



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 AM UTC

PDB ID : 1OYE / pdb_00001oye
Title : Structural Basis of Multiple 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 : 3.48 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

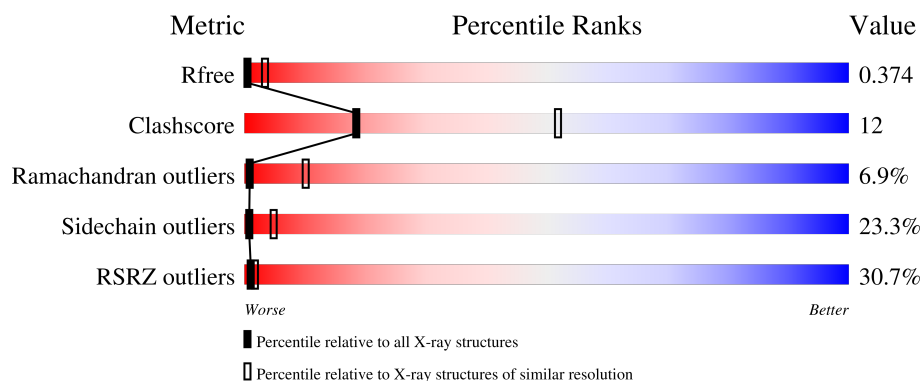
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.48 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	29% 58% 30% 8% ...

2 Entry composition [i](#)

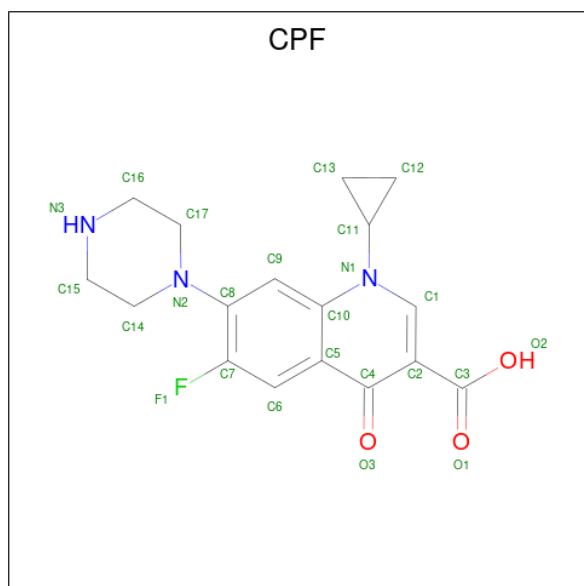
There are 2 unique types of molecules in this entry. The entry contains 7663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	1006	Total	C	N	O	S	0	0	0
			7639	4916	1262	1419	42			

- Molecule 2 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (CCD ID: CPF) (formula: C₁₇H₁₈FN₃O₃).

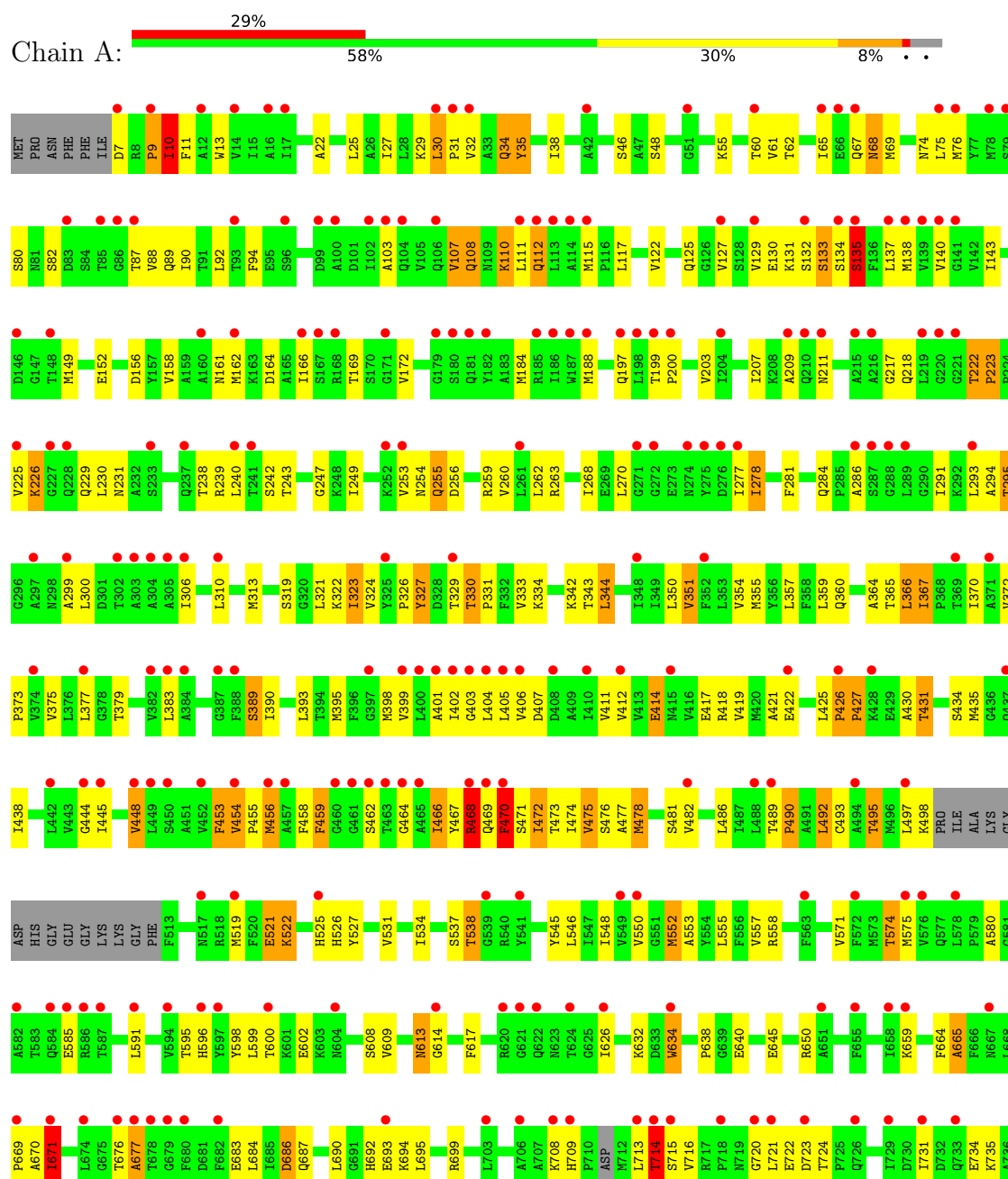


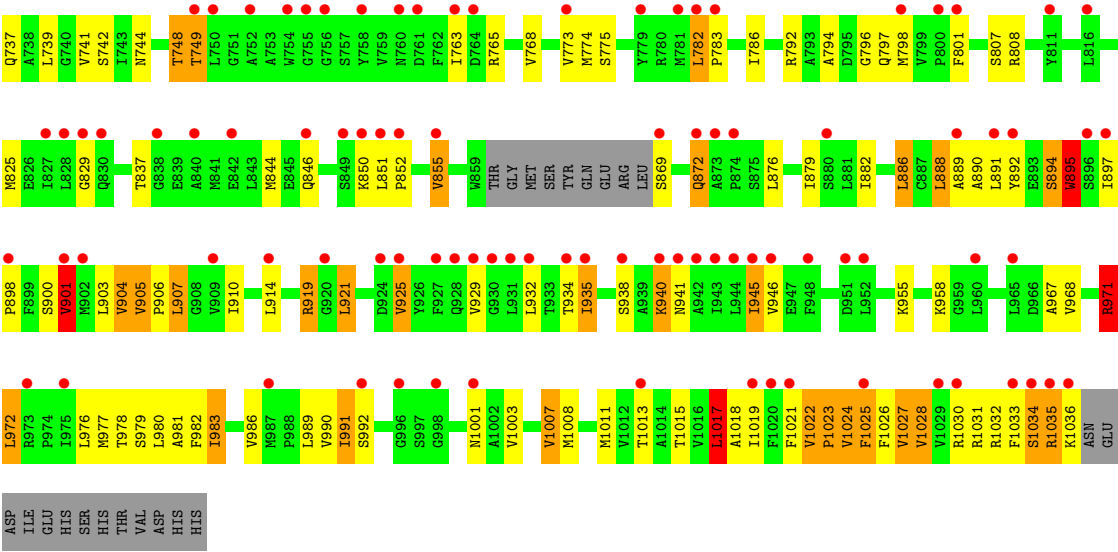
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	17	1	3	3		

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	145.11Å 145.11Å 517.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.48 46.60 – 3.48	Depositor EDS
% Data completeness (in resolution range)	99.0 (46.60-3.48) 99.0 (46.60-3.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.257 , 0.323 0.376 , 0.374	Depositor DCC
R_{free} test set	1390 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	132.4	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: 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	0.51	0/7779	0.86	3/10563 (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	1	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	PHE	N-CA-C	9.95	127.69	111.37
1	A	426	PRO	N-CA-C	7.84	120.26	110.70
1	A	454	VAL	CB-CA-C	-5.18	108.86	114.35

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	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	185	1
2	A	24	0	17	0	0
All	All	7663	0	7817	185	1

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 (185) 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	1.76	0.93
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.63	0.79
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.67	0.76
1:A:448:VAL:HG11	1:A:888:LEU:HD23	1.68	0.75
1:A:393:LEU:HD11	1:A:466:ILE:HA	1.75	0.69
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.75	0.69
1:A:354:VAL:HG13	1:A:980:LEU:HD23	1.76	0.68
1:A:910:ILE:HG23	1:A:1013:THR:HG21	1.75	0.68
1:A:613:ASN:C	1:A:613:ASN:ND2	2.49	0.68
1:A:596:HIS:O	1:A:600:THR:HG22	1.95	0.66
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.79	0.65
1:A:1015:THR:O	1:A:1019:ILE:HG22	1.97	0.65
1:A:979:SER:O	1:A:983:ILE:HG13	1.99	0.62
1:A:670:ALA:O	1:A:671:ILE:O	2.16	0.62
1:A:370:ILE:HG22	1:A:370:ILE:O	2.00	0.61
1:A:1018:ALA:HB1	1:A:1024:VAL:HG21	1.82	0.61
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.83	0.59
1:A:888:LEU:HD12	1:A:898:PRO:HA	1.84	0.59
1:A:367:ILE:HG23	1:A:492:LEU:HD13	1.84	0.59
1:A:982:PHE:CD2	1:A:1011:MET:HG3	2.37	0.59
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.37	0.59
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.84	0.59
1:A:466:ILE:H	1:A:466:ILE:HD12	1.66	0.59
1:A:454:VAL:N	1:A:455:PRO:HD2	2.18	0.59
1:A:475:VAL:HG22	1:A:478:MET:CE	2.32	0.59
1:A:575:MET:HB3	1:A:626:ILE:HD12	1.85	0.58
1:A:968:VAL:HB	1:A:1025:PHE:HZ	1.67	0.58
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.51	0.58
1:A:112:GLN:HG2	1:A:112:GLN:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ILE:HG23	1:A:395:MET:SD	2.44	0.57
1:A:291:ILE:HG21	1:A:306:ILE:HD11	1.86	0.56
1:A:359:LEU:HD13	1:A:364:ALA:HB1	1.86	0.56
1:A:613:ASN:HD22	1:A:614:GLY:N	2.03	0.56
1:A:372:VAL:N	1:A:373:PRO:HD2	2.21	0.56
1:A:188:MET:HE2	1:A:773:VAL:HG22	1.87	0.55
1:A:9:PRO:C	1:A:10:ILE:HD13	2.31	0.55
1:A:326:PRO:O	1:A:327:TYR:C	2.48	0.55
1:A:108:GLN:HB2	1:A:129:VAL:HG21	1.89	0.54
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.87	0.54
1:A:971:ARG:HD2	1:A:971:ARG:C	2.33	0.54
1:A:294:ALA:O	1:A:295:THR:C	2.51	0.53
1:A:716:VAL:HG12	1:A:829:GLY:HA3	1.89	0.53
1:A:903:LEU:O	1:A:906:PRO:HD2	2.08	0.53
1:A:527:TYR:OH	1:A:1019:ILE:O	2.24	0.53
1:A:897:ILE:HG23	1:A:946:VAL:HG11	1.91	0.53
1:A:359:LEU:HD21	1:A:977:MET:HE1	1.91	0.53
1:A:1018:ALA:CB	1:A:1024:VAL:HG21	2.39	0.53
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.92	0.52
1:A:709:HIS:CG	1:A:709:HIS:O	2.62	0.52
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.45	0.52
1:A:30:LEU:HD23	1:A:390:ILE:HG13	1.91	0.52
1:A:425:LEU:C	1:A:427:PRO:HD2	2.35	0.52
1:A:468:ARG:O	1:A:472:ILE:HG22	2.09	0.52
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.92	0.52
1:A:475:VAL:HA	1:A:478:MET:HE2	1.91	0.51
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.92	0.51
1:A:343:THR:CG2	1:A:989:LEU:HD21	2.40	0.51
1:A:401:ALA:O	1:A:405:LEU:HG	2.11	0.51
1:A:489:THR:HB	1:A:490:PRO:HD3	1.93	0.51
1:A:546:LEU:O	1:A:550:VAL:HG23	2.10	0.51
1:A:721:LEU:HD22	1:A:825:MET:CE	2.41	0.50
1:A:412:VAL:HG13	1:A:435:MET:HE1	1.94	0.50
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.94	0.50
1:A:525:HIS:O	1:A:527:TYR:N	2.43	0.50
1:A:695:LEU:HD22	1:A:825:MET:SD	2.51	0.50
1:A:402:ILE:HA	1:A:405:LEU:HD12	1.93	0.50
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.92	0.50
1:A:634:TRP:H	1:A:634:TRP:CD1	2.30	0.50
1:A:373:PRO:O	1:A:377:LEU:HG	2.12	0.49
1:A:468:ARG:HG2	1:A:469:GLN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.94	0.49
1:A:10:ILE:HG12	1:A:11:PHE:CD2	2.45	0.49
1:A:454:VAL:HG22	1:A:475:VAL:HG21	1.93	0.49
1:A:907:LEU:O	1:A:1013:THR:HG22	2.12	0.49
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.93	0.49
1:A:300:LEU:HD22	1:A:333:VAL:HG11	1.94	0.49
1:A:365:THR:O	1:A:365:THR:HG23	2.12	0.49
1:A:456:MET:HA	1:A:876:LEU:HB3	1.95	0.49
1:A:904:VAL:HG13	1:A:1024:VAL:HG22	1.95	0.49
1:A:972:LEU:C	1:A:972:LEU:HD13	2.38	0.49
1:A:466:ILE:HG23	1:A:925:VAL:HG21	1.94	0.49
1:A:897:ILE:N	1:A:898:PRO:CD	2.76	0.49
1:A:401:ALA:HB2	1:A:474:ILE:HG12	1.95	0.48
1:A:407:ASP:O	1:A:411:VAL:HG23	2.13	0.48
1:A:379:THR:HB	1:A:398:MET:HE1	1.95	0.48
1:A:92:LEU:HD22	1:A:107:VAL:HG23	1.95	0.48
1:A:211:ASN:HA	1:A:240:LEU:HD23	1.94	0.48
1:A:595:THR:HG22	1:A:599:LEU:HD12	1.96	0.48
1:A:894:SER:O	1:A:895:TRP:HB2	2.14	0.48
1:A:1033:PHE:O	1:A:1034:SER:C	2.57	0.48
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.43	0.47
1:A:967:ALA:O	1:A:971:ARG:HG3	2.14	0.47
1:A:945:ILE:HA	1:A:971:ARG:NH1	2.29	0.47
1:A:426:PRO:N	1:A:427:PRO:HD2	2.29	0.47
1:A:456:MET:HE2	1:A:932:LEU:CD1	2.45	0.47
1:A:1022:VAL:CG2	1:A:1023:PRO:HD2	2.39	0.47
1:A:482:VAL:O	1:A:486:LEU:HG	2.15	0.47
1:A:414:GLU:CD	1:A:414:GLU:C	2.83	0.47
1:A:90:ILE:N	1:A:90:ILE:HD12	2.29	0.47
1:A:664:PHE:O	1:A:665:ALA:HB2	2.15	0.47
1:A:188:MET:HE1	1:A:200:PRO:HB3	1.96	0.47
1:A:744:ASN:O	1:A:748:THR:HG22	2.16	0.46
1:A:905:VAL:HG13	1:A:935:ILE:HG12	1.96	0.46
1:A:405:LEU:HD23	1:A:481:SER:HB3	1.96	0.46
1:A:434:SER:O	1:A:438:ILE:HG13	2.15	0.46
1:A:448:VAL:CG1	1:A:888:LEU:HD23	2.43	0.46
1:A:493:CYS:O	1:A:497:LEU:HB2	2.16	0.46
1:A:405:LEU:HD21	1:A:477:ALA:HB1	1.96	0.46
1:A:466:ILE:CG2	1:A:925:VAL:HG21	2.46	0.46
1:A:721:LEU:HD22	1:A:825:MET:HE3	1.96	0.46
1:A:222:THR:HB	1:A:223:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.98	0.46
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.46	0.46
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.69	0.46
1:A:200:PRO:HD2	1:A:749:THR:HG23	1.98	0.46
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.97	0.46
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.51	0.46
1:A:472:ILE:HA	1:A:475:VAL:HB	1.97	0.45
1:A:892:TYR:HB3	1:A:897:ILE:HD13	1.98	0.45
1:A:907:LEU:HG	1:A:1017:LEU:HD23	1.98	0.45
1:A:1022:VAL:O	1:A:1023:PRO:O	2.34	0.45
1:A:453:PHE:HE2	1:A:474:ILE:HB	1.82	0.45
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.98	0.45
1:A:92:LEU:HD13	1:A:107:VAL:HG21	1.99	0.45
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.99	0.45
1:A:855:VAL:HG12	1:A:855:VAL:O	2.17	0.44
1:A:68:ASN:HD22	1:A:110:LYS:HD2	1.82	0.44
1:A:403:GLY:HA3	1:A:982:PHE:HD1	1.81	0.44
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.99	0.44
1:A:30:LEU:CD2	1:A:390:ILE:HG13	2.48	0.44
1:A:792:ARG:HA	1:A:798:MET:HE3	1.99	0.44
1:A:851:LEU:HB3	1:A:852:PRO:HD2	2.00	0.44
1:A:879:ILE:HA	1:A:882:ILE:HD12	2.00	0.44
1:A:521:GLU:O	1:A:522:LYS:C	2.61	0.43
1:A:94:PHE:CE2	1:A:103:ALA:HB1	2.53	0.43
1:A:444:GLY:HA2	1:A:891:LEU:HD23	2.00	0.43
1:A:531:VAL:O	1:A:534:ILE:HG12	2.18	0.43
1:A:919:ARG:HB3	1:A:921:LEU:HD23	2.00	0.43
1:A:929:VAL:HA	1:A:932:LEU:HD12	2.00	0.43
1:A:986:VAL:HG12	1:A:990:VAL:CG2	2.49	0.43
1:A:1033:PHE:O	1:A:1035:ARG:N	2.52	0.43
1:A:203:VAL:O	1:A:207:ILE:HG13	2.18	0.43
1:A:310:LEU:HD21	1:A:323:ILE:HD12	2.00	0.43
1:A:456:MET:O	1:A:876:LEU:HD13	2.19	0.43
1:A:475:VAL:HG22	1:A:478:MET:HE1	1.99	0.43
1:A:330:THR:HB	1:A:331:PRO:HD3	2.01	0.43
1:A:890:ALA:C	1:A:891:LEU:HD22	2.43	0.43
1:A:62:THR:OG1	1:A:88:VAL:HG21	2.19	0.43
1:A:782:LEU:HB3	1:A:783:PRO:HD2	2.01	0.43
1:A:31:PRO:HG2	1:A:389:SER:HB3	2.01	0.42
1:A:886:LEU:N	1:A:886:LEU:HD23	2.34	0.42
1:A:1003:VAL:O	1:A:1007:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:HG2	1:A:333:VAL:HG22	2.01	0.42
1:A:351:VAL:CG2	1:A:981:ALA:HB1	2.47	0.42
1:A:892:TYR:HB3	1:A:897:ILE:HG21	2.00	0.42
1:A:419:VAL:HG12	1:A:430:ALA:HB1	2.02	0.42
1:A:553:ALA:O	1:A:557:VAL:HG23	2.19	0.42
1:A:713:LEU:C	1:A:714:THR:OG1	2.62	0.42
1:A:158:VAL:HG22	1:A:162:MET:CE	2.50	0.42
1:A:458:PHE:O	1:A:459:PHE:O	2.37	0.42
1:A:941:ASN:HD21	1:A:1015:THR:HG22	1.85	0.42
1:A:1027:VAL:O	1:A:1028:VAL:C	2.63	0.41
1:A:990:VAL:O	1:A:1001:ASN:ND2	2.53	0.41
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.85	0.41
1:A:133:SER:O	1:A:135:SER:N	2.54	0.41
1:A:398:MET:O	1:A:402:ILE:HG13	2.20	0.41
1:A:470:PHE:CD1	1:A:929:VAL:HG11	2.55	0.41
1:A:686:ASP:HB2	1:A:695:LEU:HD12	2.02	0.41
1:A:108:GLN:HB3	1:A:129:VAL:HG11	2.02	0.41
1:A:383:LEU:HD11	1:A:473:THR:HG23	2.03	0.41
1:A:466:ILE:HG22	1:A:467:TYR:N	2.36	0.41
1:A:676:THR:O	1:A:677:ALA:HB3	2.21	0.41
1:A:65:ILE:O	1:A:69:MET:HB2	2.21	0.41
1:A:254:ASN:O	1:A:256:ASP:N	2.54	0.41
1:A:419:VAL:CG1	1:A:430:ALA:HB1	2.51	0.41
1:A:574:THR:HG21	1:A:598:TYR:OH	2.21	0.41
1:A:207:ILE:HG22	1:A:211:ASN:HD22	1.86	0.41
1:A:905:VAL:HB	1:A:906:PRO:CD	2.51	0.41
1:A:370:ILE:O	1:A:370:ILE:CG2	2.69	0.40
1:A:709:HIS:O	1:A:709:HIS:CD2	2.75	0.40
1:A:390:ILE:O	1:A:390:ILE:HG22	2.21	0.40
1:A:580:ALA:HB1	1:A:724:THR:HG22	2.04	0.40
1:A:968:VAL:HG22	1:A:972:LEU:HB2	2.03	0.40
1:A:469:GLN:HA	1:A:472:ILE:HG23	2.02	0.40
1:A:9:PRO:HB3	1:A:495:THR:OG1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:O	1:A:596:HIS:NE2[12_455]	2.06	0.14

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	998/1049 (95%)	788 (79%)	141 (14%)	69 (7%)	1	10

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	255	GLN
1	A	459	PHE
1	A	466	ILE
1	A	526	HIS
1	A	665	ALA
1	A	671	ILE
1	A	714	THR
1	A	794	ALA
1	A	901	VAL
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	134	SER
1	A	135	SER
1	A	152	GLU
1	A	161	ASN
1	A	169	THR
1	A	295	THR
1	A	327	TYR
1	A	427	PRO
1	A	431	THR
1	A	464	GLY
1	A	468	ARG
1	A	521	GLU

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Mol	Chain	Res	Type
1	A	775	SER
1	A	872	GLN
1	A	894	SER
1	A	900	SER
1	A	940	LYS
1	A	955	LYS
1	A	1027	VAL
1	A	34	GLN
1	A	74	ASN
1	A	110	LYS
1	A	209	ALA
1	A	366	LEU
1	A	421	ALA
1	A	495	THR
1	A	720	GLY
1	A	889	ALA
1	A	895	TRP
1	A	22	ALA
1	A	184	MET
1	A	299	ALA
1	A	522	LYS
1	A	538	THR
1	A	638	PRO
1	A	722	GLU
1	A	723	ASP
1	A	971	ARG
1	A	992	SER
1	A	35	TYR
1	A	133	SER
1	A	677	ALA
1	A	837	THR
1	A	197	GLN
1	A	552	MET
1	A	571	VAL
1	A	330	THR
1	A	223	PRO
1	A	490	PRO
1	A	669	PRO
1	A	796	GLY
1	A	217	GLY
1	A	991	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	818/855 (96%)	627 (77%)	191 (23%)	1 5

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	10	ILE
1	A	13	TRP
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
1	A	48	SER
1	A	55	LYS
1	A	67	GLN
1	A	68	ASN
1	A	75	LEU
1	A	76	MET
1	A	80	SER
1	A	82	SER
1	A	87	THR
1	A	89	GLN
1	A	107	VAL
1	A	108	GLN
1	A	111	LEU
1	A	112	GLN
1	A	115	MET
1	A	117	LEU
1	A	122	VAL
1	A	125	GLN
1	A	127	VAL

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Mol	Chain	Res	Type
1	A	130	GLU
1	A	131	LYS
1	A	132	SER
1	A	135	SER
1	A	137	LEU
1	A	138	MET
1	A	140	VAL
1	A	149	MET
1	A	156	ASP
1	A	164	ASP
1	A	166	ILE
1	A	199	THR
1	A	222	THR
1	A	225	VAL
1	A	226	LYS
1	A	229	GLN
1	A	230	LEU
1	A	238	THR
1	A	239	ARG
1	A	242	SER
1	A	243	THR
1	A	249	ILE
1	A	253	VAL
1	A	255	GLN
1	A	259	ARG
1	A	260	VAL
1	A	263	ARG
1	A	270	LEU
1	A	277	ILE
1	A	278	ILE
1	A	284	GLN
1	A	293	LEU
1	A	313	MET
1	A	319	SER
1	A	321	LEU
1	A	322	LYS
1	A	323	ILE
1	A	329	THR
1	A	334	LYS
1	A	342	LYS
1	A	344	LEU
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	351	VAL
1	A	355	MET
1	A	357	LEU
1	A	360	GLN
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	418	ARG
1	A	422	GLU
1	A	431	THR
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	470	PHE
1	A	471	SER
1	A	472	ILE
1	A	475	VAL
1	A	476	SER
1	A	478	MET
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	585	GLU
1	A	591	LEU
1	A	602	GLU
1	A	608	SER
1	A	609	VAL
1	A	613	ASN
1	A	617	PHE

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Mol	Chain	Res	Type
1	A	632	LYS
1	A	634	TRP
1	A	640	GLU
1	A	645	GLU
1	A	650	ARG
1	A	659	LYS
1	A	671	ILE
1	A	683	GLU
1	A	686	ASP
1	A	687	GLN
1	A	690	LEU
1	A	692	HIS
1	A	693	GLU
1	A	694	LYS
1	A	699	ARG
1	A	708	LYS
1	A	714	THR
1	A	715	SER
1	A	731	ILE
1	A	734	GLU
1	A	735	LYS
1	A	737	GLN
1	A	739	LEU
1	A	741	VAL
1	A	742	SER
1	A	748	THR
1	A	749	THR
1	A	763	ILE
1	A	765	ARG
1	A	768	VAL
1	A	774	MET
1	A	782	LEU
1	A	786	ILE
1	A	797	GLN
1	A	801	PHE
1	A	807	SER
1	A	808	ARG
1	A	844	MET
1	A	846	GLN
1	A	850	LYS
1	A	855	VAL
1	A	869	SER

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Mol	Chain	Res	Type
1	A	872	GLN
1	A	886	LEU
1	A	888	LEU
1	A	895	TRP
1	A	901	VAL
1	A	904	VAL
1	A	905	VAL
1	A	907	LEU
1	A	914	LEU
1	A	919	ARG
1	A	921	LEU
1	A	925	VAL
1	A	934	THR
1	A	935	ILE
1	A	938	SER
1	A	940	LYS
1	A	945	ILE
1	A	958	LYS
1	A	971	ARG
1	A	972	LEU
1	A	976	LEU
1	A	978	THR
1	A	983	ILE
1	A	991	ILE
1	A	1007	VAL
1	A	1008	MET
1	A	1017	LEU
1	A	1022	VAL
1	A	1024	VAL
1	A	1028	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG
1	A	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	112	GLN
1	A	124	GLN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	189	ASN
1	A	194	ASN
1	A	197	GLN
1	A	211	ASN
1	A	231	ASN
1	A	284	GLN
1	A	469	GLN
1	A	569	GLN
1	A	604	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	667	ASN
1	A	700	ASN
1	A	701	GLN
1	A	709	HIS
1	A	820	ASN
1	A	928	GLN
1	A	941	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 oligosaccharides 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	CPF	A	5001	-	27,27,27	0.95	2 (7%)	40,40,40	0.80	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

All (2) 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	5001	CPF	O3-C4	2.07	1.27	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	CPF	O3-C4-C5	-2.07	118.26	121.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

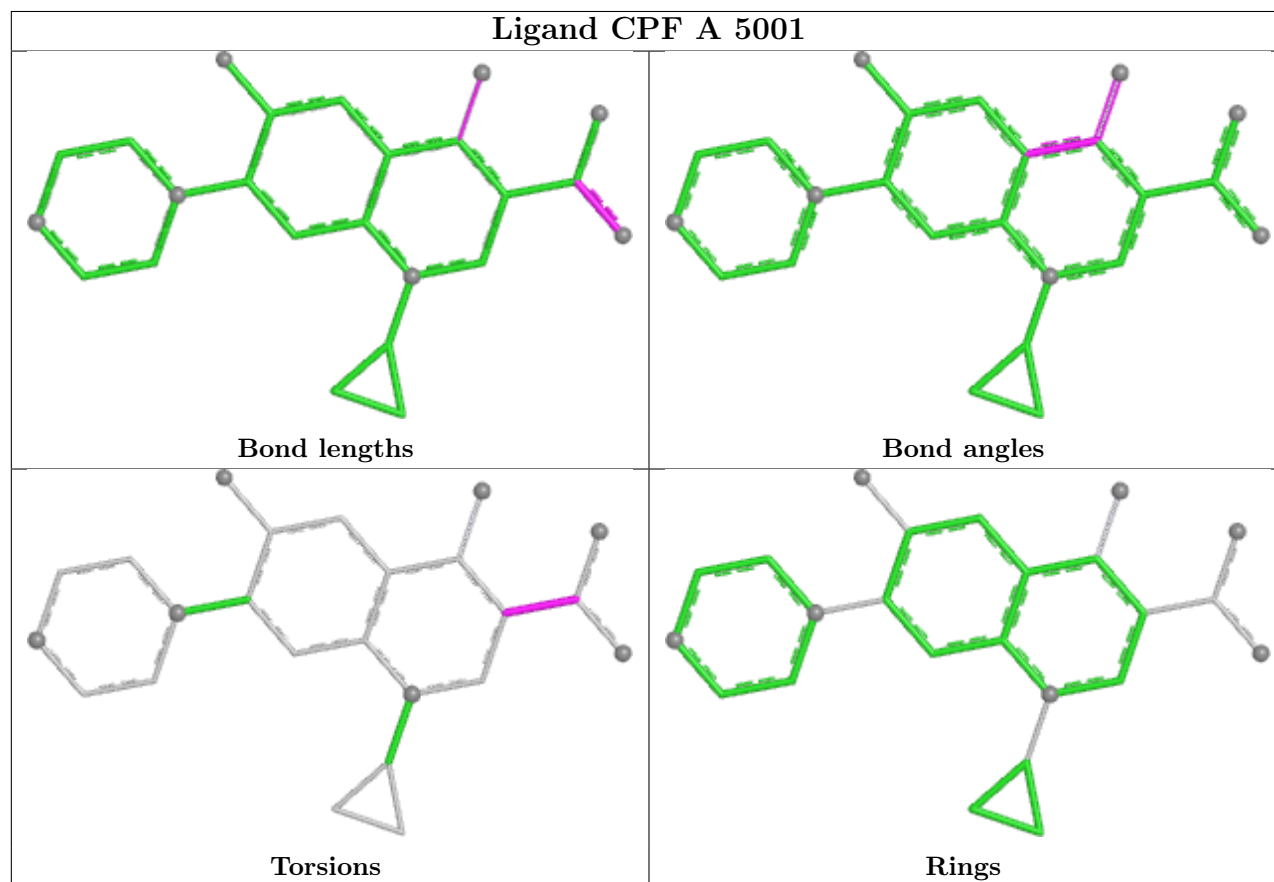
Mol	Chain	Res	Type	Atoms
2	A	5001	CPF	C4-C2-C3-O2
2	A	5001	CPF	C4-C2-C3-O1

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 [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

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%)	1.65	309 (30%) 1 2	74, 104, 116, 130	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	658	ILE	10.2
1	A	299	ALA	10.2
1	A	401	ALA	9.7
1	A	303	ALA	8.6
1	A	935	ILE	8.1
1	A	403	GLY	7.7
1	A	585	GLU	7.3
1	A	111	LEU	7.3
1	A	399	VAL	6.9
1	A	402	ILE	6.8
1	A	714	THR	6.6
1	A	494	ALA	6.4
1	A	829	GLY	6.4
1	A	241	THR	6.2
1	A	944	LEU	6.1
1	A	830	GLN	5.9
1	A	934	THR	5.8
1	A	897	ILE	5.6
1	A	721	LEU	5.4
1	A	782	LEU	5.4
1	A	519	MET	5.3
1	A	252	LYS	5.1
1	A	1029	VAL	5.0
1	A	720	GLY	5.0
1	A	1033	PHE	5.0
1	A	750	LEU	4.9
1	A	12	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	137	LEU	4.8
1	A	102	ILE	4.8
1	A	676	THR	4.7
1	A	838	GLY	4.7
1	A	306	ILE	4.6
1	A	488	LEU	4.6
1	A	951	ASP	4.6
1	A	99	ASP	4.5
1	A	134	SER	4.5
1	A	448	VAL	4.4
1	A	781	MET	4.3
1	A	293	LEU	4.2
1	A	998	GLY	4.2
1	A	723	ASP	4.2
1	A	383	LEU	4.1
1	A	992	SER	4.1
1	A	227	GLY	4.1
1	A	706	ALA	4.1
1	A	31	PRO	4.1
1	A	272	GLY	4.1
1	A	457	ALA	4.0
1	A	938	SER	4.0
1	A	816	LEU	4.0
1	A	129	VAL	4.0
1	A	929	VAL	4.0
1	A	892	TYR	4.0
1	A	85	THR	3.9
1	A	828	LEU	3.9
1	A	302	THR	3.9
1	A	1021	PHE	3.9
1	A	83	ASP	3.8
1	A	840	ALA	3.8
1	A	400	LEU	3.8
1	A	215	ALA	3.7
1	A	437	GLN	3.7
1	A	927	PHE	3.7
1	A	465	ALA	3.7
1	A	975	ILE	3.7
1	A	754	TRP	3.7
1	A	715	SER	3.6
1	A	942	ALA	3.6
1	A	801	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	452	VAL	3.6
1	A	240	LEU	3.6
1	A	731	ILE	3.6
1	A	943	ILE	3.6
1	A	733	GLN	3.6
1	A	952	LEU	3.6
1	A	604	ASN	3.5
1	A	289	LEU	3.5
1	A	925	VAL	3.5
1	A	680	PHE	3.5
1	A	679	GLY	3.5
1	A	220	GLY	3.4
1	A	960	LEU	3.4
1	A	200	PRO	3.4
1	A	659	LYS	3.4
1	A	846	GLN	3.4
1	A	404	LEU	3.4
1	A	932	LEU	3.4
1	A	671	ILE	3.4
1	A	188	MET	3.4
1	A	384	ALA	3.4
1	A	113	LEU	3.4
1	A	901	VAL	3.4
1	A	166	ILE	3.3
1	A	374	VAL	3.3
1	A	103	ALA	3.3
1	A	718	PRO	3.3
1	A	127	VAL	3.3
1	A	891	LEU	3.2
1	A	78	MET	3.2
1	A	138	MET	3.2
1	A	140	VAL	3.2
1	A	87	THR	3.2
1	A	709	HIS	3.2
1	A	305	ALA	3.2
1	A	677	ALA	3.2
1	A	461	GLY	3.2
1	A	755	GLY	3.2
1	A	233	SER	3.2
1	A	454	VAL	3.1
1	A	651	ALA	3.1
1	A	752	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	756	GLY	3.1
1	A	930	GLY	3.1
1	A	582	ALA	3.1
1	A	550	VAL	3.1
1	A	851	LEU	3.0
1	A	1001	ASN	3.0
1	A	850	LYS	3.0
1	A	842	GLU	3.0
1	A	779	TYR	3.0
1	A	655	PHE	3.0
1	A	1019	ILE	3.0
1	A	9	PRO	3.0
1	A	412	VAL	3.0
1	A	428	LYS	3.0
1	A	1020	PHE	3.0
1	A	941	ASN	3.0
1	A	1013	THR	3.0
1	A	16	ALA	2.9
1	A	896	SER	2.9
1	A	987	MET	2.9
1	A	449	LEU	2.9
1	A	621	GLY	2.9
1	A	596	HIS	2.9
1	A	469	GLN	2.9
1	A	185	ARG	2.9
1	A	167	SER	2.9
1	A	965	LEU	2.9
1	A	141	GLY	2.9
1	A	873	ALA	2.8
1	A	1030	ARG	2.8
1	A	760	ASN	2.8
1	A	572	PHE	2.8
1	A	584	GLN	2.8
1	A	219	LEU	2.8
1	A	563	PHE	2.8
1	A	678	THR	2.8
1	A	221	GLY	2.7
1	A	783	PRO	2.7
1	A	371	ALA	2.7
1	A	228	GLN	2.7
1	A	377	LEU	2.7
1	A	703	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	898	PRO	2.7
1	A	186	ILE	2.7
1	A	869	SER	2.7
1	A	115	MET	2.7
1	A	179	GLY	2.7
1	A	462	SER	2.7
1	A	100	ALA	2.7
1	A	889	ALA	2.7
1	A	7	ASP	2.7
1	A	426	PRO	2.6
1	A	872	GLN	2.6
1	A	329	THR	2.6
1	A	304	ALA	2.6
1	A	763	ILE	2.6
1	A	422	GLU	2.6
1	A	946	VAL	2.6
1	A	276	ASP	2.6
1	A	17	ILE	2.6
1	A	348	ILE	2.6
1	A	237	GLN	2.6
1	A	405	LEU	2.6
1	A	114	ALA	2.6
1	A	216	ALA	2.6
1	A	576	VAL	2.6
1	A	271	GLY	2.6
1	A	75	LEU	2.6
1	A	310	LEU	2.6
1	A	674	LEU	2.6
1	A	286	ALA	2.6
1	A	634	TRP	2.5
1	A	204	ILE	2.5
1	A	67	GLN	2.5
1	A	106	GLN	2.5
1	A	160	ALA	2.5
1	A	600	THR	2.5
1	A	182	TYR	2.5
1	A	274	ASN	2.5
1	A	415	ASN	2.5
1	A	541	TYR	2.5
1	A	135	SER	2.5
1	A	445	ILE	2.5
1	A	729	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	575	MET	2.5
1	A	30	LEU	2.5
1	A	620	ARG	2.5
1	A	382	VAL	2.5
1	A	626	ILE	2.5
1	A	525	HIS	2.5
1	A	539	GLY	2.5
1	A	726	GLN	2.5
1	A	450	SER	2.4
1	A	973	ARG	2.4
1	A	93	THR	2.4
1	A	51	GLY	2.4
1	A	920	GLY	2.4
1	A	79	SER	2.4
1	A	470	PHE	2.4
1	A	211	ASN	2.4
1	A	669	PRO	2.4
1	A	761	ASP	2.4
1	A	798	MET	2.4
1	A	1025	PHE	2.4
1	A	60	THR	2.4
1	A	800	PRO	2.4
1	A	460	GLY	2.4
1	A	162	MET	2.4
1	A	112	GLN	2.4
1	A	388	PHE	2.4
1	A	288	GLY	2.3
1	A	444	GLY	2.3
1	A	1035	ARG	2.3
1	A	682	PHE	2.3
1	A	773	VAL	2.3
1	A	287	SER	2.3
1	A	352	PHE	2.3
1	A	827	ILE	2.3
1	A	456	MET	2.3
1	A	96	SER	2.3
1	A	1034	SER	2.3
1	A	713	LEU	2.3
1	A	931	LEU	2.3
1	A	210	GLN	2.3
1	A	187	TRP	2.3
1	A	587	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	948	PHE	2.3
1	A	197	GLN	2.3
1	A	146	ASP	2.3
1	A	408	ASP	2.3
1	A	549	VAL	2.3
1	A	277	ILE	2.2
1	A	86	GLY	2.2
1	A	209	ALA	2.2
1	A	996	GLY	2.2
1	A	181	GLN	2.2
1	A	909	VAL	2.2
1	A	410	ILE	2.2
1	A	442	LEU	2.2
1	A	464	GLY	2.2
1	A	497	LEU	2.2
1	A	614	GLY	2.2
1	A	902	MET	2.2
1	A	275	TYR	2.2
1	A	132	SER	2.2
1	A	849	SER	2.2
1	A	622	GLN	2.2
1	A	693	GLU	2.2
1	A	76	MET	2.2
1	A	198	LEU	2.2
1	A	586	ARG	2.2
1	A	199	THR	2.2
1	A	749	THR	2.2
1	A	880	SER	2.2
1	A	1036	LYS	2.2
1	A	104	GLN	2.2
1	A	914	LEU	2.2
1	A	42	ALA	2.2
1	A	874	PRO	2.2
1	A	940	LYS	2.2
1	A	928	GLN	2.1
1	A	180	SER	2.1
1	A	708	LYS	2.1
1	A	66	GLU	2.1
1	A	387	GLY	2.1
1	A	517	ASN	2.1
1	A	253	VAL	2.1
1	A	624	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	397	GLY	2.1
1	A	139	VAL	2.1
1	A	406	VAL	2.1
1	A	65	ILE	2.1
1	A	758	TYR	2.1
1	A	811	TYR	2.1
1	A	852	PRO	2.1
1	A	924	ASP	2.1
1	A	463	THR	2.1
1	A	32	VAL	2.1
1	A	594	VAL	2.1
1	A	667	ASN	2.1
1	A	261	LEU	2.1
1	A	325	TYR	2.1
1	A	297	ALA	2.1
1	A	482	VAL	2.0
1	A	369	THR	2.0
1	A	489	THR	2.0
1	A	597	TYR	2.0
1	A	171	GLY	2.0
1	A	14	VAL	2.0
1	A	168	ARG	2.0
1	A	468	ARG	2.0
1	A	591	LEU	2.0
1	A	148	THR	2.0
1	A	764	ASP	2.0
1	A	225	VAL	2.0
1	A	855	VAL	2.0
1	A	578	LEU	2.0
1	A	945	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

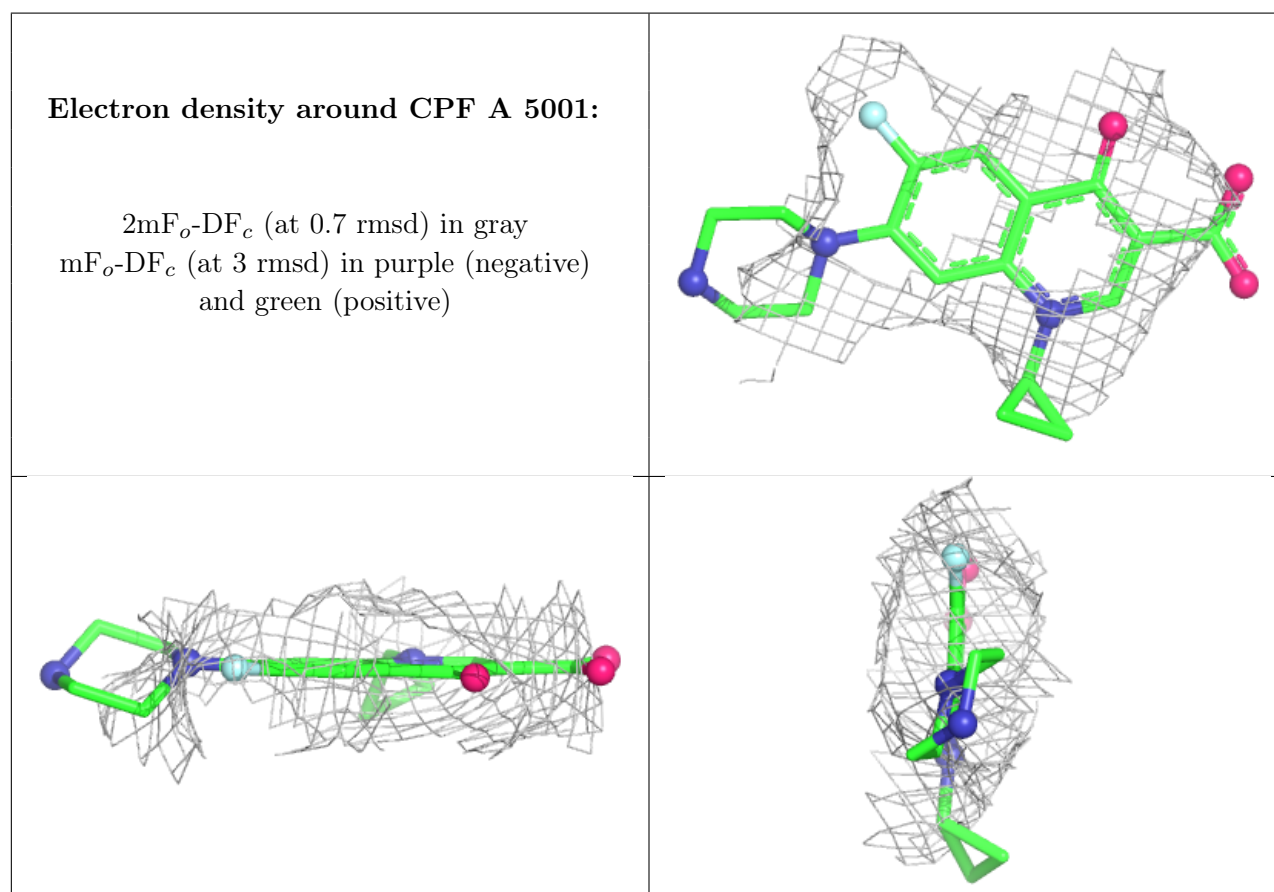
There are no oligosaccharides in this entry.

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	CPF	A	5001	24/24	0.46	0.14	150,167,172,181	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.