



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:35 AM UTC

PDB ID : 7O4B / pdb_00007o4b
Title : Crystal structure of Penicillin-Binding Protein 1 (PBP1) from *Staphylococcus aureus* in complex with penicillin G
Authors : Martinez Caballero, S.; Hermoso, J.A.
Deposited on : 2021-04-05
Resolution : 2.59 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

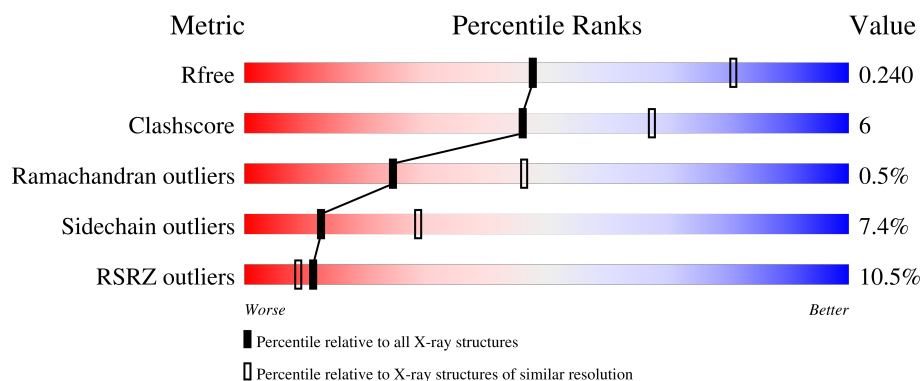
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	650	8% 63% 13% • 23%
1	C	650	8% 60% 12% • 26%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7888 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.

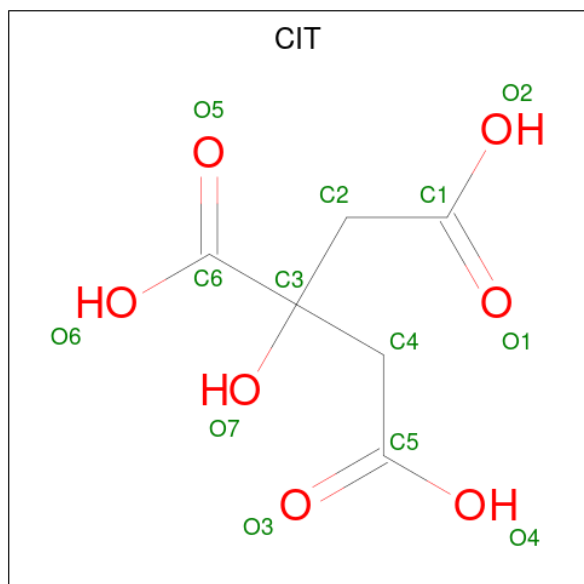
- Molecule 1 is a protein called Penicillin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3959	2512	681	750	16			
1	C	479	Total	C	N	O	S	0	0	0
			3750	2380	639	716	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	initiating methionine	UNP A0A0H2WVW5
C	64	MET	-	initiating methionine	UNP A0A0H2WVW5

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



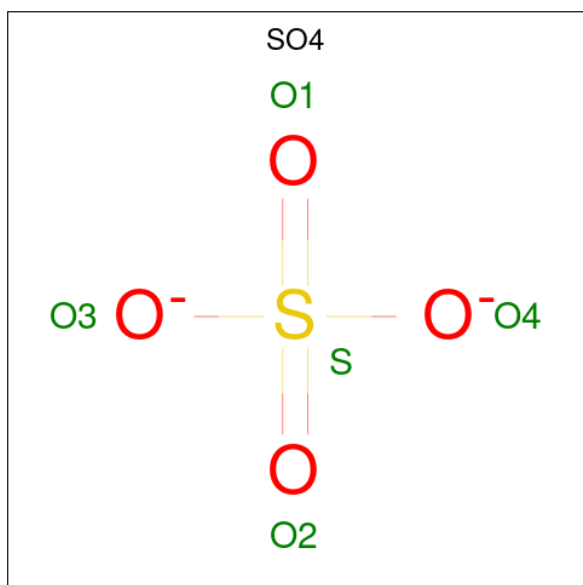
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



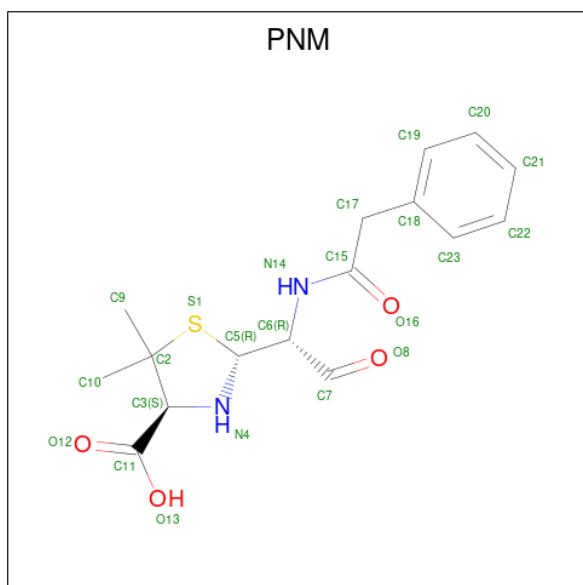
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is OPEN FORM - PENICILLIN G (CCD ID: PNM) (formula: $C_{16}H_{20}N_2O_4S$).



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

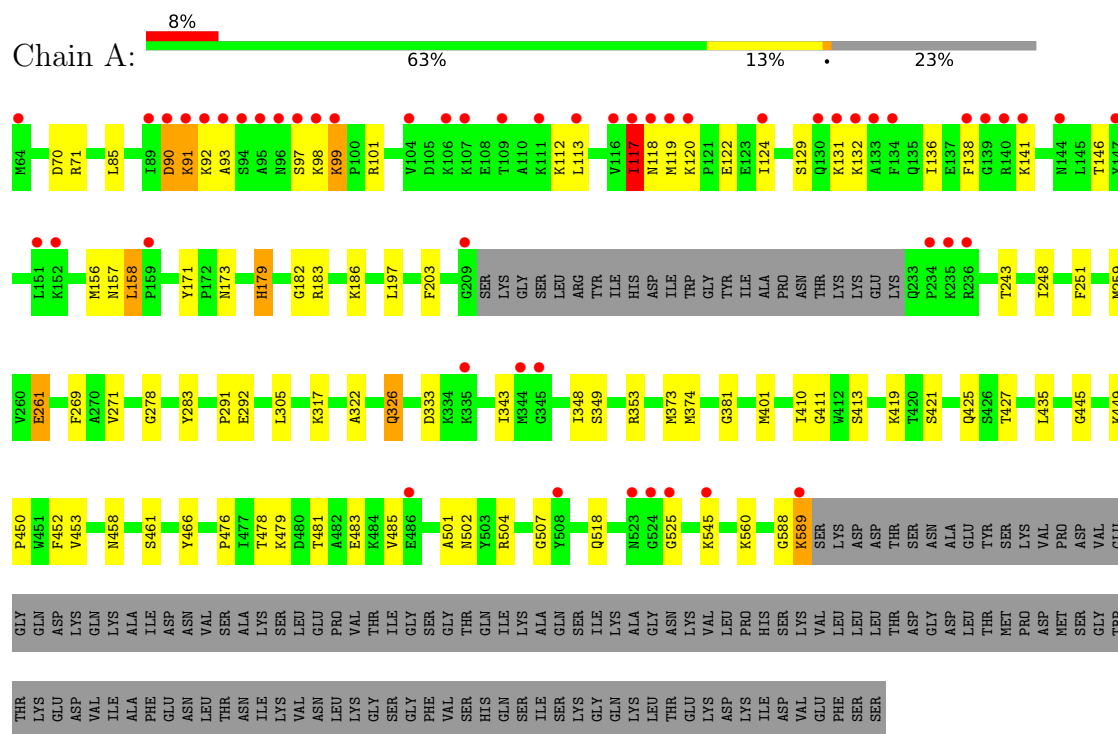
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	C	13	Total	O	0	0
			13	13		

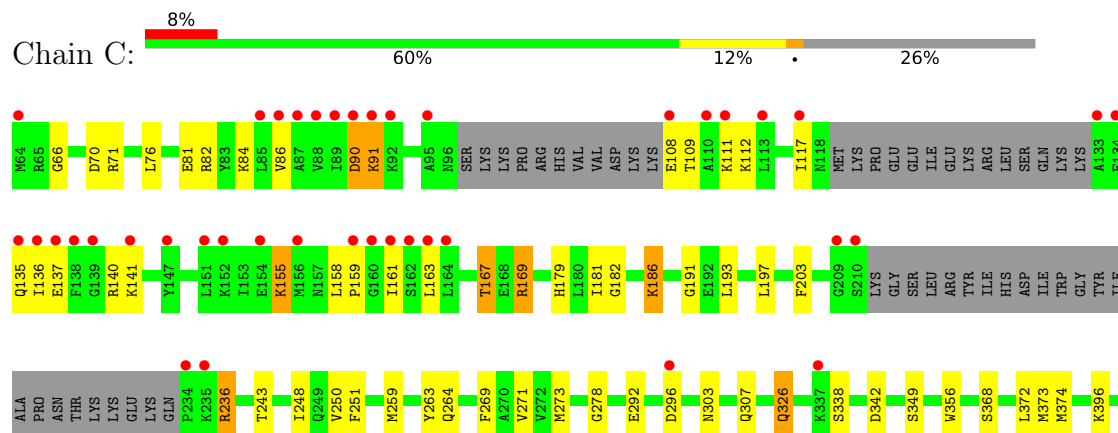
3 Residue-property plots [i](#)

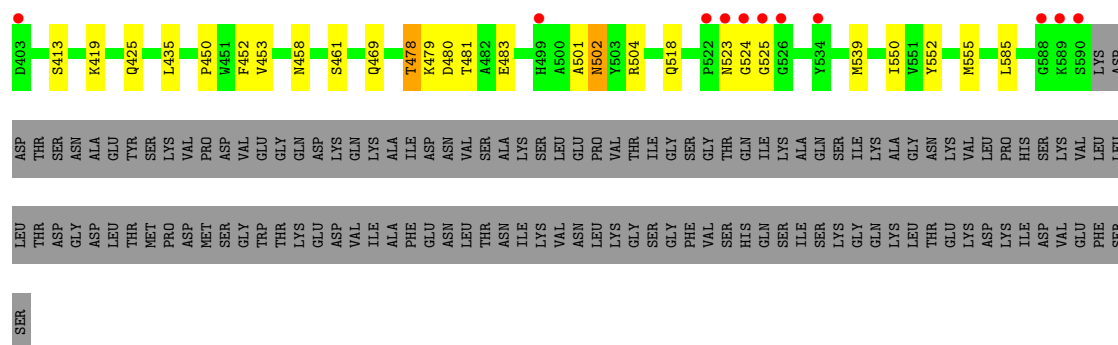
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Penicillin-binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	180.65Å 180.65Å 223.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.51 – 2.59 47.51 – 2.59	Depositor EDS
% Data completeness (in resolution range)	67.4 (47.51-2.59) 67.4 (47.51-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.241 0.207 , 0.240	Depositor DCC
R_{free} test set	2318 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7888	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PNM, SO4, CIT

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	1.03	1/4043 (0.0%)	1.41	1/5436 (0.0%)
1	C	1.01	0/3829	1.41	4/5151 (0.1%)
All	All	1.02	1/7872 (0.0%)	1.41	5/10587 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	HIS	CE1-NE2	6.00	1.38	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	478	THR	CA-CB-OG1	-6.42	99.97	109.60
1	C	296	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	342	ASP	CB-CA-C	5.21	119.12	110.78
1	A	171	TYR	CB-CA-C	5.15	116.01	110.65
1	C	90	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3959	0	3947	47	0
1	C	3750	0	3708	42	0
2	A	26	0	10	1	0
2	C	13	0	5	1	0
3	A	25	0	0	0	0
3	C	30	0	0	0	0
4	A	23	0	18	0	0
4	C	23	0	18	1	0
5	A	26	0	0	0	0
5	C	13	0	0	1	0
All	All	7888	0	7706	90	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 6.

All (90) 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:C:259:MET:HE3	1:C:555:MET:HE2	1.65	0.78
1:A:410:ILE:HA	1:A:427:THR:HG22	1.65	0.77
1:C:167:THR:O	1:C:186:LYS:NZ	2.20	0.73
1:A:411:GLY:H	1:A:427:THR:HG22	1.54	0.73
1:A:425:GLN:HE22	1:A:518:GLN:H	1.39	0.70
1:A:113:LEU:HD11	1:A:124:ILE:HG21	1.74	0.69
1:C:425:GLN:HE22	1:C:518:GLN:H	1.41	0.68
1:C:273:MET:HE2	1:C:450:PRO:HB3	1.77	0.65
1:C:273:MET:CE	1:C:450:PRO:HB3	2.30	0.61
1:A:411:GLY:N	1:A:427:THR:HG22	2.15	0.61
1:C:243:THR:OG1	1:C:452:PHE:HA	2.02	0.59
1:A:243:THR:OG1	1:A:452:PHE:HA	2.01	0.59
1:A:113:LEU:CD1	1:A:124:ILE:HD13	2.33	0.58
1:A:117:ILE:HG22	1:A:118:ASN:H	1.68	0.57
1:C:81:GLU:O	1:C:82:ARG:NH1	2.38	0.57
1:C:539:MET:CE	1:C:550:ILE:HG23	2.36	0.56
1:C:182:GLY:HA3	1:C:197:LEU:O	2.08	0.54
1:A:93:ALA:HB1	1:A:101:ARG:HB2	1.90	0.53
1:C:326:GLN:NE2	1:C:481:THR:OG1	2.42	0.52
2:C:804:CIT:O1	2:C:804:CIT:O4	2.27	0.52
1:A:85:LEU:HD23	1:A:138:PHE:CD1	2.44	0.52
1:A:112:LYS:HB3	1:A:156:MET:HE3	1.90	0.52
1:A:507:GLY:O	1:A:589:LYS:HB3	2.10	0.51
1:A:182:GLY:HA3	1:A:197:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ASN:H	1:C:307:GLN:HE21	1.58	0.50
1:C:372:LEU:HG	1:C:373:MET:HE2	1.93	0.50
1:C:539:MET:HE2	1:C:550:ILE:HG23	1.93	0.50
1:C:66:GLY:HA2	1:C:236:ARG:HH21	1.76	0.49
1:A:326:GLN:NE2	1:A:481:THR:OG1	2.42	0.49
1:C:259:MET:CE	1:C:555:MET:HE2	2.39	0.49
1:A:203:PHE:CZ	1:A:453:VAL:HG21	2.49	0.48
1:A:381:GLY:HA3	2:A:803:CIT:O1	2.13	0.48
1:A:458:ASN:HB3	1:A:461:SER:OG	2.14	0.48
1:C:278:GLY:O	1:C:450:PRO:HA	2.14	0.48
1:C:368:SER:OG	4:C:808:PNM:HC5	2.14	0.48
1:C:186:LYS:HE3	1:C:191:GLY:O	2.13	0.47
1:A:401:MET:HE2	1:A:401:MET:HA	1.94	0.47
1:C:271:VAL:HG11	1:C:435:LEU:HD11	1.96	0.47
1:A:271:VAL:HG11	1:A:435:LEU:HD11	1.97	0.47
1:A:410:ILE:CA	1:A:427:THR:HG22	2.41	0.47
1:C:539:MET:CE	1:C:550:ILE:CG2	2.93	0.47
1:C:469:GLN:HG2	5:C:902:HOH:O	2.13	0.46
1:C:91:LYS:HD3	1:C:91:LYS:HA	1.69	0.46
1:C:155:LYS:HD3	1:C:155:LYS:HA	1.65	0.46
1:A:183:ARG:NH1	1:A:291:PRO:O	2.45	0.45
1:A:278:GLY:O	1:A:450:PRO:HA	2.16	0.45
1:A:343:ILE:HD12	1:A:419:LYS:HG3	1.97	0.45
1:A:421:SER:OG	1:A:427:THR:HG23	2.16	0.45
1:C:169:ARG:HG2	1:C:193:LEU:HD13	1.99	0.45
1:C:269:PHE:CD1	1:C:269:PHE:C	2.94	0.45
1:A:99:LYS:HA	1:A:99:LYS:HD2	1.61	0.45
1:A:156:MET:O	1:A:158:LEU:HD23	2.18	0.44
1:C:203:PHE:CZ	1:C:453:VAL:HG21	2.51	0.44
1:C:458:ASN:HB3	1:C:461:SER:OG	2.17	0.44
1:A:343:ILE:HG13	1:A:348:ILE:HD12	1.99	0.44
1:A:269:PHE:C	1:A:269:PHE:CD1	2.95	0.44
1:C:76:LEU:HD13	1:C:181:ILE:HD11	1.98	0.44
1:A:326:GLN:HE22	1:A:478:THR:H	1.64	0.44
1:A:479:LYS:O	1:A:483:GLU:HG3	2.17	0.44
1:C:501:ALA:HB1	1:C:504:ARG:NH1	2.32	0.44
1:A:322:ALA:HB2	1:A:485:VAL:HG21	2.00	0.43
1:A:501:ALA:O	1:A:504:ARG:HG3	2.18	0.43
1:C:479:LYS:O	1:C:483:GLU:HG3	2.18	0.43
1:C:76:LEU:HB3	1:C:181:ILE:HD13	1.99	0.43
1:C:109:THR:HG23	1:C:158:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:MET:HG2	1:C:419:LYS:HD2	2.01	0.43
1:A:588:GLY:O	1:A:589:LYS:HB2	2.19	0.43
1:A:248:ILE:HA	1:A:251:PHE:CD2	2.54	0.42
1:C:478:THR:HG22	1:C:480:ASP:H	1.84	0.42
1:A:259:MET:HB3	1:A:259:MET:HE3	1.79	0.42
1:A:326:GLN:NE2	1:A:478:THR:HG23	2.35	0.42
1:C:338:SER:HG	1:C:356:TRP:H	1.67	0.42
1:A:445:GLY:O	1:A:476:PRO:HD2	2.19	0.41
1:C:303:ASN:H	1:C:307:GLN:NE2	2.18	0.41
1:A:91:LYS:HB3	1:A:91:LYS:HE2	1.87	0.41
1:A:374:MET:HG2	1:A:419:LYS:HD2	2.01	0.41
1:A:411:GLY:H	1:A:427:THR:CG2	2.27	0.41
1:A:449:LYS:HA	1:A:450:PRO:HD3	1.95	0.41
1:C:112:LYS:HD2	1:C:112:LYS:HA	1.92	0.41
1:A:90:ASP:C	1:A:92:LYS:H	2.27	0.41
1:C:70:ASP:OD1	1:C:70:ASP:C	2.64	0.41
1:A:317:LYS:HG2	1:A:373:MET:HG3	2.03	0.41
1:C:502:ASN:ND2	1:C:502:ASN:H	2.18	0.41
1:C:248:ILE:HA	1:C:251:PHE:CD2	2.55	0.41
1:C:539:MET:CE	1:C:552:TYR:HB2	2.50	0.41
1:C:263:TYR:O	1:C:264:GLN:C	2.64	0.40
1:A:261:GLU:O	1:A:560:LYS:HE2	2.21	0.40
1:A:283:TYR:CE1	1:A:305:LEU:HB2	2.56	0.40
1:A:466:TYR:CD1	1:A:466:TYR:C	2.99	0.40
1:A:70:ASP:OD1	1:A:70:ASP:C	2.63	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	499/650 (77%)	458 (92%)	39 (8%)	2 (0%)	30	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	471/650 (72%)	425 (90%)	43 (9%)	3 (1%)	21	42
All	All	970/1300 (75%)	883 (91%)	82 (8%)	5 (0%)	24	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	159	PRO
1	C	524	GLY
1	A	117	ILE
1	A	525	GLY
1	C	525	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	423/552 (77%)	392 (93%)	31 (7%)	13	29
1	C	399/552 (72%)	369 (92%)	30 (8%)	12	28
All	All	822/1104 (74%)	761 (93%)	61 (7%)	13	29

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	90	ASP
1	A	91	LYS
1	A	97	SER
1	A	98	LYS
1	A	99	LYS
1	A	117	ILE
1	A	119	MET
1	A	120	LYS
1	A	122	GLU
1	A	129	SER

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Mol	Chain	Res	Type
1	A	131	LYS
1	A	132	LYS
1	A	136	ILE
1	A	141	LYS
1	A	146	THR
1	A	157	ASN
1	A	158	LEU
1	A	173	ASN
1	A	179	HIS
1	A	186	LYS
1	A	261	GLU
1	A	292	GLU
1	A	326	GLN
1	A	333	ASP
1	A	349	SER
1	A	353	ARG
1	A	413	SER
1	A	502	ASN
1	A	545	LYS
1	A	589	LYS
1	C	71	ARG
1	C	84	LYS
1	C	86	VAL
1	C	90	ASP
1	C	91	LYS
1	C	108	GLU
1	C	111	LYS
1	C	117	ILE
1	C	135	GLN
1	C	136	ILE
1	C	137	GLU
1	C	140	ARG
1	C	141	LYS
1	C	155	LYS
1	C	161	ILE
1	C	163	LEU
1	C	167	THR
1	C	169	ARG
1	C	179	HIS
1	C	186	LYS
1	C	236	ARG
1	C	250	VAL

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Mol	Chain	Res	Type
1	C	292	GLU
1	C	326	GLN
1	C	349	SER
1	C	396	LYS
1	C	413	SER
1	C	502	ASN
1	C	523	ASN
1	C	585	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	185	GLN
1	A	326	GLN
1	A	425	GLN
1	A	502	ASN
1	C	307	GLN
1	C	326	GLN
1	C	409	GLN
1	C	425	GLN
1	C	436	GLN
1	C	502	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](#)

16 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	CIT	A	801	-	12,12,12	1.24	1 (8%)	17,17,17	1.34	3 (17%)
3	SO4	C	803	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	A	804	-	4,4,4	0.26	0	6,6,6	0.09	0
4	PNM	C	808	1	19,24,24	0.66	0	25,34,34	1.19	2 (8%)
3	SO4	C	802	-	4,4,4	0.29	0	6,6,6	0.11	0
4	PNM	A	808	1	19,24,24	0.72	1 (5%)	25,34,34	1.13	3 (12%)
2	CIT	A	803	-	12,12,12	1.29	1 (8%)	17,17,17	1.41	3 (17%)
3	SO4	C	807	-	4,4,4	0.33	0	6,6,6	0.29	0
3	SO4	C	805	-	4,4,4	0.28	0	6,6,6	0.09	0
3	SO4	A	802	-	4,4,4	0.31	0	6,6,6	0.15	0
3	SO4	A	805	-	4,4,4	0.33	0	6,6,6	0.05	0
3	SO4	A	806	-	4,4,4	0.29	0	6,6,6	0.12	0
3	SO4	C	806	-	4,4,4	0.31	0	6,6,6	0.07	0
3	SO4	A	807	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	C	801	-	4,4,4	0.22	0	6,6,6	0.24	0
2	CIT	C	804	-	12,12,12	1.22	1 (8%)	17,17,17	1.07	0

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	CIT	A	801	-	-	5/16/16/16	-
4	PNM	C	808	1	-	2/12/33/33	0/2/2/2
4	PNM	A	808	1	-	2/12/33/33	0/2/2/2
2	CIT	A	803	-	-	7/16/16/16	-
2	CIT	C	804	-	-	7/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	803	CIT	C3-C6	3.03	1.56	1.53
2	C	804	CIT	C3-C6	2.57	1.56	1.53
4	A	808	PNM	O12-C11	2.29	1.28	1.22
2	A	801	CIT	C2-C3	-2.20	1.51	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	808	PNM	C11-C3-N4	-3.90	104.59	110.62
4	A	808	PNM	C11-C3-N4	-3.46	105.28	110.62
2	A	803	CIT	O6-C6-C3	2.78	118.47	113.14
4	A	808	PNM	O13-C11-O12	2.54	129.84	124.08
2	A	803	CIT	O5-C6-C3	-2.42	117.40	122.09
2	A	801	CIT	O7-C3-C2	-2.27	104.19	109.38
2	A	801	CIT	O5-C6-C3	-2.20	117.83	122.09
4	C	808	PNM	C3-C2-S1	2.12	107.89	103.86
4	A	808	PNM	C9-C2-S1	-2.11	105.78	109.18
2	A	803	CIT	O3-C5-C4	-2.06	117.12	122.95
2	A	801	CIT	O1-C1-C2	-2.03	117.21	122.95

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CIT	C1-C2-C3-O7
2	A	803	CIT	C1-C2-C3-C4
2	A	803	CIT	C1-C2-C3-C6
2	A	803	CIT	C2-C3-C6-O5
2	A	803	CIT	C2-C3-C6-O6
2	A	803	CIT	O7-C3-C6-O5
2	A	803	CIT	O7-C3-C6-O6
2	C	804	CIT	C1-C2-C3-O7
2	C	804	CIT	C2-C3-C6-O5
2	C	804	CIT	C2-C3-C6-O6
2	C	804	CIT	O7-C3-C6-O5
2	C	804	CIT	O7-C3-C6-O6
4	A	808	PNM	O13-C11-C3-N4
2	A	801	CIT	C1-C2-C3-C4
2	A	801	CIT	C1-C2-C3-C6
2	A	803	CIT	C1-C2-C3-O7
2	C	804	CIT	C1-C2-C3-C4
4	C	808	PNM	O13-C11-C3-N4

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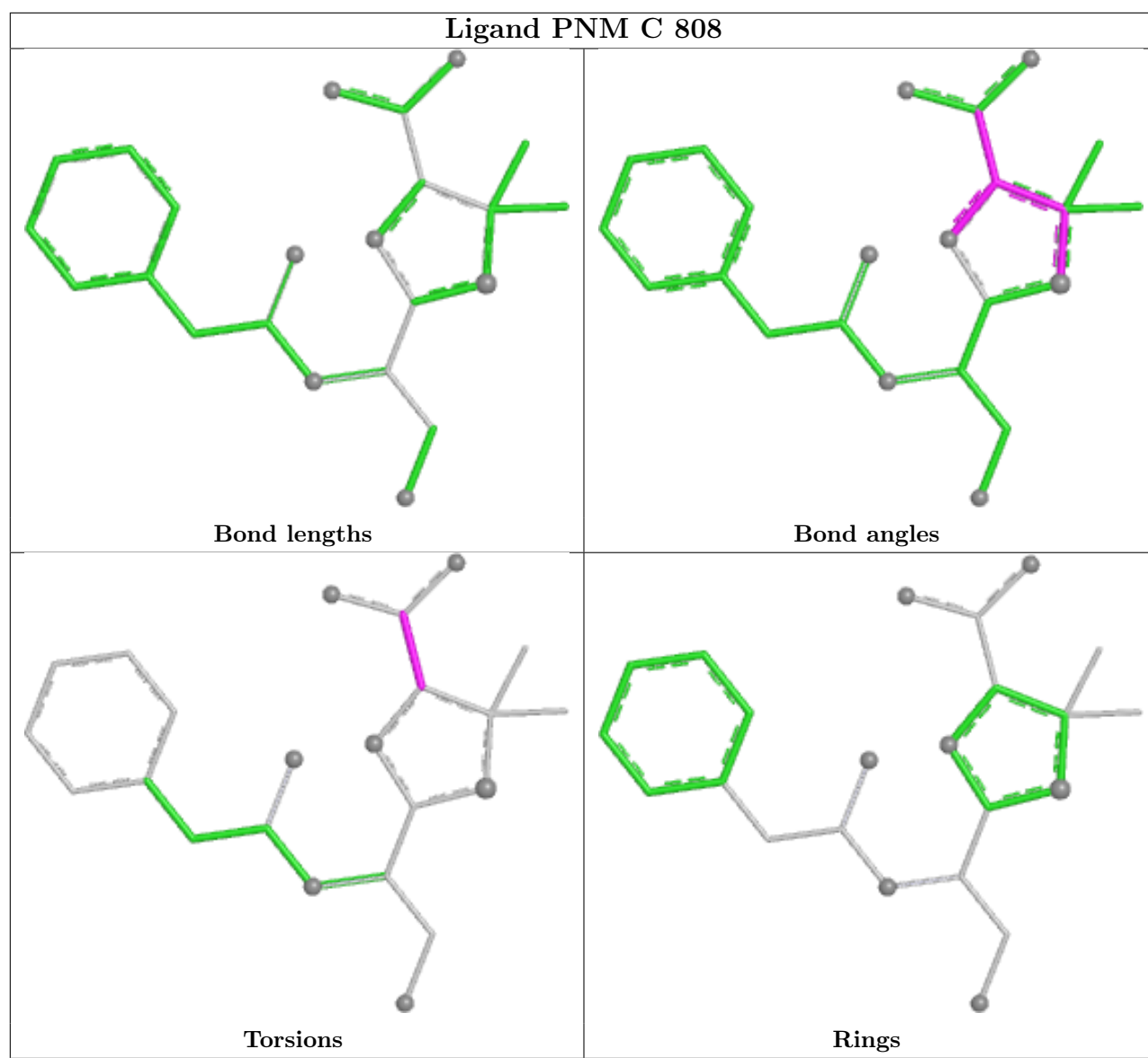
Mol	Chain	Res	Type	Atoms
4	C	808	PNM	O12-C11-C3-N4
4	A	808	PNM	O12-C11-C3-N4
2	C	804	CIT	C1-C2-C3-C6
2	A	801	CIT	C2-C3-C6-O6
2	A	801	CIT	C2-C3-C6-O5

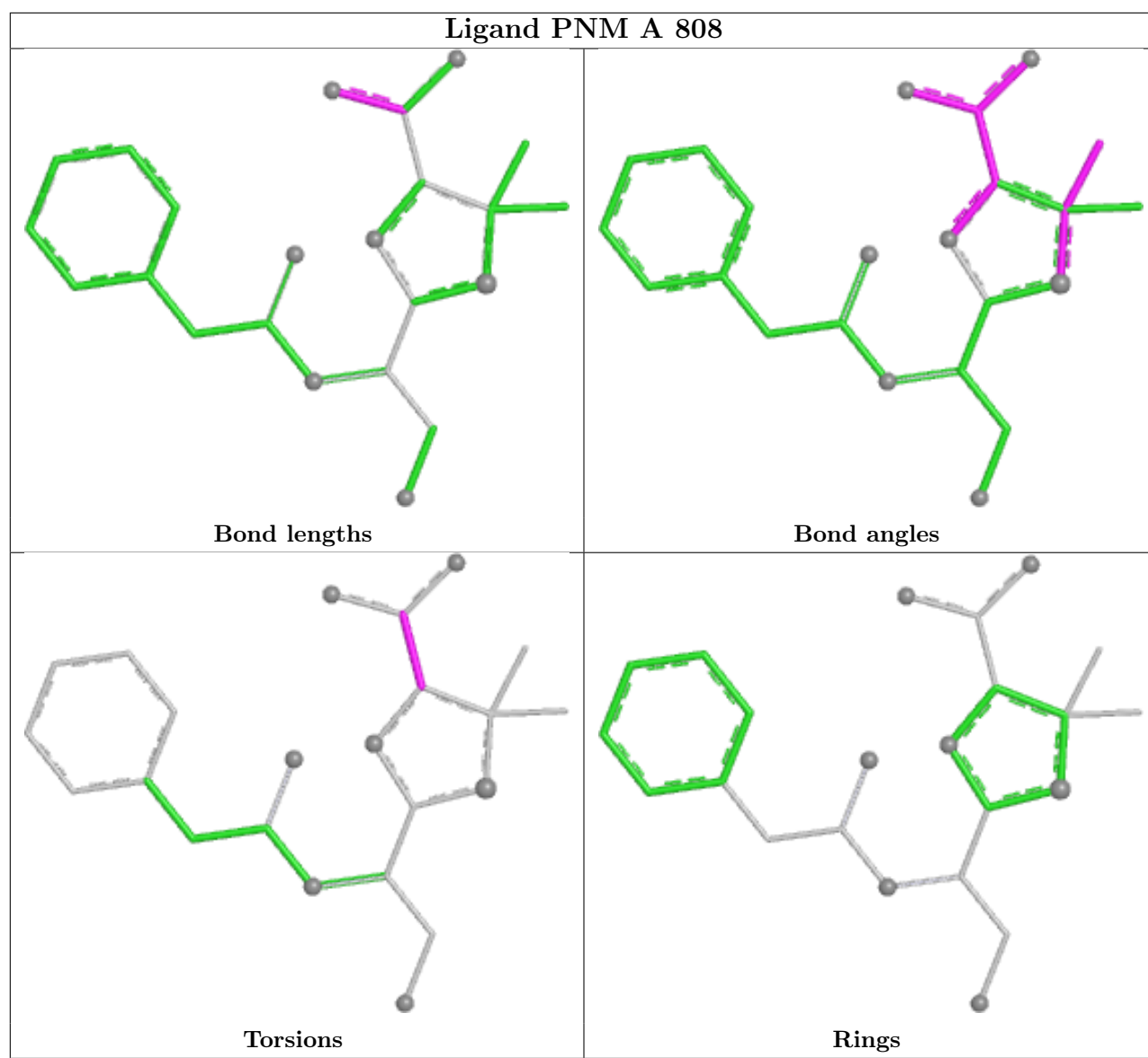
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	808	PNM	1	0
2	A	803	CIT	1	0
2	C	804	CIT	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	503/650 (77%)	0.40	52 (10%)	12 9	34, 55, 117, 174	0
1	C	479/650 (73%)	0.59	51 (10%)	11 9	40, 63, 122, 148	0
All	All	982/1300 (75%)	0.50	103 (10%)	11 9	34, 59, 120, 174	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	ILE	10.8
1	C	234	PRO	8.1
1	C	133	ALA	6.8
1	C	134	PHE	5.8
1	A	93	ALA	5.3
1	C	138	PHE	5.3
1	A	95	ALA	4.8
1	C	88	VAL	4.6
1	A	133	ALA	4.5
1	A	131	LYS	4.3
1	C	235	LYS	4.2
1	C	522	PRO	4.1
1	A	119	MET	4.1
1	C	159	PRO	4.0
1	A	139	GLY	4.0
1	A	106	LYS	3.9
1	C	403	ASP	3.9
1	C	135	GLN	3.9
1	C	296	ASP	3.8
1	A	589	LYS	3.8
1	C	164	LEU	3.7
1	A	116	VAL	3.7
1	C	87	ALA	3.6
1	A	96	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	90	ASP	3.6
1	C	136	ILE	3.6
1	C	91	LYS	3.5
1	A	64	MET	3.5
1	C	162	SER	3.4
1	C	590	SER	3.4
1	C	64	MET	3.4
1	C	113	LEU	3.4
1	C	523	ASN	3.3
1	A	234	PRO	3.2
1	C	86	VAL	3.2
1	C	161	ILE	3.2
1	A	90	ASP	3.2
1	C	534	TYR	3.2
1	A	89	ILE	3.2
1	A	94	SER	3.1
1	C	524	GLY	3.1
1	A	92	LYS	3.1
1	A	151	LEU	3.1
1	C	160	GLY	3.1
1	C	95	ALA	3.0
1	A	99	LYS	3.0
1	A	111	LYS	3.0
1	A	97	SER	3.0
1	C	588	GLY	3.0
1	A	132	LYS	2.9
1	A	235	LYS	2.9
1	A	118	ASN	2.9
1	C	163	LEU	2.9
1	A	124	ILE	2.9
1	C	110	ALA	2.9
1	A	523	ASN	2.9
1	A	98	LYS	2.9
1	A	159	PRO	2.9
1	A	141	LYS	2.8
1	C	141	LYS	2.8
1	C	525	GLY	2.7
1	A	117	ILE	2.7
1	A	525	GLY	2.7
1	C	108	GLU	2.7
1	C	151	LEU	2.7
1	A	104	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	130	GLN	2.6
1	C	137	GLU	2.6
1	C	85	LEU	2.5
1	A	345	GLY	2.5
1	A	508	TYR	2.5
1	A	134	PHE	2.5
1	C	147	TYR	2.5
1	C	154	GLU	2.4
1	C	589	LYS	2.4
1	C	526	GLY	2.4
1	C	210	SER	2.4
1	A	144	ASN	2.4
1	C	92	LYS	2.4
1	C	152	LYS	2.4
1	A	524	GLY	2.4
1	C	139	GLY	2.4
1	A	113	LEU	2.3
1	A	147	TYR	2.3
1	A	209	GLY	2.3
1	A	236	ARG	2.3
1	C	209	GLY	2.2
1	C	499	HIS	2.2
1	A	107	LYS	2.2
1	A	335	LYS	2.2
1	A	138	PHE	2.2
1	A	152	LYS	2.2
1	A	344	MET	2.2
1	C	156	MET	2.2
1	A	109	THR	2.2
1	A	545	LYS	2.2
1	A	120	LYS	2.1
1	C	111	LYS	2.1
1	A	140	ARG	2.1
1	A	91	LYS	2.1
1	C	337	LYS	2.1
1	A	486	GLU	2.0
1	C	117	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 ⓘ

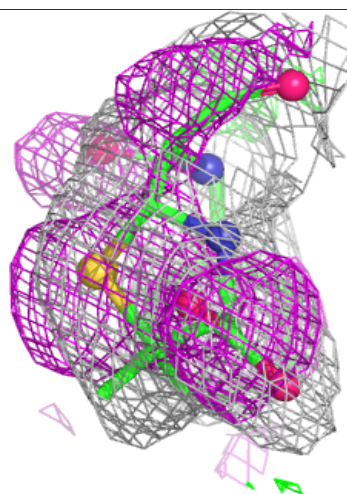
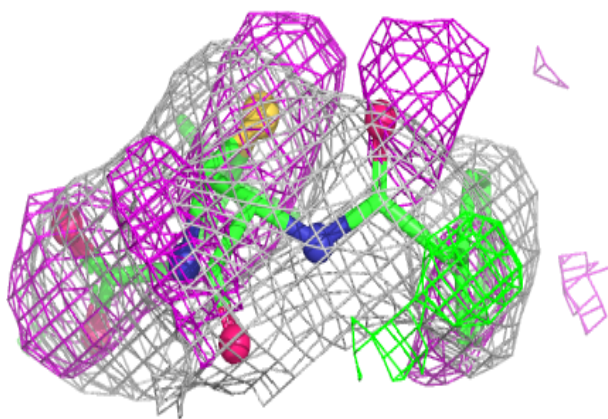
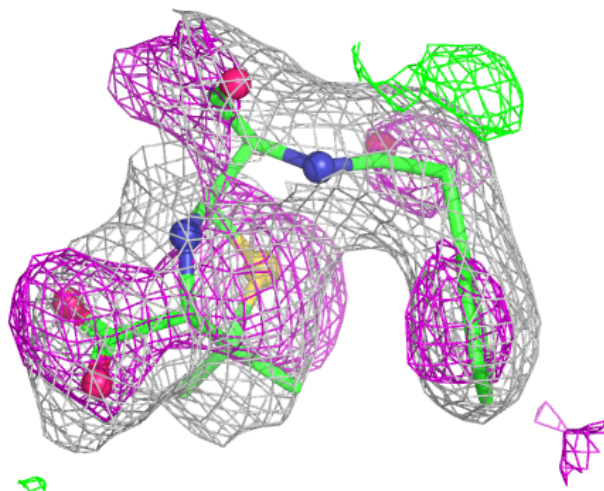
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	803	5/5	0.59	0.15	134,136,151,155	0
3	SO4	A	806	5/5	0.61	0.13	140,140,147,152	0
3	SO4	A	807	5/5	0.68	0.12	114,118,130,137	0
3	SO4	A	804	5/5	0.73	0.11	95,112,124,127	0
3	SO4	C	805	5/5	0.74	0.11	106,118,128,129	0
3	SO4	A	805	5/5	0.75	0.12	122,123,129,133	0
2	CIT	C	804	13/13	0.76	0.15	97,121,154,168	0
3	SO4	A	802	5/5	0.76	0.11	78,96,106,108	0
3	SO4	C	806	5/5	0.79	0.13	127,128,147,149	0
3	SO4	C	802	5/5	0.80	0.08	101,101,113,124	0
2	CIT	A	801	13/13	0.81	0.19	62,87,128,133	0
2	CIT	A	803	13/13	0.82	0.12	63,80,103,108	0
3	SO4	C	801	5/5	0.83	0.12	85,90,105,119	0
4	PNM	C	808	23/23	0.92	0.12	34,42,52,52	0
4	PNM	A	808	23/23	0.94	0.10	33,39,49,51	0
3	SO4	C	807	5/5	0.95	0.12	61,64,74,86	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.

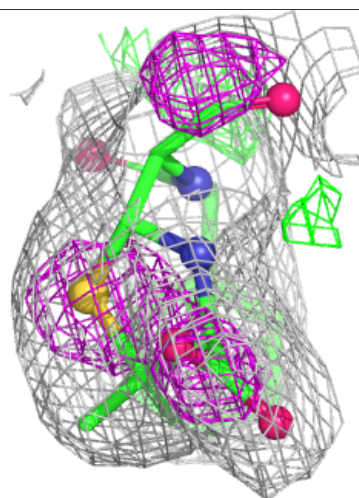
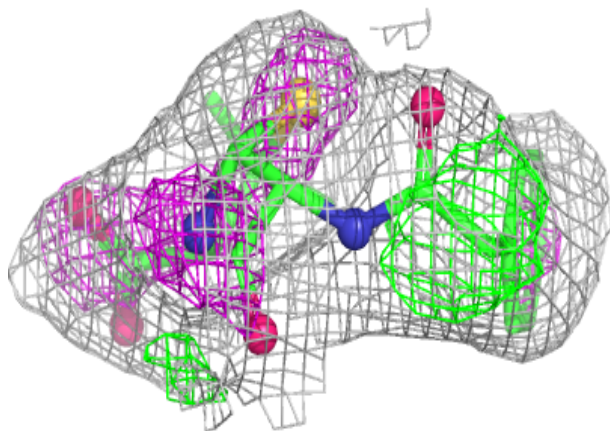
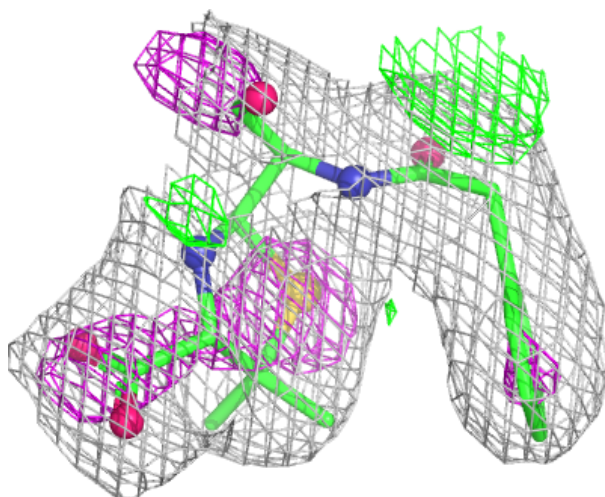
Electron density around PNM C 808:

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



Electron density around PNM A 808:

$2mF_o-DF_c$ (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.