



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:39 PM UTC

PDB ID : 6LN1 / pdb_00006ln1
Title : A natural inhibitor of DYRK1A for treatment of diabetes mellitus
Authors : Li, H.; Chen, L.X.; Zheng, M.Z.; Zhang, Q.Z.; Zhang, C.L.; Wu, C.R.; Yang, K.Y.; Song, Z.R.; Wang, Q.Q.; Li, C.; Zhou, Y.R.; Chen, J.C.
Deposited on : 2019-12-28
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

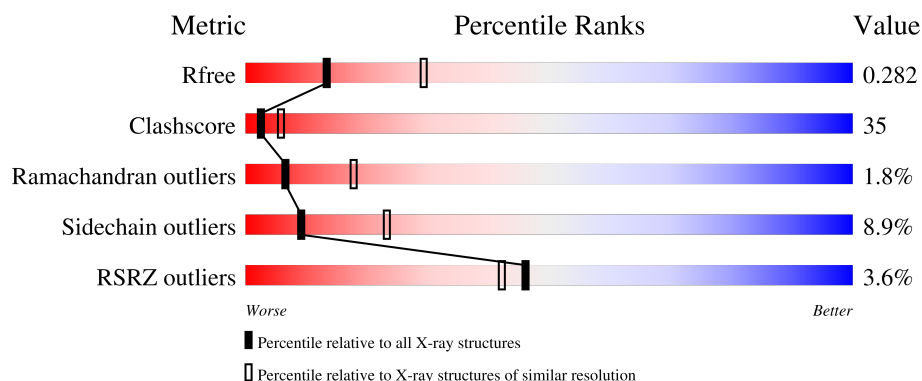
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	69% 24% • •
1	B	347	6% 43% 41% 9% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5626 atoms, of which 16 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.

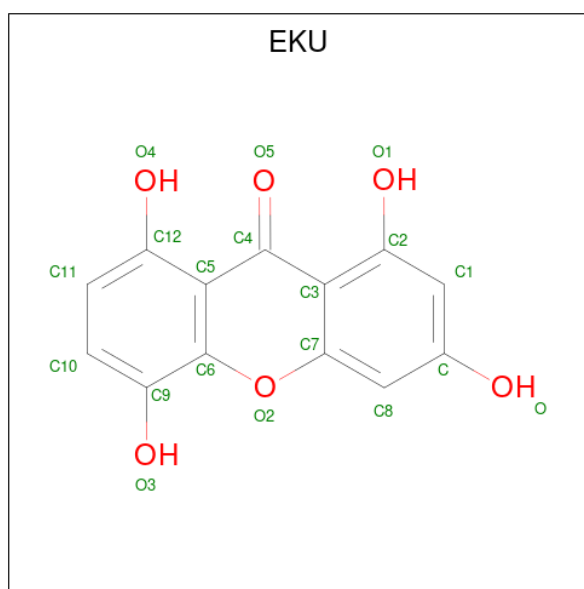
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	342	2808	1809	481	500	1	17	17	0	0
1	B	331	2720	1756	464	482	1	17	18	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	PHE	-	insertion	UNP Q13627
B	413	PHE	-	insertion	UNP Q13627

- Molecule 2 is 1,3,5,8-tetrakis(oxidanyl)xanthen-9-one (CCD ID: EKU) (formula: C₁₃H₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	27	13	8	6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			27	13	8	6		

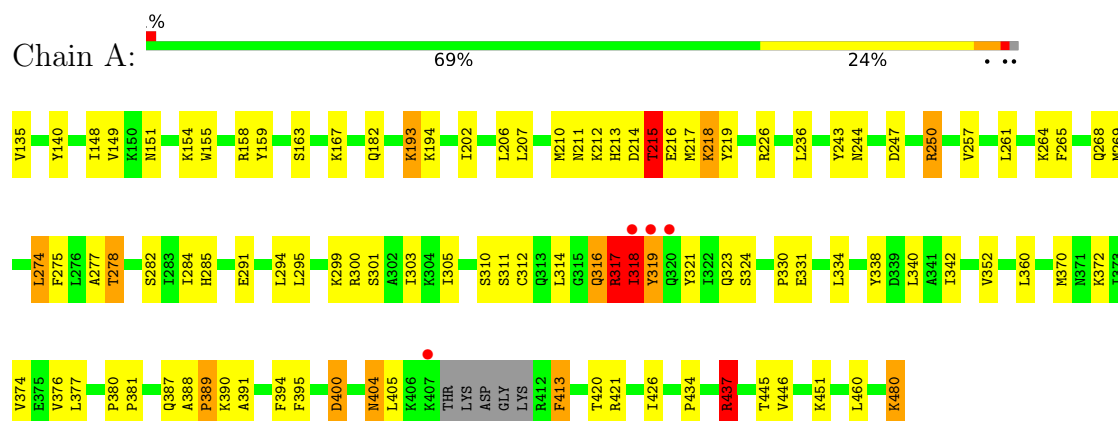
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	12	Total	O	0	0
			12	12		

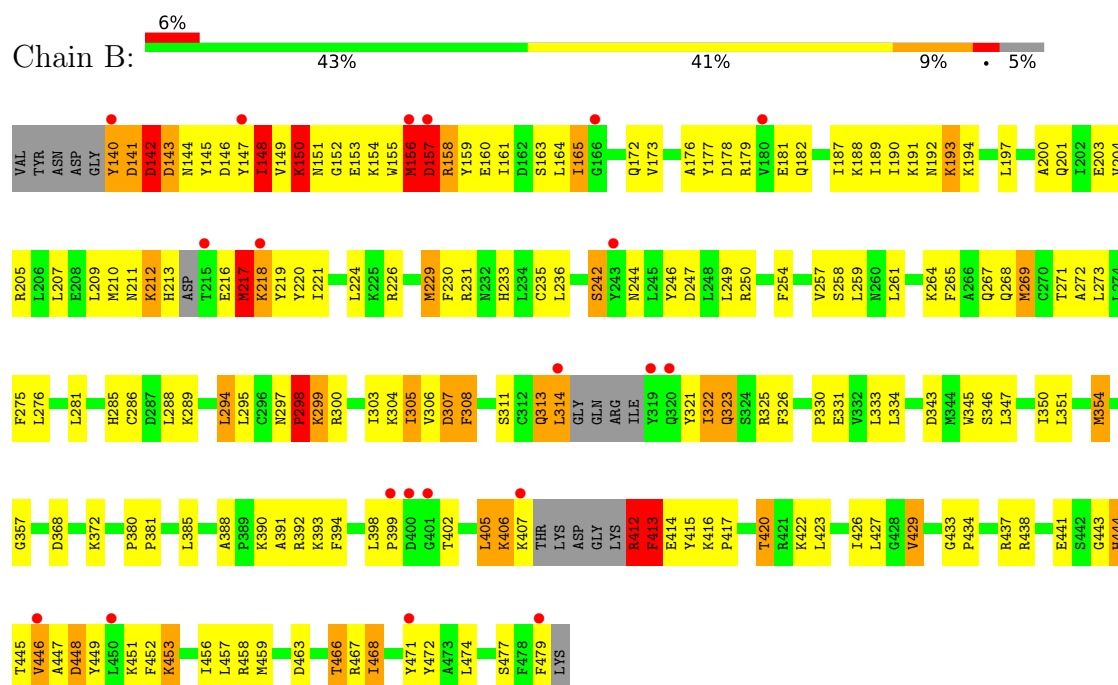
3 Residue-property plots

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: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	133.47Å 133.47Å 92.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.97 – 2.70 48.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.97-2.70) 99.9 (48.97-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.212 , 0.277 0.219 , 0.282	Depositor DCC
R_{free} test set	2016 reflections (7.80%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5626	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.93	3/2857 (0.1%)	0.98	11/3850 (0.3%)
1	B	0.93	10/2766 (0.4%)	1.20	21/3725 (0.6%)
All	All	0.93	13/5623 (0.2%)	1.10	32/7575 (0.4%)

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	5
1	B	1	2
All	All	1	7

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ASP	C-N	-33.18	0.90	1.33
1	B	313	GLN	C-N	14.33	1.53	1.33
1	A	317	ARG	C-N	-13.93	1.14	1.33
1	B	141	ASP	C-N	-8.33	1.22	1.33
1	B	405	LEU	C-N	-6.68	1.24	1.33
1	B	416	LYS	CA-C	-5.97	1.46	1.53
1	B	305	ILE	C-O	-5.84	1.17	1.24
1	B	307	ASP	CA-C	-5.56	1.47	1.53
1	B	405	LEU	C-O	-5.45	1.17	1.24
1	B	413	PHE	C-N	-5.23	1.26	1.33
1	B	405	LEU	CA-C	-5.16	1.45	1.52
1	B	141	ASP	C-O	-5.07	1.19	1.24
1	A	437	ARG	CG-CD	5.01	1.67	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASP	N-CA-CB	-23.19	71.30	110.49
1	B	414	GLU	N-CA-C	-21.58	77.46	107.88
1	B	141	ASP	CA-C-N	-17.97	87.22	121.54
1	B	141	ASP	C-N-CA	-17.97	87.22	121.54
1	B	307	ASP	N-CA-C	16.85	134.03	111.28
1	A	215	THR	CB-CA-C	-14.72	82.46	109.54
1	A	317	ARG	O-C-N	-13.31	108.88	123.52
1	B	307	ASP	CB-CA-C	-10.66	96.55	112.11
1	A	317	ARG	N-CA-C	9.83	123.31	108.46
1	B	220	TYR	N-CA-C	-9.77	99.79	114.64
1	B	314	LEU	CB-CA-C	9.58	128.30	110.10
1	A	214	ASP	CA-C-N	9.57	135.97	120.94
1	A	214	ASP	C-N-CA	9.57	135.97	120.94
1	A	214	ASP	N-CA-C	7.82	120.56	111.02
1	B	448	ASP	N-CA-C	-7.51	101.55	111.24
1	B	326	PHE	N-CA-C	-7.20	104.47	113.18
1	B	217	MET	N-CA-C	-7.06	103.52	111.14
1	A	215	THR	O-C-N	6.94	131.05	122.86
1	B	415	TYR	N-CA-C	-6.74	99.91	110.36
1	B	429	VAL	CB-CA-C	-6.64	100.40	111.29
1	A	214	ASP	O-C-N	-5.90	115.76	122.08
1	B	193	LYS	N-CA-CB	5.67	121.32	111.39
1	B	413	PHE	N-CA-C	-5.63	98.82	110.80
1	B	158	ARG	CA-C-N	5.62	131.09	123.11
1	B	158	ARG	C-N-CA	5.62	131.09	123.11
1	A	317	ARG	CA-C-N	-5.56	111.96	121.97
1	A	317	ARG	C-N-CA	-5.56	111.96	121.97
1	B	298	PRO	CA-N-CD	-5.45	104.37	112.00
1	A	243	TYR	N-CA-C	5.39	117.83	110.55
1	B	150	LYS	N-CA-C	-5.30	99.52	110.80
1	B	308	PHE	N-CA-C	5.16	120.22	113.20
1	B	148	ILE	N-CA-C	-5.10	102.16	108.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	314	LEU	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	THR	Peptide
1	A	317	ARG	Mainchain,Peptide
1	A	318	ILE	Peptide
1	A	319	TYR	Peptide
1	B	140	TYR	Peptide
1	B	412	ARG	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	2808	0	2810	98	3
1	B	2720	0	2725	291	3
2	A	19	8	0	0	0
2	B	19	8	0	0	0
3	A	32	0	0	11	0
3	B	12	0	0	9	0
All	All	5610	16	5535	382	3

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 35.

All (382) 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:438:ARG:HD2	1:B:444:HIS:CD2	1.47	1.47
1:B:151:ASN:HD21	1:B:163:SER:CA	1.35	1.36
1:B:313:GLN:O	1:B:314:LEU:HG	1.26	1.34
1:B:210:MET:HB3	1:B:218:LYS:NZ	1.42	1.30
1:B:438:ARG:HD2	1:B:444:HIS:NE2	1.48	1.28
1:B:145:TYR:HD2	1:B:191:LYS:NZ	1.17	1.25
1:B:151:ASN:ND2	1:B:163:SER:CA	1.98	1.23
1:B:151:ASN:HD21	1:B:163:SER:CB	1.51	1.22
1:B:471:TYR:CA	1:B:474:LEU:HD13	1.75	1.16
1:A:394:PHE:HA	3:A:615:HOH:O	1.44	1.16
1:A:413:PHE:CZ	3:B:605:HOH:O	1.96	1.15
1:B:380:PRO:HB2	1:B:385:LEU:HD11	1.15	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:TYR:CD2	1:B:191:LYS:NZ	1.93	1.13
1:A:413:PHE:HZ	3:B:605:HOH:O	1.31	1.11
1:B:438:ARG:CD	1:B:444:HIS:CD2	2.33	1.11
1:B:471:TYR:HA	1:B:474:LEU:HD13	1.31	1.10
1:B:141:ASP:HA	1:B:148:ILE:CD1	1.80	1.09
1:A:215:THR:CG2	1:A:215:THR:O	1.90	1.09
1:B:269:MET:HE1	1:B:305:ILE:HD11	1.32	1.09
1:B:151:ASN:ND2	1:B:163:SER:HA	1.58	1.08
1:B:447:ALA:O	1:B:451:LYS:HE2	1.53	1.07
1:B:144:ASN:O	1:B:191:LYS:NZ	1.89	1.06
1:B:471:TYR:CA	1:B:474:LEU:CD1	2.35	1.05
1:B:211:ASN:OD1	1:B:218:LYS:HE3	1.57	1.05
1:A:215:THR:O	1:A:215:THR:HG23	1.22	1.04
1:B:412:ARG:O	1:B:413:PHE:O	1.74	1.04
1:B:151:ASN:HD21	1:B:163:SER:HA	1.07	1.03
1:B:151:ASN:ND2	1:B:163:SER:CB	2.19	1.02
1:B:141:ASP:CA	1:B:148:ILE:CD1	2.36	1.02
1:B:210:MET:CB	1:B:218:LYS:NZ	2.22	1.01
1:B:210:MET:CB	1:B:218:LYS:HZ3	1.73	1.00
1:B:447:ALA:O	1:B:451:LYS:HG2	1.61	1.00
1:B:141:ASP:CA	1:B:148:ILE:HD11	1.71	1.00
1:A:211:ASN:CB	3:A:626:HOH:O	2.09	1.00
1:B:471:TYR:C	1:B:474:LEU:HD13	1.87	0.99
1:A:167:LYS:HE2	3:A:611:HOH:O	1.63	0.99
1:A:300:ARG:HD3	1:A:301:SER:H	1.23	0.99
1:B:412:ARG:C	1:B:413:PHE:O	2.04	0.98
1:B:463:ASP:HB3	1:B:466:THR:CG2	1.93	0.97
1:B:211:ASN:N	1:B:218:LYS:HE2	1.80	0.97
1:B:211:ASN:CA	1:B:218:LYS:HE2	1.95	0.97
1:B:210:MET:HB3	1:B:218:LYS:HZ3	0.90	0.97
1:B:471:TYR:C	1:B:474:LEU:CD1	2.39	0.95
1:B:148:ILE:HD12	1:B:148:ILE:H	1.27	0.95
1:B:142:ASP:OD1	1:B:144:ASN:N	1.99	0.94
1:B:269:MET:CE	1:B:305:ILE:HD11	1.97	0.92
1:B:313:GLN:O	1:B:314:LEU:CG	2.16	0.92
1:A:211:ASN:HB2	3:A:626:HOH:O	1.67	0.92
1:B:445:THR:O	1:B:448:ASP:N	2.03	0.91
1:B:144:ASN:O	1:B:191:LYS:CE	2.18	0.91
1:A:413:PHE:HE1	1:B:246:TYR:CE1	1.89	0.89
1:B:211:ASN:HA	1:B:218:LYS:HE2	1.54	0.88
1:B:249:LEU:HD11	1:B:354:MET:HE3	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:ARG:HD2	1:B:444:HIS:HD2	1.35	0.87
1:B:269:MET:HE1	1:B:305:ILE:CD1	2.04	0.86
1:B:140:TYR:HE2	3:B:610:HOH:O	1.57	0.86
1:B:141:ASP:HA	1:B:148:ILE:HD12	1.58	0.85
1:B:471:TYR:HD1	1:B:471:TYR:O	1.59	0.85
1:A:317:ARG:O	1:A:318:ILE:HG22	1.76	0.84
1:B:420:THR:HG22	3:B:609:HOH:O	1.77	0.84
1:B:380:PRO:HB2	1:B:385:LEU:CD1	2.04	0.84
1:B:447:ALA:O	1:B:451:LYS:CG	2.26	0.84
1:B:216:GLU:OE1	1:B:216:GLU:N	2.10	0.83
1:B:438:ARG:CD	1:B:444:HIS:NE2	2.35	0.83
1:B:151:ASN:ND2	1:B:163:SER:HB3	1.93	0.83
1:B:313:GLN:C	1:B:314:LEU:HG	2.02	0.82
1:B:259:LEU:H	1:B:444:HIS:CE1	1.97	0.82
1:A:480:LYS:HA	1:A:480:LYS:HE2	1.62	0.81
1:B:272:ALA:O	1:B:276:LEU:HD12	1.78	0.81
1:B:447:ALA:O	1:B:451:LYS:CE	2.26	0.81
1:B:149:VAL:C	1:B:150:LYS:HG3	2.04	0.80
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.62	0.80
1:A:300:ARG:CD	1:A:301:SER:H	1.95	0.80
1:B:145:TYR:O	1:B:191:LYS:HG3	1.81	0.79
1:B:438:ARG:HB3	1:B:444:HIS:HD2	1.47	0.79
1:B:307:ASP:CG	1:B:307:ASP:O	2.14	0.79
1:B:157:ASP:OD1	1:B:179:ARG:NH2	2.16	0.77
1:A:312:CYS:HB2	1:A:316:GLN:HG2	1.66	0.77
1:B:307:ASP:O	1:B:307:ASP:OD1	2.02	0.77
1:B:441:GLU:O	1:B:444:HIS:HB2	1.84	0.77
1:B:471:TYR:HA	1:B:474:LEU:CD1	2.06	0.76
1:B:211:ASN:CG	1:B:218:LYS:HE3	2.11	0.75
1:B:146:ASP:OD1	1:B:191:LYS:HD2	1.87	0.75
1:B:420:THR:CG2	3:B:609:HOH:O	2.32	0.75
1:B:471:TYR:O	1:B:471:TYR:CD1	2.38	0.75
1:B:149:VAL:O	1:B:150:LYS:HG3	1.87	0.74
1:B:471:TYR:C	1:B:474:LEU:HD12	2.12	0.74
1:A:434:PRO:O	1:A:437:ARG:HG2	1.88	0.74
1:B:444:HIS:O	1:B:445:THR:CG2	2.36	0.74
1:A:291:GLU:OE2	1:B:413:PHE:CD1	2.42	0.72
1:A:413:PHE:CE1	1:B:246:TYR:CE1	2.77	0.72
1:B:267:GLN:O	1:B:271:THR:HG23	1.90	0.72
1:B:434:PRO:HB2	1:B:437:ARG:HH21	1.55	0.72
1:B:209:LEU:HD23	1:B:209:LEU:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:CYS:C	1:B:236:LEU:HD23	2.15	0.71
1:B:307:ASP:OD1	1:B:307:ASP:C	2.33	0.71
1:B:155:TRP:O	1:B:158:ARG:N	2.24	0.71
1:B:438:ARG:CD	1:B:444:HIS:HD2	1.91	0.71
1:B:216:GLU:HA	1:B:219:TYR:CE1	2.26	0.70
1:A:218:LYS:HE2	1:A:219:TYR:CE1	2.27	0.70
1:B:148:ILE:HD12	1:B:148:ILE:N	2.05	0.70
1:B:463:ASP:HB3	1:B:466:THR:HG22	1.72	0.70
1:B:422:LYS:HA	3:B:602:HOH:O	1.91	0.69
1:A:264:LYS:O	1:A:268:GLN:HG3	1.92	0.69
1:B:229:MET:HE3	1:B:233:HIS:O	1.92	0.69
1:B:392:ARG:O	1:B:406:LYS:HE3	1.92	0.69
1:B:285:HIS:O	1:B:311:SER:OG	2.10	0.69
1:B:463:ASP:HB3	1:B:466:THR:HG23	1.74	0.68
1:A:291:GLU:OE2	1:B:413:PHE:HD1	1.77	0.68
1:B:285:HIS:HA	1:B:311:SER:OG	1.94	0.68
1:B:412:ARG:O	1:B:413:PHE:C	2.36	0.68
1:B:141:ASP:HB2	1:B:146:ASP:C	2.19	0.68
1:A:330:PRO:HD2	1:A:331:GLU:OE1	1.93	0.68
1:A:317:ARG:O	1:A:318:ILE:CG2	2.42	0.67
1:B:210:MET:CB	1:B:218:LYS:HZ1	2.02	0.67
1:A:202:ILE:HG21	1:A:316:GLN:HE22	1.60	0.66
1:A:413:PHE:CE2	3:B:605:HOH:O	2.30	0.66
1:B:447:ALA:C	1:B:451:LYS:HE2	2.19	0.66
1:A:317:ARG:O	1:A:318:ILE:CB	2.43	0.66
1:B:210:MET:HB3	1:B:218:LYS:CE	2.23	0.66
1:B:452:PHE:CE1	1:B:456:ILE:HD11	2.32	0.65
1:B:479:PHE:C	3:B:606:HOH:O	2.39	0.65
1:B:152:GLY:N	1:B:161:ILE:O	2.29	0.65
1:A:318:ILE:HG23	1:A:318:ILE:O	1.96	0.65
1:A:374:VAL:HG11	1:A:405:LEU:HD11	1.77	0.65
1:B:444:HIS:C	1:B:445:THR:HG23	2.21	0.65
1:B:155:TRP:C	1:B:157:ASP:N	2.54	0.65
1:B:188:LYS:HD3	1:B:190:ILE:HD11	1.80	0.64
1:A:480:LYS:HA	1:A:480:LYS:CE	2.28	0.64
1:B:148:ILE:CD1	1:B:148:ILE:H	2.02	0.64
1:B:212:LYS:O	1:B:212:LYS:HD3	1.98	0.63
1:B:216:GLU:HA	1:B:219:TYR:CD1	2.32	0.63
1:B:144:ASN:O	1:B:191:LYS:HE3	1.95	0.63
1:A:207:LEU:HD23	1:A:210:MET:HE3	1.80	0.63
1:B:144:ASN:C	1:B:191:LYS:HZ2	2.03	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:O	1:A:278:THR:HG23	1.98	0.63
1:B:380:PRO:CB	1:B:385:LEU:HD11	2.09	0.63
1:B:444:HIS:O	1:B:445:THR:HG23	1.97	0.63
1:B:242:SER:OG	1:B:298:PRO:HD3	1.98	0.62
1:B:217:MET:O	1:B:219:TYR:N	2.33	0.62
1:B:429:VAL:O	1:B:446:VAL:HG12	2.00	0.62
1:B:443:GLY:O	1:B:448:ASP:OD2	2.18	0.61
1:B:445:THR:O	1:B:448:ASP:HB2	2.00	0.61
1:B:201:GLN:O	1:B:205:ARG:HG3	1.98	0.61
1:B:447:ALA:O	1:B:451:LYS:CD	2.47	0.61
1:B:452:PHE:HE1	1:B:456:ILE:HD11	1.64	0.61
1:A:480:LYS:HE2	1:A:480:LYS:CA	2.29	0.61
1:B:259:LEU:N	1:B:444:HIS:CE1	2.68	0.61
1:B:297:ASN:HB3	1:B:300:ARG:HG3	1.83	0.61
1:B:141:ASP:HB3	1:B:147:TYR:HA	1.82	0.60
1:B:144:ASN:C	1:B:191:LYS:NZ	2.60	0.60
1:A:213:HIS:O	1:A:218:LYS:HD3	2.02	0.60
1:A:376:VAL:HG12	1:A:377:LEU:HD23	1.84	0.60
1:B:368:ASP:OD2	1:B:372:LYS:NZ	2.34	0.59
1:A:211:ASN:HB3	3:A:626:HOH:O	1.91	0.59
1:B:333:LEU:O	1:B:390:LYS:HE3	2.02	0.59
1:B:165:ILE:CG2	1:B:173:VAL:HG12	2.32	0.59
1:B:211:ASN:HA	1:B:218:LYS:CE	2.30	0.59
1:A:269:MET:HE1	1:A:305:ILE:HD11	1.84	0.58
1:B:156:MET:C	1:B:158:ARG:H	2.11	0.58
1:B:165:ILE:HG22	1:B:173:VAL:O	2.02	0.58
1:B:398:LEU:CB	1:B:399:PRO:HD2	2.34	0.58
1:A:421:ARG:HG2	1:A:426:ILE:HD11	1.86	0.58
1:B:322:ILE:O	1:B:323:GLN:CB	2.50	0.58
1:A:193:LYS:HG3	1:A:194:LYS:N	2.18	0.58
1:B:178:ASP:OD2	1:B:226:ARG:NH1	2.37	0.57
1:B:347:LEU:HD11	1:B:351:LEU:HD21	1.85	0.57
1:B:458:ARG:HG2	1:B:468:ILE:HB	1.86	0.57
1:B:176:ALA:HB3	1:B:187:ILE:HD12	1.84	0.57
1:B:443:GLY:C	1:B:448:ASP:OD2	2.47	0.57
1:B:159:TYR:HA	1:B:177:TYR:O	2.04	0.57
1:B:350:ILE:O	1:B:354:MET:HG2	2.05	0.57
1:B:264:LYS:O	1:B:268:GLN:HG3	2.05	0.56
1:B:303:ILE:O	1:B:304:LYS:HG3	2.05	0.56
1:B:333:LEU:O	1:B:390:LYS:CE	2.53	0.56
1:B:141:ASP:HB2	1:B:146:ASP:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LEU:HD13	1:B:165:ILE:N	2.21	0.56
1:B:201:GLN:O	1:B:204:VAL:HG22	2.05	0.56
1:B:308:PHE:N	1:B:308:PHE:CD1	2.74	0.56
1:A:352:VAL:HG11	1:A:360:LEU:HD13	1.87	0.56
1:A:269:MET:HE1	1:A:305:ILE:CD1	2.36	0.55
1:B:236:LEU:HD23	1:B:236:LEU:N	2.21	0.55
1:B:393:LYS:HG2	1:B:394:PHE:CE1	2.41	0.55
1:B:347:LEU:O	1:B:351:LEU:HG	2.05	0.55
1:B:444:HIS:C	1:B:445:THR:CG2	2.79	0.55
1:A:206:LEU:O	1:A:210:MET:HG3	2.06	0.55
1:A:316:GLN:O	1:A:317:ARG:HD3	2.07	0.54
1:B:210:MET:C	1:B:218:LYS:HE2	2.30	0.54
1:B:176:ALA:HB3	1:B:187:ILE:CD1	2.37	0.54
1:B:444:HIS:O	1:B:445:THR:HG22	2.04	0.54
1:B:147:TYR:CD2	1:B:148:ILE:O	2.60	0.54
1:B:155:TRP:O	1:B:157:ASP:N	2.41	0.54
1:B:259:LEU:N	1:B:444:HIS:HE1	2.04	0.54
1:B:471:TYR:C	1:B:471:TYR:CD1	2.82	0.54
1:B:322:ILE:O	1:B:323:GLN:HB2	2.08	0.54
1:B:219:TYR:CD1	1:B:219:TYR:N	2.75	0.54
1:B:249:LEU:HD11	1:B:354:MET:CE	2.33	0.54
1:B:459:MET:O	1:B:467:ARG:HD3	2.08	0.54
1:A:269:MET:HE1	1:A:305:ILE:CG1	2.39	0.53
1:A:217:MET:HB3	1:A:275:PHE:HB2	1.91	0.53
1:B:288:LEU:O	1:B:289:LYS:HB3	2.09	0.53
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.91	0.53
1:A:167:LYS:HG2	3:A:611:HOH:O	2.07	0.53
1:B:211:ASN:CG	1:B:218:LYS:CE	2.79	0.53
1:A:277:ALA:HA	1:A:340:LEU:CD2	2.39	0.52
1:B:207:LEU:HA	1:B:210:MET:HE3	1.91	0.52
1:B:212:LYS:O	1:B:213:HIS:ND1	2.42	0.52
1:B:244:ASN:HB3	1:B:294:LEU:HD13	1.91	0.52
1:B:297:ASN:C	1:B:299:LYS:H	2.16	0.52
1:B:330:PRO:HD3	1:B:345:TRP:CD2	2.44	0.52
1:A:318:ILE:CG2	1:A:318:ILE:O	2.56	0.52
1:B:229:MET:HE3	1:B:233:HIS:C	2.33	0.52
1:B:142:ASP:OD1	1:B:143:ASP:N	2.43	0.52
1:B:211:ASN:OD1	1:B:218:LYS:CE	2.46	0.52
1:B:230:PHE:CZ	1:B:231:ARG:HD2	2.45	0.52
1:B:155:TRP:O	1:B:156:MET:C	2.53	0.51
1:A:247:ASP:OD1	1:A:250:ARG:NH2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:HIS:O	1:B:286:CYS:HB2	2.10	0.51
1:B:412:ARG:N	1:B:412:ARG:CD	2.73	0.51
1:B:144:ASN:C	1:B:191:LYS:HE3	2.35	0.51
1:A:269:MET:HE1	1:A:305:ILE:HG12	1.91	0.51
1:B:453:LYS:HD3	1:B:457:LEU:HD11	1.93	0.51
1:B:438:ARG:CB	1:B:444:HIS:HD2	2.19	0.51
1:B:463:ASP:CB	1:B:466:THR:HG22	2.38	0.51
1:B:297:ASN:O	1:B:299:LYS:N	2.44	0.51
1:A:244:ASN:HA	1:A:294:LEU:HA	1.93	0.51
1:A:413:PHE:HE1	1:B:246:TYR:CZ	2.29	0.50
1:B:247:ASP:OD1	1:B:250:ARG:NH1	2.39	0.50
1:B:314:LEU:C	3:B:604:HOH:O	2.55	0.50
1:A:400:ASP:OD1	1:A:400:ASP:N	2.32	0.50
1:B:412:ARG:N	1:B:412:ARG:NE	2.60	0.50
1:B:471:TYR:O	1:B:474:LEU:HD13	2.12	0.50
1:A:334:LEU:HD21	1:A:370:MET:HE3	1.94	0.50
1:A:421:ARG:HA	3:A:623:HOH:O	2.12	0.50
1:B:157:ASP:CG	1:B:179:ARG:HH21	2.20	0.50
1:B:149:VAL:CG1	1:B:150:LYS:N	2.75	0.49
1:B:417:PRO:O	1:B:420:THR:HB	2.11	0.49
1:B:463:ASP:CG	1:B:466:THR:HG22	2.37	0.49
1:A:300:ARG:HA	1:A:300:ARG:NE	2.27	0.49
1:B:390:LYS:O	1:B:391:ALA:C	2.54	0.49
1:B:224:LEU:HD11	1:B:236:LEU:HB3	1.94	0.49
1:B:385:LEU:N	1:B:385:LEU:HD12	2.26	0.49
1:B:249:LEU:CD1	1:B:354:MET:HE3	2.35	0.49
1:B:259:LEU:HB3	1:B:444:HIS:CE1	2.47	0.49
1:B:438:ARG:HB3	1:B:444:HIS:CD2	2.35	0.49
1:B:398:LEU:HB3	1:B:399:PRO:CD	2.38	0.49
1:A:158:ARG:HD3	3:A:618:HOH:O	2.13	0.48
1:B:331:GLU:OE1	1:B:467:ARG:NH2	2.43	0.48
1:A:314:LEU:O	1:A:317:ARG:NH1	2.46	0.48
1:A:140:TYR:O	1:A:148:ILE:HG13	2.13	0.48
1:A:480:LYS:H	1:A:480:LYS:HD2	1.78	0.48
1:A:376:VAL:HG12	1:A:377:LEU:CD2	2.43	0.48
1:B:273:LEU:HD21	1:B:343:ASP:HB3	1.95	0.48
1:A:151:ASN:ND2	1:A:163:SER:HA	2.29	0.48
1:A:202:ILE:CG2	1:A:316:GLN:HE22	2.23	0.48
1:B:146:ASP:O	1:B:147:TYR:C	2.55	0.48
1:B:427:LEU:O	1:B:433:GLY:HA2	2.14	0.48
1:B:154:LYS:C	1:B:155:TRP:HD1	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:LYS:HA	1:B:193:LYS:HD3	1.50	0.48
1:A:167:LYS:CE	3:A:611:HOH:O	2.40	0.48
1:A:317:ARG:NH2	1:A:338:TYR:O	2.47	0.48
1:A:338:TYR:HB2	1:A:342:ILE:CG2	2.44	0.48
1:A:480:LYS:CE	1:A:480:LYS:CA	2.90	0.48
1:B:144:ASN:ND2	1:B:191:LYS:NZ	2.62	0.48
1:B:295:LEU:HD23	1:B:303:ILE:HG22	1.95	0.47
1:B:452:PHE:O	1:B:456:ILE:HG12	2.13	0.47
1:B:354:MET:CE	1:B:354:MET:HA	2.44	0.47
1:A:445:THR:O	1:A:446:VAL:C	2.56	0.47
1:B:474:LEU:HD12	1:B:474:LEU:H	1.80	0.47
1:B:144:ASN:ND2	1:B:191:LYS:HZ2	2.13	0.47
1:B:217:MET:C	1:B:219:TYR:H	2.23	0.47
1:B:294:LEU:N	1:B:294:LEU:CD2	2.77	0.47
1:B:445:THR:H	1:B:448:ASP:HB2	1.79	0.47
1:B:150:LYS:HD3	1:B:153:GLU:OE1	2.15	0.47
1:B:156:MET:C	1:B:158:ARG:N	2.72	0.46
1:B:230:PHE:CE1	1:B:231:ARG:HG3	2.50	0.46
1:B:381:PRO:O	1:B:385:LEU:HD13	2.15	0.46
1:B:160:GLU:OE2	1:B:179:ARG:NH1	2.49	0.46
1:B:191:LYS:O	1:B:193:LYS:N	2.46	0.46
1:B:142:ASP:O	1:B:143:ASP:C	2.56	0.46
1:B:229:MET:HE2	1:B:229:MET:HB3	1.66	0.46
1:B:244:ASN:HA	1:B:294:LEU:HA	1.96	0.46
1:A:264:LYS:HE2	3:A:629:HOH:O	2.15	0.46
1:A:269:MET:CE	1:A:305:ILE:HD11	2.45	0.46
1:B:463:ASP:CB	1:B:466:THR:CG2	2.81	0.46
1:B:147:TYR:CE2	1:B:148:ILE:O	2.68	0.46
1:B:472:TYR:C	1:B:474:LEU:N	2.72	0.46
1:B:193:LYS:CD	1:B:194:LYS:H	2.29	0.46
1:B:261:LEU:HG	1:B:265:PHE:CE2	2.50	0.46
1:A:155:TRP:HB2	1:A:159:TYR:HB2	1.98	0.45
1:B:210:MET:HB2	1:B:218:LYS:HZ1	1.77	0.45
1:B:188:LYS:HD3	1:B:190:ILE:CD1	2.44	0.45
1:B:212:LYS:O	1:B:212:LYS:CD	2.64	0.45
1:B:330:PRO:HD3	1:B:345:TRP:CE2	2.50	0.45
1:A:207:LEU:HD23	1:A:210:MET:CE	2.44	0.45
1:A:394:PHE:HB2	1:A:395:PHE:CD1	2.51	0.45
1:B:230:PHE:CZ	1:B:231:ARG:HG3	2.51	0.45
1:A:215:THR:OG1	1:A:216:GLU:N	2.47	0.45
1:A:387:GLN:OE1	1:A:387:GLN:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:O	1:B:172:GLN:OE1	2.35	0.45
1:B:297:ASN:C	1:B:299:LYS:N	2.75	0.45
1:A:285:HIS:HA	1:A:311:SER:OG	2.17	0.45
1:B:434:PRO:CB	1:B:437:ARG:HH21	2.29	0.45
1:B:142:ASP:CG	1:B:143:ASP:N	2.75	0.45
1:B:151:ASN:HD21	1:B:163:SER:HB2	1.65	0.45
1:A:257:VAL:HB	1:A:261:LEU:HD23	1.99	0.44
1:B:467:ARG:O	1:B:468:ILE:C	2.60	0.44
1:B:197:LEU:O	1:B:201:GLN:HG2	2.17	0.44
1:B:453:LYS:C	1:B:453:LYS:HD2	2.43	0.44
1:A:236:LEU:HD12	1:A:236:LEU:N	2.32	0.44
1:B:417:PRO:HB2	1:B:420:THR:OG1	2.17	0.44
1:B:211:ASN:CA	1:B:218:LYS:CE	2.82	0.44
1:A:316:GLN:O	1:A:317:ARG:HG2	2.18	0.43
1:A:338:TYR:HB2	1:A:342:ILE:HG21	1.99	0.43
1:A:388:ALA:O	1:A:389:PRO:C	2.60	0.43
1:A:480:LYS:HE2	1:A:480:LYS:N	2.33	0.43
1:B:472:TYR:C	1:B:474:LEU:H	2.25	0.43
1:A:299:LYS:HA	1:A:299:LYS:HD3	1.80	0.43
1:B:295:LEU:HD23	1:B:303:ILE:CG2	2.48	0.43
1:B:429:VAL:HG13	1:B:449:TYR:CB	2.48	0.43
1:A:215:THR:O	1:A:215:THR:HG22	2.04	0.43
1:A:420:THR:O	1:A:420:THR:HG22	2.18	0.43
1:B:273:LEU:CD2	1:B:343:ASP:HB3	2.48	0.43
1:B:331:GLU:H	1:B:331:GLU:HG3	1.42	0.43
1:B:275:PHE:CZ	1:B:281:LEU:HD11	2.53	0.43
1:B:472:TYR:N	1:B:474:LEU:HD12	2.33	0.43
1:A:265:PHE:CD1	1:A:303:ILE:HD13	2.53	0.43
1:B:154:LYS:O	1:B:155:TRP:HD1	2.01	0.43
1:B:322:ILE:O	1:B:323:GLN:HG3	2.18	0.43
1:B:217:MET:C	1:B:219:TYR:N	2.74	0.43
1:A:274:LEU:HD23	1:A:274:LEU:O	2.19	0.43
1:B:230:PHE:CZ	1:B:231:ARG:CD	3.02	0.43
1:B:145:TYR:O	1:B:191:LYS:CG	2.61	0.43
1:A:211:ASN:ND2	3:A:605:HOH:O	2.52	0.42
1:B:161:ILE:HD13	1:B:176:ALA:HB2	2.00	0.42
1:B:188:LYS:O	1:B:235:CYS:HA	2.19	0.42
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.54	0.42
1:A:413:PHE:CE1	1:B:246:TYR:CZ	3.07	0.42
1:B:203:GLU:HG3	1:B:308:PHE:HB2	2.01	0.42
1:B:249:LEU:CD1	1:B:354:MET:CE	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LYS:C	1:B:155:TRP:CD1	2.97	0.42
1:A:380:PRO:O	1:A:381:PRO:C	2.63	0.42
1:A:377:LEU:HD11	1:A:460:LEU:HB3	2.02	0.42
1:B:144:ASN:C	1:B:191:LYS:CE	2.90	0.42
1:B:190:ILE:HG22	1:B:191:LYS:N	2.33	0.42
1:B:204:VAL:HG23	1:B:205:ARG:N	2.34	0.42
1:B:224:LEU:CD1	1:B:236:LEU:HB3	2.50	0.42
1:B:346:SER:O	1:B:350:ILE:HG13	2.19	0.42
1:B:303:ILE:C	1:B:304:LYS:HG3	2.44	0.41
1:B:368:ASP:CG	1:B:372:LYS:HZ3	2.26	0.41
1:A:291:GLU:OE1	1:B:413:PHE:HE1	2.02	0.41
1:B:254:PHE:O	1:B:357:GLY:HA3	2.19	0.41
1:B:398:LEU:CB	1:B:399:PRO:CD	2.96	0.41
1:B:152:GLY:CA	1:B:161:ILE:O	2.69	0.41
1:B:190:ILE:HG13	1:B:200:ALA:CB	2.50	0.41
1:B:294:LEU:N	1:B:294:LEU:HD22	2.34	0.41
1:B:453:LYS:HE3	1:B:453:LYS:HB3	1.85	0.41
1:B:285:HIS:CA	1:B:311:SER:OG	2.65	0.41
1:B:322:ILE:C	1:B:323:GLN:HG3	2.46	0.41
1:B:429:VAL:HG13	1:B:449:TYR:HB2	2.02	0.41
1:B:141:ASP:CA	1:B:148:ILE:HD12	2.28	0.41
1:B:157:ASP:CG	1:B:179:ARG:NH2	2.78	0.41
1:A:154:LYS:HA	1:A:159:TYR:O	2.20	0.41
1:A:295:LEU:HD23	1:A:303:ILE:HG22	2.03	0.41
1:B:204:VAL:O	1:B:205:ARG:C	2.63	0.41
1:B:423:LEU:HA	1:B:426:ILE:HD12	2.02	0.41
1:A:334:LEU:HB3	1:A:388:ALA:HB1	2.02	0.41
1:B:210:MET:HB2	1:B:218:LYS:NZ	2.28	0.41
1:B:211:ASN:N	1:B:218:LYS:CE	2.68	0.41
1:B:334:LEU:HB3	1:B:388:ALA:HB1	2.03	0.41
1:B:141:ASP:CB	1:B:147:TYR:HA	2.51	0.40
1:B:217:MET:H	1:B:217:MET:HG2	1.75	0.40
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.88	0.40
1:B:210:MET:SD	1:B:221:ILE:HG21	2.62	0.40
1:B:155:TRP:O	1:B:157:ASP:C	2.65	0.40
1:B:354:MET:HA	1:B:354:MET:HE2	2.03	0.40
1:B:441:GLU:HG2	1:B:444:HIS:CD2	2.57	0.40
1:A:388:ALA:O	1:A:390:LYS:N	2.55	0.40
1:A:316:GLN:O	1:A:317:ARG:CG	2.69	0.40
1:A:404:ASN:HD22	1:A:404:ASN:HA	1.73	0.40
1:B:142:ASP:O	1:B:144:ASN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:VAL:HB	1:B:261:LEU:HD23	2.02	0.40

All (3) 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:A:319:TYR:CD1	1:B:157:ASP:CB[3_655]	1.78	0.42
1:A:319:TYR:CE1	1:B:157:ASP:CB[3_655]	2.16	0.04
1:A:193:LYS:NZ	1:B:181:GLU:OE1[3_655]	2.19	0.01

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	337/347 (97%)	314 (93%)	20 (6%)	3 (1%)	14	35
1	B	322/347 (93%)	281 (87%)	32 (10%)	9 (3%)	4	9
All	All	659/694 (95%)	595 (90%)	52 (8%)	12 (2%)	6	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	ILE
1	B	157	ASP
1	B	406	LYS
1	B	413	PHE
1	B	156	MET
1	B	218	LYS
1	B	325	ARG
1	A	323	GLN
1	B	323	GLN
1	B	298	PRO

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Mol	Chain	Res	Type
1	A	389	PRO
1	B	468	ILE

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	303/307 (99%)	280 (92%)	23 (8%)	12	30
1	B	294/307 (96%)	264 (90%)	30 (10%)	7	18
All	All	597/614 (97%)	544 (91%)	53 (9%)	9	23

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	VAL
1	A	149	VAL
1	A	182	GLN
1	A	193	LYS
1	A	212	LYS
1	A	218	LYS
1	A	226	ARG
1	A	250	ARG
1	A	274	LEU
1	A	278	THR
1	A	282	SER
1	A	284	ILE
1	A	310	SER
1	A	316	GLN
1	A	318	ILE
1	A	324	SER
1	A	372	LYS
1	A	400	ASP
1	A	404	ASN
1	A	413	PHE
1	A	437	ARG

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Mol	Chain	Res	Type
1	A	451	LYS
1	A	480	LYS
1	B	142	ASP
1	B	143	ASP
1	B	148	ILE
1	B	150	LYS
1	B	156	MET
1	B	157	ASP
1	B	165	ILE
1	B	182	GLN
1	B	189	ILE
1	B	212	LYS
1	B	217	MET
1	B	229	MET
1	B	242	SER
1	B	258	SER
1	B	269	MET
1	B	294	LEU
1	B	299	LYS
1	B	306	VAL
1	B	322	ILE
1	B	354	MET
1	B	402	THR
1	B	405	LEU
1	B	407	LYS
1	B	412	ARG
1	B	420	THR
1	B	444	HIS
1	B	446	VAL
1	B	453	LYS
1	B	466	THR
1	B	477	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	GLN
1	A	201	GLN
1	A	213	HIS
1	A	253	ASN
1	A	297	ASN
1	A	316	GLN

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	444	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PTR	A	321	1	15,16,17	1.67	2 (13%)	17,22,24	0.78	0
1	PTR	B	321	1	15,16,17	1.05	1 (6%)	17,22,24	1.96	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	2/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	PTR	OH-CZ	-5.02	1.29	1.40
1	A	321	PTR	CB-CA	-2.11	1.49	1.53
1	B	321	PTR	P-OH	2.03	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PTR	CE2-CZ-CE1	-4.06	114.23	120.16
1	B	321	PTR	CD2-CE2-CZ	3.94	124.23	119.73
1	B	321	PTR	P-OH-CZ	3.01	134.61	123.88
1	B	321	PTR	OH-CZ-CE1	2.85	127.76	119.22
1	B	321	PTR	CD2-CG-CD1	-2.25	114.89	118.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	N-CA-CB-CG
1	B	321	PTR	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EKU	B	501	-	21,21,21	4.00	14 (66%)	32,32,32	1.41	5 (15%)
2	EKU	A	501	-	21,21,21	2.65	4 (19%)	32,32,32	1.96	10 (31%)

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	EKU	B	501	-	-	-	0/3/3/3
2	EKU	A	501	-	-	-	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	EKU	O2-C6	-10.96	1.23	1.39
2	A	501	EKU	O5-C4	9.80	1.40	1.22
2	B	501	EKU	O2-C7	-9.27	1.23	1.38
2	B	501	EKU	C5-C4	-5.54	1.34	1.47
2	B	501	EKU	C3-C4	-4.39	1.37	1.47
2	B	501	EKU	C1-C	-3.76	1.33	1.39
2	B	501	EKU	C5-C12	-3.69	1.35	1.41
2	A	501	EKU	C11-C10	-3.43	1.33	1.38
2	B	501	EKU	C1-C2	-2.61	1.35	1.38
2	B	501	EKU	C3-C2	-2.58	1.37	1.41
2	A	501	EKU	O3-C9	2.53	1.41	1.36
2	B	501	EKU	C10-C9	-2.32	1.35	1.39
2	B	501	EKU	C3-C7	-2.18	1.36	1.40
2	B	501	EKU	O1-C2	-2.14	1.32	1.36
2	A	501	EKU	C1-C2	2.10	1.41	1.38
2	B	501	EKU	O-C	-2.09	1.32	1.37
2	B	501	EKU	C9-C6	-2.08	1.36	1.40
2	B	501	EKU	O3-C9	-2.02	1.32	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	EKU	O2-C6-C9	5.43	122.92	116.14
2	A	501	EKU	O2-C6-C5	-3.70	116.61	122.02
2	A	501	EKU	C2-C3-C7	3.54	120.79	117.41
2	A	501	EKU	O1-C2-C3	-3.53	114.61	121.14
2	B	501	EKU	O2-C7-C8	3.28	120.70	115.43
2	A	501	EKU	C7-C3-C4	-2.86	116.21	119.71
2	B	501	EKU	C2-C3-C7	2.82	120.10	117.41
2	A	501	EKU	C10-C11-C12	2.75	123.25	120.50
2	A	501	EKU	O1-C2-C1	2.73	126.81	119.45
2	B	501	EKU	C8-C7-C3	-2.65	117.17	121.79
2	B	501	EKU	C12-C5-C6	2.51	121.06	117.04
2	A	501	EKU	C6-C5-C4	2.21	122.37	119.73
2	B	501	EKU	C2-C1-C	-2.21	117.63	119.67
2	A	501	EKU	C7-O2-C6	2.11	122.58	117.26
2	A	501	EKU	C1-C2-C3	-2.08	118.58	120.92

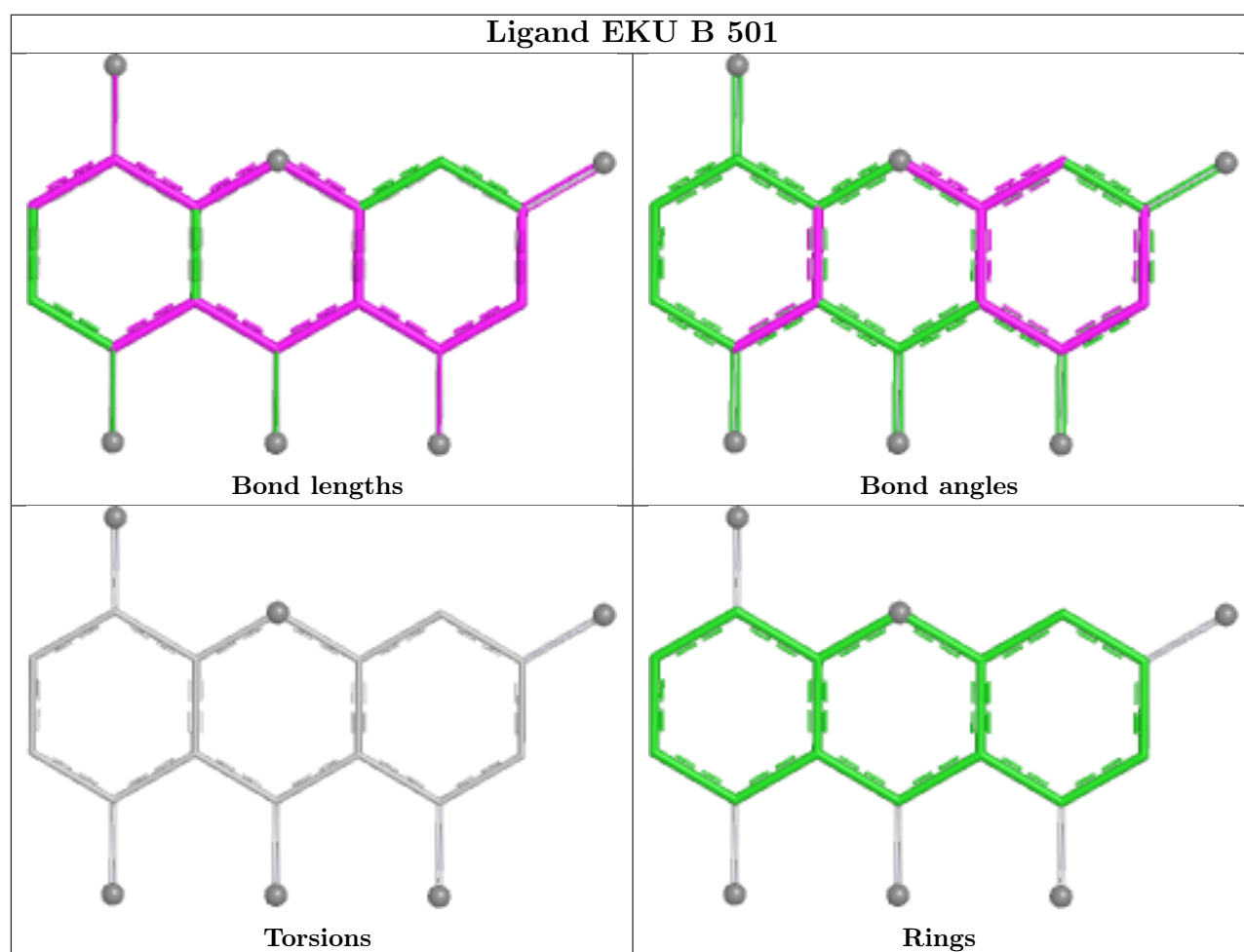
There are no chirality outliers.

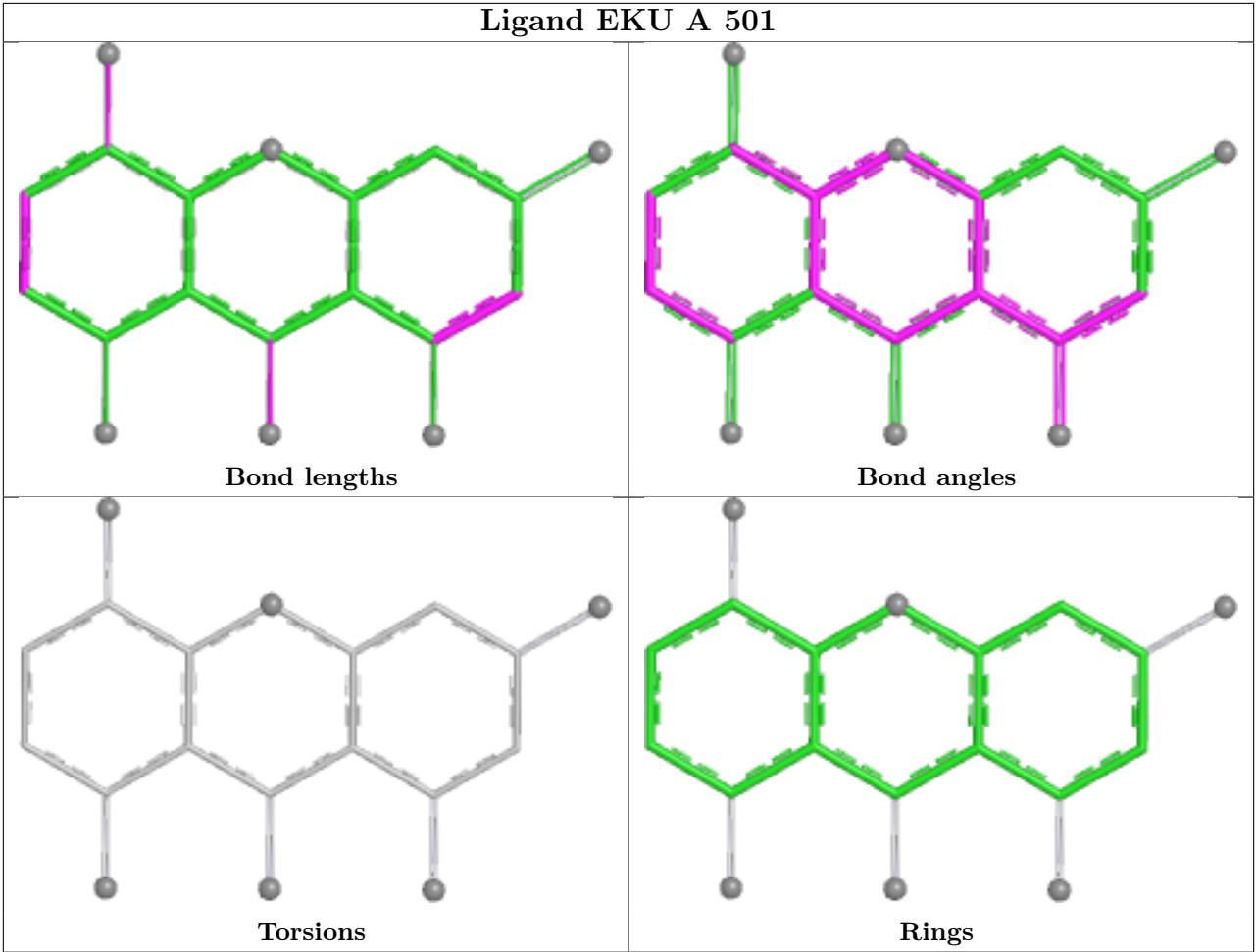
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	320:GLN	C	321:PTR	N	1.19
1	A	317:ARG	C	318:ILE	N	1.14
1	A	214:ASP	C	215:THR	N	0.90

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	341/347 (98%)	-0.22	4 (1%) 76 75	30, 46, 76, 107	1 (0%)
1	B	330/347 (95%)	0.60	20 (6%) 27 24	48, 81, 105, 117	0
All	All	671/694 (96%)	0.18	24 (3%) 46 42	30, 64, 103, 117	1 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	TYR	5.3
1	B	399	PRO	4.2
1	A	318	ILE	4.0
1	A	320	GLN	3.8
1	B	407	LYS	3.8
1	B	180	VAL	3.7
1	B	314	LEU	3.6
1	B	140	TYR	3.5
1	A	407	LYS	2.9
1	B	471	TYR	2.8
1	B	157	ASP	2.8
1	B	400	ASP	2.6
1	B	401	GLY	2.5
1	B	166	GLY	2.5
1	B	218	LYS	2.4
1	B	446	VAL	2.4
1	B	479	PHE	2.4
1	B	215	THR	2.3
1	B	156	MET	2.3
1	B	320	GLN	2.2
1	B	243	TYR	2.2
1	B	319	TYR	2.2
1	B	147	TYR	2.1
1	B	450	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PTR	A	321	16/17	-	-	53,59,67,70	16
1	PTR	B	321	16/17	-	-	64,69,77,81	16

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

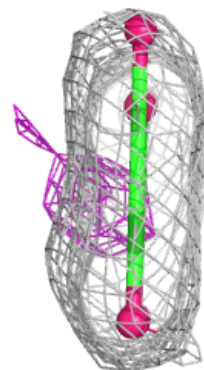
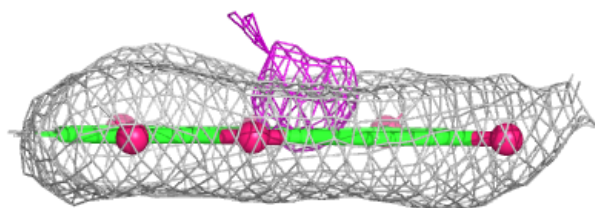
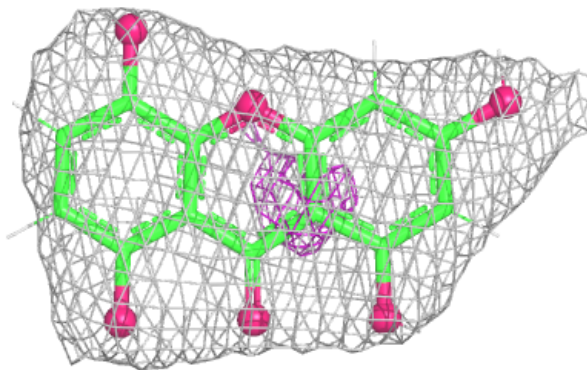
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

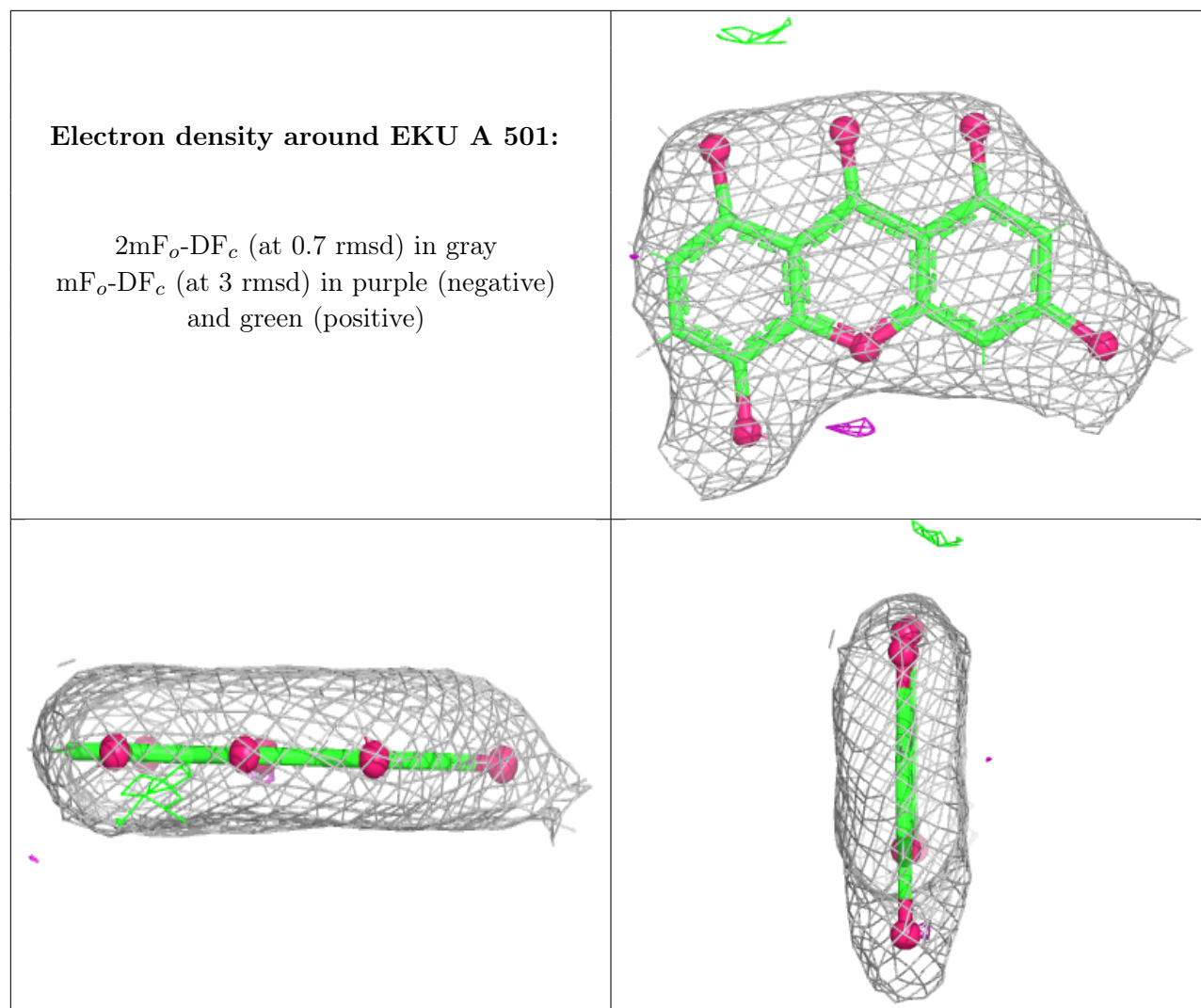
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EKU	B	501	19/19	0.88	0.10	64,74,89,91	0
2	EKU	A	501	19/19	0.93	0.09	34,42,50,53	0

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 EKV B 501:

$2mF_o-DF_c$ (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.