



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:37 PM EDT

PDB ID : 3DTW / pdb_00003dtw
Title : Crystal structure of the VEGFR2 kinase domain in complex with a benzisoxazole inhibitor
Authors : Whittington, D.A.; Long, A.M.; Rose, P.; Gu, Y.; Zhao, H.
Deposited on : 2008-07-16
Resolution : 2.90 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

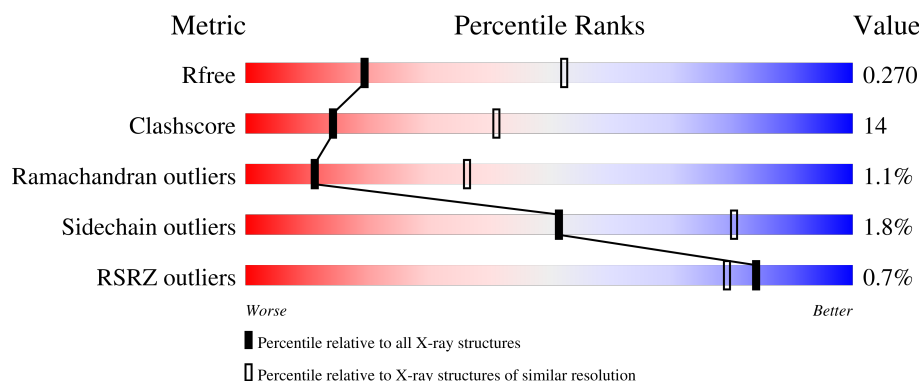
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	314	 62% 28% • 8%
1	B	314	 55% 29% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4574 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.

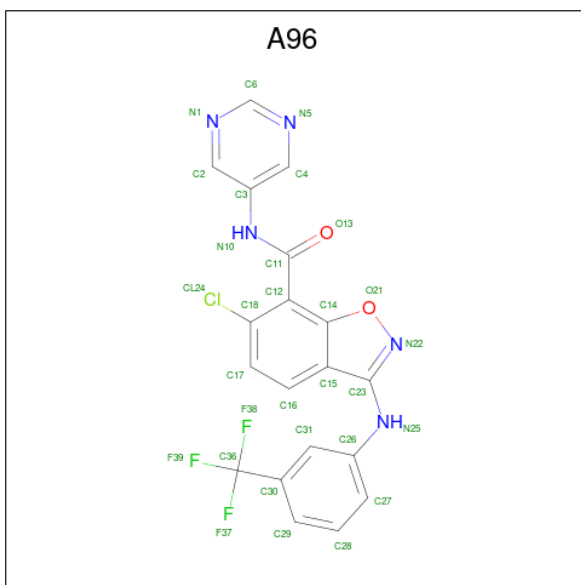
- Molecule 1 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2332	1493	412	411	16			
1	B	269	Total	C	N	O	S	0	0	0
			2167	1397	374	380	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	ALA	CYS	engineered mutation	UNP P35968
A	916	THR	VAL	engineered mutation	UNP P35968
A	990	VAL	GLU	engineered mutation	UNP P35968
A	1172	ARG	-	expression tag	UNP P35968
A	1173	HIS	-	expression tag	UNP P35968
A	1174	HIS	-	expression tag	UNP P35968
A	1175	HIS	-	expression tag	UNP P35968
A	1176	HIS	-	expression tag	UNP P35968
A	1177	HIS	-	expression tag	UNP P35968
A	1178	HIS	-	expression tag	UNP P35968
B	817	ALA	CYS	engineered mutation	UNP P35968
B	916	THR	VAL	engineered mutation	UNP P35968
B	990	VAL	GLU	engineered mutation	UNP P35968
B	1172	ARG	-	expression tag	UNP P35968
B	1173	HIS	-	expression tag	UNP P35968
B	1174	HIS	-	expression tag	UNP P35968
B	1175	HIS	-	expression tag	UNP P35968
B	1176	HIS	-	expression tag	UNP P35968
B	1177	HIS	-	expression tag	UNP P35968
B	1178	HIS	-	expression tag	UNP P35968

- Molecule 2 is 6-chloro-N-pyrimidin-5-yl-3-{[3-(trifluoromethyl)phenyl]amino}-1,2-benzisoxazole-7-carboxamide (CCD ID: A96) (formula: C₁₉H₁₁ClF₃N₅O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			30	19	1	3	5	2		
2	B	1	Total	C	Cl	F	N	O	0	0
			30	19	1	3	5	2		

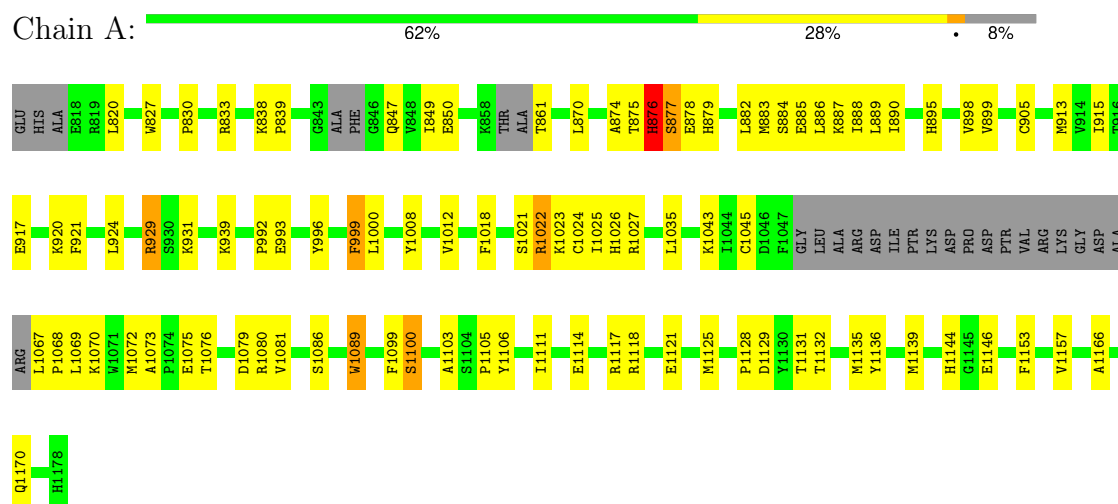
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	4	Total	O	0	0
			4	4		

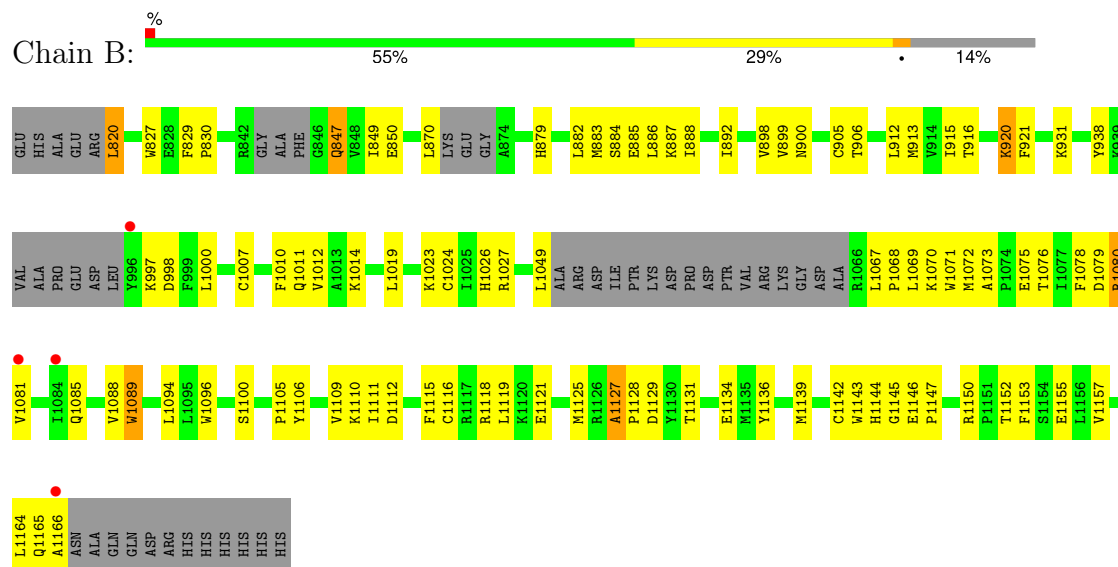
3 Residue-property plots

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: Vascular endothelial growth factor receptor 2



- Molecule 1: Vascular endothelial growth factor receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.24Å 68.36Å 88.48Å 90.00° 92.16° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.90) 97.2 (30.00-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.279 0.206 , 0.270	Depositor DCC
R_{free} test set	1460 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4574	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: A96

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	0.53	1/2391 (0.0%)	1.03	13/3227 (0.4%)
1	B	0.45	0/2218	0.99	13/2992 (0.4%)
All	All	0.49	1/4609 (0.0%)	1.01	26/6219 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	874	ALA	CA-CB	7.59	1.65	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1100	SER	N-CA-C	-7.50	102.10	112.30
1	B	1089	TRP	N-CA-C	-7.30	103.25	111.14
1	B	1129	ASP	N-CA-C	7.29	120.09	111.71
1	B	827	TRP	N-CA-C	7.10	122.11	113.38
1	B	1100	SER	N-CA-C	-6.88	103.23	112.94
1	A	915	ILE	N-CA-C	6.65	117.70	107.99
1	B	920	LYS	N-CA-C	6.54	120.71	112.87
1	A	827	TRP	N-CA-C	6.40	121.25	113.38
1	A	920	LYS	N-CA-C	6.33	118.26	111.36
1	A	1073	ALA	CA-C-N	6.17	125.66	119.24
1	A	1073	ALA	C-N-CA	6.17	125.66	119.24
1	A	1129	ASP	N-CA-C	6.10	118.73	111.71
1	A	1089	TRP	N-CA-C	-6.04	104.39	110.97
1	B	820	LEU	CA-C-N	6.03	126.22	120.31
1	B	820	LEU	C-N-CA	6.03	126.22	120.31
1	B	1073	ALA	CA-C-N	6.01	125.49	119.24
1	B	1073	ALA	C-N-CA	6.01	125.49	119.24
1	A	879	HIS	N-CA-C	-5.87	104.57	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1127	ALA	CA-C-N	5.87	125.85	120.21
1	B	1127	ALA	C-N-CA	5.87	125.85	120.21
1	B	997	LYS	N-CA-C	5.67	117.48	107.61
1	B	915	ILE	N-CA-C	5.57	115.96	108.17
1	A	1132	THR	N-CA-C	-5.44	102.09	110.58
1	A	1081	VAL	N-CA-C	5.32	115.75	107.99
1	A	921	PHE	N-CA-C	5.12	119.15	113.01
1	A	924	LEU	N-CA-C	5.07	117.54	111.71

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	2332	0	2318	66	0
1	B	2167	0	2184	62	0
2	A	30	0	11	3	0
2	B	30	0	11	1	0
3	A	11	0	0	0	0
3	B	4	0	0	1	0
All	All	4574	0	4524	128	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 14.

All (128) 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:1114:GLU:HB3	1:A:1118:ARG:HH22	1.21	1.02
1:A:1114:GLU:HB3	1:A:1118:ARG:NH2	1.86	0.89
1:B:1153:PHE:O	1:B:1157:VAL:HG23	1.72	0.89
1:A:1072:MET:HE2	1:A:1076:THR:HG22	1.58	0.83
1:B:1136:TYR:HA	1:B:1139:MET:HE3	1.63	0.79
1:B:1128:PRO:HG2	1:B:1131:THR:HB	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1152:THR:OG1	1:B:1155:GLU:HG3	1.87	0.75
1:B:1072:MET:HE2	1:B:1076:THR:HG22	1.69	0.74
1:A:849:ILE:HG22	1:A:850:GLU:O	1.90	0.71
1:B:1070:LYS:HG2	1:B:1111:ILE:HD11	1.72	0.71
1:B:1070:LYS:HE3	1:B:1105:PRO:HG2	1.74	0.70
1:A:1022:ARG:HH21	1:A:1022:ARG:HG3	1.57	0.69
1:B:885:GLU:HG3	2:B:502:A96:H27	1.77	0.67
1:A:885:GLU:HG3	2:A:501:A96:H27	1.77	0.66
1:A:1067:LEU:HD12	1:A:1068:PRO:HD2	1.78	0.65
1:A:905:CYS:SG	1:A:913:MET:HE3	2.37	0.64
1:B:1067:LEU:N	1:B:1068:PRO:HD2	2.11	0.63
1:A:1128:PRO:HG2	1:A:1131:THR:HB	1.80	0.63
1:A:1022:ARG:HH21	1:A:1022:ARG:CG	2.11	0.63
1:A:820:LEU:O	1:A:887:LYS:HD3	1.99	0.63
1:B:1079:ASP:O	1:B:1080:ARG:HB3	1.98	0.63
1:A:875:THR:HG22	1:A:877:SER:H	1.65	0.62
1:A:939:LYS:HE2	1:A:996:TYR:HB2	1.82	0.61
1:A:1153:PHE:O	1:A:1157:VAL:HG23	2.01	0.60
1:A:929:ARG:HG2	1:A:929:ARG:HH11	1.67	0.60
1:A:889:LEU:HD11	2:A:501:A96:HN25	1.67	0.60
1:B:920:LYS:HE3	1:B:921:PHE:CZ	2.37	0.60
1:B:884:SER:O	1:B:888:ILE:HG13	2.02	0.59
1:B:1144:HIS:CE1	1:B:1146:GLU:HB2	2.38	0.59
1:A:1008:TYR:O	1:A:1012:VAL:HG23	2.02	0.59
1:B:1067:LEU:HD12	1:B:1070:LYS:HE2	1.84	0.59
1:B:1164:LEU:C	1:B:1166:ALA:H	2.12	0.57
1:B:1079:ASP:O	1:B:1080:ARG:CB	2.51	0.57
1:B:1109:VAL:HG12	1:B:1110:LYS:N	2.20	0.57
1:B:1078:PHE:CE1	1:B:1116:CYS:HB3	2.40	0.57
1:B:1049:LEU:HD11	1:B:1068:PRO:HG3	1.87	0.56
1:B:1069:LEU:HD23	1:B:1072:MET:SD	2.47	0.55
1:B:1127:ALA:HB1	1:B:1131:THR:HG21	1.88	0.55
1:B:1106:TYR:CE1	1:B:1125:MET:HG3	2.43	0.54
1:B:1112:ASP:OD2	1:B:1112:ASP:C	2.50	0.54
1:B:1145:GLY:O	1:B:1147:PRO:HD3	2.08	0.54
1:A:1069:LEU:HD12	1:A:1111:ILE:HG22	1.90	0.54
1:B:931:LYS:HB2	1:B:1000:LEU:HD12	1.89	0.53
1:A:1018:PHE:O	1:A:1021:SER:OG	2.20	0.53
1:A:1117:ARG:O	1:A:1121:GLU:HG3	2.08	0.53
1:A:939:LYS:HE2	1:A:996:TYR:O	2.08	0.52
1:A:1022:ARG:CG	1:A:1022:ARG:NH2	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1026:HIS:O	1:A:1027:ARG:HB2	2.10	0.52
1:A:830:PRO:HB2	1:A:833:ARG:HG2	1.91	0.52
1:A:898:VAL:O	1:A:899:VAL:C	2.53	0.52
1:B:883:MET:O	1:B:886:LEU:HB3	2.10	0.52
1:B:906:THR:HG22	1:B:912:LEU:HD11	1.91	0.52
1:A:931:LYS:HB2	1:A:1000:LEU:HD12	1.92	0.51
1:A:1069:LEU:HD12	1:A:1111:ILE:CG2	2.41	0.51
1:A:889:LEU:HD11	2:A:501:A96:N25	2.26	0.51
1:A:1079:ASP:O	1:A:1080:ARG:HB2	2.10	0.51
1:A:939:LYS:HG2	1:A:996:TYR:CD2	2.46	0.51
1:B:905:CYS:SG	1:B:913:MET:HE3	2.51	0.50
1:B:849:ILE:HG22	1:B:850:GLU:O	2.11	0.50
1:B:1096:TRP:CD1	1:B:1128:PRO:HD3	2.46	0.50
1:B:1089:TRP:CE3	1:B:1143:TRP:HA	2.46	0.50
1:A:1070:LYS:HE3	1:A:1105:PRO:HG2	1.94	0.50
1:B:1079:ASP:HB2	1:B:1081:VAL:HG23	1.94	0.50
1:B:1134:GLU:H	1:B:1134:GLU:CD	2.20	0.49
1:A:996:TYR:O	1:A:999:PHE:HB2	2.12	0.49
1:B:1049:LEU:HD11	1:B:1068:PRO:CG	2.43	0.49
1:A:1136:TYR:O	1:A:1139:MET:HB2	2.13	0.48
1:B:1075:GLU:HG2	1:B:1076:THR:N	2.27	0.48
1:B:1088:VAL:O	1:B:1142:CYS:HB3	2.12	0.48
1:B:1078:PHE:CD1	1:B:1078:PHE:N	2.78	0.48
1:A:870:LEU:HG	1:A:882:LEU:HD22	1.95	0.48
1:B:898:VAL:O	1:B:899:VAL:C	2.56	0.48
1:A:883:MET:HE3	1:A:887:LYS:HE3	1.96	0.48
1:A:1025:ILE:O	1:A:1027:ARG:HG3	2.14	0.47
1:B:1012:VAL:HG11	1:B:1094:LEU:CD2	2.44	0.47
1:B:820:LEU:O	1:B:887:LYS:HD3	2.15	0.47
1:A:886:LEU:O	1:A:890:ILE:HG13	2.14	0.47
1:B:1026:HIS:O	1:B:1027:ARG:HB2	2.13	0.47
1:A:1114:GLU:CB	1:A:1118:ARG:HH22	2.09	0.47
1:B:1115:PHE:O	1:B:1119:LEU:HB2	2.14	0.47
1:B:888:ILE:O	1:B:892:ILE:HG13	2.15	0.46
1:B:1010:PHE:O	1:B:1014:LYS:HG3	2.16	0.46
1:B:1144:HIS:HB3	1:B:1150:ARG:HG3	1.97	0.46
1:A:1166:ALA:O	1:A:1170:GLN:HG3	2.16	0.46
1:A:1035:LEU:HG	1:A:1045:CYS:SG	2.56	0.46
1:A:1075:GLU:HG2	1:A:1076:THR:N	2.29	0.45
1:B:1079:ASP:CB	1:B:1081:VAL:HG23	2.46	0.45
1:A:1144:HIS:CE1	1:A:1146:GLU:HB2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:829:PHE:HA	1:B:830:PRO:HD3	1.85	0.45
1:B:1085:GLN:HG3	3:B:15:HOH:O	2.17	0.45
1:A:929:ARG:HH11	1:A:929:ARG:CG	2.29	0.45
1:A:884:SER:O	1:A:888:ILE:HG13	2.17	0.45
1:A:1106:TYR:CE1	1:A:1125:MET:HG3	2.52	0.45
1:B:1007:CYS:O	1:B:1011:GLN:HG3	2.16	0.45
1:B:879:HIS:CE1	1:B:912:LEU:HD22	2.52	0.44
1:A:875:THR:O	1:A:878:GLU:N	2.50	0.44
1:B:847:GLN:HE21	1:B:847:GLN:HB2	1.52	0.44
1:B:900:ASN:O	1:B:916:THR:HB	2.18	0.44
1:A:939:LYS:HE2	1:A:996:TYR:CB	2.48	0.44
1:A:1100:SER:OG	1:A:1103:ALA:HB3	2.17	0.44
1:A:875:THR:C	1:A:877:SER:N	2.76	0.43
1:A:875:THR:O	1:A:876:HIS:C	2.61	0.43
1:A:1026:HIS:O	1:A:1027:ARG:CB	2.64	0.43
1:B:1019:LEU:O	1:B:1024:CYS:HB2	2.18	0.43
1:B:1067:LEU:HG	1:B:1071:TRP:HZ3	1.83	0.43
1:A:1099:PHE:CZ	1:A:1135:MET:HE3	2.53	0.43
1:B:1112:ASP:O	1:B:1115:PHE:HB3	2.19	0.43
1:B:1139:MET:HB3	1:B:1143:TRP:CH2	2.54	0.43
1:A:895:HIS:HB2	1:A:1018:PHE:CE2	2.54	0.42
1:A:1067:LEU:HA	1:A:1068:PRO:HD2	1.78	0.42
1:A:1136:TYR:HA	1:A:1139:MET:HE3	2.01	0.42
1:A:838:LYS:HA	1:A:839:PRO:HD3	1.77	0.42
1:A:875:THR:HG22	1:A:877:SER:HB2	2.02	0.42
1:A:1114:GLU:OE1	1:A:1117:ARG:NH2	2.51	0.42
1:A:917:GLU:OE1	1:A:1043:LYS:HE3	2.20	0.41
1:A:1022:ARG:O	1:A:1023:LYS:HB2	2.21	0.41
1:B:870:LEU:HG	1:B:882:LEU:HD22	2.02	0.41
1:A:875:THR:O	1:A:877:SER:N	2.53	0.41
1:A:1128:PRO:O	1:A:1131:THR:HG22	2.21	0.41
1:B:870:LEU:HD11	1:B:879:HIS:HA	2.01	0.41
1:B:1010:PHE:CZ	1:B:1014:LYS:HD3	2.56	0.41
1:B:1023:LYS:O	1:B:1023:LYS:HG2	2.20	0.41
1:A:849:ILE:HG22	1:A:850:GLU:N	2.36	0.41
1:B:1118:ARG:HA	1:B:1121:GLU:HB2	2.02	0.41
1:A:1024:CYS:C	1:A:1025:ILE:HG13	2.46	0.40
1:B:1080:ARG:O	1:B:1080:ARG:HG2	2.21	0.40
1:A:1086:SER:O	1:A:1089:TRP:HB3	2.22	0.40
1:A:849:ILE:CG2	1:A:850:GLU:N	2.84	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	280/314 (89%)	257 (92%)	20 (7%)	3 (1%)	11	36
1	B	259/314 (82%)	232 (90%)	24 (9%)	3 (1%)	10	34
All	All	539/628 (86%)	489 (91%)	44 (8%)	6 (1%)	11	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	938	TYR
1	B	1080	ARG
1	A	993	GLU
1	B	1165	GLN
1	A	876	HIS
1	A	992	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	253/270 (94%)	246 (97%)	7 (3%)	38	72
1	B	236/270 (87%)	234 (99%)	2 (1%)	73	90
All	All	489/540 (91%)	480 (98%)	9 (2%)	51	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	847	GLN
1	A	861	THR
1	A	876	HIS
1	A	877	SER
1	A	929	ARG
1	A	999	PHE
1	A	1022	ARG
1	B	847	GLN
1	B	998	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	847	GLN
1	A	894	HIS
1	A	900	ASN
1	A	933	ASN
1	A	1137	GLN
1	A	1159	HIS
1	A	1162	ASN
1	A	1173	HIS
1	A	1175	HIS
1	A	1177	HIS
1	B	847	GLN
1	B	879	HIS
1	B	894	HIS
1	B	897	ASN
1	B	900	ASN
1	B	933	ASN
1	B	1149	GLN
1	B	1162	ASN
1	B	1165	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
2	A96	A	501	-	32,33,33	3.45	11 (34%)	42,48,48	1.44	7 (16%)
2	A96	B	502	-	32,33,33	3.13	10 (31%)	42,48,48	1.44	7 (16%)

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	A96	A	501	-	-	2/18/18/18	0/4/4/4
2	A96	B	502	-	-	2/18/18/18	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	A96	O21-N22	-11.64	1.31	1.43
2	A	501	A96	O21-N22	-11.23	1.31	1.43
2	A	501	A96	C23-N22	11.22	1.36	1.29
2	B	502	A96	C23-N22	7.92	1.34	1.29
2	A	501	A96	C23-N25	6.76	1.49	1.36
2	B	502	A96	C23-N25	5.66	1.47	1.36
2	B	502	A96	C17-C16	3.36	1.44	1.38
2	A	501	A96	C17-C16	3.15	1.43	1.38
2	B	502	A96	C31-C30	3.15	1.44	1.39
2	A	501	A96	C31-C30	3.01	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	A96	C12-C18	2.98	1.44	1.39
2	A	501	A96	C15-C14	2.89	1.44	1.39
2	A	501	A96	C12-C18	2.83	1.43	1.39
2	B	502	A96	C15-C14	2.65	1.43	1.39
2	B	502	A96	C12-C11	-2.62	1.47	1.51
2	A	501	A96	C31-C26	2.44	1.43	1.39
2	B	502	A96	C31-C26	2.44	1.43	1.39
2	A	501	A96	C12-C11	-2.42	1.47	1.51
2	B	502	A96	C17-C18	2.38	1.43	1.38
2	A	501	A96	C4-C3	2.05	1.42	1.39
2	A	501	A96	C17-C18	2.02	1.43	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A96	C18-C12-C11	3.65	125.71	121.29
2	B	502	A96	C16-C15-C23	3.26	137.11	131.38
2	A	501	A96	C16-C15-C23	3.18	136.98	131.38
2	B	502	A96	C18-C12-C11	3.11	125.06	121.29
2	B	502	A96	F39-C36-C30	-3.00	106.48	112.90
2	A	501	A96	C12-C18-CL24	3.00	123.48	119.62
2	A	501	A96	N25-C23-N22	2.79	131.38	124.35
2	B	502	A96	C12-C18-CL24	2.75	123.16	119.62
2	B	502	A96	N25-C23-N22	2.66	131.04	124.35
2	A	501	A96	C26-N25-C23	-2.58	123.06	128.24
2	A	501	A96	F39-C36-C30	-2.45	107.64	112.90
2	B	502	A96	C26-N25-C23	-2.41	123.41	128.24
2	B	502	A96	C4-C3-C2	-2.04	114.25	117.59
2	A	501	A96	C4-C3-C2	-2.04	114.26	117.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

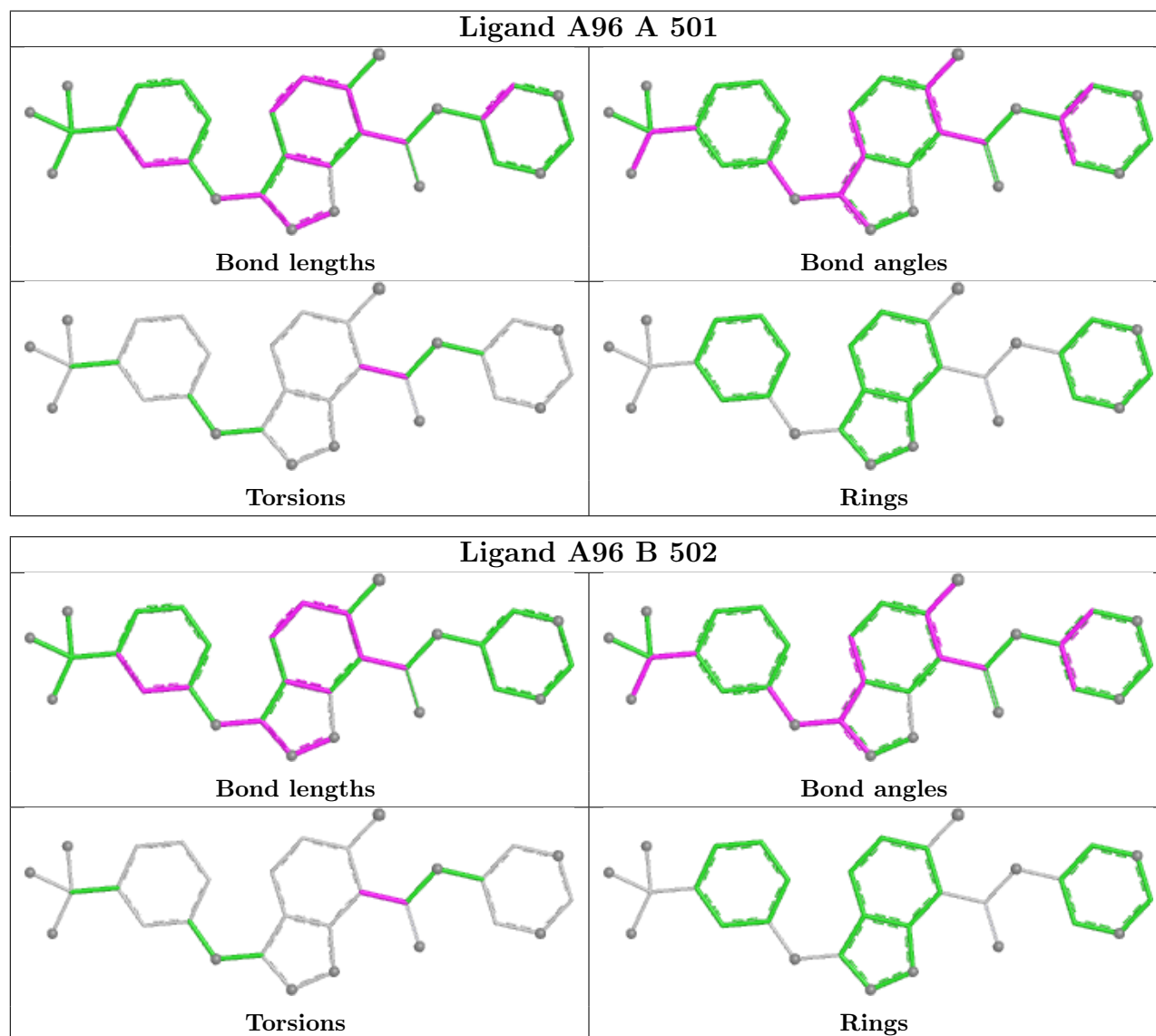
Mol	Chain	Res	Type	Atoms
2	A	501	A96	N10-C11-C12-C18
2	A	501	A96	O13-C11-C12-C18
2	B	502	A96	N10-C11-C12-C18
2	B	502	A96	O13-C11-C12-C18

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	A96	3	0
2	B	502	A96	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	288/314 (91%)	-0.22	0 100 100	19, 32, 69, 89	0
1	B	269/314 (85%)	0.13	4 (1%) 72 64	20, 48, 76, 88	0
All	All	557/628 (88%)	-0.05	4 (0%) 84 79	19, 38, 74, 89	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	996	TYR	2.8
1	B	1084	ILE	2.5
1	B	1166	ALA	2.3
1	B	1081	VAL	2.1

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(Å ²)	Q<0.9
2	A96	B	502	30/30	0.91	0.10	18,36,48,53	0

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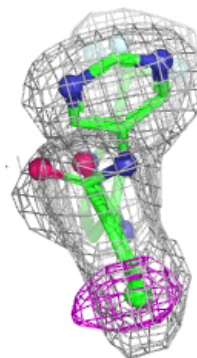
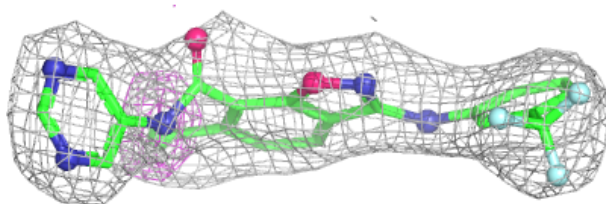
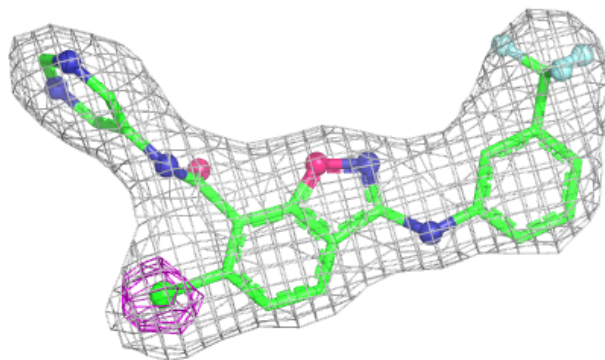
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A96	A	501	30/30	0.92	0.10	25,41,48,49	0

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.

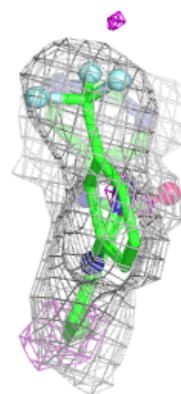
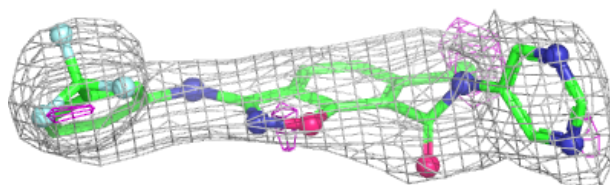
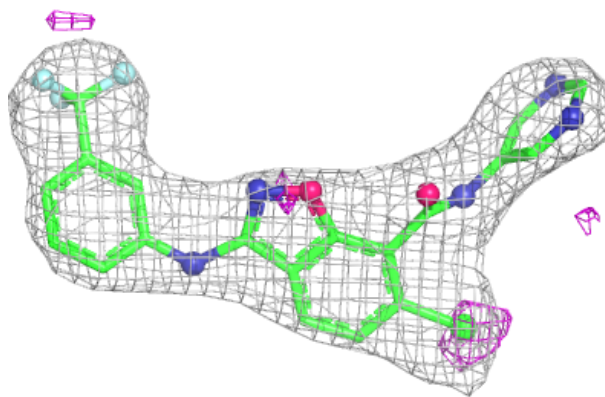
Electron density around A96 B 502:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A96 A 501:

$2mF_o-DF_c$ (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.