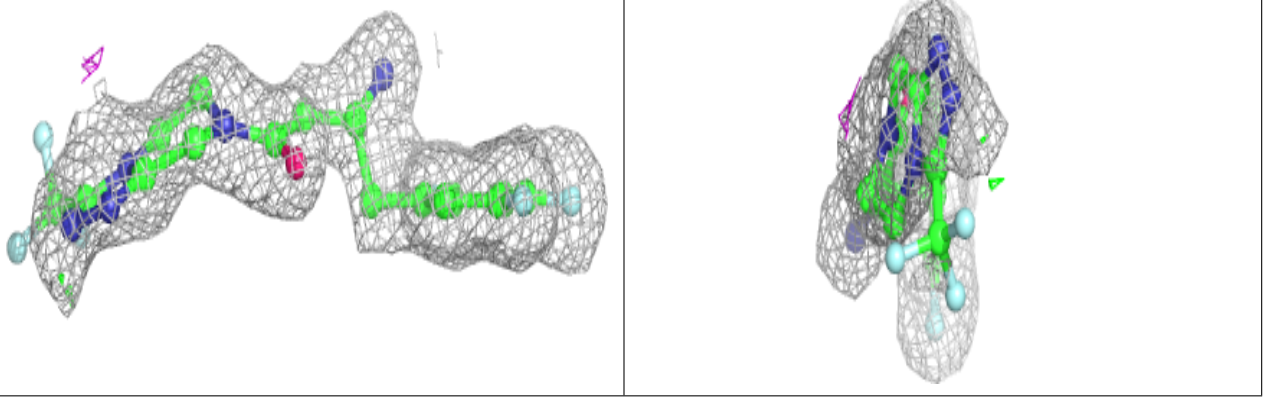




Electron density around 715 A 801:

$2mF_o$-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.