



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:06 AM UTC

PDB ID : 1T9U / pdb_00001t9u
Title : Structural Basis of Multidrug Transport by the AcrB Multidrug Efflux Pump
Authors : Yu, E.W.; McDermott, G.; Nikaido, H.
Deposited on : 2004-05-18
Resolution : 3.11 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

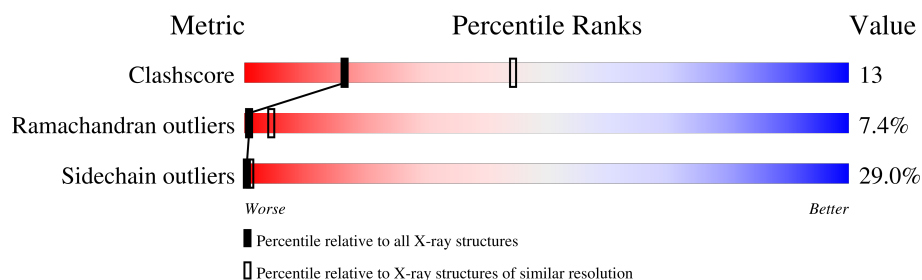
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1049	55% 31% 9% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CPF	A	5002	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7739 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.

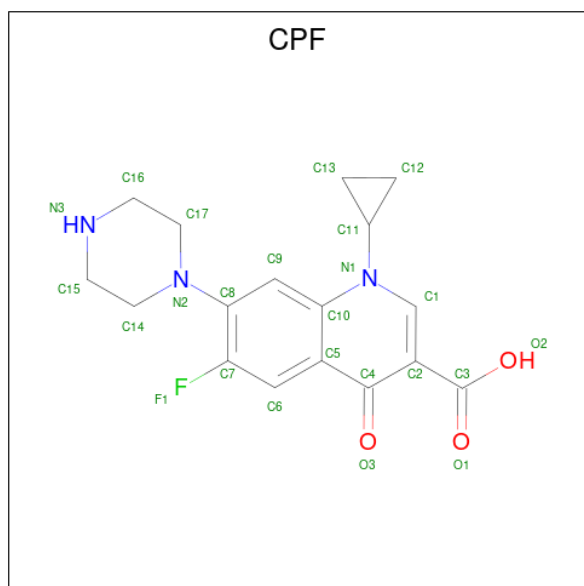
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1013	Total	C	N	O	S	0	0	0
			7691	4946	1272	1431	42			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: $C_{17}H_{18}FN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		
2	A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	TLE	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS
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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, α , β , γ	144.09Å 144.09Å 518.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.11	Depositor
% Data completeness (in resolution range)	(Not available) (182.57-3.11)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.265 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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: CPF

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	0.54	3/7830 (0.0%)	0.89	5/10630 (0.0%)

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	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	667	ASN	CG-OD1	5.32	1.33	1.23
1	A	367	ILE	CA-CB	5.29	1.57	1.54
1	A	577	GLN	CD-OE1	5.26	1.33	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ILE	N-CA-C	8.06	124.11	113.07
1	A	722	GLU	N-CA-C	7.86	127.53	110.80
1	A	426	PRO	N-CA-C	7.68	120.07	110.70
1	A	954	ASP	N-CA-C	6.37	124.37	110.80
1	A	1020	PHE	N-CA-C	5.27	114.79	107.73

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	722	GLU	CA

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Mol	Chain	Res	Type	Atom
1	A	954	ASP	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	HIS	Peptide
1	A	712	MET	Peptide
1	A	864	TYR	Peptide
1	A	867	ARG	Peptide

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	7691	0	7851	201	0
2	A	48	0	34	11	0
All	All	7739	0	7885	201	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 13.

All (201) 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:830:GLN:NE2	2:A:5002:CPF:C12	2.01	1.24
1:A:830:GLN:NE2	2:A:5002:CPF:H121	1.53	1.22
1:A:830:GLN:HE22	2:A:5002:CPF:C12	1.59	1.09
1:A:667:ASN:OD1	2:A:5002:CPF:H152	1.53	1.06
1:A:830:GLN:HE22	2:A:5002:CPF:H121	0.80	0.96
1:A:667:ASN:OD1	2:A:5002:CPF:C15	2.19	0.90
1:A:950:LYS:NZ	1:A:1028:VAL:HG11	1.94	0.83
1:A:525:HIS:HB2	1:A:526:HIS:HB2	1.65	0.78
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.65	0.78
1:A:471:SER:O	1:A:473:THR:N	2.20	0.74
1:A:830:GLN:NE2	2:A:5002:CPF:H122	2.04	0.73
1:A:830:GLN:CD	2:A:5002:CPF:C12	2.65	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:GLN:CD	2:A:5002:CPF:H122	2.17	0.68
1:A:987:MET:HE2	1:A:1008:MET:HE3	1.76	0.68
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.76	0.67
1:A:475:VAL:HG13	1:A:478:MET:HE2	1.75	0.67
1:A:990:VAL:HG21	1:A:1008:MET:SD	2.36	0.65
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.78	0.65
1:A:380:PHE:CE2	1:A:398:MET:HE2	2.32	0.64
1:A:892:TYR:CD2	1:A:897:ILE:HG21	2.33	0.64
1:A:950:LYS:HZ3	1:A:1028:VAL:HG11	1.62	0.64
1:A:459:PHE:CD1	1:A:468:ARG:HG3	2.33	0.64
1:A:950:LYS:HZ2	1:A:1028:VAL:HG11	1.60	0.63
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.81	0.63
1:A:681:ASP:O	1:A:860:THR:O	2.16	0.63
1:A:33:ALA:O	1:A:34:GLN:O	2.16	0.63
1:A:365:THR:O	1:A:365:THR:HG23	1.97	0.62
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.82	0.61
1:A:400:LEU:HD11	1:A:933:THR:HG21	1.82	0.61
1:A:709:HIS:CD2	1:A:709:HIS:O	2.55	0.60
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.56	0.59
1:A:525:HIS:HB2	1:A:526:HIS:CB	2.31	0.59
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.86	0.57
1:A:372:VAL:H	1:A:373:PRO:HD2	1.69	0.57
1:A:117:LEU:HD23	1:A:117:LEU:N	2.20	0.57
1:A:425:LEU:C	1:A:427:PRO:HD2	2.29	0.57
1:A:10:ILE:CD1	1:A:10:ILE:N	2.68	0.56
1:A:379:THR:HG22	1:A:398:MET:HE1	1.86	0.56
1:A:397:GLY:O	1:A:401:ALA:HB2	2.06	0.55
1:A:525:HIS:CB	1:A:526:HIS:HB2	2.34	0.55
1:A:527:TYR:O	1:A:531:VAL:HG23	2.06	0.55
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.89	0.55
1:A:971:ARG:HD2	1:A:971:ARG:C	2.32	0.55
1:A:717:ARG:HD2	1:A:719:ASN:HD21	1.72	0.55
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.07	0.55
1:A:188:MET:HE1	1:A:200:PRO:HB3	1.90	0.54
1:A:21:LEU:O	1:A:23:GLY:N	2.41	0.54
1:A:55:LYS:HD2	1:A:816:LEU:HD11	1.89	0.54
1:A:721:LEU:HD22	1:A:825:MET:HE2	1.89	0.54
1:A:525:HIS:HB2	1:A:526:HIS:CG	2.43	0.53
1:A:1032:ARG:CG	1:A:1032:ARG:HH11	2.20	0.53
1:A:463:THR:HG23	1:A:466:ILE:HG21	1.91	0.52
1:A:613:ASN:HD22	1:A:613:ASN:C	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.91	0.52
1:A:158:VAL:HG22	1:A:162:MET:HE2	1.91	0.52
1:A:366:LEU:O	1:A:370:ILE:HG13	2.09	0.52
1:A:872:GLN:HG2	1:A:876:LEU:HD11	1.91	0.52
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.90	0.52
1:A:90:ILE:N	1:A:90:ILE:HD12	2.24	0.52
1:A:349:ILE:HG22	1:A:350:LEU:HD23	1.91	0.52
1:A:376:LEU:HD23	1:A:398:MET:HE3	1.90	0.52
1:A:894:SER:O	1:A:895:TRP:CE3	2.63	0.51
1:A:881:LEU:HD13	1:A:902:MET:CE	2.40	0.51
1:A:710:PRO:HB2	1:A:713:LEU:CB	2.40	0.51
1:A:897:ILE:O	1:A:900:SER:OG	2.23	0.51
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.58	0.51
1:A:870:GLY:O	1:A:872:GLN:N	2.43	0.51
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.93	0.51
1:A:9:PRO:HA	1:A:491:ALA:HB1	1.92	0.51
1:A:923:ASN:C	1:A:923:ASN:HD22	2.19	0.51
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.41	0.51
1:A:10:ILE:HD13	1:A:11:PHE:H	1.77	0.50
1:A:905:VAL:HG12	1:A:935:ILE:HG12	1.94	0.50
1:A:459:PHE:CD1	1:A:459:PHE:N	2.80	0.50
1:A:1016:VAL:O	1:A:1017:LEU:HB2	2.12	0.50
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.94	0.50
1:A:415:ASN:HB3	1:A:438:ILE:HD11	1.94	0.50
1:A:338:HIS:O	1:A:338:HIS:ND1	2.45	0.49
1:A:667:ASN:OD1	2:A:5002:CPF:H151	2.08	0.49
1:A:867:ARG:C	1:A:868:LEU:HD23	2.37	0.49
1:A:534:ILE:HB	1:A:1026:PHE:CZ	2.48	0.49
1:A:709:HIS:N	1:A:710:PRO:HD3	2.27	0.49
1:A:451:ALA:CB	1:A:883:VAL:HG11	2.42	0.49
1:A:664:PHE:O	1:A:665:ALA:HB2	2.13	0.49
1:A:41:PRO:HB3	1:A:295:THR:HG22	1.95	0.49
1:A:412:VAL:O	1:A:416:VAL:HG23	2.12	0.49
1:A:133:SER:O	1:A:135:SER:N	2.46	0.49
1:A:721:LEU:O	1:A:723:ASP:N	2.45	0.48
1:A:456:MET:HA	1:A:876:LEU:HB3	1.96	0.48
1:A:596:HIS:O	1:A:600:THR:HG22	2.13	0.48
1:A:10:ILE:N	1:A:10:ILE:HD12	2.28	0.48
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.78	0.48
1:A:68:ASN:HD21	1:A:113:LEU:HB2	1.78	0.48
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:MET:N	1:A:988:PRO:HD2	2.29	0.48
1:A:394:THR:HG22	1:A:469:GLN:HB3	1.95	0.47
1:A:518:ARG:O	1:A:522:LYS:HD2	2.14	0.47
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.44	0.47
1:A:448:VAL:HG11	1:A:888:LEU:HG	1.97	0.47
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.96	0.47
1:A:463:THR:CB	1:A:868:LEU:HD22	2.45	0.47
1:A:684:LEU:C	1:A:684:LEU:HD12	2.40	0.47
1:A:450:SER:HA	1:A:478:MET:HE1	1.97	0.47
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.44	0.46
1:A:344:LEU:HD21	1:A:376:LEU:HD11	1.96	0.46
1:A:570:GLY:O	1:A:571:VAL:HG23	2.15	0.46
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.97	0.46
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.96	0.46
1:A:344:LEU:C	1:A:344:LEU:HD13	2.40	0.46
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.98	0.46
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.44	0.46
1:A:363:ARG:HG3	1:A:497:LEU:O	2.16	0.46
1:A:401:ALA:O	1:A:402:ILE:C	2.59	0.46
1:A:873:ALA:HA	1:A:876:LEU:HD12	1.98	0.46
1:A:664:PHE:O	1:A:665:ALA:CB	2.63	0.45
1:A:967:ALA:O	1:A:971:ARG:HG3	2.17	0.45
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.98	0.45
1:A:134:SER:O	1:A:135:SER:HB3	2.16	0.45
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.99	0.45
1:A:531:VAL:O	1:A:534:ILE:HG13	2.16	0.45
1:A:140:VAL:HG11	1:A:310:LEU:HD11	1.99	0.45
1:A:670:ALA:O	1:A:671:ILE:C	2.60	0.45
1:A:942:ALA:O	1:A:945:ILE:N	2.50	0.45
1:A:1021:PHE:O	1:A:1026:PHE:CE1	2.70	0.45
1:A:367:ILE:HG12	1:A:492:LEU:HD22	1.98	0.44
1:A:710:PRO:HB2	1:A:713:LEU:HB3	1.99	0.44
1:A:848:ALA:HA	1:A:851:LEU:HD12	1.99	0.44
1:A:987:MET:CE	1:A:1008:MET:HE3	2.44	0.44
1:A:365:THR:O	1:A:365:THR:CG2	2.65	0.44
1:A:979:SER:CB	1:A:1015:THR:HG21	2.47	0.44
1:A:383:LEU:HD21	1:A:473:THR:HA	1.99	0.44
1:A:905:VAL:O	1:A:909:VAL:HG23	2.17	0.44
1:A:478:MET:HG2	1:A:479:ALA:N	2.32	0.44
1:A:1024:VAL:H	1:A:1027:VAL:HG22	1.82	0.44
1:A:487:ILE:HG22	1:A:488:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.52	0.44
1:A:971:ARG:HD2	1:A:971:ARG:O	2.18	0.44
1:A:471:SER:OG	1:A:472:ILE:N	2.51	0.43
1:A:487:ILE:HG22	1:A:488:LEU:H	1.83	0.43
1:A:1018:ALA:O	1:A:1024:VAL:HB	2.18	0.43
1:A:111:LEU:O	1:A:111:LEU:HD23	2.18	0.43
1:A:669:PRO:O	1:A:670:ALA:CB	2.65	0.43
1:A:115:MET:N	1:A:116:PRO:CD	2.82	0.43
1:A:464:GLY:O	1:A:468:ARG:HB2	2.19	0.43
1:A:133:SER:O	1:A:134:SER:C	2.61	0.43
1:A:453:PHE:CD2	1:A:471:SER:HA	2.53	0.43
1:A:514:GLY:O	1:A:516:PHE:N	2.52	0.43
1:A:989:LEU:HD22	1:A:1000:GLN:HE21	1.84	0.43
1:A:144:ASN:ND2	1:A:149:MET:SD	2.92	0.43
1:A:21:LEU:O	1:A:22:ALA:C	2.62	0.43
1:A:379:THR:O	1:A:383:LEU:HG	2.18	0.43
1:A:739:LEU:HD12	1:A:799:VAL:HG11	2.00	0.43
1:A:1011:MET:HA	1:A:1014:ALA:HB3	1.99	0.43
1:A:32:VAL:HA	1:A:390:ILE:HB	2.00	0.43
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.99	0.43
1:A:713:LEU:O	1:A:832:ALA:HB2	2.19	0.43
1:A:27:ILE:HG22	1:A:28:LEU:HD12	2.01	0.42
1:A:1029:VAL:O	1:A:1033:PHE:HB2	2.19	0.42
1:A:326:PRO:O	1:A:327:TYR:C	2.62	0.42
1:A:339:GLU:O	1:A:340:VAL:HG23	2.19	0.42
1:A:684:LEU:HD23	1:A:699:ARG:HB2	2.01	0.42
1:A:458:PHE:C	1:A:459:PHE:CD1	2.97	0.42
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.53	0.42
1:A:904:VAL:O	1:A:907:LEU:HB2	2.18	0.42
1:A:188:MET:HE2	1:A:773:VAL:HG13	2.02	0.42
1:A:441:ALA:HB2	1:A:947:GLU:HG2	2.02	0.42
1:A:666:PHE:HB3	2:A:5002:CPF:F1	2.10	0.42
1:A:373:PRO:O	1:A:377:LEU:HG	2.20	0.42
1:A:895:TRP:CE3	1:A:895:TRP:HA	2.55	0.42
1:A:970:MET:O	1:A:971:ARG:HB3	2.19	0.42
1:A:450:SER:O	1:A:454:VAL:HG23	2.20	0.41
1:A:468:ARG:O	1:A:471:SER:N	2.53	0.41
1:A:968:VAL:HA	1:A:971:ARG:NE	2.35	0.41
1:A:443:VAL:HG12	1:A:443:VAL:O	2.20	0.41
1:A:420:MET:HE1	1:A:497:LEU:HG	2.03	0.41
1:A:494:ALA:O	1:A:495:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:O	1:A:207:ILE:HG13	2.21	0.41
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.56	0.41
1:A:12:ALA:HB1	1:A:487:ILE:HG22	2.02	0.41
1:A:108:GLN:HB3	1:A:129:VAL:HG11	2.03	0.41
1:A:864:TYR:CD2	1:A:865:GLN:N	2.89	0.41
1:A:892:TYR:OH	1:A:943:ILE:HG23	2.20	0.41
1:A:291:ILE:HG21	1:A:306:ILE:HD11	2.02	0.41
1:A:278:ILE:HD12	1:A:613:ASN:HB3	2.03	0.41
1:A:878:ALA:O	1:A:882:ILE:HG13	2.20	0.41
1:A:169:THR:O	1:A:170:SER:C	2.63	0.41
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.56	0.41
1:A:450:SER:CB	1:A:478:MET:HE1	2.51	0.41
1:A:864:TYR:CD2	1:A:864:TYR:N	2.89	0.41
1:A:531:VAL:HA	1:A:534:ILE:CG1	2.51	0.41
1:A:38:ILE:HG21	1:A:466:ILE:HD11	2.03	0.40
1:A:194:ASN:O	1:A:194:ASN:ND2	2.55	0.40
1:A:931:LEU:O	1:A:935:ILE:HD12	2.21	0.40
1:A:1024:VAL:N	1:A:1027:VAL:HG22	2.36	0.40
1:A:685:ILE:HD11	1:A:819:TYR:HD2	1.86	0.40
1:A:753:ALA:O	1:A:775:SER:OG	2.38	0.40
1:A:254:ASN:O	1:A:256:ASP:N	2.54	0.40
1:A:416:VAL:O	1:A:420:MET:HG3	2.21	0.40
1:A:558:ARG:HD2	1:A:558:ARG:HA	1.96	0.40
1:A:669:PRO:O	1:A:670:ALA:HB3	2.21	0.40
1:A:1032:ARG:HH11	1:A:1032:ARG:HG3	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1003/1049 (96%)	795 (79%)	134 (13%)	74 (7%)	1 4

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	22	ALA
1	A	34	GLN
1	A	134	SER
1	A	135	SER
1	A	255	GLN
1	A	459	PHE
1	A	472	ILE
1	A	515	TRP
1	A	665	ALA
1	A	670	ALA
1	A	713	LEU
1	A	722	GLU
1	A	794	ALA
1	A	871	ASN
1	A	874	PRO
1	A	889	ALA
1	A	971	ARG
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	9	PRO
1	A	110	LYS
1	A	152	GLU
1	A	161	ASN
1	A	327	TYR
1	A	340	VAL
1	A	349	ILE
1	A	421	ALA
1	A	424	GLY
1	A	495	THR
1	A	525	HIS
1	A	718	PRO
1	A	723	ASP
1	A	864	TYR
1	A	865	GLN
1	A	875	SER
1	A	954	ASP
1	A	1035	ARG
1	A	74	ASN
1	A	170	SER

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Mol	Chain	Res	Type
1	A	209	ALA
1	A	366	LEU
1	A	405	LEU
1	A	488	LEU
1	A	526	HIS
1	A	671	ILE
1	A	714	THR
1	A	955	LYS
1	A	995	ALA
1	A	1026	PHE
1	A	21	LEU
1	A	538	THR
1	A	638	PRO
1	A	677	ALA
1	A	837	THR
1	A	956	GLU
1	A	894	SER
1	A	905	VAL
1	A	940	LYS
1	A	1034	SER
1	A	372	VAL
1	A	491	ALA
1	A	571	VAL
1	A	893	GLU
1	A	1016	VAL
1	A	1027	VAL
1	A	626	ILE
1	A	943	ILE
1	A	991	ILE
1	A	411	VAL
1	A	672	VAL
1	A	514	GLY

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	823/854 (96%)	584 (71%)	239 (29%)	0 1

All (239) 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	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	44	THR
1	A	55	LYS
1	A	58	GLN
1	A	59	ASP
1	A	69	MET
1	A	72	ILE
1	A	75	LEU
1	A	80	SER
1	A	82	SER
1	A	87	THR
1	A	88	VAL
1	A	102	ILE
1	A	107	VAL
1	A	108	GLN
1	A	113	LEU
1	A	117	LEU
1	A	122	VAL
1	A	125	GLN
1	A	127	VAL
1	A	128	SER
1	A	132	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	162	MET
1	A	166	ILE
1	A	168	ARG
1	A	169	THR

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	182	TYR
1	A	185	ARG
1	A	193	LEU
1	A	197	GLN
1	A	207	ILE
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	240	LEU
1	A	243	THR
1	A	249	ILE
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	263	ARG
1	A	265	VAL
1	A	270	LEU
1	A	277	ILE
1	A	278	ILE
1	A	280	GLU
1	A	292	LYS
1	A	293	LEU
1	A	300	LEU
1	A	302	THR
1	A	307	ARG
1	A	312	LYS
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	334	LYS
1	A	335	ILE
1	A	340	VAL
1	A	342	LYS
1	A	343	THR
1	A	344	LEU
1	A	345	VAL

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Mol	Chain	Res	Type
1	A	349	ILE
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	370	ILE
1	A	376	LEU
1	A	379	THR
1	A	393	LEU
1	A	404	LEU
1	A	406	VAL
1	A	407	ASP
1	A	410	ILE
1	A	411	VAL
1	A	412	VAL
1	A	415	ASN
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	423	GLU
1	A	425	LEU
1	A	429	GLU
1	A	431	THR
1	A	433	LYS
1	A	435	MET
1	A	445	ILE
1	A	449	LEU
1	A	452	VAL
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	469	GLN
1	A	472	ILE
1	A	474	ILE
1	A	475	VAL
1	A	478	MET
1	A	484	VAL
1	A	492	LEU
1	A	497	LEU

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Mol	Chain	Res	Type
1	A	498	LYS
1	A	519	MET
1	A	526	HIS
1	A	534	ILE
1	A	546	LEU
1	A	547	ILE
1	A	548	ILE
1	A	557	VAL
1	A	558	ARG
1	A	562	SER
1	A	566	ASP
1	A	574	THR
1	A	575	MET
1	A	576	VAL
1	A	585	GLU
1	A	586	ARG
1	A	600	THR
1	A	608	SER
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE
1	A	622	GLN
1	A	632	LYS
1	A	637	ARG
1	A	640	GLU
1	A	643	LYS
1	A	645	GLU
1	A	657	GLN
1	A	659	LYS
1	A	662	MET
1	A	667	ASN
1	A	668	LEU
1	A	671	ILE
1	A	672	VAL
1	A	674	LEU
1	A	683	GLU
1	A	684	LEU
1	A	685	ILE
1	A	687	GLN
1	A	690	LEU
1	A	693	GLU
1	A	699	ARG

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Mol	Chain	Res	Type
1	A	708	LYS
1	A	713	LEU
1	A	714	THR
1	A	716	VAL
1	A	722	GLU
1	A	730	ASP
1	A	735	LYS
1	A	739	LEU
1	A	741	VAL
1	A	748	THR
1	A	757	SER
1	A	763	ILE
1	A	765	ARG
1	A	773	VAL
1	A	775	SER
1	A	782	LEU
1	A	791	VAL
1	A	798	MET
1	A	801	PHE
1	A	806	SER
1	A	817	GLU
1	A	818	ARG
1	A	828	LEU
1	A	842	GLU
1	A	844	MET
1	A	846	GLN
1	A	864	TYR
1	A	865	GLN
1	A	866	GLU
1	A	868	LEU
1	A	871	ASN
1	A	872	GLN
1	A	876	LEU
1	A	884	VAL
1	A	891	LEU
1	A	895	TRP
1	A	902	MET
1	A	903	LEU
1	A	904	VAL
1	A	905	VAL
1	A	910	ILE
1	A	914	LEU

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Mol	Chain	Res	Type
1	A	919	ARG
1	A	925	VAL
1	A	931	LEU
1	A	933	THR
1	A	934	THR
1	A	940	LYS
1	A	950	LYS
1	A	955	LYS
1	A	961	ILE
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	975	ILE
1	A	976	LEU
1	A	977	MET
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	1015	THR
1	A	1017	LEU
1	A	1019	ILE
1	A	1020	PHE
1	A	1022	VAL
1	A	1024	VAL
1	A	1027	VAL
1	A	1028	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	68	ASN
1	A	123	GLN
1	A	124	GLN
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	194	ASN
1	A	197	GLN
1	A	213	GLN
1	A	218	GLN
1	A	254	ASN
1	A	274	ASN
1	A	284	GLN
1	A	361	ASN
1	A	415	ASN
1	A	439	GLN
1	A	569	GLN
1	A	577	GLN
1	A	605	ASN
1	A	613	ASN
1	A	642	ASN
1	A	709	HIS
1	A	719	ASN
1	A	760	ASN
1	A	830	GLN
1	A	871	ASN
1	A	923	ASN
1	A	928	GLN
1	A	1001	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 ⓘ

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	CPF	A	5001	-	27,27,27	0.95	2 (7%)	40,40,40	0.80	1 (2%)
2	CPF	A	5002	-	27,27,27	0.96	2 (7%)	40,40,40	0.81	1 (2%)

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	CPF	A	5001	-	-	2/12/22/22	0/4/4/4
2	CPF	A	5002	-	-	2/12/22/22	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	CPF	O2-C3	-2.36	1.24	1.30
2	A	5002	CPF	O2-C3	-2.32	1.24	1.30
2	A	5002	CPF	O3-C4	2.17	1.27	1.23
2	A	5001	CPF	O3-C4	2.11	1.27	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5002	CPF	O3-C4-C5	-2.12	118.18	121.57
2	A	5001	CPF	O3-C4-C5	-2.10	118.21	121.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	CPF	C4-C2-C3-O2
2	A	5001	CPF	C4-C2-C3-O1
2	A	5002	CPF	C4-C2-C3-O2

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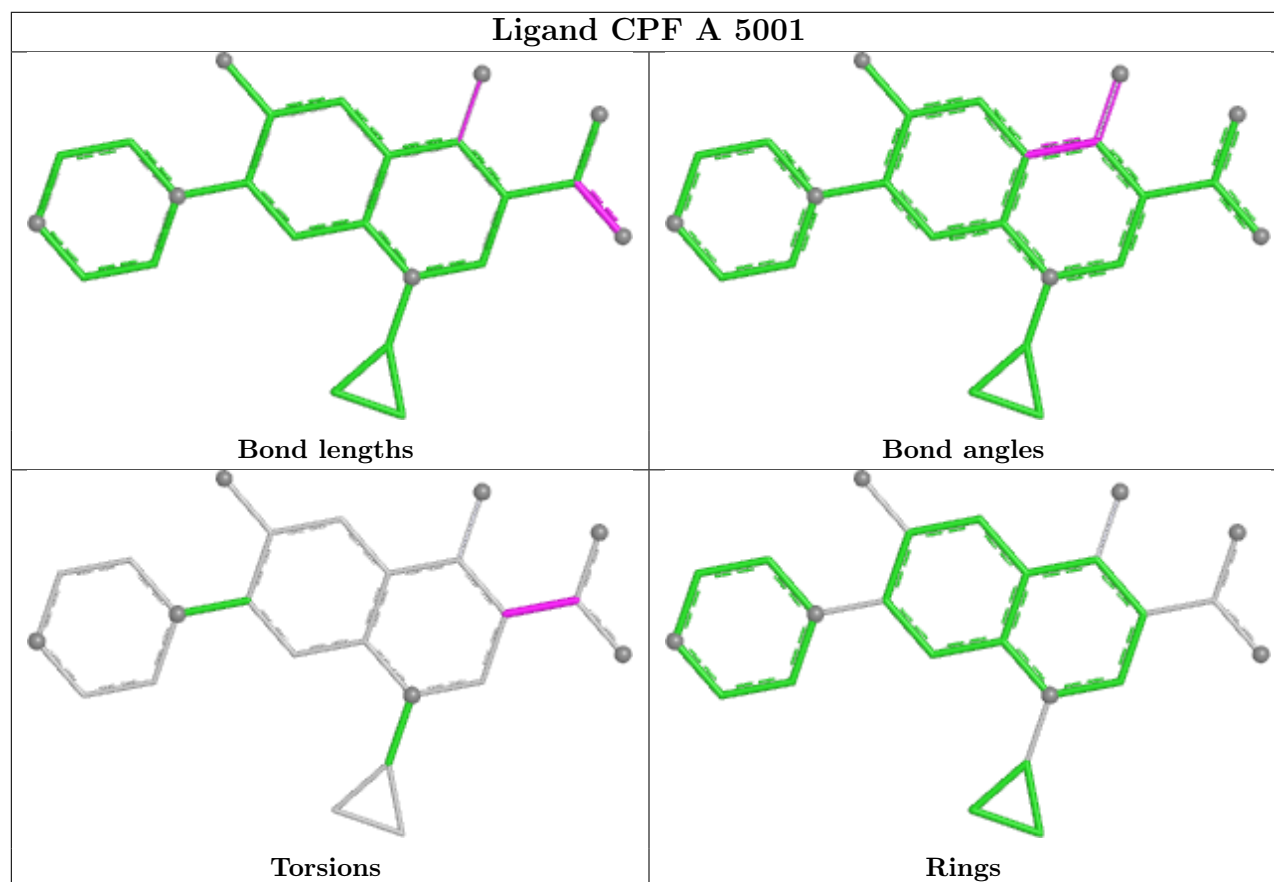
Mol	Chain	Res	Type	Atoms
2	A	5002	CPF	C4-C2-C3-O1

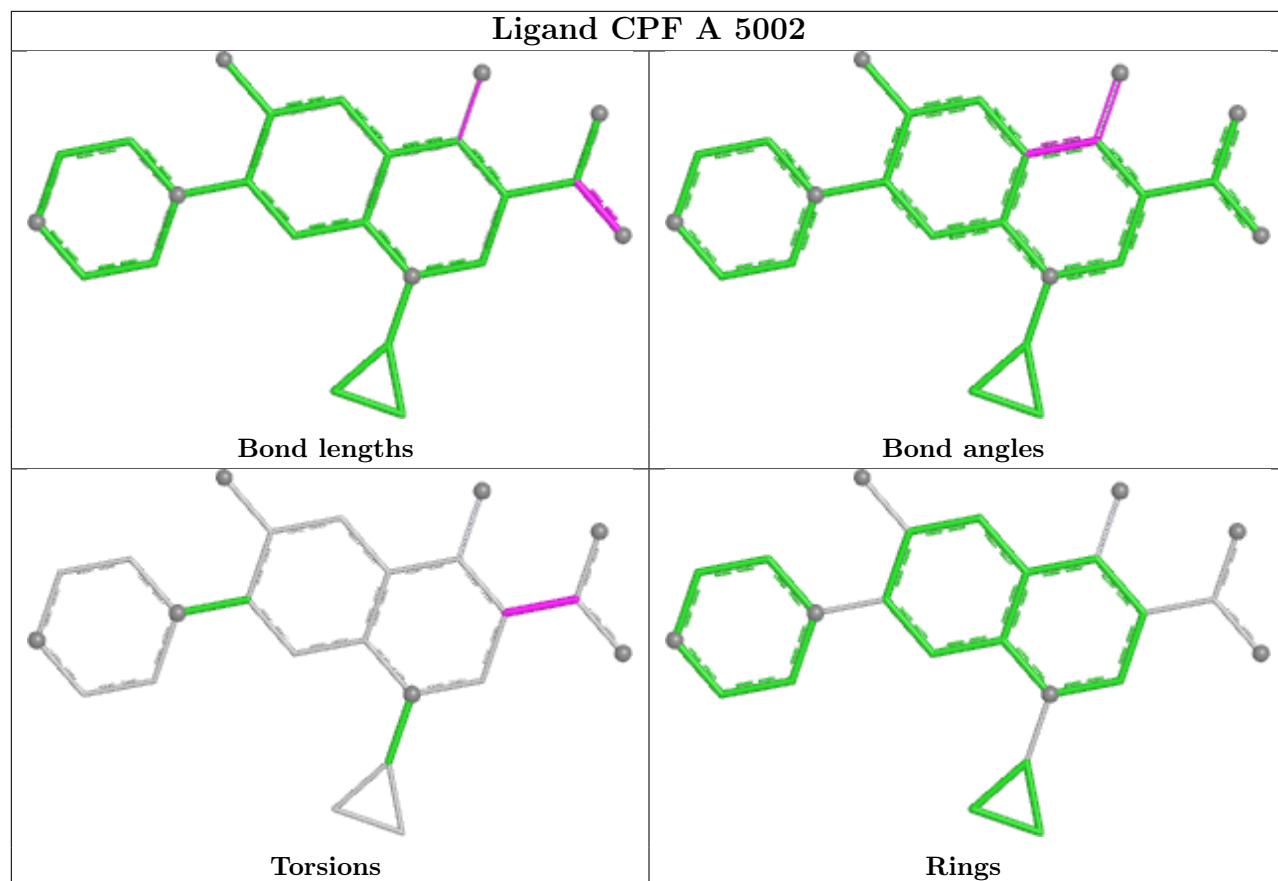
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5002	CPF	11	0

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 [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

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.