



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2017 – 07:59 AM EDT

PDB ID : 1T9W  
Title : Structural Basis of Multidrug Transport by the AcrB Multidrug Efflux Pump  
Authors : Yu, E.W.; McDermott, G.; Nikaido, H.  
Deposited on : unknown  
Resolution : 3.23 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

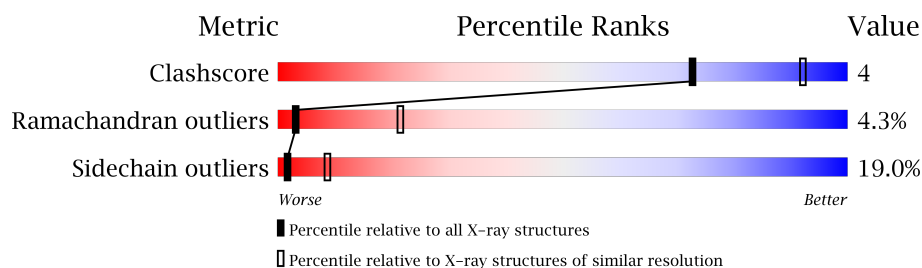
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.23 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1383 (3.28-3.20)
Ramachandran outliers	110173	1358 (3.28-3.20)
Sidechain outliers	110143	1357 (3.28-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1049	 69% 24% . .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7776 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.

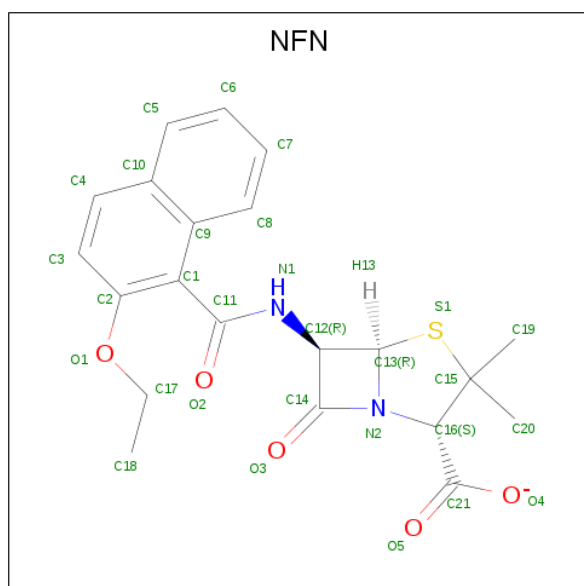
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	0	0	0
			7718	4964	1275	1436	43			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ASN	ENGINEERED	UNP P31224

- Molecule 2 is 6-[[[(2-ETHOXY-1-NAPHTHALENYL)CARBONYL]AMINO]-3,3-DIMETHYL-7-OXO-4-THIA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLATE (three-letter code: NFN) (formula: C<sub>21</sub>H<sub>21</sub>N<sub>2</sub>O<sub>5</sub>S).



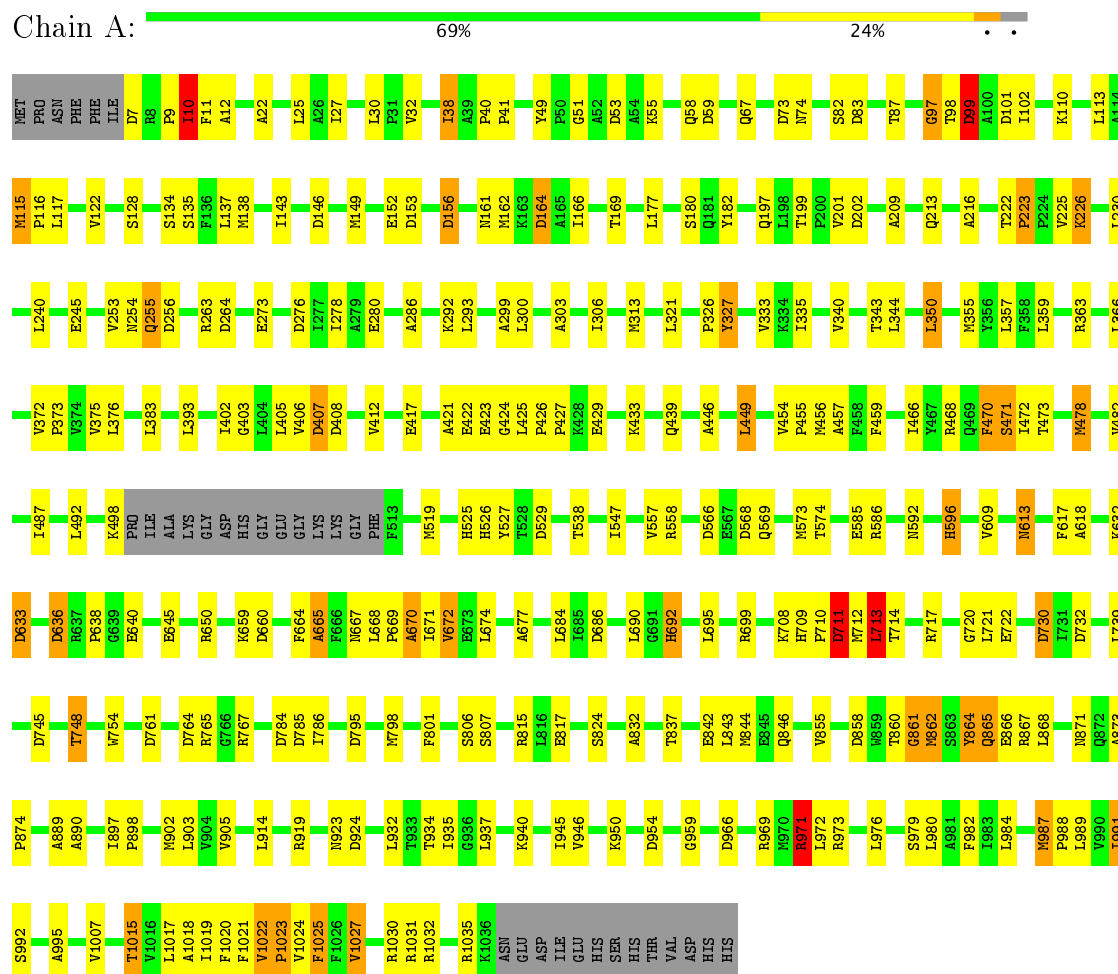
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	21	2	5	1		
2	A	1	Total	C	N	O	S	0	0
			29	21	2	5	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

Note EDS was not executed.

- Molecule 1: Acriflavine resistance protein B



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.51Å 144.51Å 519.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.23	Depositor
% Data completeness (in resolution range)	(Not available) (182.57-3.23)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.268 , 0.349	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NFN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.32	0/7861	0.65	39/10676 (0.4%)

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	A	2	2

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	795	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	568	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	924	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	407	ASP	CB-CG-OD2	5.67	123.41	118.30
1	A	276	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	59	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	53	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	745	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	156	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	660	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	966	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	101	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	764	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	256	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	784	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	83	ASP	CB-CG-OD2	5.22	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	785	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	470	PHE	N-CA-C	5.19	125.02	111.00
1	A	732	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	153	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	566	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	761	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	686	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	164	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	146	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	730	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	7	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	636	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	858	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	633	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	99	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	202	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	529	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	264	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	408	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	954	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	711	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	711	ASP	N-CA-C	5.03	124.59	111.00
1	A	73	ASP	CB-CG-OD2	5.03	122.82	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	711	ASP	CA
1	A	862	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	712	MET	Peptide
1	A	861	GLY	Peptide

## 5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7718	0	7876	60	7
2	A	58	0	39	6	0
All	All	7776	0	7915	61	7

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 4.

All (61) 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:618:ALA:HB2	2:A:6002:NFN:H203	1.75	0.69
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.76	0.67
1:A:861:GLY:O	1:A:862:MET:HB3	1.98	0.63
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.84	0.59
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.87	0.55
1:A:97:GLY:HA3	2:A:6001:NFN:H203	1.88	0.54
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.88	0.54
1:A:713:LEU:O	1:A:832:ALA:HB2	2.07	0.54
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.90	0.54
1:A:468:ARG:O	1:A:472:ILE:HG22	2.08	0.53
1:A:449:LEU:HB3	1:A:478:MET:SD	2.50	0.52
1:A:717:ARG:HG3	2:A:6002:NFN:C7	2.40	0.52
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.91	0.51
1:A:372:VAL:N	1:A:373:PRO:HD2	2.26	0.50
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.11	0.50
1:A:201:VAL:HG22	1:A:748:THR:HG23	1.94	0.50
1:A:10:ILE:HD13	1:A:10:ILE:N	2.27	0.49
1:A:932:LEU:HA	1:A:935:ILE:HD12	1.94	0.49
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.95	0.49
1:A:669:PRO:O	1:A:670:ALA:HB3	2.14	0.47
1:A:709:HIS:N	1:A:710:PRO:HD3	2.29	0.47
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.96	0.47
1:A:97:GLY:CA	2:A:6001:NFN:H203	2.43	0.47
1:A:240:LEU:HD12	1:A:245:GLU:HB3	1.96	0.47
1:A:979:SER:CB	1:A:1015:THR:HG21	2.45	0.47
1:A:97:GLY:N	2:A:6001:NFN:H203	2.31	0.46
1:A:987:MET:N	1:A:988:PRO:HD2	2.31	0.46
1:A:709:HIS:N	1:A:710:PRO:CD	2.78	0.46
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.98	0.46
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HB	1:A:223:PRO:HD3	1.98	0.46
1:A:1022:VAL:O	1:A:1023:PRO:O	2.33	0.45
2:A:6002:NFN:H183	2:A:6002:NFN:S1	2.56	0.45
1:A:425:LEU:C	1:A:427:PRO:HD2	2.37	0.45
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.99	0.45
1:A:613:ASN:HD22	1:A:613:ASN:C	2.19	0.45
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.98	0.44
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.51	0.44
1:A:38:ILE:HG21	1:A:466:ILE:HD13	2.00	0.44
1:A:664:PHE:O	1:A:665:ALA:HB2	2.16	0.44
1:A:115:MET:N	1:A:116:PRO:CD	2.81	0.44
1:A:326:PRO:O	1:A:327:TYR:C	2.56	0.44
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.48	0.43
1:A:937:LEU:HD11	1:A:982:PHE:CE1	2.54	0.43
1:A:303:ALA:HA	1:A:306:ILE:HD12	2.01	0.42
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.94	0.42
1:A:12:ALA:HB1	1:A:487:ILE:HG22	2.01	0.42
1:A:454:VAL:N	1:A:455:PRO:HD2	2.35	0.42
1:A:592:ASN:O	1:A:596:HIS:ND1	2.53	0.42
1:A:860:THR:HA	1:A:861:GLY:HA2	1.92	0.41
1:A:350:LEU:HD12	1:A:984:LEU:HB3	2.02	0.41
1:A:684:LEU:HD11	1:A:855:VAL:HG13	2.02	0.41
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.73	0.41
1:A:426:PRO:N	1:A:427:PRO:CD	2.83	0.41
1:A:525:HIS:O	1:A:527:TYR:N	2.53	0.41
1:A:897:ILE:N	1:A:898:PRO:CD	2.84	0.41
1:A:99:ASP:HB3	1:A:102:ILE:HG22	2.01	0.41
1:A:684:LEU:CD1	1:A:855:VAL:HG13	2.51	0.40
1:A:98:THR:O	1:A:99:ASP:C	2.59	0.40
1:A:692:HIS:C	1:A:692:HIS:HD1	2.24	0.40
1:A:375:VAL:HG11	1:A:405:LEU:CD2	2.52	0.40

All (7) 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:11:PHE:CE2	1:A:890:ALA:O[3_555]	1.51	0.69
1:A:226:LYS:O	1:A:596:HIS:CE1[10_445]	1.78	0.42
1:A:11:PHE:CD2	1:A:890:ALA:O[3_555]	1.86	0.34
1:A:51:GLY:O	1:A:216:ALA:O[2_555]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CZ	1:A:890:ALA:O[3_555]	1.98	0.22
1:A:226:LYS:O	1:A:596:HIS:NE2[10_445]	1.99	0.21
1:A:11:PHE:CE2	1:A:890:ALA:C[3_555]	2.03	0.17

## 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	1012/1049 (96%)	859 (85%)	109 (11%)	44 (4%)	<b>3</b> <b>21</b>

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	SER
1	A	135	SER
1	A	255	GLN
1	A	327	TYR
1	A	459	PHE
1	A	526	HIS
1	A	711	ASP
1	A	713	LEU
1	A	971	ARG
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	9	PRO
1	A	97	GLY
1	A	152	GLU
1	A	421	ALA
1	A	424	GLY
1	A	665	ALA
1	A	865	GLN
1	A	1025	PHE

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	110	LYS
1	A	161	ASN
1	A	209	ALA
1	A	720	GLY
1	A	864	TYR
1	A	223	PRO
1	A	299	ALA
1	A	538	THR
1	A	670	ALA
1	A	671	ILE
1	A	677	ALA
1	A	889	ALA
1	A	992	SER
1	A	995	ALA
1	A	10	ILE
1	A	22	ALA
1	A	638	PRO
1	A	837	THR
1	A	991	ILE
1	A	340	VAL
1	A	867	ARG
1	A	959	GLY
1	A	672	VAL

### 5.3.2 Protein sidechains ⓘ

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	826/854 (97%)	669 (81%)	157 (19%)	<b>2</b> <b>9</b>

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	67	GLN
1	A	82	SER
1	A	87	THR
1	A	99	ASP
1	A	113	LEU
1	A	115	MET
1	A	117	LEU
1	A	122	VAL
1	A	128	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET
1	A	156	ASP
1	A	162	MET
1	A	164	ASP
1	A	166	ILE
1	A	169	THR
1	A	177	LEU
1	A	180	SER
1	A	182	TYR
1	A	197	GLN
1	A	199	THR
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	263	ARG
1	A	273	GLU
1	A	278	ILE
1	A	280	GLU
1	A	292	LYS
1	A	293	LEU

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	313	MET
1	A	321	LEU
1	A	333	VAL
1	A	335	ILE
1	A	343	THR
1	A	350	LEU
1	A	355	MET
1	A	357	LEU
1	A	359	LEU
1	A	363	ARG
1	A	366	LEU
1	A	376	LEU
1	A	393	LEU
1	A	406	VAL
1	A	407	ASP
1	A	412	VAL
1	A	417	GLU
1	A	422	GLU
1	A	423	GLU
1	A	429	GLU
1	A	433	LYS
1	A	439	GLN
1	A	449	LEU
1	A	456	MET
1	A	470	PHE
1	A	471	SER
1	A	478	MET
1	A	492	LEU
1	A	498	LYS
1	A	519	MET
1	A	547	ILE
1	A	557	VAL
1	A	558	ARG
1	A	569	GLN
1	A	573	MET
1	A	574	THR
1	A	585	GLU
1	A	586	ARG
1	A	596	HIS
1	A	609	VAL
1	A	613	ASN

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Mol	Chain	Res	Type
1	A	617	PHE
1	A	632	LYS
1	A	633	ASP
1	A	636	ASP
1	A	640	GLU
1	A	645	GLU
1	A	650	ARG
1	A	659	LYS
1	A	667	ASN
1	A	668	LEU
1	A	672	VAL
1	A	674	LEU
1	A	690	LEU
1	A	692	HIS
1	A	695	LEU
1	A	699	ARG
1	A	708	LYS
1	A	711	ASP
1	A	713	LEU
1	A	714	THR
1	A	721	LEU
1	A	722	GLU
1	A	730	ASP
1	A	739	LEU
1	A	748	THR
1	A	765	ARG
1	A	767	ARG
1	A	798	MET
1	A	801	PHE
1	A	806	SER
1	A	807	SER
1	A	815	ARG
1	A	817	GLU
1	A	824	SER
1	A	842	GLU
1	A	843	LEU
1	A	844	MET
1	A	846	GLN
1	A	862	MET
1	A	864	TYR
1	A	865	GLN
1	A	866	GLU

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Mol	Chain	Res	Type
1	A	868	LEU
1	A	871	ASN
1	A	902	MET
1	A	903	LEU
1	A	905	VAL
1	A	914	LEU
1	A	919	ARG
1	A	923	ASN
1	A	934	THR
1	A	940	LYS
1	A	950	LYS
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	973	ARG
1	A	976	LEU
1	A	980	LEU
1	A	987	MET
1	A	989	LEU
1	A	991	ILE
1	A	1007	VAL
1	A	1015	THR
1	A	1020	PHE
1	A	1022	VAL
1	A	1027	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	124	GLN
1	A	194	ASN
1	A	231	ASN
1	A	391	ASN
1	A	577	GLN
1	A	605	ASN
1	A	613	ASN
1	A	657	GLN

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Mol	Chain	Res	Type
1	A	872	GLN
1	A	923	ASN
1	A	928	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NFN	A	6001	-	29,32,32	2.15	8 (27%)	44,49,49	4.85	18 (40%)
2	NFN	A	6002	-	29,32,32	2.32	8 (27%)	44,49,49	5.53	18 (40%)

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	NFN	A	6001	-	-	0/11/46/46	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NFN	A	6002	-	-	0/11/46/46	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	6001	NFN	C13-S1	-5.08	1.73	1.81
2	A	6002	NFN	C13-S1	-4.53	1.74	1.81
2	A	6002	NFN	C13-N2	-4.45	1.37	1.47
2	A	6002	NFN	C14-N2	-3.50	1.30	1.37
2	A	6001	NFN	C16-N2	-3.37	1.45	1.47
2	A	6001	NFN	C13-N2	-3.22	1.40	1.47
2	A	6002	NFN	C15-S1	-3.22	1.78	1.85
2	A	6002	NFN	C16-N2	-2.85	1.45	1.47
2	A	6001	NFN	C15-S1	-2.81	1.79	1.85
2	A	6001	NFN	C7-C8	2.01	1.41	1.36
2	A	6001	NFN	C1-C9	3.41	1.49	1.43
2	A	6002	NFN	C1-C9	3.75	1.50	1.43
2	A	6001	NFN	C1-C2	4.78	1.49	1.39
2	A	6001	NFN	C9-C10	5.38	1.52	1.43
2	A	6002	NFN	C9-C10	5.39	1.52	1.43
2	A	6002	NFN	C1-C2	5.43	1.50	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6002	NFN	C13-C12-N1	-16.67	81.50	118.25
2	A	6001	NFN	C6-C7-C8	-7.54	109.69	120.45
2	A	6002	NFN	C6-C5-C10	-7.43	108.78	120.44
2	A	6002	NFN	C6-C7-C8	-7.33	110.00	120.45
2	A	6001	NFN	C6-C5-C10	-7.22	109.11	120.44
2	A	6002	NFN	C13-C12-C14	-6.78	73.69	85.20
2	A	6001	NFN	C19-C15-S1	-3.18	103.88	109.20
2	A	6002	NFN	O3-C14-C12	-3.15	127.72	136.36
2	A	6002	NFN	C13-N2-C14	-2.96	90.04	93.92
2	A	6002	NFN	O1-C2-C3	-2.39	118.86	124.00
2	A	6002	NFN	C20-C15-S1	-2.19	105.53	109.20
2	A	6001	NFN	C12-N1-C11	-2.16	117.22	121.43
2	A	6001	NFN	C20-C15-S1	-2.15	105.61	109.20
2	A	6001	NFN	C1-C11-N1	2.03	120.98	114.77
2	A	6001	NFN	C20-C15-C16	2.16	116.39	111.57
2	A	6001	NFN	C13-N2-C14	2.23	96.85	93.92
2	A	6001	NFN	C17-O1-C2	2.37	123.56	118.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	6002	NFN	C8-C9-C10	2.50	121.12	117.89
2	A	6001	NFN	C9-C1-C11	2.60	123.38	119.41
2	A	6001	NFN	C8-C9-C10	2.89	121.63	117.89
2	A	6002	NFN	C16-C15-S1	2.97	109.17	104.11
2	A	6002	NFN	C13-N2-C16	3.44	121.55	117.26
2	A	6001	NFN	C13-C12-N1	3.91	126.86	118.25
2	A	6001	NFN	C16-C15-S1	4.46	111.70	104.11
2	A	6002	NFN	O1-C2-C1	4.74	121.26	116.19
2	A	6002	NFN	C12-C14-N2	5.92	99.94	91.87
2	A	6002	NFN	C12-C13-N2	6.20	95.96	87.98
2	A	6001	NFN	S1-C13-N2	6.71	114.12	105.10
2	A	6001	NFN	C16-N2-C14	7.19	147.28	126.35
2	A	6002	NFN	C16-N2-C14	7.52	148.23	126.35
2	A	6001	NFN	C14-C12-N1	9.94	144.08	115.38
2	A	6002	NFN	C14-C12-N1	12.44	151.28	115.38
2	A	6001	NFN	C7-C6-C5	14.35	140.91	120.45
2	A	6002	NFN	C7-C6-C5	14.43	141.01	120.45
2	A	6002	NFN	C12-C13-S1	17.49	146.87	119.40
2	A	6001	NFN	C12-C13-S1	20.04	150.88	119.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6001	NFN	3	0
2	A	6002	NFN	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.