Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 07:42 am BST

PDB ID	:	4BBF
Title	:	Aminoalkylpyrimidine Inhibitor Complexes with JAK2
Authors	:	Li, J.
Deposited on	:	2012-09-21
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

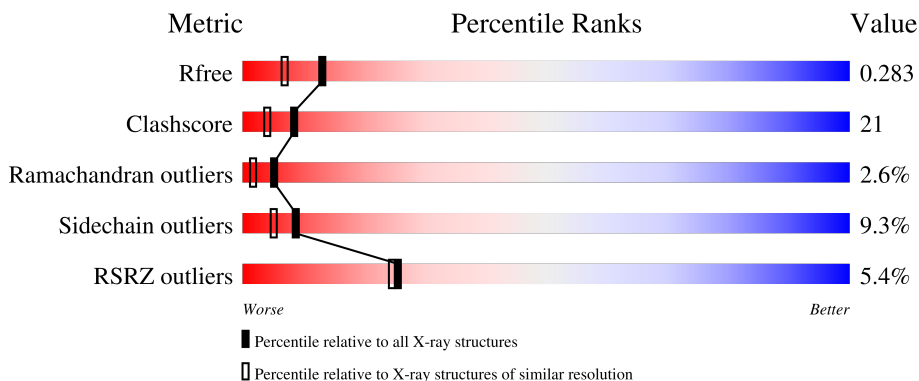|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		21
Ramachandran outliers		2.6%
Sidechain outliers		9.3%
RSRZ outliers		5.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	298	5% / 69% 21% 6% · ·
1	B	298	6% / 61% 28% 6% · ·
1	C	298	5% / 66% 21% 8% · ·
1	D	298	5% / 68% 24% · · ·

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10083 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 TYROSINE-PROTEIN KINASE JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			
1	B	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			
1	C	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			
1	D	288	Total	C	N	O	S	0	0	0
			2379	1515	415	436	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	837	GLY	-	expression tag	UNP O60674
A	838	SER	-	expression tag	UNP O60674
A	976	ASN	ASP	engineered mutation	UNP O60674
A	1133	GLU	-	expression tag	UNP O60674
A	1134	PHE	-	expression tag	UNP O60674
B	837	GLY	-	expression tag	UNP O60674
B	838	SER	-	expression tag	UNP O60674
B	976	ASN	ASP	engineered mutation	UNP O60674
B	1133	GLU	-	expression tag	UNP O60674
B	1134	PHE	-	expression tag	UNP O60674
C	837	GLY	-	expression tag	UNP O60674
C	838	SER	-	expression tag	UNP O60674
C	976	ASN	ASP	engineered mutation	UNP O60674
C	1133	GLU	-	expression tag	UNP O60674
C	1134	PHE	-	expression tag	UNP O60674
D	837	GLY	-	expression tag	UNP O60674
D	838	SER	-	expression tag	UNP O60674
D	976	ASN	ASP	engineered mutation	UNP O60674
D	1133	GLU	-	expression tag	UNP O60674
D	1134	PHE	-	expression tag	UNP O60674

- Molecule 2 is (2R)-N-[4-[2-[(4-morpholin-4-ylphenyl)amino]pyrimidin-4-yl]phenyl]pyrrolidine-2-carboxamide (three-letter code: O19) (formula: $C_{25}H_{28}N_6O_2$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 33	C 25	N 6	O 2	0	0
2	B	1	Total 33	C 25	N 6	O 2	0	0
2	C	1	Total 33	C 25	N 6	O 2	0	0
2	D	1	Total 33	C 25	N 6	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	118	Total 118	O 118	0	0
3	B	106	Total 106	O 106	0	0
3	C	110	Total 110	O 110	0	0
3	D	101	Total 101	O 101	0	0

3 Residue-property plots ⓘ

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: TYROSINE-PROTEIN KINASE JAK2
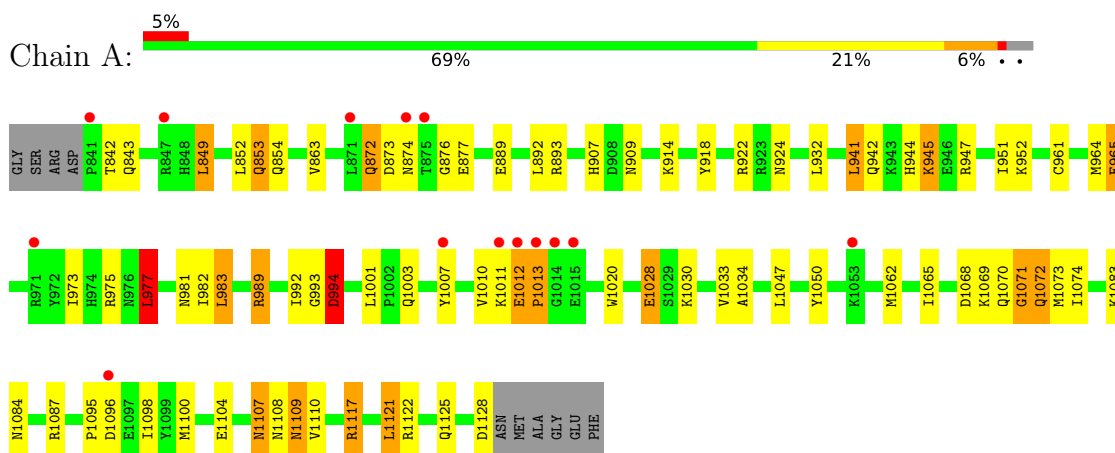
- Molecule 1: TYROSINE-PROTEIN KINASE JAK2
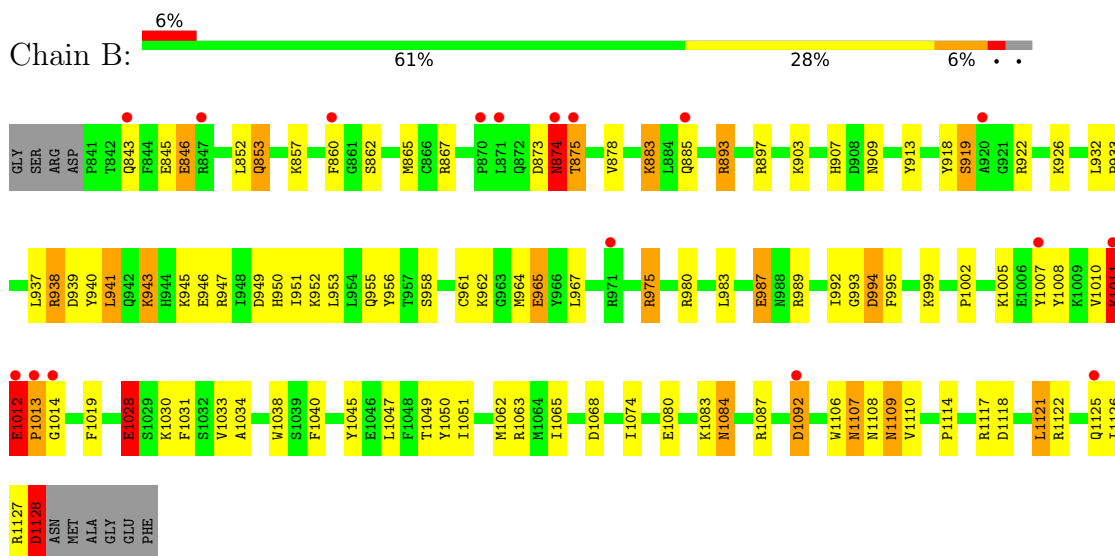
- Molecule 1: TYROSINE-PROTEIN KINASE JAK2
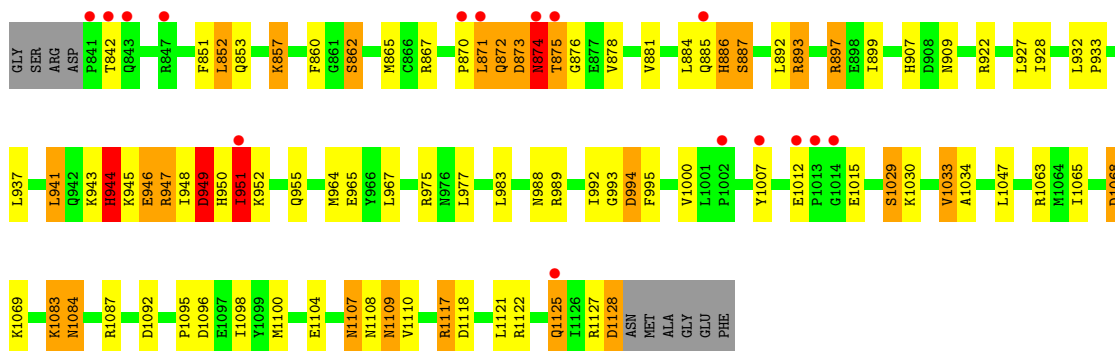
• Molecule 1: TYROSINE-PROTEIN KINASE JAK2
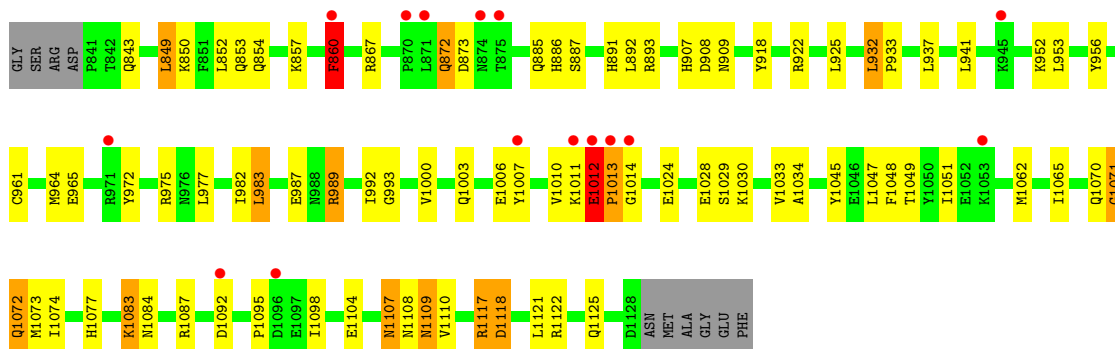
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.95Å 76.01Å 88.18Å 75.53° 67.00° 63.04°	Depositor
Resolution (Å)	80.85 – 2.00 27.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.9 (80.85-2.00) 94.9 (27.11-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.289 0.225 , 0.283	Depositor DCC
R_{free} test set	4672 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 29.5	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.467 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10083	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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 53.68 % 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 4.0709e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: O19

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	1.08	3/2432 (0.1%)	1.04	7/3274 (0.2%)
1	B	1.10	6/2432 (0.2%)	1.03	8/3274 (0.2%)
1	C	1.11	1/2432 (0.0%)	1.07	9/3274 (0.3%)
1	D	1.10	4/2432 (0.2%)	1.03	7/3274 (0.2%)
All	All	1.10	14/9728 (0.1%)	1.04	31/13096 (0.2%)

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	2
1	B	1	1
1	C	0	3
1	D	0	2
All	All	1	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1128	ASP	N-CA	8.25	1.62	1.46
1	C	1128	ASP	N-CA	7.22	1.60	1.46
1	D	1117	ARG	CB-CG	7.21	1.72	1.52
1	B	1092	ASP	CB-CG	6.10	1.64	1.51
1	A	1028	GLU	CG-CD	5.51	1.60	1.51
1	A	1020	TRP	CB-CG	5.50	1.60	1.50
1	B	1063	ARG	CG-CD	5.36	1.65	1.51
1	B	1028	GLU	CB-CG	-5.29	1.42	1.52
1	B	846	GLU	CG-CD	5.29	1.59	1.51
1	D	860	PHE	CE2-CZ	5.24	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	965	GLU	CD-OE2	-5.23	1.19	1.25
1	D	1024	GLU	CG-CD	5.14	1.59	1.51
1	A	965	GLU	CB-CG	5.08	1.61	1.52
1	D	1117	ARG	CG-CD	5.05	1.64	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	975	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	1128	ASP	N-CA-C	8.99	135.26	111.00
1	C	949	ASP	CB-CG-OD1	8.60	126.04	118.30
1	B	975	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	975	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	947	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	975	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	975	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	994	ASP	N-CA-C	6.47	128.48	111.00
1	C	975	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	D	1033	VAL	CG1-CB-CG2	6.32	121.00	110.90
1	C	951	ILE	CG1-CB-CG2	-6.26	97.63	111.40
1	D	925	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	947	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	1063	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	1033	VAL	CA-CB-CG1	5.98	119.87	110.90
1	B	938	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	947	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	849	LEU	CA-CB-CG	5.69	128.39	115.30
1	C	1128	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	977	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	C	975	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	989	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	947	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	1063	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	977	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	D	849	LEU	CB-CG-CD2	5.40	120.17	111.00
1	B	1033	VAL	CG1-CB-CG2	5.35	119.47	110.90
1	A	975	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	1033	VAL	CG1-CB-CG2	5.10	119.06	110.90
1	D	1118	ASP	CB-CG-OD1	-5.08	113.73	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	1128	ASP	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1012	GLU	Peptide
1	A	872	GLN	Peptide
1	B	1012	GLU	Peptide
1	C	1012	GLU	Peptide
1	C	1068	ASP	Peptide
1	C	1127	ARG	Peptide
1	D	1012	GLU	Peptide
1	D	872	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2379	0	2369	87	0
1	B	2379	0	2369	121	1
1	C	2379	0	2369	124	0
1	D	2379	0	2369	83	0
2	A	33	0	28	2	0
2	B	33	0	28	1	0
2	C	33	0	28	1	0
2	D	33	0	28	1	0
3	A	118	0	0	21	0
3	B	106	0	0	28	0
3	C	110	0	0	35	0
3	D	101	0	0	4	1
All	All	10083	0	9588	400	1

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 21.

All (400) 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:D:964:MET:CE	1:D:992:ILE:HD13	1.37	1.52
1:B:964:MET:CE	1:B:992:ILE:HD13	1.49	1.39
1:C:1117:ARG:HB3	1:C:1117:ARG:NH1	1.40	1.35
1:D:860:PHE:CZ	1:D:891:HIS:HD2	1.48	1.29
1:B:1084:ASN:HB3	3:B:2076:HOH:O	1.35	1.27
1:D:860:PHE:CE2	1:D:891:HIS:HD2	1.54	1.26
1:C:964:MET:CE	1:C:992:ILE:HD13	1.64	1.25
1:B:1118:ASP:HB3	3:B:2093:HOH:O	1.07	1.24
1:A:1083:LYS:HB2	3:A:2097:HOH:O	1.08	1.23
1:C:1118:ASP:HB3	3:C:2100:HOH:O	1.05	1.22
1:D:964:MET:CE	1:D:992:ILE:CD1	2.20	1.20
1:B:1117:ARG:HB3	1:B:1117:ARG:NH1	1.58	1.18
1:B:1092:ASP:HB2	3:B:2084:HOH:O	1.45	1.16
1:C:1092:ASP:HB2	3:C:2091:HOH:O	1.38	1.16
1:A:1007:TYR:HB3	3:A:2073:HOH:O	1.45	1.16
1:C:1084:ASN:HB3	3:C:2083:HOH:O	1.44	1.15
1:D:964:MET:HE3	1:D:992:ILE:CD1	1.76	1.14
1:D:860:PHE:CZ	1:D:891:HIS:CD2	2.36	1.13
1:C:1117:ARG:HH11	1:C:1117:ARG:CB	1.62	1.13
3:A:2047:HOH:O	1:C:1125:GLN:HG2	1.49	1.12
1:B:1117:ARG:HD3	3:B:2096:HOH:O	1.49	1.10
1:D:965:GLU:OE1	1:D:1117:ARG:HG2	1.48	1.10
1:D:860:PHE:CE2	1:D:891:HIS:CD2	2.37	1.10
1:B:964:MET:HE2	1:B:992:ILE:HD13	1.16	1.09
1:B:946:GLU:HG3	1:C:949:ASP:HB2	1.09	1.09
1:A:964:MET:HE2	1:A:977:LEU:HD11	1.35	1.08
1:C:893:ARG:HG3	1:C:893:ARG:HH11	1.15	1.08
1:B:1019:PHE:HZ	1:B:1062:MET:HE1	1.15	1.07
1:C:964:MET:HE2	1:C:992:ILE:HD13	1.22	1.07
1:D:1065:ILE:HG21	3:D:2079:HOH:O	1.53	1.07
1:B:964:MET:CE	1:B:992:ILE:CD1	2.34	1.05
1:B:1117:ARG:HB3	1:B:1117:ARG:HH11	1.08	1.05
1:C:1117:ARG:HB3	1:C:1117:ARG:HH11	0.90	1.05
1:C:1117:ARG:NH1	1:C:1117:ARG:CB	2.20	1.04
1:C:1117:ARG:HD2	3:C:2047:HOH:O	1.58	1.04
1:C:951:ILE:HB	3:C:2109:HOH:O	1.59	1.01
1:B:964:MET:HE3	1:B:992:ILE:HD13	1.36	1.01
1:C:865:MET:HG2	3:C:2005:HOH:O	1.60	1.00
1:C:945:LYS:O	1:C:947:ARG:N	1.94	0.99
1:D:964:MET:HE3	1:D:992:ILE:HD13	1.01	0.99
1:B:964:MET:HE3	1:B:992:ILE:CD1	1.93	0.98
1:B:946:GLU:CG	1:C:949:ASP:HB2	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:GLN:HG2	1:B:853:GLN:NE2	1.79	0.98
1:B:1011:LYS:HE2	1:B:1012:GLU:HA	1.45	0.97
1:C:964:MET:HE3	1:C:992:ILE:HD13	1.47	0.96
1:B:1019:PHE:HZ	1:B:1062:MET:CE	1.78	0.95
1:B:946:GLU:HG3	1:C:949:ASP:CB	1.97	0.95
1:D:964:MET:HE2	1:D:992:ILE:HD13	1.44	0.95
1:B:1117:ARG:NH1	1:B:1117:ARG:CB	2.29	0.95
1:B:964:MET:HE2	1:B:992:ILE:CD1	1.97	0.94
1:A:964:MET:CE	1:A:977:LEU:CD1	2.46	0.93
1:D:964:MET:HE2	1:D:992:ILE:CD1	1.95	0.93
1:A:964:MET:CE	1:A:977:LEU:HD11	1.98	0.93
1:A:1096:ASP:HB2	3:A:2107:HOH:O	1.67	0.92
1:A:853:GLN:HG2	1:B:853:GLN:HE22	1.35	0.91
1:A:1083:LYS:HD3	1:A:1084:ASN:ND2	1.85	0.90
1:A:1007:TYR:HD2	1:A:1030:LYS:HB3	1.33	0.90
1:B:1128:ASP:HA	3:B:2103:HOH:O	1.71	0.90
1:C:964:MET:CE	1:C:992:ILE:CD1	2.50	0.89
1:C:1117:ARG:HG2	3:C:2047:HOH:O	1.72	0.89
1:A:1117:ARG:HD2	3:A:2061:HOH:O	1.73	0.89
1:A:1071:GLY:C	3:A:2096:HOH:O	2.12	0.88
1:A:964:MET:HE3	1:A:977:LEU:HD13	1.54	0.88
1:B:1084:ASN:ND2	3:B:2076:HOH:O	1.96	0.88
1:D:1007:TYR:HD2	1:D:1030:LYS:HB3	1.39	0.88
1:C:1117:ARG:CG	3:C:2047:HOH:O	2.20	0.88
1:A:1104:GLU:OE1	1:A:1122:ARG:NH1	2.07	0.87
1:B:1125:GLN:HG2	3:B:2102:HOH:O	1.75	0.86
1:C:1117:ARG:CD	3:C:2047:HOH:O	2.20	0.86
1:B:1117:ARG:NH2	3:B:2097:HOH:O	2.04	0.86
1:A:964:MET:HE3	1:A:977:LEU:CD1	2.05	0.85
1:C:946:GLU:HB3	3:C:2039:HOH:O	1.75	0.84
1:C:951:ILE:HG13	1:C:952:LYS:N	1.90	0.84
1:B:922:ARG:O	1:B:922:ARG:HG3	1.77	0.84
1:C:872:GLN:O	1:C:873:ASP:HB2	1.75	0.83
1:B:1012:GLU:O	1:B:1014:GLY:N	2.10	0.83
1:A:1007:TYR:OH	1:A:1110:VAL:HG11	1.77	0.83
1:A:1007:TYR:CD2	1:A:1030:LYS:HB3	2.13	0.83
1:B:1117:ARG:NE	3:B:2097:HOH:O	2.08	0.83
1:C:1084:ASN:ND2	3:C:2083:HOH:O	1.92	0.83
1:A:1072:GLN:N	3:A:2096:HOH:O	2.12	0.82
1:B:1019:PHE:CZ	1:B:1062:MET:HE1	2.08	0.82
1:C:945:LYS:C	1:C:947:ARG:H	1.82	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:964:MET:HE3	1:C:992:ILE:CD1	2.10	0.82
1:B:860:PHE:O	1:B:885:GLN:N	2.12	0.81
1:C:943:LYS:O	1:C:944:HIS:HB2	1.79	0.81
1:D:860:PHE:O	1:D:860:PHE:CD1	2.33	0.81
1:C:907:HIS:HD1	1:C:909:ASN:H	1.30	0.80
1:D:1083:LYS:HD3	3:D:2082:HOH:O	1.80	0.79
1:D:1083:LYS:CE	1:D:1084:ASN:HD21	1.96	0.79
1:D:1083:LYS:HE2	1:D:1084:ASN:HD21	1.46	0.79
1:D:1007:TYR:OH	1:D:1110:VAL:HG11	1.83	0.79
1:B:951:ILE:HG23	3:B:2040:HOH:O	1.82	0.78
1:D:1007:TYR:CD2	1:D:1030:LYS:HB3	2.18	0.77
1:B:1019:PHE:CZ	1:B:1062:MET:CE	2.65	0.77
1:B:1084:ASN:CB	3:B:2076:HOH:O	2.05	0.77
1:C:964:MET:HE2	1:C:992:ILE:CD1	2.09	0.76
1:B:1128:ASP:O	3:B:2101:HOH:O	2.01	0.76
1:B:1117:ARG:CZ	3:B:2097:HOH:O	2.34	0.75
1:B:885:GLN:HG2	3:B:2009:HOH:O	1.87	0.74
1:B:897:ARG:HG3	3:B:2013:HOH:O	1.86	0.73
1:C:922:ARG:HG3	1:C:922:ARG:O	1.89	0.73
1:D:1107:ASN:HD22	1:D:1109:ASN:H	1.33	0.73
1:B:965:GLU:OE1	1:B:1117:ARG:HG2	1.89	0.73
1:B:1117:ARG:HH11	1:B:1117:ARG:CB	1.91	0.73
1:C:1096:ASP:O	1:C:1100:MET:HG3	1.88	0.73
1:C:1117:ARG:HH11	1:C:1117:ARG:CG	2.02	0.73
1:D:860:PHE:O	1:D:860:PHE:HD1	1.68	0.73
1:D:850:LYS:HG3	1:D:867:ARG:HH21	1.54	0.72
1:C:885:GLN:HG2	3:C:2014:HOH:O	1.89	0.72
1:A:1062:MET:HE1	1:A:1074:ILE:HD13	1.71	0.72
1:C:860:PHE:O	1:C:885:GLN:N	2.16	0.72
1:C:945:LYS:HG2	1:C:946:GLU:N	2.03	0.72
1:D:860:PHE:CE2	1:D:886:HIS:O	2.44	0.71
3:A:2047:HOH:O	1:C:1125:GLN:CG	2.21	0.71
1:C:1084:ASN:CB	3:C:2083:HOH:O	2.16	0.71
1:D:1065:ILE:CG2	3:D:2079:HOH:O	2.21	0.71
1:C:941:LEU:O	1:C:945:LYS:HB2	1.91	0.70
1:A:1117:ARG:CG	3:A:2061:HOH:O	2.38	0.70
1:A:1117:ARG:CD	3:A:2061:HOH:O	2.36	0.70
3:A:2024:HOH:O	1:C:1128:ASP:O	2.10	0.70
1:A:1062:MET:CE	1:A:1074:ILE:HD13	2.22	0.69
1:D:1012:GLU:O	1:D:1014:GLY:N	2.19	0.68
1:B:846:GLU:OE1	1:B:919:SER:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1062:MET:HE1	1:B:1074:ILE:HG21	1.74	0.68
1:D:922:ARG:O	1:D:922:ARG:HG3	1.93	0.68
1:D:1118:ASP:O	1:D:1122:ARG:HG3	1.94	0.68
1:A:1010:VAL:CG1	1:A:1013:PRO:HD3	2.23	0.67
1:C:893:ARG:HG3	1:C:893:ARG:NH1	1.94	0.67
1:D:1083:LYS:CD	3:D:2082:HOH:O	2.39	0.67
1:C:872:GLN:O	1:C:873:ASP:CB	2.43	0.67
1:C:1128:ASP:OD1	1:C:1128:ASP:N	2.28	0.67
1:A:1010:VAL:HG12	1:A:1013:PRO:HD3	1.76	0.66
3:C:2031:HOH:O	1:D:1083:LYS:NZ	2.18	0.66
1:C:951:ILE:CD1	3:C:2043:HOH:O	2.44	0.66
1:D:1104:GLU:OE1	1:D:1122:ARG:NH1	2.27	0.65
1:A:924:ASN:HB2	1:C:1125:GLN:NE2	2.10	0.65
1:C:1104:GLU:OE1	1:C:1122:ARG:NH2	2.23	0.65
1:A:1071:GLY:CA	3:A:2096:HOH:O	2.45	0.65
1:B:1128:ASP:C	3:B:2103:HOH:O	2.31	0.65
1:C:876:GLY:HA3	3:C:2007:HOH:O	1.96	0.65
1:A:1010:VAL:HG12	1:A:1013:PRO:CD	2.27	0.64
1:D:965:GLU:CD	1:D:1117:ARG:HG2	2.18	0.64
1:C:951:ILE:HD12	3:C:2043:HOH:O	1.97	0.64
1:A:945:LYS:HB3	3:A:2053:HOH:O	1.96	0.64
1:A:964:MET:CE	1:A:977:LEU:HD13	2.18	0.63
1:B:1028:GLU:HG2	1:B:1030:LYS:HD2	1.79	0.63
1:A:1083:LYS:HD2	3:A:2098:HOH:O	1.97	0.63
1:B:1092:ASP:CB	3:B:2084:HOH:O	2.20	0.63
2:C:2229:O19:H27	2:C:2229:O19:N20	2.13	0.63
1:D:918:TYR:HB3	1:D:922:ARG:HD2	1.80	0.63
1:B:1007:TYR:HE1	3:B:2061:HOH:O	1.82	0.62
1:B:1002:PRO:HG2	1:B:1005:LYS:HD2	1.80	0.62
2:B:2229:O19:H27	2:B:2229:O19:N20	2.14	0.62
1:A:1007:TYR:CB	3:A:2073:HOH:O	2.21	0.62
1:D:1107:ASN:ND2	1:D:1109:ASN:H	1.98	0.62
1:B:1062:MET:HE3	1:B:1074:ILE:HD13	1.83	0.61
1:A:924:ASN:HB2	1:C:1125:GLN:HE21	1.62	0.61
1:A:1121:LEU:O	1:A:1125:GLN:OE1	2.19	0.61
1:C:945:LYS:HG2	1:C:946:GLU:H	1.64	0.61
1:C:852:LEU:CD2	3:C:2005:HOH:O	2.49	0.60
1:C:852:LEU:HD23	3:C:2005:HOH:O	2.01	0.60
1:A:1083:LYS:HD3	1:A:1084:ASN:HD21	1.64	0.60
1:A:1117:ARG:NH1	1:A:1117:ARG:HB3	2.15	0.60
1:A:1117:ARG:CG	1:A:1117:ARG:HH11	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:GLU:OE1	1:C:1117:ARG:HG2	2.02	0.60
1:D:860:PHE:CZ	1:D:887:SER:HA	2.37	0.60
1:C:1034:ALA:CB	1:C:1110:VAL:HG13	2.32	0.60
1:A:922:ARG:HG3	1:A:922:ARG:O	2.02	0.60
1:A:1071:GLY:O	1:A:1073:MET:N	2.33	0.60
1:C:1087:ARG:HH22	1:C:1108:ASN:ND2	1.99	0.59
1:C:878:VAL:HG13	3:C:2005:HOH:O	2.02	0.59
1:A:889:GLU:HG3	1:D:1073:MET:HE3	1.83	0.59
1:B:1062:MET:CE	1:B:1074:ILE:HG21	2.32	0.59
1:B:1117:ARG:CB	1:B:1117:ARG:CZ	2.81	0.59
1:D:860:PHE:CZ	1:D:886:HIS:O	2.56	0.59
1:C:945:LYS:CG	1:C:946:GLU:H	2.15	0.59
1:C:1007:TYR:HE1	3:C:2063:HOH:O	1.86	0.59
1:C:872:GLN:CA	3:C:2011:HOH:O	2.51	0.59
1:A:1083:LYS:HD3	1:A:1084:ASN:CG	2.24	0.58
1:B:883:LYS:HE2	3:B:2003:HOH:O	2.02	0.58
1:D:1087:ARG:HH22	1:D:1108:ASN:ND2	2.01	0.58
1:B:1034:ALA:CB	1:B:1110:VAL:HG13	2.34	0.58
1:D:907:HIS:HE1	1:D:909:ASN:HD22	1.51	0.57
1:C:937:LEU:HD21	1:C:1047:LEU:HD21	1.86	0.57
1:B:1126:ILE:C	1:B:1128:ASP:N	2.56	0.57
1:A:1117:ARG:HG2	3:A:2061:HOH:O	2.02	0.57
1:C:952:LYS:NZ	1:C:955:GLN:HE22	2.03	0.57
1:A:1070:GLN:O	1:A:1071:GLY:O	2.22	0.57
1:B:950:HIS:HE1	3:B:2042:HOH:O	1.87	0.56
1:D:1062:MET:HE1	1:D:1074:ILE:HG21	1.86	0.56
1:B:964:MET:HE3	1:B:992:ILE:HD11	1.85	0.56
1:B:897:ARG:CG	3:B:2013:HOH:O	2.47	0.56
1:B:952:LYS:HZ3	1:B:955:GLN:HE22	1.55	0.55
1:D:1010:VAL:HG12	1:D:1013:PRO:HD2	1.88	0.55
1:B:1008:TYR:CE1	1:B:1010:VAL:HG22	2.41	0.55
1:B:1011:LYS:HE2	1:B:1012:GLU:CA	2.28	0.55
1:B:1019:PHE:CZ	1:B:1062:MET:HE2	2.41	0.55
1:B:1062:MET:HE1	1:B:1074:ILE:CG2	2.36	0.55
1:B:883:LYS:HB2	1:B:926:LYS:HE2	1.88	0.55
1:B:952:LYS:NZ	1:B:955:GLN:HE22	2.04	0.55
1:C:952:LYS:HZ3	1:C:955:GLN:HE22	1.54	0.55
1:B:1012:GLU:HG2	1:B:1013:PRO:N	2.22	0.55
1:A:892:LEU:HD23	1:D:1073:MET:HE2	1.88	0.55
1:B:1087:ARG:HH22	1:B:1108:ASN:ND2	2.04	0.55
1:C:1118:ASP:CB	3:C:2100:HOH:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1117:ARG:HG3	3:B:2094:HOH:O	2.07	0.54
1:D:1083:LYS:O	1:D:1083:LYS:HG2	2.07	0.54
1:A:941:LEU:HD11	1:A:1047:LEU:HD23	1.89	0.54
1:C:1083:LYS:CD	1:C:1084:ASN:ND2	2.71	0.54
1:A:1117:ARG:HH11	1:A:1117:ARG:HG2	1.72	0.54
1:B:1051:ILE:HG22	1:B:1051:ILE:O	2.07	0.54
1:A:1100:MET:O	1:A:1104:GLU:HG3	2.08	0.54
1:A:1013:PRO:HB3	3:A:2067:HOH:O	2.08	0.53
1:C:922:ARG:HG3	1:C:922:ARG:HH11	1.73	0.53
1:D:1012:GLU:C	1:D:1014:GLY:H	2.06	0.53
1:C:947:ARG:HD2	3:C:2037:HOH:O	2.06	0.53
1:B:983:LEU:HD23	1:B:993:GLY:HA3	1.90	0.53
1:A:907:HIS:HE1	1:A:909:ASN:HD22	1.57	0.53
1:D:1117:ARG:NH1	1:D:1117:ARG:HB3	2.24	0.53
1:A:918:TYR:HB3	1:A:922:ARG:HD2	1.91	0.53
1:A:944:HIS:ND1	1:A:947:ARG:NH1	2.57	0.53
1:C:1007:TYR:CD1	1:C:1030:LYS:HB3	2.43	0.53
1:A:914:LYS:HG3	3:A:2019:HOH:O	2.08	0.53
1:C:881:VAL:HG22	1:C:928:ILE:HD12	1.91	0.53
1:C:873:ASP:OD2	1:C:875:THR:OG1	2.27	0.52
1:C:873:ASP:CG	1:C:874:ASN:H	2.11	0.52
1:C:897:ARG:HH21	1:C:1000:VAL:HG21	1.75	0.52
1:B:1080:GLU:O	1:B:1084:ASN:OD1	2.28	0.52
1:D:1083:LYS:HE3	1:D:1084:ASN:ND2	2.25	0.52
1:A:853:GLN:NE2	1:B:853:GLN:HE21	2.07	0.52
1:B:1045:TYR:O	1:B:1049:THR:HG23	2.09	0.52
1:C:893:ARG:HH11	1:C:893:ARG:CG	2.05	0.52
1:C:1083:LYS:HD3	1:C:1084:ASN:ND2	2.25	0.51
1:A:853:GLN:HE21	1:B:853:GLN:HE21	1.59	0.51
1:B:1117:ARG:NH2	3:B:2098:HOH:O	2.44	0.51
1:D:1011:LYS:HD3	1:D:1012:GLU:CA	2.40	0.51
1:B:893:ARG:HG3	1:B:893:ARG:HH11	1.76	0.51
1:D:1095:PRO:HD2	1:D:1098:ILE:HD12	1.92	0.51
1:B:939:ASP:O	1:B:943:LYS:HD3	2.11	0.51
1:B:1126:ILE:O	1:B:1128:ASP:N	2.42	0.51
1:A:964:MET:HE1	1:A:992:ILE:HD13	1.93	0.51
1:D:1109:ASN:C	1:D:1109:ASN:HD22	2.14	0.51
1:C:1034:ALA:HB1	1:C:1110:VAL:HG13	1.93	0.51
1:D:1083:LYS:CE	1:D:1084:ASN:ND2	2.69	0.51
1:B:1083:LYS:HD3	1:B:1084:ASN:ND2	2.26	0.50
1:A:981:ASN:HB3	3:A:2065:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:ASP:OD1	1:C:874:ASN:N	2.45	0.50
1:C:1117:ARG:HH22	1:D:1077:HIS:HB3	1.76	0.50
1:D:937:LEU:HD21	1:D:1047:LEU:HD21	1.93	0.50
1:A:1010:VAL:HG11	1:A:1013:PRO:HD3	1.94	0.50
1:A:1107:ASN:HD22	1:A:1109:ASN:H	1.59	0.50
1:B:1087:ARG:HH22	1:B:1108:ASN:HD21	1.60	0.50
1:D:860:PHE:CE1	1:D:891:HIS:CD2	2.98	0.50
1:A:874:ASN:ND2	1:B:878:VAL:H	2.10	0.49
1:B:958:SER:O	1:B:962:LYS:HG3	2.12	0.49
1:D:961:CYS:O	1:D:965:GLU:HG3	2.12	0.49
1:B:941:LEU:HD21	1:B:953:LEU:HD21	1.94	0.49
1:A:973:ILE:HD11	1:A:1001:LEU:HD11	1.95	0.49
1:B:952:LYS:HD2	1:B:956:TYR:CZ	2.48	0.49
1:C:1083:LYS:HD3	3:C:2083:HOH:O	2.11	0.49
1:B:1125:GLN:CG	3:B:2102:HOH:O	2.47	0.49
1:C:944:HIS:CE1	1:C:947:ARG:NH1	2.81	0.49
1:C:885:GLN:CG	3:C:2014:HOH:O	2.55	0.49
1:C:994:ASP:OD1	3:C:2012:HOH:O	2.20	0.49
1:B:946:GLU:HB3	3:B:2034:HOH:O	2.13	0.49
1:C:1122:ARG:HG3	3:C:2104:HOH:O	2.12	0.49
1:C:1083:LYS:HD3	1:C:1084:ASN:HD22	1.77	0.49
1:A:853:GLN:CG	1:B:853:GLN:NE2	2.64	0.48
1:A:918:TYR:CB	1:A:922:ARG:HD2	2.43	0.48
1:B:940:TYR:OH	1:B:987:GLU:HG2	2.13	0.48
1:B:937:LEU:HD21	1:B:1047:LEU:HD21	1.94	0.48
1:D:860:PHE:CD2	1:D:891:HIS:CD2	2.99	0.48
1:B:1114:PRO:HB2	1:B:1118:ASP:OD1	2.14	0.48
1:C:1125:GLN:O	1:C:1128:ASP:C	2.52	0.48
1:A:853:GLN:HG2	1:B:853:GLN:HE21	1.75	0.48
1:B:987:GLU:HG2	3:B:2029:HOH:O	2.14	0.48
1:A:922:ARG:NH2	1:D:1072:GLN:OE1	2.45	0.47
1:C:1107:ASN:HD22	1:C:1109:ASN:H	1.61	0.47
1:A:1117:ARG:CG	1:A:1117:ARG:NH1	2.76	0.47
1:D:941:LEU:HD21	1:D:953:LEU:HD21	1.96	0.47
1:A:1007:TYR:HH	1:A:1110:VAL:HG11	1.79	0.47
1:C:983:LEU:HD23	1:C:993:GLY:HA3	1.95	0.47
1:D:918:TYR:CB	1:D:922:ARG:HD2	2.44	0.47
1:A:982:ILE:C	1:A:983:LEU:HD22	2.35	0.47
1:C:952:LYS:NZ	1:C:955:GLN:NE2	2.63	0.47
1:C:1095:PRO:HG2	1:C:1098:ILE:HD13	1.96	0.47
1:C:884:LEU:HB3	1:C:887:SER:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:TYR:O	1:B:922:ARG:HA	2.15	0.47
1:B:994:ASP:CG	3:B:2008:HOH:O	2.53	0.47
1:C:1087:ARG:HH22	1:C:1108:ASN:HD21	1.63	0.47
1:C:967:LEU:HD21	1:C:995:PHE:CE1	2.50	0.47
1:C:1083:LYS:CD	1:C:1084:ASN:HD22	2.27	0.47
1:A:1095:PRO:HG2	1:A:1098:ILE:HD12	1.97	0.47
1:C:945:LYS:C	1:C:947:ARG:N	2.55	0.47
1:A:951:ILE:HD12	1:A:952:LYS:N	2.31	0.46
1:C:951:ILE:HD13	3:C:2043:HOH:O	2.12	0.46
1:A:941:LEU:O	1:A:945:LYS:HG3	2.15	0.46
1:A:914:LYS:HE3	3:A:2019:HOH:O	2.15	0.46
1:A:961:CYS:O	1:A:965:GLU:HG3	2.16	0.46
1:D:1062:MET:CE	1:D:1074:ILE:HD13	2.45	0.46
1:C:873:ASP:CG	1:C:874:ASN:N	2.68	0.46
1:B:1121:LEU:O	1:B:1125:GLN:OE1	2.33	0.46
1:C:943:LYS:HB2	1:C:943:LYS:NZ	2.31	0.46
1:C:945:LYS:HA	1:C:948:ILE:HD12	1.97	0.46
1:C:1117:ARG:CB	1:C:1117:ARG:CZ	2.91	0.46
1:B:952:LYS:NZ	1:B:955:GLN:NE2	2.63	0.46
1:B:903:LYS:HG3	1:B:913:TYR:CE2	2.50	0.45
1:D:983:LEU:HD23	1:D:993:GLY:HA3	1.98	0.45
1:A:863:VAL:HG21	2:A:2229:O19:C6	2.46	0.45
1:A:1011:LYS:C	1:A:1013:PRO:HD2	2.37	0.45
1:A:1107:ASN:ND2	1:A:1109:ASN:H	2.14	0.45
1:B:946:GLU:HG2	3:B:2030:HOH:O	2.15	0.45
1:D:857:LYS:HE3	1:D:885:GLN:HE21	1.81	0.45
1:B:961:CYS:SG	1:B:1040:PHE:CZ	3.10	0.45
1:B:949:ASP:CB	1:C:946:GLU:HG3	2.46	0.45
2:D:2229:O19:N20	2:D:2229:O19:H27	2.31	0.45
1:B:1007:TYR:CD1	1:B:1030:LYS:HB3	2.51	0.45
1:C:1117:ARG:NH2	3:C:2103:HOH:O	2.49	0.45
1:D:1083:LYS:HE3	1:D:1084:ASN:HD21	1.74	0.45
1:C:932:LEU:HA	1:C:933:PRO:HD3	1.68	0.45
1:D:860:PHE:HZ	1:D:887:SER:HA	1.81	0.45
1:C:876:GLY:CA	3:C:2007:HOH:O	2.61	0.45
1:B:1038:TRP:CE3	1:B:1106:TRP:HA	2.52	0.45
1:C:945:LYS:HE2	1:C:945:LYS:HB3	1.28	0.45
1:D:952:LYS:HD2	1:D:956:TYR:CZ	2.52	0.45
1:A:1096:ASP:O	1:A:1100:MET:HG3	2.17	0.44
1:D:1010:VAL:O	1:D:1029:SER:HB3	2.17	0.44
1:D:1011:LYS:HD3	1:D:1012:GLU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:944:HIS:CE1	1:A:947:ARG:HH12	2.34	0.44
1:A:1087:ARG:HH22	1:A:1108:ASN:ND2	2.15	0.44
1:C:907:HIS:HE1	1:C:909:ASN:HD22	1.64	0.44
1:D:1012:GLU:C	1:D:1014:GLY:N	2.67	0.44
1:D:1071:GLY:O	1:D:1073:MET:N	2.43	0.44
1:A:1083:LYS:CD	1:A:1084:ASN:HD21	2.30	0.44
1:D:1117:ARG:NH1	1:D:1117:ARG:CB	2.80	0.44
1:D:1048:PHE:CZ	1:D:1098:ILE:HD13	2.52	0.44
1:D:1034:ALA:CB	1:D:1110:VAL:HG13	2.48	0.44
2:A:2229:O19:H27	2:A:2229:O19:N20	2.33	0.44
1:B:980:ARG:NH1	1:B:980:ARG:HB2	2.33	0.44
1:B:967:LEU:HD11	1:B:995:PHE:HE1	1.82	0.44
1:B:1109:ASN:C	1:B:1109:ASN:HD22	2.21	0.44
1:C:876:GLY:N	3:C:2007:HOH:O	2.50	0.44
1:B:857:LYS:HE3	1:B:885:GLN:OE1	2.18	0.43
1:B:932:LEU:HA	1:B:933:PRO:HD3	1.90	0.43
1:A:1010:VAL:HG12	1:A:1013:PRO:HD2	1.98	0.43
1:B:1107:ASN:HD22	1:B:1108:ASN:N	2.16	0.43
1:B:975:ARG:HD2	1:B:1031:PHE:CG	2.54	0.43
1:C:950:HIS:HE1	3:C:2021:HOH:O	2.01	0.43
1:C:1095:PRO:CG	1:C:1098:ILE:HD13	2.47	0.43
1:B:1008:TYR:CD1	1:B:1010:VAL:HG22	2.54	0.43
1:D:972:TYR:CD1	1:D:1000:VAL:HG22	2.53	0.43
1:C:899:ILE:HG12	1:C:927:LEU:HD13	2.00	0.43
1:B:907:HIS:HE1	1:B:909:ASN:HD22	1.67	0.43
1:C:922:ARG:O	1:C:922:ARG:CG	2.62	0.43
1:B:1107:ASN:ND2	1:B:1109:ASN:H	2.16	0.43
1:A:843:GLN:HB2	1:D:1011:LYS:HE2	2.00	0.43
1:B:853:GLN:HB3	1:B:865:MET:HE3	2.00	0.43
1:B:1012:GLU:HG2	1:B:1013:PRO:CA	2.49	0.43
1:D:908:ASP:CG	1:D:989:ARG:HH21	2.21	0.43
1:D:964:MET:HE3	1:D:992:ILE:HD11	1.88	0.43
1:D:1045:TYR:O	1:D:1049:THR:HG23	2.18	0.43
1:A:941:LEU:HD22	1:A:1050:TYR:HA	2.00	0.43
1:C:1107:ASN:ND2	1:C:1109:ASN:H	2.16	0.43
1:A:964:MET:CE	1:A:992:ILE:HD13	2.49	0.43
1:C:870:PRO:C	1:C:872:GLN:H	2.23	0.43
1:C:857:LYS:HG3	1:C:862:SER:OG	2.19	0.42
1:B:1126:ILE:O	1:B:1127:ARG:C	2.57	0.42
1:C:994:ASP:CG	3:C:2012:HOH:O	2.57	0.42
1:A:983:LEU:HD23	1:A:993:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:LYS:NZ	1:C:988:ASN:ND2	2.68	0.42
1:B:941:LEU:HD13	1:B:1050:TYR:HA	2.02	0.42
1:B:952:LYS:HZ3	1:B:955:GLN:NE2	2.17	0.42
1:D:1087:ARG:HH22	1:D:1108:ASN:HD21	1.65	0.42
1:B:867:ARG:NH1	1:B:874:ASN:HA	2.35	0.41
1:C:860:PHE:C	1:C:885:GLN:HB2	2.41	0.41
1:C:1109:ASN:HD22	1:C:1109:ASN:C	2.24	0.41
1:D:893:ARG:HA	1:D:893:ARG:HD2	1.85	0.41
1:A:874:ASN:HD22	1:B:878:VAL:H	1.68	0.41
1:A:1028:GLU:OE1	1:A:1030:LYS:HD2	2.19	0.41
1:D:932:LEU:HA	1:D:933:PRO:HD3	1.93	0.41
1:B:860:PHE:C	1:B:885:GLN:HB2	2.40	0.41
1:C:885:GLN:O	1:C:886:HIS:C	2.58	0.41
1:A:1034:ALA:CB	1:A:1110:VAL:HG13	2.51	0.41
1:B:1008:TYR:HE1	1:B:1010:VAL:HG22	1.84	0.41
1:C:851:PHE:CZ	1:C:853:GLN:HA	2.56	0.41
1:B:867:ARG:HH11	1:B:874:ASN:HA	1.86	0.41
1:B:999:LYS:HD2	1:B:1008:TYR:CZ	2.55	0.41
1:D:1028:GLU:CG	1:D:1030:LYS:HE3	2.51	0.41
1:B:938:ARG:HA	1:B:1051:ILE:HD13	2.03	0.41
1:C:1083:LYS:HD2	1:C:1084:ASN:ND2	2.36	0.41
1:D:1062:MET:HE3	1:D:1074:ILE:HD13	2.03	0.41
1:A:1117:ARG:NH1	1:A:1117:ARG:CB	2.83	0.40
1:D:982:ILE:C	1:D:983:LEU:HD22	2.42	0.40
1:C:867:ARG:NH1	1:C:874:ASN:HA	2.36	0.40
1:C:964:MET:HE3	1:C:977:LEU:HD11	2.03	0.40
3:A:2034:HOH:O	1:D:1071:GLY:O	2.22	0.40
1:D:952:LYS:NZ	1:D:987:GLU:O	2.55	0.40
1:C:1092:ASP:CB	3:C:2091:HOH:O	2.24	0.40
1:C:1095:PRO:HD2	1:C:1098:ILE:HD13	2.02	0.40

All (1) 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)
1:B:1128:ASP:OD2	3:D:2039:HOH:O[1_645]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	286/298 (96%)	268 (94%)	11 (4%)	7 (2%)	6	2
1	B	286/298 (96%)	264 (92%)	15 (5%)	7 (2%)	6	2
1	C	286/298 (96%)	266 (93%)	10 (4%)	10 (4%)	3	1
1	D	286/298 (96%)	269 (94%)	11 (4%)	6 (2%)	7	2
All	All	1144/1192 (96%)	1067 (93%)	47 (4%)	30 (3%)	5	2

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1071	GLY
1	A	1072	GLN
1	B	873	ASP
1	B	874	ASN
1	B	994	ASP
1	B	1013	PRO
1	C	873	ASP
1	C	874	ASN
1	C	944	HIS
1	C	946	GLU
1	C	994	ASP
1	C	1069	LYS
1	D	1013	PRO
1	D	1071	GLY
1	D	1072	GLN
1	A	872	GLN
1	A	876	GLY
1	C	872	GLN
1	D	872	GLN
1	D	873	ASP
1	B	875	THR
1	C	871	LEU

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Mol	Chain	Res	Type
1	C	886	HIS
1	C	1029	SER
1	A	873	ASP
1	A	994	ASP
1	A	1013	PRO
1	B	919	SER
1	B	1011	LYS
1	D	1012	GLU

5.3.2 Protein sidechains ⓘ

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	263/271 (97%)	238 (90%)	25 (10%)	8	5
1	B	263/271 (97%)	238 (90%)	25 (10%)	8	5
1	C	263/271 (97%)	235 (89%)	28 (11%)	6	3
1	D	263/271 (97%)	243 (92%)	20 (8%)	13	8
All	All	1052/1084 (97%)	954 (91%)	98 (9%)	9	5

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	842	THR
1	A	849	LEU
1	A	852	LEU
1	A	853	GLN
1	A	854	GLN
1	A	877	GLU
1	A	893	ARG
1	A	932	LEU
1	A	941	LEU
1	A	942	GLN
1	A	945	LYS
1	A	977	LEU
1	A	983	LEU

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Mol	Chain	Res	Type
1	A	989	ARG
1	A	994	ASP
1	A	1003	GLN
1	A	1012	GLU
1	A	1065	ILE
1	A	1068	ASP
1	A	1069	LYS
1	A	1107	ASN
1	A	1109	ASN
1	A	1117	ARG
1	A	1121	LEU
1	A	1128	ASP
1	B	843	GLN
1	B	845	GLU
1	B	852	LEU
1	B	853	GLN
1	B	862	SER
1	B	874	ASN
1	B	875	THR
1	B	883	LYS
1	B	893	ARG
1	B	941	LEU
1	B	943	LYS
1	B	945	LYS
1	B	987	GLU
1	B	989	ARG
1	B	1011	LYS
1	B	1012	GLU
1	B	1028	GLU
1	B	1065	ILE
1	B	1068	ASP
1	B	1084	ASN
1	B	1107	ASN
1	B	1109	ASN
1	B	1121	LEU
1	B	1122	ARG
1	B	1128	ASP
1	C	842	THR
1	C	852	LEU
1	C	857	LYS
1	C	862	SER
1	C	871	LEU

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Mol	Chain	Res	Type
1	C	874	ASN
1	C	875	THR
1	C	887	SER
1	C	892	LEU
1	C	893	ARG
1	C	897	ARG
1	C	941	LEU
1	C	944	HIS
1	C	949	ASP
1	C	951	ILE
1	C	989	ARG
1	C	1015	GLU
1	C	1029	SER
1	C	1033	VAL
1	C	1065	ILE
1	C	1068	ASP
1	C	1083	LYS
1	C	1084	ASN
1	C	1107	ASN
1	C	1109	ASN
1	C	1117	ARG
1	C	1121	LEU
1	C	1125	GLN
1	D	843	GLN
1	D	849	LEU
1	D	852	LEU
1	D	853	GLN
1	D	854	GLN
1	D	860	PHE
1	D	892	LEU
1	D	932	LEU
1	D	983	LEU
1	D	989	ARG
1	D	1003	GLN
1	D	1006	GLU
1	D	1051	ILE
1	D	1070	GLN
1	D	1083	LYS
1	D	1092	ASP
1	D	1107	ASN
1	D	1109	ASN
1	D	1121	LEU

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Mol	Chain	Res	Type
1	D	1125	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	874	ASN
1	A	891	HIS
1	A	909	ASN
1	A	942	GLN
1	A	955	GLN
1	A	988	ASN
1	A	1003	GLN
1	A	1084	ASN
1	A	1107	ASN
1	A	1108	ASN
1	A	1109	ASN
1	A	1112	GLN
1	A	1125	GLN
1	B	853	GLN
1	B	854	GLN
1	B	906	GLN
1	B	909	ASN
1	B	950	HIS
1	B	955	GLN
1	B	988	ASN
1	B	1107	ASN
1	B	1108	ASN
1	B	1109	ASN
1	B	1112	GLN
1	B	1125	GLN
1	C	843	GLN
1	C	874	ASN
1	C	885	GLN
1	C	906	GLN
1	C	909	ASN
1	C	924	ASN
1	C	944	HIS
1	C	950	HIS
1	C	955	GLN
1	C	988	ASN
1	C	1070	GLN
1	C	1107	ASN

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Mol	Chain	Res	Type
1	C	1108	ASN
1	C	1109	ASN
1	C	1125	GLN
1	D	854	GLN
1	D	885	GLN
1	D	891	HIS
1	D	909	ASN
1	D	955	GLN
1	D	988	ASN
1	D	1003	GLN
1	D	1084	ASN
1	D	1107	ASN
1	D	1108	ASN
1	D	1109	ASN
1	D	1111	ASN
1	D	1125	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	O19	C	2229	-	37,37,37	1.02	1 (2%)	50,50,50	2.43	9 (18%)
2	O19	B	2229	-	37,37,37	0.90	0	50,50,50	2.41	10 (20%)
2	O19	D	2229	-	37,37,37	0.76	0	50,50,50	2.77	11 (22%)
2	O19	A	2229	-	37,37,37	0.79	0	50,50,50	2.60	15 (30%)

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	O19	C	2229	-	-	0/20/35/35	0/5/5/5
2	O19	B	2229	-	-	0/20/35/35	0/5/5/5
2	O19	D	2229	-	-	0/20/35/35	0/5/5/5
2	O19	A	2229	-	-	0/20/35/35	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2229	O19	C26-C25	2.03	1.43	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2229	O19	C17-N18-C19	10.86	125.08	115.45
2	D	2229	O19	C17-N18-C19	10.72	124.95	115.45
2	D	2229	O19	N18-C19-N20	-10.10	116.98	126.55
2	C	2229	O19	C17-N18-C19	9.32	123.72	115.45
2	C	2229	O19	N18-C19-N20	-9.04	117.98	126.55
2	A	2229	O19	N18-C19-N20	-8.23	118.76	126.55
2	B	2229	O19	N18-C19-N20	-7.92	119.05	126.55
2	B	2229	O19	C17-N18-C19	7.78	122.35	115.45
2	B	2229	O19	C7-N20-C19	6.64	122.16	116.69
2	D	2229	O19	C7-N20-C19	6.63	122.15	116.69
2	D	2229	O19	C29-N28-C33	6.03	124.84	111.52
2	A	2229	O19	C29-N28-C33	5.90	124.54	111.52
2	C	2229	O19	C7-N20-C19	5.32	121.07	116.69
2	C	2229	O19	C29-N28-C33	4.79	122.09	111.52
2	B	2229	O19	C15-C11-C9	-4.78	103.84	111.16
2	A	2229	O19	C16-C17-N18	-4.35	118.55	123.96
2	B	2229	O19	C29-N28-C33	4.21	120.81	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2229	O19	C16-C17-N18	-4.07	118.91	123.96
2	C	2229	O19	C16-C17-N18	-4.06	118.91	123.96
2	D	2229	O19	C16-C17-N18	-3.61	119.47	123.96
2	A	2229	O19	C7-N20-C19	3.46	119.55	116.69
2	A	2229	O19	C15-C11-C9	-3.42	105.92	111.16
2	C	2229	O19	C15-C11-C9	-3.39	105.96	111.16
2	D	2229	O19	C5-C6-C1	2.92	123.02	119.03
2	D	2229	O19	C15-C11-C9	-2.65	107.10	111.16
2	A	2229	O19	C30-C29-N28	-2.55	105.31	110.02
2	A	2229	O19	C5-C4-C3	-2.53	117.49	121.13
2	C	2229	O19	O31-C32-C33	-2.49	106.32	111.80
2	A	2229	O19	N21-C19-N20	2.45	125.23	116.92
2	D	2229	O19	C24-C25-N28	-2.43	118.03	121.38
2	A	2229	O19	C2-C3-C7	-2.34	117.58	121.28
2	D	2229	O19	C5-C4-C3	-2.32	117.80	121.13
2	B	2229	O19	C5-C4-C3	-2.27	117.86	121.13
2	A	2229	O19	C2-C1-C6	-2.27	117.68	120.30
2	C	2229	O19	C13-N12-C11	2.26	113.32	107.08
2	A	2229	O19	C32-C33-N28	2.22	114.12	110.02
2	B	2229	O19	C4-C3-C7	-2.21	117.79	121.28
2	B	2229	O19	C16-C7-N20	-2.18	119.14	121.97
2	D	2229	O19	C2-C3-C4	2.16	121.89	117.59
2	D	2229	O19	C13-N12-C11	2.12	112.92	107.08
2	A	2229	O19	C13-N12-C11	2.11	112.88	107.08
2	A	2229	O19	C2-C3-C4	2.10	121.77	117.59
2	C	2229	O19	C3-C7-N20	2.03	118.90	116.02
2	A	2229	O19	O31-C30-C29	-2.03	107.33	111.80
2	B	2229	O19	C2-C3-C4	2.02	121.62	117.59

There are no chirality outliers.

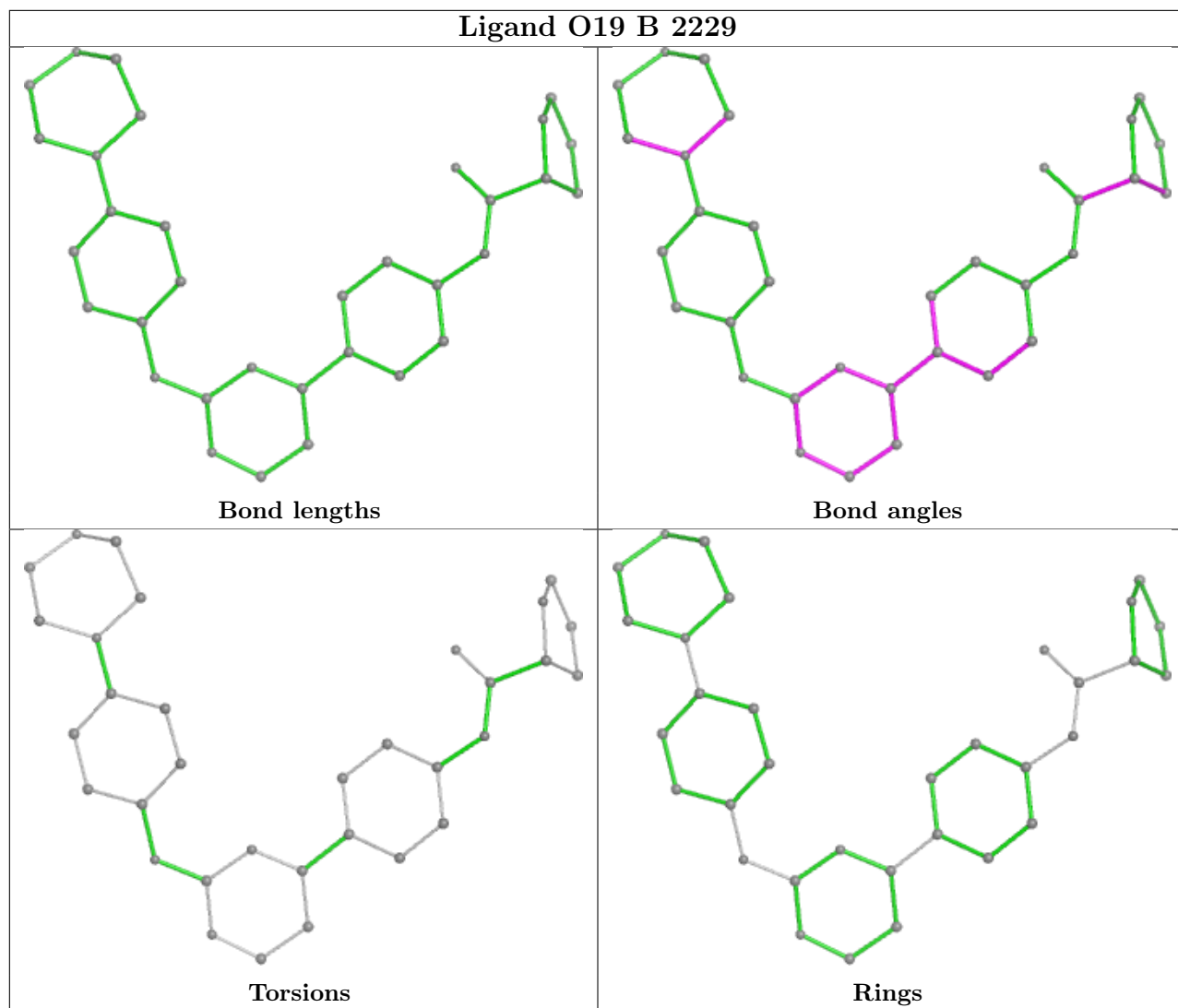There are no torsion outliers.

There are no ring outliers.
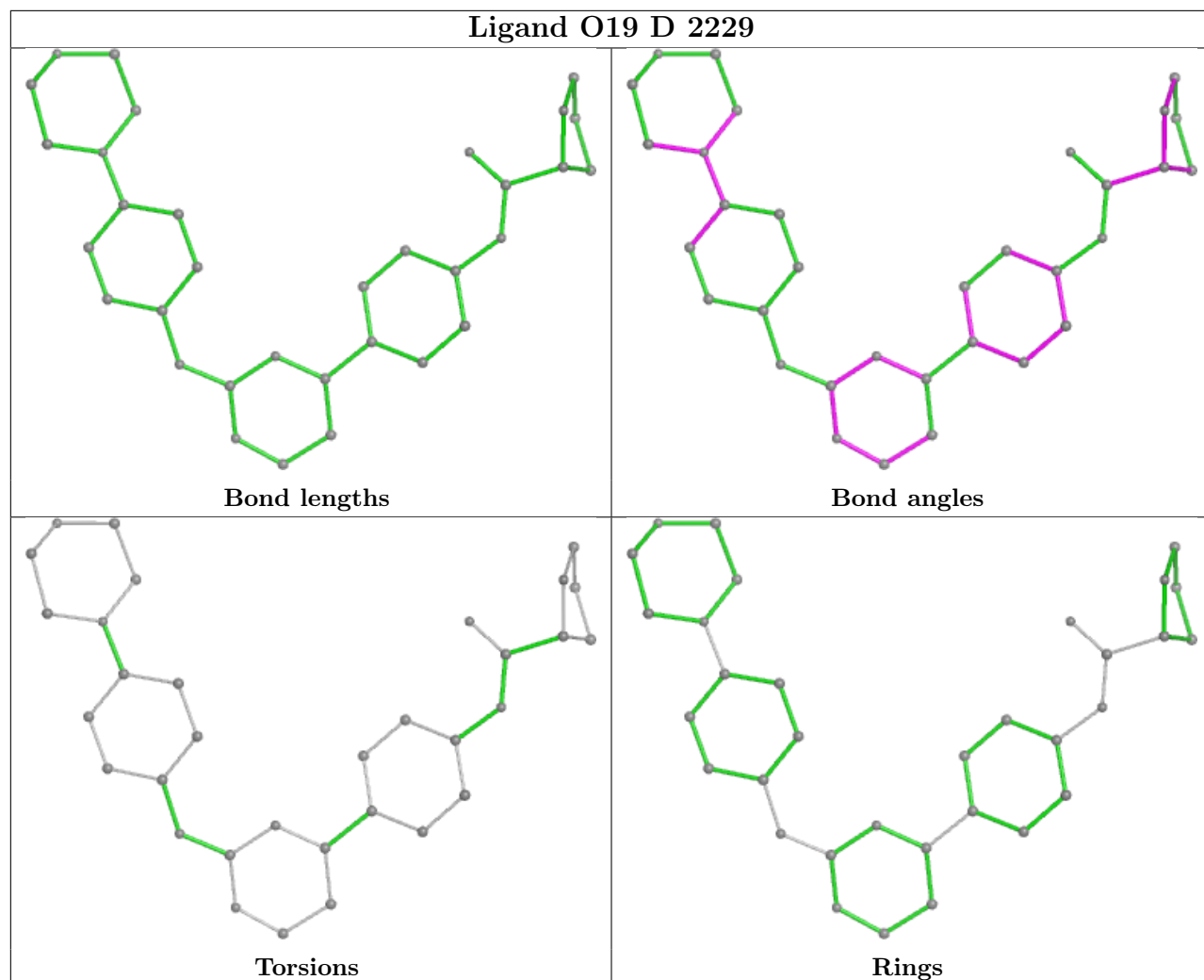
4 monomers are involved in 5 short contacts:

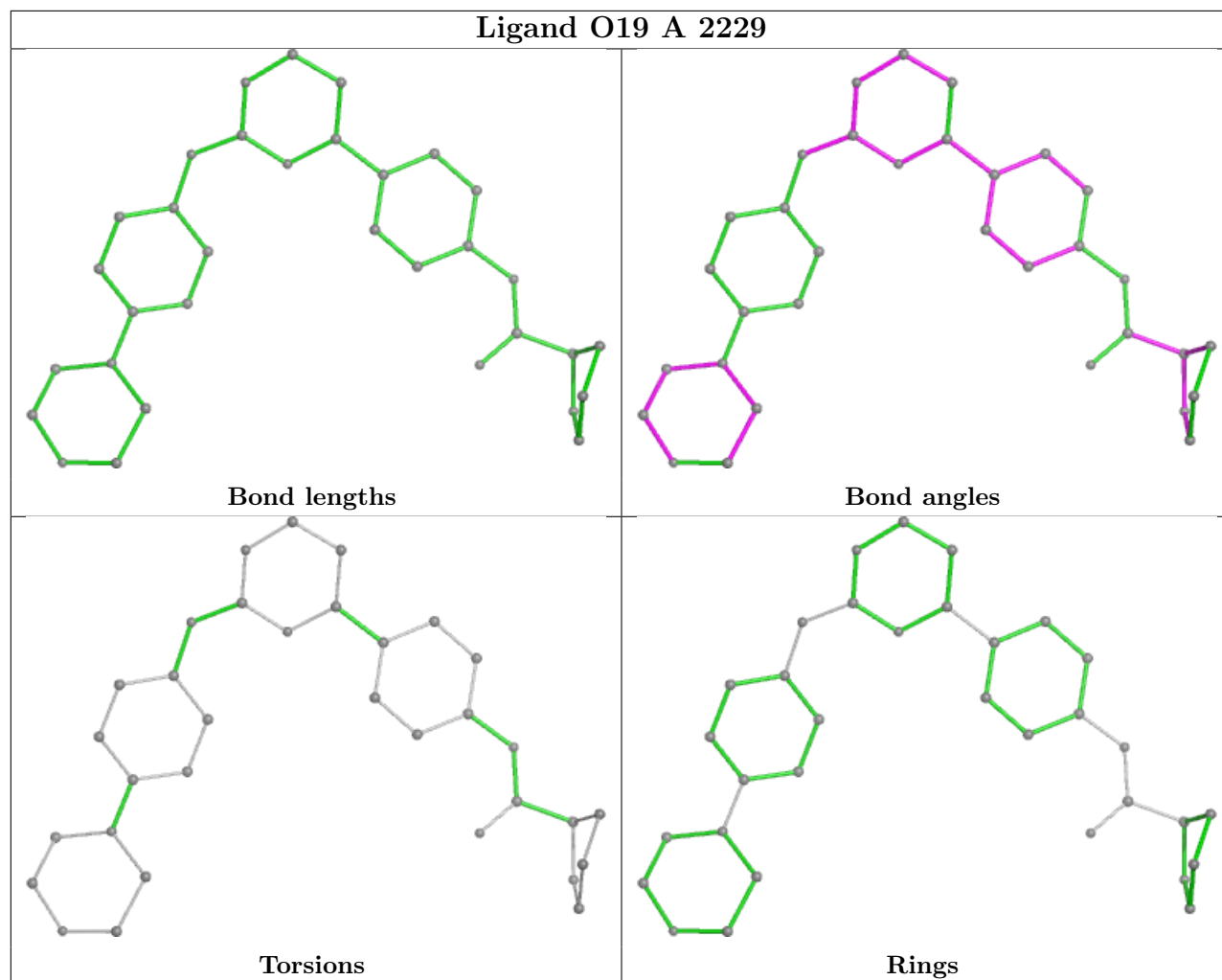| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2229	O19	1	0
2	B	2229	O19	1	0
2	D	2229	O19	1	0
2	A	2229	O19	2	0

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 O19 C 2229

Bond lengths

Bond angles

Torsions

Rings

Ligand O19 B 2229

Bond lengths

Bond angles

Torsions

Rings

Ligand O19 D 2229

Bond lengths

Bond angles

Torsions

Rings

Ligand O19 A 2229

Bond lengths

Bond angles

Torsions

Rings
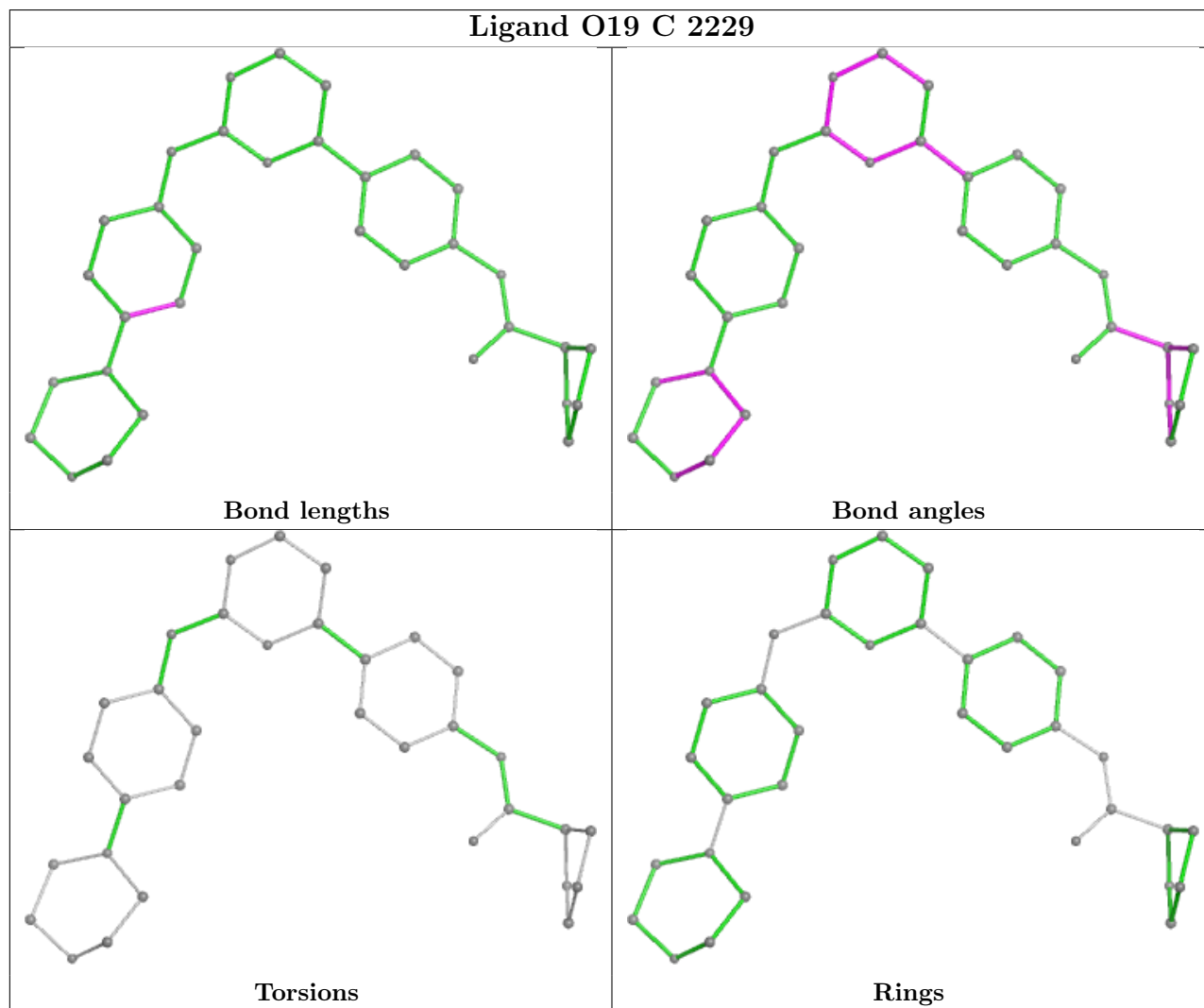
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	288/298 (96%)	0.07	14 (4%)	29	28	14, 25, 46, 67	3 (1%)
1	B	288/298 (96%)	0.09	17 (5%)	22	21	14, 26, 52, 64	3 (1%)
1	C	288/298 (96%)	0.13	16 (5%)	24	23	15, 26, 50, 67	3 (1%)
1	D	288/298 (96%)	0.05	15 (5%)	27	26	12, 25, 46, 62	3 (1%)
All	All	1152/1192 (96%)	0.09	62 (5%)	25	24	12, 26, 49, 67	12 (1%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1013	PRO	7.7
1	D	1014	GLY	6.9
1	C	1013	PRO	6.5
1	C	875	THR	6.3
1	A	1014	GLY	6.0
1	C	871	LEU	5.6
1	D	1013	PRO	5.6
1	D	874	ASN	5.6
1	B	1007	TYR	5.5
1	B	1013	PRO	5.0
1	D	871	LEU	4.9
1	D	1007	TYR	4.8
1	A	871	LEU	4.8
1	C	1007	TYR	4.8
1	A	1007	TYR	4.7
1	B	871	LEU	4.5
1	B	920	ALA	4.4
1	C	841	PRO	4.2
1	B	1014	GLY	4.1
1	D	860	PHE	4.1
1	C	885	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1012	GLU	3.9
1	A	841	PRO	3.7
1	C	1014	GLY	3.7
1	D	1011	LYS	3.3
1	C	843	GLN	3.2
1	D	1012	GLU	3.2
1	D	1053	LYS	3.2
1	A	875	THR	3.1
1	B	875	THR	3.1
1	C	842	THR	3.1
1	D	870	PRO	3.1
1	A	1011	LYS	3.0
1	B	1011	LYS	2.9
1	C	1012	GLU	2.8
1	C	1002	PRO	2.8
1	B	1125	GLN	2.7
1	B	860	PHE	2.7
1	B	1092	ASP	2.7
1	C	1125	GLN	2.6
1	A	874	ASN	2.6
1	D	875	THR	2.6
1	B	885	GLN	2.5
1	A	1053	LYS	2.5
1	B	870	PRO	2.4
1	A	1015	GLU	2.4
1	A	1096	ASP	2.4
1	B	843	GLN	2.3
1	D	971	ARG	2.3
1	B	874	ASN	2.3
1	A	971	ARG	2.3
1	D	1096	ASP	2.3
1	B	1012	GLU	2.2
1	D	945	LYS	2.2
1	A	847	ARG	2.2
1	B	847	ARG	2.2
1	B	971	ARG	2.2
1	C	847	ARG	2.2
1	C	951	ILE	2.1
1	C	870	PRO	2.1
1	D	1092	ASP	2.1
1	C	874	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	O19	B	2229	33/33	0.92	0.11	23,27,39,40	0
2	O19	C	2229	33/33	0.93	0.12	22,26,40,42	0
2	O19	D	2229	33/33	0.94	0.11	19,24,35,37	0
2	O19	A	2229	33/33	0.95	0.11	19,24,35,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
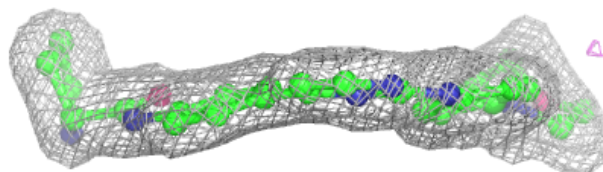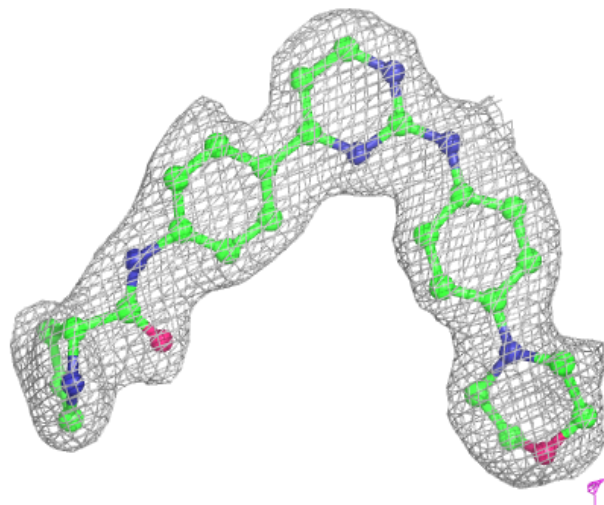
Electron density around O19 B 2229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
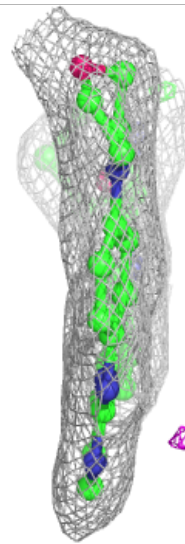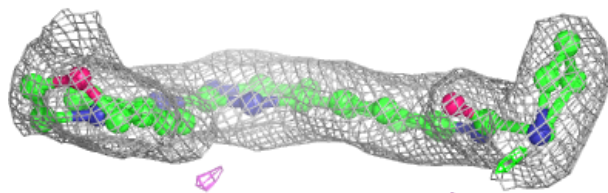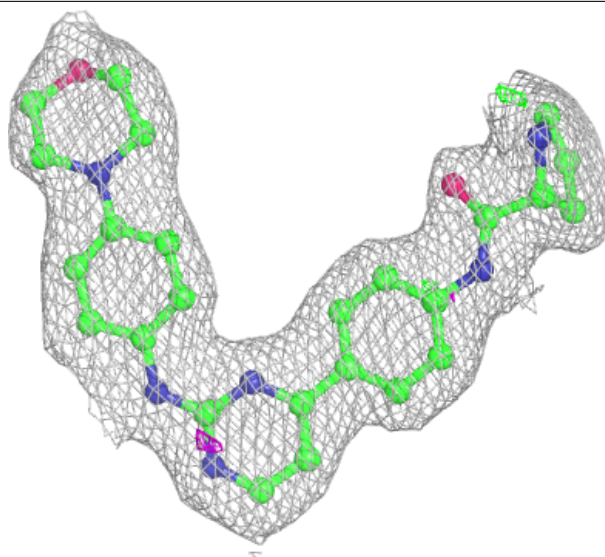
Electron density around O19 C 2229:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
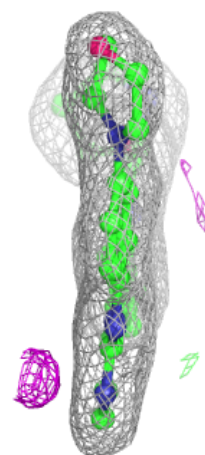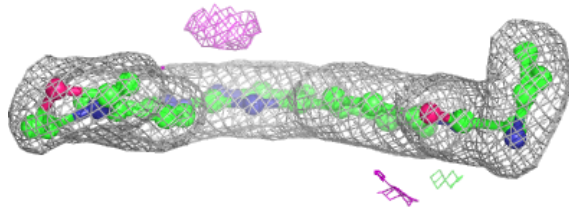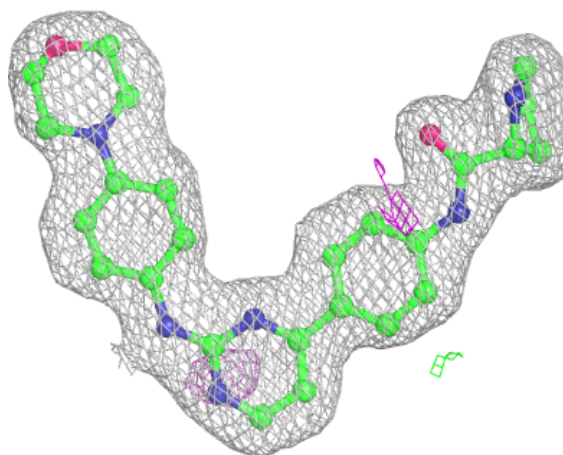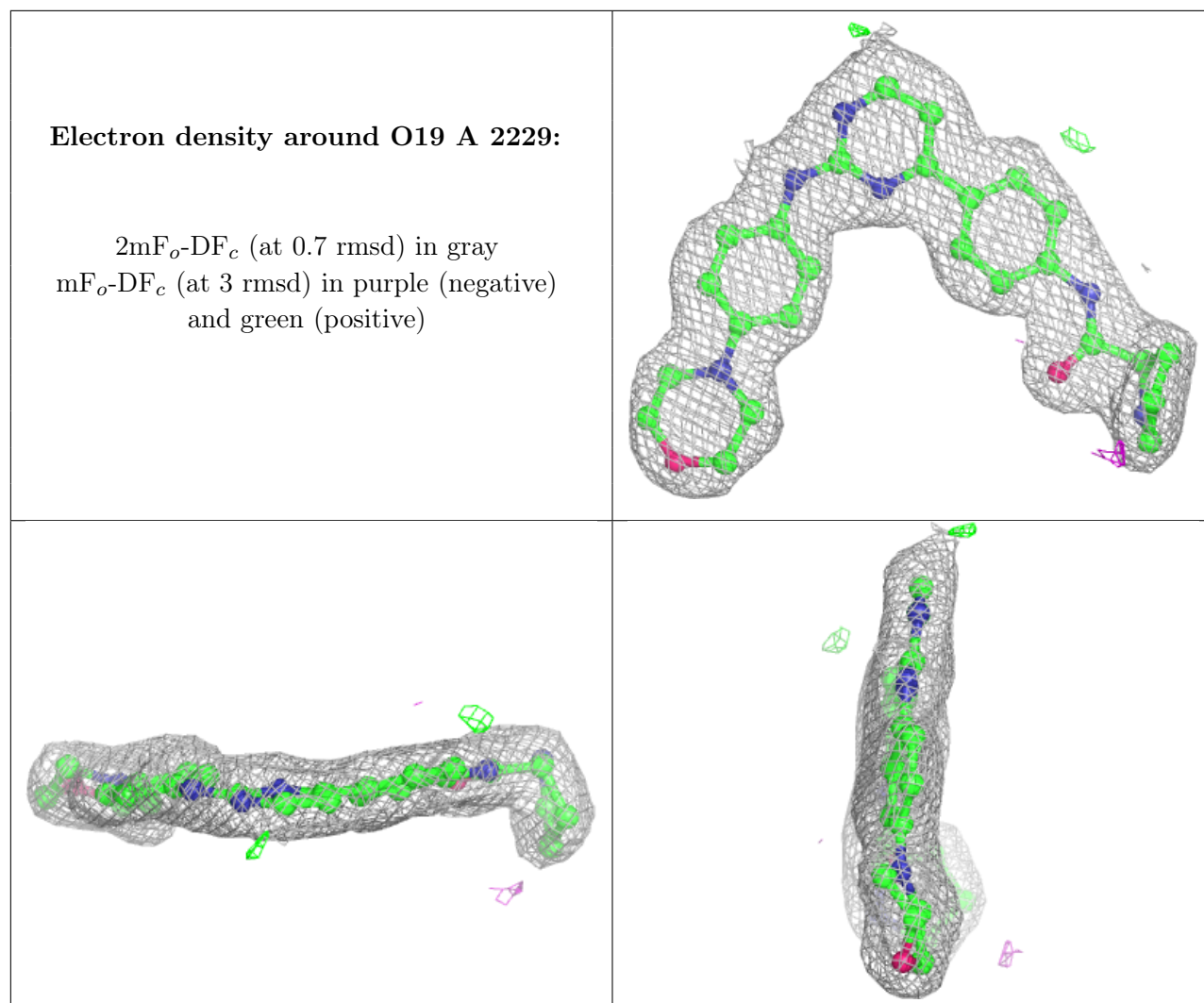mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
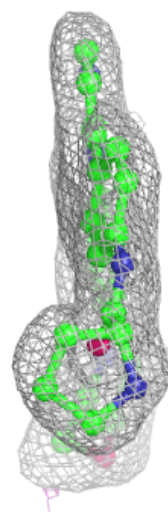
Electron density around O19 D 2229:

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

Electron density around O19 A 2229:

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.