Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 12:18 AM EDT

PDB ID	:	2QU6
Title	:	Crystal structure of the VEGFR2 kinase domain in complex with a benzoxazole inhibitor
Authors	:	Whittington, D.A.; Kim, J.L.; Long, A.M.; Rose, P.; Gu, Y.; Zhao, H.
Deposited on	:	2007-08-03
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

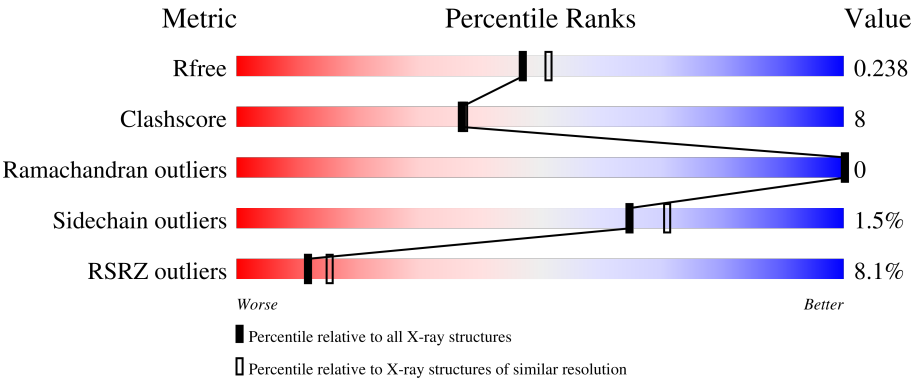
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	4% 77% 13% 10%
1	B	314	11% 64% 18% · 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4698 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.

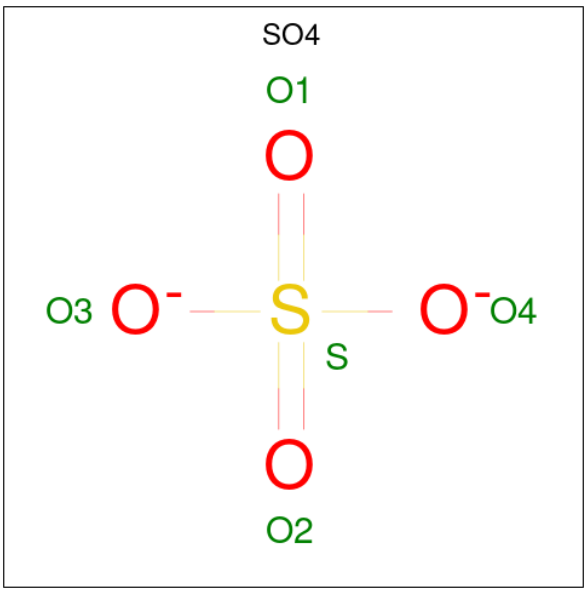
- Molecule 1 is a protein called Vascular endothelial growth factor receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2297	1472	404	405	16			
1	B	260	Total	C	N	O	S	0	0	0
			2092	1346	361	369	16			

There are 24 discrepancies between the modelled and reference sequences:

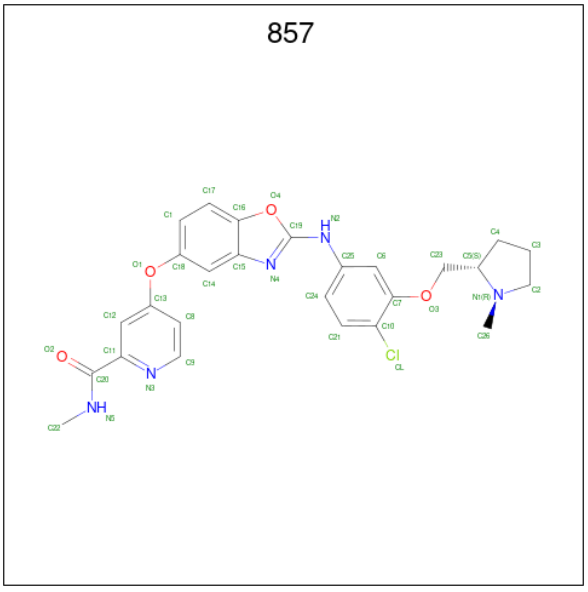
Chain	Residue	Modelled	Actual	Comment	Reference
A	817	ALA	CYS	engineered mutation	UNP P35968
A	916	THR	VAL	engineered mutation	UNP P35968
A	990	VAL	GLU	engineered mutation	UNP P35968
A	1054	PTR	TYR	modified residue	UNP P35968
A	1059	PTR	TYR	modified residue	UNP P35968
A	1172	ARG	-	expression tag	UNP 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	1054	PTR	TYR	modified residue	UNP P35968
B	1059	PTR	TYR	modified residue	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 4-({2-[(4-chloro-3-{[(2S)-1-methylpyrrolidin-2-yl]methoxy}phenyl)amino]-1,3-benzoxazol-5-yl}oxy)-N-methylpyridine-2-carboxamide (three-letter code: 857) (formula: $C_{26}H_{26}ClN_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			36	26	1	5	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			36	26	1	5	4		

- Molecule 4 is water.

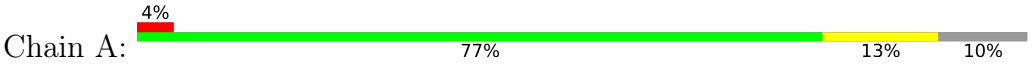
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		
4	B	56	Total	O	0	0
			56	56		

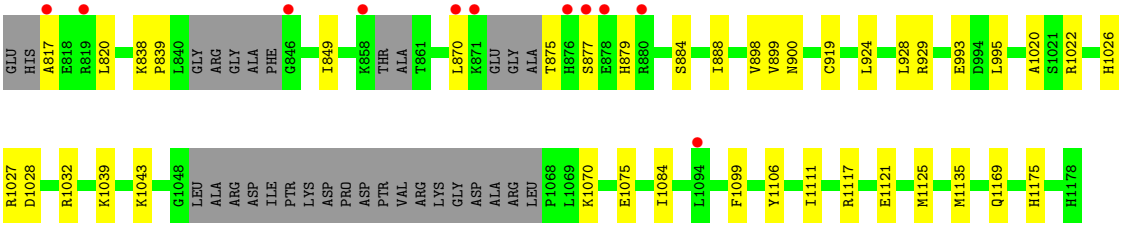
3 Residue-property plots (i)

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: Vascular endothelial growth factor receptor 2

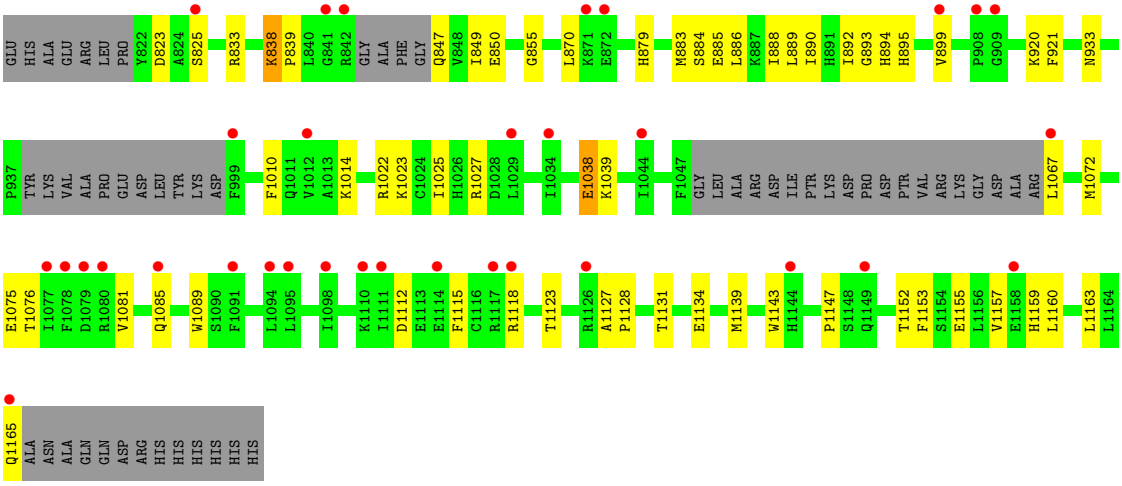
Chain A:





• Molecule 1: Vascular endothelial growth factor receptor 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.37Å 67.37Å 89.62Å 90.00° 92.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (30.00-2.10) 93.4 (29.83-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.272 0.208 , 0.238	Depositor DCC
R_{free} test set	1755 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4698	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 857, SO4

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	0.39	0/2355	0.63	0/3176
1	B	0.37	0/2141	0.59	0/2889
All	All	0.38	0/4496	0.61	0/6065

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

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	2297	0	2282	29	0
1	B	2092	0	2106	44	0
2	A	5	0	0	1	0
3	A	36	0	26	0	0
3	B	36	0	26	2	0
4	A	176	0	0	2	0
4	B	56	0	0	2	0
All	All	4698	0	4440	69	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 8.

All (69) 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:838:LYS:HD2	1:B:1039:LYS:HE2	1.64	0.78
1:B:1027:ARG:HH22	3:B:502:857:H22	1.59	0.67
1:B:1159:HIS:NE2	1:B:1163:LEU:HD11	2.10	0.66
1:B:1160:LEU:HD23	1:B:1163:LEU:HD12	1.79	0.64
1:A:839:PRO:HA	1:A:849:ILE:HG22	1.80	0.61
1:B:920:LYS:HD2	1:B:921:PHE:CE1	2.36	0.61
1:A:884:SER:O	1:A:888:ILE:HG13	2.02	0.60
1:A:875:THR:HG22	1:A:877:SER:H	1.66	0.59
1:B:1128:PRO:HG2	1:B:1131:THR:HB	1.84	0.59
1:B:833:ARG:HH21	1:B:855:GLY:HA3	1.69	0.57
1:A:924:LEU:O	1:A:928:LEU:HG	2.05	0.57
1:A:993:GLU:OE1	1:A:1175:HIS:HE1	1.88	0.57
1:B:870:LEU:HD11	1:B:879:HIS:HA	1.87	0.56
1:B:920:LYS:HD2	1:B:921:PHE:CZ	2.40	0.56
1:B:933:ASN:HB2	4:B:263:HOH:O	2.05	0.56
1:A:1026:HIS:O	1:A:1027:ARG:HB2	2.06	0.56
1:B:1152:THR:OG1	1:B:1155:GLU:HG3	2.07	0.54
1:A:838:LYS:HB3	1:B:1038:GLU:HG2	1.89	0.53
1:B:1067:LEU:HB3	1:B:1072:MET:CE	2.39	0.53
1:B:899:VAL:HG13	1:B:899:VAL:O	2.08	0.53
1:B:1075:GLU:HG2	1:B:1076:THR:N	2.23	0.53
1:A:1070:LYS:HD3	1:A:1111:ILE:HD11	1.90	0.53
1:A:1169:GLN:HG3	2:A:503:SO4:O2	2.09	0.51
1:A:900:ASN:HD22	1:A:900:ASN:N	2.06	0.51
1:B:1067:LEU:HB3	1:B:1072:MET:HE1	1.90	0.51
1:B:1081:VAL:O	1:B:1081:VAL:HG23	2.10	0.51
1:B:1085:GLN:NE2	1:B:1147:PRO:O	2.43	0.51
1:A:1022:ARG:HH21	1:A:1022:ARG:HG3	1.76	0.50
1:A:1099:PHE:CE2	1:A:1135:MET:HG2	2.48	0.49
1:A:1117:ARG:O	1:A:1121:GLU:HG3	2.11	0.49
1:B:849:ILE:HG22	1:B:850:GLU:N	2.28	0.49
1:B:894:HIS:CG	1:B:895:HIS:N	2.81	0.49
1:B:892:ILE:HG13	1:B:893:GLY:N	2.27	0.48
1:B:1153:PHE:O	1:B:1157:VAL:HG23	2.13	0.48
1:B:888:ILE:O	1:B:892:ILE:HG23	2.14	0.47
1:A:899:VAL:O	1:A:899:VAL:HG13	2.15	0.46
1:B:1027:ARG:NH2	3:B:502:857:H22	2.27	0.46
1:A:838:LYS:HD3	1:B:1038:GLU:HG2	1.97	0.46
1:A:993:GLU:OE1	1:A:1175:HIS:CE1	2.69	0.45
1:A:1028:ASP:CG	1:A:1032:ARG:HH22	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:GLY:HA2	4:B:241:HOH:O	2.17	0.45
1:B:1159:HIS:CD2	1:B:1163:LEU:HD11	2.52	0.44
1:A:870:LEU:HD11	1:A:879:HIS:HA	2.00	0.44
1:B:1022:ARG:O	1:B:1023:LYS:HB2	2.17	0.44
1:B:1118:ARG:HD3	1:B:1123:THR:OG1	2.17	0.44
1:B:892:ILE:O	1:B:1022:ARG:NE	2.51	0.44
1:A:1020:ALA:HB1	1:A:1084:ILE:HD13	2.00	0.43
1:B:1127:ALA:HB1	1:B:1131:THR:HG21	2.00	0.43
1:B:1134:GLU:OE1	1:B:1134:GLU:N	2.38	0.43
1:B:885:GLU:O	1:B:889:LEU:HG	2.17	0.43
1:B:847:GLN:HG2	1:B:849:ILE:HD11	2.00	0.43
1:B:838:LYS:HA	1:B:839:PRO:HD3	1.83	0.43
1:B:1112:ASP:O	1:B:1115:PHE:HB3	2.19	0.43
1:A:838:LYS:CD	1:B:1039:LYS:HE2	2.42	0.42
1:B:884:SER:O	1:B:888:ILE:HG13	2.19	0.42
1:B:1010:PHE:CZ	1:B:1014:LYS:HD3	2.54	0.42
1:B:1139:MET:HB3	1:B:1143:TRP:CH2	2.54	0.42
1:A:817:ALA:O	1:A:820:LEU:HB2	2.19	0.42
1:A:1075:GLU:HB3	4:A:204:HOH:O	2.19	0.42
1:B:1089:TRP:CE3	1:B:1143:TRP:HA	2.55	0.42
1:A:898:VAL:O	1:A:899:VAL:C	2.56	0.42
1:B:823:ASP:OD1	1:B:825:SER:HB3	2.20	0.42
1:B:1025:ILE:O	1:B:1027:ARG:NH2	2.54	0.41
1:A:817:ALA:HA	1:A:820:LEU:HD12	2.03	0.41
1:A:1027:ARG:HD2	4:A:13:HOH:O	2.21	0.41
1:B:886:LEU:O	1:B:890:ILE:HG13	2.21	0.41
1:A:1106:TYR:CE1	1:A:1125:MET:HG3	2.57	0.40
1:A:899:VAL:O	1:A:899:VAL:CG1	2.68	0.40
1:A:919:CYS:SG	1:A:1043:LYS:HD2	2.61	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	Percentiles	
1	A	273/314 (87%)	267 (98%)	6 (2%)	0	100	100
1	B	252/314 (80%)	246 (98%)	6 (2%)	0	100	100
All	All	525/628 (84%)	513 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	250/270 (93%)	247 (99%)	3 (1%)	71	77
1	B	229/270 (85%)	225 (98%)	4 (2%)	60	67
All	All	479/540 (89%)	472 (98%)	7 (2%)	65	71

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	929	ARG
1	A	995	LEU
1	A	1039	LYS
1	B	838	LYS
1	B	883	MET
1	B	1038	GLU
1	B	1165	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	894	HIS
1	A	900	ASN
1	A	933	ASN
1	A	1040	ASN
1	A	1162	ASN
1	A	1165	GLN

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Mol	Chain	Res	Type
1	A	1167	ASN
1	A	1173	HIS
1	A	1175	HIS
1	B	847	GLN
1	B	933	ASN
1	B	1040	ASN
1	B	1165	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 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	857	B	502	-	37,40,40	2.31	11 (29%)	45,56,56	2.72	18 (40%)
3	857	A	501	-	37,40,40	2.22	13 (35%)	45,56,56	2.79	17 (37%)
2	SO4	A	503	-	4,4,4	0.20	0	6,6,6	0.31	0

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	857	B	502	-	-	1/17/29/29	0/5/5/5
3	857	A	501	-	-	2/17/29/29	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	857	C14-C18	5.51	1.46	1.37
3	B	502	857	C14-C18	5.39	1.46	1.37
3	B	502	857	C19-N2	5.06	1.45	1.36
3	B	502	857	C24-C25	4.80	1.47	1.39
3	A	501	857	C19-N2	4.55	1.44	1.36
3	B	502	857	C17-C1	4.17	1.45	1.36
3	A	501	857	C24-C25	4.08	1.46	1.39
3	B	502	857	C1-C18	3.98	1.46	1.38
3	A	501	857	C17-C1	3.92	1.44	1.36
3	A	501	857	C1-C18	3.91	1.46	1.38
3	A	501	857	C8-C13	3.61	1.45	1.38
3	B	502	857	C8-C13	3.60	1.45	1.38
3	A	501	857	C7-C10	3.46	1.45	1.39
3	A	501	857	C6-C7	2.80	1.43	1.38
3	B	502	857	C6-C7	2.62	1.43	1.38
3	B	502	857	C7-C10	2.50	1.44	1.39
3	B	502	857	C11-N3	2.46	1.39	1.34
3	A	501	857	C21-C10	2.30	1.43	1.38
3	A	501	857	C25-N2	-2.29	1.35	1.40
3	B	502	857	C11-C20	-2.26	1.45	1.50
3	B	502	857	C6-C25	2.16	1.43	1.39
3	A	501	857	C24-C21	2.15	1.42	1.38
3	A	501	857	C11-N3	2.15	1.38	1.34
3	A	501	857	C5-N1	2.05	1.51	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	857	C22-N5-C20	-8.88	111.83	121.89
3	A	501	857	C9-N3-C11	8.58	128.06	116.93
3	B	502	857	C9-N3-C11	7.72	126.95	116.93
3	A	501	857	C8-C9-N3	-7.10	115.14	123.96
3	A	501	857	C22-N5-C20	-7.00	113.96	121.89
3	B	502	857	C8-C9-N3	-6.63	115.72	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	857	C20-C11-N3	4.91	123.27	117.48
3	A	501	857	O3-C7-C10	4.41	121.85	116.40
3	B	502	857	C24-C21-C10	-3.82	114.48	120.00
3	A	501	857	C20-C11-N3	3.74	121.90	117.48
3	A	501	857	C18-C14-C15	-3.69	115.40	119.27
3	A	501	857	C24-C25-C6	3.68	124.01	119.65
3	A	501	857	C24-C21-C10	-3.46	115.00	120.00
3	B	502	857	C21-C10-C7	3.44	125.62	120.78
3	A	501	857	C1-C18-C14	3.30	125.25	120.81
3	A	501	857	O1-C13-C12	-3.14	109.26	119.10
3	B	502	857	C18-C14-C15	-3.13	115.98	119.27
3	A	501	857	C21-C10-C7	3.08	125.12	120.78
3	A	501	857	C8-C13-C12	3.01	124.67	120.53
3	B	502	857	C3-C4-C5	2.97	111.58	104.68
3	B	502	857	O1-C13-C12	-2.96	109.82	119.10
3	B	502	857	C11-C20-N5	-2.79	113.84	115.67
3	A	501	857	C3-C4-C5	2.75	111.08	104.68
3	A	501	857	C6-C25-N2	-2.67	111.28	120.32
3	B	502	857	C12-C11-N3	-2.64	119.86	123.19
3	A	501	857	C17-C1-C18	-2.52	116.79	120.17
3	B	502	857	C8-C13-C12	2.49	123.96	120.53
3	B	502	857	C1-C18-C14	2.45	124.10	120.81
3	A	501	857	C25-C6-C7	-2.38	116.24	119.45
3	B	502	857	C18-O1-C13	2.37	124.36	118.80
3	B	502	857	C24-C25-C6	2.36	122.44	119.65
3	B	502	857	C6-C25-N2	-2.29	112.57	120.32
3	A	501	857	C12-C11-N3	-2.28	120.32	123.19
3	B	502	857	C7-C10-CL	-2.21	116.83	119.43
3	B	502	857	C25-C6-C7	-2.19	116.49	119.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

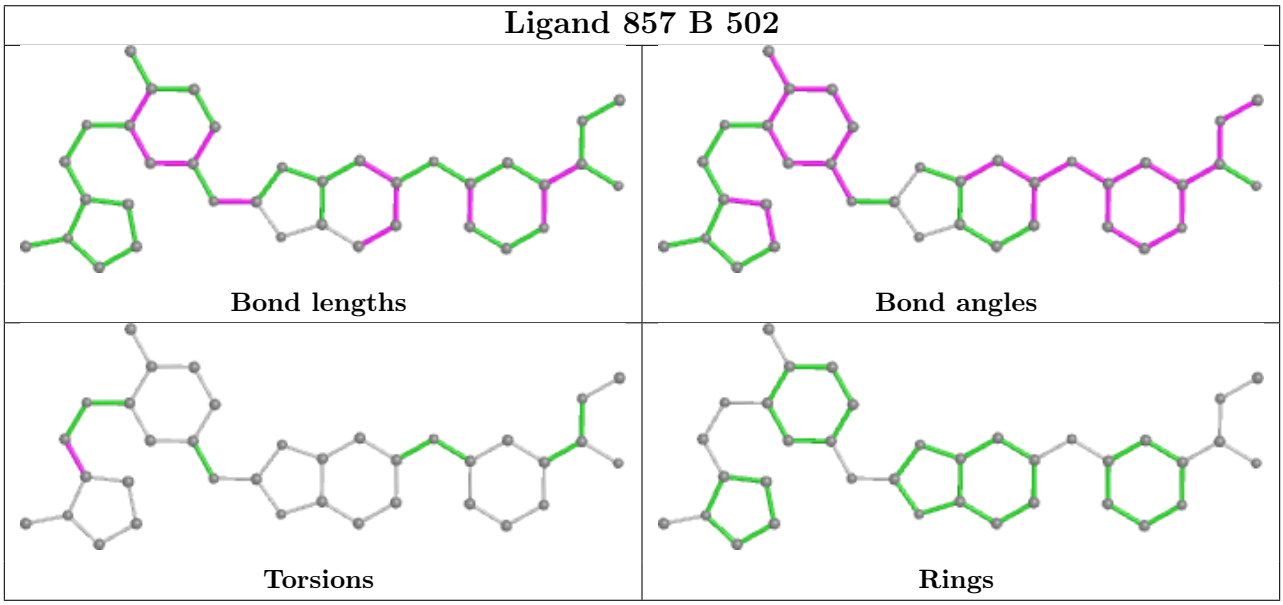
Mol	Chain	Res	Type	Atoms
3	A	501	857	O3-C23-C5-C4
3	B	502	857	O3-C23-C5-N1
3	A	501	857	O3-C23-C5-N1

There are no ring outliers.

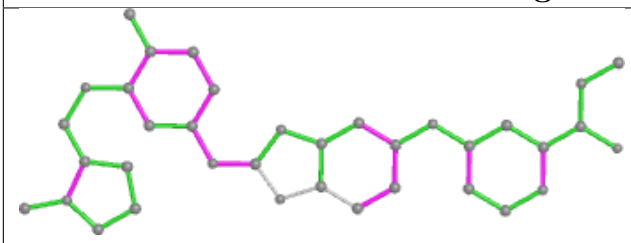
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	857	2	0
2	A	503	SO4	1	0

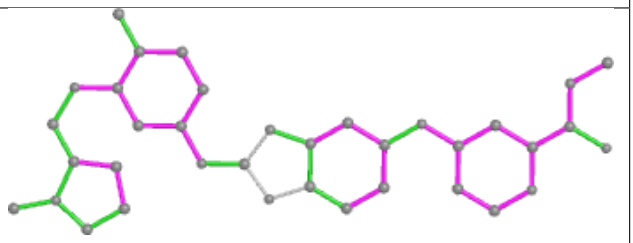
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



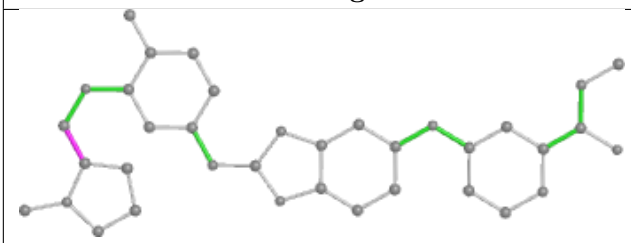
Ligand 857 A 501



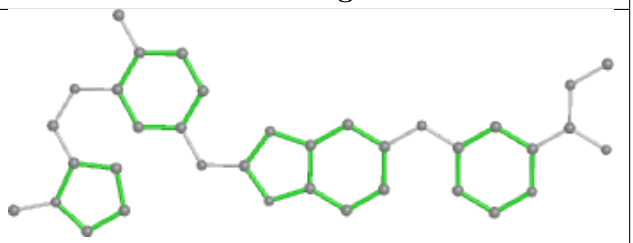
Bond lengths



Bond angles



Torsions



Rings

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

6.1 Protein, DNA and RNA chains

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)	Q<0.9
1	A	283/314 (90%)	0.08	11 (3%) 39 45	18, 29, 51, 68	0
1	B	260/314 (82%)	0.60	33 (12%) 3 5	26, 44, 64, 73	0
All	All	543/628 (86%)	0.33	44 (8%) 12 15	18, 35, 61, 73	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	842	ARG	5.2
1	B	1078	PHE	5.1
1	A	846	GLY	5.1
1	A	858	LYS	4.7
1	A	819	ARG	4.5
1	B	872	GLU	4.4
1	B	841	GLY	4.2
1	B	871	LYS	3.9
1	B	908	PRO	3.7
1	B	1080	ARG	3.7
1	A	870	LEU	3.7
1	B	1094	LEU	3.6
1	A	871	LYS	3.6
1	B	1067	LEU	3.5
1	B	1110	LYS	3.5
1	B	1095	LEU	3.5
1	A	876	HIS	3.4
1	B	1126	ARG	3.4
1	B	1079	ASP	3.0
1	B	1118	ARG	2.9
1	A	878	GLU	2.9
1	B	1111	ILE	2.9
1	B	1165	GLN	2.9
1	B	1091	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	880	ARG	2.7
1	B	1044	ILE	2.6
1	B	1117	ARG	2.5
1	B	1012	VAL	2.5
1	B	999	PHE	2.5
1	B	909	GLY	2.5
1	B	1098	ILE	2.5
1	B	825	SER	2.4
1	B	1034	ILE	2.3
1	B	1158	GLU	2.3
1	B	1029	LEU	2.2
1	B	899	VAL	2.2
1	B	1085	GLN	2.2
1	A	1094	LEU	2.1
1	A	817	ALA	2.1
1	A	877	SER	2.1
1	B	1077	ILE	2.1
1	B	1114	GLU	2.1
1	B	1144	HIS	2.0
1	B	1149	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

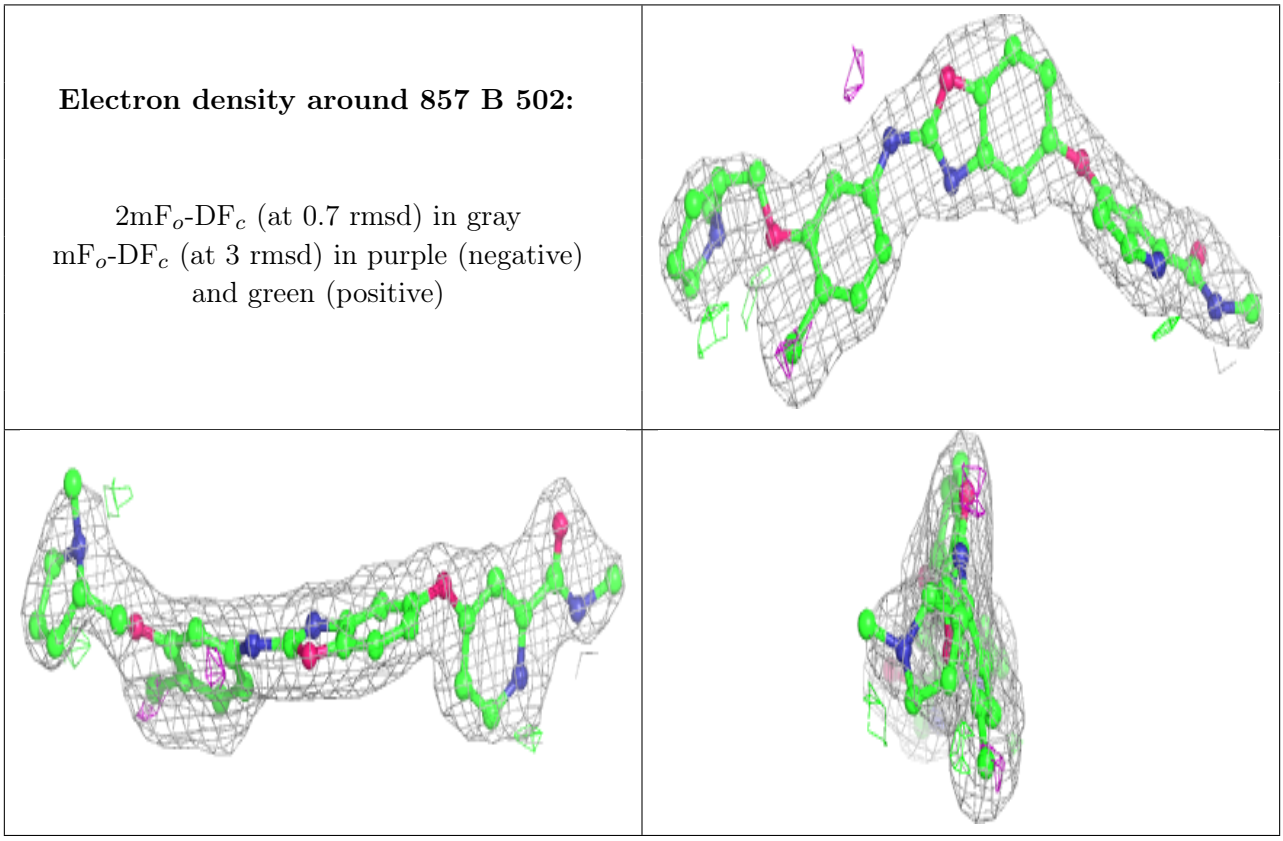
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	503	5/5	0.76	0.33	69,70,70,72	0
3	857	B	502	36/36	0.91	0.14	32,37,51,52	0
3	857	A	501	36/36	0.94	0.11	27,33,44,46	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.

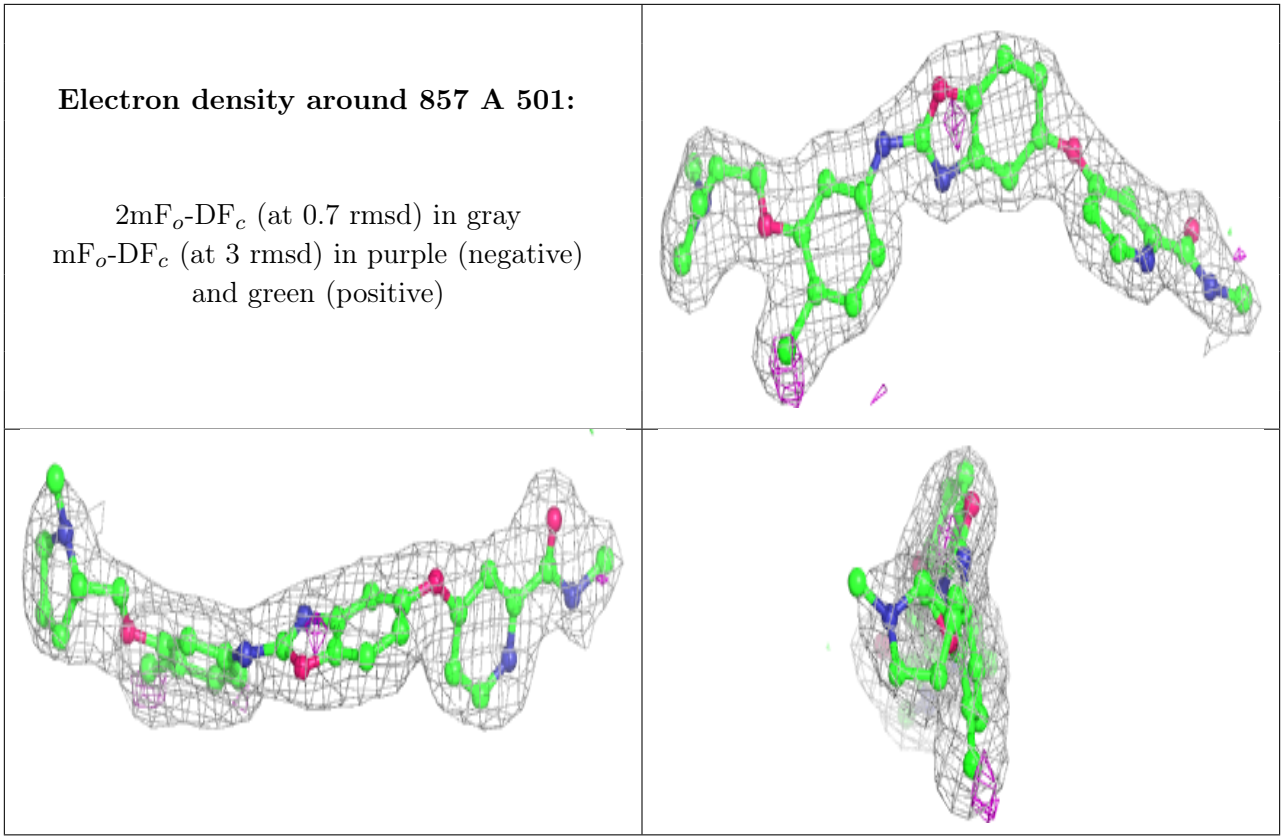
Electron density around 857 B 502:

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



Electron density around 857 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.