

Full wwPDB X-ray Structure Validation Report (i)

May 18, 2020 – 06:37 pm BST

PDB ID : 4ACH

Title: GSK3b in complex with inhibitor

Authors : Xue, Y.; Ormo, M.

Deposited on : 2011-12-15

Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.11

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)

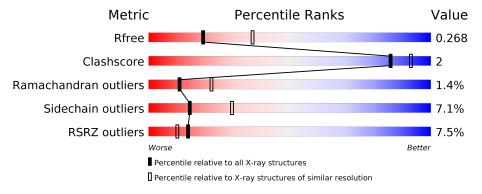
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	$3163 \ (2.60 - 2.60)$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60 - 2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain				
1	A	465	8% 67%	7%		25%	
1	В	465	66%	8%	•	25%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5838 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 GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	351	Total 2805	C 1804	N 482	O 508	S 11	0	0	1
1	В	351	Total 2805	C 1804	N 482	O 508	S 11	0	0	1

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	expression tag	UNP P49841
A	-43	SER	_	expression tag	UNP P49841
A	-42	TYR	-	expression tag	UNP P49841
A	-41	TYR	-	expression tag	UNP P49841
A	-40	HIS	_	expression tag	UNP P49841
A	-39	HIS	-	expression tag	UNP P49841
A	-38	HIS	-	expression tag	UNP P49841
A	-37	HIS	_	expression tag	UNP P49841
A	-36	HIS	-	expression tag	UNP P49841
A	-35	HIS	_	expression tag	UNP P49841
A	-34	ASP	_	expression tag	UNP P49841
A	-33	TYR	-	expression tag	UNP P49841
A	-32	ASP	_	expression tag	UNP P49841
A	-31	ILE	-	expression tag	UNP P49841
A	-30	PRO	_	expression tag	UNP P49841
A	-29	THR	_	expression tag	UNP P49841
A	-28	THR	_	expression tag	UNP P49841
A	-27	GLU	_	expression tag	UNP P49841
A	-26	ASN	-	expression tag	UNP P49841
A	-25	LEU	_	expression tag	UNP P49841
A	-24	TYR	=	expression tag	UNP P49841
A	-23	PHE	-	expression tag	UNP P49841
A	-22	GLN	-	expression tag	UNP P49841
A	-21	GLY	-	expression tag	UNP P49841
A	-20	ALA	_	expression tag	UNP P49841



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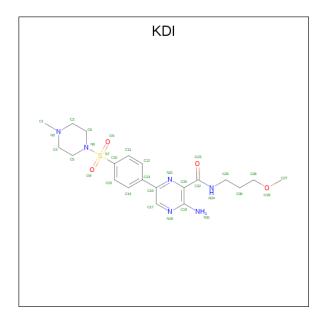
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P49841
A	-18	GLY	-	expression tag	UNP P49841
A	-17	SER	-	expression tag	UNP P49841
A	-16	SER	-	expression tag	UNP P49841
A	-15	HIS	-	expression tag	UNP P49841
A	-14	HIS	-	expression tag	UNP P49841
A	-13	HIS	-	expression tag	UNP P49841
A	-12	HIS	-	expression tag	UNP P49841
A	-11	HIS	-	expression tag	UNP P49841
A	-10	HIS	-	expression tag	UNP P49841
A	-9	SER	-	expression tag	UNP P49841
A	-8	SER	_	expression tag	UNP P49841
A	-7	GLY	-	expression tag	UNP P49841
A	-6	LEU	-	expression tag	UNP P49841
A	-5	VAL	_	expression tag	UNP P49841
A	-4	PRO	-	expression tag	UNP P49841
A	-3	ARG	_	expression tag	UNP P49841
A	-2	GLY	-	expression tag	UNP P49841
A	-1	SER	-	expression tag	UNP P49841
A	0	HIS	-	expression tag	UNP P49841
В	-44	MET	-	expression tag	UNP P49841
В	-43	SER	_	expression tag	UNP P49841
В	-42	TYR	-	expression tag	UNP P49841
В	-41	TYR	_	expression tag	UNP P49841
В	-40	HIS	-	expression tag	UNP P49841
В	-39	HIS	-	expression tag	UNP P49841
В	-38	HIS	-	expression tag	UNP P49841
В	-37	HIS	-	expression tag	UNP P49841
В	-36	HIS	-	expression tag	UNP P49841
В	-35	HIS	-	expression tag	UNP P49841
В	-34	ASP	-	expression tag	UNP P49841
В	-33	TYR	-	expression tag	UNP P49841
В	-32	ASP	-	expression tag	UNP P49841
В	-31	ILE	-	expression tag	UNP P49841
В	-30	PRO	-	expression tag	UNP P49841
В	-29	THR	-	expression tag	UNP P49841
В	-28	THR	-	expression tag	UNP P49841
В	-27	GLU	-	expression tag	UNP P49841
В	-26	ASN	-	expression tag	UNP P49841
В	-25	LEU	-	expression tag	UNP P49841
В	-24	TYR	-	expression tag	UNP P49841
В	-23	PHE	-	expression tag	UNP P49841



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Chain	Residue	Modelled	Actual	Comment	Reference
В	-22	GLN	-	expression tag	UNP P49841
В	-21	GLY	-	expression tag	UNP P49841
В	-20	ALA	-	expression tag	UNP P49841
В	-19	MET	-	expression tag	UNP P49841
В	-18	GLY	-	expression tag	UNP P49841
В	-17	SER	_	expression tag	UNP P49841
В	-16	SER	-	expression tag	UNP P49841
В	-15	HIS	-	expression tag	UNP P49841
В	-14	HIS	-	expression tag	UNP P49841
В	-13	HIS	-	expression tag	UNP P49841
В	-12	HIS	_	expression tag	UNP P49841
В	-11	HIS	-	expression tag	UNP P49841
В	-10	HIS	_	expression tag	UNP P49841
В	-9	SER	-	expression tag	UNP P49841
В	-8	SER	_	expression tag	UNP P49841
В	-7	GLY	-	expression tag	UNP P49841
В	-6	LEU	-	expression tag	UNP P49841
В	-5	VAL	_	expression tag	UNP P49841
В	-4	PRO	-	expression tag	UNP P49841
В	-3	ARG		expression tag	UNP P49841
В	-2	GLY	-	expression tag	UNP P49841
В	-1	SER	-	expression tag	UNP P49841
В	0	HIS	-	expression tag	UNP P49841

• Molecule 2 is 3-AMINO-N-(3-METHOXYPROPYL)-6- $\{4-[(4-METHYLPIPERAZIN-1-YL) SULFONYL]PHENYL\}PYRAZINE-2-CARBOXAMIDE (three-letter code: KDI) (formula: <math>C_{20}H_{28}N_6O_4S$).





Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf			
9	Λ	1	Total	С	Ν	О	O S		0	
	A	1	31	20	6	4	1	0		
9	D	1	Total	С	N	О	S	0	0	
	D	1	31	20	6	4	1	0	U	

$\bullet\,$ Molecule 3 is water.

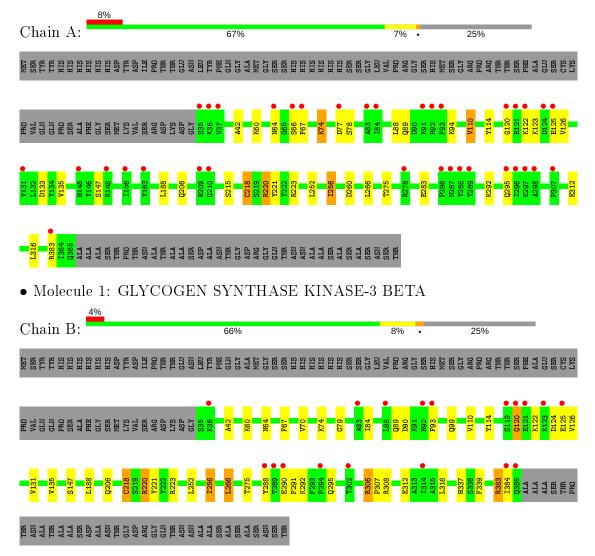
N	/Iol	Chain	Residues	Atoms	ZeroOcc	AltConf
	3	A	65	Total O 65 65	0	0
	3	В	101	Total O 101 101	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: GLYCOGEN SYNTHASE KINASE-3 BETA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	83.95Å 85.17Å 178.39Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 - 2.60	Depositor
Resolution (A)	19.93 - 2.60	EDS
% Data completeness	97.0 (19.94-2.60)	Depositor
(in resolution range)	97.1 (19.93-2.60)	EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.36 (at 2.59Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
D D	0.230 , 0.252	Depositor
R, R_{free}	0.254 , 0.268	DCC
R_{free} test set	1556 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.27 , 63.0	EDS
L-test for twinning ²	$< L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5838	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: KDI

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		
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.50	0/2876	0.72	$2/3913 \ (0.1\%)$	
1	В	0.52	0/2876	0.70	$1/3913 \ (0.0\%)$	
All	All	0.51	0/5752	0.71	$3/7826 \ (0.0\%)$	

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	77	ASP	C-N-CA	5.82	136.25	121.70
1	В	120	GLY	N-CA-C	5.14	125.96	113.10
1	A	74	LYS	CD-CE-NZ	-5.01	100.18	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2805	0	2833	8	0
1	В	2805	0	2833	17	0
2	A	31	0	28	0	0
2	В	31	0	28	1	0
3	A	65	0	0	0	0
3	В	101	0	0	1	0



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\mathbf{Mol}	Chain	Non-H	H(model)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
All	All	5838	0	5722	25	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 2.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({f \AA})$	overlap (\AA)
1:B:306:ARG:HD2	1:B:308:ARG:HB2	1.74	0.69
1:B:74:LYS:HE2	1:B:79:GLY:HA2	1.87	0.56
1:B:337:HIS:HD2	1:B:339:PHE:H	1.55	0.55
1:B:383:ARG:NH1	1:B:383:ARG:HB2	2.25	0.51
1:B:288:TYR:HA	1:B:291:PHE:HD2	1.77	0.50
1:B:135:VAL:HB	1:B:188:LEU:HB3	1.94	0.49
1:A:135:VAL:HB	1:A:188:LEU:HB3	1.94	0.48
1:B:383:ARG:HH11	1:B:383:ARG:HB2	1.80	0.47
1:A:218:CYS:HB3	1:A:223:ARG:HG2	1.97	0.47
1:A:42:ALA:HB1	1:A:114:TYR:HB3	1.96	0.47
1:A:88:LEU:HD11	1:A:125:GLU:HB3	1.98	0.46
1:B:307:PRO:HD2	3:B:2069:HOH:O	2.15	0.46
1:A:110:VAL:HG22	1:A:133:ASP:HB2	1.98	0.46
1:B:218:CYS:HB3	1:B:223:ARG:HG2	1.97	0.46
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.97	0.45
1:A:215:SER:O	1:A:223:ARG:NH2	2.52	0.43
1:B:67:PHE:CE2	1:B:70:VAL:HG23	2.53	0.43
1:A:252:LEU:HD11	1:A:256:ILE:HD12	2.02	0.41
1:B:252:LEU:HD11	1:B:256:ILE:HD12	2.03	0.41
1:B:266:LEU:HA	1:B:266:LEU:HD12	1.94	0.40
1:B:84:ILE:HG12	1:B:131:VAL:HG22	2.02	0.40
1:B:67:PHE:HE2	1:B:70:VAL:HG23	1.86	0.40
1:B:89:GLN:HG3	1:B:90:ASP:O	2.21	0.40
1:A:220:ARG:HD3	1:B:220:ARG:HD3	2.03	0.40
2:B:1386:KDI:H281	2:B:1386:KDI:H24	1.75	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	Percentil	les
1	A	349/465~(75%)	325 (93%)	18 (5%)	6 (2%)	9 18	
1	В	349/465~(75%)	330 (95%)	15 (4%)	4 (1%)	14 30	
All	All	698/930 (75%)	655 (94%)	33 (5%)	10 (1%)	11 22	

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	SER
1	A	122	LYS
1	В	120	GLY
1	A	221	TYR
1	В	221	TYR
1	A	120	GLY
1	A	123	LYS
1	В	295	GLN
1	A	295	GLN
1	В	384	ILE

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	Rotameric Outliers		Percentiles		
1	A	312/404 (77%)	290 (93%)	22 (7%)	14	29		
1	В	312/404 (77%)	290 (93%)	22 (7%)	14	29		
All	All	624/808 (77%)	580 (93%)	44 (7%)	14	29		



All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	64	ASN
1	A	66	SER
1	A	67	PHE
1	A	74	LYS
1	A	89	GLN
1	A A	94	LYS
1	A	110	VAL
1	A	126	VAL
1	A	147	SER
1	A	206	GLN
1	A	218	CYS
1	A	220	ARG
1	A	256	ARG ILE
1	A	260	ASP
1	A	266	LEU
1	A	275	THR
1	A	283	GLU
1	A	292	LYS
1	A	312	GLU
1	A	316	LEU
1	A	383	ARG
1	В	60	LYS
1	В	64	ASN
1	В	93	PHE
1	В	99	GLN
1	В	110	VAL
1	В	122	LYS
1	В	124	ASP
1	В	125	GLU
1	В	126	VAL
1	В	147	SER
1	В	206	GLN
1	В	218	CYS
1	В	220	ARG
1	В	256	ILE
1	В	266	LEU
1	В	275	THR
1	В	290	GLU
1	В	292	LYS
1	В	306	ARG
1	В	312	GLU



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Mol	Chain	Res	Type
1	В	316	LEU
1	В	383	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	A	381	HIS
1	В	99	GLN
1	В	337	HIS
1	В	381	HIS

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 carbohydrates 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	T	Chain	Dog	Link	Во	ond leng	$ ag{ths}$	В	ond ang	gles
	MIOI	l Type	Chain	m Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
Ī	2	KDI	В	1386	-	33,33,33	1.00	1 (3%)	43,46,46	2.30	11 (25%)
	2	KDI	A	1386	-	33,33,33	1.09	4 (12%)	43,46,46	2.49	12 (27%)



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	${f Torsions}$	Rings
2	KDI	В	1386	-	-	11/26/36/36	0/3/3/3
2	KDI	A	1386	-	-	7/26/36/36	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(ext{\AA})$
2	A	1386	KDI	S7-N6	3.43	1.68	1.63
2	В	1386	KDI	S7-N6	2.96	1.67	1.63
2	A	1386	KDI	C5-N6	2.36	1.50	1.47
2	A	1386	KDI	C6-N6	2.17	1.50	1.47
2	A	1386	KDI	C19-N31	2.03	1.39	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	1386	KDI	C6-N6-C5	8.88	121.99	112.17
2	В	1386	KDI	C6-N6-C5	8.40	121.47	112.17
2	A	1386	KDI	C4-C5-N6	7.19	114.41	108.91
2	В	1386	KDI	C4-C5-N6	5.65	113.24	108.91
2	A	1386	KDI	C3-C6-N6	5.57	113.17	108.91
2	В	1386	KDI	C22-C20-N21	4.92	120.59	115.99
2	A	1386	KDI	C22-C20-N21	4.38	120.08	115.99
2	В	1386	KDI	C3-C6-N6	4.08	112.03	108.91
2	В	1386	KDI	C13-C16-N21	3.43	120.89	116.02
2	A	1386	KDI	C13-C16-N21	3.23	120.61	116.02
2	A	1386	KDI	C10-S7-N6	-2.84	103.92	107.30
2	В	1386	KDI	C20-N21-C16	2.64	122.12	118.19
2	В	1386	KDI	C10-S7-N6	-2.62	104.18	107.30
2	A	1386	KDI	C20-N21-C16	2.52	121.95	118.19
2	В	1386	KDI	C6-C3-N2	-2.48	108.00	110.80
2	В	1386	KDI	O9-S7-C10	-2.48	104.91	108.05
2	В	1386	KDI	C25-N24-C22	2.43	127.63	122.08
2	В	1386	KDI	C14-C13-C16	-2.20	117.81	121.28
2	A	1386	KDI	O8-S7-N6	2.20	108.69	106.69
2	A	1386	KDI	O9-S7-O8	2.18	123.05	119.52
2	A	1386	KDI	C17-N18-C19	2.17	120.93	118.70
2	A	1386	KDI	C25-N24-C22	2.12	126.92	122.08
2	A	1386	KDI	O9-S7-C10	-2.04	105.47	108.05



There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	1386	KDI	C12-C13-C16-C17
2	В	1386	KDI	C14-C13-C16-C17
2	В	1386	KDI	O29-C28-C30-C25
2	В	1386	KDI	C12-C13-C16-N21
2	В	1386	KDI	C14-C13-C16-N21
2	В	1386	KDI	N24-C25-C30-C28
2	В	1386	KDI	C6-N6-S7-O9
2	В	1386	KDI	C30-C28-O29-C27
2	A	1386	KDI	C30-C28-O29-C27
2	A	1386	KDI	C6-N6-S7-O9
2	В	1386	KDI	C6-N6-S7-O8
2	A	1386	KDI	O29-C28-C30-C25
2	A	1386	KDI	C5-N6-S7-O8
2	A	1386	KDI	C12-C13-C16-N21
2	В	1386	KDI	C6-N6-S7-C10
2	В	1386	KDI	N21-C20-C22-N24
2	A	1386	KDI	C14-C13-C16-N21
2	A	1386	KDI	C6-N6-S7-O8

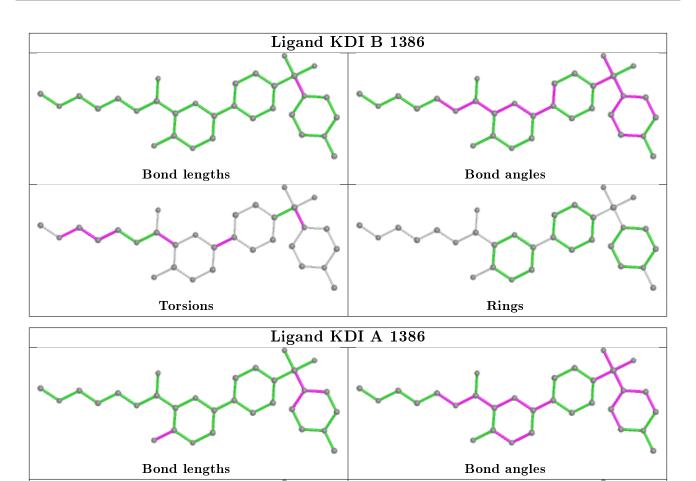
There are no ring outliers.

1 monomer is involved in 1 short contact:

\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1386	KDI	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Rings

5.7 Other polymers (i)

There are no such residues in this entry.

Torsions

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, 95^{th} 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	${f Analysed}$	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	351/465~(75%)	0.48	35 (9%) 7 4	51, 84, 147, 165	0
1	В	351/465~(75%)	0.19	18 (5%) 28 22	48, 71, 131, 158	0
All	All	702/930 (75%)	0.33	53 (7%) 14 10	48, 77, 142, 165	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	PRO	6.1
1	A	120	GLY	6.0
1	В	120	GLY	5.8
1	A	93	PHE	5.7
1	A	35	SER	4.6
1	В	93	PHE	4.5
1	A	289	THR	4.2
1	A	125	GLU	4.1
1	A	297	LYS	4.0
1	В	290	GLU	3.8
1	A	383	ARG	3.7
1	В	121	GLU	3.7
1	A	122	LYS	3.6
1	В	385	GLN	3.5
1	A	66	SER	3.5
1	A	296	ILE	3.4
1	В	289	THR	3.4
1	A	83	ALA	3.4
1	В	92	ARG	3.4
1	A	278	ARG	3.4
1	A	298	ALA	3.4
1	A	36	LYS	3.2
1	A	77	ASP	3.2
1	В	288	TYR	3.2



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Mol	Chain	Res	Type	RSRZ
1	A	64	ASN	3.2
1	A	288	TYR	3.1
1	A	84	ILE	2.9
1	A	121	GLU	2.9
1	В	384	ILE	2.7
1	В	123	LYS	2.6
1	A	131	VAL	2.5
1	A	148	ARG	2.5
1	В	88	LEU	2.4
1	В	119	SER	2.4
1	A	307	PRO	2.4
1	A	124	ASP	2.4
1	A	145	HIS	2.4
1	A	210	GLY	2.4
1	A	92	ARG	2.4
1	A	67	PHE	2.3
1	A	209	ARG	2.3
1	A	91	LYS	2.3
1	A	37	VAL	2.3
1	A	295	GLN	2.2
1	В	294	PRO	2.2
1	В	36	LYS	2.2
1	A	287	ASN	2.2
1	A	156	ILE	2.2
1	В	83	ALA	2.2
1	В	302	THR	2.2
1	В	125	GLU	2.1
1	В	314	ILE	2.0
1	A	163	TYR	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 carbohydrates in this entry.

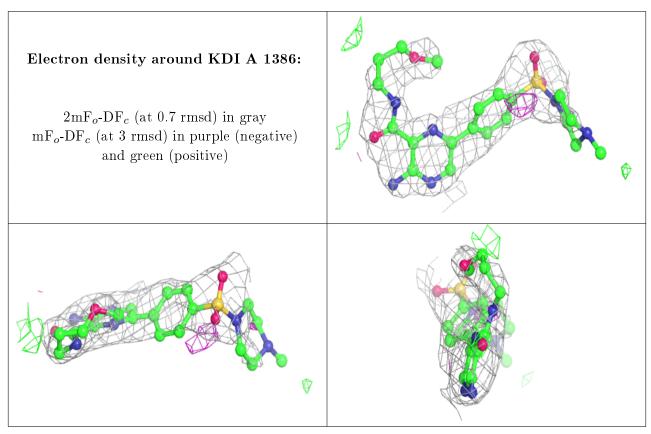


6.4 Ligands (i)

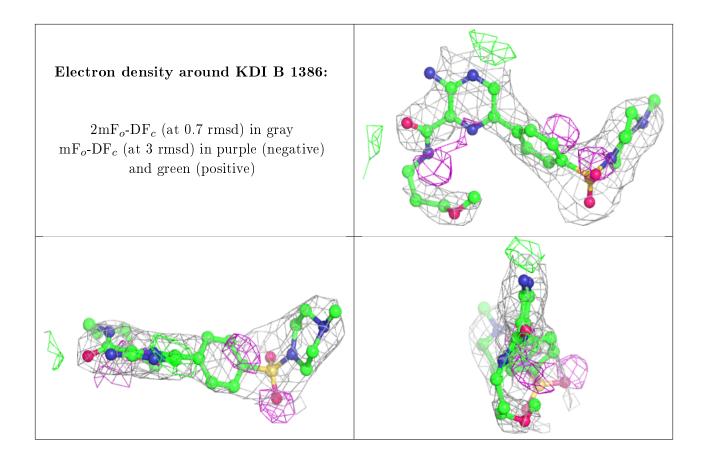
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
2	KDI	A	1386	31/31	0.80	0.29	87,102,137,138	0
2	KDI	В	1386	31/31	0.84	0.31	74,106,108,109	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.

