



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:21 PM GMT

PDB ID : 1T9X  
Title : Structural Basis of Multidrug Transport by the AcrB Multidrug Efflux Pump  
Authors : Yu, E.W.; McDermott, G.; Nikaido, H.  
Deposited on : 2004-05-19  
Resolution : 3.08 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

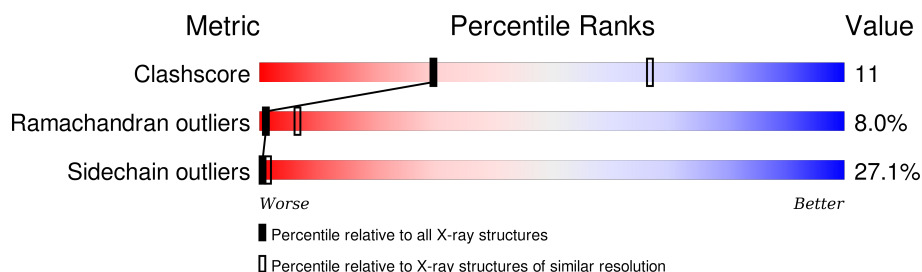
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)

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	 55% 31% 9% . .

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7747 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.

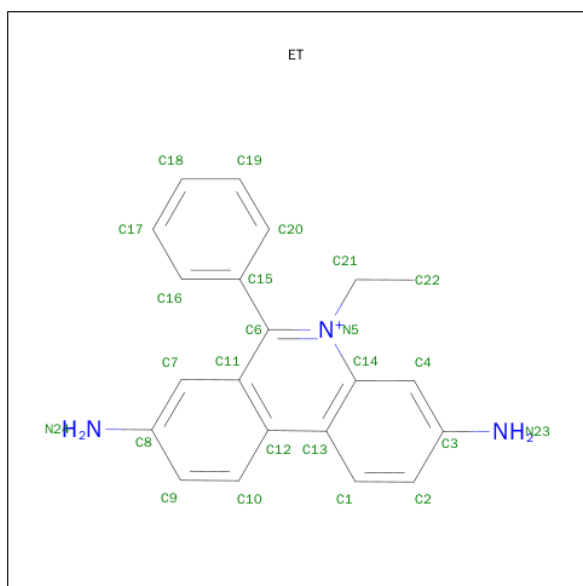
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1014	7699	4950	1273	1434	42	0	0	0

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 ETHIDIUM (three-letter code: ET) (formula:  $C_{21}H_{20}N_3$ ).



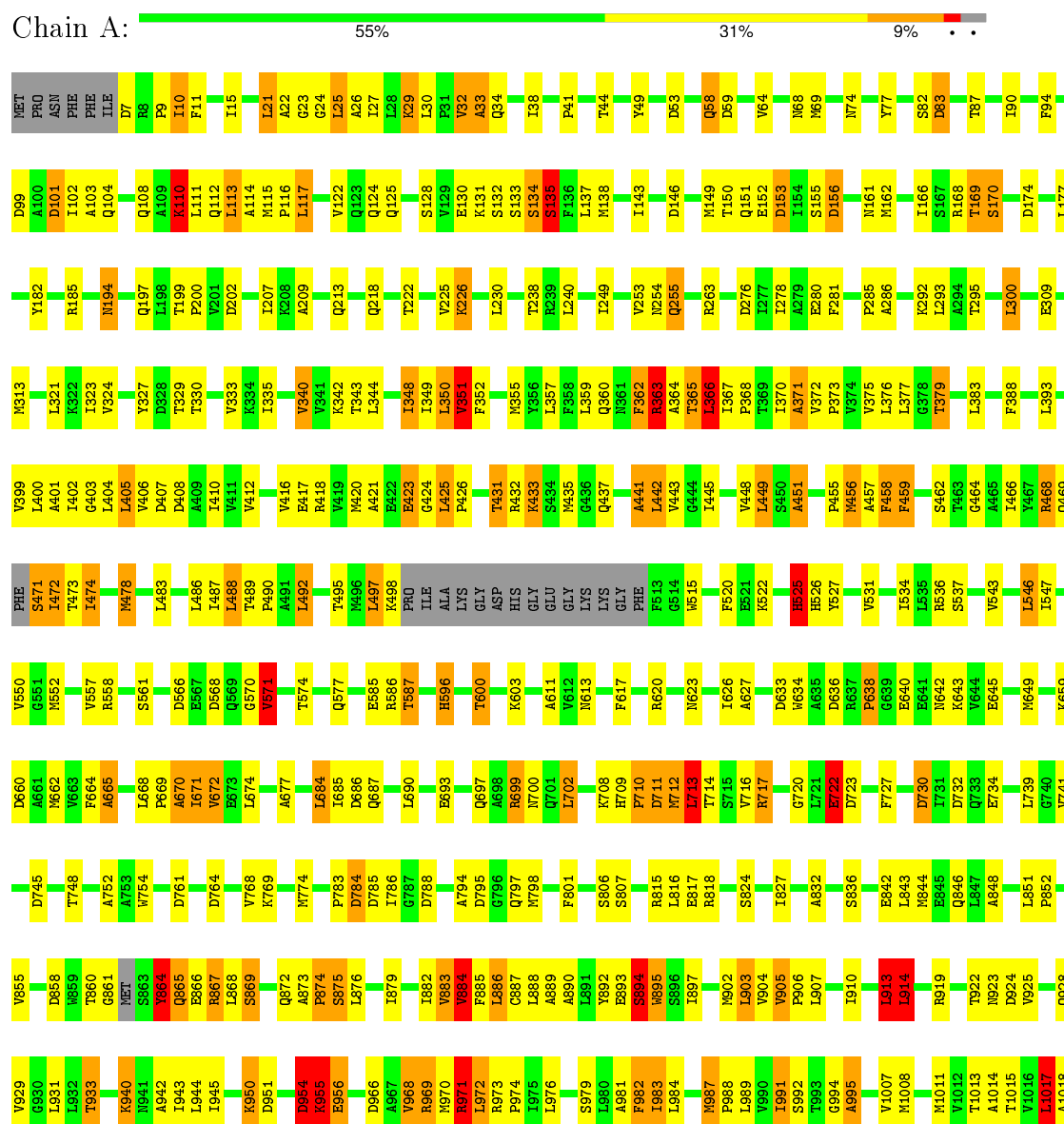
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	24	21	3	0	0
2	A	1	24	21	3	0	0

### 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 errors 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



I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ASP	ILE	GLU	HIS	VAL	HIS	THR	VAL	ASP	HIS	HIS
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.97Å 144.97Å 519.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	3.28 – 3.08	Depositor
% Data completeness (in resolution range)	(Not available) (3.28-3.08)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.272 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7747	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: ET

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	0.37	0/7839	0.75	38/10644 (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	5	8

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	711	ASP	N-CA-C	7.20	130.44	111.00
1	A	33	ALA	N-CA-C	6.70	129.10	111.00
1	A	407	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	795	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	568	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	351	VAL	CB-CA-C	5.86	122.53	111.40
1	A	924	ASP	CB-CG-OD2	5.78	123.51	118.30
1	A	869	SER	CB-CA-C	5.63	120.81	110.10
1	A	966	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	53	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	7	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	174	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	723	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	745	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	660	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	711	ASP	CB-CG-OD2	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	408	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	99	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	869	SER	N-CA-CB	5.29	118.43	110.50
1	A	858	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	686	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	784	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	788	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	276	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	785	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	83	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	153	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	146	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	566	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	722	GLU	N-CA-C	5.15	124.91	111.00
1	A	764	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	761	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	636	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	730	ASP	CB-CG-OD2	5.08	122.88	118.30
1	A	732	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	202	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	954	ASP	CB-CG-OD2	5.01	122.81	118.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	351	VAL	CA
1	A	474	ILE	CA
1	A	711	ASP	CA
1	A	722	GLU	CA
1	A	869	SER	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1022	VAL	Peptide
1	A	426	PRO	Peptide
1	A	451	ALA	Peptide
1	A	525	HIS	Peptide
1	A	712	MET	Peptide
1	A	864	TYR	Peptide
1	A	867	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	894	SER	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	7699	0	7856	175	0
2	A	48	0	40	4	0
All	All	7747	0	7896	175	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 11.

All (175) 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:717:ARG:HG3	2:A:3002:ET:C2	1.93	0.98
1:A:525:HIS:HB3	1:A:526:HIS:HB2	1.52	0.89
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.55	0.88
1:A:950:LYS:NZ	1:A:1028:VAL:HG11	1.89	0.85
1:A:717:ARG:HG3	2:A:3002:ET:C3	2.10	0.82
1:A:587:THR:HG23	1:A:613:ASN:HD21	1.45	0.81
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.63	0.80
1:A:950:LYS:HZ3	1:A:1028:VAL:HG11	1.51	0.75
1:A:471:SER:O	1:A:473:THR:N	2.19	0.75
1:A:348:ILE:O	1:A:350:LEU:N	2.21	0.74
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.71	0.72
1:A:883:VAL:O	1:A:885:PHE:N	2.23	0.70
1:A:400:LEU:HD11	1:A:933:THR:HG21	1.74	0.70
1:A:68:ASN:HD21	1:A:113:LEU:HB2	1.56	0.70
1:A:713:LEU:O	1:A:832:ALA:HB2	1.94	0.67
1:A:449:LEU:HB3	1:A:478:MET:SD	2.37	0.65
1:A:982:PHE:O	1:A:984:LEU:N	2.30	0.65
1:A:365:THR:HG23	1:A:365:THR:O	1.99	0.63
1:A:525:HIS:HB3	1:A:526:HIS:CB	2.27	0.63
1:A:77:TYR:OH	1:A:861:GLY:O	2.06	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:HIS:CB	1:A:526:HIS:HB2	2.26	0.61
1:A:451:ALA:CB	1:A:883:VAL:HG11	2.31	0.61
1:A:950:LYS:HZ2	1:A:1028:VAL:HG11	1.62	0.61
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.82	0.61
1:A:684:LEU:HD13	1:A:855:VAL:HG13	1.84	0.60
1:A:1013:THR:O	1:A:1013:THR:HG22	2.02	0.59
1:A:883:VAL:HG13	1:A:884:VAL:N	2.18	0.59
1:A:1022:VAL:HG22	1:A:1023:PRO:CD	2.32	0.59
1:A:709:HIS:N	1:A:710:PRO:HD3	2.17	0.59
1:A:717:ARG:HD2	2:A:3002:ET:C4	2.33	0.59
1:A:366:LEU:O	1:A:370:ILE:HG13	2.04	0.58
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.86	0.58
1:A:32:VAL:HG23	1:A:300:LEU:HD21	1.85	0.57
1:A:64:VAL:HG12	1:A:114:ALA:HB1	1.86	0.57
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.87	0.56
1:A:867:ARG:C	1:A:868:LEU:HD23	2.25	0.56
1:A:451:ALA:HB3	1:A:883:VAL:HG21	1.87	0.56
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.87	0.56
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.87	0.55
1:A:860:THR:HG22	1:A:861:GLY:HA3	1.87	0.55
1:A:404:LEU:HD11	1:A:449:LEU:HD21	1.88	0.55
1:A:883:VAL:HG13	1:A:884:VAL:H	1.71	0.55
1:A:684:LEU:C	1:A:684:LEU:HD12	2.27	0.55
1:A:717:ARG:CG	2:A:3002:ET:C3	2.84	0.54
1:A:68:ASN:ND2	1:A:110:LYS:O	2.40	0.54
1:A:892:TYR:CD2	1:A:897:ILE:HG21	2.42	0.54
1:A:117:LEU:N	1:A:117:LEU:HD23	2.23	0.53
1:A:464:GLY:O	1:A:468:ARG:HB2	2.09	0.53
1:A:972:LEU:O	1:A:972:LEU:HD22	2.09	0.53
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.91	0.52
1:A:684:LEU:HD23	1:A:699:ARG:HB2	1.91	0.52
1:A:527:TYR:O	1:A:531:VAL:HG23	2.10	0.52
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.40	0.51
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.11	0.51
1:A:483:LEU:O	1:A:487:ILE:HD12	2.10	0.51
1:A:459:PHE:CD1	1:A:468:ARG:HG3	2.46	0.51
1:A:25:LEU:HD13	1:A:26:ALA:N	2.26	0.51
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.64	0.50
1:A:68:ASN:HD21	1:A:113:LEU:CB	2.21	0.50
1:A:887:CYS:HA	1:A:890:ALA:HB3	1.92	0.50
1:A:350:LEU:HD12	1:A:984:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.40	0.50
1:A:525:HIS:CB	1:A:526:HIS:CB	2.89	0.49
1:A:451:ALA:HB1	1:A:883:VAL:HG11	1.94	0.49
1:A:727:PHE:CZ	1:A:783:PRO:HB3	2.47	0.49
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.94	0.49
1:A:363:ARG:HG3	1:A:497:LEU:O	2.11	0.49
1:A:1011:MET:HA	1:A:1014:ALA:HB3	1.93	0.49
1:A:371:ALA:O	1:A:375:VAL:HG23	2.12	0.49
1:A:451:ALA:HB3	1:A:883:VAL:HG11	1.95	0.49
1:A:925:VAL:O	1:A:929:VAL:HG23	2.13	0.49
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.48	0.48
1:A:979:SER:CB	1:A:1015:THR:HG21	2.43	0.48
1:A:41:PRO:HB3	1:A:295:THR:HG22	1.96	0.48
1:A:684:LEU:HD12	1:A:685:ILE:N	2.28	0.48
1:A:971:ARG:C	1:A:971:ARG:HD2	2.34	0.48
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.48	0.48
1:A:951:ASP:O	1:A:955:LYS:HG3	2.13	0.48
1:A:913:LEU:O	1:A:914:LEU:C	2.52	0.48
1:A:664:PHE:O	1:A:665:ALA:CB	2.61	0.47
1:A:1024:VAL:N	1:A:1027:VAL:HG22	2.29	0.47
1:A:868:LEU:O	1:A:873:ALA:HB2	2.15	0.47
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.45	0.47
1:A:710:PRO:HB2	1:A:713:LEU:HA	1.95	0.47
1:A:21:LEU:O	1:A:23:GLY:N	2.47	0.47
1:A:104:GLN:HE21	1:A:130:GLU:HA	1.79	0.47
1:A:487:ILE:HG22	1:A:488:LEU:H	1.80	0.47
1:A:942:ALA:O	1:A:945:ILE:N	2.48	0.47
1:A:638:PRO:HD2	1:A:642:ASN:HD22	1.80	0.47
1:A:372:VAL:HG23	1:A:373:PRO:HD3	1.96	0.47
1:A:393:LEU:HD11	1:A:466:ILE:HA	1.96	0.47
1:A:895:TRP:CE3	1:A:895:TRP:HA	2.49	0.47
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.97	0.47
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.98	0.46
1:A:451:ALA:HA	1:A:455:PRO:HD2	1.97	0.46
1:A:456:MET:HG2	1:A:876:LEU:HD13	1.97	0.46
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.97	0.46
1:A:90:ILE:N	1:A:90:ILE:HD12	2.31	0.46
1:A:907:LEU:HG	1:A:1017:LEU:HD23	1.97	0.46
1:A:587:THR:CG2	1:A:613:ASN:HD21	2.22	0.46
1:A:365:THR:O	1:A:365:THR:CG2	2.64	0.46
1:A:970:MET:O	1:A:971:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ILE:HG23	1:A:1013:THR:HG21	1.97	0.45
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.98	0.45
1:A:487:ILE:HG22	1:A:488:LEU:N	2.32	0.45
1:A:1024:VAL:H	1:A:1027:VAL:HG22	1.80	0.45
1:A:864:TYR:CD2	1:A:865:GLN:N	2.85	0.45
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.80	0.45
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.49	0.45
1:A:402:ILE:HA	1:A:405:LEU:HD12	1.99	0.45
1:A:457:ALA:HB2	1:A:471:SER:HB2	1.97	0.45
1:A:25:LEU:HD13	1:A:25:LEU:C	2.37	0.45
1:A:979:SER:O	1:A:982:PHE:HB3	2.17	0.45
1:A:468:ARG:O	1:A:471:SER:N	2.50	0.44
1:A:886:LEU:N	1:A:886:LEU:HD23	2.32	0.44
1:A:10:ILE:HG12	1:A:11:PHE:CD2	2.53	0.44
1:A:379:THR:O	1:A:383:LEU:HG	2.18	0.44
1:A:894:SER:O	1:A:895:TRP:CE3	2.71	0.44
1:A:669:PRO:O	1:A:670:ALA:HB3	2.17	0.44
1:A:884:VAL:HG12	1:A:885:PHE:N	2.33	0.44
1:A:669:PRO:O	1:A:670:ALA:CB	2.66	0.44
1:A:894:SER:HB3	1:A:897:ILE:HD12	2.00	0.43
1:A:21:LEU:O	1:A:24:GLY:N	2.51	0.43
1:A:151:GLN:HG2	1:A:285:PRO:HB3	2.00	0.43
1:A:664:PHE:O	1:A:665:ALA:HB3	2.18	0.43
1:A:672:VAL:HG23	1:A:674:LEU:HD23	2.00	0.43
1:A:895:TRP:HA	1:A:895:TRP:HE3	1.83	0.43
1:A:367:ILE:HG12	1:A:492:LEU:HD22	2.00	0.43
1:A:954:ASP:O	1:A:955:LYS:C	2.57	0.43
1:A:611:ALA:HA	1:A:627:ALA:HA	2.01	0.43
1:A:441:ALA:O	1:A:443:VAL:N	2.52	0.43
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.53	0.43
1:A:489:THR:HB	1:A:490:PRO:CD	2.49	0.42
1:A:981:ALA:C	1:A:982:PHE:O	2.57	0.42
1:A:373:PRO:O	1:A:377:LEU:HG	2.20	0.42
1:A:412:VAL:O	1:A:416:VAL:HG23	2.20	0.42
1:A:133:SER:O	1:A:134:SER:C	2.58	0.42
1:A:596:HIS:O	1:A:600:THR:HG22	2.19	0.42
1:A:670:ALA:O	1:A:671:ILE:C	2.57	0.42
1:A:543:VAL:HA	1:A:546:LEU:HD12	2.01	0.42
1:A:752:ALA:O	1:A:774:MET:HA	2.20	0.42
1:A:199:THR:HB	1:A:200:PRO:HD2	2.01	0.42
1:A:58:GLN:HE21	1:A:816:LEU:HD13	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HA	1:A:445:ILE:HD11	2.02	0.42
1:A:468:ARG:HB3	1:A:469:GLN:H	1.60	0.42
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.34	0.41
1:A:987:MET:N	1:A:988:PRO:CD	2.83	0.41
1:A:994:GLY:O	1:A:995:ALA:HB2	2.20	0.41
1:A:940:LYS:O	1:A:944:LEU:HG	2.20	0.41
1:A:115:MET:N	1:A:116:PRO:CD	2.83	0.41
1:A:903:LEU:O	1:A:907:LEU:HD13	2.18	0.41
1:A:10:ILE:HG12	1:A:11:PHE:HD2	1.84	0.41
1:A:169:THR:O	1:A:170:SER:C	2.59	0.41
1:A:433:LYS:N	1:A:433:LYS:HD3	2.36	0.41
1:A:362:PHE:O	1:A:365:THR:N	2.53	0.41
1:A:851:LEU:HB3	1:A:852:PRO:HD2	2.02	0.41
1:A:94:PHE:CZ	1:A:103:ALA:HB1	2.56	0.41
1:A:458:PHE:O	1:A:459:PHE:O	2.38	0.41
1:A:527:TYR:OH	1:A:968:VAL:HG21	2.21	0.41
1:A:848:ALA:HA	1:A:851:LEU:HD12	2.02	0.41
1:A:431:THR:HG22	1:A:435:MET:HE3	2.01	0.41
1:A:886:LEU:C	1:A:888:LEU:H	2.24	0.41
1:A:133:SER:O	1:A:135:SER:N	2.54	0.41
1:A:570:GLY:O	1:A:571:VAL:HG23	2.21	0.41
1:A:401:ALA:HB2	1:A:474:ILE:HG23	2.02	0.41
1:A:194:ASN:ND2	1:A:194:ASN:O	2.54	0.41
1:A:1033:PHE:O	1:A:1034:SER:OG	2.36	0.41
1:A:362:PHE:O	1:A:364:ALA:N	2.54	0.41
1:A:367:ILE:CG1	1:A:492:LEU:HD22	2.51	0.41
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.50	0.41
1:A:1014:ALA:O	1:A:1018:ALA:HB3	2.21	0.40
1:A:954:ASP:O	1:A:956:GLU:N	2.54	0.40
1:A:412:VAL:HG23	1:A:489:THR:HG21	2.02	0.40
1:A:423:GLU:O	1:A:425:LEU:HB2	2.22	0.40
1:A:448:VAL:HG12	1:A:884:VAL:HA	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1006/1049 (96%)	781 (78%)	145 (14%)	80 (8%)	<b>1</b> <b>6</b>

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ALA
1	A	33	ALA
1	A	134	SER
1	A	170	SER
1	A	255	GLN
1	A	340	VAL
1	A	349	ILE
1	A	351	VAL
1	A	352	PHE
1	A	363	ARG
1	A	441	ALA
1	A	442	LEU
1	A	459	PHE
1	A	515	TRP
1	A	670	ALA
1	A	711	ASP
1	A	713	LEU
1	A	874	PRO
1	A	875	SER
1	A	883	VAL
1	A	884	VAL
1	A	889	ALA
1	A	893	GLU
1	A	914	LEU
1	A	955	LYS
1	A	969	ARG
1	A	971	ARG
1	A	995	ALA
1	A	1021	PHE
1	A	1023	PRO
1	A	110	LYS
1	A	135	SER
1	A	152	GLU
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	209	ALA
1	A	327	TYR
1	A	348	ILE
1	A	366	LEU
1	A	405	LEU
1	A	421	ALA
1	A	424	GLY
1	A	472	ILE
1	A	495	THR
1	A	665	ALA
1	A	671	ILE
1	A	794	ALA
1	A	968	VAL
1	A	1017	LEU
1	A	1025	PHE
1	A	74	ASN
1	A	468	ARG
1	A	488	LEU
1	A	525	HIS
1	A	722	GLU
1	A	894	SER
1	A	956	GLU
1	A	982	PHE
1	A	983	ILE
1	A	9	PRO
1	A	29	LYS
1	A	571	VAL
1	A	633	ASP
1	A	638	PRO
1	A	677	ALA
1	A	954	ASP
1	A	21	LEU
1	A	226	LYS
1	A	362	PHE
1	A	550	VAL
1	A	626	ILE
1	A	720	GLY
1	A	913	LEU
1	A	991	ILE
1	A	365	THR
1	A	371	ALA
1	A	497	LEU

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Mol	Chain	Res	Type
1	A	943	ILE
1	A	1027	VAL
1	A	710	PRO
1	A	410	ILE

### 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	824/854 (96%)	601 (73%)	223 (27%)	<b>0</b> <b>1</b>

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS
1	A	30	LEU
1	A	32	VAL
1	A	34	GLN
1	A	38	ILE
1	A	44	THR
1	A	49	TYR
1	A	58	GLN
1	A	59	ASP
1	A	69	MET
1	A	82	SER
1	A	83	ASP
1	A	87	THR
1	A	101	ASP
1	A	102	ILE
1	A	108	GLN
1	A	110	LYS
1	A	111	LEU

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	113	LEU
1	A	117	LEU
1	A	122	VAL
1	A	124	GLN
1	A	125	GLN
1	A	128	SER
1	A	131	LYS
1	A	132	SER
1	A	135	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET
1	A	150	THR
1	A	153	ASP
1	A	155	SER
1	A	156	ASP
1	A	162	MET
1	A	166	ILE
1	A	168	ARG
1	A	169	THR
1	A	177	LEU
1	A	182	TYR
1	A	185	ARG
1	A	194	ASN
1	A	197	GLN
1	A	207	ILE
1	A	213	GLN
1	A	218	GLN
1	A	222	THR
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	240	LEU
1	A	249	ILE
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	263	ARG
1	A	278	ILE
1	A	280	GLU

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Mol	Chain	Res	Type
1	A	292	LYS
1	A	293	LEU
1	A	300	LEU
1	A	309	GLU
1	A	313	MET
1	A	321	LEU
1	A	323	ILE
1	A	329	THR
1	A	330	THR
1	A	333	VAL
1	A	335	ILE
1	A	340	VAL
1	A	342	LYS
1	A	343	THR
1	A	350	LEU
1	A	355	MET
1	A	357	LEU
1	A	359	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU
1	A	376	LEU
1	A	379	THR
1	A	388	PHE
1	A	406	VAL
1	A	417	GLU
1	A	418	ARG
1	A	420	MET
1	A	423	GLU
1	A	425	LEU
1	A	431	THR
1	A	432	ARG
1	A	433	LYS
1	A	437	GLN
1	A	449	LEU
1	A	456	MET
1	A	458	PHE
1	A	462	SER
1	A	471	SER
1	A	472	ILE
1	A	474	ILE
1	A	478	MET

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Mol	Chain	Res	Type
1	A	486	LEU
1	A	492	LEU
1	A	498	LYS
1	A	520	PHE
1	A	522	LYS
1	A	525	HIS
1	A	536	ARG
1	A	537	SER
1	A	546	LEU
1	A	547	ILE
1	A	552	MET
1	A	557	VAL
1	A	558	ARG
1	A	561	SER
1	A	571	VAL
1	A	574	THR
1	A	577	GLN
1	A	585	GLU
1	A	586	ARG
1	A	587	THR
1	A	596	HIS
1	A	600	THR
1	A	603	LYS
1	A	617	PHE
1	A	620	ARG
1	A	623	ASN
1	A	634	TRP
1	A	640	GLU
1	A	643	LYS
1	A	645	GLU
1	A	649	MET
1	A	659	LYS
1	A	662	MET
1	A	668	LEU
1	A	672	VAL
1	A	684	LEU
1	A	687	GLN
1	A	690	LEU
1	A	693	GLU
1	A	697	GLN
1	A	699	ARG
1	A	700	ASN

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	708	LYS
1	A	712	MET
1	A	713	LEU
1	A	714	THR
1	A	716	VAL
1	A	717	ARG
1	A	722	GLU
1	A	730	ASP
1	A	734	GLU
1	A	739	LEU
1	A	741	VAL
1	A	748	THR
1	A	768	VAL
1	A	784	ASP
1	A	797	GLN
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	818	ARG
1	A	824	SER
1	A	827	ILE
1	A	836	SER
1	A	842	GLU
1	A	843	LEU
1	A	844	MET
1	A	846	GLN
1	A	864	TYR
1	A	865	GLN
1	A	866	GLU
1	A	869	SER
1	A	872	GLN
1	A	875	SER
1	A	879	ILE
1	A	882	ILE
1	A	884	VAL
1	A	886	LEU
1	A	895	TRP
1	A	902	MET

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Mol	Chain	Res	Type
1	A	903	LEU
1	A	904	VAL
1	A	905	VAL
1	A	913	LEU
1	A	914	LEU
1	A	919	ARG
1	A	922	THR
1	A	923	ASN
1	A	928	GLN
1	A	931	LEU
1	A	933	THR
1	A	940	LYS
1	A	950	LYS
1	A	955	LYS
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	983	ILE
1	A	987	MET
1	A	989	LEU
1	A	991	ILE
1	A	992	SER
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1020	PHE
1	A	1022	VAL
1	A	1024	VAL
1	A	1027	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1035	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	GLN
1	A	68	ASN
1	A	104	GLN
1	A	161	ASN

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Mol	Chain	Res	Type
1	A	194	ASN
1	A	218	GLN
1	A	254	ASN
1	A	284	GLN
1	A	415	ASN
1	A	577	GLN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	642	ASN
1	A	657	GLN
1	A	709	HIS
1	A	760	ASN
1	A	872	GLN
1	A	923	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	ET	A	3001	-	26,27,27	3.64	16 (61%)	33,39,39	1.65	6 (18%)
2	ET	A	3002	-	26,27,27	3.65	16 (61%)	33,39,39	1.65	6 (18%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ET	A	3001	-	-	0/6/6/6	0/4/4/4
2	ET	A	3002	-	-	0/6/6/6	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3002	ET	C6-C11	-2.93	1.38	1.43
2	A	3001	ET	C6-C11	-2.81	1.38	1.43
2	A	3001	ET	C17-C16	2.00	1.43	1.38
2	A	3002	ET	C17-C16	2.00	1.43	1.38
2	A	3002	ET	C10-C12	2.02	1.45	1.41
2	A	3001	ET	C10-C12	2.02	1.45	1.41
2	A	3002	ET	C19-C20	2.14	1.43	1.38
2	A	3001	ET	C19-C20	2.26	1.43	1.38
2	A	3002	ET	C13-C14	2.31	1.45	1.41
2	A	3001	ET	C13-C14	2.35	1.45	1.41
2	A	3002	ET	C10-C9	2.48	1.41	1.36
2	A	3001	ET	C10-C9	2.55	1.42	1.36
2	A	3002	ET	C4-C3	3.02	1.44	1.39
2	A	3001	ET	C4-C3	3.07	1.44	1.39
2	A	3002	ET	C7-C11	3.17	1.48	1.42
2	A	3001	ET	C7-C11	3.18	1.48	1.42
2	A	3001	ET	C14-N5	3.52	1.45	1.40
2	A	3002	ET	C14-N5	3.56	1.45	1.40
2	A	3001	ET	C11-C12	3.89	1.48	1.42
2	A	3002	ET	C11-C12	3.98	1.48	1.42
2	A	3001	ET	C1-C13	4.12	1.49	1.41
2	A	3002	ET	C1-C13	4.13	1.49	1.41
2	A	3001	ET	C20-C15	4.15	1.48	1.39
2	A	3002	ET	C20-C15	4.22	1.48	1.39
2	A	3002	ET	C16-C15	4.28	1.48	1.39
2	A	3001	ET	C16-C15	4.33	1.48	1.39
2	A	3001	ET	C4-C14	4.50	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3002	ET	C4-C14	4.55	1.50	1.40
2	A	3001	ET	C15-C6	6.29	1.57	1.48
2	A	3002	ET	C15-C6	6.38	1.57	1.48
2	A	3002	ET	C6-N5	11.48	1.59	1.35
2	A	3001	ET	C6-N5	11.50	1.59	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	ET	C11-C6-N5	-3.15	114.91	119.47
2	A	3002	ET	C11-C6-N5	-3.11	114.97	119.47
2	A	3001	ET	C20-C15-C16	-2.69	112.46	117.55
2	A	3002	ET	C20-C15-C16	-2.69	112.47	117.55
2	A	3002	ET	C19-C20-C15	2.37	123.69	120.56
2	A	3001	ET	C19-C20-C15	2.39	123.72	120.56
2	A	3001	ET	C8-C7-C11	2.64	123.69	120.81
2	A	3002	ET	C8-C7-C11	2.66	123.72	120.81
2	A	3002	ET	C20-C15-C6	3.51	126.14	120.19
2	A	3001	ET	C20-C15-C6	3.54	126.20	120.19
2	A	3001	ET	C6-C11-C12	5.02	125.29	117.94
2	A	3002	ET	C6-C11-C12	5.05	125.33	117.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3002	ET	4	0

## 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](#)

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.