



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 PM UTC

PDB ID : 3UDI / pdb_00003udi
Title : Crystal structure of Acinetobacter baumannii PBP1a in complex with penicillin G
Authors : Han, S.
Deposited on : 2011-10-28
Resolution : 2.60 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

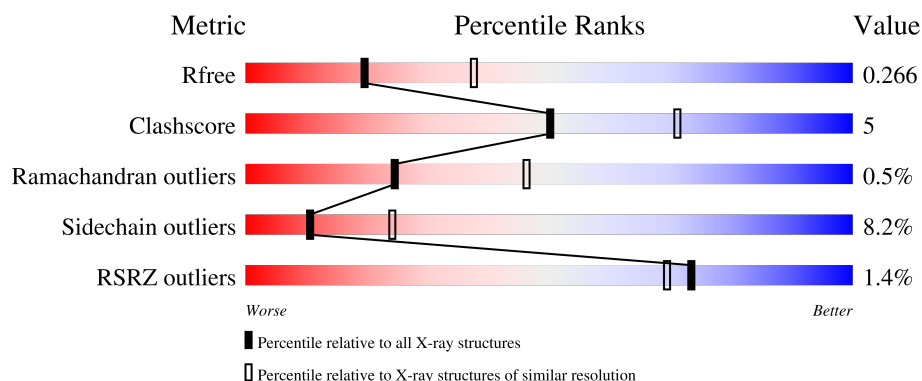
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	731	2% 64% 15% • 18%
1	B	731	% 66% 14% • 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9726 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 Penicillin-binding protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4723	3010	834	863	16			
1	B	601	Total	C	N	O	S	0	0	0
			4734	3014	837	867	16			

There are 32 discrepancies between the modelled and reference sequences:

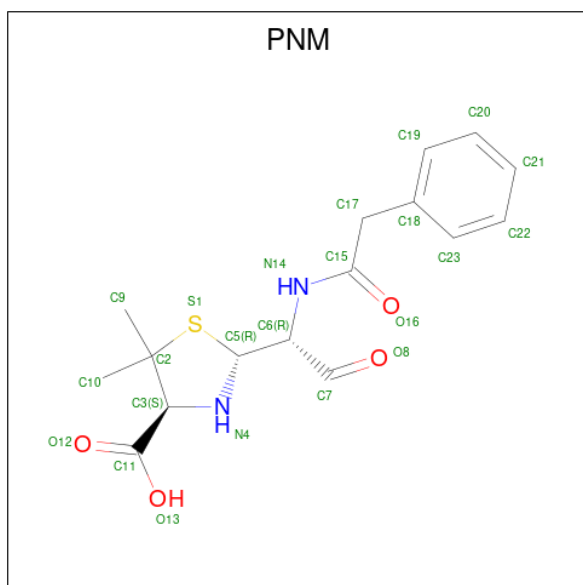
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP G1C794
A	10	HIS	-	expression tag	UNP G1C794
A	11	HIS	-	expression tag	UNP G1C794
A	12	HIS	-	expression tag	UNP G1C794
A	13	HIS	-	expression tag	UNP G1C794
A	14	HIS	-	expression tag	UNP G1C794
A	15	HIS	-	expression tag	UNP G1C794
A	16	GLU	-	expression tag	UNP G1C794
A	17	ASN	-	expression tag	UNP G1C794
A	18	LEU	-	expression tag	UNP G1C794
A	19	TYR	-	expression tag	UNP G1C794
A	20	PHE	-	expression tag	UNP G1C794
A	21	GLN	-	expression tag	UNP G1C794
A	22	SER	-	expression tag	UNP G1C794
A	23	HIS	-	expression tag	UNP G1C794
A	24	MET	-	expression tag	UNP G1C794
B	9	MET	-	expression tag	UNP G1C794
B	10	HIS	-	expression tag	UNP G1C794
B	11	HIS	-	expression tag	UNP G1C794
B	12	HIS	-	expression tag	UNP G1C794
B	13	HIS	-	expression tag	UNP G1C794
B	14	HIS	-	expression tag	UNP G1C794
B	15	HIS	-	expression tag	UNP G1C794
B	16	GLU	-	expression tag	UNP G1C794
B	17	ASN	-	expression tag	UNP G1C794

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Chain	Residue	Modelled	Actual	Comment	Reference
B	18	LEU	-	expression tag	UNP G1C794
B	19	TYR	-	expression tag	UNP G1C794
B	20	PHE	-	expression tag	UNP G1C794
B	21	GLN	-	expression tag	UNP G1C794
B	22	SER	-	expression tag	UNP G1C794
B	23	HIS	-	expression tag	UNP G1C794
B	24	MET	-	expression tag	UNP G1C794

- Molecule 2 is OPEN FORM - PENICILLIN G (CCD ID: PNM) (formula: $C_{16}H_{20}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	16	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			23	16	2	4	1		

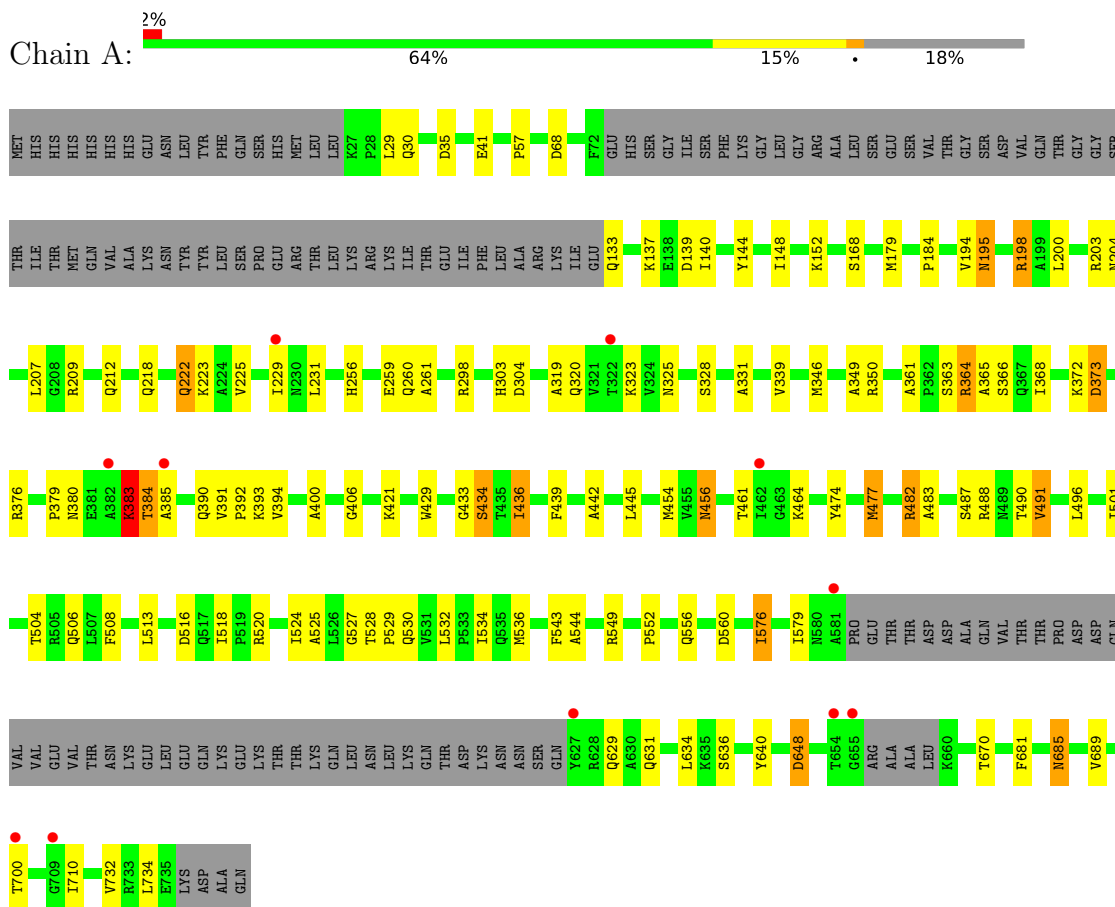
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	146	Total	O	0	0
			146	146		

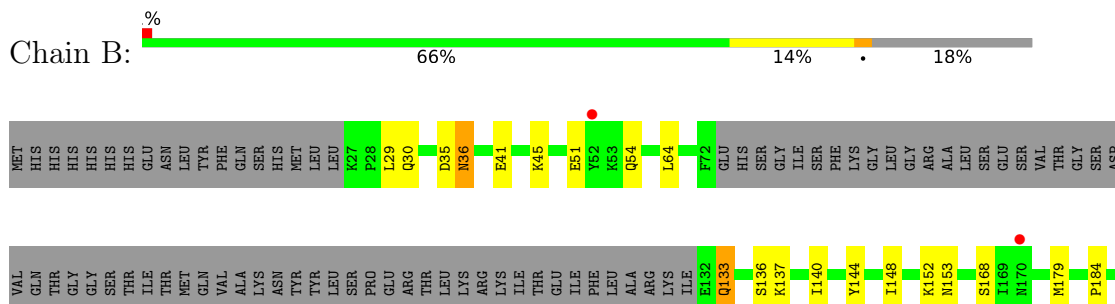
3 Residue-property plots

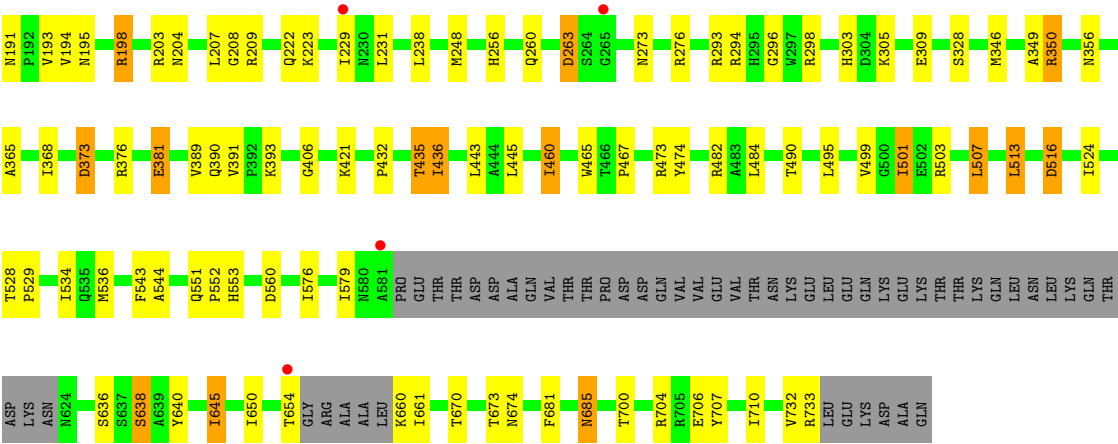
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Penicillin-binding protein 1a



- Molecule 1: Penicillin-binding protein 1a





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 242.68Å 49.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.08 – 2.60 48.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.08-2.60) 91.5 (48.08-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.187 , 0.250 0.201 , 0.266	Depositor DCC
R_{free} test set	2060 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9726	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: PNM

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	0.84	0/4832	1.33	22/6552 (0.3%)
1	B	0.87	1/4843 (0.0%)	1.35	27/6567 (0.4%)
All	All	0.85	1/9675 (0.0%)	1.34	49/13119 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	248	MET	SD-CE	6.07	1.94	1.79

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	706	GLU	N-CA-C	7.43	120.76	109.62
1	B	576	ILE	N-CA-CB	7.35	116.19	110.45
1	B	674	ASN	CA-CB-CG	7.18	119.78	112.60
1	A	393	LYS	N-CA-C	-6.94	103.49	112.23
1	A	456	ASN	CA-CB-CG	6.73	119.33	112.60
1	B	393	LYS	N-CA-C	-6.72	104.56	112.89
1	A	576	ILE	N-CA-CB	6.71	115.69	110.45
1	B	685	ASN	CA-CB-CG	6.53	119.13	112.60
1	A	685	ASN	CA-CB-CG	6.34	118.94	112.60
1	A	464	LYS	CA-C-N	6.18	131.63	121.86
1	A	464	LYS	C-N-CA	6.18	131.63	121.86
1	A	456	ASN	N-CA-C	5.94	118.21	108.52
1	B	516	ASP	CA-CB-CG	5.83	118.43	112.60
1	B	168	SER	N-CA-C	-5.69	102.10	110.52
1	B	36	ASN	N-CA-C	5.63	119.73	112.86
1	B	560	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	532	LEU	N-CA-C	-5.58	102.61	110.31
1	A	648	ASP	CA-CB-CG	5.55	118.15	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	685	ASN	N-CA-C	-5.53	101.06	108.86
1	A	543	PHE	CA-C-N	5.52	128.44	120.38
1	A	543	PHE	C-N-CA	5.52	128.44	120.38
1	A	139	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	153	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	184	PRO	CA-C-N	5.46	127.91	120.54
1	A	184	PRO	C-N-CA	5.46	127.91	120.54
1	A	168	SER	N-CA-C	-5.44	102.47	110.52
1	B	350	ARG	N-CA-C	-5.43	101.65	109.48
1	A	373	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	560	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	373	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	198	ARG	CA-C-N	5.35	127.45	120.28
1	B	198	ARG	C-N-CA	5.35	127.45	120.28
1	B	296	GLY	CA-C-N	5.33	128.41	120.95
1	B	296	GLY	C-N-CA	5.33	128.41	120.95
1	A	685	ASN	N-CA-C	-5.32	101.36	108.86
1	B	208	GLY	CA-C-N	5.24	127.31	120.28
1	B	208	GLY	C-N-CA	5.24	127.31	120.28
1	A	482	ARG	CA-C-N	5.23	127.29	120.28
1	A	482	ARG	C-N-CA	5.23	127.29	120.28
1	B	650	ILE	N-CA-C	5.20	116.67	111.00
1	B	645	ILE	N-CA-C	-5.17	105.46	110.42
1	A	501	ILE	CA-C-N	5.12	127.09	120.44
1	A	501	ILE	C-N-CA	5.12	127.09	120.44
1	B	184	PRO	CA-C-N	5.08	127.40	120.54
1	B	184	PRO	C-N-CA	5.08	127.40	120.54
1	B	543	PHE	CA-C-N	5.06	127.77	120.38
1	B	543	PHE	C-N-CA	5.06	127.77	120.38
1	B	482	ARG	CA-C-N	5.05	127.05	120.28
1	B	482	ARG	C-N-CA	5.05	127.05	120.28

There are no chirality outliers.

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	4723	0	4707	55	0
1	B	4734	0	4712	50	0
2	A	23	0	18	1	0
2	B	23	0	18	3	0
3	A	77	0	0	1	0
3	B	146	0	0	1	0
All	All	9726	0	9455	101	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 5.

All (101) 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:298:ARG:H	1:A:390:GLN:HE22	1.19	0.90
1:B:298:ARG:H	1:B:390:GLN:HE22	1.17	0.89
1:A:323:LYS:HE3	1:A:325:ASN:HD21	1.53	0.73
1:B:435:THR:HG22	1:B:536:MET:HE2	1.73	0.70
1:A:350:ARG:HG2	1:A:361:ALA:HA	1.79	0.64
1:B:707:TYR:HE1	2:B:999:PNM:H21	1.62	0.64
1:B:328:SER:HA	1:B:346:MET:HE1	1.80	0.63
1:A:137:LYS:NZ	1:B:256:HIS:HD2	1.96	0.63
1:A:436:ILE:HG12	1:A:508:PHE:HZ	1.63	0.63
1:A:488:ARG:HB2	1:A:491:VAL:HG12	1.81	0.62
1:A:488:ARG:HB2	1:A:491:VAL:CG1	2.30	0.62
1:A:303:HIS:HD2	1:A:373:ASP:OD1	1.83	0.61
1:B:528:THR:N	1:B:529:PRO:HD2	2.15	0.61
1:B:303:HIS:HD2	1:B:373:ASP:OD1	1.83	0.60
1:A:229:ILE:HG22	1:A:231:LEU:HG	1.84	0.59
1:A:436:ILE:HG12	1:A:508:PHE:CZ	2.37	0.59
1:B:707:TYR:CE1	2:B:999:PNM:H21	2.38	0.58
1:A:57:PRO:HD2	3:A:759:HOH:O	2.04	0.57
1:B:229:ILE:HG22	1:B:231:LEU:HG	1.84	0.57
1:B:435:THR:CG2	1:B:536:MET:HE2	2.34	0.57
1:B:406:GLY:O	1:B:552:PRO:HA	2.05	0.57
1:A:524:ILE:HG22	1:A:529:PRO:HG3	1.87	0.56
1:A:218:GLN:O	1:A:222:GLN:HG2	2.06	0.56
1:B:551:GLN:O	1:B:553:HIS:HD2	1.89	0.56
1:A:406:GLY:O	1:A:552:PRO:HA	2.08	0.54
1:A:209:ARG:NH2	1:A:212:GLN:HE22	2.06	0.54
1:A:483:ALA:HB1	1:A:491:VAL:HG11	1.89	0.53
1:B:524:ILE:HG22	1:B:529:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:MET:HE2	1:B:203:ARG:HD3	1.91	0.52
1:A:496:LEU:HD22	1:A:525:ALA:HB2	1.93	0.51
1:B:294:ARG:HA	1:B:350:ARG:HH22	1.75	0.51
1:B:654:THR:HG21	1:B:660:LYS:N	2.27	0.50
1:A:179:MET:HE2	1:A:203:ARG:HD3	1.93	0.50
1:A:376:ARG:HD2	1:A:391:VAL:HG23	1.94	0.50
1:A:195:ASN:HD21	1:A:198:ARG:HD2	1.77	0.49
1:B:229:ILE:HG21	1:B:231:LEU:CD1	2.42	0.49
1:A:229:ILE:HG21	1:A:231:LEU:HD11	1.94	0.48
1:A:487:SER:HB2	2:A:998:PNM:HC5	1.93	0.48
1:A:670:THR:HG22	1:A:681:PHE:HD1	1.79	0.48
1:A:229:ILE:HG21	1:A:231:LEU:CD1	2.44	0.48
1:A:504:THR:O	1:A:508:PHE:HD1	1.97	0.48
1:A:328:SER:HA	1:A:346:MET:HE1	1.95	0.48
1:B:376:ARG:HD2	1:B:391:VAL:HG23	1.97	0.47
1:A:433:GLY:O	1:A:527:GLY:HA3	2.15	0.47
1:B:229:ILE:HG21	1:B:231:LEU:HD12	1.97	0.46
1:B:673:THR:O	2:B:999:PNM:H19	2.15	0.46
1:B:356:ASN:HD21	1:B:704:ARG:H	1.63	0.46
1:B:191:ASN:HB3	1:B:194:VAL:HB	1.96	0.45
1:B:670:THR:HG22	1:B:681:PHE:HD1	1.80	0.45
1:A:454:MET:HB3	1:A:477:MET:HG3	1.98	0.45
1:B:551:GLN:O	1:B:553:HIS:CD2	2.69	0.45
1:B:293:ARG:HH12	1:B:389:VAL:HG12	1.82	0.45
1:A:365:ALA:HA	1:A:368:ILE:HD12	1.99	0.45
1:B:484:LEU:HD23	1:B:645:ILE:HG21	1.98	0.45
1:B:495:LEU:O	1:B:499:VAL:HG22	2.17	0.44
1:B:365:ALA:HA	1:B:368:ILE:HD12	1.99	0.44
1:A:195:ASN:ND2	1:A:198:ARG:HD2	2.33	0.44
1:A:528:THR:N	1:A:529:PRO:HD2	2.32	0.44
1:A:30:GLN:HG2	1:A:41:GLU:HG2	2.00	0.44
1:A:204:ASN:HA	1:A:207:LEU:HD12	2.00	0.44
1:B:474:TYR:HE1	1:B:490:THR:HG21	1.83	0.44
1:A:364:ARG:HE	1:A:366:SER:HG	1.65	0.44
1:B:432:PRO:O	1:B:435:THR:HB	2.18	0.44
1:B:443:LEU:HB2	1:B:507:LEU:HD22	2.00	0.43
1:A:474:TYR:HE1	1:A:490:THR:HG21	1.83	0.43
1:A:640:TYR:CD1	1:A:732:VAL:HG23	2.53	0.43
1:A:544:ALA:HA	1:A:732:VAL:HG12	1.99	0.43
1:A:261:ALA:HA	1:B:144:TYR:CE1	2.54	0.43
1:B:465:TRP:CZ2	1:B:467:PRO:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:HD21	1:A:385:ALA:HB3	1.84	0.42
1:A:640:TYR:CD1	1:A:734:LEU:HB2	2.54	0.42
1:B:501:ILE:H	1:B:501:ILE:HG13	1.57	0.42
1:B:273:ASN:HB3	1:B:276:ARG:HB2	2.01	0.42
1:B:544:ALA:HA	1:B:732:VAL:HG12	2.01	0.42
1:A:392:PRO:HB3	1:A:394:VAL:HG12	2.00	0.42
1:B:640:TYR:CD1	1:B:732:VAL:HG23	2.54	0.42
1:A:442:ALA:HB1	1:A:634:LEU:HD21	2.01	0.42
1:B:51:GLU:HB2	1:B:54:GLN:HG3	2.02	0.42
1:A:319:ALA:HB1	1:A:331:ALA:HB1	2.01	0.42
1:B:707:TYR:HB3	3:B:881:HOH:O	2.18	0.42
1:B:460:ILE:HG22	1:B:490:THR:HG22	2.02	0.42
1:A:144:TYR:O	1:A:148:ILE:HG13	2.20	0.41
1:A:576:ILE:HD11	1:A:629:GLN:HB2	2.02	0.41
1:B:204:ASN:HA	1:B:207:LEU:HD12	2.01	0.41
1:B:445:LEU:HB3	1:B:638:SER:HB3	2.01	0.41
1:A:229:ILE:CG2	1:A:231:LEU:CD1	2.98	0.41
1:A:434:SER:OG	1:A:487:SER:HB3	2.19	0.41
1:A:256:HIS:HD2	1:B:137:LYS:NZ	2.18	0.41
1:B:356:ASN:ND2	1:B:704:ARG:H	2.18	0.41
1:A:400:ALA:HA	1:A:689:VAL:O	2.20	0.41
1:A:429:TRP:HB3	1:A:530:GLN:HB3	2.02	0.41
1:A:439:PHE:HE2	1:A:536:MET:HE1	1.85	0.41
1:B:30:GLN:HG2	1:B:41:GLU:HG2	2.03	0.41
1:B:144:TYR:O	1:B:148:ILE:HG13	2.20	0.41
1:A:320:GLN:HE21	1:A:372:LYS:HG2	1.86	0.41
1:A:383:LYS:HB3	1:A:384:THR:H	1.66	0.41
1:B:45:LYS:H	1:B:263:ASP:HB3	1.86	0.41
1:B:436:ILE:HD11	1:B:513:LEU:HD21	2.02	0.41
1:B:381:GLU:H	1:B:381:GLU:CD	2.29	0.40
1:A:549:ARG:HH22	1:B:133:GLN:HE22	1.68	0.40
1:A:488:ARG:O	1:A:491:VAL:HG13	2.22	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	592/731 (81%)	557 (94%)	30 (5%)	5 (1%)	16	34
1	B	593/731 (81%)	560 (94%)	32 (5%)	1 (0%)	43	66
All	All	1185/1462 (81%)	1117 (94%)	62 (5%)	6 (0%)	24	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	LYS
1	A	349	ALA
1	B	349	ALA
1	A	384	THR
1	A	379	PRO
1	A	579	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	490/608 (81%)	448 (91%)	42 (9%)	10	22
1	B	492/608 (81%)	453 (92%)	39 (8%)	11	26
All	All	982/1216 (81%)	901 (92%)	81 (8%)	10	24

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	35	ASP
1	A	68	ASP
1	A	133	GLN
1	A	140	ILE
1	A	152	LYS

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Mol	Chain	Res	Type
1	A	194	VAL
1	A	195	ASN
1	A	198	ARG
1	A	200	LEU
1	A	222	GLN
1	A	223	LYS
1	A	225	VAL
1	A	259	GLU
1	A	260	GLN
1	A	304	ASP
1	A	339	VAL
1	A	363	SER
1	A	364	ARG
1	A	383	LYS
1	A	421	LYS
1	A	434	SER
1	A	436	ILE
1	A	445	LEU
1	A	456	ASN
1	A	461	THR
1	A	477	MET
1	A	482	ARG
1	A	491	VAL
1	A	506	GLN
1	A	513	LEU
1	A	516	ASP
1	A	518	ILE
1	A	520	ARG
1	A	534	ILE
1	A	556	GLN
1	A	631	GLN
1	A	636	SER
1	A	648	ASP
1	A	685	ASN
1	A	700	THR
1	A	710	ILE
1	B	29	LEU
1	B	35	ASP
1	B	36	ASN
1	B	64	LEU
1	B	133	GLN
1	B	136	SER

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Mol	Chain	Res	Type
1	B	140	ILE
1	B	152	LYS
1	B	193	VAL
1	B	195	ASN
1	B	198	ARG
1	B	209	ARG
1	B	222	GLN
1	B	223	LYS
1	B	238	LEU
1	B	260	GLN
1	B	263	ASP
1	B	305	LYS
1	B	309	GLU
1	B	381	GLU
1	B	421	LYS
1	B	435	THR
1	B	436	ILE
1	B	460	ILE
1	B	473	ARG
1	B	501	ILE
1	B	503	ARG
1	B	507	LEU
1	B	513	LEU
1	B	516	ASP
1	B	534	ILE
1	B	579	ILE
1	B	636	SER
1	B	638	SER
1	B	661	ILE
1	B	685	ASN
1	B	700	THR
1	B	710	ILE
1	B	733	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	36	ASN
1	A	170	ASN
1	A	195	ASN
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	256	HIS
1	A	303	HIS
1	A	320	GLN
1	A	325	ASN
1	A	380	ASN
1	A	390	GLN
1	A	402	ASN
1	A	456	ASN
1	A	530	GLN
1	A	553	HIS
1	A	556	GLN
1	A	629	GLN
1	A	722	GLN
1	A	725	GLN
1	B	30	GLN
1	B	170	ASN
1	B	195	ASN
1	B	256	HIS
1	B	303	HIS
1	B	320	GLN
1	B	356	ASN
1	B	390	GLN
1	B	402	ASN
1	B	456	ASN
1	B	553	HIS
1	B	722	GLN

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	PNM	B	999	1	19,24,24	0.82	1 (5%)	25,34,34	1.46	5 (20%)
2	PNM	A	998	1	19,24,24	0.88	1 (5%)	25,34,34	1.40	2 (8%)

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	PNM	B	999	1	-	4/12/33/33	0/2/2/2
2	PNM	A	998	1	-	4/12/33/33	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	998	PNM	O13-C11	-2.47	1.22	1.30
2	B	999	PNM	O13-C11	-2.32	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	PNM	C2-C3-C11	3.80	119.55	112.37
2	A	998	PNM	C2-C3-C11	3.35	118.71	112.37
2	A	998	PNM	C17-C15-N14	3.04	120.61	115.88
2	B	999	PNM	C17-C15-N14	2.84	120.30	115.88
2	B	999	PNM	C3-C2-S1	-2.34	99.41	103.86
2	B	999	PNM	C2-S1-C5	2.20	99.00	93.41
2	B	999	PNM	O8-C7-C6	-2.07	119.38	124.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

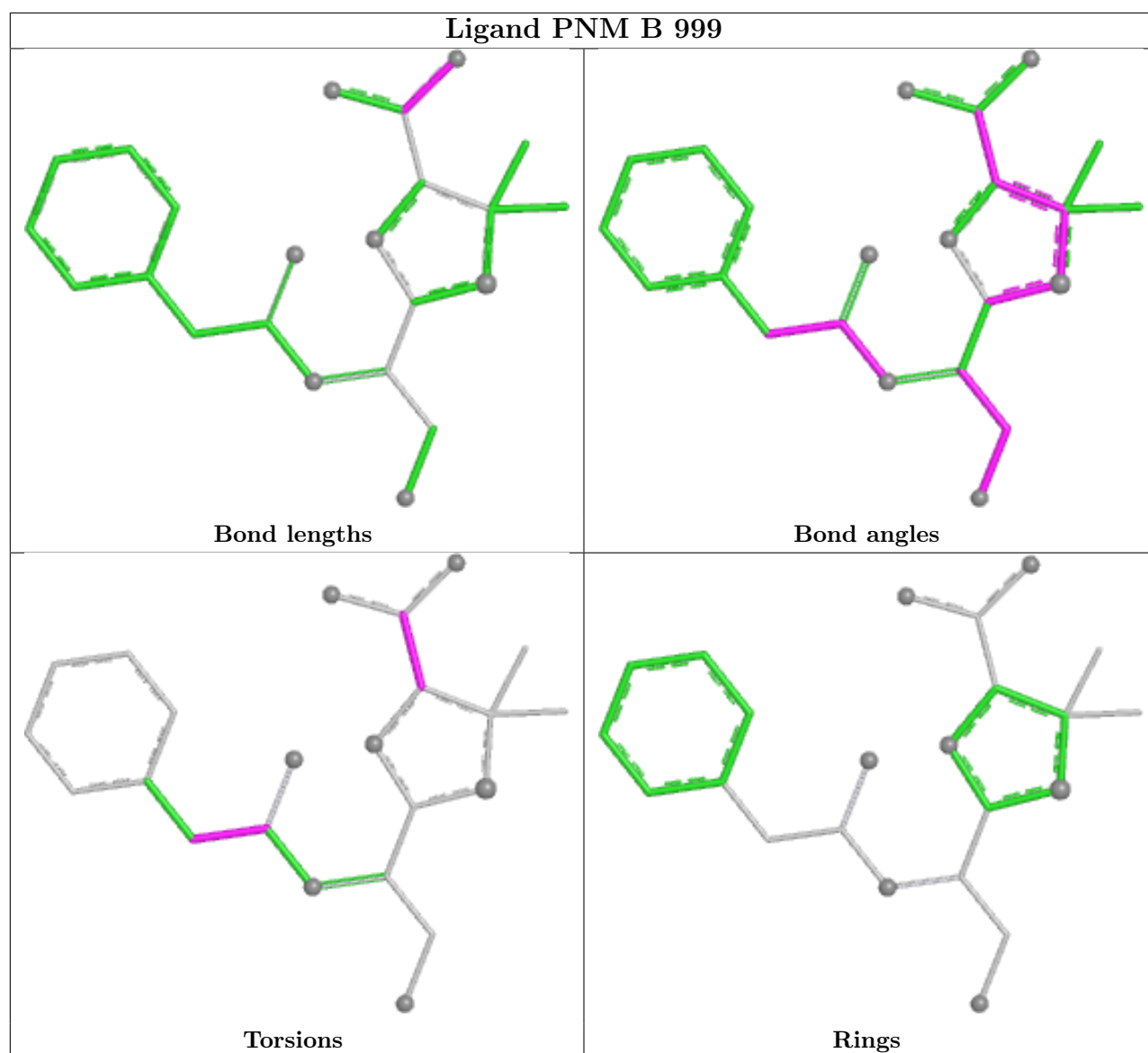
Mol	Chain	Res	Type	Atoms
2	A	998	PNM	O12-C11-C3-N4
2	B	999	PNM	O13-C11-C3-C2
2	B	999	PNM	O12-C11-C3-C2
2	A	998	PNM	O13-C11-C3-N4
2	A	998	PNM	C15-C17-C18-C19
2	A	998	PNM	C15-C17-C18-C23
2	B	999	PNM	O16-C15-C17-C18
2	B	999	PNM	N14-C15-C17-C18

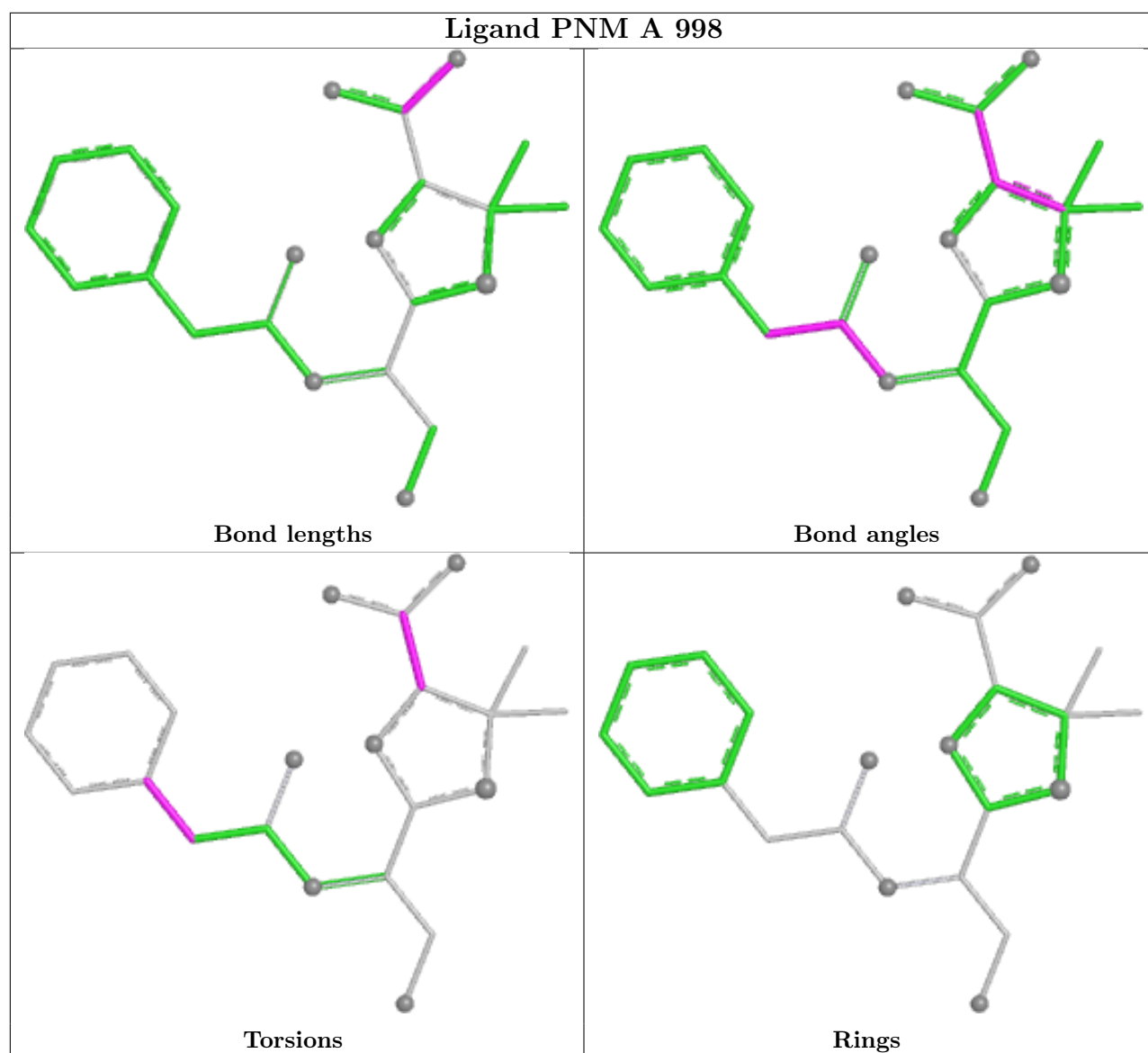
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	999	PNM	3	0
2	A	998	PNM	1	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 ⓘ

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	600/731 (82%)	0.17	11 (1%) 67 63	43, 77, 129, 165	0
1	B	601/731 (82%)	-0.07	6 (0%) 79 76	26, 66, 113, 141	0
All	All	1201/1462 (82%)	0.05	17 (1%) 73 69	26, 73, 122, 165	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	655	GLY	3.9
1	A	462	ILE	3.1
1	B	581	ALA	2.7
1	A	581	ALA	2.6
1	A	654	THR	2.5
1	B	654	THR	2.4
1	B	265	GLY	2.4
1	A	322	THR	2.3
1	B	170	ASN	2.2
1	A	382	ALA	2.1
1	A	229	ILE	2.1
1	B	229	ILE	2.1
1	A	700	THR	2.1
1	A	385	ALA	2.0
1	A	709	GLY	2.0
1	A	627	TYR	2.0
1	B	52	TYR	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

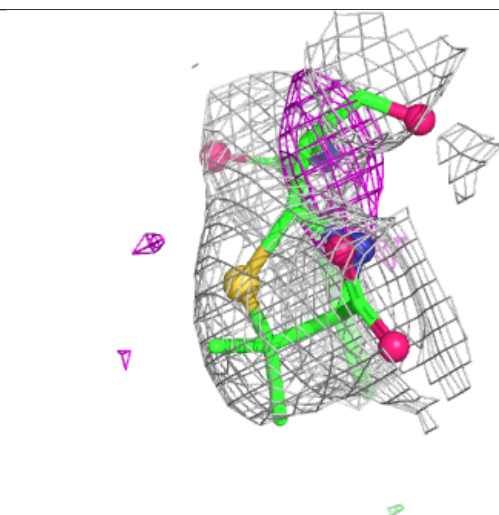
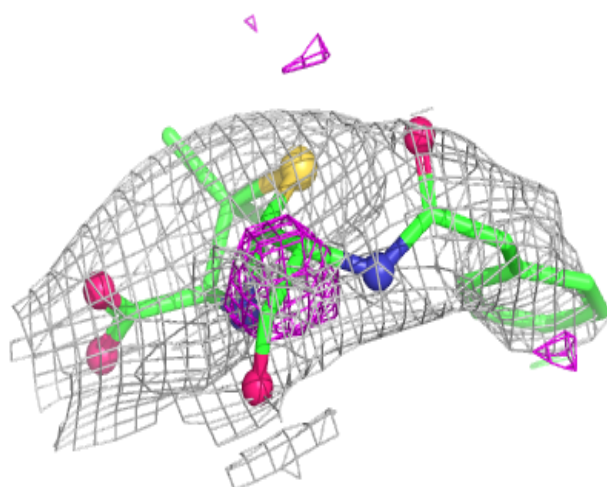
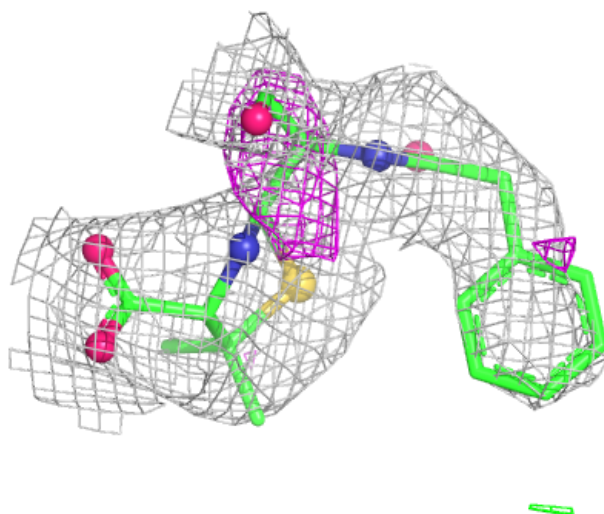
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

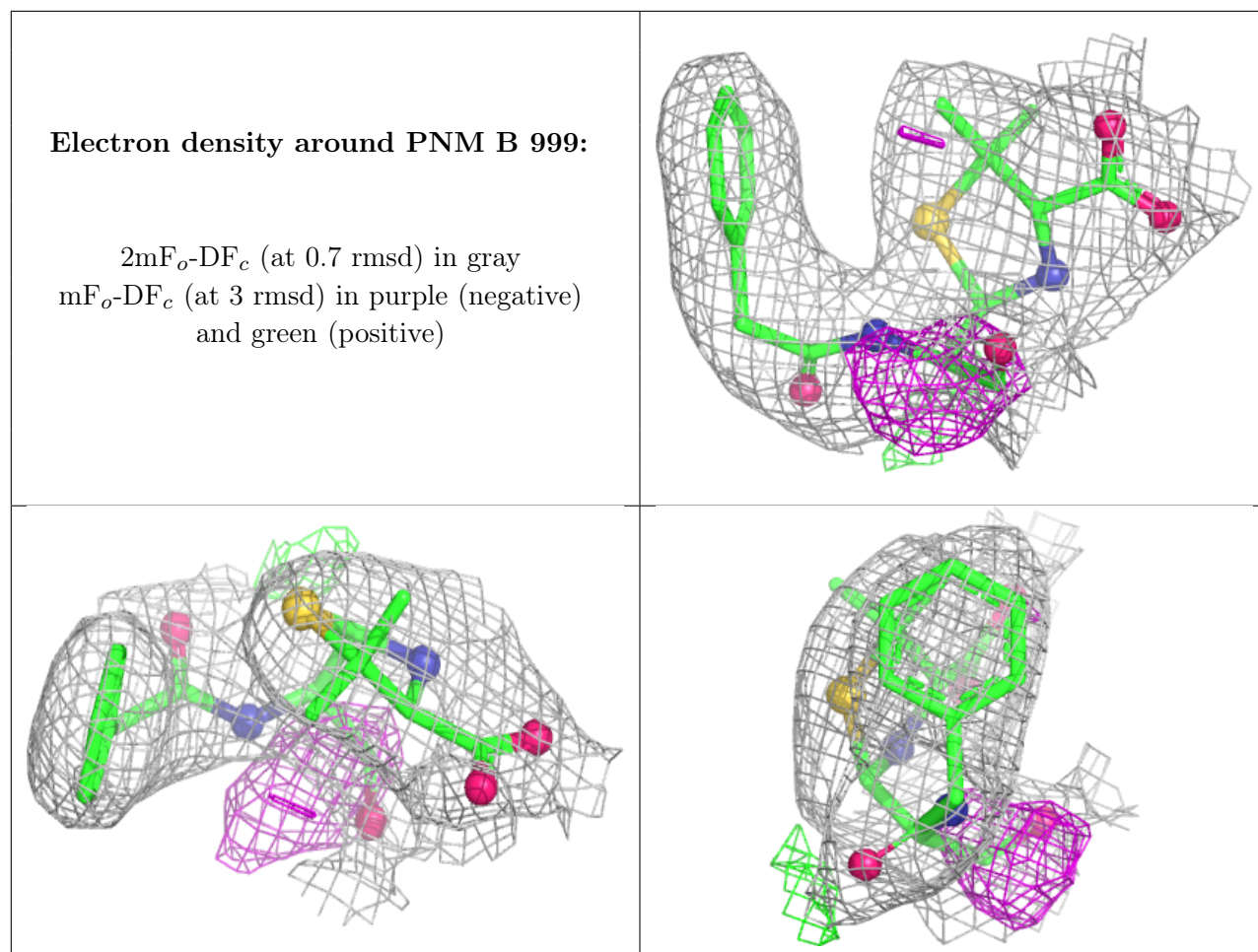
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PNM	A	998	23/23	0.82	0.15	97,100,101,101	0
2	PNM	B	999	23/23	0.87	0.11	55,74,78,81	0

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 PNM A 998:

$2mF_o-DF_c$ (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.