

Full wwPDB X-ray Structure Validation Report (i)

Jun 4, 2024 – 10:20 PM EDT

PDB ID : 8SC7

Title: Structure of EGFR in complex with MTX-531

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Deposited on : 2023-04-05

Resolution : 1.98 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.36.2buster-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)

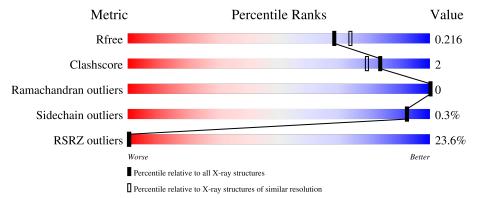
Validation Pipeline (wwPDB-VP) : 2.36.2

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 1.98 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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					
			23%					
1	A	330	93%	5% •				



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2922 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.

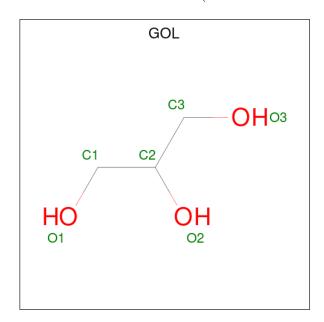
• Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	326	Total	С	N	О	S	0	6	0
1	A	320	2657	1700	451	486	20	0	U	U

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLY	-	expression tag	UNP P00533
A	694	ALA	-	expression tag	UNP P00533
A	695	MET	-	expression tag	UNP P00533

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



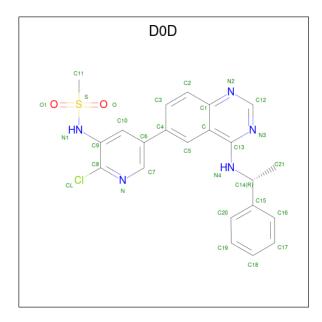
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0



• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0

• Molecule 4 is N-[(5P)-2-chloro-5-(4-{[(1R)-1-phenylethyl]amino}quinazolin-6-yl)pyridin -3-yl]methanesulfonamide (three-letter code: D0D) (formula: $C_{22}H_{20}ClN_5O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
1	Δ	1	Total	С	Cl	N	О	S	0	1
T	11	1	41	24	1	7	6	3		1

• Molecule 5 is water.

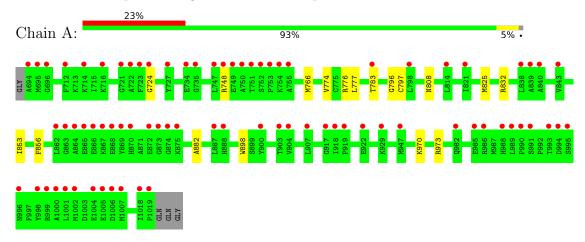
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	217	Total O 217 217	0	0



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: Epidermal growth factor receptor





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants	145.52Å 145.52Å 145.52Å	Danagitan
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.30 - 1.98	Depositor
Resolution (A)	34.30 - 1.98	EDS
% Data completeness	96.5 (34.30-1.98)	Depositor
(in resolution range)	96.6 (34.30-1.98)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.82 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
D.D.	0.186 , 0.216	Depositor
R, R_{free}	0.192 , 0.216	DCC
R_{free} test set	1439 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 59.7	EDS
L-test for twinning ²	$< L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2922	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: D0D, CL, GOL

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	$\mathbf{lengths}$	Bond angles		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.29	0/2718	0.54	0/3678	

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	A	2657	0	2681	13	0
2	A	6	0	8	0	0
3	A	1	0	0	0	0
4	A	41	0	0	3	0
5	A	217	0	0	3	0
All	All	2922	0	2689	13	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:783:THR:HA	5:A:1319:HOH:O	1.84	0.77
1:A:796:GLY:HA3	4:A:1103[A]:D0D:C11	2.22	0.69
1:A:797:CYS:H	4:A:1103[B]:D0D:C11	2.17	0.57
1:A:796:GLY:HA3	4:A:1103[B]:D0D:O1	2.06	0.55
1:A:766:MET:HB3	1:A:777:LEU:HB2	1.90	0.54
1:A:970:LYS:HA	1:A:973:ARG:NH2	2.27	0.48
1:A:776[B]:ARG:HE	1:A:776[B]:ARG:HB2	1.49	0.47
1:A:774[B]:VAL:HG13	1:A:856:PHE:HZ	1.80	0.46
1:A:724:GLY:HA2	1:A:748:ARG:HG2	1.97	0.45
1:A:808:ASN:HB3	5:A:1232:HOH:O	2.18	0.43
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.54	0.42
1:A:825:MET:SD	1:A:853:ILE:HD13	2.61	0.40
1:A:783:THR:HG22	5:A:1319:HOH:O	2.20	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	330/330 (100%)	321 (97%)	9 (3%)	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	292/288 (101%)	291 (100%)	1 (0%)	92 92	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	832	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	812	GLN
1	A	816	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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).

ſ	Mol	Mol Type Chain Res		Link	Во	Bond lengths			Bond angles		
	MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	4	D0D	A	1103[C]	-	33,34,34	1.54	6 (18%)	46,49,49	1.21	3 (6%)



Mol	Type	Chain	Res	Dog Link		Res Link Bond lengths			Bond angles		
WIOI	туре	Chain	nes	Lilik	Counts	RMSZ	$\mid \# Z > 2$	Counts	RMSZ	# Z > 2	
4	D0D	A	1103[B]	-	33,34,34	1.49	5 (15%)	46,49,49	1.24	4 (8%)	
2	GOL	A	1101	-	5,5,5	0.10	0	5,5,5	0.31	0	
4	D0D	A	1103[A]	-	33,34,34	1.62	6 (18%)	46,49,49	1.25	4 (8%)	

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
4	D0D	A	1103[C]	-	-	2/17/17/17	0/4/4/4
4	D0D	A	1103[B]	-	-	3/17/17/17	0/4/4/4
2	GOL	A	1101	-	-	2/4/4/4	-
4	D0D	A	1103[A]	-	-	3/17/17/17	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\textup{\AA})$	Ideal(Å)
4	A	1103[A]	D0D	C9-N1	3.99	1.49	1.42
4	A	1103[A]	D0D	C10-C9	3.70	1.45	1.39
4	A	1103[B]	D0D	C10-C9	3.70	1.45	1.39
4	A	1103[C]	D0D	C10-C9	3.70	1.45	1.39
4	A	1103[A]	D0D	C8-C9	3.63	1.43	1.40
4	A	1103[B]	D0D	C8-C9	3.63	1.43	1.40
4	A	1103[C]	D0D	C8-C9	3.63	1.43	1.40
4	A	1103[A]	D0D	C11-S	-3.41	1.67	1.75
4	A	1103[B]	D0D	C11-S	-3.38	1.67	1.75
4	A	1103[C]	D0D	C9-N1	3.28	1.48	1.42
4	A	1103[C]	D0D	C11-S	-3.05	1.68	1.75
4	A	1103[A]	D0D	C8-N	2.60	1.35	1.32
4	A	1103[B]	D0D	C8-N	2.60	1.35	1.32
4	A	1103[C]	D0D	C8-N	2.60	1.35	1.32
4	A	1103[A]	D0D	C6-C4	-2.16	1.43	1.49
4	A	1103[B]	D0D	C6-C4	-2.16	1.43	1.49
4	A	1103[C]	D0D	C6-C4	-2.16	1.43	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	1103[A]	D0D	C10-C9-C8	-3.45	112.35	116.06
4	A	1103[B]	D0D	C10-C9-C8	-3.45	112.35	116.06

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-	110116	DICULUUS	Duuc
	J	1	1

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^{o})$
4	A	1103[C]	D0D	C10-C9-C8	-3.45	112.35	116.06
4	A	1103[A]	D0D	C10-C6-C7	3.13	120.21	117.11
4	A	1103[B]	D0D	C10-C6-C7	3.13	120.21	117.11
4	A	1103[C]	D0D	C10-C6-C7	3.13	120.21	117.11
4	A	1103[A]	D0D	C11-S-N1	-3.00	103.21	106.63
4	A	1103[B]	D0D	C11-S-N1	-2.42	103.87	106.63
4	A	1103[A]	D0D	C5-C-C13	-2.32	122.78	124.88
4	A	1103[B]	D0D	C5-C-C13	-2.32	122.78	124.88
4	A	1103[C]	D0D	C5-C-C13	-2.32	122.78	124.88

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	GOL	O1-C1-C2-C3
4	A	1103[B]	D0D	C9-N1-S-O1
4	A	1103[B]	D0D	C9-N1-S-C11
4	A	1103[C]	D0D	C9-N1-S-C11
4	A	1103[C]	D0D	C9-N1-S-O
4	A	1103[B]	D0D	C9-N1-S-O
2	A	1101	GOL	O1-C1-C2-O2
4	A	1103[A]	D0D	C9-N1-S-O
4	A	1103[A]	D0D	C9-N1-S-O1
4	A	1103[A]	D0D	C9-N1-S-C11

There are no ring outliers.

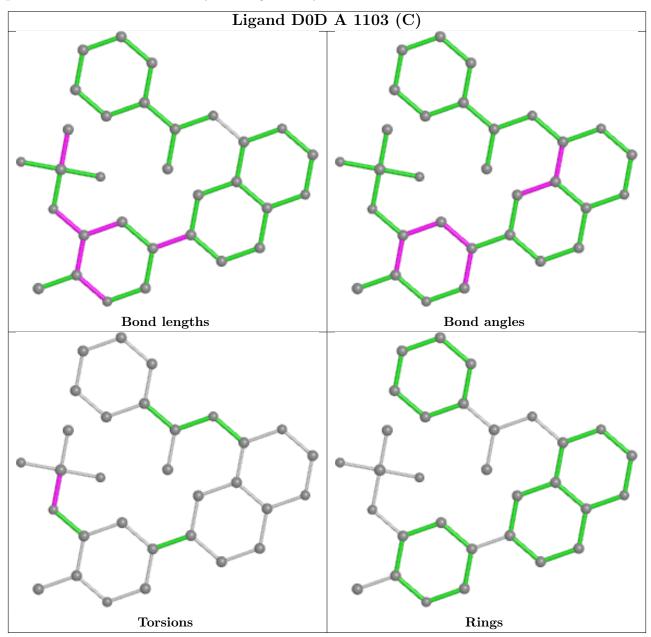
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1103[B]	D0D	2	0
4	A	1103[A]	D0D	1	0

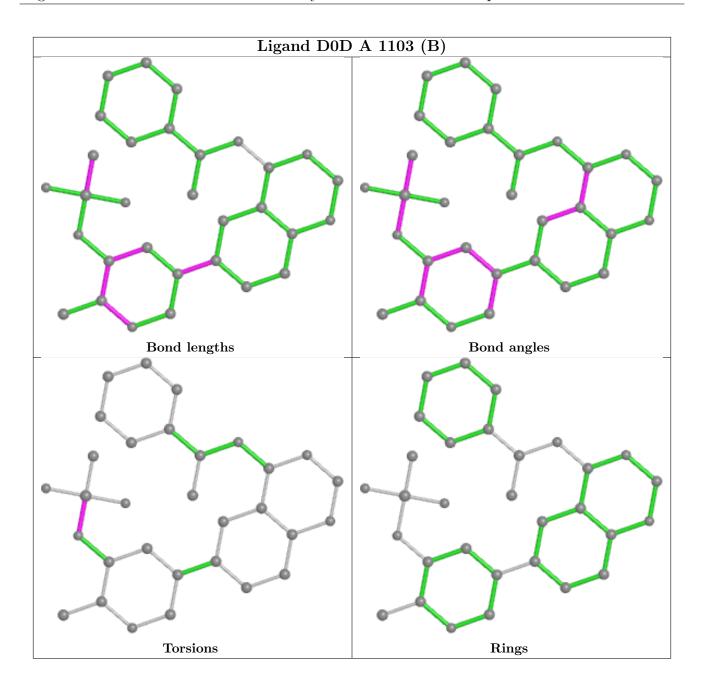
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



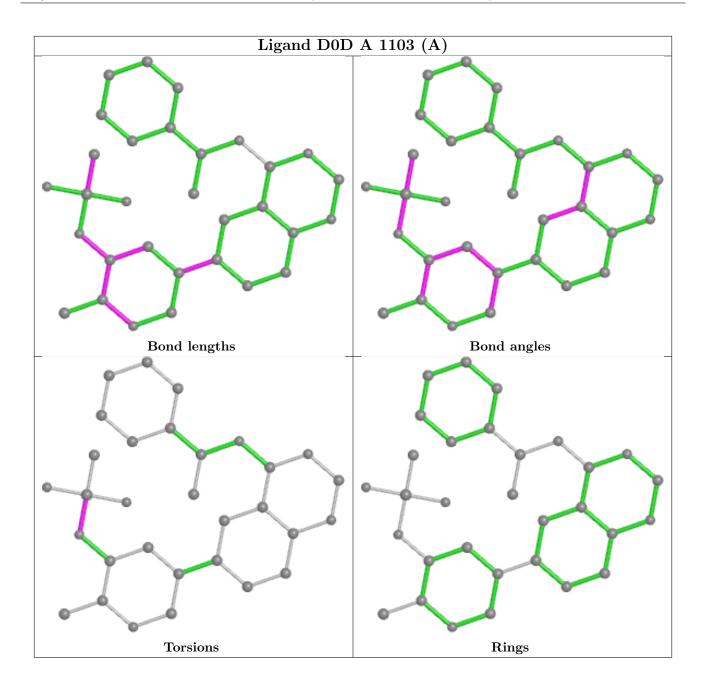
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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>	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	A	326/330 (98%)	1.31	77 (23%) 0 0	36, 54, 117, 139	0

All (77) RSRZ outliers are listed below:

Mol	Chain			RSRZ
1	A	723	PHE	9.1
1	A	1002	MET	9.0
1	A	864	ALA	8.6
1	A	863	GLY	7.5
1	A	1000	ALA	7.2
1	A	995	SER	7.0
1	A	751	THR	6.9
1	A	873	GLY	6.8
1	A	998	TYR	6.3
1	A	999	ARG	6.2
1	A	747	LEU	6.1
1	A	1004	GLU	5.8
1	A	988	HIS	5.7
1	A	865	GLU	5.6
1	A	867	LYS	5.5
1	A	1005	GLU	5.4
1	A	722	ALA	5.3
1	A	753	PRO	5.3
1	A	748	ARG	5.2
1	A	875	LYS	5.2
1	A	696	GLY	5.1
1	A	917	GLY	5.0
1	A	750	ALA	4.7
1	A	874	GLY	4.6
1	A	991	SER	4.6
1	A	993	THR	4.4
1	A	1006	ASP	4.2

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Mol	Mol Chain		Type	RSRZ	
1	A	869			
1	A	996	ASN	4.0	
1	A	749	GLU	4.0	
1	A	870[A]	HIS	4.0	
1	A	986	ARG	3.8	
1	A	990	PRO	3.8	
1	A	735	GLY	3.7	
1	A	1001	LEU	3.6	
1	A	994	ASP	3.5	
1	A	862	LEU	3.5	
1	A	695	MET	3.5	
1	A	755	ALA	3.3	
1	A	922	GLU	3.3	
1	A	752	SER	3.3	
1	A	712	PHE	3.3	
1	A	754	LYS	3.3	
1	A	843	VAL	3.3	
1	A	694	ALA	3.2	
1	A	904	VAL	3.2	
1	A	1018	ILE	3.2	
1	A	724	GLY	3.1	
1	A	839	ALA	3.0	
1	A	838	LEU	3.0	
1	A	1019	PRO	2.9	
1	A	872	GLU	2.9	
1	A	734	GLU	2.8	
1	A	919	PRO	2.8	
1	A	783	THR	2.8	
1	A	868	GLU	2.8	
1	A	866	GLU	2.8	
1	A	985	GLU	2.7	
1	A	821	ILE	2.6	
1	A	798	LEU	2.6	
1	A	887	LEU	2.6	
1	A	714	LYS	2.5	
1	A	903	THR	2.4	
1	A	716	LYS	2.4	
1	A	907	LEU	2.4	
1	A	989	LEU	2.4	
1	A	727	TYR	2.4	
1	A	721	GLY	2.3	
1	A	982	GLN	2.3	

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Mol	Chain	Res	Type	RSRZ
1	A	840	ALA	2.3
1	A	918	ILE	2.3
1	A	1007	MET	2.2
1	A	888	HIS	2.1
1	A	900	TYR	2.1
1	A	929	LYS	2.1
1	A	947	MET	2.1
1	A	814	LEU	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)

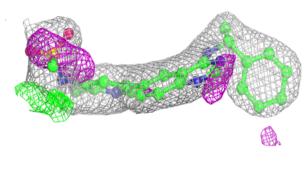
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

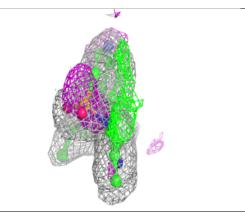
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{ ilde{A}}^2)$	Q<0.9
3	CL	A	1102	1/1	0.84	0.13	83,83,83,83	0
2	GOL	A	1101	6/6	0.85	0.18	83,84,85,89	0
4	D0D	A	1103[A]	31/31	0.90	0.15	44,49,82,89	5
4	D0D	A	1103[B]	31/31	0.90	0.15	44,49,85,89	5
4	D0D	A	1103[C]	31/31	0.90	0.15	44,49,81,89	5

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.



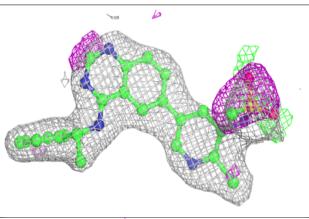
Electron density around D0D A 1103 (A): 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

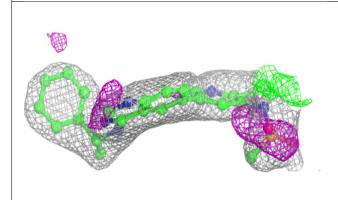


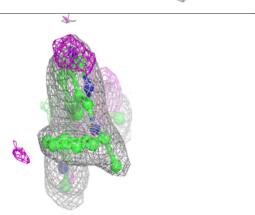


Electron density around D0D A 1103 (B):

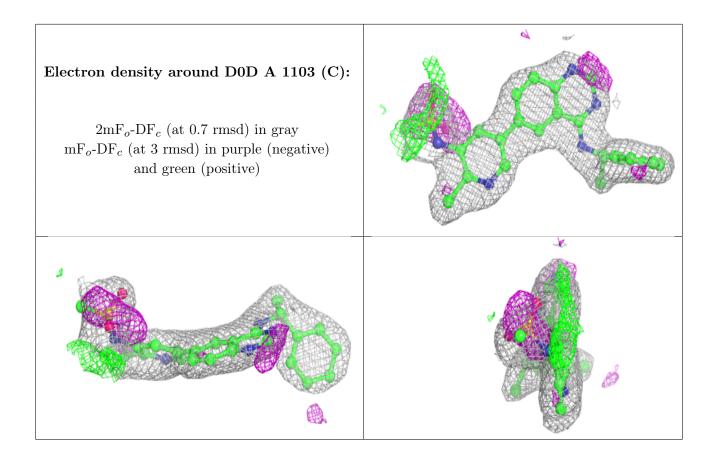
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

