

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	5U6B
Title	:	Structure of the Axl kinase domain in complex with a macrocyclic inhibitor
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Deposited on	:	2016-12-07
Resolution	:	2.84 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:

MolProbity	:	4.02b-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
$\operatorname{CCP4}$:	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 2.84 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	$1031 \ (2.86-2.82)$
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	$1050 \ (2.86-2.82)$
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (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 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	А	307	4%	12% •	12%
1	В	307	5%	16%	• 5%
1	С	307	3% 75%	11% •	12%
1	D	307	7%	16%	• 5%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9046 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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	270	Total	С	Ν	Ο	\mathbf{S}	0	0	0	
	A	270	2143	1363	363	397	20	0			
1	р	291	Total	С	Ν	Ο	S	0	0	0	
	I D		2316	1474	393	428	21	0	0	U	
1	1 C 270	0 970	270	Total	С	Ν	Ο	S	0	0	0
		270	2143	1363	363	397	20	0			
1	1 D	20.1	Total	С	Ν	Ο	S	0	0	0	
I D	291	2316	1474	393	428	21	0	0	U		

• Molecule 1 is a protein called Tyrosine-protein kinase receptor UFO.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	512	GLY	-	expression tag	UNP P30530
А	513	SER	-	expression tag	UNP P30530
В	512	GLY	-	expression tag	UNP P30530
В	513	SER	-	expression tag	UNP P30530
С	512	GLY	-	expression tag	UNP P30530
С	513	SER	-	expression tag	UNP P30530
D	512	GLY	-	expression tag	UNP P30530
D	513	SER	-	expression tag	UNP P30530

• Molecule 2 is (10R)-7-amino-11-chloro-12-fluoro-1-(2-hydroxyethyl)-3,10,16-trimethyl-16,1 7-dihydro-1H-8,4-(azeno)pyrazolo[4,3-h][2,5,11]benzoxadiazacyclotetradecin-15(10H)-one (three-letter code: 7YS) (formula: $C_{21}H_{22}ClFN_6O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	Δ	1	Total C Cl F N O	0	0
	A	L	32 21 1 1 6 3	0	0
9	В	1	Total C Cl F N O	0	0
	D	T	32 21 1 1 6 3	0	0
9	C	1	Total C Cl F N O	0	0
		T	32 21 1 1 6 3	0	0
9	П	1	Total C Cl F N O	0	0
			32 21 1 1 6 3	0	U



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: Tyrosine-protein kinase receptor UFO

GLU PRO ASP GLU

• Molecule 1: Tyrosine-protein kinase receptor UFO





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	81.68Å 100.70Å 81.92 Å	Deperitor
a, b, c, α , β , γ	90.00° 93.97° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	59.81 - 2.84	Depositor
Resolution (A)	81.72 - 2.84	EDS
% Data completeness	99.3(59.81-2.84)	Depositor
(in resolution range)	$99.3 \ (81.72 - 2.84)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$2.12 (at 2.82 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
D D .	0.211 , 0.239	Depositor
Π, Π_{free}	0.229 , 0.237	DCC
R_{free} test set	771 reflections (2.45%)	wwPDB-VP
Wilson B-factor $(Å^2)$	52.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35 , 53.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9046	wwPDB-VP
Average B, all atoms $(Å^2)$	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: 7YS

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).

Mal	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.46	0/2186	0.66	0/2950
1	В	0.48	0/2361	0.69	0/3181
1	С	0.46	0/2186	0.66	0/2950
1	D	0.47	0/2361	0.69	0/3181
All	All	0.47	0/9094	0.68	0/12262

There are no bond length outliers.

There are no bond angle outliers.

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	А	2143	0	2144	16	0
1	В	2316	0	2316	27	0
1	С	2143	0	2144	12	0
1	D	2316	0	2316	28	0
2	А	32	0	0	0	0
2	В	32	0	0	0	0
2	С	32	0	0	0	0
2	D	32	0	0	0	0
All	All	9046	0	8920	79	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 4.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	At0111-2	${f distance} \ ({ m \AA})$	overlap (Å)
1:D:713:VAL:HB	1:D:755:ASN:HD22	1.59	0.67
1:C:667:ARG:HD3	1:D:754:GLU:HG3	1.78	0.66
1:B:713:VAL:HB	1:B:755:ASN:HD22	1.60	0.66
1:A:667:ARG:HD3	1:B:754:GLU:HG3	1.79	0.63
1:B:589:MET:HB3	1:B:600:LEU:HB2	1.81	0.61
1:A:573:ILE:HD13	1:A:579:LEU:HD23	1.81	0.60
1:B:610:ARG:HB2	1:B:614:PRO:HA	1.83	0.59
1:B:512:GLY:N	1:B:513:SER:HG	2.00	0.58
1:D:740:TRP:HD1	1:D:782:MET:HE1	1.69	0.58
1:D:781:LEU:HD22	1:D:799:LEU:HD23	1.86	0.58
1:B:519:SER:HA	1:B:576:ARG:HH21	1.69	0.58
1:B:740:TRP:HD1	1:B:782:MET:HE1	1.68	0.57
1:A:713:VAL:HB	1:A:755:ASN:HD22	1.69	0.57
1:B:533:ARG:HA	1:B:604:CYS:SG	2.44	0.57
1:C:713:VAL:HB	1:C:755:ASN:HD22	1.69	0.57
1:D:533:ARG:HA	1:D:604:CYS:SG	2.45	0.56
1:C:541:THR:HA	1:C:551:MET:HG3	1.87	0.56
1:A:812:PRO:HB2	1:A:813:ALA:HB2	1.87	0.56
1:D:519:SER:HA	1:D:576:ARG:HH21	1.69	0.56
1:A:604:CYS:HB2	1:A:617:VAL:HB	1.86	0.56
1:B:781:LEU:HD22	1:B:799:LEU:HD23	1.88	0.55
1:D:512:GLY:N	1:D:513:SER:HG	2.04	0.55
1:C:812:PRO:HB2	1:C:813:ALA:HB2	1.89	0.54
1:B:740:TRP:HB2	1:B:782:MET:HE3	1.91	0.53
1:B:568:THR:HG22	1:B:617:VAL:HG22	1.91	0.53
1:A:592:PHE:O	1:A:599:ARG:HG2	2.09	0.52
1:A:713:VAL:HA	1:A:716:ILE:HD12	1.91	0.52
1:B:589:MET:HE1	1:B:598:MET:HG3	1.92	0.51
1:D:740:TRP:HB2	1:D:782:MET:HE3	1.93	0.51
1:C:568:THR:HG22	1:C:617:VAL:HG22	1.93	0.50
1:B:541:THR:HA	1:B:551:MET:HG2	1.94	0.50
1:D:585:GLU:HG3	1:D:691:PHE:HB2	1.94	0.49
1:C:713:VAL:HA	1:C:716:ILE:HD12	1.94	0.49
1:D:659:GLY:O	1:D:663:LEU:HD22	2.11	0.49
1:C:784:ARG:HB3	1:C:794:PRO:HD3	1.94	0.49
1:A:784:ARG:HB3	1:A:794:PRO:HD3	1.94	0.48
1:D:610:ARG:O	1:D:610:ARG:HG2	2.14	0.47



	louis pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:568:THR:HG22	1:A:617:VAL:HG22	1.96	0.47
1:B:681:ASN:ND2	1:B:685:SER:H	2.12	0.47
1:A:667:ARG:CD	1:B:754:GLU:HG3	2.44	0.47
1:C:667:ARG:CD	1:D:754:GLU:HG3	2.44	0.46
1:D:589:MET:HE1	1:D:598:MET:HG3	1.97	0.46
1:D:671:ARG:NH2	1:D:704:ARG:HE	2.13	0.46
1:D:541:THR:HA	1:D:551:MET:HG2	1.98	0.46
1:A:541:THR:HA	1:A:551:MET:HG3	1.97	0.46
1:B:610:ARG:HG2	1:B:610:ARG:O	2.15	0.45
1:B:659:GLY:O	1:B:663:LEU:HD22	2.16	0.45
1:B:671:ARG:NH2	1:B:704:ARG:HE	2.15	0.45
1:B:740:TRP:HD1	1:B:782:MET:CE	2.30	0.45
1:D:517:GLY:O	1:D:576:ARG:HG3	2.17	0.45
1:D:784:ARG:HB3	1:D:794:PRO:HD3	1.99	0.45
1:C:652:PHE:O	1:C:656:ILE:HG12	2.16	0.44
1:B:784:ARG:HB3	1:B:794:PRO:HD3	2.00	0.44
1:D:740:TRP:HD1	1:D:782:MET:CE	2.29	0.44
1:C:558:ASP:O	1:C:559:ASP:HB2	2.18	0.44
1:D:713:VAL:HB	1:D:755:ASN:ND2	2.31	0.43
1:D:671:ARG:HH22	1:D:704:ARG:HE	1.65	0.43
1:A:652:PHE:O	1:A:656:ILE:HG12	2.19	0.43
1:D:604:CYS:O	1:D:616:PRO:HA	2.19	0.43
1:C:532:ASP:HB3	1:C:535:LYS:HD2	2.01	0.43
1:D:722:ALA:HB2	1:D:759:TYR:CE1	2.54	0.43
1:A:573:ILE:HD12	1:A:616:PRO:HD3	2.01	0.43
1:A:548:GLY:HA2	1:A:570:LYS:HB2	2.01	0.42
1:B:722:ALA:HB2	1:B:759:TYR:CE1	2.54	0.42
1:B:652:PHE:O	1:B:656:ILE:HG12	2.19	0.42
1:B:704:ARG:HG2	1:B:724:ARG:HB3	2.02	0.42
1:A:651:LYS:HD2	1:A:807:LEU:HD21	2.02	0.42
1:B:671:ARG:HH22	1:B:704:ARG:HE	1.66	0.42
1:C:529:VAL:HG22	1:C:603:VAL:HG22	2.02	0.42
1:D:512:GLY:HA3	1:D:513:SER:HA	1.92	0.42
1:D:652:PHE:O	1:D:656:ILE:HG12	2.20	0.42
1:A:635:SER:HB3	1:A:745:ARG:HH21	1.85	0.42
1:B:548:GLY:HA2	1:B:570:LYS:HB2	2.00	0.42
1:D:514:ASN:HB3	1:D:576:ARG:NH1	2.35	0.41
1:D:669:ILE:HG22	1:D:671:ARG:HG3	2.02	0.41
1:B:517:GLY:O	1:B:576:ARG:HG3	2.20	0.41
1:D:704:ARG:HG2	1:D:724:ARG:HB3	2.02	0.41
1:B:656:ILE:HB	1:B:735:PHE:HE1	1.86	0.40



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Atom-1	Atom-1 Atom-2		Clash overlap (Å)
1:D:521:GLU:H	1:D:521:GLU:HG2	1.72	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	Perce	\mathbf{ntiles}
1	А	264/307~(86%)	255~(97%)	7 (3%)	2 (1%)	19	38
1	В	283/307~(92%)	265~(94%)	17~(6%)	1 (0%)	34	56
1	С	264/307~(86%)	250~(95%)	12 (4%)	2 (1%)	19	38
1	D	283/307~(92%)	267~(94%)	15~(5%)	1 (0%)	34	56
All	All	1094/1228~(89%)	1037 (95%)	51 (5%)	6 (0%)	29	51

All (6) Ramachandran outliers are listed below:

\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	А	558	ASP
1	А	559	ASP
1	С	558	ASP
1	С	559	ASP
1	В	700	GLY
1	D	700	GLY

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	237/268~(88%)	219~(92%)	18 (8%)	13 28
1	В	255/268~(95%)	232~(91%)	23 (9%)	9 19
1	С	237/268~(88%)	215 (91%)	22 (9%)	9 18
1	D	255/268~(95%)	232~(91%)	23 (9%)	9 19
All	All	984/1072~(92%)	898 (91%)	86 (9%)	10 21

analysed, and the total number of residues.

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	522	LEU
1	А	523	LYS
1	А	525	LYS
1	А	526	LEU
1	А	527	ARG
1	А	541	THR
1	А	544	GLU
1	А	556	ASN
1	А	558	ASP
1	А	571	ILE
1	А	579	LEU
1	А	599	ARG
1	А	623	MET
1	А	633	LEU
1	А	636	ARG
1	А	647	GLN
1	А	728	SER
1	А	781	LEU
1	В	521	GLU
1	В	526	LEU
1	В	541	THR
1	В	575	THR
1	В	576	ARG
1	В	580	GLU
1	В	590	LYS
1	В	600	LEU
1	В	610	ARG
1	В	623	MET
1	В	633	LEU
1	В	647	GLN
1	В	663	LEU



Mol	Chain	Res	Type
1	В	664	SER
1	В	666	LYS
1	В	667	ARG
1	В	681	ASN
1	В	697	ILE
1	В	704	ARG
1	В	710	LYS
1	В	718	ILE
1	В	728	SER
1	В	787	GLU
1	С	523	LYS
1	С	525	LYS
1	С	526	LEU
1	С	527	ARG
1	С	528	ASP
1	С	541	THR
1	С	551	MET
1	С	556	ASN
1	С	558	ASP
1	С	561	ILE
1	С	569	MET
1	С	573	ILE
1	С	579	LEU
1	С	599	ARG
1	С	623	MET
1	С	633	LEU
1	С	636	ARG
1	С	647	GLN
1	С	723	ASP
1	С	728	SER
1	C	781	LEU
1	С	803	LEU
1	D	521	GLU
1	D	526	LEU
1	D	541	THR
1	D	575	THR
1	D	580	GLU
1	D	590	LYS
1	D	600	LEU
1	D	610	ARG
1	D	623	MET
1	D	633	LEU



Mol	Chain	Res	Type
1	D	647	GLN
1	D	663	LEU
1	D	664	SER
1	D	666	LYS
1	D	667	ARG
1	D	681	ASN
1	D	690	ASP
1	D	697	ILE
1	D	704	ARG
1	D	710	LYS
1	D	718	ILE
1	D	728	SER
1	D	787	GLU

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

Mol	Chain	Res	Type
1	А	681	ASN
1	А	755	ASN
1	В	681	ASN
1	В	755	ASN
1	С	755	ASN
1	D	557	GLN
1	D	681	ASN
1	D	755	ASN

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)

4 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).

Mal	Tune	Chain	Dog	Tink	Bo	ond leng	\mathbf{ths}	B	ond ang	gles
INIOI	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7YS	А	9001	-	31,35,35	0.55	0	35,52,52	1.11	2 (5%)
2	7YS	В	9001	-	31,35,35	0.47	0	35,52,52	1.08	2 (5%)
2	7YS	С	9001	-	31,35,35	0.60	1 (3%)	35,52,52	1.06	2 (5%)
2	7YS	D	9001	-	31,35,35	0.46	0	35,52,52	1.07	2 (5%)

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	7YS	А	9001	-	-	2/22/27/27	0/3/4/4
2	7YS	В	9001	-	-	2/22/27/27	0/3/4/4
2	7YS	С	9001	-	-	2/22/27/27	0/3/4/4
2	7YS	D	9001	-	-	2/22/27/27	0/3/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	С	9001	7YS	C20-C21	-2.38	1.35	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	А	9001	7YS	C1-O18-C17	3.71	122.13	116.79
2	В	9001	7YS	C1-O18-C17	3.49	121.82	116.79
2	С	9001	7YS	C1-O18-C17	3.38	121.65	116.79
2	D	9001	7YS	C1-O18-C17	3.18	121.37	116.79
2	D	9001	7YS	O18-C17-C16	2.84	111.84	107.64



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	В	9001	7YS	O18-C17-C16	2.69	111.62	107.64
2	А	9001	7YS	O18-C17-C16	2.50	111.33	107.64
2	С	9001	7YS	O18-C17-C16	2.26	110.98	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	9001	7YS	C11-C12-N13-C14
2	В	9001	7YS	C11-C12-N13-C14
2	С	9001	7YS	C11-C12-N13-C14
2	D	9001	7YS	C11-C12-N13-C14
2	А	9001	7YS	C11-C12-N13-C27
2	В	9001	7YS	C11-C12-N13-C27
2	С	9001	7YS	C11-C12-N13-C27
2	D	9001	7YS	C11-C12-N13-C27

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 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 sufficient 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, 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	Analysed	<RSRZ $>$	# RSRZ > 2	$OWAB(Å^2)$	$\mathbf{Q}{<}0.9$
1	А	270/307~(87%)	0.34	11 (4%) 37 29	29, 52, 82, 105	0
1	В	291/307~(94%)	0.51	16 (5%) 25 18	30, 54, 87, 101	0
1	С	270/307~(87%)	0.36	10 (3%) 41 33	31, 53, 87, 100	0
1	D	291/307~(94%)	0.57	22 (7%) 13 8	32, 57, 91, 108	0
All	All	1122/1228~(91%)	0.45	59 (5%) 26 20	29, 54, 88, 108	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	682	GLU	5.9
1	С	559	ASP	4.9
1	С	547	PHE	4.8
1	D	643	TYR	4.5
1	В	810	LEU	4.5
1	А	572	ALA	4.4
1	С	573	ILE	4.4
1	D	644	LEU	4.3
1	А	573	ILE	4.0
1	А	571	ILE	3.9
1	D	811	PRO	3.9
1	D	708	ILE	3.8
1	А	640	GLN	3.8
1	А	547	PHE	3.7
1	А	574	CYS	3.7
1	D	699	ASN	3.5
1	D	646	THR	3.5
1	С	546	GLU	3.4
1	D	698	TYR	3.4
1	D	611	GLU	3.3
1	С	534	HIS	3.3



Mol

1

1

1

1

1

1

1

1

1

1

1

1

1

1

RSRZ

3.3

3.2

2.9

2.9

PRO	2.9
SER	2.8
TYR	2.8
THR	2.7
LEU	2.7
GLN	2.6
GLN	2.6
LYS	2.5
GLY	2.5
TYR	2.5
ILE	2.5
SER	2.4
GLN	2.4
ASN	2.3
ALA	2.3
TVR	0.3

Continued from previous page...

 \mathbf{Res}

811

611

556

647

641

694

698

646

810

647

640

570

512

643

Type

PRO

GLU

ASN

 GLN

Chain

В

В

В

А

D

С

В

В

D

В

С

В

D

В

ILI В 1 571D SE. 1 515GL 1 D 647 D AS 1 681D AL 1 709TYR1 С 6342.3В LYS1 5632.3GLU 1 А 5462.3D SER 2.21 612 $\overline{\mathbf{C}}$ 1 571ILE 2.2GLU 2.21 А 524В THR 1 5412.21 D ILE 697 2.2D ASP 1 2.25321 А 521GLU 2.2В 1 560SER 2.2В ASN 1 5142.11 А 694SER 2.1D 1 560SER 2.11 $\overline{\mathbf{C}}$ 813 ALA 2.11 D 622 PHE2.1GLY 1 В 5122.0В 1 760ASP 2.01 D 514ASN 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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
2	7YS	D	9001	32/32	0.93	0.28	$41,\!52,\!59,\!61$	0
2	7YS	В	9001	32/32	0.94	0.24	$48,\!58,\!63,\!67$	0
2	7YS	С	9001	32/32	0.95	0.20	$37,\!45,\!50,\!52$	0
2	7YS	А	9001	32/32	0.96	0.20	39,43,49,51	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.

