

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2024 - 04:11 pm GMT

PDB ID	:	8QZD
Title	:	Soluble epoxide hydrolase in complex with Epoxykinin
Authors	:	Kumar, A.; Ehrler, J.M.H.; Ziegler, S.; Doetsch, L.; Proschak, E.; Knapp, S.;
		Structural Genomics Consortium (SGC)
Deposited on	:	2023-10-27
Resolution	:	1.30 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 (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:

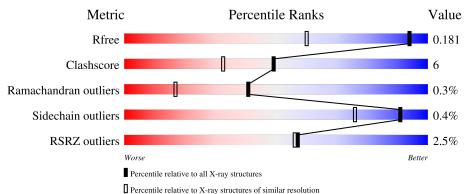
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.30 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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			
			2%			
1	А	367	78%	8%	•	13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	А	606	-	-	Х	-



	3	Chain	1 0		Geometry	Clashes	Electron density
2	EDO	А	614	-	-	Х	-
4	BR	А	612	-	-	Х	-

Continued from previous page...



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3013 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 Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	A	320	Total 2679	C 1717	N 450	0 486	S 26	0	16	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	198	MET	-	initiating methionine	UNP P34913
А	199	GLY	-	expression tag	UNP P34913
А	200	SER	-	expression tag	UNP P34913
А	201	SER	-	expression tag	UNP P34913
А	202	HIS	-	expression tag	UNP P34913
А	203	HIS	-	expression tag	UNP P34913
А	204	HIS	-	expression tag	UNP P34913
А	205	HIS	-	expression tag	UNP P34913
А	206	HIS	-	expression tag	UNP P34913
A	207	HIS	-	expression tag	UNP P34913
А	208	SER	-	expression tag	UNP P34913
A	209	SER	-	expression tag	UNP P34913
A	210	GLY	-	expression tag	UNP P34913
А	211	LEU	-	expression tag	UNP P34913
А	212	VAL	-	expression tag	UNP P34913
А	213	PRO	-	expression tag	UNP P34913
A	214	ARG	-	expression tag	UNP P34913
А	215	GLY	-	expression tag	UNP P34913
A	216	SER	-	expression tag	UNP P34913
А	217	HIS	-	expression tag	UNP P34913
А	218	MET	-	expression tag	UNP P34913
А	219	ALA	-	expression tag	UNP P34913
А	220	SER	-	expression tag	UNP P34913
А	221	MET	-	expression tag	UNP P34913
А	556	LEU	-	expression tag	UNP P34913
А	557	LEU	-	expression tag	UNP P34913
А	558	GLU	-	expression tag	UNP P34913

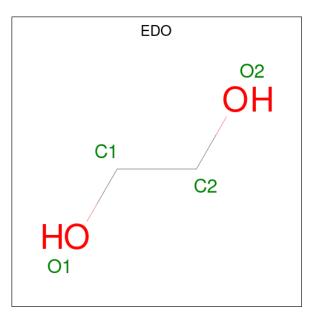
There are 33 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	559	HIS	-	expression tag	UNP P34913
А	560	HIS	-	expression tag	UNP P34913
А	561	HIS	-	expression tag	UNP P34913
А	562	HIS	-	expression tag	UNP P34913
А	563	HIS	-	expression tag	UNP P34913
А	564	HIS	-	expression tag	UNP P34913

Continued from previous page...

• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



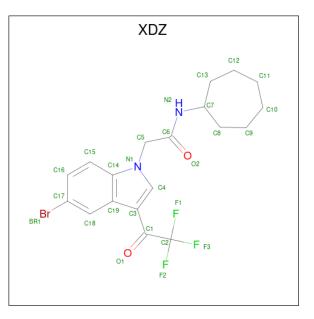
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 3 is 2-[5-bromanyl-3-[2,2,2-tris(fluoranyl)ethanoyl]indol-1-yl]-N-cycloheptyl-ethana mide (three-letter code: XDZ) (formula: C₁₉H₂₀BrF₃N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
3	Δ	1	Total	Br	С	F	Ν	0	0	0
0	Л	I	27	1	19	3	2	2	0	0

• Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Br 1 1	0	0

• Molecule 5 is water.



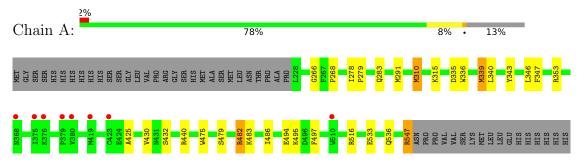
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	258	Total O 258 258	0	0



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: Bifunctional epoxide hydrolase 2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	45.92Å 80.31Å 89.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.54 - 1.30	Depositor
Resolution (A)	44.54 - 1.30	EDS
% Data completeness	99.6 (44.54-1.30)	Depositor
(in resolution range)	99.6(44.54-1.30)	EDS
R _{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.40 (at 1.31 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
D D.	0.163 , 0.180	Depositor
R, R_{free}	0.163 , 0.181	DCC
R_{free} test set	4091 reflections $(5.07%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	16.0	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.36 , 37.6	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3013	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XDZ, BR, EDO

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	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.62	0/2757	0.98	9/3742~(0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	$\operatorname{rs} \mid \# \operatorname{Planarity} \operatorname{outliers}$	
1	А	0	1	

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	482	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	А	339[A]	MET	CG-SD-CE	-6.27	90.16	100.20
1	А	339[B]	MET	CG-SD-CE	-6.27	90.16	100.20
1	А	516	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	А	494	GLU	CG-CD-OE2	5.52	129.34	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide



5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2679	0	2578	25	0
2	А	48	0	70	14	0
3	А	27	0	0	1	0
4	А	1	0	0	4	0
5	А	258	0	0	9	0
All	All	3013	0	2648	32	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 6.

The worst 5 of 32 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:315:LYS:HG3	5:A:833:HOH:O	1.68	0.92
1:A:310[B]:MET:HE1	1:A:340:LEU:HA	1.68	0.75
3:A:609:XDZ:BR1	4:A:612:BR:BR	3.14	0.74
1:A:483:LYS:H	2:A:614:EDO:H11	1.54	0.71
1:A:283[B]:GLN:HG2	5:A:734:HOH:O	1.92	0.69

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	А	334/367~(91%)	328~(98%)	5(2%)	1 (0%)	41 17



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	268	PRO

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	А	291/323~(90%)	290 (100%)	1 (0%)	92 78

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

Mol	Chain	Res	Type
1	А	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	513	HIS

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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	Turne	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	les
1VIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	XDZ	А	609	-	26,29,29	1.13	2 (7%)	34,42,42	1.32	2 (5%)
2	EDO	А	606	-	3,3,3	1.04	0	2,2,2	0.89	0
2	EDO	А	601	-	3,3,3	0.28	0	2,2,2	0.68	0
2	EDO	А	610	-	3,3,3	0.17	0	2,2,2	0.26	0
2	EDO	А	611	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	А	603	-	3, 3, 3	0.29	0	2,2,2	0.85	0
2	EDO	А	614	-	3, 3, 3	0.33	0	2,2,2	0.25	0
2	EDO	А	605	-	3, 3, 3	0.31	0	2,2,2	1.06	0
2	EDO	А	604	-	3, 3, 3	0.32	0	2,2,2	0.19	0
2	EDO	А	608	-	$3,\!3,\!3$	0.40	0	2,2,2	0.62	0
2	EDO	А	607	-	3, 3, 3	1.25	0	2,2,2	0.33	0
2	EDO	А	613	-	3,3,3	0.11	0	2,2,2	0.13	0
2	EDO	А	602	_	$3,\!3,\!3$	0.18	0	2,2,2	0.60	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	XDZ	А	609	-	-	0/15/27/27	0/3/3/3
2	EDO	А	606	-	-	0/1/1/1	-
2	EDO	А	601	-	-	1/1/1/1	-
2	EDO	А	610	-	-	1/1/1/1	-
2	EDO	А	611	-	-	1/1/1/1	-
2	EDO	А	603	-	-	1/1/1/1	-
2	EDO	А	614	-	-	1/1/1/1	-
2	EDO	А	605	-	-	1/1/1/1	-
2	EDO	А	604	-	-	0/1/1/1	-
2	EDO	А	608	-	-	1/1/1/1	-
2	EDO	А	607	-	-	1/1/1/1	-



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	А	613	-	-	1/1/1/1	-
2	EDO	А	602	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
3	А	609	XDZ	C3-C19	3.00	1.45	1.42
3	А	609	XDZ	C13-C7	2.96	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	609	XDZ	C7-N2-C6	5.57	131.13	122.92
3	А	609	XDZ	C17-C18-C19	-2.64	116.52	119.79

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	607	EDO	O1-C1-C2-O2
2	А	613	EDO	O1-C1-C2-O2
2	А	601	EDO	O1-C1-C2-O2
2	А	608	EDO	O1-C1-C2-O2
2	А	611	EDO	O1-C1-C2-O2

There are no ring outliers.

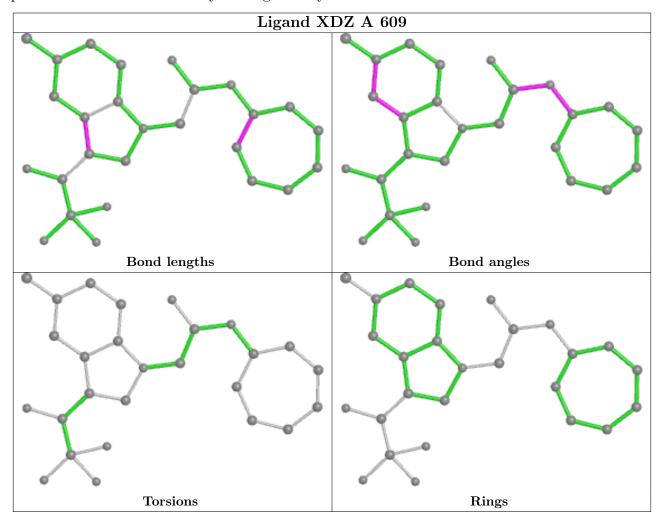
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	609	XDZ	1	0
2	А	606	EDO	5	0
2	А	610	EDO	1	0
2	А	603	EDO	2	0
2	А	614	EDO	5	0
2	А	608	EDO	1	0
2	А	602	EDO	2	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 $>$	#RSI	RZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	320/367~(87%)	-0.01	8 (2%)	57 56	12, 17, 37, 57	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	423	CYS	4.4
1	А	510	TRP	3.7
1	А	380	VAL	3.6
1	А	375	ILE	3.4
1	А	376	LYS	3.4

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.

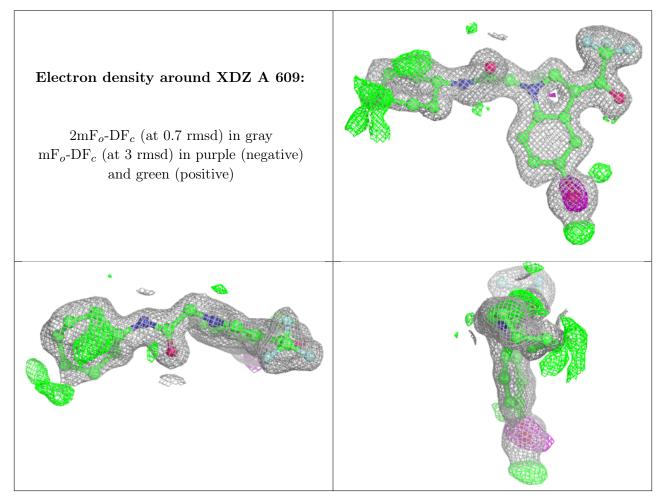
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	EDO	А	611	4/4	0.64	0.12	41,42,43,44	0
2	EDO	А	608	4/4	0.67	0.18	26,32,34,42	4



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	А	610	4/4	0.76	0.13	27,27,28,30	4
2	EDO	А	601	4/4	0.76	0.19	26,28,36,39	4
2	EDO	А	613	4/4	0.81	0.12	40,44,46,48	0
2	EDO	А	614	4/4	0.87	0.16	40,42,45,46	0
2	EDO	А	606	4/4	0.90	0.20	16, 18, 24, 28	4
2	EDO	А	607	4/4	0.92	0.17	19,20,21,24	4
2	EDO	А	604	4/4	0.92	0.15	16,18,19,20	4
4	BR	А	612	1/1	0.92	0.12	32,32,32,32	1
2	EDO	А	602	4/4	0.94	0.11	17,20,23,23	4
2	EDO	А	603	4/4	0.95	0.17	$16,\!24,\!26,\!27$	4
3	XDZ	А	609	27/27	0.95	0.12	17,20,30,34	27
2	EDO	А	605	4/4	0.95	0.10	17,18,19,19	4

Continued from previous page...

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.

