



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:54 AM UTC

PDB ID : 4KIK / pdb_00004kik
Title : Human I κ B kinase beta
Authors : Liu, S.; Mosyak, L.
Deposited on : 2013-05-02
Resolution : 2.83 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

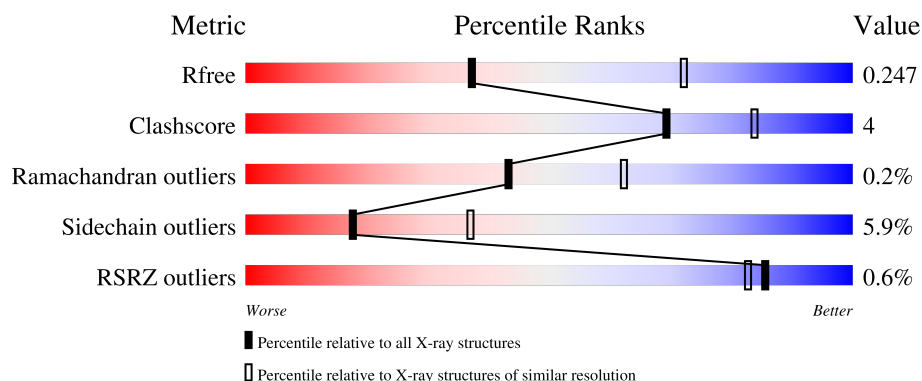
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	677	
2	B	677	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10602 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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	P	S	0	1	0
			5041	3166	894	947	1	33			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP O14920
A	-4	HIS	-	expression tag	UNP O14920
A	-3	HIS	-	expression tag	UNP O14920
A	-2	HIS	-	expression tag	UNP O14920
A	-1	HIS	-	expression tag	UNP O14920
A	0	HIS	-	expression tag	UNP O14920
A	1	HIS	-	expression tag	UNP O14920
A	665	SER	-	expression tag	UNP O14920
A	666	PRO	-	expression tag	UNP O14920
A	667	GLY	-	expression tag	UNP O14920
A	668	ARG	-	expression tag	UNP O14920
A	669	PRO	-	expression tag	UNP O14920
A	670	LEU	-	expression tag	UNP O14920
A	671	ASN	-	expression tag	UNP O14920

- Molecule 2 is a protein called Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	650	Total	C	N	O	P	S	0	0	0
			5270	3311	928	995	2	34			

There are 14 discrepancies between the modelled and reference sequences:

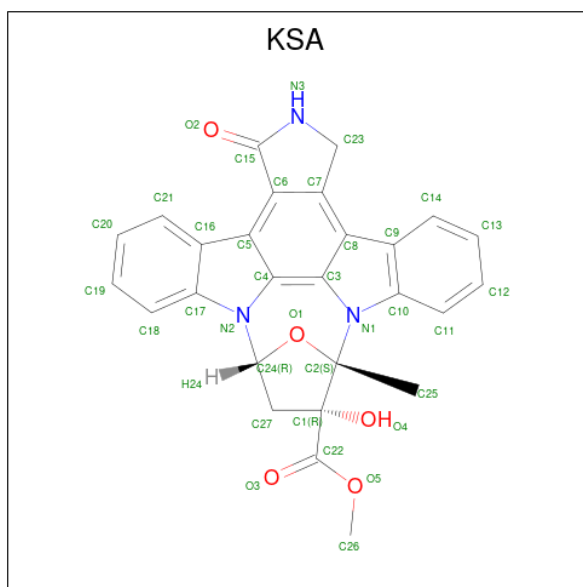
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	MET	-	expression tag	UNP O14920
B	-4	HIS	-	expression tag	UNP O14920

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP O14920
B	-2	HIS	-	expression tag	UNP O14920
B	-1	HIS	-	expression tag	UNP O14920
B	0	HIS	-	expression tag	UNP O14920
B	1	HIS	-	expression tag	UNP O14920
B	665	SER	-	expression tag	UNP O14920
B	666	PRO	-	expression tag	UNP O14920
B	667	GLY	-	expression tag	UNP O14920
B	668	ARG	-	expression tag	UNP O14920
B	669	PRO	-	expression tag	UNP O14920
B	670	LEU	-	expression tag	UNP O14920
B	671	ASN	-	expression tag	UNP O14920

- Molecule 3 is K-252A (CCD ID: KSA) (formula: $C_{27}H_{21}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	27	3	5		
3	B	1	Total	C	N	O	0	0
			35	27	3	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		

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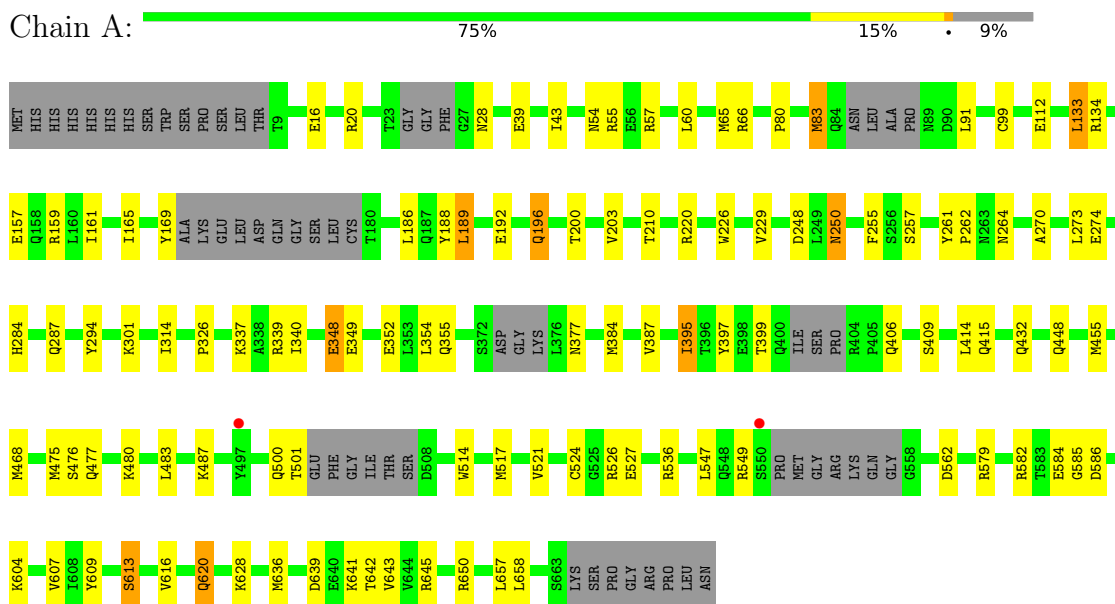
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	89	Total	O	0	0
			89	89		

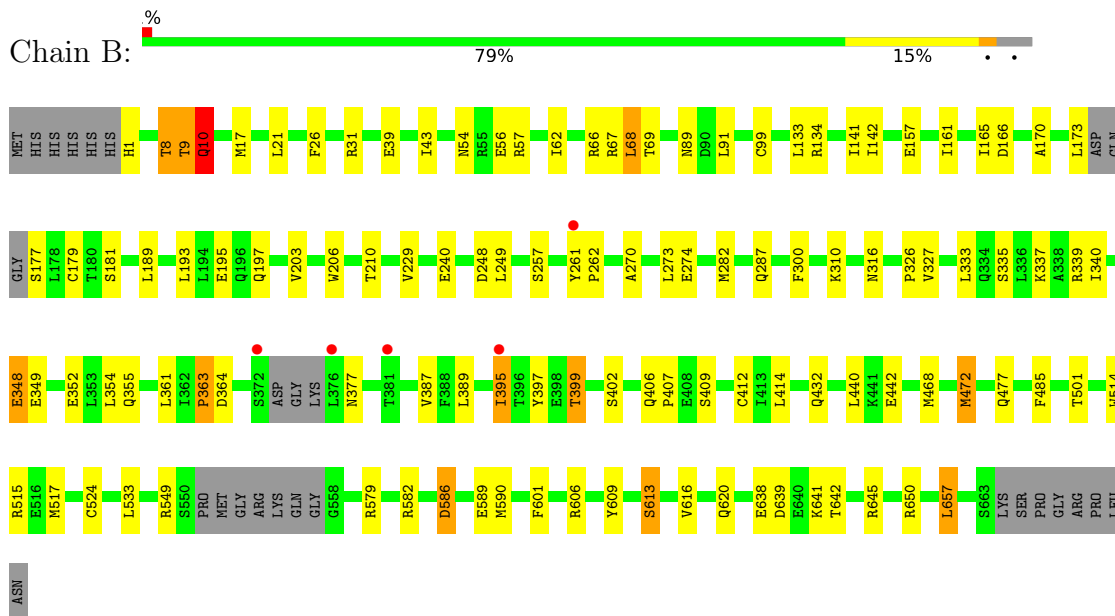
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta



- Molecule 2: Inhibitor of nuclear factor kappa-B kinase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.95Å 68.69Å 107.40Å 90.00° 107.03° 90.00°	Depositor
Resolution (Å)	47.17 – 2.83 47.17 – 2.83	Depositor EDS
% Data completeness (in resolution range)	93.7 (47.17-2.83) 94.1 (47.17-2.83)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.184 , 0.236 0.192 , 0.247	Depositor DCC
R_{free} test set	1742 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10602	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.86	2/5110 (0.0%)	1.42	33/6889 (0.5%)
2	B	0.85	2/5340 (0.0%)	1.41	36/7211 (0.5%)
All	All	0.85	4/10450 (0.0%)	1.42	69/14100 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	590	MET	SD-CE	-7.56	1.60	1.79
2	B	472	MET	SD-CE	-5.31	1.66	1.79
1	A	314	ILE	CG1-CD1	-5.04	1.32	1.51
1	A	83	MET	SD-CE	-5.02	1.67	1.79

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	363	PRO	CA-C-N	10.52	140.63	121.70
2	B	363	PRO	C-N-CA	10.52	140.63	121.70
1	A	250	ASN	CA-C-N	8.89	137.71	121.70
1	A	250	ASN	C-N-CA	8.89	137.71	121.70
2	B	586	ASP	CA-CB-CG	7.96	120.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	THR	CA-C-N	7.91	130.88	120.28
2	B	8	THR	C-N-CA	7.91	130.88	120.28
1	A	250	ASN	N-CA-C	7.88	123.05	112.88
2	B	485	PHE	CA-CB-CG	6.53	120.33	113.80
2	B	210	THR	CA-C-N	6.30	128.63	120.44
2	B	210	THR	C-N-CA	6.30	128.63	120.44
1	A	210	THR	CA-C-N	6.13	128.41	120.44
1	A	210	THR	C-N-CA	6.13	128.41	120.44
1	A	255	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	99	CYS	CA-C-N	5.97	129.09	120.38
1	A	99	CYS	C-N-CA	5.97	129.09	120.38
2	B	248	ASP	CA-CB-CG	5.95	118.55	112.60
2	B	363	PRO	N-CA-C	-5.93	100.48	110.21
1	A	248	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	586	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	549	ARG	CA-C-N	5.79	132.12	121.70
1	A	549	ARG	C-N-CA	5.79	132.12	121.70
2	B	363	PRO	O-C-N	-5.78	117.32	122.93
2	B	99	CYS	CA-C-N	5.77	128.59	120.28
2	B	99	CYS	C-N-CA	5.77	128.59	120.28
1	A	585	GLY	N-CA-C	5.74	118.97	110.42
1	A	273	LEU	CA-C-N	5.71	127.86	120.44
1	A	273	LEU	C-N-CA	5.71	127.86	120.44
2	B	62	ILE	CA-C-N	5.54	127.64	120.44
2	B	62	ILE	C-N-CA	5.54	127.64	120.44
2	B	68	LEU	CA-C-N	5.51	129.04	121.33
2	B	68	LEU	C-N-CA	5.51	129.04	121.33
2	B	340	ILE	CA-C-N	5.36	127.78	120.54
2	B	340	ILE	C-N-CA	5.36	127.78	120.54
1	A	643	VAL	CA-C-N	5.36	127.31	120.56
1	A	643	VAL	C-N-CA	5.36	127.31	120.56
2	B	26	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	340	ILE	CA-C-N	5.33	127.69	120.38
1	A	340	ILE	C-N-CA	5.33	127.69	120.38
2	B	195	GLU	CA-C-N	5.28	129.64	122.19
2	B	195	GLU	C-N-CA	5.28	129.64	122.19
1	A	620	GLN	CA-C-N	5.27	127.34	120.28
1	A	620	GLN	C-N-CA	5.27	127.34	120.28
2	B	273	LEU	CA-C-N	5.26	127.28	120.44
2	B	273	LEU	C-N-CA	5.26	127.28	120.44
1	A	229	VAL	CA-C-N	5.21	127.53	120.44
1	A	229	VAL	C-N-CA	5.21	127.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	MET	CA-C-N	5.20	131.06	121.70
1	A	83	MET	C-N-CA	5.20	131.06	121.70
2	B	377	ASN	CA-CB-CG	5.20	117.80	112.60
2	B	517	MET	CA-C-N	5.18	127.17	120.44
2	B	517	MET	C-N-CA	5.18	127.17	120.44
2	B	229	VAL	CA-C-N	5.15	127.14	120.44
2	B	229	VAL	C-N-CA	5.15	127.14	120.44
2	B	206	TRP	CA-C-N	5.15	127.13	120.44
2	B	206	TRP	C-N-CA	5.15	127.13	120.44
2	B	549	ARG	CA-C-N	5.13	130.93	121.70
2	B	549	ARG	C-N-CA	5.13	130.93	121.70
1	A	517	MET	CA-C-N	5.07	127.03	120.44
1	A	517	MET	C-N-CA	5.07	127.03	120.44
2	B	348	GLU	CA-C-N	5.06	127.57	120.28
2	B	348	GLU	C-N-CA	5.06	127.57	120.28
1	A	348	GLU	CA-C-N	5.06	127.56	120.28
1	A	348	GLU	C-N-CA	5.06	127.56	120.28
1	A	526	ARG	CA-C-N	5.04	127.34	120.54
1	A	526	ARG	C-N-CA	5.04	127.34	120.54
1	A	250	ASN	O-C-N	-5.03	116.26	122.25
1	A	250	ASN	CA-C-O	-5.01	113.67	119.59
2	B	442	GLU	CB-CG-CD	5.01	121.11	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	ASN	Mainchain,Peptide
2	B	363	PRO	Mainchain,Peptide

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	5041	0	5064	37	1
2	B	5270	0	5300	37	1
3	A	35	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	35	0	21	0	0
4	A	132	0	0	1	0
4	B	89	0	0	1	0
All	All	10602	0	10406	73	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (73) 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:604:LYS:O	1:A:607:VAL:HG22	1.90	0.72
2:B:638:GLU:O	2:B:642:THR:HG23	1.96	0.66
2:B:9:THR:HG21	2:B:17:MET:O	1.96	0.65
1:A:536:ARG:HH12	1:A:628:LYS:HE3	1.63	0.63
2:B:68:LEU:HD21	2:B:141:ILE:HD13	1.80	0.62
2:B:134:ARG:HH21	2:B:300:PHE:HB3	1.67	0.59
1:A:55:ARG:HG2	1:A:91:LEU:HD21	1.84	0.58
1:A:483:LEU:CD2	1:A:521:VAL:HG13	2.34	0.58
1:A:200:THR:O	1:A:203:VAL:HG22	2.04	0.58
2:B:397:TYR:HB3	2:B:609:TYR:HD1	1.69	0.57
2:B:399:THR:HB	2:B:606:ARG:HG2	1.87	0.56
2:B:524:CYS:HB2	2:B:639:ASP:CG	2.32	0.55
1:A:159:ARG:HB3	1:A:377:ASN:HB3	1.88	0.55
1:A:524:CYS:HB2	1:A:639:ASP:CG	2.34	0.53
1:A:409:SER:HB2	1:A:432:GLN:HE22	1.74	0.52
1:A:397:TYR:HB3	1:A:609:TYR:HD1	1.76	0.51
1:A:112:GLU:HB3	4:A:997:HOH:O	2.09	0.51
1:A:80:PRO:HD2	1:A:83:MET:HE2	1.94	0.50
1:A:455:MET:HE1	1:A:547:LEU:HB3	1.93	0.50
2:B:579:ARG:HA	2:B:582:ARG:HD2	1.93	0.50
1:A:186:LEU:HA	1:A:189:LEU:HD22	1.95	0.49
2:B:326:PRO:HD2	2:B:339:ARG:HH22	1.77	0.48
2:B:333:LEU:HD11	2:B:361:LEU:HD23	1.96	0.48
1:A:397:TYR:H	1:A:613:SER:HB3	1.79	0.48
1:A:395:ILE:HG22	1:A:620:GLN:HE22	1.79	0.48
1:A:192:GLU:HB2	1:A:196:GLN:HE21	1.79	0.47
2:B:54:ASN:HA	2:B:57:ARG:HB2	1.96	0.47
1:A:54:ASN:HA	1:A:57:ARG:HB2	1.95	0.47
2:B:514:TRP:CE2	2:B:650:ARG:HG3	2.50	0.47
1:A:579:ARG:HA	1:A:582:ARG:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:SER:HA	1:A:616:VAL:HG22	1.97	0.47
1:A:20:ARG:HD2	1:A:28:ASN:OD1	2.15	0.47
2:B:613:SER:HA	2:B:616:VAL:HG22	1.96	0.47
2:B:395:ILE:HG22	2:B:620:GLN:HE22	1.79	0.46
2:B:261:TYR:CD1	2:B:262:PRO:HA	2.50	0.46
2:B:142:ILE:O	2:B:170:ALA:HA	2.16	0.46
1:A:326:PRO:HD2	1:A:339:ARG:HH22	1.81	0.45
2:B:270:ALA:O	2:B:274:GLU:HB2	2.15	0.45
2:B:409:SER:HB2	2:B:432:GLN:HE22	1.82	0.45
2:B:9:THR:CG2	2:B:17:MET:O	2.64	0.45
1:A:270:ALA:O	1:A:274:GLU:HB2	2.16	0.45
2:B:316:ASN:HD22	2:B:389:LEU:HD23	1.82	0.45
2:B:337:LYS:HB3	2:B:348:GLU:HG2	1.99	0.45
1:A:337:LYS:HB3	1:A:348:GLU:HG2	1.99	0.44
1:A:55:ARG:CG	1:A:91:LEU:HD21	2.47	0.44
1:A:514:TRP:CE2	1:A:650:ARG:HG3	2.52	0.44
2:B:240:GLU:HG3	2:B:282:MET:HE1	1.98	0.44
1:A:352:GLU:HG2	1:A:354:LEU:HD13	1.99	0.44
1:A:294:TYR:CE1	1:A:301:LYS:HG3	2.53	0.44
2:B:262:PRO:HD3	2:B:407:PRO:HG3	1.99	0.44
2:B:352:GLU:HG2	2:B:354:LEU:HD13	1.99	0.44
1:A:658:LEU:HD11	2:B:657:LEU:HB3	2.00	0.43
2:B:10:GLN:HB3	2:B:17:MET:HE2	2.01	0.43
1:A:641:LYS:HB3	1:A:645:ARG:NH1	2.35	0.42
2:B:21:LEU:HD21	2:B:31:ARG:HB2	2.01	0.42
1:A:476:SER:OG	1:A:636:MET:HE1	2.20	0.42
1:A:355:GLN:HG3	1:A:387:VAL:HG22	2.02	0.41
1:A:487:LYS:HE3	1:A:521:VAL:HG12	2.02	0.41
2:B:56:GLU:HG3	4:B:876:HOH:O	2.20	0.41
2:B:440:LEU:HD22	2:B:601:PHE:CG	2.55	0.41
1:A:261:TYR:CG	1:A:262:PRO:HA	2.56	0.41
2:B:89:ASN:OD1	2:B:91:LEU:HB2	2.21	0.41
1:A:284:HIS:HB3	1:A:287:GLN:HB3	2.01	0.41
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.89	0.41
1:A:57:ARG:HG2	1:A:169:TYR:C	2.46	0.41
2:B:641:LYS:HB3	2:B:645:ARG:NH1	2.36	0.41
1:A:188:TYR:CZ	1:A:220:ARG:HD3	2.56	0.41
2:B:189:LEU:HD12	2:B:193:LEU:HD13	2.03	0.41
2:B:249:LEU:HD12	2:B:412:CYS:SG	2.61	0.41
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.88	0.40
2:B:9:THR:H	2:B:9:THR:HG22	1.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:GLN:HG3	2:B:387:VAL:HG22	2.03	0.40
2:B:472:MET:HE1	2:B:533:LEU:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:THR:CG2	2:B:515:ARG:CD[2_542]	2.05	0.15

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	603/677 (89%)	587 (97%)	16 (3%)	0	100	100
2	B	641/677 (95%)	623 (97%)	15 (2%)	3 (0%)	24	43
All	All	1244/1354 (92%)	1210 (97%)	31 (2%)	3 (0%)	43	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	GLN
2	B	166	ASP
2	B	402	SER

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	562/611 (92%)	528 (94%)	34 (6%)	17	36
2	B	588/610 (96%)	554 (94%)	34 (6%)	18	38
All	All	1150/1221 (94%)	1082 (94%)	68 (6%)	18	37

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	39	GLU
1	A	43	ILE
1	A	60	LEU
1	A	65	MET
1	A	66	ARG
1	A	133	LEU
1	A	134	ARG
1	A	157	GLU
1	A	161	ILE
1	A	165	ILE
1	A	189	LEU
1	A	196	GLN
1	A	226	TRP
1	A	264	ASN
1	A	349	GLU
1	A	384	MET
1	A	395	ILE
1	A	399	THR
1	A	406	GLN
1	A	414	LEU
1	A	415	GLN
1	A	448	GLN
1	A	468	MET
1	A	475	MET
1	A	477	GLN
1	A	480	LYS
1	A	500	GLN
1	A	527	GLU
1	A	562	ASP
1	A	584	GLU
1	A	613	SER
1	A	642	THR
1	A	657	LEU

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Mol	Chain	Res	Type
2	B	1	HIS
2	B	8	THR
2	B	9	THR
2	B	10	GLN
2	B	39	GLU
2	B	43	ILE
2	B	66	ARG
2	B	67	ARG
2	B	69	THR
2	B	157	GLU
2	B	161	ILE
2	B	165	ILE
2	B	173	LEU
2	B	179	CYS
2	B	197	GLN
2	B	203	VAL
2	B	257	SER
2	B	287	GLN
2	B	310	LYS
2	B	327	VAL
2	B	335	SER
2	B	349	GLU
2	B	364	ASP
2	B	395	ILE
2	B	399	THR
2	B	406	GLN
2	B	414	LEU
2	B	468	MET
2	B	477	GLN
2	B	501	THR
2	B	586	ASP
2	B	589	GLU
2	B	613	SER
2	B	657	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	150	ASN
1	A	196	GLN
1	A	197	GLN

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Mol	Chain	Res	Type
1	A	232	HIS
1	A	250	ASN
1	A	287	GLN
1	A	308	ASN
1	A	316	ASN
1	A	432	GLN
1	A	448	GLN
1	A	477	GLN
1	A	500	GLN
1	A	548	GLN
1	A	581	GLN
1	A	588	GLN
1	A	611	GLN
1	A	620	GLN
2	B	54	ASN
2	B	196	GLN
2	B	197	GLN
2	B	232	HIS
2	B	287	GLN
2	B	308	ASN
2	B	432	GLN
2	B	478	GLN
2	B	581	GLN
2	B	588	GLN
2	B	620	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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
2	SEP	B	177	2	8,9,10	1.01	0	7,12,14	1.99	2 (28%)
2	SEP	B	181	2	8,9,10	1.14	1 (12%)	7,12,14	3.00	3 (42%)
1	SEP	A	257	1	8,9,10	2.22	4 (50%)	7,12,14	3.70	3 (42%)

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	SEP	B	177	2	-	5/6/8/10	-
2	SEP	B	181	2	-	3/6/8/10	-
1	SEP	A	257	1	-	3/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	SEP	P-O1P	3.56	1.61	1.50
1	A	257	SEP	P-OG	3.36	1.70	1.60
2	B	181	SEP	P-O1P	2.52	1.58	1.50
1	A	257	SEP	CB-CA	2.47	1.59	1.52
1	A	257	SEP	OG-CB	2.41	1.53	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	SEP	OG-CB-CA	8.10	116.03	108.14
2	B	181	SEP	OG-CB-CA	7.08	115.03	108.14
1	A	257	SEP	O3P-P-OG	4.17	117.54	106.67
2	B	177	SEP	OG-CB-CA	3.60	111.65	108.14
2	B	177	SEP	O3P-P-OG	2.66	113.60	106.67
2	B	181	SEP	OG-P-O1P	2.54	113.30	106.44
2	B	181	SEP	O2P-P-OG	2.17	112.32	106.67
1	A	257	SEP	O3P-P-O2P	-2.08	100.01	107.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	257	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	A	257	SEP	C-CA-CB-OG
2	B	177	SEP	N-CA-CB-OG
2	B	177	SEP	C-CA-CB-OG
2	B	177	SEP	CB-OG-P-O2P
2	B	181	SEP	CB-OG-P-O2P
2	B	177	SEP	CB-OG-P-O3P
2	B	181	SEP	CB-OG-P-O3P
1	A	257	SEP	CA-CB-OG-P
2	B	181	SEP	CA-CB-OG-P
2	B	177	SEP	CB-OG-P-O1P

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	$\# Z > 2$
3	KSA	A	800	-	40,42,42	1.61	4 (10%)	54,70,70	0.93	4 (7%)
3	KSA	B	700	-	40,42,42	1.13	4 (10%)	54,70,70	1.05	7 (12%)

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	KSA	A	800	-	-	1/8/46/46	-
3	KSA	B	700	-	-	2/8/46/46	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	KSA	C15-N3	7.59	1.41	1.35
3	A	800	KSA	C24-N2	4.99	1.49	1.45
3	B	700	KSA	C24-N2	4.54	1.49	1.45
3	B	700	KSA	C15-N3	3.76	1.38	1.35
3	B	700	KSA	C3-N1	2.74	1.42	1.40
3	A	800	KSA	C23-N3	2.24	1.47	1.45
3	A	800	KSA	O1-C2	-2.10	1.41	1.42
3	B	700	KSA	C10-N1	2.01	1.43	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	700	KSA	C5-C6-C7	2.94	122.81	120.76
3	A	800	KSA	C8-C7-C6	-2.91	119.33	121.25
3	B	700	KSA	C8-C7-C6	-2.89	119.34	121.25
3	A	800	KSA	C23-C7-C6	2.74	110.89	109.88
3	A	800	KSA	C5-C6-C7	2.50	122.51	120.76
3	B	700	KSA	C23-N3-C15	-2.32	111.74	113.86
3	B	700	KSA	C23-C7-C6	2.31	110.73	109.88
3	A	800	KSA	C23-N3-C15	-2.19	111.86	113.86
3	B	700	KSA	O4-C1-C22	2.14	112.64	109.40
3	B	700	KSA	O2-C15-N3	-2.13	122.98	125.35
3	B	700	KSA	C6-C15-N3	2.06	108.34	106.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

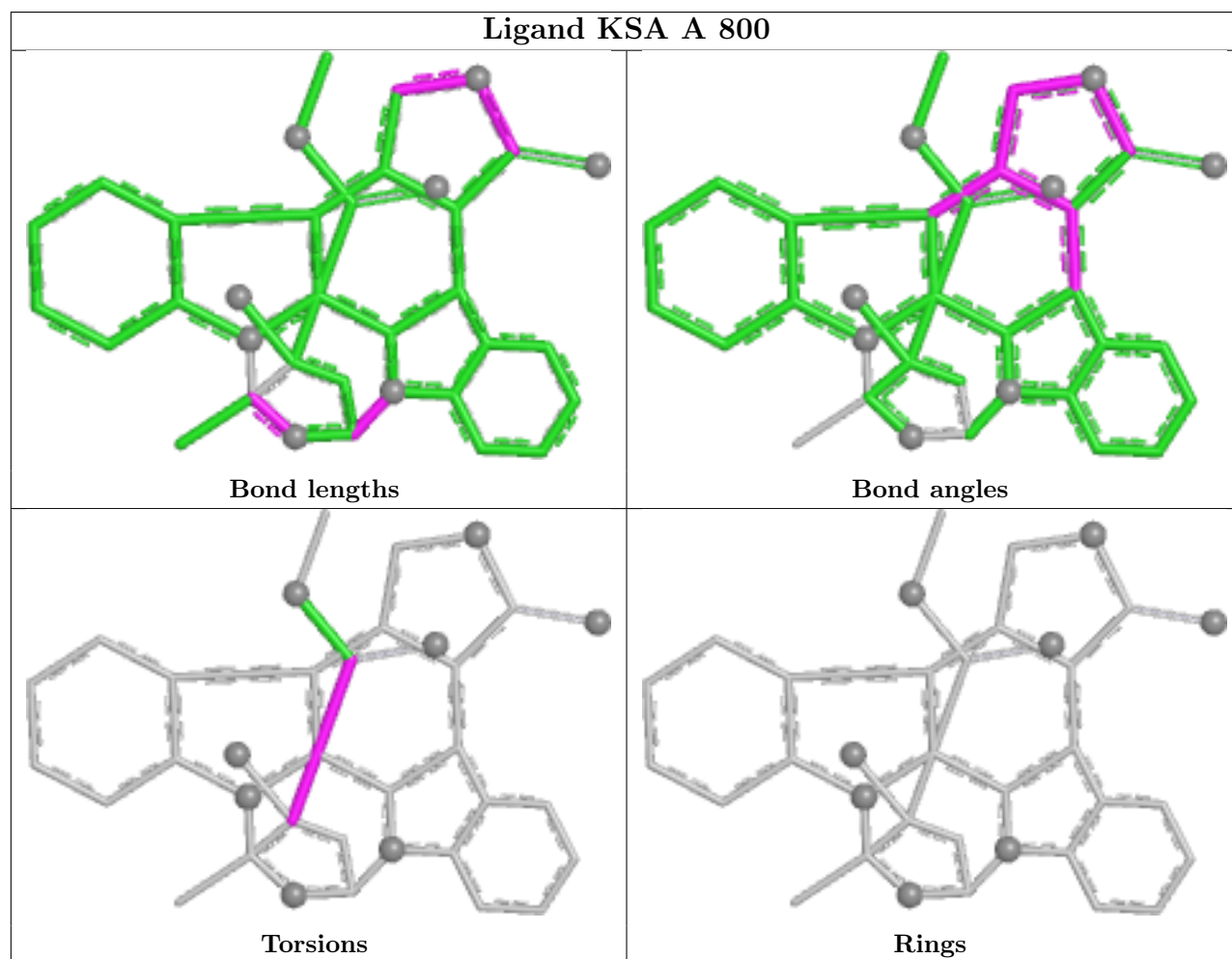
Mol	Chain	Res	Type	Atoms
3	A	800	KSA	O4-C1-C22-O3
3	B	700	KSA	O4-C1-C22-O3
3	B	700	KSA	O4-C1-C22-O5

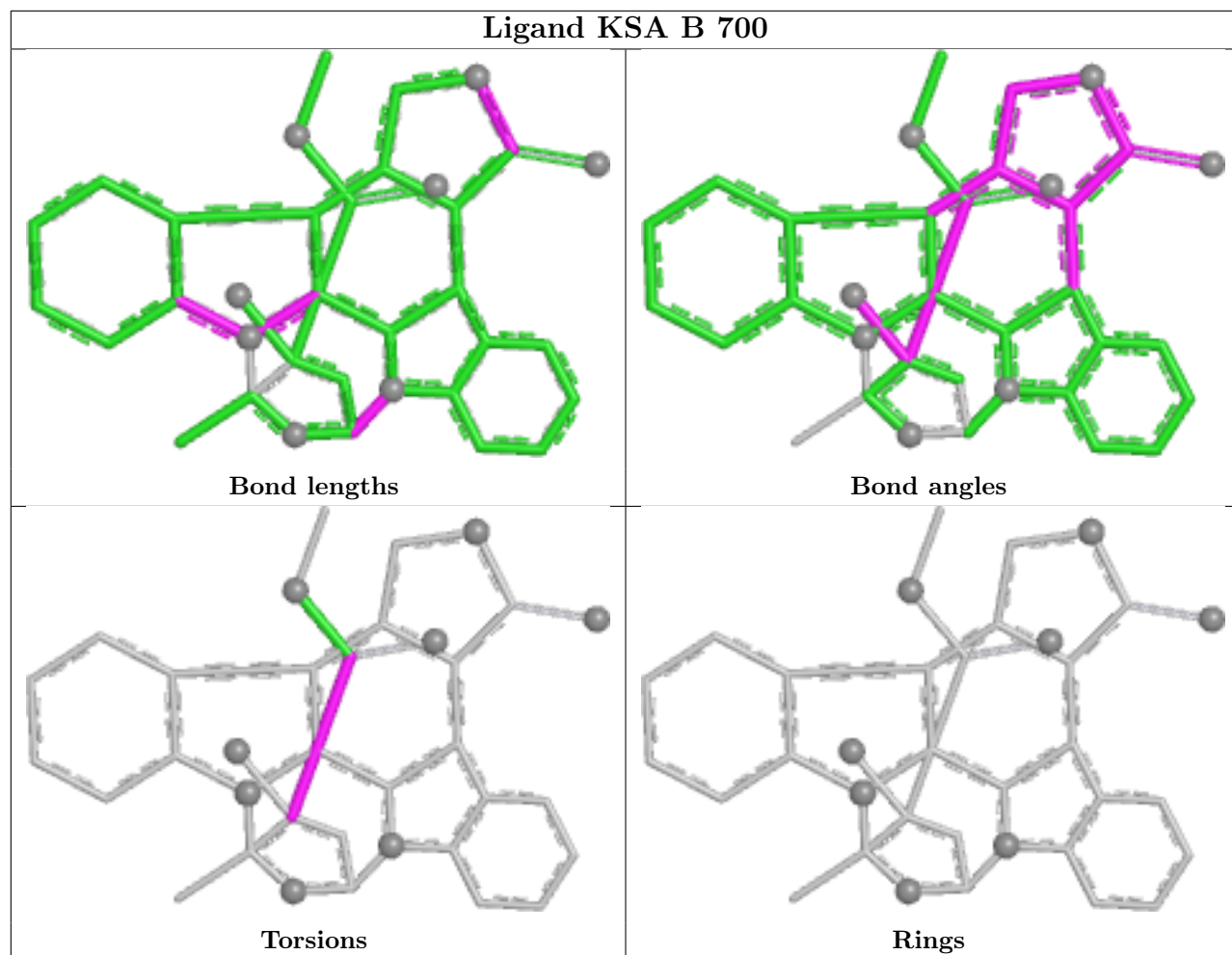
There are no ring outliers.

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 [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	618/677 (91%)	-0.32	2 (0%)	90 89	20, 45, 80, 126	1 (0%)
2	B	648/677 (95%)	-0.16	5 (0%)	82 78	27, 55, 88, 138	0
All	All	1266/1354 (93%)	-0.24	7 (0%)	85 83	20, 50, 84, 138	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	550	SER	3.3
2	B	261	TYR	3.2
2	B	376	LEU	2.6
2	B	395	ILE	2.5
1	A	497	TYR	2.4
2	B	372	SER	2.1
2	B	381	THR	2.1

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(Å ²)	Q < 0.9
2	SEP	B	177	10/11	0.71	0.12	85,98,112,113	0
1	SEP	A	257	10/11	0.79	0.14	40,52,72,73	0
2	SEP	B	181	10/11	0.95	0.06	49,56,65,67	0

6.3 Carbohydrates [i](#)

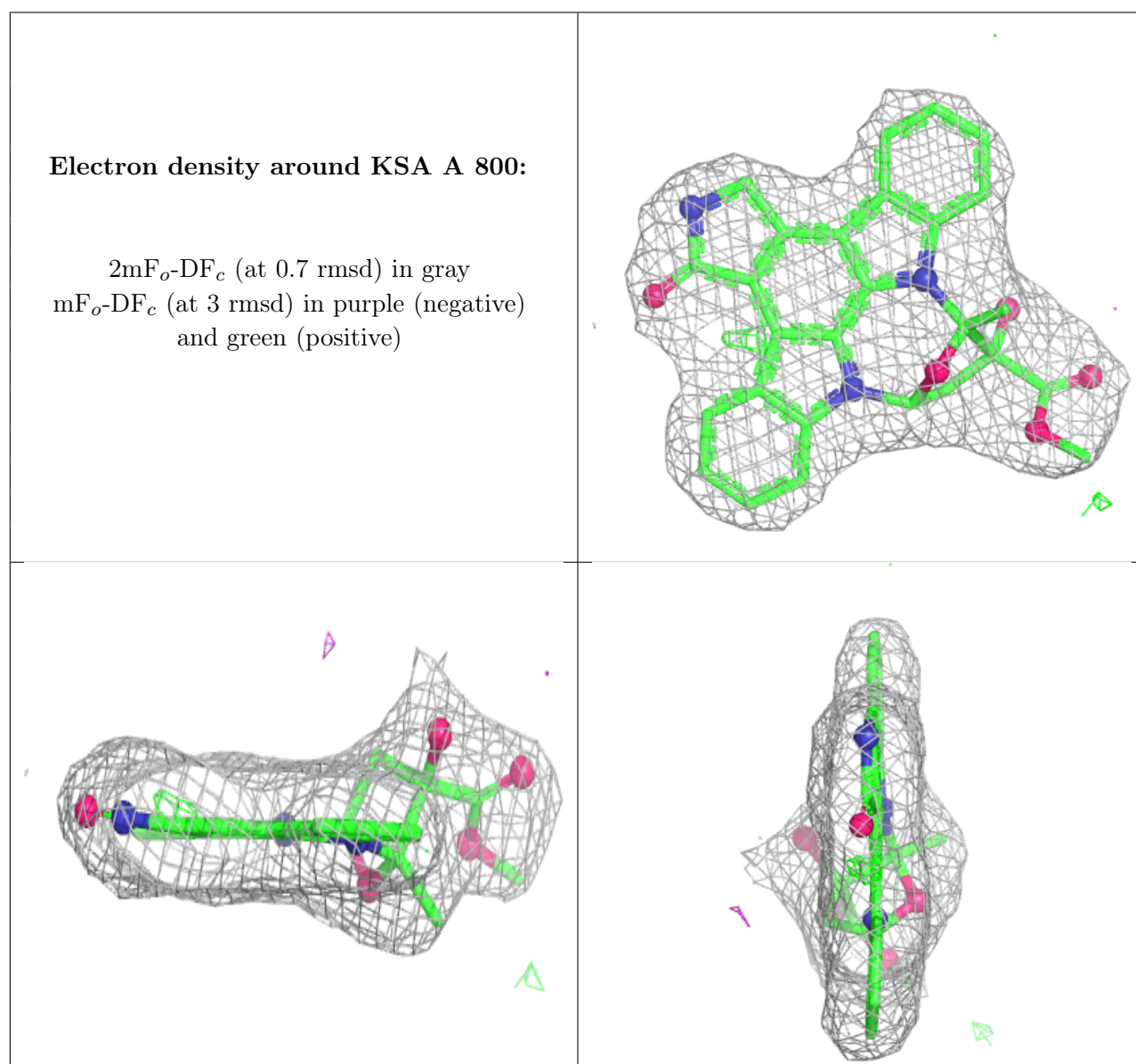
There are no oligosaccharides in this entry.

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.

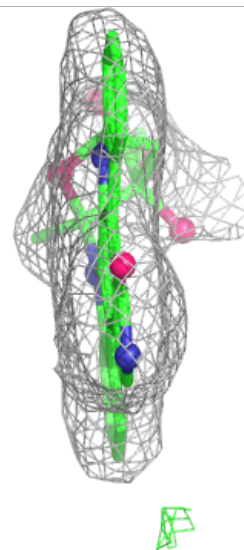
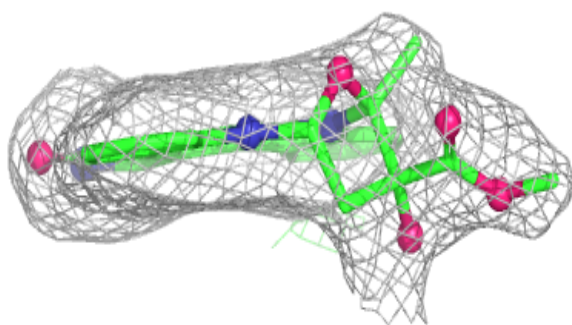
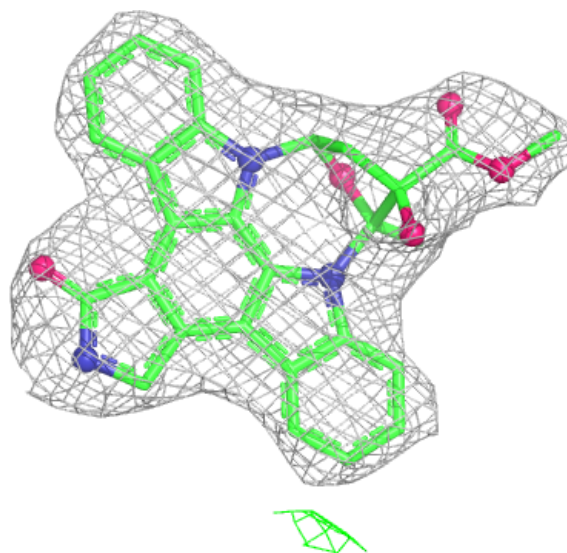
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	KSA	A	800	35/35	0.96	0.07	19,27,36,39	0
3	KSA	B	700	35/35	0.96	0.07	29,37,43,44	0

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 KSA B 700:

$2mF_o-DF_c$ (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.