



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 09:11 AM JST

PDB ID : 6LEJ  
Title : Structure of E. coli beta-glucuronidase complex with C6-propyl uronic isofagomine  
Authors : Lin, H.-Y.; Kuo, Y.-H.; Lin, C.-H.  
Deposited on : 2019-11-25  
Resolution : 2.62 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](mailto: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>.

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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 : 2.36  
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

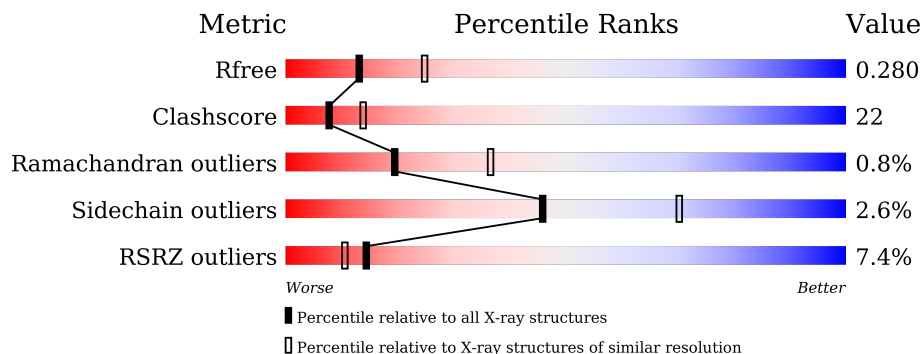
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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  $\geq 3$ , 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	606	
2	B	603	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9600 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 Beta-D-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	600	4809	3055	829	903	22	0	0	0

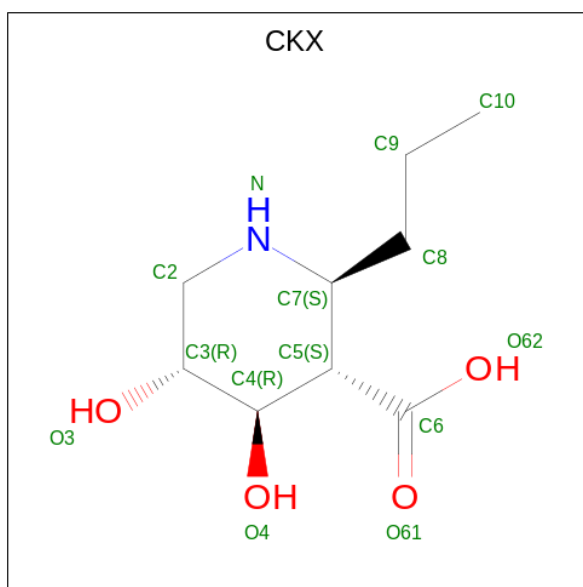
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP W8SYR0
A	-1	SER	-	expression tag	UNP W8SYR0
A	0	HIS	-	expression tag	UNP W8SYR0

- Molecule 2 is a protein called Beta-D-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	587	4698	2987	806	884	21	0	0	0

- Molecule 3 is (2 {S},3 {S},4 {R},5 {R})-4,5-bis(oxidanyl)-2-propyl-piperidine-3-carboxylic acid (three-letter code: CKX) (formula: C<sub>9</sub>H<sub>17</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	9	1	4	0	0
3	B	1	14	9	1	4	0	0

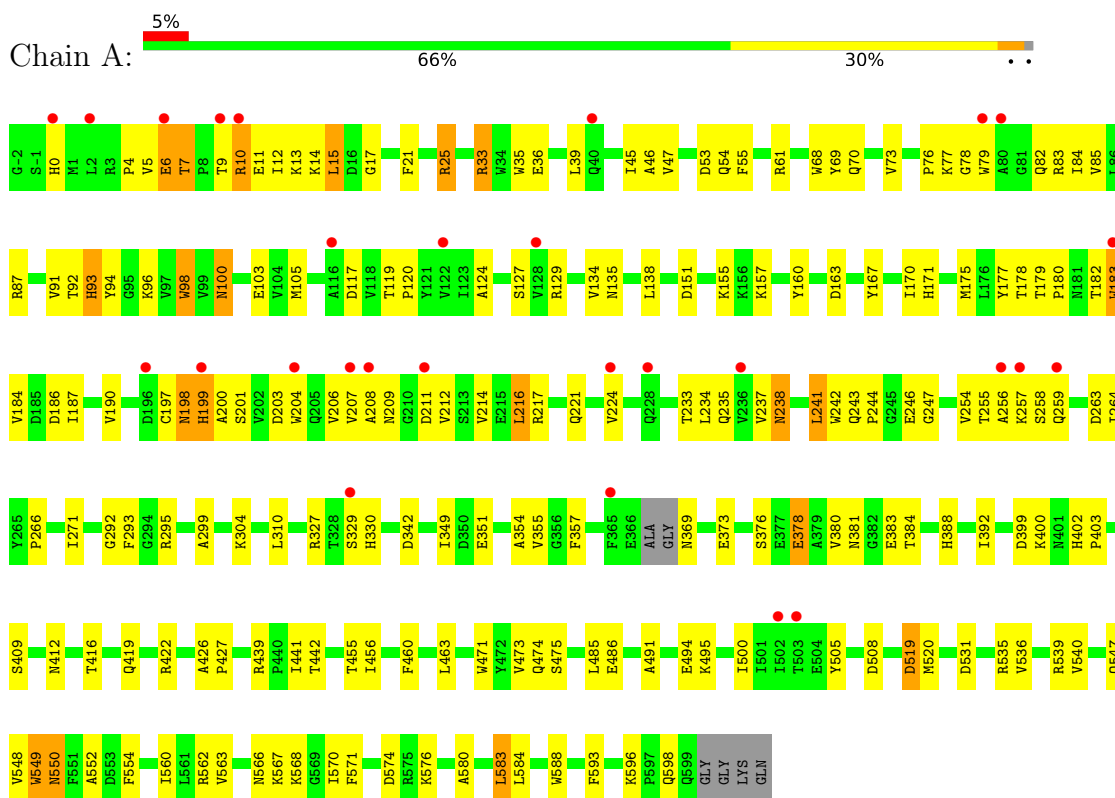
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	40	40	40	0	0
4	B	25	25	25	0	0

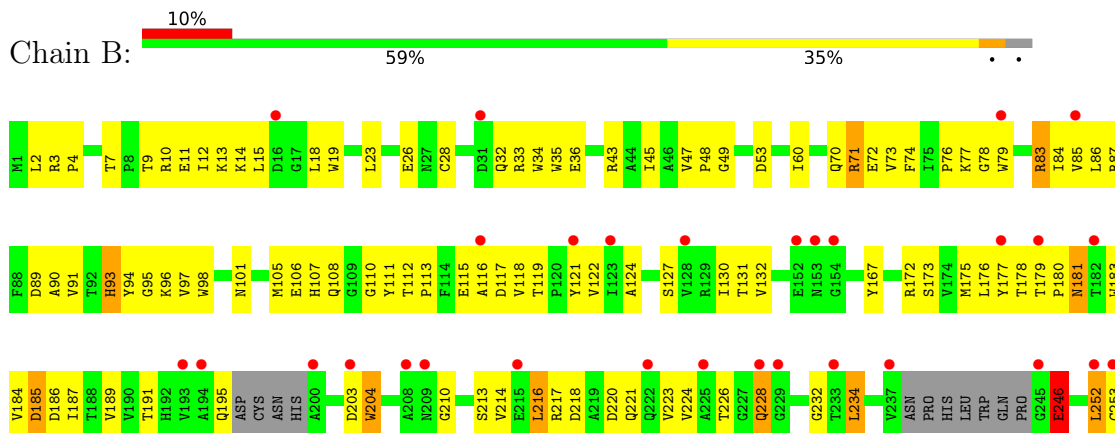
### 3 Residue-property plots

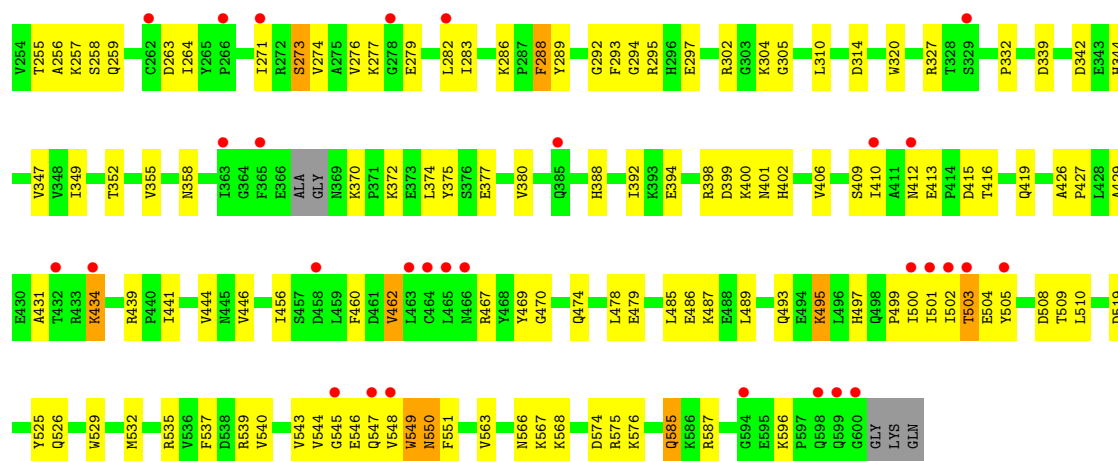
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-D-glucuronidase



- Molecule 2: Beta-D-glucuronidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.69Å 76.55Å 125.43Å 90.00° 124.85° 90.00°	Depositor
Resolution (Å)	29.75 – 2.62 29.75 – 2.62	Depositor EDS
% Data completeness (in resolution range)	80.0 (29.75-2.62) 80.0 (29.75-2.62)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.61Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.237 , 0.280 0.237 , 0.280	Depositor DCC
$R_{free}$ test set	1999 reflections (6.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.8	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9600	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.58	2/4938 (0.0%)	0.80	8/6719 (0.1%)
2	B	0.61	3/4818 (0.1%)	0.87	15/6549 (0.2%)
All	All	0.59	5/9756 (0.1%)	0.84	23/13268 (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
2	B	0	4
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	246	GLU	CB-CG	6.69	1.64	1.52
1	A	6	GLU	CB-CG	6.64	1.64	1.52
2	B	479	GLU	CD-OE1	6.06	1.32	1.25
1	A	98	TRP	CB-CG	-5.42	1.40	1.50
2	B	495	LYS	CD-CE	5.24	1.64	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	252	LEU	CA-CB-CG	12.27	143.52	115.30
2	B	487	LYS	CA-CB-CG	11.72	139.18	113.40
1	A	10	ARG	NE-CZ-NH2	-10.76	114.92	120.30
2	B	487	LYS	CB-CA-C	-10.58	89.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ILE	CG1-CB-CG2	-9.39	90.73	111.40
1	A	10	ARG	NE-CZ-NH1	8.85	124.73	120.30
2	B	487	LYS	CB-CG-CD	8.05	132.52	111.60
1	A	216	LEU	CA-CB-CG	7.96	133.61	115.30
2	B	83	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	10	ARG	CD-NE-CZ	7.27	133.78	123.60
2	B	495	LYS	CA-CB-CG	6.90	128.59	113.40
2	B	234	LEU	CA-CB-CG	6.42	130.06	115.30
2	B	83	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	B	495	LYS	CD-CE-NZ	5.99	125.49	111.70
2	B	462	VAL	CG1-CB-CG2	5.95	120.41	110.90
1	A	549	TRP	C-N-CA	5.78	136.14	121.70
2	B	83	ARG	CG-CD-NE	5.77	123.91	111.80
2	B	487	LYS	CG-CD-CE	-5.72	94.74	111.90
2	B	487	LYS	N-CA-CB	5.68	120.83	110.60
2	B	549	TRP	C-N-CA	5.52	135.50	121.70
1	A	519	ASP	CB-CG-OD2	-5.37	113.46	118.30
2	B	185	ASP	C-N-CA	5.13	134.51	121.70
1	A	6	GLU	C-N-CA	5.11	134.47	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	ASN	Peptide
1	A	199	HIS	Peptide
2	B	246	GLU	Peptide
2	B	273	SER	Peptide
2	B	293	PHE	Peptide
2	B	503	THR	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4809	0	4585	175	0
2	B	4698	0	4494	241	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	0	1	0
3	B	14	0	0	0	0
4	A	40	0	0	5	0
4	B	25	0	0	12	0
All	All	9600	0	9079	406	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (406) 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)
2:B:274:VAL:HG21	2:B:283:ILE:HA	1.28	1.14
2:B:289:TYR:CE1	2:B:596:LYS:HE3	1.86	1.11
1:A:216:LEU:HD12	1:A:224:VAL:HG13	1.33	1.10
2:B:327:ARG:HH21	2:B:504:GLU:HG2	1.15	1.05
2:B:83:ARG:NH2	2:B:183:TRP:O	1.91	1.04
1:A:381:ASN:HD21	1:A:383:GLU:HB2	1.22	1.01
1:A:10:ARG:HG3	1:A:11:GLU:H	1.22	1.00
1:A:10:ARG:NH1	2:B:74:PHE:HB2	1.75	1.00
1:A:10:ARG:HH12	2:B:74:PHE:CB	1.76	0.98
2:B:327:ARG:NH2	2:B:504:GLU:HG2	1.77	0.98
1:A:10:ARG:NH1	2:B:74:PHE:CB	2.29	0.95
2:B:115:GLU:HB2	2:B:177:TYR:OH	1.66	0.94
2:B:85:VAL:HG23	2:B:117:ASP:HA	1.45	0.94
2:B:204:TRP:CZ2	2:B:234:LEU:HD22	2.03	0.94
1:A:77:LYS:HA	1:A:124:ALA:HB1	1.47	0.93
2:B:543:VAL:O	2:B:596:LYS:NZ	2.00	0.93
2:B:83:ARG:HH22	2:B:184:VAL:HA	1.34	0.93
2:B:289:TYR:HE1	2:B:596:LYS:HE3	1.32	0.90
1:A:216:LEU:CD1	1:A:224:VAL:HG13	2.04	0.87
1:A:7:THR:O	1:A:10:ARG:NH2	2.08	0.87
2:B:509:THR:HG21	2:B:526:GLN:HB2	1.54	0.87
2:B:85:VAL:HG13	2:B:177:TYR:CE2	2.09	0.86
1:A:33:ARG:HG3	1:A:36:GLU:HG3	1.58	0.86
2:B:274:VAL:HG11	2:B:282:LEU:O	1.76	0.85
2:B:412:ASN:HA	2:B:444:VAL:HG23	1.57	0.85
1:A:197:CYS:O	1:A:238:ASN:ND2	2.11	0.84
2:B:85:VAL:HG23	2:B:117:ASP:CA	2.06	0.84
1:A:10:ARG:HH11	2:B:74:PHE:HB2	1.43	0.82
2:B:253:CYS:SG	2:B:264:ILE:HD11	2.21	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HB2	1:A:349:ILE:HB	1.64	0.80
1:A:531:ASP:OD1	4:A:801:HOH:O	1.99	0.79
2:B:204:TRP:HZ2	2:B:234:LEU:HD22	1.47	0.79
2:B:566:ASN:HD21	2:B:568:LYS:HB2	1.47	0.79
1:A:83:ARG:NH2	1:A:183:TRP:HA	1.98	0.78
2:B:409:SER:O	4:B:801:HOH:O	2.00	0.78
2:B:327:ARG:HH21	2:B:504:GLU:CG	1.97	0.77
2:B:83:ARG:HH12	2:B:184:VAL:HG13	1.49	0.77
2:B:85:VAL:HG13	2:B:177:TYR:CD2	2.20	0.77
2:B:288:PHE:HD2	2:B:289:TYR:N	1.81	0.77
2:B:97:VAL:HG12	2:B:105:MET:HB2	1.65	0.76
1:A:299:ALA:HB2	1:A:310:LEU:HD11	1.68	0.76
1:A:381:ASN:ND2	1:A:383:GLU:HB2	1.99	0.75
1:A:10:ARG:HB2	1:A:10:ARG:CZ	2.16	0.75
2:B:3:ARG:HD2	2:B:4:PRO:HD2	1.69	0.75
1:A:203:ASP:HB3	1:A:233:THR:HB	1.69	0.75
2:B:83:ARG:NH2	2:B:184:VAL:HA	2.02	0.75
2:B:273:SER:OG	2:B:274:VAL:HG23	1.85	0.74
2:B:26:GLU:OE1	2:B:26:GLU:N	2.16	0.74
1:A:491:ALA:O	1:A:494:GLU:HG2	1.88	0.74
2:B:289:TYR:HE1	2:B:596:LYS:CE	2.01	0.74
2:B:213:SER:HA	2:B:228:GLN:HB2	1.70	0.73
1:A:79:TRP:CD2	1:A:178:THR:HG21	2.24	0.73
1:A:33:ARG:HB2	1:A:35:TRP:CE2	2.24	0.73
1:A:9:THR:HG21	1:A:180:PRO:HD3	1.70	0.73
2:B:107:HIS:O	4:B:802:HOH:O	2.07	0.72
1:A:416:THR:HG21	1:A:456:ILE:HG12	1.70	0.72
1:A:83:ARG:HG3	1:A:179:THR:HG23	1.69	0.72
2:B:71:ARG:NH1	2:B:72:GLU:O	2.23	0.71
1:A:10:ARG:CG	1:A:11:GLU:H	1.95	0.70
1:A:0:HIS:HB3	1:A:186:ASP:HB2	1.72	0.70
2:B:255:THR:HG22	2:B:264:ILE:HD13	1.72	0.70
1:A:216:LEU:HD12	1:A:224:VAL:CG1	2.19	0.70
2:B:355:VAL:HG12	2:B:412:ASN:HB3	1.73	0.70
2:B:15:LEU:HD11	2:B:173:SER:HA	1.74	0.70
2:B:85:VAL:CG1	2:B:177:TYR:CE2	2.74	0.70
2:B:220:ASP:HB2	4:B:813:HOH:O	1.91	0.70
1:A:369:ASN:N	4:A:805:HOH:O	2.24	0.69
1:A:7:THR:HG21	1:A:264:ILE:O	1.92	0.69
1:A:87:ARG:HB3	1:A:175:MET:HE1	1.75	0.69
2:B:274:VAL:CG2	2:B:283:ILE:HA	2.15	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:LEU:HD23	2:B:224:VAL:CG1	2.23	0.68
2:B:216:LEU:N	2:B:252:LEU:HD13	2.08	0.68
1:A:151:ASP:OD1	1:A:157:LYS:NZ	2.28	0.67
2:B:486:GLU:OE1	2:B:539:ARG:NH2	2.26	0.67
2:B:320:TRP:O	4:B:803:HOH:O	2.13	0.66
1:A:560:ILE:O	4:A:802:HOH:O	2.12	0.66
1:A:155:LYS:NZ	4:A:808:HOH:O	2.28	0.66
2:B:289:TYR:CD1	2:B:596:LYS:HB2	2.31	0.66
1:A:46:ALA:H	1:A:54:GLN:HE22	1.44	0.66
2:B:83:ARG:CZ	2:B:179:THR:HG23	2.26	0.66
1:A:17:GLY:HA2	1:A:47:VAL:H	1.61	0.65
1:A:78:GLY:HA3	2:B:78:GLY:HA3	1.77	0.65
2:B:85:VAL:HG23	2:B:117:ASP:N	2.11	0.65
1:A:563:VAL:O	1:A:567:LYS:NZ	2.30	0.64
2:B:96:LYS:HD3	2:B:106:GLU:HB2	1.79	0.64
1:A:560:ILE:HB	4:A:802:HOH:O	1.97	0.64
2:B:83:ARG:NH2	2:B:179:THR:HG23	2.13	0.64
2:B:112:THR:HG21	2:B:394:GLU:HB3	1.79	0.64
2:B:283:ILE:O	2:B:286:LYS:HB3	1.98	0.64
1:A:211:ASP:HB2	1:A:257:LYS:HG3	1.80	0.63
2:B:563:VAL:O	2:B:567:LYS:NZ	2.31	0.63
1:A:540:VAL:O	1:A:596:LYS:NZ	2.31	0.63
1:A:237:VAL:HG12	1:A:238:ASN:H	1.62	0.63
2:B:532:MET:HB2	2:B:535:ARG:HH21	1.64	0.63
2:B:532:MET:HA	2:B:535:ARG:HE	1.64	0.63
2:B:288:PHE:HD2	2:B:289:TYR:H	1.45	0.62
1:A:505:TYR:CZ	1:A:548:VAL:HG12	2.34	0.62
2:B:210:GLY:HA3	2:B:258:SER:OG	1.99	0.62
1:A:92:THR:HG1	1:A:171:HIS:HD1	1.47	0.62
2:B:289:TYR:HE2	2:B:546:GLU:HG2	1.65	0.62
2:B:510:LEU:HD23	2:B:510:LEU:H	1.63	0.62
2:B:279:GLU:OE1	2:B:493:GLN:NE2	2.24	0.61
2:B:85:VAL:HG13	2:B:177:TYR:CZ	2.35	0.61
1:A:92:THR:OG1	1:A:171:HIS:ND1	2.32	0.61
1:A:354:ALA:HB1	1:A:357:PHE:HE1	1.66	0.61
1:A:566:ASN:OD1	1:A:568:LYS:HB2	2.00	0.61
2:B:410:ILE:HD12	2:B:460:PHE:HE1	1.66	0.61
2:B:375:TYR:HA	2:B:380:VAL:HG13	1.83	0.61
1:A:184:VAL:HG13	1:A:207:VAL:HG22	1.83	0.61
2:B:574:ASP:OD1	2:B:576:LYS:HE3	2.01	0.61
1:A:182:THR:HA	1:A:209:ASN:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:O	1:A:127:SER:HA	2.01	0.60
1:A:441:ILE:HG22	1:A:460:PHE:HD2	1.65	0.60
2:B:502:ILE:HD12	2:B:537:PHE:CE2	2.36	0.60
1:A:96:LYS:HE3	1:A:98:TRP:HZ2	1.67	0.60
2:B:79:TRP:HB3	2:B:84:ILE:HD11	1.82	0.60
2:B:347:VAL:HG13	2:B:406:VAL:HG21	1.83	0.60
1:A:6:GLU:HG2	1:A:10:ARG:HD2	1.83	0.60
2:B:15:LEU:HD11	2:B:173:SER:CA	2.31	0.59
2:B:549:TRP:HD1	2:B:568:LYS:HD3	1.68	0.59
2:B:327:ARG:NH2	2:B:503:THR:O	2.36	0.59
2:B:310:LEU:HD11	2:B:575:ARG:NH1	2.18	0.59
2:B:314:ASP:OD1	2:B:551:PHE:HE2	1.84	0.59
2:B:2:LEU:HD23	2:B:3:ARG:N	2.16	0.58
2:B:181:ASN:O	2:B:181:ASN:ND2	2.35	0.58
2:B:497:HIS:O	4:B:804:HOH:O	2.16	0.58
1:A:244:PRO:HB2	1:A:593:PHE:HE1	1.68	0.58
2:B:485:LEU:O	2:B:489:LEU:HG	2.03	0.58
2:B:276:VAL:HG21	2:B:462:VAL:CG2	2.34	0.58
1:A:7:THR:HG22	1:A:266:PRO:HD3	1.84	0.58
2:B:97:VAL:CG1	2:B:105:MET:HB2	2.33	0.58
1:A:94:TYR:HB3	1:A:135:ASN:HB3	1.84	0.58
2:B:370:LYS:O	2:B:372:LYS:HE3	2.03	0.58
2:B:355:VAL:CG1	2:B:412:ASN:HB3	2.34	0.57
2:B:462:VAL:HG22	2:B:499:PRO:HD2	1.84	0.57
2:B:566:ASN:ND2	2:B:568:LYS:HB2	2.16	0.57
2:B:32:GLN:HE21	2:B:34:TRP:HE1	1.53	0.57
2:B:352:THR:HG22	4:B:801:HOH:O	2.03	0.57
2:B:470:GLY:H	2:B:474:GLN:HB2	1.68	0.57
1:A:293:PHE:HE1	1:A:570:ILE:HG13	1.70	0.57
1:A:10:ARG:HG3	1:A:11:GLU:N	2.06	0.57
1:A:299:ALA:CB	1:A:310:LEU:HD11	2.34	0.57
2:B:486:GLU:CD	2:B:539:ARG:HH21	2.07	0.56
2:B:218:ASP:O	2:B:221:GLN:HG3	2.05	0.56
2:B:502:ILE:HD12	2:B:537:PHE:CZ	2.41	0.56
2:B:398:ARG:NH1	2:B:399:ASP:OD2	2.37	0.56
2:B:310:LEU:HD21	2:B:575:ARG:HH12	1.70	0.56
1:A:45:ILE:HD13	1:A:55:PHE:HZ	1.70	0.56
2:B:416:THR:HG21	2:B:456:ILE:HG12	1.88	0.56
1:A:76:PRO:HD2	1:A:79:TRP:CZ3	2.40	0.56
1:A:566:ASN:HD21	1:A:568:LYS:HD2	1.69	0.56
2:B:33:ARG:NH2	2:B:36:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:HIS:NE2	4:B:808:HOH:O	2.33	0.56
1:A:10:ARG:HH12	2:B:74:PHE:HB3	1.69	0.55
2:B:83:ARG:NH2	2:B:179:THR:CG2	2.69	0.55
2:B:183:TRP:CE3	2:B:256:ALA:HB2	2.41	0.55
2:B:32:GLN:NE2	2:B:34:TRP:HE1	2.04	0.55
2:B:113:PRO:HD2	2:B:398:ARG:HD3	1.87	0.55
1:A:21:PHE:HD2	1:A:69:TYR:CE1	2.24	0.55
1:A:45:ILE:HD13	1:A:55:PHE:CZ	2.42	0.55
1:A:10:ARG:NH1	2:B:74:PHE:CG	2.68	0.55
1:A:342:ASP:CG	1:A:403:PRO:HD2	2.27	0.55
2:B:183:TRP:HB3	2:B:263:ASP:OD2	2.07	0.55
1:A:550:ASN:OD1	1:A:554:PHE:CE2	2.59	0.55
2:B:277:LYS:HG3	2:B:282:LEU:CD1	2.37	0.55
1:A:199:HIS:CG	1:A:200:ALA:H	2.24	0.55
1:A:293:PHE:CD1	1:A:548:VAL:HG22	2.42	0.55
2:B:288:PHE:CD2	2:B:289:TYR:N	2.70	0.55
2:B:216:LEU:HA	2:B:252:LEU:HA	1.88	0.54
1:A:183:TRP:HB3	1:A:208:ALA:HB3	1.89	0.54
2:B:183:TRP:CZ2	2:B:187:ILE:HD11	2.42	0.54
2:B:398:ARG:NH2	4:B:805:HOH:O	2.39	0.54
1:A:77:LYS:C	1:A:79:TRP:H	2.10	0.54
2:B:73:VAL:O	2:B:127:SER:HA	2.07	0.54
2:B:89:ASP:OD1	2:B:175:MET:HE2	2.08	0.54
2:B:23:LEU:HD11	2:B:60:ILE:HG12	1.88	0.54
2:B:111:TYR:HB2	2:B:332:PRO:HD2	1.88	0.54
2:B:204:TRP:CE2	2:B:234:LEU:HD22	2.43	0.54
1:A:203:ASP:OD1	1:A:204:TRP:N	2.40	0.54
1:A:486:GLU:OE1	1:A:539:ARG:NH2	2.37	0.54
1:A:583:LEU:HD23	1:A:584:LEU:HD12	1.89	0.54
2:B:501:ILE:HG23	2:B:545:GLY:HA3	1.90	0.54
2:B:543:VAL:HG23	2:B:596:LYS:NZ	2.23	0.54
2:B:191:THR:HG21	2:B:271:ILE:HA	1.91	0.53
2:B:97:VAL:HG23	2:B:132:VAL:HG22	1.90	0.53
2:B:246:GLU:HB3	2:B:344:HIS:O	2.07	0.53
1:A:4:PRO:HG2	1:A:175:MET:HE3	1.90	0.53
2:B:13:LYS:HG3	2:B:15:LEU:HD13	1.91	0.53
2:B:413:GLU:HB3	2:B:446:VAL:HB	1.90	0.53
2:B:2:LEU:HD23	2:B:3:ARG:H	1.74	0.53
2:B:70:GLN:NE2	2:B:131:THR:OG1	2.30	0.53
2:B:87:ARG:N	2:B:177:TYR:HE1	2.07	0.53
2:B:85:VAL:CG1	2:B:177:TYR:CD2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ASN:HA	2:B:444:VAL:CG2	2.34	0.52
2:B:327:ARG:CZ	2:B:503:THR:O	2.57	0.52
1:A:241:LEU:O	1:A:243:GLN:HG2	2.10	0.52
1:A:399:ASP:HA	1:A:402:HIS:HD2	1.74	0.52
2:B:431:ALA:O	2:B:434:LYS:HB2	2.09	0.52
2:B:587:ARG:NE	4:B:812:HOH:O	2.42	0.52
2:B:94:TYR:CD1	2:B:108:GLN:HG2	2.44	0.52
1:A:87:ARG:HD3	1:A:175:MET:HE1	1.90	0.52
1:A:199:HIS:CG	1:A:200:ALA:N	2.78	0.52
2:B:217:ARG:HB3	2:B:221:GLN:HA	1.92	0.52
1:A:163:ASP:OD1	1:A:562:ARG:NH2	2.43	0.51
1:A:83:ARG:NH2	1:A:179:THR:OG1	2.44	0.51
1:A:486:GLU:CD	1:A:539:ARG:HH21	2.11	0.51
2:B:183:TRP:HZ2	2:B:187:ILE:HD11	1.74	0.51
2:B:314:ASP:OD1	2:B:551:PHE:CE2	2.63	0.51
2:B:388:HIS:CD2	2:B:392:ILE:HD11	2.46	0.51
1:A:258:SER:OG	1:A:259:GLN:N	2.43	0.51
2:B:93:HIS:H	2:B:110:GLY:CA	2.23	0.51
1:A:580:ALA:O	1:A:584:LEU:HD13	2.11	0.51
2:B:277:LYS:HG3	2:B:282:LEU:HD11	1.92	0.50
2:B:83:ARG:NE	2:B:179:THR:HG23	2.27	0.50
2:B:441:ILE:HG22	2:B:460:PHE:HD1	1.77	0.50
1:A:199:HIS:CE1	1:A:200:ALA:HB3	2.46	0.50
2:B:279:GLU:C	2:B:499:PRO:HG3	2.31	0.50
1:A:241:LEU:HB2	1:A:271:ILE:O	2.12	0.50
2:B:18:LEU:HA	2:B:45:ILE:O	2.10	0.50
2:B:374:LEU:HD22	2:B:415:ASP:HB3	1.93	0.50
1:A:204:TRP:CZ2	1:A:206:VAL:HG23	2.46	0.50
1:A:473:VAL:HG23	1:A:474:GLN:OE1	2.12	0.50
2:B:549:TRP:HA	2:B:549:TRP:CE3	2.45	0.50
1:A:100:ASN:OD1	1:A:129:ARG:NH2	2.45	0.49
2:B:462:VAL:HG13	2:B:499:PRO:O	2.11	0.49
2:B:467:ARG:HG3	2:B:467:ARG:HH11	1.77	0.49
1:A:237:VAL:HG12	1:A:238:ASN:N	2.26	0.49
1:A:355:VAL:HG12	1:A:412:ASN:HB3	1.93	0.49
2:B:2:LEU:HD12	2:B:401:ASN:HD22	1.78	0.49
2:B:94:TYR:HD1	2:B:108:GLN:HG2	1.77	0.49
2:B:3:ARG:HD2	2:B:4:PRO:CD	2.42	0.49
1:A:83:ARG:NH1	1:A:183:TRP:CE2	2.81	0.49
2:B:358:ASN:HA	2:B:415:ASP:HB2	1.95	0.49
1:A:91:VAL:HG22	1:A:170:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HG3	1:A:105:MET:O	2.12	0.49
1:A:10:ARG:O	1:A:178:THR:OG1	2.20	0.49
2:B:274:VAL:HG21	2:B:283:ILE:HD12	1.94	0.49
2:B:563:VAL:O	2:B:563:VAL:HG23	2.13	0.49
1:A:96:LYS:HE3	1:A:98:TRP:CZ2	2.48	0.48
1:A:214:VAL:HG21	1:A:233:THR:CG2	2.43	0.48
1:A:36:GLU:O	1:A:129:ARG:NH2	2.37	0.48
2:B:327:ARG:HB2	2:B:349:ILE:HB	1.95	0.48
2:B:339:ASP:O	2:B:342:ASP:HB2	2.12	0.48
2:B:2:LEU:CD1	2:B:401:ASN:HD22	2.26	0.48
1:A:549:TRP:HD1	1:A:568:LYS:HD3	1.78	0.48
1:A:233:THR:HG22	1:A:233:THR:O	2.14	0.48
1:A:584:LEU:HD23	1:A:588:TRP:CH2	2.48	0.48
1:A:33:ARG:HB2	1:A:35:TRP:NE1	2.28	0.48
1:A:12:ILE:HD12	2:B:12:ILE:HG13	1.96	0.48
2:B:79:TRP:CD2	2:B:178:THR:HG21	2.48	0.48
2:B:84:ILE:H	2:B:119:THR:HB	1.78	0.48
2:B:467:ARG:HD3	2:B:469:TYR:HE2	1.79	0.48
2:B:246:GLU:HB3	2:B:344:HIS:C	2.35	0.47
1:A:292:GLY:O	1:A:547:GLN:HA	2.14	0.47
1:A:25:ARG:HH22	1:A:155:LYS:HD3	1.77	0.47
2:B:85:VAL:CG2	2:B:117:ASP:HA	2.32	0.47
2:B:74:PHE:CE1	2:B:127:SER:HB2	2.50	0.47
2:B:118:VAL:O	2:B:122:VAL:HG22	2.14	0.47
2:B:14:LYS:HD3	2:B:176:LEU:HG	1.96	0.47
2:B:15:LEU:HD11	2:B:173:SER:CB	2.43	0.47
1:A:5:VAL:HG22	1:A:6:GLU:N	2.28	0.47
1:A:91:VAL:CG1	1:A:134:VAL:HG22	2.44	0.47
2:B:19:TRP:CD1	2:B:47:VAL:HG21	2.50	0.47
2:B:500:ILE:O	2:B:543:VAL:HA	2.15	0.47
1:A:11:GLU:HA	1:A:177:TYR:HA	1.96	0.47
1:A:246:GLU:OE2	1:A:246:GLU:N	2.48	0.47
2:B:118:VAL:CG2	2:B:121:TYR:HB2	2.45	0.47
2:B:210:GLY:HA3	2:B:258:SER:CB	2.45	0.47
1:A:373:GLU:HB3	1:A:376:SER:HB2	1.97	0.46
2:B:85:VAL:HG12	2:B:177:TYR:O	2.15	0.46
1:A:234:LEU:HD23	1:A:235:GLN:N	2.30	0.46
2:B:90:ALA:HB3	2:B:172:ARG:HB2	1.97	0.46
2:B:118:VAL:O	2:B:118:VAL:HG22	2.15	0.46
2:B:292:GLY:O	2:B:547:GLN:HA	2.16	0.46
2:B:10:ARG:HG3	2:B:11:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:TRP:CD1	2:B:183:TRP:C	2.88	0.46
1:A:485:LEU:HG	1:A:536:VAL:HG11	1.98	0.46
2:B:70:GLN:HA	2:B:130:ILE:O	2.15	0.46
1:A:295:ARG:O	1:A:329:SER:HB2	2.16	0.46
2:B:478:LEU:HD11	2:B:529:TRP:HD1	1.80	0.46
1:A:330:HIS:NE2	3:A:701:CKX:O3	2.48	0.46
1:A:409:SER:HB2	1:A:442:THR:HG23	1.97	0.46
2:B:282:LEU:HA	2:B:286:LYS:O	2.16	0.46
1:A:574:ASP:OD1	1:A:576:LYS:HE3	2.17	0.46
2:B:183:TRP:HE3	2:B:256:ALA:HB2	1.81	0.45
2:B:493:GLN:O	2:B:497:HIS:N	2.27	0.45
1:A:380:VAL:HG13	1:A:384:THR:HG21	1.98	0.45
2:B:13:LYS:HE3	2:B:15:LEU:HD13	1.98	0.45
2:B:310:LEU:HD11	2:B:575:ARG:HH12	1.79	0.45
2:B:203:ASP:OD1	2:B:232:GLY:O	2.34	0.45
2:B:86:LEU:C	2:B:177:TYR:HE1	2.19	0.45
2:B:189:VAL:HA	2:B:203:ASP:O	2.16	0.45
2:B:510:LEU:HD23	2:B:510:LEU:N	2.31	0.45
1:A:184:VAL:HG23	1:A:263:ASP:OD2	2.17	0.45
1:A:187:ILE:HD11	1:A:254:VAL:HG21	1.98	0.45
2:B:95:GLY:N	4:B:802:HOH:O	2.49	0.45
1:A:53:ASP:OD2	1:A:61:ARG:NH1	2.50	0.45
1:A:351:GLU:OE2	1:A:409:SER:OG	2.26	0.45
2:B:15:LEU:HG	2:B:48:PRO:HG3	1.97	0.45
2:B:113:PRO:CD	2:B:398:ARG:HD3	2.47	0.45
1:A:378:GLU:H	1:A:378:GLU:HG3	1.39	0.45
1:A:182:THR:OG1	1:A:209:ASN:O	2.33	0.45
2:B:76:PRO:O	2:B:124:ALA:HB1	2.16	0.45
2:B:289:TYR:HA	2:B:544:VAL:O	2.17	0.45
1:A:10:ARG:CG	1:A:11:GLU:N	2.73	0.45
1:A:21:PHE:HA	1:A:68:TRP:O	2.16	0.45
1:A:494:GLU:HG3	1:A:495:LYS:N	2.32	0.45
2:B:167:TYR:HB2	2:B:304:LYS:HD2	1.98	0.44
2:B:540:VAL:HG23	2:B:543:VAL:HG22	1.99	0.44
1:A:98:TRP:CD1	1:A:103:GLU:HB3	2.52	0.44
1:A:535:ARG:O	1:A:539:ARG:HG3	2.17	0.44
1:A:212:VAL:HA	1:A:255:THR:O	2.17	0.44
1:A:562:ARG:NH2	1:A:566:ASN:HD22	2.15	0.44
2:B:410:ILE:HD11	2:B:429:ALA:HA	1.99	0.44
1:A:190:VAL:O	1:A:201:SER:HA	2.18	0.44
2:B:96:LYS:HG2	2:B:98:TRP:CH2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:SER:HA	2:B:228:GLN:CB	2.40	0.44
2:B:85:VAL:HG22	2:B:177:TYR:OH	2.17	0.44
2:B:214:VAL:O	2:B:226:THR:HG23	2.17	0.44
2:B:217:ARG:HG2	2:B:223:VAL:HA	1.98	0.44
1:A:552:ALA:HA	1:A:571:PHE:O	2.18	0.44
2:B:327:ARG:NH1	2:B:327:ARG:HG2	2.33	0.44
1:A:9:THR:HG21	1:A:180:PRO:CD	2.46	0.44
1:A:211:ASP:O	1:A:256:ALA:HA	2.18	0.44
1:A:4:PRO:HG2	1:A:175:MET:CE	2.47	0.44
1:A:98:TRP:NE1	1:A:103:GLU:HB3	2.32	0.44
2:B:185:ASP:HB3	2:B:186:ASP:H	1.59	0.44
1:A:400:LYS:O	1:A:439:ARG:NH2	2.49	0.44
2:B:26:GLU:HG2	2:B:28:CYS:SG	2.57	0.44
2:B:115:GLU:HB2	2:B:177:TYR:HH	1.77	0.44
1:A:463:LEU:HD23	1:A:500:ILE:HG12	2.00	0.43
2:B:85:VAL:HG13	2:B:177:TYR:CG	2.53	0.43
2:B:508:ASP:OD2	2:B:568:LYS:NZ	2.36	0.43
1:A:426:ALA:HB3	1:A:427:PRO:HD3	2.01	0.43
2:B:101:ASN:N	4:B:809:HOH:O	2.51	0.43
1:A:6:GLU:HG2	1:A:10:ARG:CD	2.47	0.43
2:B:105:MET:HE3	2:B:115:GLU:HA	2.01	0.43
1:A:471:TRP:O	1:A:475:SER:OG	2.28	0.43
2:B:374:LEU:CD2	2:B:415:ASP:HB3	2.49	0.43
2:B:426:ALA:HB3	2:B:427:PRO:HD3	2.00	0.43
2:B:519:ASP:O	2:B:525:TYR:HB2	2.18	0.43
1:A:14:LYS:HZ1	1:A:73:VAL:HG21	1.84	0.43
2:B:49:GLY:HA2	2:B:305:GLY:HA3	2.00	0.43
2:B:87:ARG:HB2	2:B:177:TYR:CE1	2.53	0.43
2:B:216:LEU:HD23	2:B:224:VAL:HG13	2.01	0.43
1:A:9:THR:HG21	1:A:179:THR:HA	2.00	0.43
2:B:76:PRO:HD2	2:B:79:TRP:CE3	2.54	0.43
1:A:36:GLU:C	1:A:129:ARG:HH12	2.22	0.42
1:A:53:ASP:OD1	1:A:167:TYR:HE1	2.01	0.42
2:B:53:ASP:OD2	2:B:53:ASP:N	2.52	0.42
2:B:327:ARG:NE	2:B:503:THR:HB	2.34	0.42
1:A:117:ASP:HB2	1:A:183:TRP:HH2	1.84	0.42
2:B:505:TYR:CZ	2:B:548:VAL:HG12	2.54	0.42
1:A:76:PRO:HA	2:B:10:ARG:NH2	2.35	0.42
1:A:167:TYR:HB2	1:A:304:LYS:HD2	2.01	0.42
1:A:574:ASP:N	1:A:574:ASP:OD2	2.47	0.42
2:B:14:LYS:HD2	2:B:73:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:VAL:HG23	2:B:116:ALA:C	2.39	0.42
1:A:9:THR:C	1:A:10:ARG:HH21	2.22	0.42
1:A:85:VAL:HB	1:A:177:TYR:CE2	2.54	0.42
2:B:71:ARG:HD3	2:B:73:VAL:HG22	2.01	0.42
1:A:9:THR:HA	2:B:77:LYS:NZ	2.34	0.42
1:A:119:THR:HG22	1:A:120:PRO:HD3	2.01	0.42
2:B:255:THR:CG2	2:B:264:ILE:HD13	2.45	0.42
2:B:327:ARG:HG2	2:B:327:ARG:HH11	1.85	0.42
1:A:14:LYS:NZ	1:A:73:VAL:HG21	2.34	0.42
1:A:15:LEU:C	1:A:17:GLY:H	2.23	0.42
1:A:77:LYS:O	1:A:79:TRP:N	2.53	0.42
1:A:471:TRP:CZ2	1:A:508:ASP:HB2	2.55	0.42
1:A:83:ARG:HG3	1:A:179:THR:O	2.20	0.41
1:A:388:HIS:O	1:A:392:ILE:HD12	2.21	0.41
1:A:471:TRP:CZ3	1:A:520:MET:HB3	2.55	0.41
2:B:180:PRO:HG2	2:B:263:ASP:HB2	2.00	0.41
1:A:598:GLN:HG2	1:A:598:GLN:O	2.20	0.41
2:B:91:VAL:O	2:B:110:GLY:HA2	2.19	0.41
1:A:79:TRP:O	1:A:82:GLN:HB2	2.20	0.41
1:A:381:ASN:ND2	1:A:383:GLU:N	2.69	0.41
2:B:118:VAL:HG23	2:B:121:TYR:HB2	2.01	0.41
2:B:177:TYR:N	2:B:177:TYR:CD1	2.88	0.41
2:B:84:ILE:HB	2:B:122:VAL:HG21	2.01	0.41
2:B:294:GLY:O	2:B:550:ASN:HA	2.20	0.41
1:A:39:LEU:H	1:A:70:GLN:NE2	2.18	0.41
2:B:15:LEU:CG	2:B:48:PRO:HG3	2.51	0.41
2:B:410:ILE:HD12	2:B:460:PHE:CE1	2.51	0.41
1:A:13:LYS:HE3	1:A:15:LEU:HG	2.02	0.41
2:B:19:TRP:CG	2:B:47:VAL:HG21	2.56	0.41
1:A:182:THR:HG23	1:A:263:ASP:HB2	2.03	0.41
1:A:422:ARG:HB2	1:A:455:THR:HG22	2.02	0.41
1:A:471:TRP:CZ3	1:A:520:MET:HE3	2.55	0.41
2:B:35:TRP:HD1	2:B:101:ASN:HA	1.86	0.41
2:B:388:HIS:O	2:B:392:ILE:HD12	2.21	0.41
1:A:93:HIS:CD2	1:A:138:LEU:HD21	2.56	0.41
2:B:585:GLN:HB2	4:B:803:HOH:O	2.20	0.41
1:A:83:ARG:CG	1:A:179:THR:HG23	2.45	0.40
1:A:242:TRP:CD1	1:A:247:GLY:HA2	2.56	0.40
2:B:89:ASP:OD1	2:B:175:MET:CE	2.69	0.40
2:B:9:THR:HG23	2:B:179:THR:HA	2.04	0.40
1:A:98:TRP:N	1:A:98:TRP:CE3	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:HIS:H	2:B:110:GLY:HA2	1.85	0.40
1:A:96:LYS:HB3	1:A:96:LYS:HE2	1.84	0.40
1:A:217:ARG:HB3	1:A:221:GLN:HA	2.02	0.40
2:B:74:PHE:CD1	2:B:127:SER:HB2	2.56	0.40
2:B:228:GLN:NE2	2:B:257:LYS:HZ1	2.20	0.40
2:B:297:GLU:O	2:B:304:LYS:HG2	2.22	0.40
2:B:400:LYS:O	2:B:439:ARG:NH1	2.49	0.40
2:B:478:LEU:HD11	2:B:529:TRP:CD1	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	596/606 (98%)	548 (92%)	43 (7%)	5 (1%)	19	36
2	B	579/603 (96%)	529 (91%)	46 (8%)	4 (1%)	22	41
All	All	1175/1209 (97%)	1077 (92%)	89 (8%)	9 (1%)	19	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	7	THR
2	B	550	ASN
1	A	93	HIS
2	B	93	HIS
1	A	100	ASN
1	A	550	ASN
2	B	259	GLN
1	A	7	THR
1	A	33	ARG

### 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	509/513 (99%)	498 (98%)	11 (2%)	52	74
2	B	496/511 (97%)	481 (97%)	15 (3%)	41	66
All	All	1005/1024 (98%)	979 (97%)	26 (3%)	46	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	25	ARG
1	A	160	TYR
1	A	183	TRP
1	A	198	ASN
1	A	238	ASN
1	A	241	LEU
1	A	378	GLU
1	A	419	GLN
1	A	519	ASP
1	A	583	LEU
2	B	43	ARG
2	B	71	ARG
2	B	181	ASN
2	B	195	GLN
2	B	204	TRP
2	B	216	LEU
2	B	228	GLN
2	B	288	PHE
2	B	295	ARG
2	B	302	ARG
2	B	377	GLU
2	B	419	GLN
2	B	434	LYS
2	B	495	LYS
2	B	585	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	238	ASN
1	A	381	ASN
1	A	466	ASN
1	A	558	GLN
2	B	32	GLN
2	B	228	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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CKX	B	701	-	14,14,14	1.35	2 (14%)	14,19,19	1.44	2 (14%)
3	CKX	A	701	-	14,14,14	1.35	2 (14%)	14,19,19	1.14	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CKX	B	701	-	-	1/7/24/24	0/1/1/1
3	CKX	A	701	-	-	3/7/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	CKX	O61-C6	4.23	1.35	1.22
3	B	701	CKX	O61-C6	3.48	1.32	1.22
3	B	701	CKX	O62-C6	-2.72	1.21	1.30
3	A	701	CKX	O62-C6	-2.33	1.22	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	CKX	O3-C3-C4	-2.80	104.53	110.14
3	B	701	CKX	O62-C6-O61	-2.47	118.47	124.09
3	A	701	CKX	O62-C6-O61	-2.27	118.93	124.09
3	A	701	CKX	C9-C8-C7	-2.16	110.10	114.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	CKX	C4-C5-C6-O62
3	A	701	CKX	N-C7-C8-C9
3	B	701	CKX	N-C7-C8-C9
3	A	701	CKX	C4-C5-C6-O61

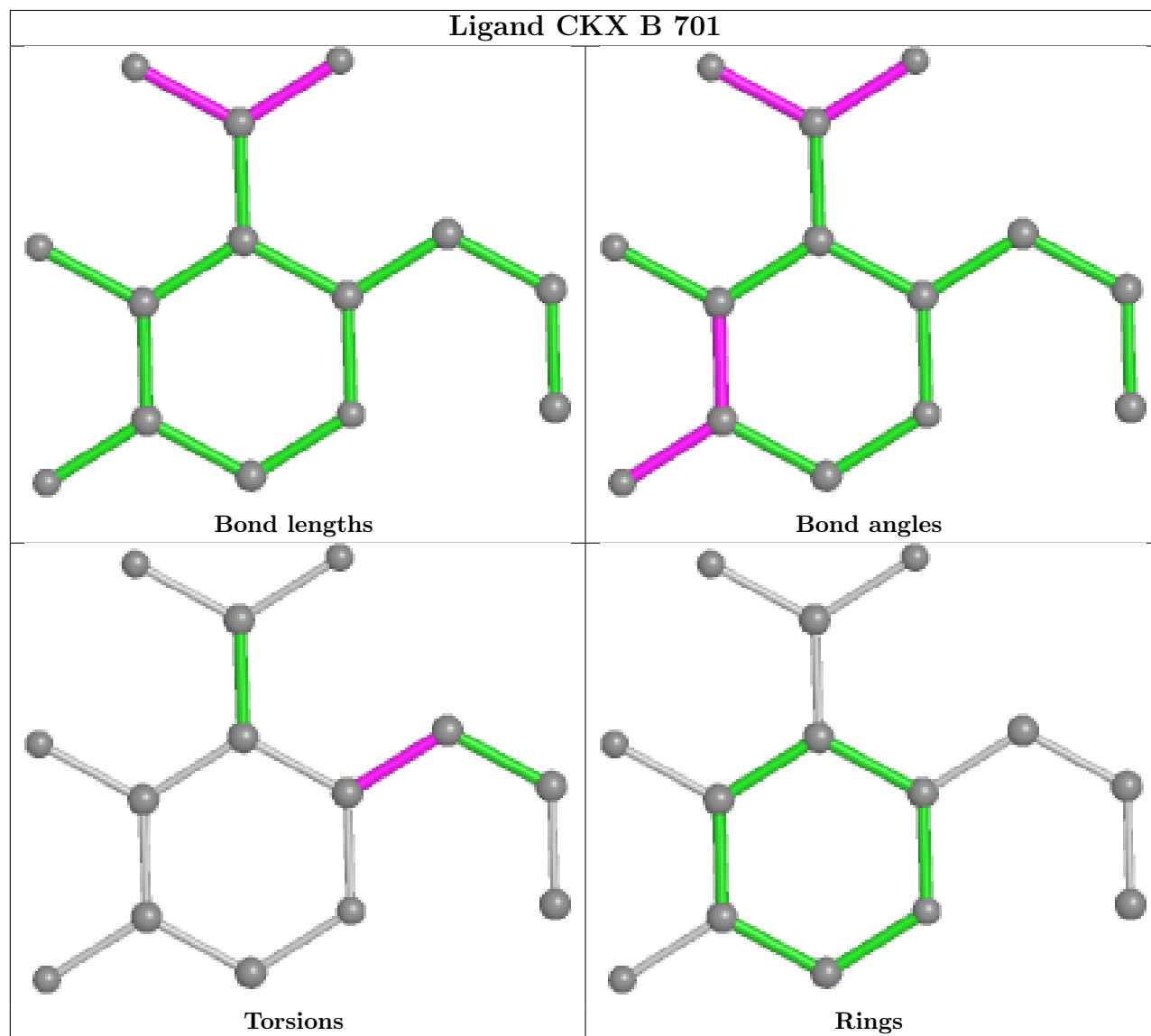
There are no ring outliers.

1 monomer is involved in 1 short contact:

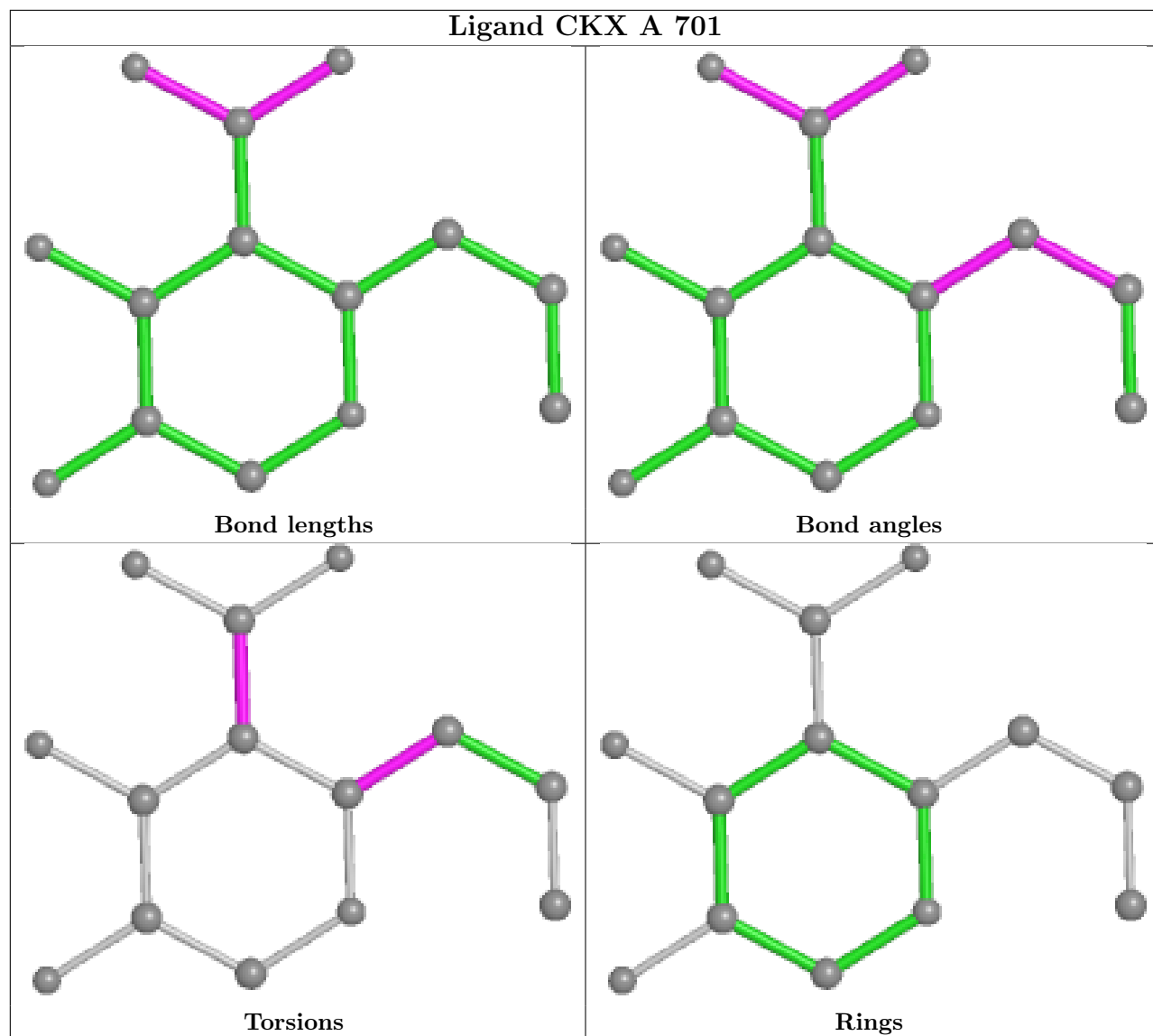
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	CKX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	600/606 (99%)	0.19	28 (4%) 31 25	19, 43, 87, 121	0
2	B	587/603 (97%)	0.59	60 (10%) 6 4	26, 66, 100, 112	0
All	All	1187/1209 (98%)	0.39	88 (7%) 14 10	19, 57, 93, 121	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	6.4
2	B	600	GLY	6.1
1	A	208	ALA	5.3
2	B	282	LEU	4.7
1	A	211	ASP	4.4
1	A	236	VAL	4.0
2	B	271	ILE	3.8
2	B	177	TYR	3.8
1	A	256	ALA	3.8
2	B	278	GLY	3.7
1	A	40	GLN	3.6
2	B	252	LEU	3.6
1	A	10	ARG	3.6
2	B	85	VAL	3.5
2	B	123	ILE	3.4
1	A	365	PHE	3.4
2	B	464	CYS	3.4
2	B	262	CYS	3.3
2	B	208	ALA	3.3
2	B	599	GLN	3.3
2	B	501	ILE	3.2
2	B	229	GLY	3.2
2	B	253	CYS	3.1
2	B	116	ALA	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	463	LEU	2.9
1	A	6	GLU	2.8
2	B	222	GLN	2.8
2	B	547	GLN	2.7
2	B	245	GLY	2.7
2	B	503	THR	2.7
1	A	128	VAL	2.7
2	B	193	VAL	2.7
2	B	209	ASN	2.7
2	B	16	ASP	2.6
2	B	31	ASP	2.6
2	B	458	ASP	2.6
1	A	116	ALA	2.6
2	B	121	TYR	2.6
1	A	80	ALA	2.6
2	B	545	GLY	2.6
2	B	153	ASN	2.6
2	B	505	TYR	2.6
1	A	196	ASP	2.5
1	A	204	TRP	2.5
1	A	228	GLN	2.5
1	A	183	TRP	2.5
2	B	203	ASP	2.5
2	B	154	GLY	2.5
2	B	432	THR	2.5
2	B	502	ILE	2.5
2	B	466	ASN	2.5
1	A	122	VAL	2.4
1	A	259	GLN	2.4
1	A	329	SER	2.4
2	B	500	ILE	2.4
2	B	365	PHE	2.4
2	B	410	ILE	2.3
2	B	128	VAL	2.3
2	B	434	LYS	2.3
1	A	2	LEU	2.3
2	B	412	ASN	2.3
2	B	194	ALA	2.3
2	B	548	VAL	2.2
1	A	199	HIS	2.2
2	B	215	GLU	2.2
2	B	237	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	2.2
2	B	266	PRO	2.2
2	B	465	LEU	2.2
1	A	9	THR	2.2
2	B	329	SER	2.2
1	A	224	VAL	2.2
1	A	79	TRP	2.2
2	B	200	ALA	2.2
2	B	594	GLY	2.1
2	B	179	THR	2.1
2	B	233	THR	2.1
1	A	257	LYS	2.1
2	B	385	GLN	2.1
1	A	503	THR	2.1
1	A	502	ILE	2.1
2	B	598	GLN	2.1
2	B	363	ILE	2.0
2	B	182	THR	2.0
2	B	79	TRP	2.0
2	B	228	GLN	2.0
2	B	225	ALA	2.0
2	B	152	GLU	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<sup>th</sup> 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.

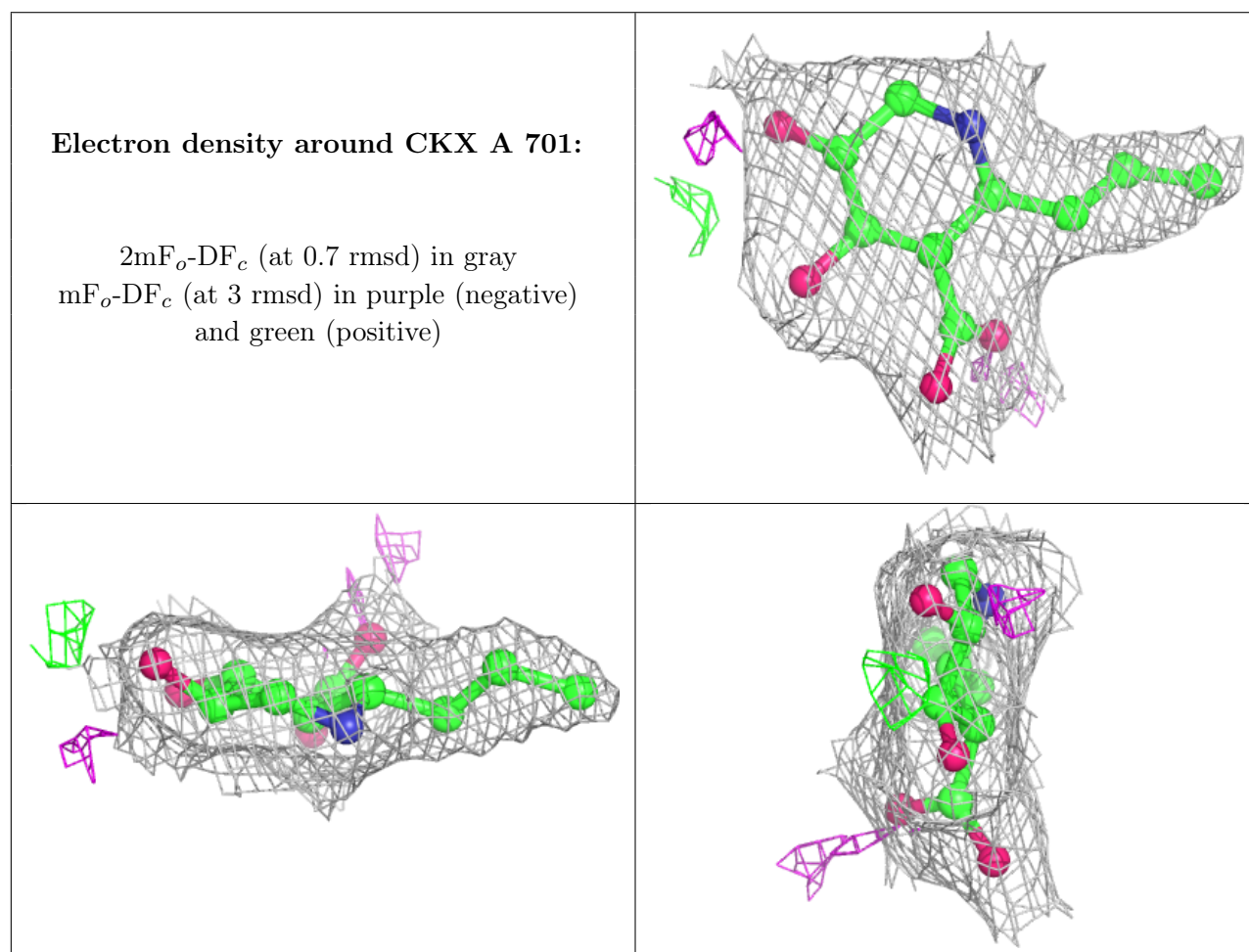
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CKX	A	701	14/14	0.92	0.20	25,26,26,27	0

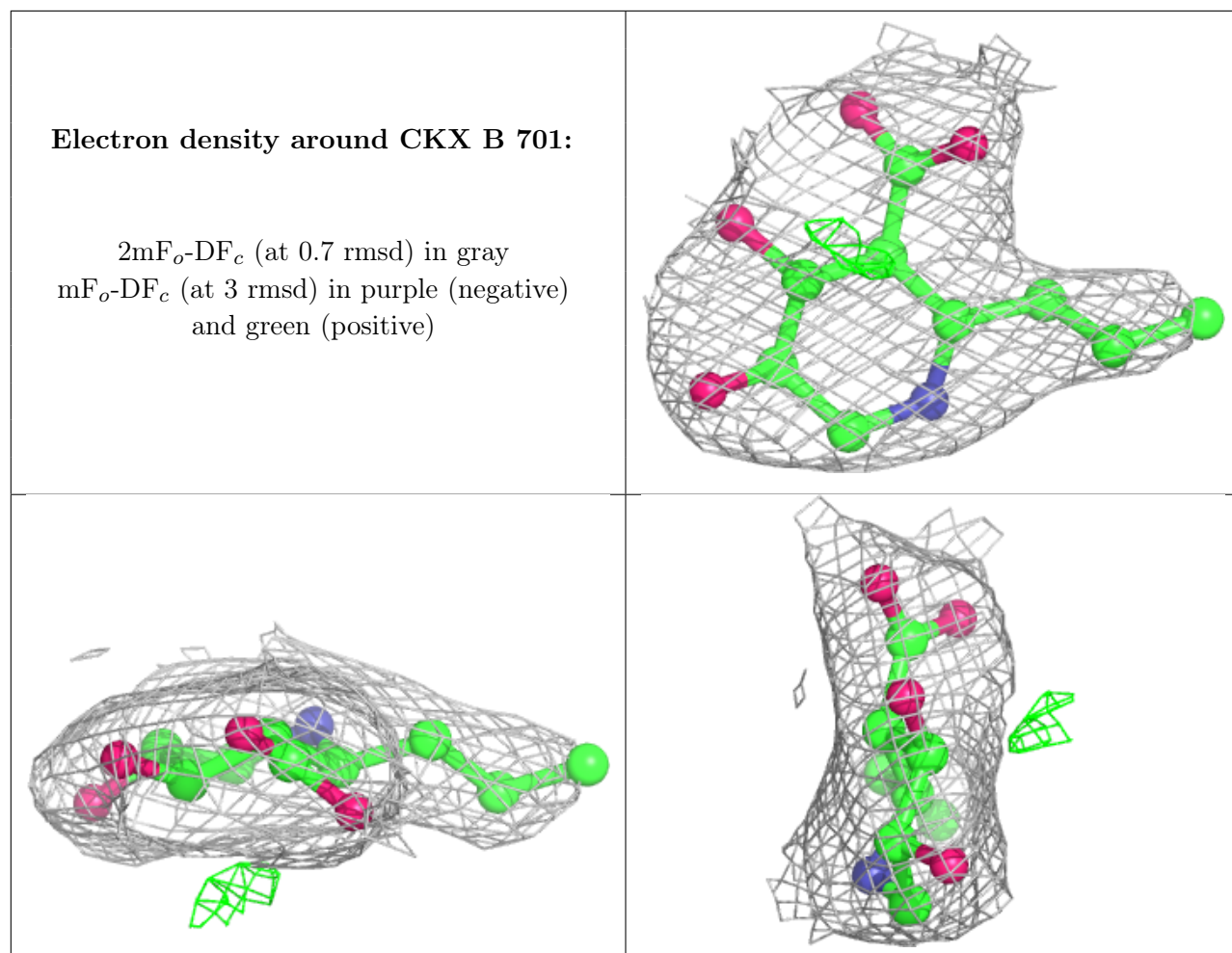
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CKX	B	701	14/14	0.93	0.25	42,48,50,50	0

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.