



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:06 PM UTC

PDB ID : 4EIQ / pdb_00004eiq
Title : Chromopyrrolic acid-soaked RebC-10x with bound 7-carboxy-K252c
Authors : Goldman, P.J.; Ryan, K.S.; Howard-Jones, A.R.; Hamill, M.J.; Elliott, S.J.;
Walsh, C.T.; Drennan, C.L.
Deposited on : 2012-04-05
Resolution : 2.76 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

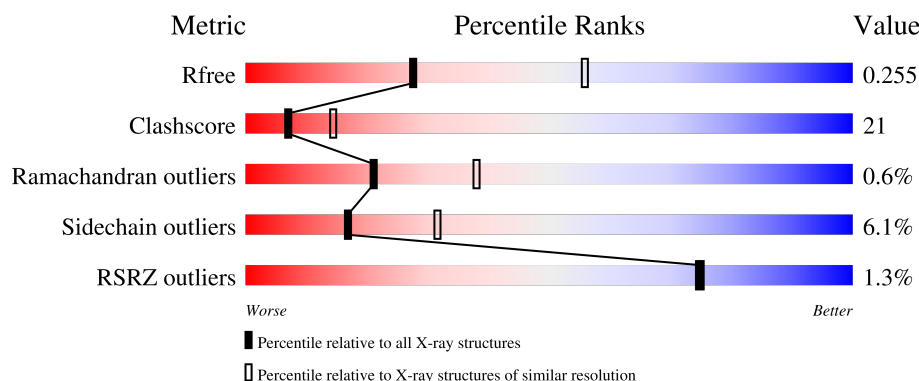
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

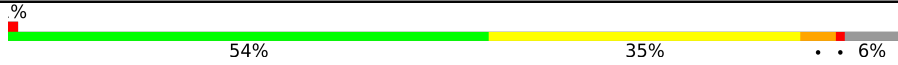
The reported resolution of this entry is 2.76 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	549	
1	B	549	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7928 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 Putative FAD-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3925	2463	742	710	10			
1	B	511	Total	C	N	O	S	0	0	0
			3887	2444	735	699	9			

There are 60 discrepancies between the modelled and reference sequences:

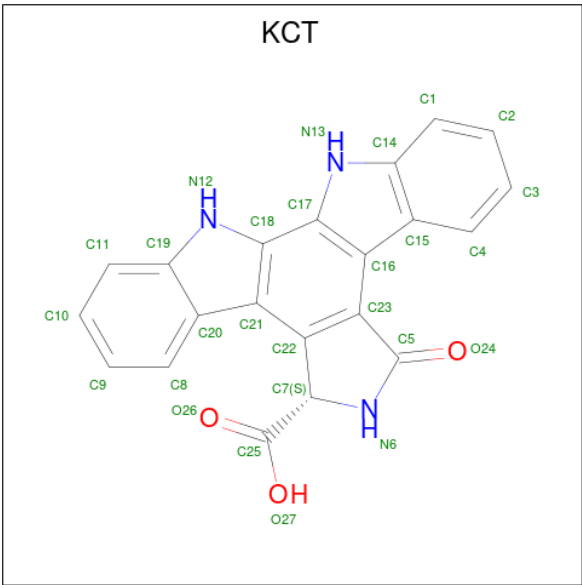
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8KI25
A	-18	GLY	-	expression tag	UNP Q8KI25
A	-17	SER	-	expression tag	UNP Q8KI25
A	-16	SER	-	expression tag	UNP Q8KI25
A	-15	HIS	-	expression tag	UNP Q8KI25
A	-14	HIS	-	expression tag	UNP Q8KI25
A	-13	HIS	-	expression tag	UNP Q8KI25
A	-12	HIS	-	expression tag	UNP Q8KI25
A	-11	HIS	-	expression tag	UNP Q8KI25
A	-10	HIS	-	expression tag	UNP Q8KI25
A	-9	SER	-	expression tag	UNP Q8KI25
A	-8	SER	-	expression tag	UNP Q8KI25
A	-7	GLY	-	expression tag	UNP Q8KI25
A	-6	LEU	-	expression tag	UNP Q8KI25
A	-5	VAL	-	expression tag	UNP Q8KI25
A	-4	PRO	-	expression tag	UNP Q8KI25
A	-3	ARG	-	expression tag	UNP Q8KI25
A	-2	GLY	-	expression tag	UNP Q8KI25
A	-1	SER	-	expression tag	UNP Q8KI25
A	0	HIS	-	expression tag	UNP Q8KI25
A	36	ASP	GLU	engineered mutation	UNP Q8KI25
A	37	ALA	GLN	engineered mutation	UNP Q8KI25
A	38	GLY	THR	engineered mutation	UNP Q8KI25
A	46	LYS	ARG	engineered mutation	UNP Q8KI25
A	48	SER	GLY	engineered mutation	UNP Q8KI25

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ALA	GLN	engineered mutation	UNP Q8KI25
A	216	VAL	PHE	engineered mutation	UNP Q8KI25
A	231	SER	ALA	engineered mutation	UNP Q8KI25
A	239	ASN	ARG	engineered mutation	UNP Q8KI25
A	241	VAL	THR	engineered mutation	UNP Q8KI25
B	-19	MET	-	expression tag	UNP Q8KI25
B	-18	GLY	-	expression tag	UNP Q8KI25
B	-17	SER	-	expression tag	UNP Q8KI25
B	-16	SER	-	expression tag	UNP Q8KI25
B	-15	HIS	-	expression tag	UNP Q8KI25
B	-14	HIS	-	expression tag	UNP Q8KI25
B	-13	HIS	-	expression tag	UNP Q8KI25
B	-12	HIS	-	expression tag	UNP Q8KI25
B	-11	HIS	-	expression tag	UNP Q8KI25
B	-10	HIS	-	expression tag	UNP Q8KI25
B	-9	SER	-	expression tag	UNP Q8KI25
B	-8	SER	-	expression tag	UNP Q8KI25
B	-7	GLY	-	expression tag	UNP Q8KI25
B	-6	LEU	-	expression tag	UNP Q8KI25
B	-5	VAL	-	expression tag	UNP Q8KI25
B	-4	PRO	-	expression tag	UNP Q8KI25
B	-3	ARG	-	expression tag	UNP Q8KI25
B	-2	GLY	-	expression tag	UNP Q8KI25
B	-1	SER	-	expression tag	UNP Q8KI25
B	0	HIS	-	expression tag	UNP Q8KI25
B	36	ASP	GLU	engineered mutation	UNP Q8KI25
B	37	ALA	GLN	engineered mutation	UNP Q8KI25
B	38	GLY	THR	engineered mutation	UNP Q8KI25
B	46	LYS	ARG	engineered mutation	UNP Q8KI25
B	48	SER	GLY	engineered mutation	UNP Q8KI25
B	117	ALA	GLN	engineered mutation	UNP Q8KI25
B	216	VAL	PHE	engineered mutation	UNP Q8KI25
B	231	SER	ALA	engineered mutation	UNP Q8KI25
B	239	ASN	ARG	engineered mutation	UNP Q8KI25
B	241	VAL	THR	engineered mutation	UNP Q8KI25

- Molecule 2 is (5S)-7-oxo-6,7,12,13-tetrahydro-5H-indolo[2,3-a]pyrrolo[3,4-c]carbazole-5-carboxylic acid (CCD ID: KCT) (formula: C₂₁H₁₃N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	21	3	3		
2	B	1	Total	C	N	O	0	0
			27	21	3	3		

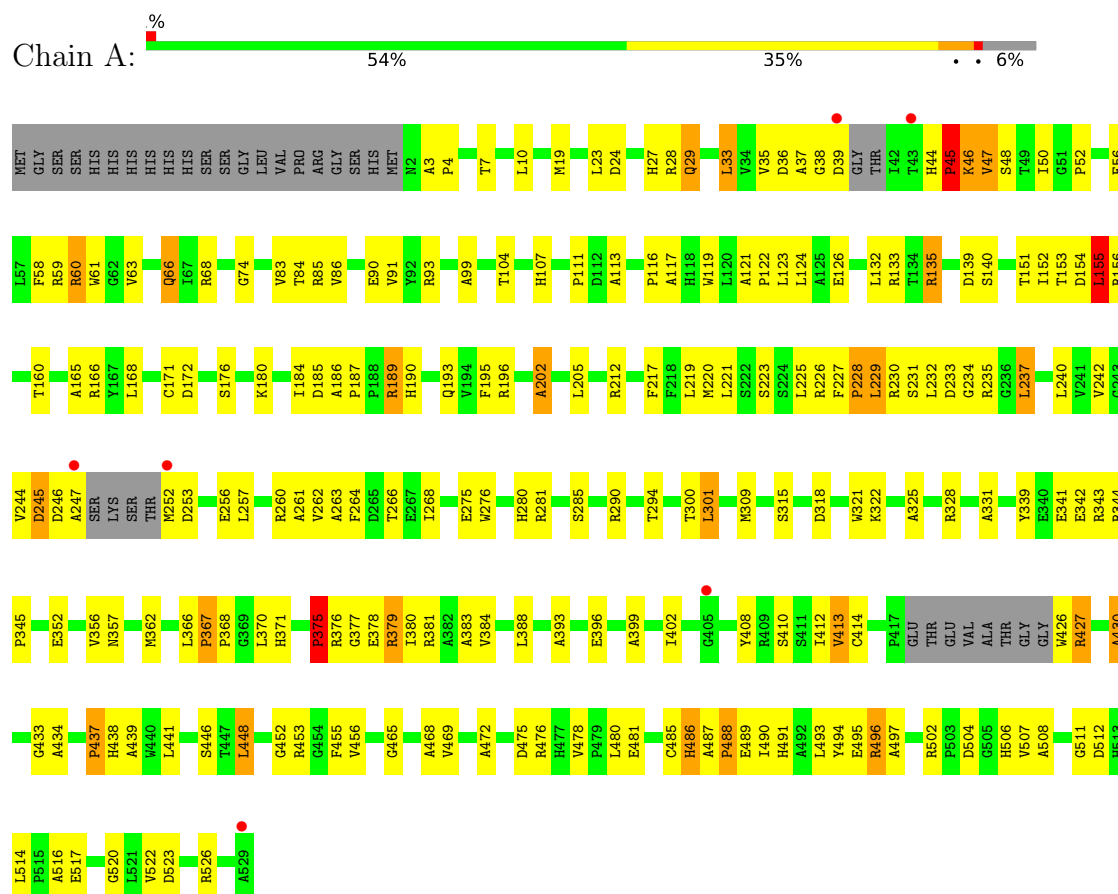
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	26	Total	O	0	0
			26	26		

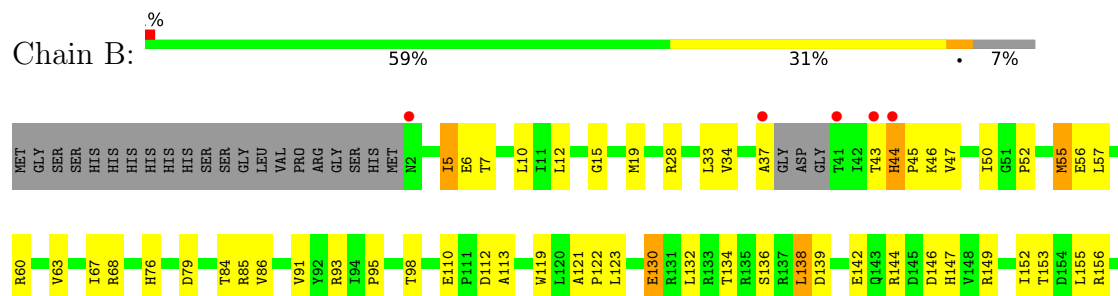
3 Residue-property plots

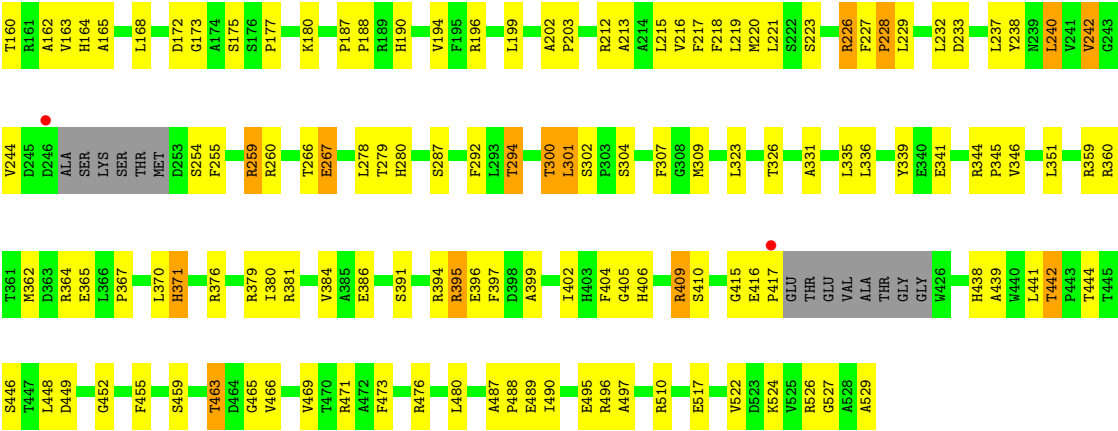
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Putative FAD-monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.18Å 77.70Å 123.14Å 90.00° 98.78° 90.00°	Depositor
Resolution (Å)	47.30 – 2.76 47.30 – 2.76	Depositor EDS
% Data completeness (in resolution range)	94.4 (47.30-2.76) 94.5 (47.30-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.255 0.206 , 0.255	Depositor DCC
R_{free} test set	1458 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7928	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: KCT

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	0.52	1/4020 (0.0%)	1.07	35/5469 (0.6%)
1	B	0.57	1/3983 (0.0%)	1.00	15/5423 (0.3%)
All	All	0.55	2/8003 (0.0%)	1.04	50/10892 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	HIS	CA-C	-5.64	1.46	1.52
1	B	46	LYS	C-O	-5.06	1.18	1.24

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	486	HIS	N-CA-C	9.45	124.81	112.72
1	A	496	ARG	N-CA-C	-9.32	96.66	110.46
1	A	516	ALA	N-CA-C	8.62	125.51	111.37
1	B	405	GLY	N-CA-C	8.14	124.01	114.16
1	A	245	ASP	N-CA-C	-7.76	100.32	110.33
1	B	415	GLY	N-CA-C	7.26	120.28	111.93
1	A	486	HIS	CB-CA-C	-7.14	98.67	110.37
1	A	430	ALA	N-CA-C	-6.92	104.15	112.59
1	B	173	GLY	N-CA-C	6.88	120.66	112.33
1	B	232	LEU	N-CA-C	6.76	118.30	111.07
1	A	375	PRO	N-CA-C	6.67	126.21	112.47
1	A	47	VAL	N-CA-C	6.62	123.11	109.34
1	A	48	SER	N-CA-C	6.58	121.38	113.23
1	A	171	CYS	N-CA-C	-6.46	102.54	110.61
1	A	45	PRO	CB-CA-C	6.37	122.07	111.56
1	A	366	LEU	CA-C-N	6.36	126.93	120.38
1	A	366	LEU	C-N-CA	6.36	126.93	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CB-CA-C	6.29	120.69	110.95
1	B	228	PRO	N-CA-C	6.22	121.27	111.38
1	B	463	THR	N-CA-C	-6.20	105.65	112.72
1	A	441	LEU	N-CA-C	-6.16	104.47	112.23
1	A	46	LYS	CB-CA-C	-6.12	99.49	110.70
1	B	441	LEU	N-CA-C	-6.12	104.89	112.90
1	A	46	LYS	N-CA-C	6.09	119.18	111.69
1	A	139	ASP	N-CA-C	-6.06	104.30	111.03
1	B	202	ALA	CA-C-N	5.96	125.66	119.05
1	B	202	ALA	C-N-CA	5.96	125.66	119.05
1	B	229	LEU	N-CA-C	-5.86	97.77	108.02
1	A	413	VAL	N-CA-C	-5.83	97.21	109.34
1	A	367	PRO	N-CA-C	5.82	117.80	110.70
1	A	140	SER	N-CA-CB	-5.77	102.57	111.46
1	A	228	PRO	N-CA-C	5.74	120.23	111.11
1	A	229	LEU	N-CA-C	-5.57	98.11	108.02
1	B	79	ASP	N-CA-C	5.54	117.69	110.43
1	A	516	ALA	CB-CA-C	-5.53	101.66	110.84
1	A	83	VAL	N-CA-C	5.51	115.26	108.53
1	A	84	THR	N-CA-C	-5.51	105.69	112.90
1	B	86	VAL	N-CA-C	-5.49	101.60	108.84
1	A	202	ALA	CA-C-N	5.46	125.55	119.32
1	A	202	ALA	C-N-CA	5.46	125.55	119.32
1	A	437	PRO	N-CA-C	5.37	119.66	111.34
1	A	230	ARG	N-CA-C	5.36	118.22	109.59
1	A	59	ARG	N-CA-C	-5.35	105.53	111.36
1	B	495	GLU	N-CA-C	5.33	119.62	113.38
1	A	367	PRO	CA-C-N	5.32	126.49	119.84
1	A	367	PRO	C-N-CA	5.32	126.49	119.84
1	B	386	GLU	N-CA-C	-5.28	105.44	111.14
1	B	442	THR	N-CA-C	-5.21	101.39	108.11
1	A	104	THR	CA-C-N	5.06	125.06	119.89
1	A	104	THR	C-N-CA	5.06	125.06	119.89

There are no chirality outliers.

There are no planarity outliers.

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	3925	0	3857	180	0
1	B	3887	0	3811	147	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
3	A	36	0	0	5	0
3	B	26	0	0	0	0
All	All	7928	0	7692	327	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 21.

All (327) 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:A:399:ALA:HB1	1:A:402:ILE:HD13	1.14	1.13
1:B:44:HIS:HB3	1:B:45:PRO:CD	1.79	1.11
1:B:44:HIS:CB	1:B:45:PRO:CD	2.28	1.11
1:A:46:LYS:C	1:A:47:VAL:HG22	1.75	1.09
1:B:44:HIS:HB3	1:B:45:PRO:HD3	1.36	1.06
1:B:44:HIS:HB2	1:B:45:PRO:HD2	1.40	0.99
1:A:46:LYS:O	1:A:47:VAL:CG2	2.13	0.96
1:B:44:HIS:CB	1:B:45:PRO:HD2	1.93	0.94
1:B:43:THR:O	1:B:44:HIS:HB2	1.67	0.94
1:A:489:GLU:HG2	1:A:490:ILE:HD12	1.50	0.93
1:A:315:SER:HA	1:A:343:ARG:HD2	1.50	0.92
1:A:46:LYS:O	1:A:47:VAL:HG22	1.68	0.91
1:A:496:ARG:HD2	1:A:511:GLY:HA2	1.53	0.91
1:A:86:VAL:HG21	1:A:229:LEU:HD13	1.54	0.89
1:A:46:LYS:C	1:A:47:VAL:CG2	2.45	0.89
1:B:194:VAL:O	1:B:244:VAL:HG22	1.72	0.86
1:A:219:LEU:O	1:A:226:ARG:HA	1.76	0.84
1:B:130:GLU:CD	1:B:130:GLU:H	1.85	0.83
1:B:522:VAL:O	1:B:526:ARG:HG2	1.79	0.82
1:A:344:ARG:HB3	1:A:345:PRO:HD3	1.62	0.81
1:A:66:GLN:H	1:A:66:GLN:NE2	1.80	0.79
1:A:10:LEU:HD23	1:A:168:LEU:HD12	1.66	0.78
1:A:135:ARG:HD2	1:A:156:ARG:HE	1.49	0.77
1:A:52:PRO:O	1:A:56:GLU:HG3	1.85	0.77
1:B:409:ARG:HE	1:B:409:ARG:HA	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:MET:HE1	1:A:132:LEU:HD22	1.67	0.76
1:A:121:ALA:HB3	1:A:122:PRO:HD3	1.69	0.74
1:B:365:GLU:O	1:B:367:PRO:HD3	1.85	0.74
1:B:175:SER:O	1:B:177:PRO:HD3	1.87	0.74
1:A:189:ARG:HG2	1:A:189:ARG:HH11	1.53	0.73
1:A:437:PRO:HG2	1:A:494:TYR:CE1	2.25	0.72
1:B:130:GLU:CD	1:B:130:GLU:N	2.47	0.72
1:B:138:LEU:HD12	1:B:152:ILE:HD11	1.70	0.72
1:B:5:ILE:HG22	1:B:162:ALA:O	1.90	0.72
1:B:52:PRO:O	1:B:56:GLU:HG3	1.89	0.72
1:B:194:VAL:HB	1:B:244:VAL:CG2	2.20	0.72
1:A:66:GLN:HE21	1:A:66:GLN:N	1.88	0.71
1:A:135:ARG:HG3	1:A:135:ARG:HH11	1.56	0.70
1:A:66:GLN:H	1:A:66:GLN:HE21	1.37	0.70
1:B:91:VAL:HG21	1:B:220:MET:CE	2.21	0.70
1:B:144:ARG:NH2	1:B:149:ARG:HD2	2.06	0.70
1:A:24:ASP:HB2	1:A:61:TRP:CZ2	2.27	0.70
1:A:156:ARG:HH11	1:A:156:ARG:HG2	1.58	0.69
1:A:275:GLU:HG2	1:A:276:TRP:N	2.06	0.69
1:B:5:ILE:C	1:B:5:ILE:HD13	2.17	0.69
1:B:60:ARG:HD2	1:B:452:GLY:HA3	1.74	0.69
1:A:46:LYS:O	1:A:47:VAL:HG23	1.90	0.68
1:A:217:PHE:O	1:A:228:PRO:HA	1.94	0.68
1:B:91:VAL:HG21	1:B:220:MET:HE2	1.74	0.67
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.60	0.67
1:A:244:VAL:HG12	1:A:245:ASP:O	1.94	0.67
1:B:399:ALA:O	1:B:402:ILE:HG22	1.96	0.66
1:B:43:THR:O	1:B:44:HIS:CB	2.40	0.66
1:A:91:VAL:HG21	1:A:220:MET:CE	2.25	0.66
1:A:502:ARG:HG3	1:A:506:HIS:O	1.96	0.66
1:B:28:ARG:HG2	1:B:28:ARG:HH11	1.60	0.66
1:A:399:ALA:HB1	1:A:402:ILE:CD1	2.09	0.66
1:A:487:ALA:HB1	1:A:489:GLU:OE1	1.96	0.65
1:B:394:ARG:HB3	1:B:394:ARG:NH1	2.12	0.65
1:B:227:PHE:HB3	1:B:228:PRO:HD2	1.79	0.64
1:A:60:ARG:HD3	1:A:452:GLY:HA3	1.80	0.64
1:B:212:ARG:HB3	1:B:212:ARG:NH1	2.11	0.64
1:A:522:VAL:O	1:A:526:ARG:HG2	1.97	0.64
1:A:375:PRO:HA	1:A:378:GLU:HB2	1.78	0.64
1:B:5:ILE:HG23	1:B:163:VAL:HA	1.79	0.64
1:A:227:PHE:HB3	1:A:228:PRO:HD2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ARG:HB3	1:B:345:PRO:HD3	1.78	0.63
1:A:47:VAL:HA	2:A:600:KCT:O27	1.98	0.63
1:B:489:GLU:N	1:B:489:GLU:OE1	2.31	0.62
1:A:221:LEU:HD13	1:A:221:LEU:O	1.99	0.62
1:A:262:VAL:HG12	1:A:264:PHE:H	1.64	0.61
1:B:199:LEU:HD11	1:B:237:LEU:HD22	1.81	0.61
1:A:91:VAL:HG21	1:A:220:MET:HE2	1.82	0.61
1:A:10:LEU:HD23	1:A:168:LEU:CD1	2.30	0.61
1:B:300:THR:C	1:B:301:LEU:HD23	2.26	0.60
1:A:184:ILE:HD13	1:A:285:SER:HB2	1.84	0.60
1:A:344:ARG:NH2	3:A:736:HOH:O	2.34	0.60
1:A:135:ARG:O	1:A:155:LEU:HB2	2.02	0.60
1:A:388:LEU:CD2	1:A:393:ALA:HB2	2.32	0.60
1:A:33:LEU:HD21	1:A:133:ARG:HG2	1.84	0.59
1:A:402:ILE:N	1:A:402:ILE:HD12	2.18	0.59
1:A:315:SER:CA	1:A:343:ARG:HD2	2.27	0.59
1:B:364:ARG:HH11	1:B:364:ARG:HG2	1.67	0.59
1:B:527:GLY:C	1:B:529:ALA:H	2.11	0.59
1:A:220:MET:HE3	1:A:370:LEU:HD21	1.85	0.58
1:A:153:THR:OG1	1:A:160:THR:HG22	2.03	0.58
1:B:370:LEU:HD22	1:B:381:ARG:HG2	1.85	0.58
1:A:189:ARG:NH1	3:A:735:HOH:O	2.37	0.58
1:B:5:ILE:HD13	1:B:5:ILE:O	2.03	0.58
1:B:12:LEU:HD22	1:B:172:ASP:HB3	1.86	0.58
1:A:294:THR:HG22	1:A:339:TYR:OH	2.04	0.57
1:B:144:ARG:HH22	1:B:149:ARG:HD2	1.68	0.57
1:A:35:VAL:HG11	1:A:152:ILE:HG12	1.87	0.57
1:B:476:ARG:HG3	1:B:476:ARG:NH1	2.20	0.57
1:B:394:ARG:NH1	1:B:394:ARG:CB	2.67	0.57
1:A:488:PRO:N	1:A:489:GLU:OE1	2.37	0.57
1:B:446:SER:O	1:B:449:ASP:HB2	2.05	0.57
1:B:394:ARG:CB	1:B:394:ARG:HH11	2.18	0.57
1:A:517:GLU:HG2	1:A:520:GLY:H	1.69	0.57
1:B:255:PHE:CE1	1:B:259:ARG:HD2	2.39	0.56
1:A:244:VAL:C	1:A:245:ASP:O	2.46	0.56
1:B:190:HIS:HB2	1:B:280:HIS:CG	2.40	0.56
1:A:376:ARG:O	1:A:380:ILE:HG13	2.05	0.56
1:A:50:ILE:HG12	1:A:309:MET:HE1	1.88	0.56
1:A:107:HIS:HB2	3:A:726:HOH:O	2.04	0.56
1:B:360:ARG:NE	1:B:391:SER:O	2.38	0.56
1:A:489:GLU:OE1	1:A:489:GLU:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:THR:HG23	1:B:339:TYR:OH	2.05	0.56
1:B:84:THR:O	1:B:221:LEU:HG	2.05	0.56
1:A:68:ARG:NH2	1:A:111:PRO:O	2.33	0.56
1:A:185:ASP:OD2	1:A:187:PRO:HD3	2.05	0.56
1:A:455:PHE:O	1:A:480:LEU:HD12	2.06	0.56
1:B:341:GLU:OE2	1:B:410:SER:HB2	2.06	0.56
1:A:375:PRO:C	1:A:377:GLY:N	2.62	0.55
1:B:6:GLU:OE2	1:B:164:HIS:ND1	2.39	0.55
1:A:28:ARG:CZ	1:A:321:TRP:HB3	2.36	0.55
1:A:7:THR:O	1:A:165:ALA:HA	2.07	0.55
1:A:223:SER:O	1:A:226:ARG:NH1	2.40	0.55
1:B:28:ARG:HG2	1:B:28:ARG:NH1	2.19	0.55
1:A:342:GLU:HB3	1:A:408:TYR:CD1	2.41	0.55
1:A:375:PRO:C	1:A:377:GLY:H	2.15	0.55
1:B:255:PHE:HE1	1:B:259:ARG:HD2	1.72	0.55
1:B:47:VAL:HG21	1:B:309:MET:SD	2.47	0.54
1:A:172:ASP:OD1	1:A:176:SER:OG	2.21	0.54
1:A:341:GLU:OE2	1:A:410:SER:HB2	2.06	0.54
1:B:194:VAL:HB	1:B:244:VAL:HG21	1.89	0.54
1:B:190:HIS:HB2	1:B:280:HIS:CD2	2.43	0.54
1:B:7:THR:O	1:B:165:ALA:HA	2.08	0.54
1:B:55:MET:HB3	1:B:110:GLU:HB3	1.90	0.53
1:B:144:ARG:CZ	1:B:149:ARG:HD2	2.38	0.53
1:B:226:ARG:NH2	1:B:362:MET:O	2.41	0.53
1:A:412:ILE:HG13	1:A:412:ILE:O	2.07	0.53
1:A:50:ILE:HG12	1:A:309:MET:CE	2.39	0.53
1:B:217:PHE:O	1:B:228:PRO:HA	2.09	0.53
1:A:352:GLU:O	1:A:356:VAL:HG23	2.09	0.52
1:A:427:ARG:HG2	1:A:427:ARG:HH21	1.75	0.52
1:A:3:ALA:HB1	1:A:4:PRO:HD2	1.91	0.52
1:B:219:LEU:O	1:B:226:ARG:HA	2.10	0.52
1:B:279:THR:OG1	1:B:300:THR:HG21	2.09	0.52
1:B:346:VAL:HG13	1:B:406:HIS:CD2	2.45	0.52
1:B:394:ARG:HH11	1:B:394:ARG:HB2	1.73	0.51
1:A:502:ARG:HB2	1:A:504:ASP:OD1	2.09	0.51
1:A:190:HIS:HB2	1:A:280:HIS:CG	2.45	0.51
1:B:93:ARG:O	1:B:95:PRO:HD3	2.11	0.51
1:B:142:GLU:OE2	1:B:144:ARG:NH1	2.44	0.50
1:A:453:ARG:HB2	3:A:720:HOH:O	2.12	0.50
1:B:215:LEU:HG	1:B:216:VAL:HG23	1.92	0.50
1:B:359:ARG:HG3	1:B:359:ARG:HH11	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ARG:HB2	1:A:242:VAL:CG1	2.42	0.50
1:A:328:ARG:HG3	1:A:328:ARG:HH11	1.76	0.50
1:A:456:VAL:HG22	1:A:481:GLU:HB2	1.92	0.50
1:B:395:ARG:CG	1:B:395:ARG:HH21	2.24	0.50
1:B:438:HIS:CG	1:B:439:ALA:N	2.80	0.50
1:A:219:LEU:O	1:A:226:ARG:CA	2.55	0.50
1:A:378:GLU:HA	1:A:381:ARG:NH1	2.26	0.50
1:A:502:ARG:HG2	1:A:508:ALA:HB2	1.94	0.49
1:A:375:PRO:O	1:A:377:GLY:N	2.45	0.49
1:A:202:ALA:HB1	1:A:205:LEU:HB2	1.95	0.49
1:A:357:ASN:CG	1:A:396:GLU:HG3	2.37	0.49
1:B:473:PHE:CD1	1:B:480:LEU:HD22	2.47	0.49
1:A:257:LEU:O	1:A:260:ARG:HB2	2.13	0.49
1:B:370:LEU:CD2	1:B:381:ARG:HG2	2.42	0.49
1:A:497:ALA:HB3	1:A:512:ASP:HA	1.95	0.49
1:B:5:ILE:C	1:B:5:ILE:CD1	2.86	0.49
1:A:375:PRO:O	1:A:376:ARG:C	2.55	0.49
1:A:221:LEU:HD12	1:A:225:LEU:HD12	1.95	0.49
1:B:438:HIS:HA	1:B:448:LEU:HD13	1.95	0.49
1:A:27:HIS:HB3	3:A:705:HOH:O	2.11	0.49
1:A:300:THR:C	1:A:301:LEU:HD23	2.38	0.48
1:A:465:GLY:O	1:A:468:ALA:HB3	2.13	0.48
1:B:331:ALA:HB1	1:B:335:LEU:HD22	1.93	0.48
1:A:38:GLY:HA3	1:A:135:ARG:HH12	1.79	0.48
1:A:189:ARG:HG2	1:A:189:ARG:NH1	2.22	0.48
1:B:68:ARG:NH1	1:B:113:ALA:HB2	2.28	0.48
1:B:119:TRP:O	1:B:122:PRO:HD2	2.14	0.48
1:A:44:HIS:O	1:A:45:PRO:O	2.32	0.48
1:B:394:ARG:HB3	1:B:394:ARG:CZ	2.43	0.48
1:B:444:THR:HG22	1:B:444:THR:O	2.14	0.48
1:B:47:VAL:HG13	1:B:47:VAL:O	2.12	0.48
1:A:74:GLY:HA2	1:A:99:ALA:HB3	1.95	0.47
1:B:409:ARG:HA	1:B:409:ARG:NE	2.26	0.47
1:A:487:ALA:HB1	1:A:489:GLU:CD	2.38	0.47
1:A:472:ALA:O	1:A:475:ASP:HB2	2.13	0.47
1:B:37:ALA:HA	1:B:136:SER:O	2.13	0.47
1:B:144:ARG:HG3	1:B:147:HIS:NE2	2.29	0.47
1:A:156:ARG:HG2	1:A:156:ARG:NH1	2.27	0.47
1:A:266:THR:O	1:A:268:ILE:HG13	2.14	0.47
1:A:66:GLN:NE2	1:A:66:GLN:N	2.51	0.47
1:A:246:ASP:O	1:A:247:ALA:HB3	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HD12	1:A:402:ILE:H	1.80	0.47
1:A:412:ILE:C	1:A:413:VAL:CG2	2.88	0.47
1:A:90:GLU:CD	1:A:93:ARG:HE	2.22	0.47
1:A:370:LEU:HD12	1:A:381:ARG:HG2	1.97	0.47
1:A:437:PRO:HB2	1:A:493:LEU:HD21	1.96	0.47
1:A:523:ASP:OD1	1:A:526:ARG:NH1	2.48	0.47
1:A:38:GLY:HA3	1:A:135:ARG:NH1	2.30	0.47
1:A:135:ARG:HH11	1:A:135:ARG:CG	2.25	0.46
1:B:15:GLY:O	1:B:19:MET:HG2	2.16	0.46
1:B:138:LEU:HA	1:B:152:ILE:HD13	1.97	0.46
1:B:459:SER:HA	1:B:497:ALA:O	2.14	0.46
1:A:193:GLN:HE22	1:A:362:MET:CE	2.28	0.46
1:A:339:TYR:O	1:A:343:ARG:HB2	2.15	0.46
1:A:344:ARG:HB3	1:A:345:PRO:CD	2.41	0.46
1:A:119:TRP:O	1:A:122:PRO:HD2	2.16	0.46
1:A:68:ARG:NH1	1:A:113:ALA:HB2	2.31	0.46
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.80	0.46
1:B:346:VAL:HG13	1:B:406:HIS:NE2	2.31	0.46
1:B:351:LEU:C	1:B:351:LEU:HD23	2.41	0.46
1:A:488:PRO:HA	1:A:491:HIS:HB3	1.97	0.46
1:B:307:PHE:CE1	1:B:402:ILE:HG21	2.51	0.46
1:A:388:LEU:HD23	1:A:393:ALA:HB2	1.98	0.46
1:A:485:CYS:SG	1:A:486:HIS:N	2.89	0.46
1:B:376:ARG:O	1:B:380:ILE:HG13	2.16	0.46
1:A:28:ARG:C	1:A:29:GLN:HG2	2.40	0.45
1:A:35:VAL:HG23	1:A:35:VAL:O	2.16	0.45
1:B:203:PRO:HD2	1:B:267:GLU:HG2	1.98	0.45
1:A:380:ILE:O	1:A:383:ALA:HB3	2.15	0.45
1:B:218:PHE:HE1	1:B:397:PHE:HZ	1.63	0.45
1:A:186:ALA:O	1:A:281:ARG:CZ	2.65	0.45
1:B:10:LEU:O	1:B:168:LEU:HD12	2.16	0.45
1:A:253:ASP:O	1:A:257:LEU:HG	2.17	0.45
1:B:85:ARG:HG2	1:B:221:LEU:HD21	1.99	0.45
1:B:489:GLU:HG2	1:B:490:ILE:N	2.32	0.45
1:A:116:PRO:HD2	1:A:119:TRP:CE3	2.51	0.45
1:B:279:THR:O	1:B:300:THR:HG22	2.17	0.45
1:B:156:ARG:NH1	1:B:156:ARG:HB3	2.32	0.45
1:A:44:HIS:C	1:A:45:PRO:O	2.59	0.45
1:A:151:THR:C	1:A:152:ILE:HD12	2.41	0.45
1:B:121:ALA:HB3	1:B:122:PRO:HD3	1.98	0.45
1:A:325:ALA:HB1	1:A:331:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HG3	1:A:135:ARG:NH1	2.27	0.44
1:A:233:ASP:O	1:A:235:ARG:HG3	2.17	0.44
1:A:154:ASP:C	1:A:156:ARG:H	2.24	0.44
1:A:379:ARG:HD3	1:A:379:ARG:HA	1.76	0.44
1:B:371:HIS:CD2	1:B:371:HIS:N	2.85	0.44
1:B:63:VAL:O	1:B:67:ILE:HG13	2.18	0.44
1:B:527:GLY:C	1:B:529:ALA:N	2.75	0.44
1:A:28:ARG:NH2	1:A:321:TRP:HB3	2.32	0.44
1:B:359:ARG:HG3	1:B:359:ARG:NH1	2.33	0.44
1:B:119:TRP:CH2	1:B:233:ASP:HB2	2.53	0.44
1:B:196:ARG:HG3	1:B:244:VAL:CG1	2.48	0.44
1:A:412:ILE:O	1:A:413:VAL:HG22	2.17	0.44
1:B:138:LEU:HD12	1:B:152:ILE:CD1	2.45	0.44
1:A:172:ASP:OD1	1:A:172:ASP:N	2.45	0.44
1:B:199:LEU:HD12	1:B:238:TYR:O	2.17	0.44
1:A:195:PHE:HB2	1:A:276:TRP:CE2	2.53	0.43
1:A:58:PHE:HB3	1:A:63:VAL:HG23	1.99	0.43
1:A:413:VAL:HG11	1:A:433:GLY:CA	2.48	0.43
1:B:5:ILE:CG2	1:B:162:ALA:O	2.62	0.43
1:B:278:LEU:HD21	1:B:302:SER:HB2	2.00	0.43
1:A:85:ARG:CZ	1:A:263:ALA:HA	2.47	0.43
1:A:438:HIS:ND1	1:A:446:SER:OG	2.48	0.43
1:B:144:ARG:NH1	1:B:149:ARG:HD2	2.33	0.43
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.81	0.43
1:A:495:GLU:HB3	1:A:496:ARG:HH12	1.84	0.43
1:B:91:VAL:CG2	1:B:220:MET:HE2	2.44	0.43
1:A:29:GLN:HB2	1:A:328:ARG:HH22	1.84	0.43
1:B:93:ARG:NH2	1:B:213:ALA:O	2.51	0.43
1:A:152:ILE:HD12	1:A:152:ILE:N	2.33	0.43
1:B:156:ARG:HB3	1:B:156:ARG:HH11	1.84	0.43
1:B:416:GLU:HB3	1:B:417:PRO:HD2	2.00	0.43
1:B:146:ASP:OD1	1:B:146:ASP:N	2.50	0.43
1:B:446:SER:O	1:B:449:ASP:N	2.45	0.43
1:B:50:ILE:HD12	1:B:67:ILE:HG21	2.01	0.42
1:B:180:LYS:HA	1:B:180:LYS:HD2	1.72	0.42
1:A:378:GLU:OE1	1:A:381:ARG:NH1	2.48	0.42
1:B:76:HIS:O	1:B:98:THR:HG22	2.19	0.42
1:A:117:ALA:C	1:A:119:TRP:H	2.26	0.42
1:B:212:ARG:HH11	1:B:212:ARG:CB	2.32	0.42
1:A:237:LEU:HD23	1:A:237:LEU:HA	1.80	0.42
1:A:245:ASP:C	1:A:247:ALA:H	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:N	1:A:256:GLU:OE1	2.53	0.42
1:A:412:ILE:C	1:A:413:VAL:HG23	2.44	0.42
1:A:430:ALA:C	1:A:507:VAL:HG21	2.45	0.42
1:B:112:ASP:C	1:B:112:ASP:OD1	2.62	0.42
1:A:36:ASP:C	1:A:38:GLY:N	2.78	0.42
1:B:346:VAL:HG22	1:B:406:HIS:CD2	2.54	0.42
1:B:463:THR:O	1:B:466:VAL:HG23	2.20	0.42
1:A:23:LEU:O	1:A:27:HIS:HD2	2.03	0.42
1:A:232:LEU:HD12	1:A:237:LEU:HD13	2.02	0.42
1:B:226:ARG:NH2	1:B:362:MET:HA	2.34	0.42
1:B:381:ARG:HA	1:B:384:VAL:HG22	2.02	0.42
1:A:301:LEU:HD23	1:A:301:LEU:N	2.35	0.41
1:A:378:GLU:HA	1:A:381:ARG:HH12	1.85	0.41
1:A:219:LEU:HD11	1:A:261:ALA:HB1	2.01	0.41
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.79	0.41
1:B:496:ARG:HG3	1:B:510:ARG:HD2	2.03	0.41
1:B:34:VAL:O	1:B:132:LEU:HD12	2.20	0.41
1:B:402:ILE:HD12	1:B:402:ILE:HA	1.92	0.41
1:A:196:ARG:HG3	1:A:244:VAL:CG2	2.50	0.41
1:B:187:PRO:HA	1:B:188:PRO:HD3	1.77	0.41
1:B:442:THR:C	1:B:444:THR:N	2.78	0.41
1:B:455:PHE:O	1:B:480:LEU:HA	2.19	0.41
1:B:487:ALA:HA	1:B:488:PRO:HD2	1.85	0.41
1:A:19:MET:HE3	1:A:124:LEU:C	2.45	0.41
1:A:44:HIS:O	1:A:45:PRO:C	2.64	0.41
1:B:266:THR:OG1	1:B:267:GLU:N	2.54	0.41
1:A:318:ASP:OD2	1:A:322:LYS:NZ	2.48	0.41
1:A:135:ARG:NH1	1:A:135:ARG:CG	2.81	0.41
1:A:384:VAL:O	1:A:388:LEU:HB2	2.20	0.41
1:A:448:LEU:HA	1:A:448:LEU:HD12	1.86	0.41
1:B:326:THR:HA	1:B:331:ALA:HB3	2.03	0.41
1:B:395:ARG:CG	1:B:395:ARG:NH2	2.82	0.41
1:B:465:GLY:O	1:B:469:VAL:HG23	2.19	0.41
1:A:46:LYS:HA	1:A:46:LYS:HD2	1.83	0.41
1:A:430:ALA:O	1:A:507:VAL:HG21	2.20	0.41
1:A:231:SER:OG	1:A:234:GLY:HA2	2.21	0.41
1:B:57:LEU:HD23	1:B:57:LEU:HA	1.80	0.41
1:B:196:ARG:HB2	1:B:242:VAL:HG22	2.03	0.41
1:B:153:THR:HA	1:B:160:THR:HG22	2.03	0.41
1:A:37:ALA:C	1:A:39:ASP:H	2.28	0.40
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.32	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:HD2	1:A:370:LEU:HD22	2.03	0.40
1:A:434:ALA:O	1:A:506:HIS:HA	2.21	0.40
1:B:323:LEU:HD23	1:B:336:LEU:HD21	2.03	0.40
1:A:166:ARG:O	1:A:290:ARG:NH1	2.51	0.40
1:B:52:PRO:HB2	1:B:404:PHE:HZ	1.87	0.40
1:A:119:TRP:C	1:A:122:PRO:HD2	2.46	0.40
1:A:229:LEU:HD23	1:A:229:LEU:C	2.46	0.40
1:A:476:ARG:HB2	1:A:478:VAL:HG23	2.03	0.40
1:A:488:PRO:O	1:A:489:GLU:C	2.64	0.40
1:A:439:ALA:HB1	1:A:490:ILE:HG13	2.04	0.40
1:B:223:SER:O	1:B:226:ARG:HD3	2.22	0.40
1:B:287:SER:HB3	1:B:292:PHE:CD2	2.56	0.40
1:A:24:ASP:HB2	1:A:61:TRP:HZ2	1.80	0.40
1:B:240:LEU:C	1:B:240:LEU:HD22	2.46	0.40
1:B:396:GLU:O	2:B:600:KCT:H10	2.21	0.40

There are no symmetry-related clashes.

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	506/549 (92%)	454 (90%)	48 (10%)	4 (1%)	16	30
1	B	503/549 (92%)	471 (94%)	30 (6%)	2 (0%)	30	50
All	All	1009/1098 (92%)	925 (92%)	78 (8%)	6 (1%)	21	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	HIS
1	A	155	LEU
1	A	45	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	304	SER
1	A	368	PRO
1	A	488	PRO

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	396/432 (92%)	373 (94%)	23 (6%)	18	34
1	B	390/432 (90%)	365 (94%)	25 (6%)	16	29
All	All	786/864 (91%)	738 (94%)	48 (6%)	17	31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	33	LEU
1	A	60	ARG
1	A	66	GLN
1	A	123	LEU
1	A	126	GLU
1	A	135	ARG
1	A	155	LEU
1	A	180	LYS
1	A	189	ARG
1	A	212	ARG
1	A	237	LEU
1	A	240	LEU
1	A	301	LEU
1	A	371	HIS
1	A	375	PRO
1	A	379	ARG
1	A	414	CYS
1	A	426	TRP
1	A	427	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	448	LEU
1	A	469	VAL
1	A	514	LEU
1	B	5	ILE
1	B	33	LEU
1	B	55	MET
1	B	123	LEU
1	B	130	GLU
1	B	134	THR
1	B	138	LEU
1	B	139	ASP
1	B	155	LEU
1	B	226	ARG
1	B	240	LEU
1	B	242	VAL
1	B	254	SER
1	B	259	ARG
1	B	267	GLU
1	B	294	THR
1	B	300	THR
1	B	301	LEU
1	B	371	HIS
1	B	379	ARG
1	B	395	ARG
1	B	409	ARG
1	B	471	ARG
1	B	517	GLU
1	B	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	29	GLN
1	A	66	GLN
1	A	193	GLN
1	A	403	HIS
1	B	107	HIS
1	B	193	GLN
1	B	280	HIS
1	B	371	HIS
1	B	406	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	486	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	KCT	B	600	-	31,32,32	2.05	8 (25%)	43,50,50	2.03	16 (37%)
2	KCT	A	600	-	31,32,32	1.96	11 (35%)	43,50,50	1.97	16 (37%)

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	KCT	B	600	-	-	3/4/16/16	0/6/6/6
2	KCT	A	600	-	-	3/4/16/16	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	KCT	C16-C23	6.73	1.52	1.40
2	A	600	KCT	C16-C23	6.10	1.51	1.40
2	B	600	KCT	C21-C22	3.45	1.46	1.40
2	A	600	KCT	C20-C21	-3.28	1.39	1.46
2	B	600	KCT	C20-C21	-3.15	1.39	1.46
2	A	600	KCT	C21-C22	2.88	1.45	1.40
2	B	600	KCT	O24-C5	2.85	1.30	1.23
2	B	600	KCT	C3-C4	2.43	1.43	1.38
2	A	600	KCT	O27-C25	-2.36	1.23	1.30
2	A	600	KCT	C7-N6	2.36	1.48	1.46
2	A	600	KCT	O24-C5	2.35	1.28	1.23
2	A	600	KCT	C3-C2	2.26	1.43	1.38
2	A	600	KCT	C3-C4	2.10	1.42	1.38
2	B	600	KCT	C10-C9	2.09	1.42	1.38
2	A	600	KCT	C2-C1	2.09	1.42	1.38
2	B	600	KCT	C9-C8	2.07	1.42	1.38
2	A	600	KCT	C10-C9	2.05	1.42	1.38
2	B	600	KCT	C10-C11	2.04	1.42	1.38
2	A	600	KCT	C10-C11	2.02	1.42	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	KCT	C22-C7-C25	5.67	118.33	109.83
2	A	600	KCT	C25-C7-N6	-4.80	105.46	112.05
2	B	600	KCT	C17-C18-N12	-3.99	124.85	130.50
2	A	600	KCT	C23-C5-N6	3.87	109.68	106.76
2	B	600	KCT	C23-C5-N6	3.83	109.64	106.76
2	A	600	KCT	C17-C18-N12	-3.34	125.77	130.50
2	A	600	KCT	C4-C15-C14	3.27	122.68	119.07
2	A	600	KCT	C22-C7-C25	3.13	114.53	109.83
2	A	600	KCT	C1-C14-N13	3.12	133.52	129.07
2	B	600	KCT	C1-C14-N13	3.04	133.41	129.07
2	A	600	KCT	C1-C14-C15	-3.02	118.53	121.68
2	B	600	KCT	C25-C7-N6	-2.94	108.02	112.05
2	B	600	KCT	C4-C15-C14	2.92	122.29	119.07
2	B	600	KCT	C1-C14-C15	-2.87	118.69	121.68
2	A	600	KCT	C11-C19-N12	2.85	133.14	129.07
2	B	600	KCT	C11-C19-N12	2.70	132.93	129.07
2	B	600	KCT	C21-C20-C19	2.61	108.74	106.21
2	B	600	KCT	C21-C18-N12	2.56	111.60	108.89
2	A	600	KCT	C21-C20-C19	2.56	108.69	106.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	KCT	C18-C17-N13	-2.51	126.94	130.50
2	A	600	KCT	C16-C17-N13	2.50	111.54	108.89
2	B	600	KCT	C18-C17-N13	-2.49	126.97	130.50
2	B	600	KCT	C16-C17-N13	2.46	111.49	108.89
2	A	600	KCT	C23-C16-C17	-2.36	115.52	118.61
2	A	600	KCT	O24-C5-N6	-2.33	123.98	125.97
2	A	600	KCT	C11-C19-C20	-2.31	119.27	121.68
2	B	600	KCT	C23-C16-C17	-2.31	115.58	118.61
2	A	600	KCT	C21-C18-N12	2.22	111.24	108.89
2	A	600	KCT	C8-C20-C19	2.21	121.51	119.07
2	B	600	KCT	O24-C5-N6	-2.18	124.10	125.97
2	B	600	KCT	C11-C19-C20	-2.09	119.50	121.68
2	B	600	KCT	C21-C18-C17	2.07	123.54	120.65

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	KCT	O27-C25-C7-N6
2	A	600	KCT	O26-C25-C7-N6
2	A	600	KCT	O26-C25-C7-C22
2	B	600	KCT	O27-C25-C7-N6
2	B	600	KCT	O26-C25-C7-N6
2	B	600	KCT	O26-C25-C7-C22

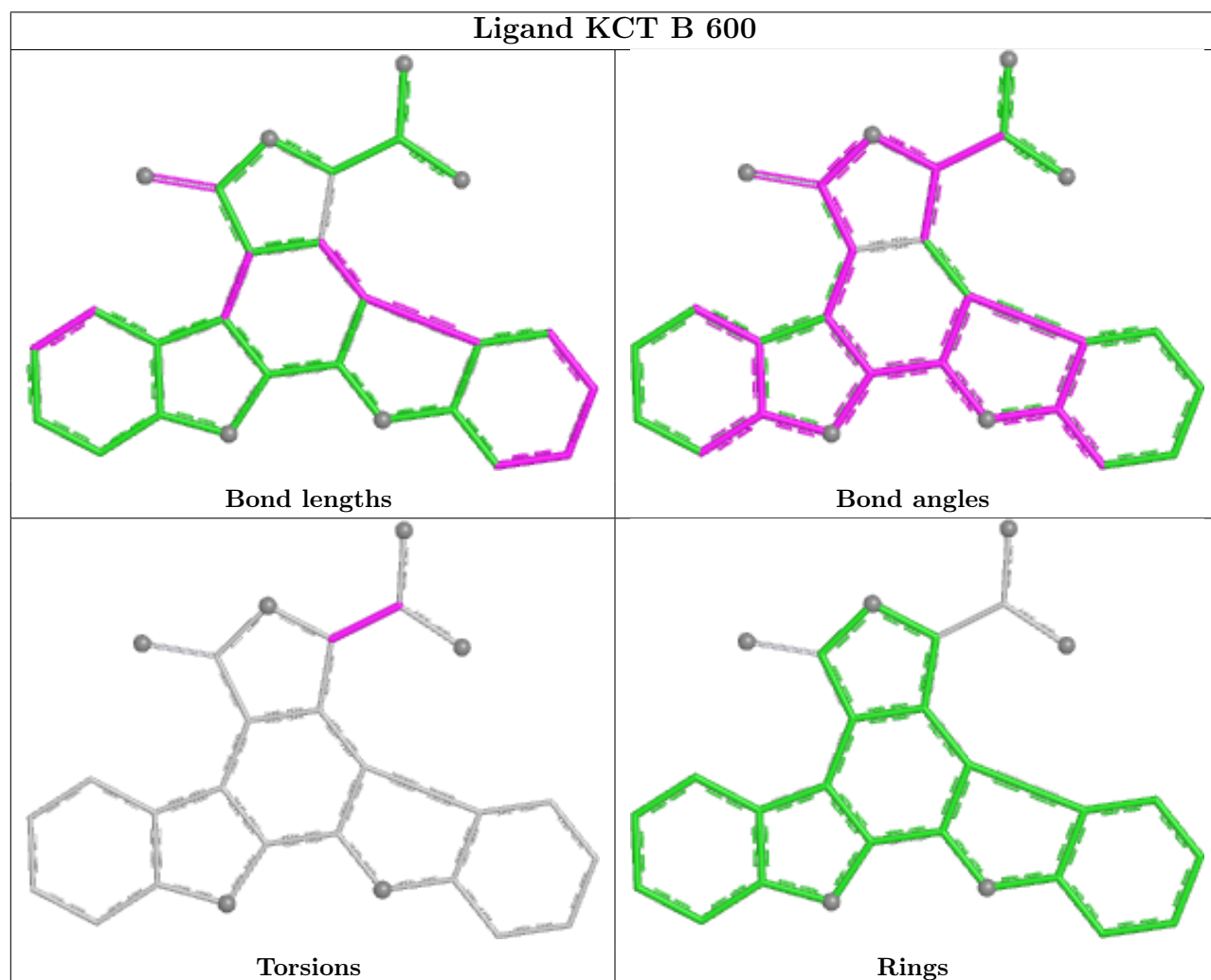
There are no ring outliers.

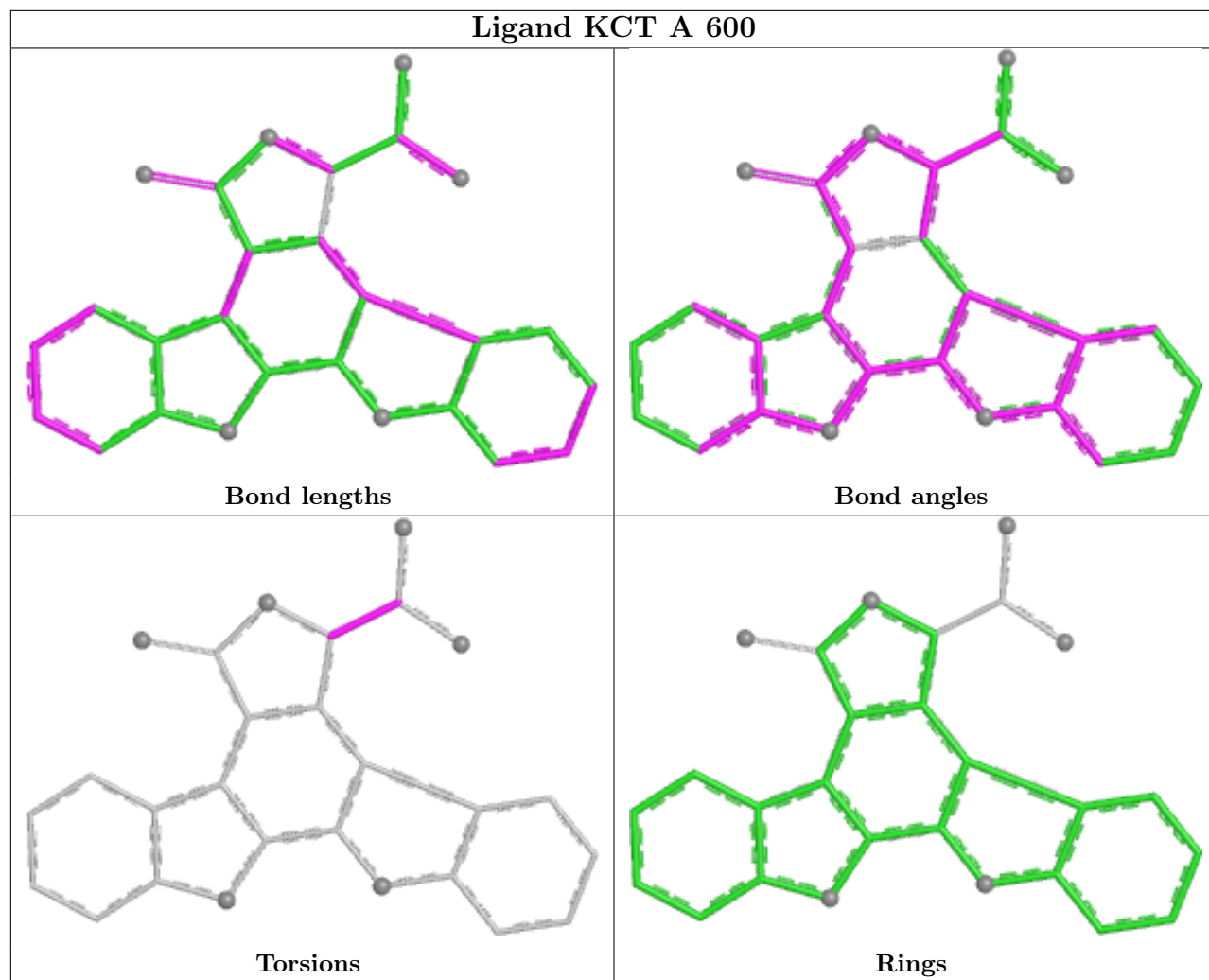
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	KCT	1	0
2	A	600	KCT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	514/549 (93%)	0.04	6 (1%) 76 76	45, 66, 91, 117	0
1	B	511/549 (93%)	-0.15	7 (1%) 73 73	34, 52, 80, 108	0
All	All	1025/1098 (93%)	-0.06	13 (1%) 75 75	34, 59, 88, 117	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ASP	3.2
1	B	44	HIS	3.1
1	B	41	THR	3.1
1	A	39	ASP	2.7
1	B	43	THR	2.5
1	A	43	THR	2.3
1	A	405	GLY	2.3
1	A	247	ALA	2.3
1	A	529	ALA	2.2
1	A	252	MET	2.2
1	B	37	ALA	2.1
1	B	2	ASN	2.0
1	B	417	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

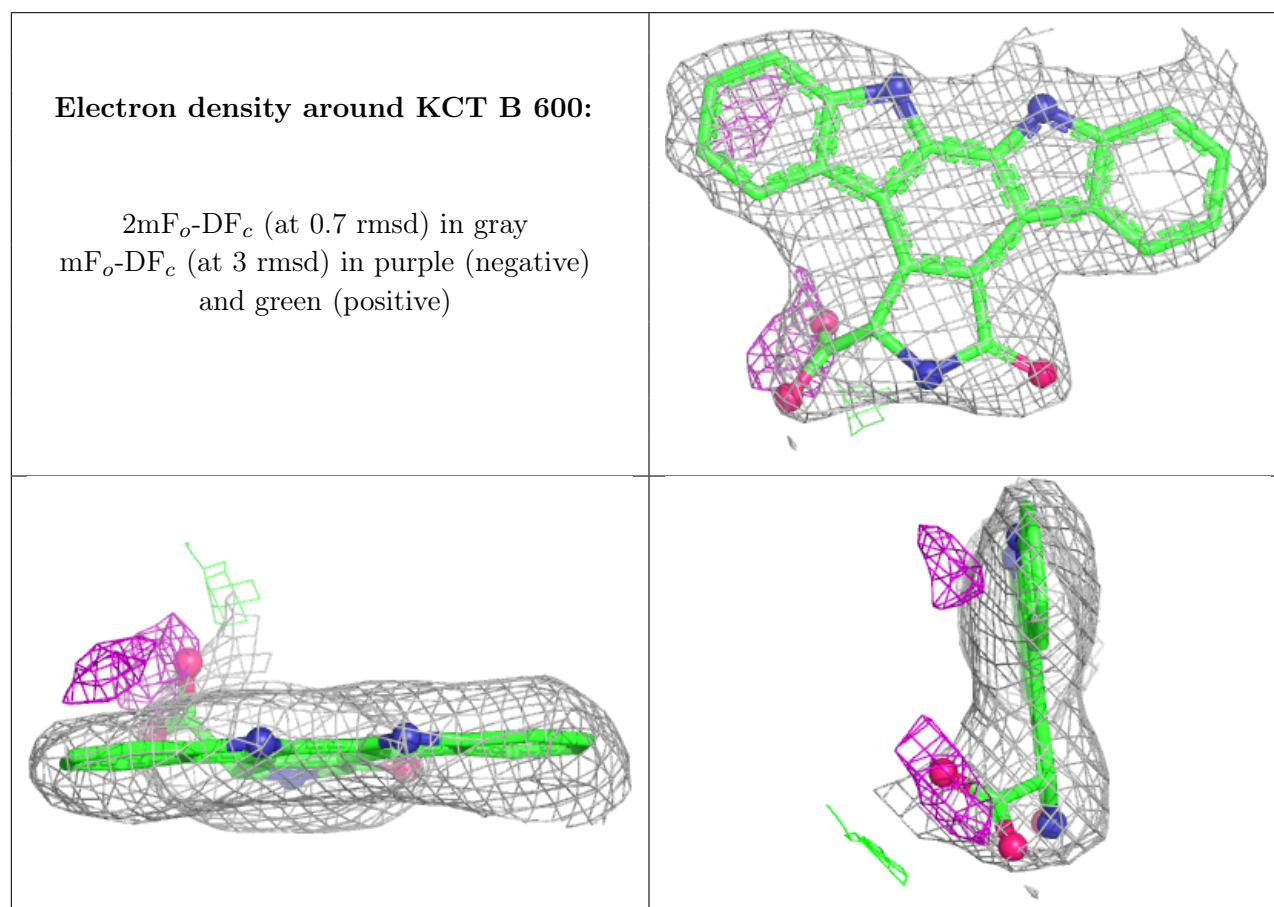
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

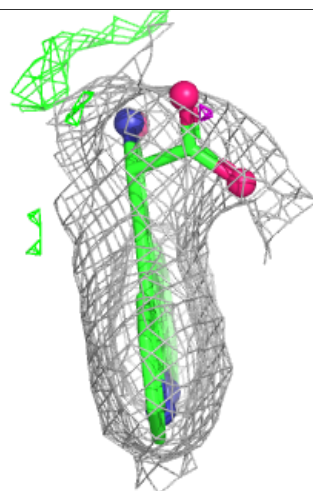
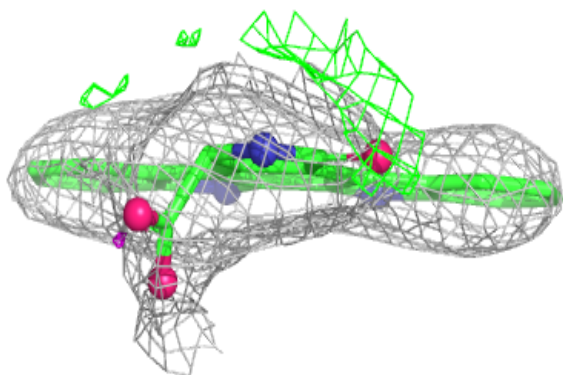
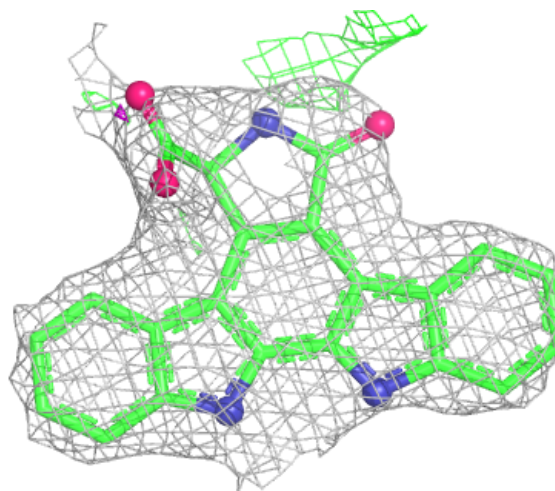
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KCT	B	600	27/27	0.90	0.13	59,64,75,80	0
2	KCT	A	600	27/27	0.92	0.11	69,71,80,84	0

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 KCT A 600:

$2mF_o-DF_c$ (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.