

wwPDB X-ray Structure Validation Summary Report (i)

Aug 18, 2021 - 05:07 am BST

PDB ID	:	7B2Y
Title	:	Notum complex with ARUK3003910
Authors	:	Zhao, Y.; Jone, E.Y.
Deposited on		
Resolution	:	1.23 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 following versions of software and data (see references (1)) were used in the production of this report:

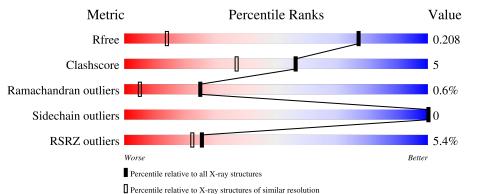
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac	::	1.8.5 (274361), CSD as541be (2020) 1.13 2.23.1 1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)	:	Parkinson et al. (1996) 2.23.1
, , , , , , , , , , , , , , , , ,		

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 1.23 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
R _{free}	130704	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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		
			5%		
1	А	383	83%	9%	• 7%

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
3	SO4	А	503	-	-	Х	-



α \cdot \cdot \cdot	C		
Continued	trom	nromanie	naao
Continucu	110116	$p_{I} c_{U} c_{U} c_{U} c_{U}$	p_{uy}
		1	1 0

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	А	509	-	-	Х	-
7	GOL	А	511	-	Х	-	-



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3063 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 Palmitoleoyl-protein carboxylesterase NOTUM.

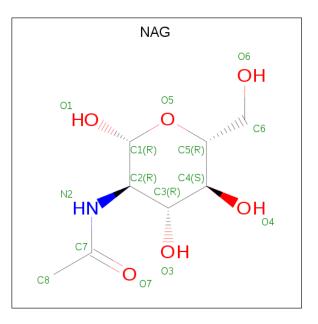
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	355	Total	С	Ν	Ο	\mathbf{S}	0	4	0
	Л	000	2859	1810	513	518	18	0	4	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	78	GLU	-	expression tag	UNP Q6P988
A	79	THR	-	expression tag	UNP Q6P988
А	80	GLY	-	expression tag	UNP Q6P988
А	330	SER	CYS	engineered mutation	UNP Q6P988
A	452	GLY	-	expression tag	UNP Q6P988
А	453	THR	-	expression tag	UNP Q6P988
A	454	LYS	-	expression tag	UNP Q6P988
A	455	HIS	-	expression tag	UNP Q6P988
A	456	HIS	-	expression tag	UNP Q6P988
А	457	HIS	-	expression tag	UNP Q6P988
А	458	HIS	-	expression tag	UNP Q6P988
А	459	HIS	-	expression tag	UNP Q6P988
А	460	HIS	-	expression tag	UNP Q6P988

There are 13 discrepancies between the modelled and reference sequences:

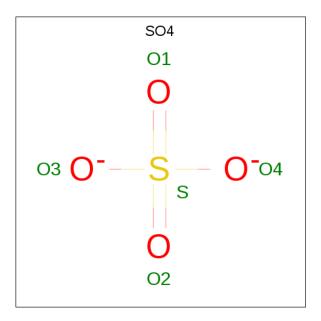
• Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	А	1	Total 14	C 8	N 1	O 5	0	0

 $\bullet\,$ Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: ${\rm O_4S}).$



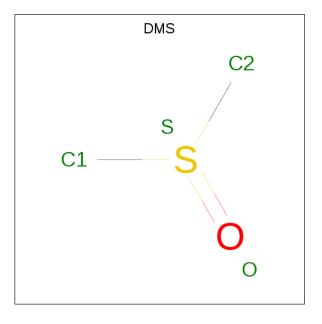
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	A	1	$\begin{array}{ccc} {\rm Total} & {\rm O} & {\rm S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

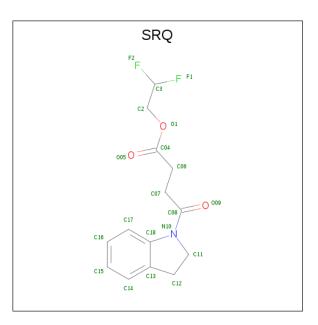
• Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	A	ton	ıs		ZeroOcc	AltConf
4	А	1	Total 4	$\begin{array}{c} \mathrm{C} \\ \mathrm{2} \end{array}$	0 1	${ m S}$ 1	0	0

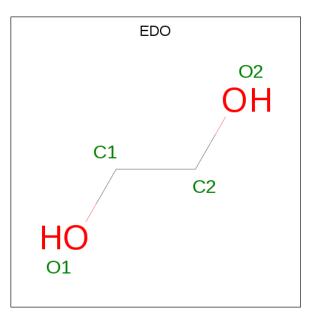
• Molecule 5 is 2,2-bis(fluoranyl)ethyl 4-(2,3-dihydroindol-1-yl)-4-oxidanylidene-butano ate (three-letter code: SRQ) (formula: $C_{14}H_{15}F_2NO_3$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	А	1	Total 15	C 12	N 1	$\begin{array}{c} 0\\ 2\end{array}$	0	0
			10	12	T	2		

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



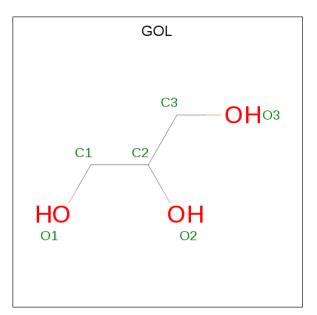
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 4 2 2 \end{array}$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



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Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
6	А	1	Total 4	${ m C} 2$	O 2	0	0

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	А	1	Total 6	${ m C} { m 3}$	O 3	0	0

• Molecule 8 is water.

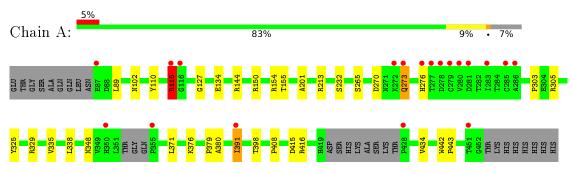
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	114	Total O 114 114	0	0



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: Palmitoleoyl-protein carboxylesterase NOTUM





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	60.01Å 71.54Å 78.02Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.61 - 1.23	Depositor
Resolution (A)	52.73 - 1.23	EDS
% Data completeness	99.8 (39.61-1.23)	Depositor
(in resolution range)	99.9 (52.73-1.23)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$0.96 (at 1.23 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D.	0.186 , 0.208	Depositor
R, R_{free}	0.186 , 0.208	DCC
R_{free} test set	5003 reflections $(5.11%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	17.3	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.40 , 43.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.51, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3063	wwPDB-VP
Average B, all atoms $(Å^2)$	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.28% 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: SRQ, EDO, NAG, DMS, SO4, 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).

[Mol	Chain	Boı	nd lengths	Bond angles		
	INIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
	1	А	0.71	1/2948~(0.0%)	0.89	5/4005~(0.1%)	

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	#Planarity outliers
1	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	134	GLU	CG-CD	7.53	1.63	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	115	ARG	CD-NE-CZ	12.01	140.41	123.60
1	А	115	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	А	416	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	А	415	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	А	273	GLN	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	115	ARG	Sidechain



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	2859	0	2773	26	1
2	А	14	0	13	0	0
3	А	35	0	0	3	0
4	А	4	0	6	0	0
5	А	15	0	0	0	0
6	А	16	0	24	7	0
7	А	6	0	5	2	0
8	А	114	0	0	0	1
All	All	3063	0	2821	29	1

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 5.

The worst 5 of 29 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:303:PRO:HA	6:A:509:EDO:H11	1.56	0.87
1:A:325:TYR:OH	7:A:511:GOL:H32	1.91	0.70
1:A:338:LEU:HA	1:A:371[A]:LEU:HD23	1.75	0.68
1:A:398:THR:HG22	1:A:408:PRO:HG2	1.77	0.67
3:A:503:SO4:O2	6:A:509:EDO:O1	2.15	0.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH2	8:A:604:HOH:O[2_575]	2.06	0.14



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	353/383~(92%)	333~(94%)	18 (5%)	2(1%)	25 5	

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	127	GLY
1	А	391	ILE

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	313/333~(94%)	313~(100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	А	273	GLN
1	А	276	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)

15 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	Tune	Chain	Res	Link	Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	А	511	-	$5,\!5,\!5$	<mark>3.98</mark>	3 (60%)	5, 5, 5	2.14	<mark>3 (60%)</mark>
3	SO4	А	513	-	4,4,4	0.15	0	$6,\!6,\!6$	0.14	0
3	SO4	А	503	-	4,4,4	0.18	0	$6,\!6,\!6$	0.13	0
3	SO4	А	514	-	4,4,4	0.22	0	$6,\!6,\!6$	0.28	0
3	SO4	А	504	-	4,4,4	0.20	0	6, 6, 6	0.30	0
2	NAG	А	501	1	14,14,15	0.50	0	17,19,21	0.53	0
3	SO4	А	502	-	4,4,4	0.30	0	$6,\!6,\!6$	0.49	0
3	SO4	А	515	-	4,4,4	0.21	0	6,6,6	1.50	1(16%)
6	EDO	А	508	-	$3,\!3,\!3$	0.44	0	2,2,2	0.61	0
3	SO4	А	512	-	4,4,4	0.42	0	6, 6, 6	0.29	0
6	EDO	A	507	-	$3,\!3,\!3$	0.59	0	2,2,2	0.51	0
6	EDO	А	509	-	$3,\!3,\!3$	0.42	0	2,2,2	0.41	0
6	EDO	А	510	-	3,3,3	0.31	0	2,2,2	1.21	0
5	SRQ	А	506	1	16, 16, 21	1.20	3 (18%)	$20,\!21,\!28$	1.64	<mark>5 (25%)</mark>
4	DMS	А	505	-	3,3,3	0.49	0	3, 3, 3	0.39	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.



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Mol	Type	Chain	\mathbf{Res}	\mathbf{Link}	Chirals	Torsions	Rings
7	GOL	А	511	-	-	3/4/4/4	-
2	NAG	А	501	1	-	0/6/23/26	0/1/1/1
6	EDO	А	508	-	-	0/1/1/1	-
6	EDO	А	507	-	-	1/1/1/1	-
6	EDO	А	509	-	-	0/1/1/1	-
6	EDO	А	510	-	-	1/1/1/1	-
5	SRQ	А	506	1	-	1/7/17/23	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
7	А	511	GOL	C3-C2	-6.86	1.23	1.51
7	А	511	GOL	O3-C3	-5.08	1.21	1.42
5	А	506	SRQ	C08-N10	2.73	1.40	1.36
5	А	506	SRQ	C11-C12	-2.35	1.49	1.53
5	А	506	SRQ	C18-N10	2.30	1.44	1.39

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

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
5	А	506	SRQ	C12-C11-N10	3.30	107.82	104.94
7	А	511	GOL	O2-C2-C1	2.86	121.74	109.12
7	А	511	GOL	O2-C2-C3	2.86	121.73	109.12
5	А	506	SRQ	C14-C13-C18	2.85	121.89	119.80
5	А	506	SRQ	C11-N10-C18	-2.74	107.22	109.22

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	А	511	GOL	O1-C1-C2-C3
7	А	511	GOL	C1-C2-C3-O3
6	А	507	EDO	O1-C1-C2-O2
7	А	511	GOL	O1-C1-C2-O2
6	А	510	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	511	GOL	2	0
3	А	503	SO4	3	0

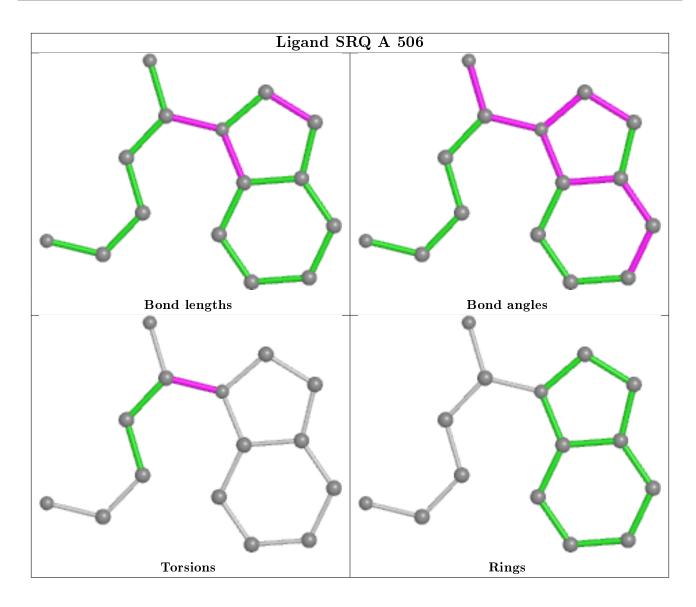


0 0 1 0 0 0		ricer			
Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
6	А	508	EDO	1	0
6	А	507	EDO	2	0
6	А	509	EDO	4	0

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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 sufficient 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, 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	А	355/383~(92%)	0.12	19 (5%) 25 22	14, 20, 37, 51	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	283	ILE	7.2
1	А	280	VAL	6.0
1	А	115	ARG	5.9
1	А	276	HIS	4.2
1	А	350	HIS	3.6

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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
6	EDO	А	507	4/4	0.72	0.13	$35,\!35,\!36,\!41$	0
6	EDO	А	508	4/4	0.84	0.16	17,29,31,44	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	А	510	4/4	0.84	0.24	$28,\!32,\!35,\!35$	0
2	NAG	А	501	14/15	0.87	0.20	$25,\!35,\!47,\!48$	0
3	SO4	А	513	5/5	0.90	0.15	$65,\!74,\!81,\!86$	0
6	EDO	А	509	4/4	0.90	0.19	$29,\!36,\!39,\!40$	0
3	SO4	А	503	5/5	0.90	0.14	$53,\!57,\!63,\!71$	0
3	SO4	А	502	5/5	0.94	0.11	$23,\!24,\!28,\!30$	0
3	SO4	А	514	5/5	0.94	0.24	$30,\!31,\!34,\!44$	0
3	SO4	А	515	5/5	0.95	0.28	$24,\!25,\!40,\!45$	0
5	SRQ	А	506	15/20	0.95	0.06	$15,\!17,\!22,\!22$	0
3	SO4	А	504	5/5	0.95	0.18	32,32,39,40	0
7	GOL	А	511	6/6	0.96	0.17	$14,\!31,\!37,\!38$	0
4	DMS	А	505	4/4	0.98	0.08	23,27,27,28	0
3	SO4	А	512	5/5	0.99	0.04	$18,\!18,\!21,\!22$	0

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6.5 Other polymers (i)

There are no such residues in this entry.

