

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:16 AM EDT

PDB ID	:	6V8S
Title	:	Crystal structure of Ara h 8.0201
Authors	:	Pote, S.; Offermann, L.R.; Hurlburt, B.K.; McBride, J.K.; Chruszcz, M.
Deposited on	:	2019-12-12
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 (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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
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 (i)

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

The reported resolution of this entry is 2.10 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 21480 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.

Mol	Chain	Residues	At	oms		ZeroOcc	AltConf	Trace
1	А	152	Total C 1146 729	N) 182	O 235	0	0	0
1	В	152	Total C 1143 728	N 8 182	O 233	0	0	0
1	С	152	Total C 1138 723	N 3 180	O 235	0	0	0
1	D	152	Total C 1145 729	N) 182	0 234	0	1	0
1	Е	152	Total C 1138 725	N 5 182	O 231	0	0	0
1	F	152	Total C 1146 729	N) 182	O 235	0	0	0
1	G	152	Total C 1155 734	N 4 184	O 237	0	2	0
1	Н	152	Total C 1155 734	N 4 184	O 237	0	1	0
1	Ι	152	Total C 1143 728	N 3 182	O 233	0	0	0
1	J	151	Total C 1136 725	N 5 181	O 230	0	0	0
1	K	151	Total C 1118 713	N 3 179	O 226	0	0	0
1	L	152	Total C 1139 726	N 5 182	O 231	0	0	0
1	М	152	Total C 1142 726	N 3 181	O 235	0	0	0
1	N	152	Total C 1135 723	N 3 181	0 231	0	0	0
1	Ο	152	Total C 1146 729	N) 182	O 235	0	0	0
1	Р	152	Total C 1142 727	N 7 182	O 233	0	0	0

• Molecule 1 is a protein called Ara h 8 allergen isoform.



• Molecule 2 is 8-ANILINO-1-NAPHTHALENE SULFONATE (three-letter code: 2AN) (formula: C₁₆H₁₃NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf
0	٨	1	Total	С	Ν	Ο	S	0	0
	А	1	21	16	1	3	1	0	0
0	٨	1	Total	С	Ν	Ο	S	0	0
	А	1	21	16	1	3	1	0	0
0	٨	1	Total	С	Ν	0	S	0	0
	A	1	21	16	1	3	1	0	0
0	۸	1	Total	С	Ν	Ο	S	0	0
	Л	1	21	16	1	3	1	0	0
2	Δ	1	Total	С	Ν	0	S	0	0
2	Л	T	21	16	1	3	1	0	0
2	B	1	Total	С	Ν	Ο	\mathbf{S}	0	0
2	D	1	21	16	1	3	1	0	0
2	В	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	D	1	21	16	1	3	1	0	0
2	В	1	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	D	1	21	16	1	3	1	0	0
2	В	1	Total	\mathbf{C}	Ν	Ο	\mathbf{S}	0	0
	D	I	21	16	1	3	1	0	0
2	С	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	U	1	21	16	1	3	1	0	0
2	С	1	Total	\mathbf{C}	Ν	0	S	0	0
		1	21	16	1	3	1	0	0
2	С	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	U	1	21	16	1	3	1	0	



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Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf
0	C	1	Total	С	Ν	0	S	0	0
2	C	1	21	16	1	3	1	0	0
0	C	1	Total	С	Ν	0	S	0	0
	C	1	21	16	1	3	1	0	0
0	C	1	Total	С	Ν	0	S	0	0
	C	1	21	16	1	3	1	0	0
0	C	1	Total	С	Ν	0	S	0	0
	U	L	21	16	1	3	1	0	0
0	C	1	Total	С	Ν	0	S	0	0
	U	L	21	16	1	3	1	0	0
0	С	1	Total	С	Ν	0	S	0	0
	U	L	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	0	S	0	0
	D	L	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	0	S	0	0
	D	L	21	16	1	3	1	0	0
0	Л	1	Total	С	Ν	Ο	S	0	0
	D	L	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	0	S	0	0
	D	1	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	0	S	0	0
	D	L	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	0	S	0	0
	D	L	21	16	1	3	1	0	0
0	Б	1	Total	С	Ν	Ο	S	0	0
	E	L	21	16	1	3	1	0	0
0	Б	1	Total	С	Ν	Ο	S	0	0
	Ľ	L	21	16	1	3	1	0	0
0	F	1	Total	С	Ν	0	S	0	0
	Ľ	L	21	16	1	3	1	0	0
0	F	1	Total	С	Ν	0	S	0	0
	Ľ	I	21	16	1	3	1	0	0
0	F	1	Total	С	Ν	0	S	0	0
	Ľ	I	21	16	1	3	1	0	0
9	F	1	Total	С	Ν	0	S	0	0
	<u>ت</u>		21	16	1	3	1	U	
2	F	1	Total	С	Ν	0	S	0	0
	Ľ	L	21	16	1	3	1	U	
9	F	1	Total	С	Ν	0	S	0	Ο
	Г	1	21	16	1	3	1	U	U
9	F	1	Total	С	Ν	0	S	0	0
	Ľ		21	16	1	3	1	0	



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Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf
0	Б	1	Total	С	Ν	0	S	0	0
2	F	1	21	16	1	3	1	0	0
0	F	1	Total	С	Ν	Ο	S	0	0
2	F	1	21	16	1	3	1	0	0
0	F	1	Total	С	Ν	Ο	S	0	0
	Г	L	21	16	1	3	1	0	0
0	Б	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	Г	L	21	16	1	3	1	0	0
9	F	1	Total	С	Ν	0	\mathbf{S}	0	0
	Г	L	21	16	1	3	1	0	0
9	F	1	Total	С	Ν	0	S	0	0
	Г	L	21	16	1	3	1	0	0
9	С	1	Total	С	Ν	0	S	0	0
	G	L	21	16	1	3	1	0	0
0	С	1	Total	С	Ν	Ο	S	0	0
	G	L	21	16	1	3	1	0	0
0	С	1	Total	С	Ν	Ο	S	0	0
	G	L	21	16	1	3	1	0	0
0	C	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	G	L	21	16	1	3	1	0	0
0	С	1	Total	С	Ν	0	S	0	0
	G	1	21	16	1	3	1	0	0
0	C	1	Total	С	Ν	0	S	0	0
	G	L	21	16	1	3	1	0	0
0	тт	1	Total	С	Ν	0	S	0	0
	П	L	21	16	1	3	1	0	0
0	тт	1	Total	С	Ν	Ο	S	0	0
	п	L	21	16	1	3	1	0	0
0	и	1	Total	С	Ν	Ο	S	0	0
	11	L	21	16	1	3	1	0	0
0	ц	1	Total	С	Ν	Ο	S	0	0
	п	L	21	16	1	3	1	0	0
0	ц	1	Total	С	Ν	Ο	S	0	0
	11	L	21	16	1	3	1	0	0
0	Ц	1	Total	С	Ν	Ο	S	0	0
	11	L	21	16	1	3	1	0	0
0	Ц	1	Total	С	Ν	Ο	S	0	0
	11	L 1	21	16	1	3	1	U	U
9	Ц	1	Total	С	Ν	0	\mathbf{S}	0	Ο
	11		21	16	1	3	1	U	U
0	ч	1	Total	С	Ν	0	S	0	0
	п	1	21	16	1	3	1	U	U



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Mol	Chain	Residues		Atc	ms			ZeroOcc	AltConf
0	т	1	Total	С	Ν	Ο	S	0	0
2	1	1	21	16	1	3	1	0	0
0	т	1	Total	С	Ν	0	S	0	0
	1	L	21	16	1	3	1	0	0
0	т	1	Total	С	Ν	0	S	0	0
	1	L	21	16	1	3	1	0	0
9	Т	1	Total	С	Ν	0	S	0	0
	1	I	21	16	1	3	1	0	0
2	T	1	Total	С	Ν	Ο	\mathbf{S}	0	0
2	1	T	21	16	1	3	1	0	0
2	T	1	Total	С	Ν	0	\mathbf{S}	0	0
	J	I	21	16	1	3	1	0	0
2	T	1	Total	С	Ν	0	\mathbf{S}	0	0
	J	I	21	16	1	3	1	0	0
2	т	1	Total	С	Ν	0	S	0	0
	J	I	21	16	1	3	1	0	0
2	т	1	Total	С	Ν	0	S	0	0
	J	L	21	16	1	3	1	0	0
0	т	1	Total	С	Ν	Ο	\mathbf{S}	0	0
	J	L	21	16	1	3	1	0	0
0	т	1	Total	С	Ν	0	S	0	0
	J	L	21	16	1	3	1	0	0
0	K	1	Total	С	Ν	Ο	S	0	0
	Λ	L	21	16	1	3	1	0	0
0	K	1	Total	С	Ν	0	S	0	0
	Λ	L	21	16	1	3	1	0	0
0	K	1	Total	С	Ν	Ο	S	0	0
	Γ	L	21	16	1	3	1	0	0
0	V	1	Total	С	Ν	Ο	S	0	0
	Γ	L	21	16	1	3	1	0	0
0	V	1	Total	С	Ν	0	S	0	0
	Λ	L	21	16	1	3	1	0	0
0	V	1	Total	С	Ν	0	S	0	0
	Λ	L	21	16	1	3	1	0	0
0	V	1	Total	С	Ν	0	S	0	0
	ñ	L	21	16	1	3	1	0	0
0	т	1	Total	С	Ν	0	S	0	0
	L		21	16	1	3	1	U	
0	т	1	Total	С	Ν	Ο	S	0	0
			21	16	1	3	1	U	U
0	т	1	Total	С	Ν	0	S	0	0
			21	16	1	3	1	U	U



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Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf
0	т	1	Total	С	Ν	0	S	0	0
2		1	21	16	1	3	1	0	0
0	м	1	Total	С	Ν	Ο	S	0	0
2	IVI	1	21	16	1	3	1	0	0
0	м	1	Total	С	Ν	0	S	0	0
	IVI	L	21	16	1	3	1	0	0
0	М	1	Total	С	Ν	Ο	S	0	0
	111	L	21	16	1	3	1	0	0
9	М	1	Total	С	Ν	0	\mathbf{S}	0	0
	111	T	21	16	1	3	1	0	0
9	М	1	Total	С	Ν	0	S	0	0
	111	T	21	16	1	3	1	0	0
9	М	1	Total	С	Ν	0	S	0	0
	IVI	L	21	16	1	3	1	0	0
0	М	1	Total	С	Ν	0	S	0	0
	IVI	L	21	16	1	3	1	0	0
0	М	1	Total	С	Ν	Ο	S	0	0
	IVI	L	21	16	1	3	1	0	0
0	М	1	Total	С	Ν	0	\mathbf{S}	0	0
	IVI	L	21	16	1	3	1	0	0
0	N	1	Total	С	Ν	0	\mathbf{S}	0	0
	IN	L	21	16	1	3	1	0	0
0	N	1	Total	С	Ν	0	S	0	0
	IN	L	21	16	1	3	1	0	0
0	N	1	Total	С	Ν	0	S	0	0
	11	L	21	16	1	3	1	0	0
0	N	1	Total	С	Ν	0	S	0	0
	11	L	21	16	1	3	1	0	0
0	0	1	Total	С	Ν	0	S	0	0
	0	T	21	16	1	3	1	0	0
0	0	1	Total	С	Ν	0	S	0	0
	0	L	21	16	1	3	1	0	0
9	0	1	Total	С	Ν	0	S	0	0
	0	L	21	16	1	3	1	0	0
0	0	1	Total	С	Ν	0	S	0	0
	0	T	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	Ο	S	0	0
	1	L	21	16	1	3	1	0	0
0	D	1	Total	С	Ν	0	S	0	0
	Г		21	16	1	3	1	0	
0	Б	1	Total	С	Ν	0	S	0	0
	Г		21	16	1	3	1	U	U



Mol	Chain	Residues	_	Atc	\mathbf{ms}			ZeroOcc	AltConf	
2	P	1	Total	С	Ν	0	S	0	0	
	2 1	1	21	16	1	3	1	0	U	
9	D	1	Total	С	Ν	0	S	0	0	
	1	1	21	16	1	3	1	0	0	
2	D	1	Total	С	Ν	0	\mathbf{S}	0	0	
	1	I	21	16	1	3	1	0	0	
2	D	1	Total	С	Ν	0	\mathbf{S}	0	0	
	1	1	21	16	1	3	1	0	0	
2	D	1	Total	С	Ν	0	\mathbf{S}	0	0	
	I	I	21	16	1	3	1	0	0	
2	Р	1	Total	С	N	0	S	0	0	
	L	1	21	16	1	3	1	0		

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Ato	\mathbf{ms}		ZeroOcc	AltConf
3	Н	1	Total 5	0 4	S 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	83	Total O 83 83	0	0
4	В	88	Total O 88 88	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	63	Total O 63 63	0	0
4	D	61	Total O 61 61	0	0
4	Е	67	Total O 67 67	0	0
4	F	58	Total O 58 58	0	0
4	G	60	Total O 60 60	0	0
4	Н	63	Total O 63 63	0	0
4	Ι	79	Total O 79 79	0	0
4	J	62	Total O 62 62	0	0
4	К	57	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	0
4	L	90	Total O 90 90	0	0
4	М	71	Total O 71 71	0	0
4	Ν	63	Total O 63 63	0	0
4	Ο	51	Total O 51 51	0	0
4	Р	50	$\begin{array}{c c} \hline Total & O \\ 50 & 50 \end{array}$	0	0

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MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	78.16Å 90.03Å 94.25Å	Depositor
a, b, c, α , β , γ	94.13° 106.91° 97.23°	Depositor
Resolution (Å)	38.09 - 2.10	Depositor
% Data completeness	91 5 (38 09-2 10)	Depositor
(in resolution range)	51.5 (50.05-2.10)	
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) > 1$	$3.92 (at 2.10 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.232 , 0.266	Depositor
Wilson B-factor $(Å^2)$	19.6	Xtriage
Anisotropy	0.092	Xtriage
L-test for twinning ²	$ < L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21480	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 77.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9513e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

103 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



					Bond lengths			Bond angles			
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	2AN	N	202	-	22,23,23	0.96	1 (4%)	29,33,33	0.91	2 (6%)	
2	2AN	Ο	203	-	22,23,23	0.74	1 (4%)	29,33,33	1.04	2 (6%)	
2	2AN	F	206	-	22,23,23	0.77	1 (4%)	29,33,33	0.96	1 (3%)	
2	2AN	J	203	-	22,23,23	0.95	2 (9%)	29,33,33	0.83	1 (3%)	
2	2AN	Р	504	-	22,23,23	0.74	0	29,33,33	0.80	0	
2	2AN	G	301	-	22,23,23	0.63	1 (4%)	29,33,33	0.79	0	
2	2AN	Н	1102	-	22,23,23	0.66	0	29,33,33	0.91	0	
2	2AN	А	201	-	22,23,23	0.86	1 (4%)	29,33,33	0.86	0	
2	2AN	G	302	-	22,23,23	0.72	1 (4%)	29,33,33	0.81	1 (3%)	
2	2AN	F	204	-	22,23,23	0.76	1 (4%)	29,33,33	0.83	0	
2	2AN	L	202	-	22,23,23	0.81	1 (4%)	29,33,33	0.87	1 (3%)	
2	2AN	Ν	204	-	22,23,23	0.95	1 (4%)	29,33,33	0.81	0	
2	2AN	А	203	-	22,23,23	0.79	1 (4%)	29,33,33	0.90	1 (3%)	
2	2AN	В	204	-	22,23,23	0.77	1 (4%)	29,33,33	0.85	0	
2	2AN	С	303	-	22,23,23	0.90	1 (4%)	29,33,33	0.91	1 (3%)	
2	2AN	D	706	-	22,23,23	0.81	1 (4%)	29,33,33	0.76	0	
2	2AN	D	702	-	22,23,23	0.86	2 (9%)	29,33,33	0.76	0	
2	2AN	D	704	-	22,23,23	0.75	1 (4%)	29,33,33	0.80	0	
2	2AN	Р	508	-	22,23,23	0.68	1 (4%)	29,33,33	0.74	0	
2	2AN	L	203	-	22,23,23	0.80	1 (4%)	29,33,33	0.78	0	
2	2AN	Е	504	-	22,23,23	0.81	1 (4%)	29,33,33	0.77	0	
2	2AN	С	302	-	22,23,23	0.76	0	29,33,33	0.80	0	
2	2AN	Е	505	-	22,23,23	0.75	1 (4%)	29,33,33	0.72	0	
2	2AN	F	207	-	22,23,23	0.72	1 (4%)	29,33,33	0.77	1 (3%)	
2	2AN	N	203	-	22,23,23	0.83	1 (4%)	29,33,33	0.81	1 (3%)	
2	2AN	Е	506	-	22,23,23	0.83	1 (4%)	29,33,33	0.88	1 (3%)	
2	2AN	Ι	204	-	22,23,23	0.73	1 (4%)	29,33,33	0.87	1 (3%)	
2	2AN	Р	502	-	22,23,23	0.63	0	29,33,33	0.77	0	
2	2AN	L	201	-	22,23,23	0.68	1 (4%)	29,33,33	0.95	2 (6%)	
2	2AN	Р	505	-	22,23,23	0.73	0	29,33,33	0.97	2(6%)	
2	2AN	K	202	-	22,23,23	0.74	1 (4%)	29,33,33	1.02	2 (6%)	
2	2AN	N	201	-	22,23,23	0.57	0	29,33,33	0.66	0	
2	2AN	J	201	-	22,23,23	0.73	0	29,33,33	0.88	0	

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).



Mal	Tune	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	2AN	Р	506	-	22,23,23	0.80	1 (4%)	29,33,33	0.84	0
2	2AN	Р	509	-	22,23,23	0.89	1 (4%)	29,33,33	0.71	0
2	2AN	Ι	205	-	22,23,23	0.71	1 (4%)	29,33,33	0.77	1 (3%)
2	2AN	Н	1109	-	22,23,23	0.92	2 (9%)	29,33,33	0.90	1 (3%)
2	2AN	М	502	-	22,23,23	0.89	1 (4%)	29,33,33	1.06	3 (10%)
2	2AN	K	201	-	22,23,23	0.94	1 (4%)	29,33,33	0.82	0
2	2AN	J	205	-	22,23,23	0.80	1 (4%)	29,33,33	0.88	1 (3%)
2	2AN	K	205	-	22,23,23	0.67	1 (4%)	29,33,33	1.17	2 (6%)
2	2AN	В	202	-	22,23,23	0.72	1 (4%)	29,33,33	0.82	0
2	2AN	Е	502	-	22,23,23	0.80	1 (4%)	29,33,33	1.00	2 (6%)
2	2AN	J	206	-	22,23,23	0.68	1 (4%)	29,33,33	0.83	2(6%)
2	2AN	С	307	-	22,23,23	0.74	1 (4%)	29,33,33	0.80	0
2	2AN	J	202	-	22,23,23	0.84	1 (4%)	29,33,33	0.95	1 (3%)
2	2AN	М	506	-	22,23,23	0.75	1 (4%)	29,33,33	0.81	0
2	2AN	М	509	-	22,23,23	0.62	0	29,33,33	0.80	0
2	2AN	L	204	-	22,23,23	0.69	1 (4%)	29,33,33	0.76	0
2	2AN	G	306	-	22,23,23	0.77	1 (4%)	29,33,33	0.77	0
2	2AN	С	306	-	22,23,23	0.63	1 (4%)	29,33,33	1.16	3 (10%)
2	2AN	G	305	-	22,23,23	0.76	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	G	303	-	22,23,23	0.75	0	29,33,33	0.75	0
2	2AN	J	204	-	22,23,23	0.82	1 (4%)	29,33,33	0.74	0
2	2AN	Н	1107	-	22,23,23	0.72	1 (4%)	29,33,33	0.74	0
3	SO4	Н	1110	-	4,4,4	0.34	0	6,6,6	0.08	0
2	2AN	С	301	-	22,23,23	0.98	1 (4%)	29,33,33	0.94	0
2	2AN	D	701	-	22,23,23	0.97	1 (4%)	29,33,33	0.84	0
2	2AN	K	204	-	22,23,23	0.83	1 (4%)	29,33,33	0.76	0
2	2AN	F	201	-	22,23,23	0.62	0	29,33,33	0.73	0
2	2AN	В	203	-	22,23,23	0.73	1 (4%)	29,33,33	0.80	0
2	2AN	Ι	203	-	22,23,23	0.84	1 (4%)	29,33,33	0.95	1 (3%)
2	2AN	D	705	-	22,23,23	0.78	1 (4%)	29,33,33	0.73	0
2	2AN	С	308	-	22,23,23	0.99	3 (13%)	29,33,33	0.89	1 (3%)
2	2AN	А	204	-	22,23,23	0.68	1 (4%)	29,33,33	0.78	0
2	2AN	Н	1101	-	22,23,23	0.73	1 (4%)	29,33,33	0.99	1 (3%)
2	2AN	В	201	-	22,23,23	0.85	1 (4%)	29,33,33	0.93	1 (3%)
2	2AN	0	201	-	22,23,23	0.85	1 (4%)	29,33,33	0.88	0



Mal	Tune	Chain	Dec	Tink	Bo	ond leng	ths	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	2AN	Н	1103	-	22,23,23	0.83	1 (4%)	29,33,33	0.72	0
2	2AN	А	202	-	22,23,23	0.78	1 (4%)	29,33,33	0.77	0
2	2AN	М	505	-	22,23,23	0.77	1 (4%)	29,33,33	1.16	2(6%)
2	2AN	Ι	201	-	22,23,23	0.49	0	29,33,33	0.90	1 (3%)
2	2AN	М	508	-	22,23,23	0.73	1 (4%)	29,33,33	0.85	0
2	2AN	Р	501	-	22,23,23	0.71	1 (4%)	29,33,33	0.81	0
2	2AN	Н	1108	-	22,23,23	0.81	1 (4%)	29,33,33	0.81	1 (3%)
2	2AN	М	503	-	22,23,23	0.86	1 (4%)	29,33,33	0.86	0
2	2AN	F	205	-	22,23,23	0.76	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	F	208	-	22,23,23	0.97	3 (13%)	29,33,33	0.85	1 (3%)
2	2AN	М	504	-	22,23,23	0.84	0	29,33,33	0.80	1 (3%)
2	2AN	Р	507	-	22,23,23	0.72	1 (4%)	29,33,33	0.70	0
2	2AN	K	203	-	22,23,23	0.76	1 (4%)	29,33,33	0.75	1 (3%)
2	2AN	G	304	-	22,23,23	0.69	1 (4%)	29,33,33	0.92	1 (3%)
2	2AN	С	304	-	22,23,23	0.70	1 (4%)	29,33,33	0.63	0
2	2AN	С	309	-	22,23,23	0.75	1 (4%)	29,33,33	0.85	0
2	2AN	М	501	-	22,23,23	0.77	1 (4%)	29,33,33	0.79	0
2	2AN	А	205	_	22,23,23	0.63	0	29,33,33	0.82	1 (3%)
2	2AN	K	207	-	22,23,23	0.71	1 (4%)	29,33,33	0.73	0
2	2AN	Р	503	-	22,23,23	0.78	1 (4%)	29,33,33	0.89	1 (3%)
2	2AN	М	507	_	22,23,23	0.89	1 (4%)	29,33,33	0.71	0
2	2AN	Е	501	-	22,23,23	0.66	0	29,33,33	0.79	0
2	2AN	F	202	-	22,23,23	0.70	1 (4%)	29,33,33	0.80	0
2	2AN	Н	1104	-	22,23,23	0.68	0	29,33,33	0.88	0
2	2AN	0	204	-	22,23,23	0.79	1 (4%)	29,33,33	0.89	2(6%)
2	2AN	D	703	-	22,23,23	0.72	0	29,33,33	1.05	2(6%)
2	2AN	Ι	202	-	22,23,23	0.71	1 (4%)	29,33,33	0.84	0
2	2AN	К	206	-	22,23,23	1.17	3 (13%)	29,33,33	0.95	1 (3%)
2	2AN	Е	507	-	22,23,23	1.09	3 (13%)	29,33,33	1.14	1 (3%)
2	2AN	Н	1105	-	22,23,23	0.68	1 (4%)	29,33,33	0.80	0
2	2AN	0	202	-	22,23,23	0.74	1 (4%)	29,33,33	0.72	0
2	2AN	С	305	-	22,23,23	0.78	1 (4%)	29,33,33	0.84	0
2	2AN	Е	503	-	22,23,23	0.89	2(9%)	29,33,33	0.95	2(6%)
2	2AN	F	203	-	22,23,23	0.80	1 (4%)	29,33,33	0.74	0
2	2AN	Н	1106	-	22,23,23	0.77	1 (4%)	29,33,33	0.99	1 (3%)



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
2	2AN	N	202	-	-	0/10/10/10	0/3/3/3
2	2AN	0	203	-	-	0/10/10/10	0/3/3/3
2	2AN	F	206	-	-	0/10/10/10	0/3/3/3
2	2AN	J	203	-	-	1/10/10/10	0/3/3/3
2	2AN	Р	504	-	-	0/10/10/10	0/3/3/3
2	2AN	G	301	-	-	1/10/10/10	0/3/3/3
2	2AN	Н	1102	-	-	0/10/10/10	0/3/3/3
2	2AN	А	201	-	-	0/10/10/10	0/3/3/3
2	2AN	G	302	-	-	0/10/10/10	0/3/3/3
2	2AN	F	204	-	-	0/10/10/10	0/3/3/3
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Ν	204	-	-	2/10/10/10	0/3/3/3
2	2AN	А	203	-	-	0/10/10/10	0/3/3/3
2	2AN	В	204	-	-	0/10/10/10	0/3/3/3
2	2AN	С	303	-	_	0/10/10/10	0/3/3/3
2	2AN	D	706	-	-	2/10/10/10	0/3/3/3
2	2AN	D	702	-	-	2/10/10/10	0/3/3/3
2	2AN	D	704	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	508	-	-	0/10/10/10	0/3/3/3
2	2AN	L	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Е	504	-	-	1/10/10/10	0/3/3/3
2	2AN	С	302	-	-	0/10/10/10	0/3/3/3
2	2AN	Е	505	-	-	0/10/10/10	0/3/3/3
2	2AN	F	207	-	-	2/10/10/10	0/3/3/3
2	2AN	N	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Е	506	-	-	2/10/10/10	0/3/3/3
2	2AN	Ι	204	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	502	-	-	0/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	505	-	-	0/10/10/10	0/3/3/3
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	506	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	509	-	-	2/10/10/10	0/3/3/3
2	2AN	Ι	205	-	-	0/10/10/10	0/3/3/3
2	2AN	Н	1109	-	-	2/10/10/10	0/3/3/3



Mol		Chain	Res	 Link	Chirals	Torsions	Rings
2	$\frac{1}{2}$ AN	M	502	-	-	0/10/10/10	0/3/3/3
2	24N	K	201	_	_	0/10/10/10	0/3/3/3
2	2AN	.I	201	_	_	0/10/10/10	0/3/3/3
2	2AN	K	205	_	_	8/10/10/10	0/3/3/3
2	2AN	B	202	_	_	0/10/10/10	0/3/3/3
2	2AN	E	502	_	_	$\frac{0/10/10/10}{0/10/10}$	0/3/3/3
2	2AN	J	206	_	_	$\frac{7}{10}$	0/3/3/3
2	2AN	C	307	_	-	0/10/10/10	0/3/3/3
2	2AN	J	202	-	_	3/10/10/10	0/3/3/3
2	2AN	М	506	_	-	2/10/10/10	0/3/3/3
2	2AN	М	509	_	_	$\frac{5}{10}$	0/3/3/3
2	2AN		204	_	_	$\frac{2}{10}$	0/3/3/3
2	2 AN	G	306	_		0/10/10/10	0/3/3/3
2	2AN	C	306	_	_	0/10/10/10	0/3/3/3
2	2AN	G	305	_	_	$\frac{0/10/10/10}{0/10/10}$	0/3/3/3
2	2AN	G	303	_	-	$\frac{0/10/10/10}{0/10/10}$	0/3/3/3
2	2AN	J	204	-	-	0/10/10/10	0/3/3/3
2	2AN	Н	1107	-	-	0/10/10/10	0/3/3/3
2	2AN	С	301	-	-	0/10/10/10	0/3/3/3
2	2AN	D	701	-	-	2/10/10/10	0/3/3/3
2	2AN	K	204	-	-	0/10/10/10	0/3/3/3
2	2AN	F	201	-	-	0/10/10/10	0/3/3/3
2	2AN	В	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Ι	203	-	-	0/10/10/10	0/3/3/3
2	2AN	D	705	-	-	0/10/10/10	0/3/3/3
2	2AN	С	308	-	-	2/10/10/10	0/3/3/3
2	2AN	A	204	_	-	0/10/10/10	0/3/3/3
2	2AN	Н	1101	-	-	2/10/10/10	0/3/3/3
2	2AN	В	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Ο	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Н	1103	-	-	5/10/10/10	0/3/3/3
2	2AN	А	202	_	-	2/10/10/10	0/3/3/3
2	2AN	М	505	-	-	1/10/10/10	0/3/3/3
2	2AN	Ι	201	-	-	0/10/10/10	0/3/3/3
2	2AN	М	508	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	501	-	-	0/10/10/10	0/3/3/3
2	2AN	Н	1108	-	-	0/10/10/10	$\overline{0/3/3/3}$
2	2AN	М	503	-	-	0/10/10/10	0/3/3/3
2	2AN	F	205		-	0/10/10/10	0/3/3/3
2	2AN	F	208	_	-	1/10/10/10	0/3/3/3



Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	2AN	М	504	-	-	0/10/10/10	0/3/3/3
2	2AN	Р	507	-	-	0/10/10/10	0/3/3/3
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	304	-	-	1/10/10/10	0/3/3/3
2	2AN	С	304	-	-	0/10/10/10	0/3/3/3
2	2AN	С	309	-	-	2/10/10/10	0/3/3/3
2	2AN	М	501	-	-	2/10/10/10	0/3/3/3
2	2AN	А	205	-	-	0/10/10/10	0/3/3/3
2	2AN	K	207	-	-	2/10/10/10	0/3/3/3
2	2AN	Р	503	-	-	8/10/10/10	0/3/3/3
2	2AN	М	507	-	-	0/10/10/10	0/3/3/3
2	2AN	Е	501	-	-	2/10/10/10	0/3/3/3
2	2AN	F	202	-	-	1/10/10/10	0/3/3/3
2	2AN	Н	1104	-	-	2/10/10/10	0/3/3/3
2	2AN	0	204	-	-	0/10/10/10	0/3/3/3
2	2AN	D	703	-	-	0/10/10/10	0/3/3/3
2	2AN	Ι	202	-	-	1/10/10/10	0/3/3/3
2	2AN	K	206	-	-	0/10/10/10	0/3/3/3
2	2AN	Е	507	-	-	6/10/10/10	0/3/3/3
2	2AN	Н	1105	-	-	0/10/10/10	0/3/3/3
2	2AN	0	202	-	-	0/10/10/10	0/3/3/3
2	2AN	C	305	-	-	2/10/10/10	0/3/3/3
2	2AN	Е	503	-	-	0/10/10/10	0/3/3/3
2	2AN	F	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Н	1106	-	-	0/10/10/10	0/3/3/3

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	L	203	2AN	O1-S	3.34	1.60	1.43
2	Κ	206	2AN	C1-N	3.30	1.47	1.38
2	Ν	202	2AN	O1-S	3.21	1.59	1.43
2	М	507	2AN	O1-S	3.13	1.59	1.43
2	В	201	2AN	O2-S	3.07	1.59	1.43
2	J	202	2AN	O2-S	3.07	1.59	1.43
2	Ε	502	2AN	O2-S	3.07	1.59	1.43
2	F	204	2AN	O2-S	3.05	1.59	1.43
2	D	706	2AN	O2-S	3.04	1.59	1.43
2	В	203	2AN	O1-S	2.98	1.58	1.43
2	М	505	2AN	O2-S	2.91	1.58	1.43



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Р	509	2AN	O1-S	2.90	1.58	1.43
2	D	701	2AN	O1-S	2.90	1.58	1.43
2	J	204	2AN	O1-S	2.90	1.58	1.43
2	С	301	2AN	O2-S	2.86	1.58	1.43
2	А	201	2AN	O1-S	2.85	1.58	1.43
2	Н	1109	2AN	O1-S	2.82	1.57	1.43
2	F	207	2AN	O2-S	2.82	1.57	1.43
2	Р	501	2AN	O2-S	2.78	1.57	1.43
2	Е	506	2AN	O1-S	2.78	1.57	1.43
2	Ν	204	2AN	O2-S	2.78	1.57	1.43
2	Н	1108	2AN	O1-S	2.77	1.57	1.43
2	Κ	203	2AN	O1-S	2.75	1.57	1.43
2	J	205	2AN	O2-S	2.75	1.57	1.43
2	D	705	2AN	O2-S	2.75	1.57	1.43
2	L	202	2AN	O2-S	2.75	1.57	1.43
2	Ι	202	2AN	O2-S	2.73	1.57	1.43
2	Е	505	2AN	O1-S	2.73	1.57	1.43
2	F	208	2AN	O2-S	2.72	1.57	1.43
2	Е	504	2AN	O1-S	2.72	1.57	1.43
2	Κ	206	2AN	O2-S	2.72	1.57	1.43
2	J	203	2AN	O1-S	2.70	1.57	1.43
2	М	506	2AN	O1-S	2.68	1.57	1.43
2	Е	507	2AN	C1-N	2.67	1.45	1.38
2	Н	1106	2AN	O2-S	2.67	1.57	1.43
2	С	308	2AN	O1-S	2.66	1.57	1.43
2	М	503	2AN	O2-S	2.64	1.57	1.43
2	С	303	2AN	O2-S	2.64	1.57	1.43
2	Е	507	2AN	O1-S	2.63	1.56	1.43
2	С	307	2AN	O3-S	2.63	1.58	1.45
2	0	204	2AN	O1-S	2.62	1.56	1.43
2	Н	1107	2AN	O1-S	2.60	1.56	1.43
2	С	304	2AN	O1-S	2.60	1.56	1.43
2	Ι	203	2AN	O1-S	2.60	1.56	1.43
2	М	502	2AN	O2-S	2.59	1.56	1.43
2	G	302	2AN	O1-S	2.57	1.56	1.43
2	В	204	2AN	O2-S	2.56	1.56	1.43
2	D	704	2AN	O2-S	2.55	1.56	1.43
2	K	201	2AN	O2-S	2.55	1.56	1.43
2	A	204	2AN	O1-S	2.54	1.56	1.43
2	G	306	2AN	O2-S	2.54	1.56	1.43
2	K	202	2AN	O2-S	2.54	1.56	1.43
2	0	202	2AN	O3-S	2.51	1.58	1.45



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	Р	503	2AN	O3-S	2.50	1.57	1.45
2	С	305	2AN	O1-S	2.49	1.56	1.43
2	М	501	2AN	O3-S	2.47	1.57	1.45
2	Н	1105	2AN	O1-S	2.47	1.56	1.43
2	Ι	205	2AN	O2-S	2.44	1.56	1.43
2	F	205	2AN	O2-S	2.42	1.55	1.43
2	Н	1101	2AN	O2-S	2.41	1.55	1.43
2	С	306	2AN	O2-S	2.41	1.55	1.43
2	F	203	2AN	O1-S	2.40	1.55	1.43
2	0	203	2AN	O1-S	2.39	1.55	1.43
2	А	203	2AN	O3-S	2.39	1.57	1.45
2	D	702	2AN	O3-S	2.35	1.57	1.45
2	J	206	2AN	O3-S	2.35	1.57	1.45
2	Κ	205	2AN	O1-S	2.34	1.55	1.43
2	Н	1109	2AN	C1-N	2.34	1.44	1.38
2	F	202	2AN	O3-S	2.34	1.57	1.45
2	G	305	2AN	O1-S	2.32	1.55	1.43
2	Е	507	2AN	C1-C10	2.30	1.46	1.42
2	Κ	204	2AN	O1-S	2.30	1.55	1.43
2	Ν	203	2AN	O3-S	2.29	1.56	1.45
2	Ι	204	2AN	O2-S	2.28	1.55	1.43
2	Р	506	2AN	O3-S	2.28	1.56	1.45
2	Р	508	2AN	O3-S	2.27	1.56	1.45
2	А	202	2AN	O2-S	2.26	1.55	1.43
2	0	201	2AN	O2-S	2.25	1.55	1.43
2	Ε	503	2AN	C1-C10	2.21	1.46	1.42
2	Κ	206	2AN	C1-C10	2.21	1.46	1.42
2	Р	507	2AN	O3-S	2.21	1.56	1.45
2	L	201	2AN	O1-S	2.20	1.54	1.43
2	J	203	2AN	C1-C10	2.20	1.46	1.42
2	С	308	2AN	C1-C10	2.20	1.46	1.42
2	М	508	2AN	O3-S	2.20	1.56	1.45
2	G	304	2AN	O3-S	2.19	1.56	1.45
2	В	202	2AN	O1-S	2.15	1.54	1.43
2	L	204	2AN	O3-S	2.14	1.56	1.45
2	С	308	2AN	C1-N	2.14	1.44	1.38
2	K	207	2AN	O3-S	2.13	1.56	1.45
2	F	206	2AN	O3-S	2.13	1.56	1.45
2	F	208	2AN	C1-C10	2.11	1.45	1.42
2	D	702	2AN	C1-N	2.11	1.44	1.38
2	G	301	2AN	O2-S	2.11	1.54	1.43
2	F	208	2AN	C1-N	2.10	1.44	1.38



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	Е	503	2AN	O2-S	2.10	1.54	1.43
2	С	309	2AN	O3-S	2.09	1.55	1.45
2	Н	1103	2AN	O3-S	2.05	1.55	1.45

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All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	K	205	2AN	C11-N-C1	-4.21	116.25	126.71
2	М	505	2AN	C10-C1-N	-3.55	115.41	120.71
2	С	306	2AN	C10-C1-N	-3.48	115.52	120.71
2	Е	507	2AN	C11-N-C1	3.03	134.24	126.71
2	K	202	2AN	C11-N-C1	2.83	133.74	126.71
2	С	308	2AN	C11-N-C1	2.78	133.62	126.71
2	М	505	2AN	C11-N-C1	2.76	133.56	126.71
2	Н	1109	2AN	C11-N-C1	2.72	133.47	126.71
2	D	703	2AN	02-S-01	-2.65	99.11	112.86
2	0	203	2AN	C11-N-C1	2.65	133.28	126.71
2	K	206	2AN	C11-N-C1	2.52	132.96	126.71
2	F	206	2AN	C11-N-C1	2.47	132.85	126.71
2	Е	503	2AN	C2-C1-N	-2.46	117.20	123.92
2	Е	502	2AN	C10-C1-N	-2.44	117.07	120.71
2	D	703	2AN	C1-C10-C5	-2.38	115.49	118.92
2	0	203	2AN	C10-C1-N	-2.36	117.18	120.71
2	В	201	2AN	C11-N-C1	2.33	132.51	126.71
2	0	204	2AN	C11-N-C1	2.31	132.45	126.71
2	J	202	2AN	C11-N-C1	2.26	132.33	126.71
2	J	206	2AN	C10-C1-N	-2.26	117.34	120.71
2	Н	1101	2AN	C2-C1-N	-2.24	117.81	123.92
2	G	304	2AN	C11-N-C1	2.24	132.26	126.71
2	N	203	2AN	C11-N-C1	2.23	132.24	126.71
2	Р	503	2AN	C2-C1-N	-2.22	117.86	123.92
2	G	302	2AN	C11-N-C1	2.22	132.23	126.71
2	Е	502	2AN	C11-N-C1	2.20	132.18	126.71
2	М	502	2AN	O3-S-O2	-2.20	100.99	111.54
2	С	306	2AN	C11-N-C1	2.19	132.14	126.71
2	А	203	2AN	C11-N-C1	2.17	132.09	126.71
2	F	208	2AN	C2-C1-N	-2.16	118.03	123.92
2	K	205	2AN	C2-C1-N	-2.15	118.05	123.92
2	Е	503	2AN	C1-C10-C5	-2.14	115.85	118.92
2	G	305	2AN	C11-N-C1	2.13	132.01	126.71
2	Н	1106	2AN	O2-S-O1	-2.13	101.81	112.86
2	Ι	204	2AN	C2-C1-N	-2.12	118.13	123.92



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	N	202	2AN	C1-C10-C5	-2.11	115.88	118.92
2	N	202	2AN	C2-C1-N	-2.10	118.19	123.92
2	L	201	2AN	C1-C10-C5	-2.10	115.90	118.92
2	J	203	2AN	C2-C1-N	-2.10	118.20	123.92
2	0	204	2AN	C10-C1-N	-2.08	117.60	120.71
2	Κ	203	2AN	C2-C1-N	-2.07	118.27	123.92
2	J	205	2AN	C11-N-C1	2.07	131.85	126.71
2	F	205	2AN	O3-S-O2	-2.07	101.63	111.54
2	L	202	2AN	C11-N-C1	2.07	131.84	126.71
2	Κ	202	2AN	C10-C1-N	-2.07	117.62	120.71
2	Е	506	2AN	C2-C1-N	-2.07	118.28	123.92
2	Ι	205	2AN	C2-C1-N	-2.05	118.33	123.92
2	L	201	2AN	O2-S-O1	-2.05	102.23	112.86
2	Р	505	2AN	C2-C1-N	-2.04	118.35	123.92
2	М	502	2AN	C1-C10-C5	-2.04	115.99	118.92
2	С	303	2AN	C1-C10-C5	-2.04	115.99	118.92
2	J	206	2AN	C11-N-C1	2.03	131.75	126.71
2	А	205	2AN	C1-C10-C5	-2.03	116.00	118.92
2	Р	505	2AN	C1-C10-C5	-2.03	116.00	118.92
2	М	504	2AN	C2-C1-N	-2.02	118.40	123.92
2	F	207	2AN	C10-C1-N	-2.02	117.69	120.71
2	Ι	203	2AN	C2-C1-N	-2.02	118.41	123.92
2	Н	1108	2AN	C2-C1-N	-2.01	118.43	123.92
2	М	502	2AN	C11-N-C1	2.01	131.70	126.71
2	Ι	201	2AN	C2-C1-N	-2.01	118.45	123.92
2	С	306	2AN	C9-C10-C5	2.00	118.31	116.29

There are no chirality outliers.

All (88) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	Е	507	2AN	C8-C9-S-O1
2	Е	507	2AN	C10-C9-S-O1
2	Е	507	2AN	C8-C9-S-O2
2	Е	507	2AN	C10-C9-S-O2
2	J	206	2AN	C10-C9-S-O2
2	Κ	205	2AN	C8-C9-S-O1
2	Κ	205	2AN	C10-C9-S-O1
2	Κ	205	2AN	C10-C9-S-O3
2	М	509	2AN	C10-C9-S-O3
2	P	503	2AN	C8-C9-S-O1
2	Р	503	2AN	C10-C9-S-O1



Mol	Chain	Res	Type	Atoms
2	Р	503	2AN	C8-C9-S-O2
2	Р	503	2AN	C10-C9-S-O2
2	Р	503	2AN	C8-C9-S-O3
2	J	206	2AN	C12-C11-N-C1
2	G	304	2AN	C10-C9-S-O1
2	Н	1103	2AN	C10-C9-S-O1
2	J	202	2AN	C10-C9-S-O1
2	J	202	2AN	C10-C9-S-O2
2	K	205	2AN	C10-C9-S-O2
2	J	206	2AN	C16-C11-N-C1
2	Р	509	2AN	C16-C11-N-C1
2	Р	509	2AN	C12-C11-N-C1
2	Н	1103	2AN	C8-C9-S-O1
2	J	202	2AN	C8-C9-S-O1
2	F	207	2AN	C16-C11-N-C1
2	Н	1109	2AN	C12-C11-N-C1
2	F	207	2AN	C12-C11-N-C1
2	Н	1109	2AN	C16-C11-N-C1
2	Ν	204	2AN	C16-C11-N-C1
2	D	702	2AN	C12-C11-N-C1
2	D	702	2AN	C16-C11-N-C1
2	Ν	204	2AN	C12-C11-N-C1
2	D	706	2AN	C10-C9-S-O1
2	F	202	2AN	C10-C9-S-O1
2	J	206	2AN	C10-C9-S-O1
2	М	509	2AN	C10-C9-S-O2
2	Е	501	2AN	C12-C11-N-C1
2	Е	507	2AN	C8-C9-S-O3
2	Ε	507	2AN	C10-C9-S-O3
2	Н	1103	2AN	C10-C9-S-O3
2	J	206	2AN	C10-C9-S-O3
2	Κ	205	2AN	C8-C9-S-O3
2	М	509	2AN	C8-C9-S-O3
2	Р	503	2AN	C10-C9-S-O3
2	C	305	2AN	C2-C1-N-C11
2	D	701	2AN	C2-C1-N-C11
2	Ι	202	2AN	C2-C1-N-C11
2	Р	503	2AN	C2-C1-N-C11
2	Е	501	2AN	C16-C11-N-C1
2	Е	506	2AN	C12-C11-N-C1
2	H	1101	2AN	C10-C1-N-C11
2	Р	503	2AN	C10-C1-N-C11

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Mol	Chain	Res	Type	Atoms
2	Κ	205	2AN	C12-C11-N-C1
2	D	706	2AN	C8-C9-S-O1
2	J	206	2AN	C8-C9-S-O1
2	J	206	2AN	C8-C9-S-O2
2	K	205	2AN	C8-C9-S-O2
2	С	308	2AN	C16-C11-N-C1
2	С	308	2AN	C12-C11-N-C1
2	G	301	2AN	C2-C1-N-C11
2	Н	1101	2AN	C2-C1-N-C11
2	F	208	2AN	C10-C9-S-O1
2	М	509	2AN	C10-C9-S-O1
2	С	309	2AN	C12-C11-N-C1
2	Κ	207	2AN	C12-C11-N-C1
2	K	205	2AN	C16-C11-N-C1
2	М	501	2AN	C16-C11-N-C1
2	М	501	2AN	C12-C11-N-C1
2	С	309	2AN	C16-C11-N-C1
2	А	202	2AN	C2-C1-N-C11
2	Е	504	2AN	C2-C1-N-C11
2	Н	1103	2AN	C2-C1-N-C11
2	Н	1104	2AN	C2-C1-N-C11
2	L	204	2AN	C2-C1-N-C11
2	М	506	2AN	C2-C1-N-C11
2	А	202	2AN	C10-C1-N-C11
2	С	305	2AN	C10-C1-N-C11
2	D	701	2AN	C10-C1-N-C11
2	Н	1103	2AN	C10-C1-N-C11
2	Н	1104	2AN	C10-C1-N-C11
2	J	203	2AN	C10-C1-N-C11
2	L	204	2AN	C10-C1-N-C11
2	М	506	2AN	C10-C1-N-C11
2	М	509	2AN	C16-C11-N-C1
2	K	207	2AN	C16-C11-N-C1
2	М	505	2AN	C10-C9-S-O1
2	Е	506	2AN	C16-C11-N-C1

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There are no ring outliers.

No monomer is involved in short contacts.

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.




















































































































































































































































































































































































































4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

