



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:10 PM UTC

PDB ID : 1OY9 / pdb_00001oy9
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)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

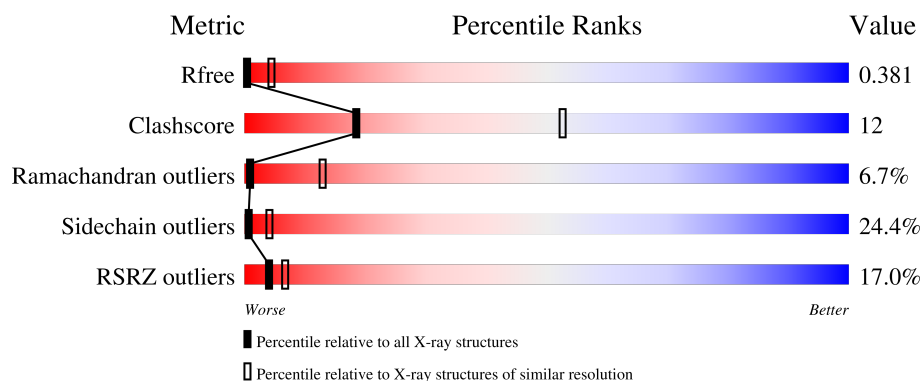
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	1049	16% 58% 29% 8% ••

2 Entry composition [i](#)

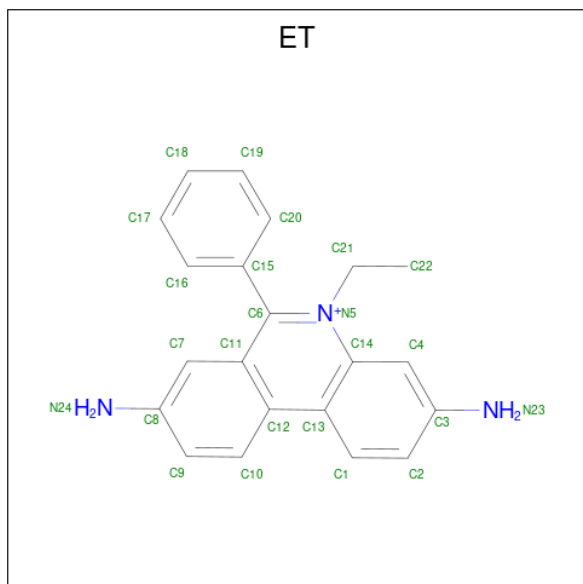
There are 2 unique types of molecules in this entry. The entry contains 7663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: ET) (formula: $C_{21}H_{20}N_3$).

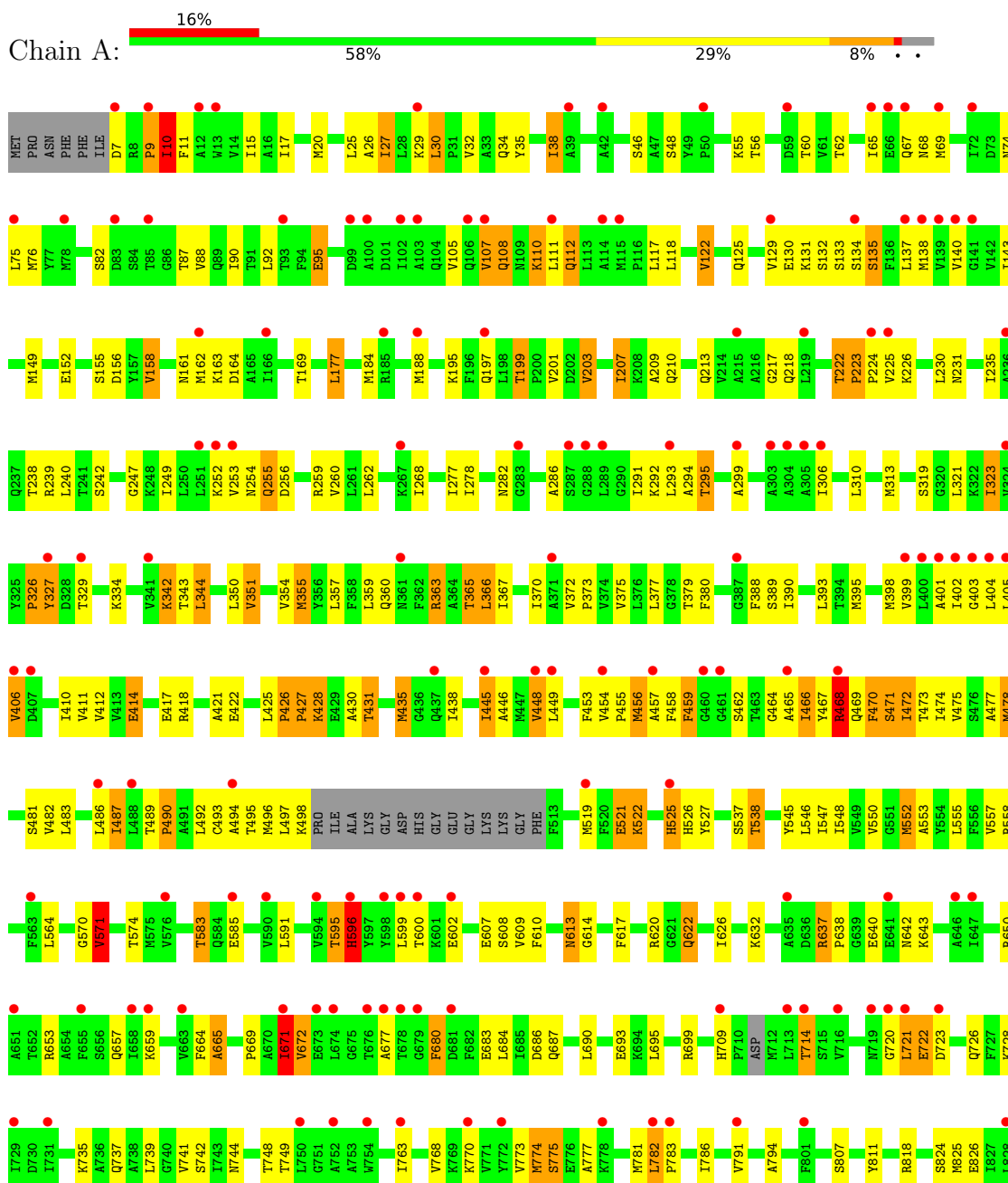


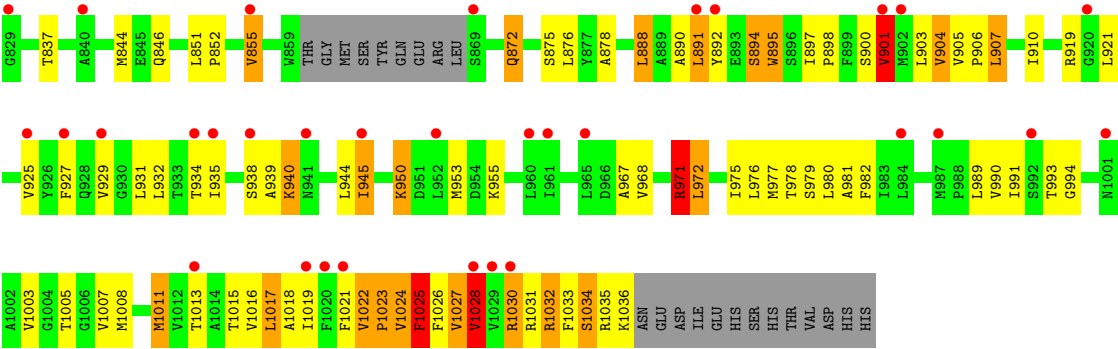
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	24	21	3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

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 46.60 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.80) 98.8 (46.60-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.283 , 0.344 0.381 , 0.381	Depositor DCC
R_{free} test set	1562 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	142.8	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 106.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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.

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	0.70	5/7779 (0.1%)	0.90	9/10563 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	596	HIS	CG-CD2	27.61	1.66	1.35
1	A	596	HIS	CE1-NE2	19.78	1.52	1.32
1	A	596	HIS	CG-ND1	14.38	1.54	1.38
1	A	596	HIS	ND1-CE1	13.76	1.46	1.32
1	A	596	HIS	CD2-NE2	8.12	1.46	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	PHE	N-CA-C	14.20	128.15	111.11
1	A	680	PHE	N-CA-C	10.57	125.98	109.81
1	A	596	HIS	CG-CD2-NE2	-9.42	97.78	107.20
1	A	672	VAL	CB-CA-C	8.27	122.69	111.28
1	A	596	HIS	ND1-CG-CD2	7.56	113.66	106.10
1	A	426	PRO	N-CA-C	6.97	119.21	110.70
1	A	672	VAL	N-CA-C	6.21	118.06	109.80
1	A	110	LYS	N-CA-C	-5.46	108.39	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	HIS	CB-CG-CD2	-5.16	124.50	131.20

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 ⓘ

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	186	0
2	A	24	0	20	0	0
All	All	7663	0	7820	186	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 12.

All (186) 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	0.86
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:O	1:A:365:THR:HG23	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:1023:PRO:HA	1:A:1026:PHE:HB2	1.80	0.63
1:A:613:ASN:C	1:A:613:ASN:ND2	2.47	0.63
1:A:291:ILE:HG21	1:A:306:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:A:709:HIS:O	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:359:LEU:HD21	1:A:977:MET:HE1	1.85	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
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:370:ILE:HG22	1:A:370:ILE:O	2.05	0.57
1:A:967:ALA:O	1:A:971:ARG:HG3	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:326:PRO:O	1:A:327:TYR:C	2.49	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:379:THR:HB	1:A:398:MET:HE1	1.89	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:294:ALA:O	1:A:295:THR:C	2.51	0.53
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.92	0.52
1:A:472:ILE:HA	1:A:475:VAL:HB	1.91	0.52
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.90	0.52
1:A:428:LYS:HZ2	1:A:494:ALA:HB1	1.74	0.52
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.91	0.51
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.92	0.51
1:A:363:ARG:HB2	1:A:496:MET:SD	2.51	0.51
1:A:475:VAL:HA	1:A:478:MET:HE2	1.92	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: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:425:LEU:C	1:A:427:PRO:HD2	2.37	0.49
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.46	0.49
1:A:380:PHE:CE2	1:A:398:MET:HE2	2.47	0.49
1:A:456:MET:O	1:A:876:LEU:HD13	2.12	0.49
1:A:56:THR:O	1:A:60:THR:HG22	2.13	0.49
1:A:372:VAL:HG12	1:A:405:LEU:HB3	1.93	0.49
1:A:1035:ARG:HD3	1:A:1035:ARG:H	1.78	0.49
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:38:ILE:HD13	1:A:672:VAL:HG21	1.93	0.48
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.42	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:426:PRO:N	1:A:427:PRO:HD2	2.28	0.48
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.96	0.48
1:A:521:GLU:O	1:A:522:LYS:C	2.57	0.48
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.48	0.48
1:A:1032:ARG:HH11	1:A:1032:ARG:HG2	1.78	0.48
1:A:890:ALA:C	1:A:891:LEU:HD22	2.39	0.47
1:A:1022:VAL:O	1:A:1023:PRO:O	2.32	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:95:GLU:OE1	1:A:95:GLU:CA	2.62	0.47
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ALA:HA	1:A:468:ARG:HB3	1.96	0.47
1:A:1026:PHE:O	1:A:1030:ARG:HG2	2.14	0.47
1:A:163:LYS:HD2	1:A:177:LEU:HD23	1.97	0.47
1:A:310:LEU:HD21	1:A:323:ILE:HD12	1.97	0.47
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.45	0.47
1:A:414:GLU:CD	1:A:414:GLU:C	2.83	0.47
1:A:971:ARG:HD2	1:A:971:ARG:C	2.40	0.47
1:A:855:VAL:HG12	1:A:855:VAL:O	2.14	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:1033:PHE:O	1:A:1034:SER:C	2.58	0.45
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:26:ALA:O	1:A:30:LEU:HB2	2.17	0.45
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.97	0.45
1:A:112:GLN:HG2	1:A:112:GLN:O	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:342:LYS:CE	1:A:342:LYS:HA	2.47	0.44
1:A:469:GLN:HA	1:A:472:ILE:CG2	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
1:A:158:VAL:HG22	1:A:162:MET:HE3	2.00	0.44
1:A:472:ILE:O	1:A:473:THR:C	2.61	0.44
1:A:90:ILE:N	1:A:90:ILE:HD12	2.33	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:527:TYR:OH	1:A:1019:ILE:HG13	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD22	1:A:470:PHE:CD2	2.54	0.43
1:A:684:LEU:HG	1:A:695:LEU:HD21	2.01	0.43
1:A:388:PHE:N	1:A:388:PHE:CD2	2.87	0.43
1:A:1022:VAL:CG2	1:A:1023:PRO:HD2	2.41	0.43
1:A:474:ILE:HA	1:A:477:ALA:HB3	2.01	0.43
1:A:203:VAL:O	1:A:207:ILE:HG13	2.19	0.42
1:A:344:LEU:HD23	1:A:402:ILE:HD11	2.01	0.42
1:A:188:MET:HE2	1:A:773:VAL:HG22	2.01	0.42
1:A:470:PHE:CD1	1:A:929:VAL:HG11	2.54	0.42
1:A:27:ILE:CD1	1:A:390:ILE:HD11	2.49	0.42
1:A:695:LEU:HD22	1:A:825:MET:SD	2.60	0.42
1:A:891:LEU:HD22	1:A:891:LEU:N	2.34	0.42
1:A:254:ASN:O	1:A:256:ASP:N	2.52	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:1003:VAL:O	1:A:1007:VAL:HG23	2.20	0.42
1:A:721:LEU:HD22	1:A:825:MET:HE2	2.01	0.42
1:A:475:VAL:HG22	1:A:478:MET:CE	2.49	0.42
1:A:939:ALA:O	1:A:940:LYS:C	2.62	0.42
1:A:493:CYS:O	1:A:497:LEU:HB2	2.20	0.41
1:A:553:ALA:O	1:A:557:VAL:HG23	2.20	0.41
1:A:875:SER:O	1:A:878:ALA:HB3	2.20	0.41
1:A:950:LYS:HA	1:A:953:MET:HB3	2.01	0.41
1:A:9:PRO:HB3	1:A:495:THR:OG1	2.20	0.41
1:A:95:GLU:OE1	1:A:95:GLU:N	2.52	0.41
1:A:344:LEU:C	1:A:344:LEU:HD13	2.46	0.41
1:A:401:ALA:O	1:A:405:LEU:HG	2.20	0.41
1:A:546:LEU:O	1:A:550:VAL:HG23	2.20	0.41
1:A:921:LEU:CD2	1:A:1005:THR:HG21	2.48	0.41
1:A:445:ILE:O	1:A:449:LEU:HG	2.20	0.41
1:A:466:ILE:HG22	1:A:467:TYR:N	2.35	0.41
1:A:552:MET:HG3	1:A:910:ILE:HB	2.01	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:1027:VAL:O	1:A:1028:VAL:C	2.63	0.41
1:A:851:LEU:HB3	1:A:852:PRO:HD2	2.03	0.41
1:A:412:VAL:HG13	1:A:435:MET:HE1	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:199:THR:HG21	1:A:791:VAL:HG13	2.03	0.41
1:A:388:PHE:HE1	1:A:472:ILE:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:MET:HA	1:A:438:ILE:HB	2.01	0.41
1:A:971:ARG:HD2	1:A:971:ARG:O	2.20	0.41
1:A:342:LYS:HA	1:A:342:LYS:HE2	2.02	0.41
1:A:888:LEU:HD13	1:A:897:ILE:HG22	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:9:PRO:O	1:A:10:ILE:C	2.64	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	13

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	618 (76%)	200 (24%)	1 4

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE
1	A	15	ILE
1	A	17	ILE
1	A	25	LEU
1	A	27	ILE
1	A	29	LYS
1	A	30	LEU
1	A	32	VAL
1	A	35	TYR
1	A	38	ILE
1	A	46	SER

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Mol	Chain	Res	Type
1	A	48	SER
1	A	55	LYS
1	A	65	ILE
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	122	VAL
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	140	VAL
1	A	149	MET
1	A	155	SER
1	A	156	ASP
1	A	158	VAL
1	A	164	ASP
1	A	177	LEU
1	A	195	LYS
1	A	199	THR
1	A	203	VAL
1	A	207	ILE
1	A	210	GLN
1	A	213	GLN
1	A	222	THR
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	235	ILE

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Mol	Chain	Res	Type
1	A	238	THR
1	A	239	ARG
1	A	240	LEU
1	A	242	SER
1	A	249	ILE
1	A	252	LYS
1	A	253	VAL
1	A	255	GLN
1	A	259	ARG
1	A	260	VAL
1	A	277	ILE
1	A	278	ILE
1	A	292	LYS
1	A	293	LEU
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	323	ILE
1	A	329	THR
1	A	334	LYS
1	A	342	LYS
1	A	344	LEU
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	365	THR
1	A	366	LEU
1	A	367	ILE
1	A	389	SER
1	A	404	LEU
1	A	406	VAL
1	A	411	VAL
1	A	414	GLU
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	428	LYS
1	A	431	THR
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	462	SER
1	A	468	ARG
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	547	ILE
1	A	552	MET
1	A	555	LEU
1	A	558	ARG
1	A	571	VAL
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	653	ARG
1	A	657	GLN
1	A	659	LYS
1	A	671	ILE
1	A	680	PHE

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Mol	Chain	Res	Type
1	A	683	GLU
1	A	686	ASP
1	A	687	GLN
1	A	690	LEU
1	A	693	GLU
1	A	699	ARG
1	A	714	THR
1	A	721	LEU
1	A	722	GLU
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	763	ILE
1	A	768	VAL
1	A	770	LYS
1	A	774	MET
1	A	782	LEU
1	A	786	ILE
1	A	807	SER
1	A	811	TYR
1	A	818	ARG
1	A	824	SER
1	A	826	GLU
1	A	844	MET
1	A	846	GLN
1	A	855	VAL
1	A	872	GLN
1	A	888	LEU
1	A	891	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	935	ILE

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Mol	Chain	Res	Type
1	A	938	SER
1	A	944	LEU
1	A	945	ILE
1	A	950	LYS
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	978	THR
1	A	990	VAL
1	A	991	ILE
1	A	1008	MET
1	A	1011	MET
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	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	68	ASN
1	A	108	GLN
1	A	109	ASN
1	A	112	GLN
1	A	123	GLN
1	A	124	GLN
1	A	181	GLN
1	A	194	ASN
1	A	197	GLN
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	282	ASN
1	A	284	GLN
1	A	338	HIS
1	A	391	ASN
1	A	569	GLN

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Mol	Chain	Res	Type
1	A	588	GLN
1	A	613	ASN
1	A	622	GLN
1	A	642	ASN
1	A	657	GLN
1	A	667	ASN
1	A	700	ASN
1	A	709	HIS
1	A	760	ASN
1	A	923	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3.10	16 (61%)	35,39,39	2.82	9 (25%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	ET	C15-C6	7.66	1.57	1.49
2	A	3001	ET	C4-C14	5.17	1.50	1.40
2	A	3001	ET	C16-C15	4.65	1.48	1.39
2	A	3001	ET	C20-C15	4.50	1.48	1.39
2	A	3001	ET	C1-C13	4.09	1.49	1.41
2	A	3001	ET	C14-N5	3.91	1.45	1.40
2	A	3001	ET	C4-C3	3.54	1.44	1.39
2	A	3001	ET	C11-C12	3.51	1.48	1.42
2	A	3001	ET	C7-C11	3.22	1.48	1.42
2	A	3001	ET	C6-C11	-2.75	1.38	1.43
2	A	3001	ET	C19-C20	2.63	1.43	1.38
2	A	3001	ET	C17-C16	2.35	1.42	1.38
2	A	3001	ET	C10-C9	2.35	1.41	1.36
2	A	3001	ET	C19-C18	2.08	1.42	1.38
2	A	3001	ET	C10-C12	2.05	1.45	1.41
2	A	3001	ET	C13-C14	2.01	1.45	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	ET	C21-N5-C14	8.89	124.65	118.31
2	A	3001	ET	C21-N5-C6	-8.58	114.38	119.47
2	A	3001	ET	C6-C11-C12	6.38	125.36	118.81
2	A	3001	ET	C20-C15-C6	4.23	126.11	120.25
2	A	3001	ET	C7-C11-C6	-3.67	115.87	122.66
2	A	3001	ET	C13-C14-N5	3.10	120.46	118.46
2	A	3001	ET	C20-C15-C16	-2.90	112.49	117.68
2	A	3001	ET	C19-C20-C15	2.73	123.64	120.54
2	A	3001	ET	C17-C16-C15	2.10	122.93	120.54

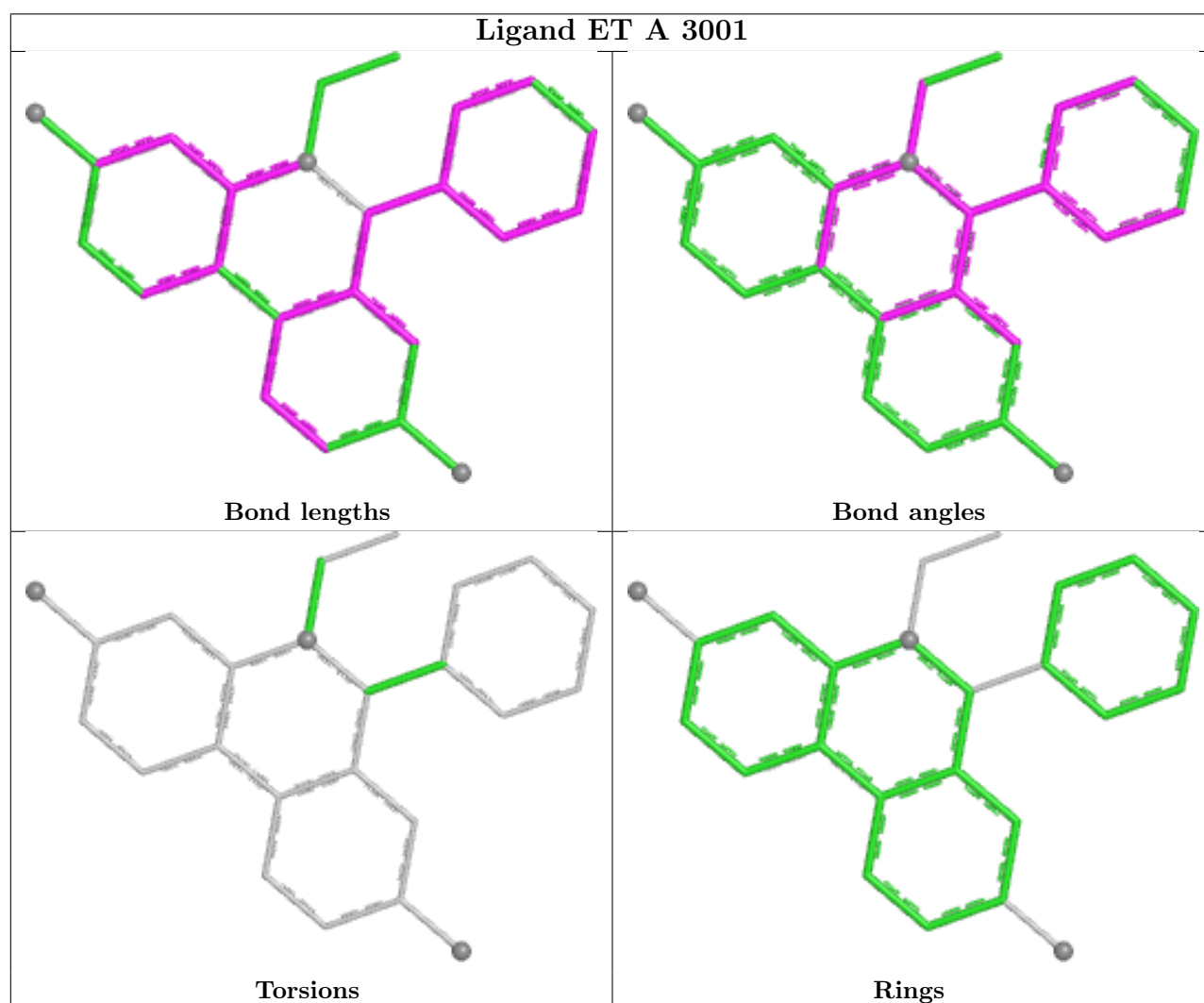
There are no chirality outliers.

There are no torsion outliers.

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 than 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.



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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1006/1049 (95%)	1.15	171 (16%) 4 7	115, 152, 166, 182	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	GLY	7.9
1	A	401	ALA	6.6
1	A	134	SER	6.5
1	A	111	LEU	5.9
1	A	935	ILE	5.9
1	A	402	ILE	5.9
1	A	99	ASP	5.7
1	A	960	LEU	5.4
1	A	600	THR	5.1
1	A	303	ALA	5.1
1	A	772	TYR	5.0
1	A	1021	PHE	4.9
1	A	399	VAL	4.8
1	A	671	ILE	4.8
1	A	563	PHE	4.7
1	A	461	GLY	4.7
1	A	107	VAL	4.5
1	A	778	LYS	4.3
1	A	215	ALA	4.2
1	A	585	GLU	4.1
1	A	599	LEU	4.1
1	A	676	THR	4.0
1	A	782	LEU	4.0
1	A	404	LEU	3.9
1	A	449	LEU	3.8
1	A	721	LEU	3.8
1	A	714	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	723	ASP	3.7
1	A	400	LEU	3.6
1	A	50	PRO	3.6
1	A	519	MET	3.5
1	A	299	ALA	3.5
1	A	658	ILE	3.5
1	A	283	GLY	3.4
1	A	103	ALA	3.4
1	A	78	MET	3.4
1	A	100	ALA	3.4
1	A	938	SER	3.3
1	A	709	HIS	3.3
1	A	720	GLY	3.3
1	A	829	GLY	3.3
1	A	252	LYS	3.3
1	A	405	LEU	3.2
1	A	42	ALA	3.2
1	A	457	ALA	3.2
1	A	596	HIS	3.2
1	A	102	ILE	3.1
1	A	678	THR	3.1
1	A	236	ALA	3.1
1	A	448	VAL	3.1
1	A	855	VAL	3.1
1	A	674	LEU	3.1
1	A	445	ILE	3.1
1	A	952	LEU	3.1
1	A	65	ILE	3.0
1	A	655	PHE	2.9
1	A	460	GLY	2.9
1	A	659	LYS	2.9
1	A	251	LEU	2.9
1	A	752	ALA	2.8
1	A	69	MET	2.8
1	A	961	ILE	2.8
1	A	13	TRP	2.8
1	A	406	VAL	2.8
1	A	494	ALA	2.8
1	A	83	ASP	2.8
1	A	992	SER	2.8
1	A	267	LYS	2.8
1	A	289	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	361	ASN	2.8
1	A	59	ASP	2.7
1	A	454	VAL	2.7
1	A	1030	ARG	2.7
1	A	754	TRP	2.7
1	A	140	VAL	2.7
1	A	576	VAL	2.7
1	A	783	PRO	2.7
1	A	801	PHE	2.7
1	A	141	GLY	2.7
1	A	488	LEU	2.7
1	A	929	VAL	2.7
1	A	677	ALA	2.7
1	A	840	ALA	2.7
1	A	602	GLU	2.7
1	A	750	LEU	2.7
1	A	486	LEU	2.7
1	A	306	ILE	2.6
1	A	304	ALA	2.6
1	A	29	LYS	2.6
1	A	987	MET	2.6
1	A	93	THR	2.6
1	A	185	ARG	2.6
1	A	197	GLN	2.6
1	A	651	ALA	2.6
1	A	902	MET	2.6
1	A	341	VAL	2.6
1	A	828	LEU	2.6
1	A	598	TYR	2.5
1	A	719	ASN	2.5
1	A	1020	PHE	2.5
1	A	525	HIS	2.5
1	A	85	THR	2.5
1	A	137	LEU	2.5
1	A	869	SER	2.5
1	A	106	GLN	2.5
1	A	731	ILE	2.5
1	A	663	VAL	2.5
1	A	941	ASN	2.5
1	A	673	GLU	2.4
1	A	729	ILE	2.4
1	A	791	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	934	THR	2.4
1	A	219	LEU	2.4
1	A	371	ALA	2.4
1	A	927	PHE	2.4
1	A	594	VAL	2.4
1	A	984	LEU	2.4
1	A	188	MET	2.4
1	A	139	VAL	2.4
1	A	901	VAL	2.4
1	A	7	ASP	2.4
1	A	162	MET	2.4
1	A	387	GLY	2.3
1	A	647	ILE	2.3
1	A	1028	VAL	2.3
1	A	305	ALA	2.3
1	A	114	ALA	2.3
1	A	646	ALA	2.3
1	A	679	GLY	2.3
1	A	770	LYS	2.3
1	A	945	ILE	2.3
1	A	465	ALA	2.2
1	A	892	TYR	2.2
1	A	138	MET	2.2
1	A	763	ILE	2.2
1	A	965	LEU	2.2
1	A	9	PRO	2.2
1	A	329	THR	2.2
1	A	39	ALA	2.2
1	A	1019	ILE	2.2
1	A	66	GLU	2.2
1	A	407	ASP	2.1
1	A	293	LEU	2.1
1	A	716	VAL	2.1
1	A	288	GLY	2.1
1	A	468	ARG	2.1
1	A	1001	ASN	2.1
1	A	324	VAL	2.1
1	A	327	TYR	2.1
1	A	224	PRO	2.1
1	A	641	GLU	2.1
1	A	287	SER	2.1
1	A	67	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	2.1
1	A	590	VAL	2.1
1	A	925	VAL	2.1
1	A	920	GLY	2.1
1	A	72	ILE	2.1
1	A	635	ALA	2.1
1	A	891	LEU	2.1
1	A	681	ASP	2.1
1	A	166	ILE	2.1
1	A	129	VAL	2.1
1	A	253	VAL	2.1
1	A	1029	VAL	2.1
1	A	115	MET	2.1
1	A	75	LEU	2.0
1	A	713	LEU	2.0
1	A	437	GLN	2.0
1	A	1013	THR	2.0
1	A	12	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

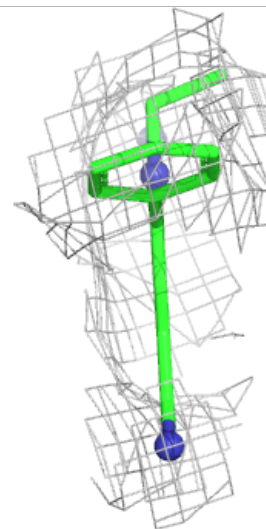
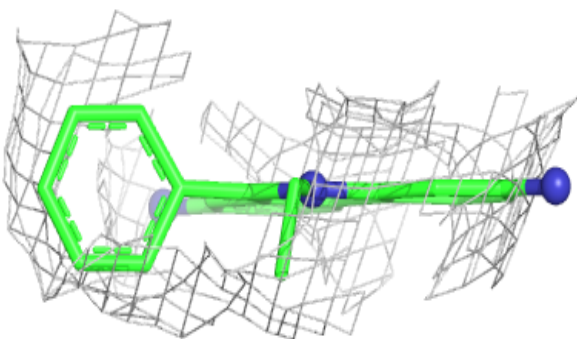
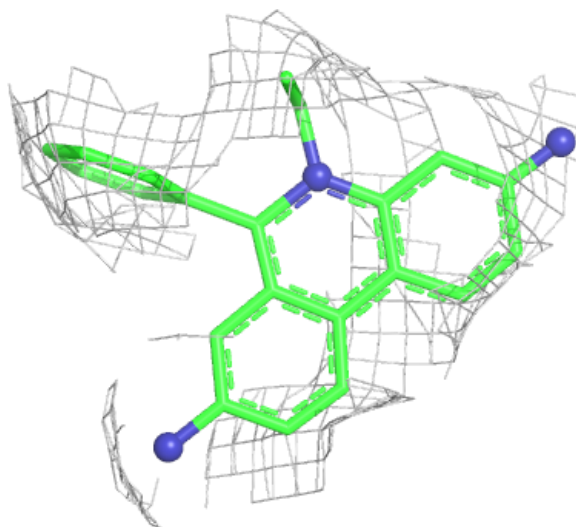
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ET	A	3001	24/24	0.73	0.14	194,216,226,229	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ET A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.