



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 10:43 PM EDT

PDB ID : 7K1D
Title : Crystal structure of human insulin degrading enzyme (IDE) in complex with compound BDM_77291
Authors : Liang, W.G.; Deprez, R.; Bosc, D.; Tang, W.
Deposited on : 2020-09-07
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

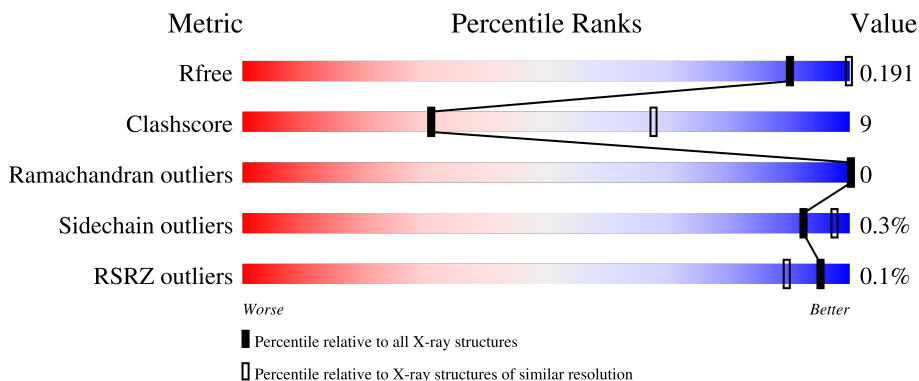
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	990	 75% 21%
1	B	990	 79% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15889 atoms, of which 82 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	957	7829	5042	1314	1451	22	0	0	0
1	B	958	7834	5047	1315	1449	23	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735

Continued on next page...

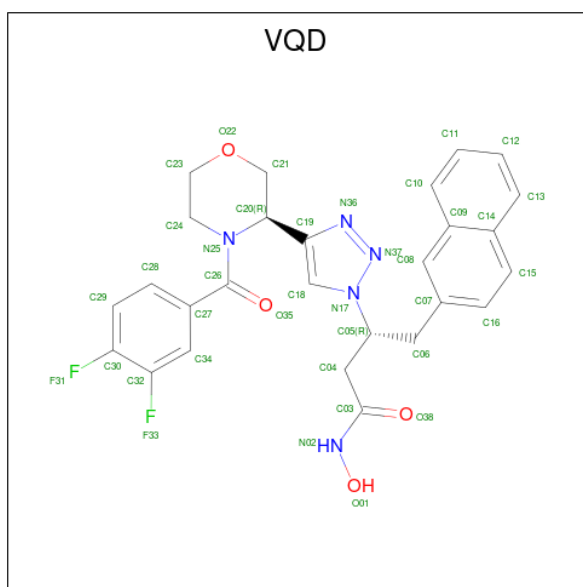
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	MET	-	initiating methionine	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

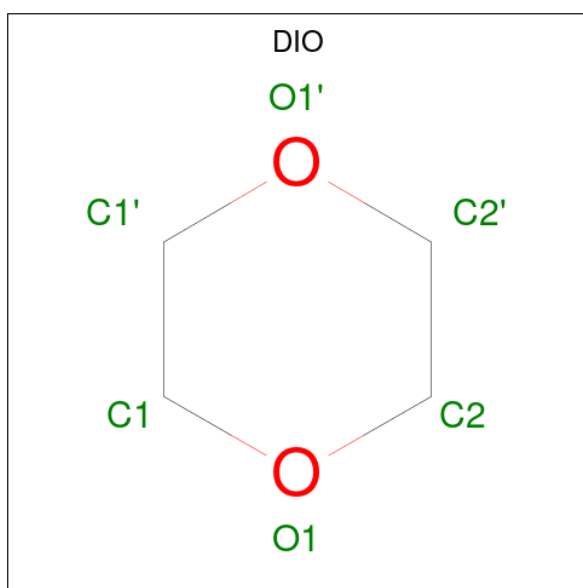
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0

- Molecule 3 is (3R)-3-{4-[(3R)-4-(3,4-difluorobenzene-1-carbonyl)morpholin-3-yl]-1H-1,2,3-triazol-1-yl}-N-hydroxy-4-(naphthalen-2-yl)butanamide (three-letter code: VQD) (formula: C₂₇H₂₅F₂N₅O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	F	N	O	0	0
			38	27	2	5	4		
3	B	1	Total	C	F	N	O	0	0
			38	27	2	5	4		

- Molecule 4 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



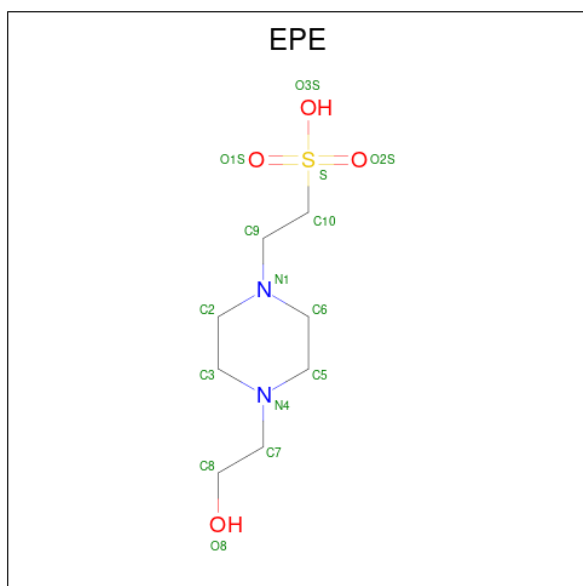
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	A	1	Total	C	H	O	0	0
			14	4	8	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		
4	B	1	Total	C	H	O	0	0
			14	4	8	2		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
5	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

N376	E598	W776	E862
L392	L599	F777	N963
Q396	L600	N787	ASP
R431	L604	E792	SER
L441	L616	I793	ASN
V449	L620	Q796	PRO
L450	G626	M799	VAL
T451	L629	L808	VAL
L455	N635	E817	GLY
P473	D636	P818	GLU
V476	K637	F820	PHE
V481	Q638	R824	PRO
K483	K643	I843	ALA
E486	E647	Q844	GLN
D507	K648	G845	ASN
I510	F659	I846	ASP
K511	Q677	R847	ILE
T526	M683	I868	N979
K527	T696	K872	L980
L538	E689	M877	P984
P548	L709	L894	E990
K552	P710	Y907	V1008
S557	A714	Q914	K1009
K558	F715	Q915	P1010
L559	I716	Y916	H1011
D565	P717	V925	ILE
K566	R722	K833	ASN
L574	I725	Y940	PHE
E577	L729	E942	MET
F578	N732	A945	ALA
P579	I733	V946	LYS
A583	T734	D947	LEU
D586	M742	A948	
P587	L758	P949	
Y594	L771	R950	
	R774	R951	
	G775	H952	
		K953	
		R961	

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	264.31Å 264.31Å 90.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.42 – 3.00 45.42 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.2 (45.42-3.00) 89.9 (45.42-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.156 , 0.192 0.158 , 0.191	Depositor DCC
R_{free} test set	1990 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtrriage
Anisotropy	0.009	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15889	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DIO, EPE, VQD, ZN

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	0.47	0/8024	0.63	0/10854
1	B	0.49	0/8030	0.65	0/10862
All	All	0.48	0/16054	0.64	0/21716

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	7829	0	7769	162	0
1	B	7834	0	7779	123	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	38	0	0	0	0
3	B	38	0	0	0	0
4	A	18	24	24	0	0
4	B	18	24	24	1	0
5	A	15	17	17	1	0
5	B	15	17	17	0	0
All	All	15807	82	15630	285	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 9.

The worst 5 of 285 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:B:153:VAL:HG22	1:B:154:SER:H	1.00	1.15
1:B:153:VAL:HG22	1:B:154:SER:N	1.70	0.98
1:B:153:VAL:CG2	1:B:154:SER:H	1.76	0.98
1:B:716:ILE:HB	1:B:717:PRO:HD3	1.46	0.94
1:A:545:THR:HG22	1:A:546:PRO:HD2	1.50	0.93

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	953/990 (96%)	920 (96%)	33 (4%)	0	100	100
1	B	954/990 (96%)	915 (96%)	39 (4%)	0	100	100
All	All	1907/1980 (96%)	1835 (96%)	72 (4%)	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	853/879 (97%)	849 (100%)	4 (0%)	88	96
1	B	853/879 (97%)	852 (100%)	1 (0%)	93	98
All	All	1706/1758 (97%)	1701 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	457	GLU
1	A	460	ARG
1	A	756	LYS
1	B	774	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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	VQD	A	1102	2	41,42,42	2.80	9 (21%)	47,59,59	1.85	9 (19%)
4	DIO	A	1105	-	6,6,6	0.74	0	6,6,6	0.86	0
4	DIO	B	1103	-	6,6,6	0.68	0	6,6,6	0.74	0
4	DIO	A	1104	-	6,6,6	0.71	0	6,6,6	1.45	2 (33%)
5	EPE	B	1106	-	15,15,15	1.18	1 (6%)	18,20,20	1.91	4 (22%)
5	EPE	A	1106	-	15,15,15	0.88	1 (6%)	18,20,20	1.90	5 (27%)
4	DIO	A	1103	-	6,6,6	0.66	0	6,6,6	0.71	0
3	VQD	B	1102	2	41,42,42	2.72	8 (19%)	47,59,59	1.58	7 (14%)
4	DIO	B	1105	-	6,6,6	0.74	0	6,6,6	0.86	0
4	DIO	B	1104	-	6,6,6	0.75	0	6,6,6	0.93	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	VQD	A	1102	2	-	2/18/37/37	0/5/5/5
4	DIO	A	1105	-	-	-	0/1/1/1
4	DIO	B	1103	-	-	-	0/1/1/1
5	EPE	B	1106	-	-	5/9/19/19	0/1/1/1
4	DIO	A	1104	-	-	-	0/1/1/1
5	EPE	A	1106	-	-	7/9/19/19	0/1/1/1
4	DIO	A	1103	-	-	-	0/1/1/1
3	VQD	B	1102	2	-	2/18/37/37	0/5/5/5
4	DIO	B	1105	-	-	-	0/1/1/1
4	DIO	B	1104	-	-	-	0/1/1/1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	VQD	C03-N02	13.65	1.47	1.32
3	B	1102	VQD	C03-N02	13.64	1.47	1.32
3	B	1102	VQD	C18-C19	5.59	1.44	1.36
3	A	1102	VQD	C20-N25	-5.30	1.42	1.47
3	A	1102	VQD	C18-C19	4.83	1.43	1.36

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	VQD	C23-O22-C21	6.53	119.02	109.97
3	B	1102	VQD	C23-O22-C21	5.03	116.94	109.97
3	A	1102	VQD	O01-N02-C03	4.39	126.28	119.79
5	B	1106	EPE	C5-N4-C3	4.15	118.17	108.83
5	A	1106	EPE	C5-N4-C3	4.03	117.89	108.83

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

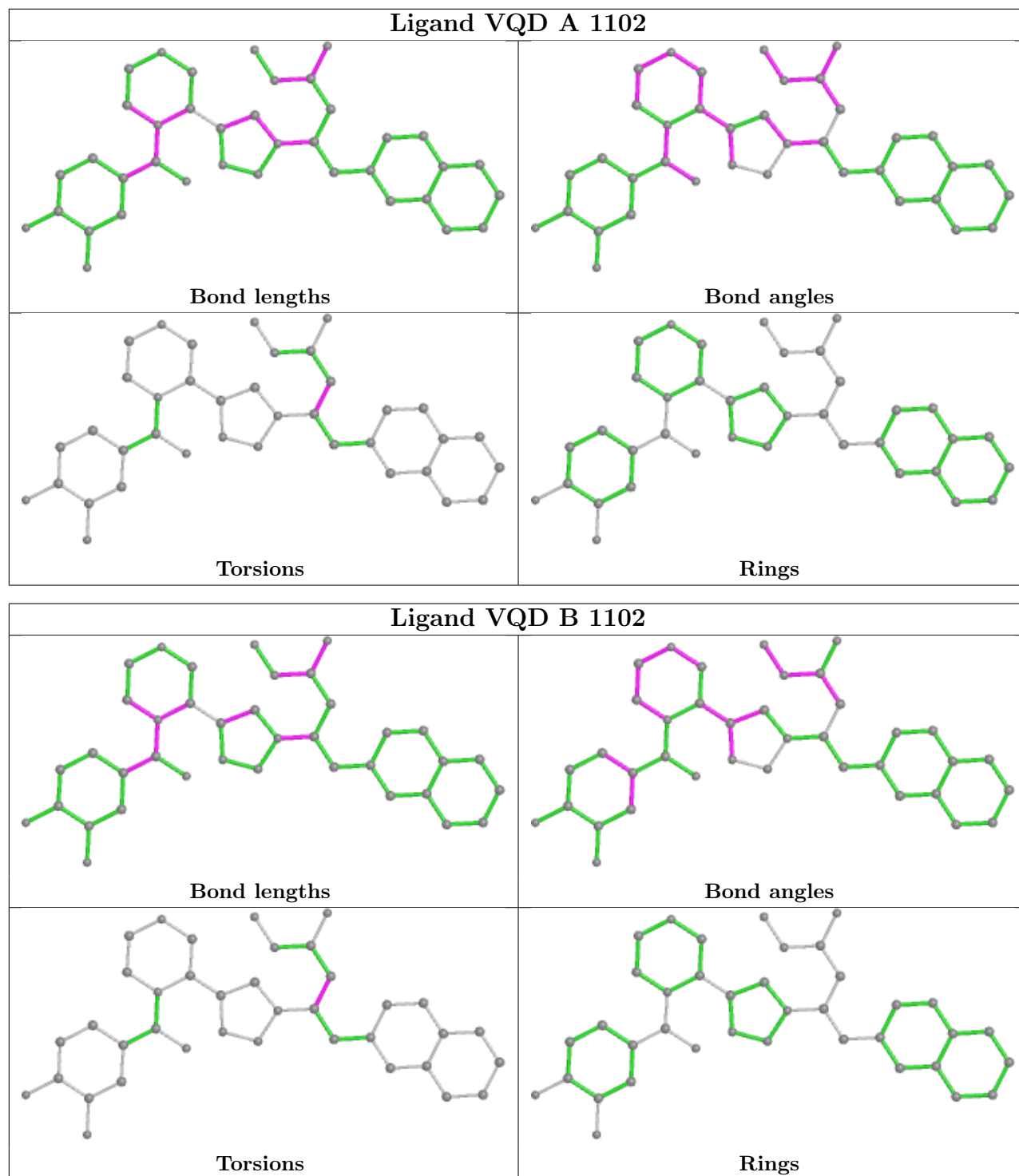
Mol	Chain	Res	Type	Atoms
3	A	1102	VQD	C03-C04-C05-C06
3	A	1102	VQD	C03-C04-C05-N17
3	B	1102	VQD	C03-C04-C05-C06
3	B	1102	VQD	C03-C04-C05-N17
5	A	1106	EPE	C9-C10-S-O1S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1106	EPE	1	0
4	B	1105	DIO	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 [i](#)

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	957/990 (96%)	-0.48	1 (0%) 95 89	30, 53, 76, 115	0
1	B	958/990 (96%)	-0.53	1 (0%) 95 89	27, 45, 70, 127	0
All	All	1915/1980 (96%)	-0.50	2 (0%) 95 89	27, 49, 74, 127	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	GLY	2.3
1	A	52	ASN	2.2

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, 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.

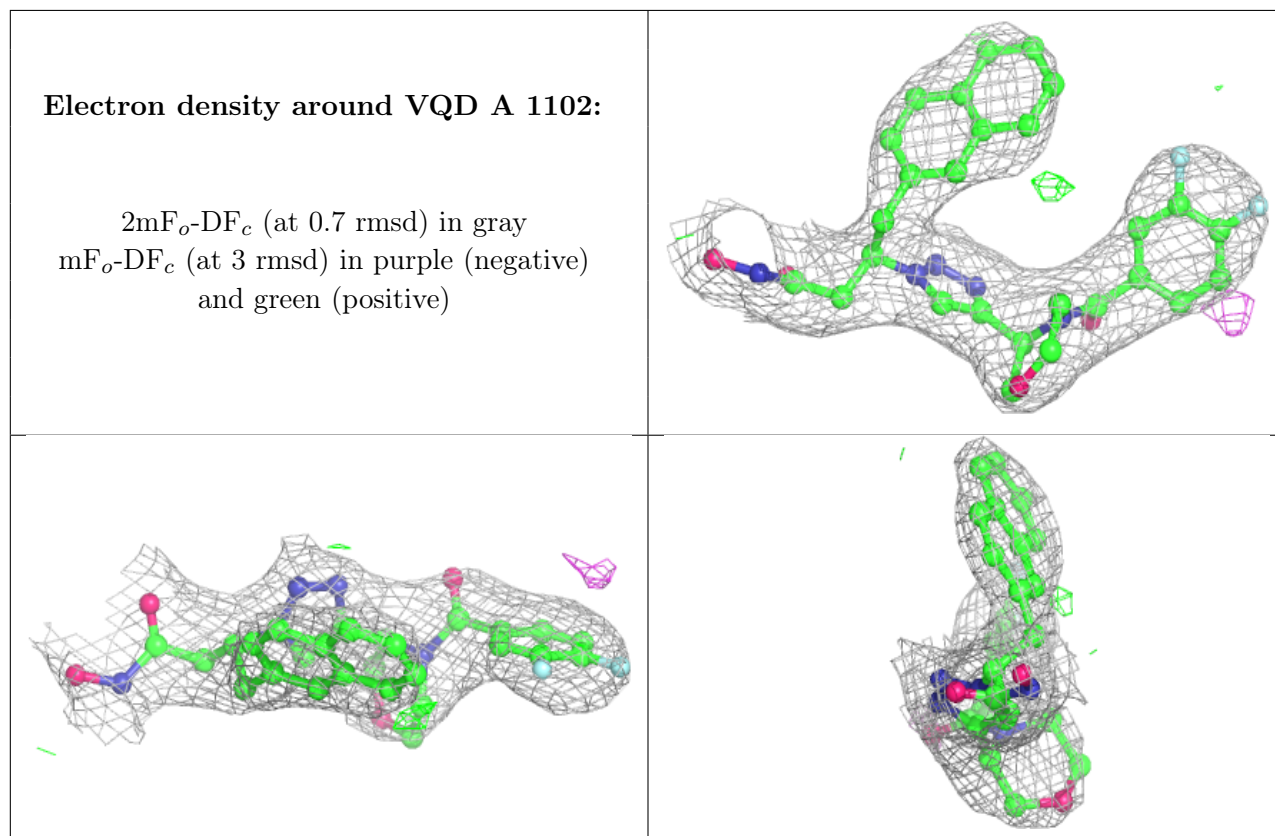
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DIO	A	1104	6/6	0.74	0.31	71,91,129,129	0
4	DIO	A	1103	6/6	0.78	0.36	81,97,120,120	0
4	DIO	B	1103	6/6	0.80	0.39	75,102,120,120	0

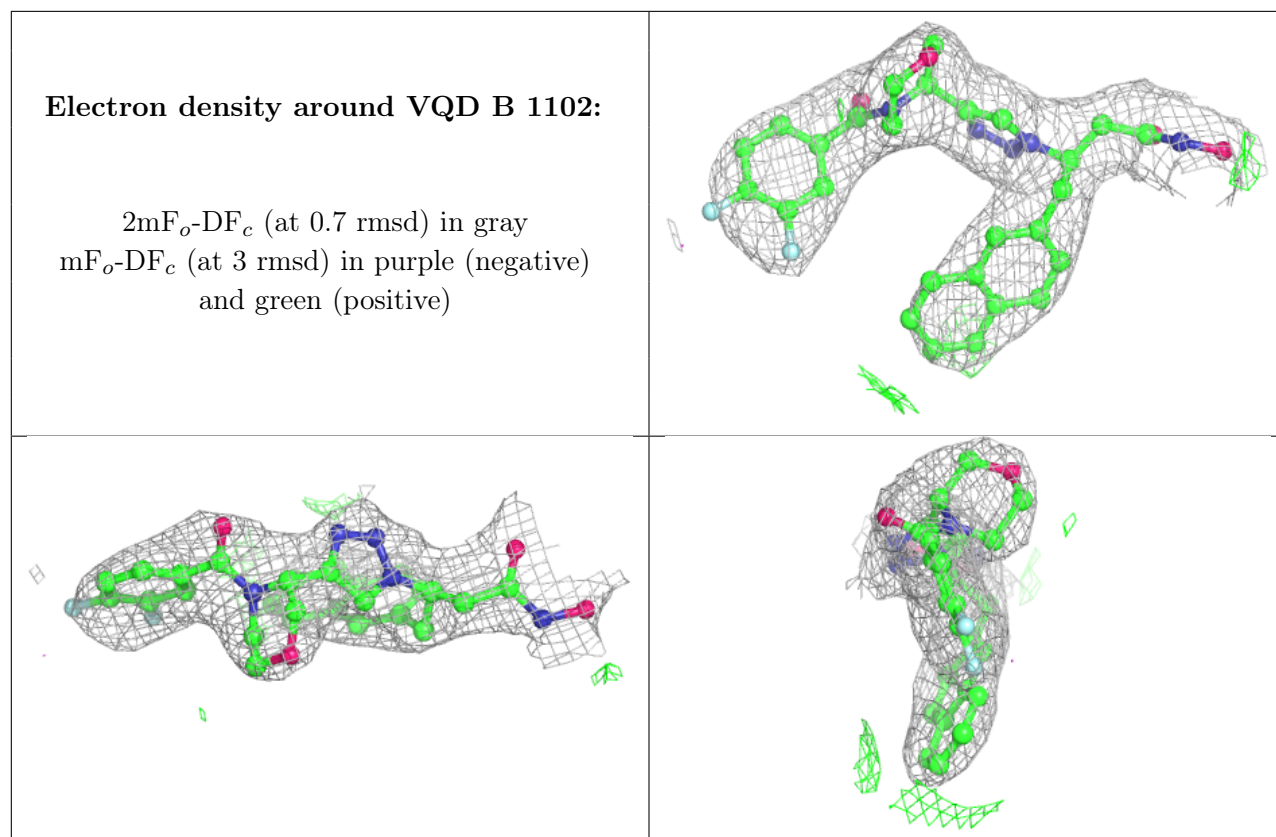
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DIO	A	1105	6/6	0.82	0.26	65,88,129,129	0
4	DIO	B	1104	6/6	0.83	0.33	57,80,117,117	0
4	DIO	B	1105	6/6	0.86	0.30	51,65,120,120	0
5	EPE	A	1106	15/15	0.94	0.18	54,90,108,108	0
5	EPE	B	1106	15/15	0.94	0.22	54,79,103,109	0
3	VQD	A	1102	38/38	0.96	0.19	41,54,72,73	0
3	VQD	B	1102	38/38	0.96	0.17	41,49,62,76	0
2	ZN	A	1101	1/1	0.99	0.12	52,52,52,52	0
2	ZN	B	1101	1/1	0.99	0.17	42,42,42,42	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.