WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:25 PM GMT

PDB ID : 1OY9
Title : Structural Basis of Multiple Drug Binding Capacity of the AcrB Multidrug Efflux Pump
Authors : Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on : 2003-04-03
Resolution : 3.80 Å(reported)

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

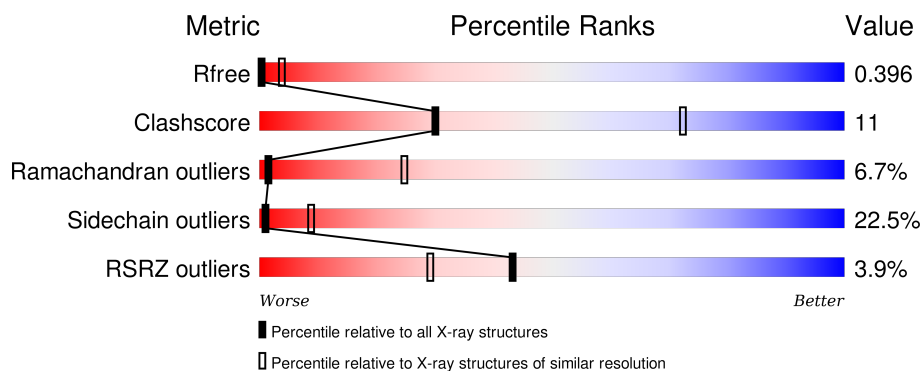|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	Percentile Ranks	Value
Rfree		0.396
Clashscore		11
Ramachandran outliers		6.7%
Sidechain outliers		22.5%
RSRZ outliers		3.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 >=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 <=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.

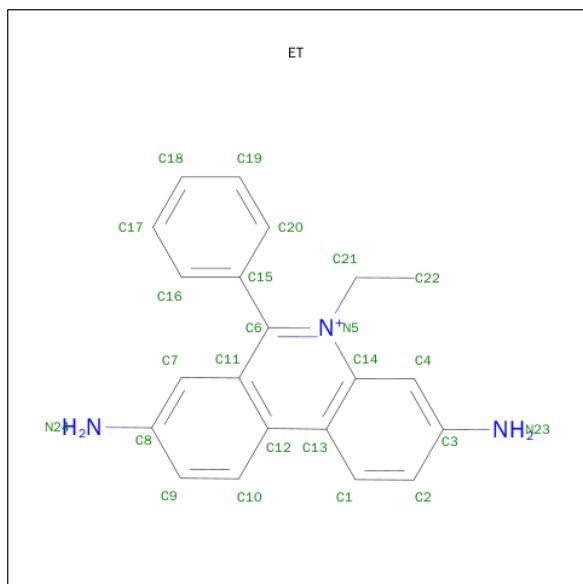| Mol	Chain	Length	Quality of chain
1	A	1049	4% / 57% / 31% / 8% · ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7663 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	1006	7639	4916	1262	1419	42	0	0	0

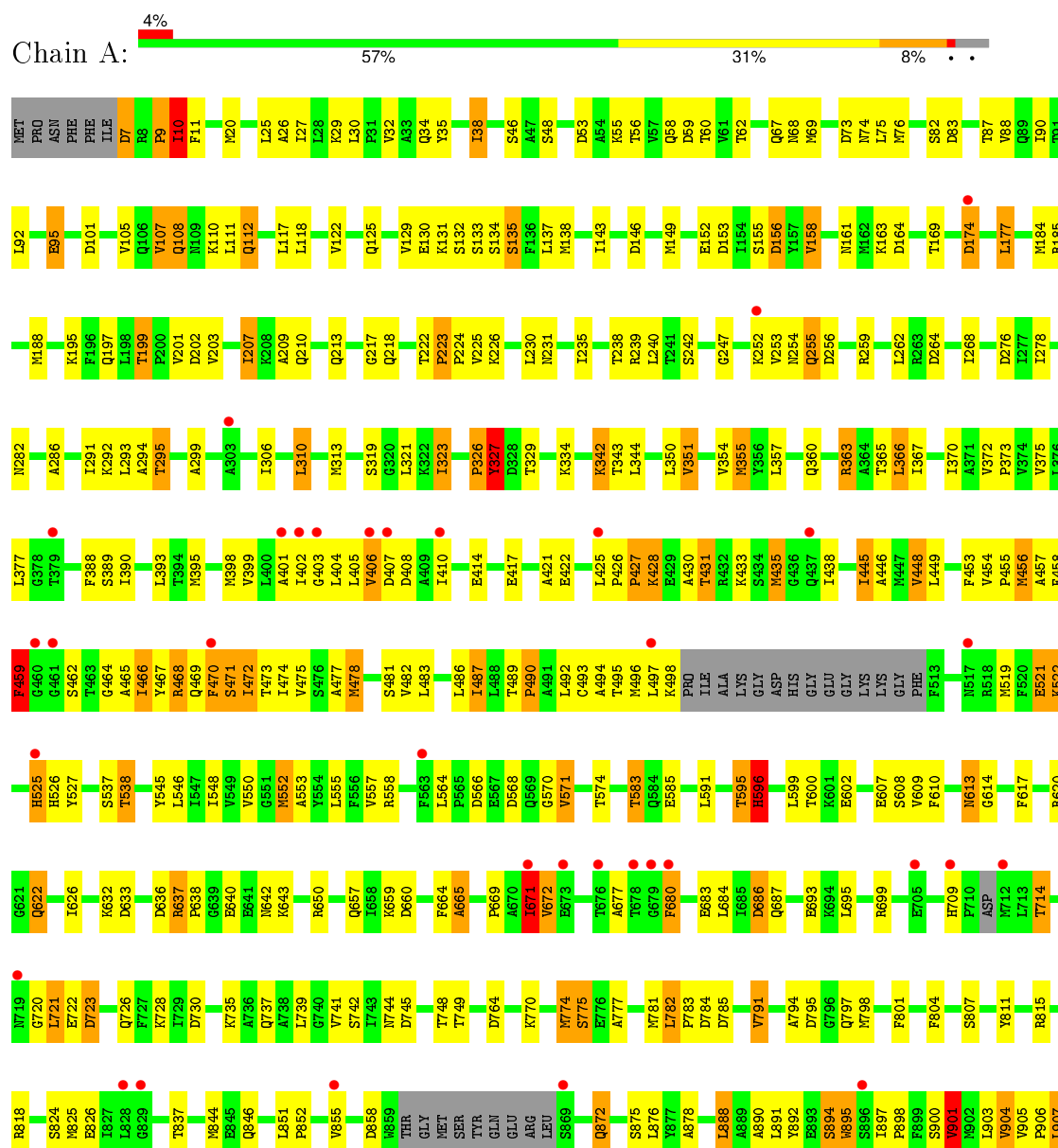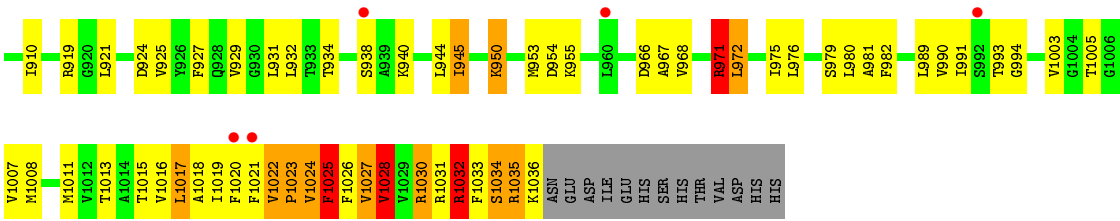- Molecule 2 is ETHIDIUM (three-letter code: ET) (formula: $C_{21}H_{20}N_3$).

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

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.

- Molecule 1: Acriflavine resistance protein B

Chain A:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.68Å 144.68Å 517.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.80 46.58 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.80) 84.3 (46.58-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.283 , 0.344 0.390 , 0.396	Depositor DCC
R_{free} test set	1072 reflections (5.42%)	DCC
Wilson B-factor (Å²)	142.8	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.27 , 88.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Outliers	1 of 30764 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: 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	0.43	3/7779 (0.0%)	0.72	38/10563 (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	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	596	HIS	CG-CD2	17.93	1.66	1.35
1	A	596	HIS	CE1-NE2	8.56	1.52	1.32
1	A	596	HIS	CG-ND1	6.96	1.54	1.38

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	407	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	470	PHE	N-CA-C	6.35	128.15	111.00
1	A	568	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	723	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	791	VAL	CG1-CB-CG2	6.02	120.53	110.90
1	A	596	HIS	CG-CD2-NE2	-6.01	97.78	109.20
1	A	672	VAL	CB-CA-C	5.94	122.69	111.40
1	A	795	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	858	ASP	CB-CG-OD2	5.78	123.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	174	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	924	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	680	PHE	N-CA-C	5.55	125.98	111.00
1	A	146	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	7	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	264	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	83	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	101	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	636	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	408	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	660	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	153	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	633	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	784	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	785	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	566	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	966	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	745	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	156	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	73	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	764	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	276	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	53	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	202	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	954	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	686	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	730	ASP	CB-CG-OD2	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	PHE	CA
1	A	680	PHE	CA

There are no planarity outliers.

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	A	7639	0	7800	172	0
2	A	24	0	20	0	0
All	All	7663	0	7820	172	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 (172) 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:613:ASN:HD22	1:A:613:ASN:C	1.81	0.82
1:A:596:HIS:O	1:A:600:THR:HG22	1.81	0.80
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.65	0.78
1:A:613:ASN:HD22	1:A:614:GLY:N	1.84	0.74
1:A:483:LEU:O	1:A:487:ILE:HG13	1.90	0.72
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.74	0.70
1:A:365:THR:HG23	1:A:365:THR:O	1.92	0.69
1:A:468:ARG:O	1:A:472:ILE:HG22	1.93	0.69
1:A:921:LEU:HD23	1:A:1005:THR:HG21	1.76	0.67
1:A:613:ASN:C	1:A:613:ASN:ND2	2.47	0.67
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.80	0.63
1:A:291:ILE:HG21	1:A:306:ILE:HD11	1.81	0.63
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.79	0.63
1:A:910:ILE:HG23	1:A:1013:THR:HG21	1.80	0.62
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.82	0.61
1:A:993:THR:HB	1:A:994:GLY:HA2	1.82	0.61
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.82	0.60
1:A:709:HIS:O	1:A:709:HIS:CG	2.54	0.60
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.82	0.60
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.83	0.59
1:A:201:VAL:HG22	1:A:748:THR:HG23	1.84	0.59
1:A:591:LEU:O	1:A:595:THR:OG1	2.20	0.59
1:A:637:ARG:HG2	1:A:642:ASN:HB3	1.85	0.58
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.03	0.58
1:A:372:VAL:HG11	1:A:406:VAL:HG22	1.86	0.58
1:A:975:ILE:HG21	1:A:1019:ILE:HD13	1.85	0.58
1:A:454:VAL:N	1:A:455:PRO:HD2	2.19	0.57
1:A:92:LEU:HD13	1:A:107:VAL:HG21	1.86	0.57
1:A:448:VAL:HG11	1:A:888:LEU:HD23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.87	0.57
1:A:493:CYS:SG	1:A:497:LEU:HD22	2.44	0.57
1:A:456:MET:SD	1:A:932:LEU:HD11	2.45	0.57
1:A:967:ALA:O	1:A:971:ARG:HG3	2.05	0.57
1:A:370:ILE:O	1:A:370:ILE:HG22	2.05	0.57
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.86	0.56
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.54	0.56
1:A:372:VAL:N	1:A:373:PRO:HD2	2.21	0.56
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.87	0.56
1:A:570:GLY:O	1:A:571:VAL:HG23	2.06	0.56
1:A:894:SER:O	1:A:895:TRP:HB2	2.06	0.56
1:A:1032:ARG:CG	1:A:1032:ARG:HH11	2.20	0.55
1:A:365:THR:O	1:A:365:THR:CG2	2.55	0.55
1:A:458:PHE:O	1:A:459:PHE:O	2.24	0.55
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.89	0.55
1:A:133:SER:O	1:A:135:SER:N	2.40	0.54
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	1.89	0.54
1:A:979:SER:CB	1:A:1015:THR:HG21	2.38	0.54
1:A:477:ALA:O	1:A:481:SER:HB3	2.08	0.53
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.90	0.52
1:A:472:ILE:HA	1:A:475:VAL:HB	1.91	0.52
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.92	0.52
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.90	0.52
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.92	0.51
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.91	0.51
1:A:363:ARG:HB2	1:A:496:MET:SD	2.51	0.51
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.11	0.51
1:A:903:LEU:O	1:A:906:PRO:HD2	2.10	0.50
1:A:972:LEU:HD23	1:A:1019:ILE:HG12	1.92	0.50
1:A:390:ILE:HG23	1:A:395:MET:SD	2.52	0.50
1:A:326:PRO:O	1:A:327:TYR:C	2.49	0.50
1:A:525:HIS:O	1:A:527:TYR:N	2.45	0.50
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.42	0.50
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.47	0.50
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.26	0.50
1:A:904:VAL:HA	1:A:907:LEU:HB2	1.94	0.50
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.46	0.49
1:A:456:MET:O	1:A:876:LEU:HD13	2.12	0.49
1:A:372:VAL:HG12	1:A:405:LEU:HB3	1.93	0.49
1:A:1035:ARG:H	1:A:1035:ARG:HD3	1.78	0.49
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HG23	1:A:473:THR:H	1.77	0.49
1:A:1016:VAL:O	1:A:1017:LEU:HB2	2.13	0.49
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.42	0.48
1:A:38:ILE:HD13	1:A:672:VAL:HG21	1.93	0.48
1:A:744:ASN:O	1:A:748:THR:HG22	2.13	0.48
1:A:1033:PHE:O	1:A:1035:ARG:N	2.47	0.48
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.96	0.48
1:A:426:PRO:N	1:A:427:PRO:HD2	2.28	0.48
1:A:294:ALA:O	1:A:295:THR:C	2.51	0.48
1:A:1032:ARG:HG2	1:A:1032:ARG:HH11	1.78	0.48
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.48	0.48
1:A:1022:VAL:O	1:A:1023:PRO:O	2.32	0.47
1:A:855:VAL:O	1:A:855:VAL:HG12	2.14	0.47
1:A:449:LEU:HB2	1:A:478:MET:SD	2.55	0.47
1:A:664:PHE:O	1:A:665:ALA:HB2	2.14	0.47
1:A:1026:PHE:O	1:A:1030:ARG:HG2	2.14	0.47
1:A:465:ALA:HA	1:A:468:ARG:HB3	1.96	0.47
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.95	0.47
1:A:428:LYS:HZ2	1:A:494:ALA:HB1	1.79	0.47
1:A:95:GLU:CA	1:A:95:GLU:OE1	2.62	0.47
1:A:310:LEU:HD21	1:A:323:ILE:HD12	1.97	0.47
1:A:163:LYS:HD2	1:A:177:LEU:HD23	1.97	0.47
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.45	0.47
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.97	0.46
1:A:709:HIS:O	1:A:709:HIS:CD2	2.69	0.46
1:A:468:ARG:HG2	1:A:469:GLN:N	2.31	0.46
1:A:457:ALA:HB2	1:A:471:SER:CB	2.45	0.46
1:A:188:MET:N	1:A:775:SER:HA	2.31	0.46
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.46	0.45
1:A:118:LEU:HD13	1:A:122:VAL:HG11	1.97	0.45
1:A:897:ILE:N	1:A:898:PRO:CD	2.79	0.45
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.97	0.45
1:A:26:ALA:O	1:A:30:LEU:HB2	2.17	0.45
1:A:425:LEU:C	1:A:427:PRO:HD2	2.37	0.45
1:A:112:GLN:O	1:A:112:GLN:HG2	2.16	0.45
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.97	0.45
1:A:10:ILE:HD13	1:A:11:PHE:H	1.81	0.45
1:A:469:GLN:HA	1:A:472:ILE:CG2	2.47	0.44
1:A:342:LYS:HA	1:A:342:LYS:CE	2.47	0.44
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.99	0.44
1:A:545:TYR:HA	1:A:548:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:OH	1:A:1019:ILE:HG13	2.17	0.44
1:A:158:VAL:HG12	1:A:177:LEU:HD21	2.00	0.44
1:A:489:THR:HB	1:A:490:PRO:HD3	1.99	0.44
1:A:90:ILE:N	1:A:90:ILE:HD12	2.33	0.44
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.82	0.44
1:A:448:VAL:HG21	1:A:888:LEU:HD23	2.00	0.44
1:A:774:MET:O	1:A:775:SER:HB3	2.18	0.43
1:A:927:PHE:CZ	1:A:931:LEU:HD21	2.53	0.43
1:A:583:THR:HA	1:A:622:GLN:HE21	1.83	0.43
1:A:782:LEU:HB3	1:A:783:PRO:HD2	1.99	0.43
1:A:521:GLU:O	1:A:522:LYS:C	2.57	0.43
1:A:222:THR:HB	1:A:223:PRO:HD3	2.00	0.43
1:A:20:MET:HA	1:A:377:LEU:HD13	1.99	0.43
1:A:355:MET:HB3	1:A:365:THR:OG1	2.18	0.43
1:A:684:LEU:HG	1:A:695:LEU:HD21	2.01	0.43
1:A:890:ALA:C	1:A:891:LEU:HD22	2.39	0.43
1:A:393:LEU:HD22	1:A:470:PHE:CD2	2.54	0.43
1:A:1022:VAL:CG2	1:A:1023:PRO:HD2	2.41	0.43
1:A:388:PHE:CD2	1:A:388:PHE:N	2.87	0.43
1:A:474:ILE:HA	1:A:477:ALA:HB3	2.01	0.43
1:A:344:LEU:HD23	1:A:402:ILE:HD11	2.01	0.42
1:A:203:VAL:O	1:A:207:ILE:HG13	2.19	0.42
1:A:470:PHE:CD1	1:A:929:VAL:HG11	2.54	0.42
1:A:695:LEU:HD22	1:A:825:MET:SD	2.60	0.42
1:A:27:ILE:CD1	1:A:390:ILE:HD11	2.49	0.42
1:A:891:LEU:N	1:A:891:LEU:HD22	2.34	0.42
1:A:399:VAL:HA	1:A:402:ILE:HD12	2.01	0.42
1:A:456:MET:HA	1:A:876:LEU:HB3	2.00	0.42
1:A:254:ASN:O	1:A:256:ASP:N	2.52	0.42
1:A:1003:VAL:O	1:A:1007:VAL:HG23	2.20	0.42
1:A:971:ARG:C	1:A:971:ARG:HD2	2.40	0.42
1:A:475:VAL:HG22	1:A:478:MET:CE	2.49	0.42
1:A:493:CYS:O	1:A:497:LEU:HB2	2.20	0.41
1:A:950:LYS:HA	1:A:953:MET:HB3	2.01	0.41
1:A:875:SER:O	1:A:878:ALA:HB3	2.20	0.41
1:A:553:ALA:O	1:A:557:VAL:HG23	2.20	0.41
1:A:401:ALA:O	1:A:405:LEU:HG	2.20	0.41
1:A:921:LEU:CD2	1:A:1005:THR:HG21	2.48	0.41
1:A:95:GLU:N	1:A:95:GLU:OE1	2.52	0.41
1:A:546:LEU:O	1:A:550:VAL:HG23	2.20	0.41
1:A:9:PRO:HB3	1:A:495:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:O	1:A:449:LEU:HG	2.20	0.41
1:A:552:MET:HG3	1:A:910:ILE:HB	2.01	0.41
1:A:466:ILE:HG22	1:A:467:TYR:N	2.35	0.41
1:A:282:ASN:HD21	1:A:608:SER:HA	1.84	0.41
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.50	0.41
1:A:851:LEU:HB3	1:A:852:PRO:HD2	2.03	0.41
1:A:398:MET:O	1:A:402:ILE:HG13	2.20	0.41
1:A:721:LEU:HD22	1:A:825:MET:CE	2.51	0.41
1:A:388:PHE:HE1	1:A:472:ILE:HG21	1.86	0.41
1:A:971:ARG:O	1:A:971:ARG:HD2	2.20	0.41
1:A:1033:PHE:O	1:A:1034:SER:C	2.58	0.41
1:A:435:MET:HA	1:A:438:ILE:HB	2.01	0.41
1:A:199:THR:HG21	1:A:791:VAL:HG13	2.03	0.41
1:A:888:LEU:HD13	1:A:897:ILE:HG22	2.02	0.41
1:A:342:LYS:HA	1:A:342:LYS:HE2	2.02	0.41
1:A:777:ALA:O	1:A:781:MET:HG2	2.21	0.40
1:A:112:GLN:O	1:A:112:GLN:CG	2.70	0.40
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.86	0.40
1:A:38:ILE:HD13	1:A:672:VAL:CG2	2.51	0.40
1:A:564:LEU:HB3	1:A:671:ILE:HG23	2.03	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	998/1049 (95%)	782 (78%)	149 (15%)	67 (7%)	1 25

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE

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Mol	Chain	Res	Type
1	A	134	SER
1	A	255	GLN
1	A	327	TYR
1	A	431	THR
1	A	459	PHE
1	A	526	HIS
1	A	665	ALA
1	A	671	ILE
1	A	714	THR
1	A	872	GLN
1	A	900	SER
1	A	901	VAL
1	A	955	LYS
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	1034	SER
1	A	9	PRO
1	A	105	VAL
1	A	135	SER
1	A	152	GLU
1	A	161	ASN
1	A	197	GLN
1	A	295	THR
1	A	410	ILE
1	A	427	PRO
1	A	521	GLU
1	A	522	LYS
1	A	571	VAL
1	A	610	PHE
1	A	723	ASP
1	A	775	SER
1	A	794	ALA
1	A	940	LYS
1	A	1027	VAL
1	A	74	ASN
1	A	169	THR
1	A	184	MET
1	A	209	ALA
1	A	366	LEU
1	A	421	ALA

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Mol	Chain	Res	Type
1	A	472	ILE
1	A	538	THR
1	A	720	GLY
1	A	722	GLU
1	A	894	SER
1	A	971	ARG
1	A	430	ALA
1	A	466	ILE
1	A	468	ARG
1	A	490	PRO
1	A	525	HIS
1	A	638	PRO
1	A	1028	VAL
1	A	224	PRO
1	A	677	ALA
1	A	837	THR
1	A	34	GLN
1	A	299	ALA
1	A	217	GLY
1	A	626	ILE
1	A	223	PRO
1	A	464	GLY
1	A	669	PRO
1	A	326	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	818/855 (96%)	634 (78%)	184 (22%)	1	9

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE

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Mol	Chain	Res	Type
1	A	25	LEU
1	A	29	LYS
1	A	32	VAL
1	A	35	TYR
1	A	38	ILE
1	A	46	SER
1	A	48	SER
1	A	55	LYS
1	A	58	GLN
1	A	67	GLN
1	A	68	ASN
1	A	69	MET
1	A	75	LEU
1	A	76	MET
1	A	82	SER
1	A	87	THR
1	A	95	GLU
1	A	107	VAL
1	A	108	GLN
1	A	110	LYS
1	A	111	LEU
1	A	112	GLN
1	A	117	LEU
1	A	125	GLN
1	A	130	GLU
1	A	131	LYS
1	A	132	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET
1	A	155	SER
1	A	156	ASP
1	A	158	VAL
1	A	164	ASP
1	A	174	ASP
1	A	177	LEU
1	A	185	ARG
1	A	195	LYS
1	A	199	THR
1	A	207	ILE
1	A	210	GLN
1	A	213	GLN

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Mol	Chain	Res	Type
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	235	ILE
1	A	238	THR
1	A	239	ARG
1	A	240	LEU
1	A	242	SER
1	A	252	LYS
1	A	253	VAL
1	A	255	GLN
1	A	259	ARG
1	A	278	ILE
1	A	292	LYS
1	A	293	LEU
1	A	310	LEU
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	323	ILE
1	A	327	TYR
1	A	329	THR
1	A	334	LYS
1	A	342	LYS
1	A	350	LEU
1	A	351	VAL
1	A	355	MET
1	A	357	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU
1	A	367	ILE
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	414	GLU
1	A	417	GLU
1	A	422	GLU
1	A	428	LYS
1	A	431	THR
1	A	433	LYS
1	A	435	MET

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Mol	Chain	Res	Type
1	A	445	ILE
1	A	448	VAL
1	A	453	PHE
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	471	SER
1	A	478	MET
1	A	486	LEU
1	A	487	ILE
1	A	492	LEU
1	A	498	LYS
1	A	519	MET
1	A	537	SER
1	A	538	THR
1	A	552	MET
1	A	555	LEU
1	A	558	ARG
1	A	574	THR
1	A	583	THR
1	A	585	GLU
1	A	595	THR
1	A	596	HIS
1	A	602	GLU
1	A	607	GLU
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	620	ARG
1	A	622	GLN
1	A	632	LYS
1	A	637	ARG
1	A	640	GLU
1	A	643	LYS
1	A	650	ARG
1	A	657	GLN
1	A	659	LYS
1	A	671	ILE
1	A	680	PHE
1	A	683	GLU
1	A	686	ASP
1	A	687	GLN

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Mol	Chain	Res	Type
1	A	693	GLU
1	A	699	ARG
1	A	714	THR
1	A	721	LEU
1	A	726	GLN
1	A	728	LYS
1	A	735	LYS
1	A	737	GLN
1	A	739	LEU
1	A	741	VAL
1	A	742	SER
1	A	749	THR
1	A	770	LYS
1	A	774	MET
1	A	782	LEU
1	A	797	GLN
1	A	798	MET
1	A	801	PHE
1	A	804	PHE
1	A	807	SER
1	A	811	TYR
1	A	815	ARG
1	A	818	ARG
1	A	824	SER
1	A	826	GLU
1	A	844	MET
1	A	846	GLN
1	A	872	GLN
1	A	888	LEU
1	A	895	TRP
1	A	901	VAL
1	A	904	VAL
1	A	907	LEU
1	A	919	ARG
1	A	925	VAL
1	A	934	THR
1	A	938	SER
1	A	944	LEU
1	A	945	ILE
1	A	950	LYS
1	A	971	ARG
1	A	972	LEU

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Mol	Chain	Res	Type
1	A	976	LEU
1	A	990	VAL
1	A	991	ILE
1	A	1008	MET
1	A	1020	PHE
1	A	1022	VAL
1	A	1024	VAL
1	A	1025	PHE
1	A	1028	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG
1	A	1036	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	124	GLN
1	A	161	ASN
1	A	181	GLN
1	A	194	ASN
1	A	228	GLN
1	A	231	ASN
1	A	338	HIS
1	A	391	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	642	ASN
1	A	657	GLN
1	A	667	ASN
1	A	760	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)

1 ligand is 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	15 (57%)	33,39,39	1.66	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 Torsion 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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	ET	C6-C11	-2.77	1.38	1.43
2	A	3001	ET	C10-C12	2.08	1.45	1.41
2	A	3001	ET	C19-C20	2.19	1.43	1.38
2	A	3001	ET	C13-C14	2.21	1.45	1.41
2	A	3001	ET	C10-C9	2.44	1.41	1.36
2	A	3001	ET	C4-C3	3.02	1.44	1.39
2	A	3001	ET	C7-C11	3.24	1.48	1.42
2	A	3001	ET	C14-N5	3.58	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	ET	C11-C12	3.85	1.48	1.42
2	A	3001	ET	C1-C13	4.11	1.49	1.41
2	A	3001	ET	C20-C15	4.21	1.48	1.39
2	A	3001	ET	C16-C15	4.35	1.48	1.39
2	A	3001	ET	C4-C14	4.56	1.50	1.40
2	A	3001	ET	C15-C6	6.31	1.57	1.48
2	A	3001	ET	C6-N5	11.46	1.59	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3001	ET	C11-C6-N5	-3.19	114.84	119.47
2	A	3001	ET	C20-C15-C16	-2.68	112.49	117.55
2	A	3001	ET	C19-C20-C15	2.33	123.64	120.56
2	A	3001	ET	C8-C7-C11	2.66	123.71	120.81
2	A	3001	ET	C20-C15-C6	3.49	126.11	120.19
2	A	3001	ET	C6-C11-C12	5.07	125.36	117.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9
1	A	1006/1049 (95%)	0.15	39 (3%)	43	29	115, 152, 166, 182	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	PHE	6.8
1	A	403	GLY	5.9
1	A	679	GLY	5.0
1	A	678	THR	4.8
1	A	497	LEU	4.5
1	A	402	ILE	4.4
1	A	460	GLY	4.4
1	A	676	THR	4.0
1	A	461	GLY	4.0
1	A	563	PHE	3.9
1	A	401	ALA	3.7
1	A	992	SER	3.3
1	A	303	ALA	3.1
1	A	406	VAL	3.0
1	A	525	HIS	3.0
1	A	712	MET	2.9
1	A	896	SER	2.9
1	A	719	ASN	2.9
1	A	673	GLU	2.7
1	A	252	LYS	2.7
1	A	1020	PHE	2.7
1	A	517	ASN	2.7
1	A	938	SER	2.5
1	A	671	ILE	2.5
1	A	379	THR	2.5
1	A	425	LEU	2.4
1	A	437	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	855	VAL	2.4
1	A	960	LEU	2.3
1	A	470	PHE	2.3
1	A	410	ILE	2.3
1	A	828	LEU	2.3
1	A	407	ASP	2.2
1	A	829	GLY	2.2
1	A	680	PHE	2.2
1	A	869	SER	2.2
1	A	705	GLU	2.2
1	A	709	HIS	2.1
1	A	174	ASP	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
2	ET	A	3001	24/24	0.68	0.26	-	194,216,226,229	0

6.5 Other polymers (i)

There are no such residues in this entry.