Full wwPDB X-ray Structure Validation Report (i)

May 23, 2022 – 01:13 pm BST

PDB ID	:	7O4B
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

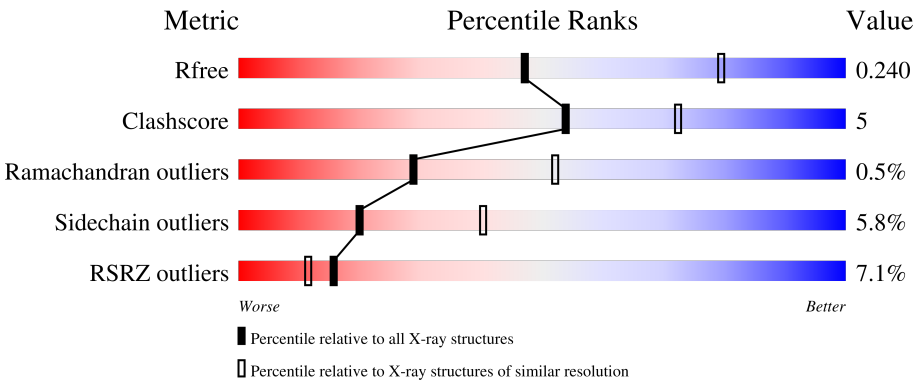
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	4% 65% 12% 23%
1	C	650	7% 62% 11% • 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.

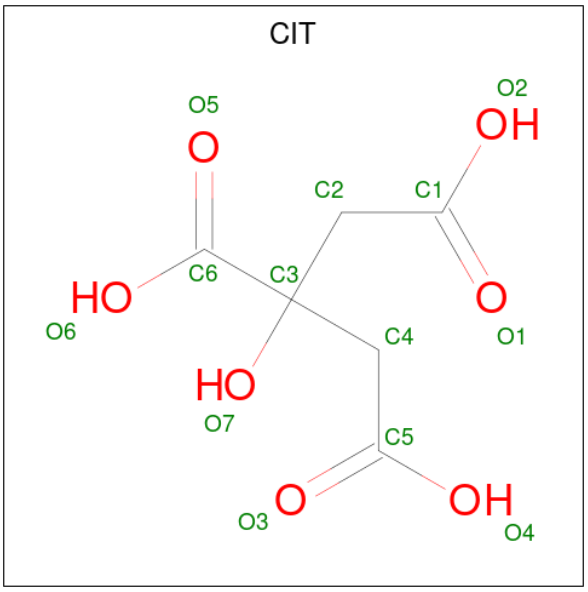
- Molecule 1 is a protein called Penicillin-binding protein 1.

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

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 (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

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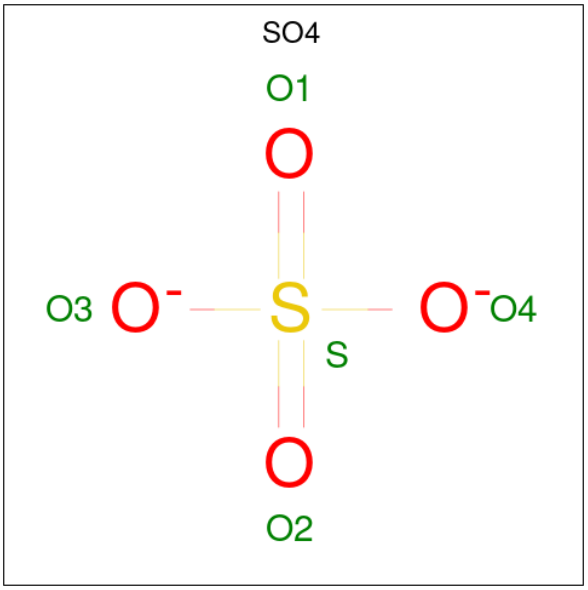
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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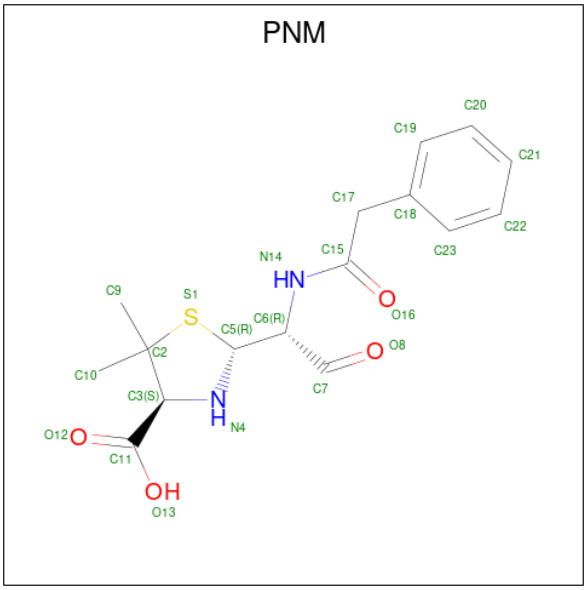
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0

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



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

- Molecule 5 is water.

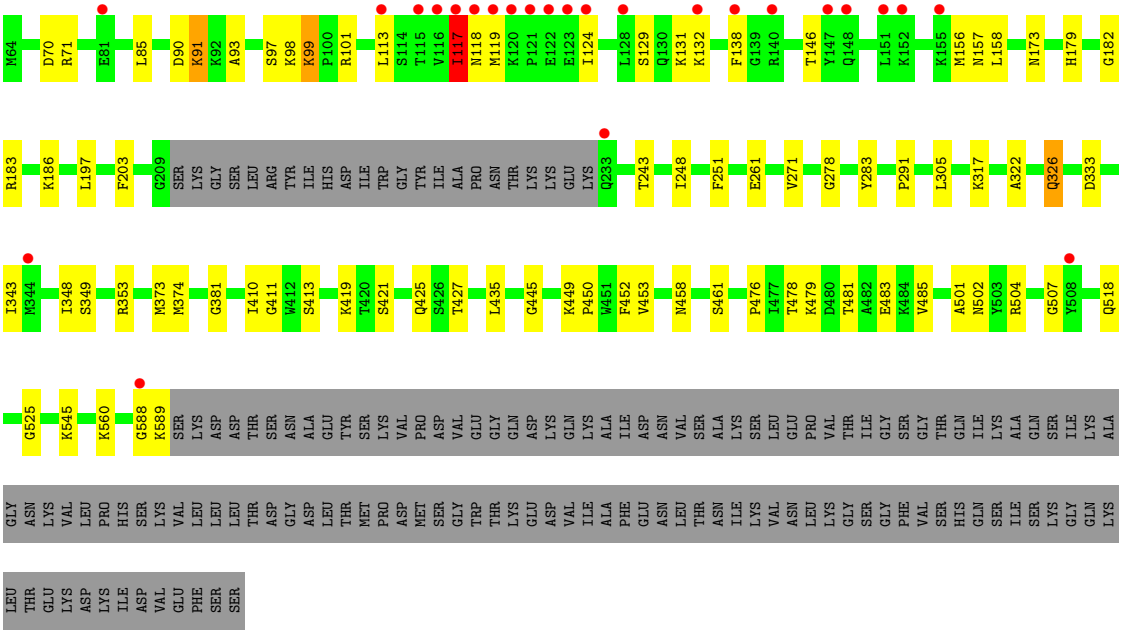
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	26	26	26	0	0
			Total	O		
5	C	13	13	13	0	0

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.

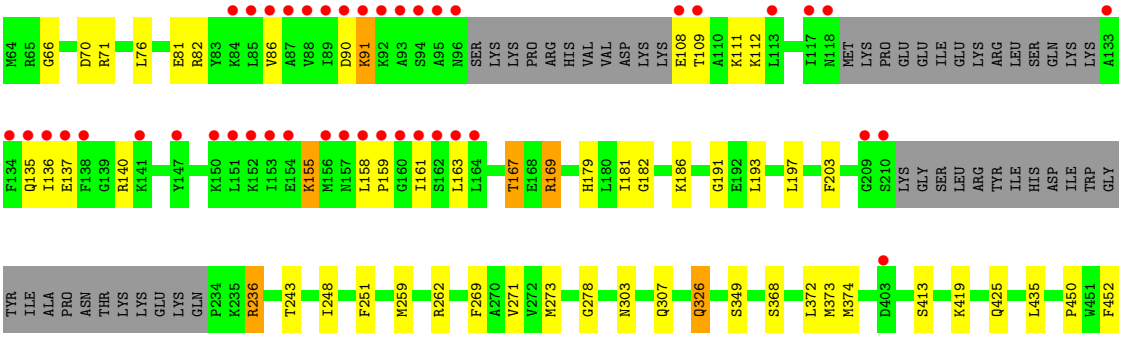
• Molecule 1: Penicillin-binding protein 1

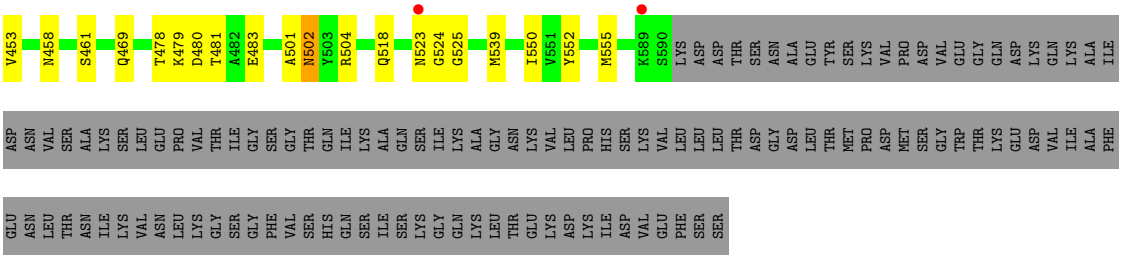
Chain A:



• Molecule 1: Penicillin-binding protein 1

Chain C:




V453
N458
S461
Q469
T478
K479
D480
T481
A482
E483
A501
N502
Y503
R504
Q518
N523
G524
G525
M539
I550
V551
Y552
M555
K589
S590
LYS
ASP
ASP
THR
SER
ASN
ALA
GLU
TYR
SER
LYS
VAL
PRO
ASP
VAL
GLU
GLY
GLN
ASP
LYS
GLN
LYS
ALA
ILE
ASP
ASN
VAL
SER
ALA
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SER
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LEU
LEU
THR
ASP
GLY
ASP
LEU
THR
MET
PRO
ASP
MET
SER
GLY
TRP
THR
LYS
GLU
ASP
VAL
ILE
ALA
PHE
GLU
ASN
LEU
THR
ASN
ILE
LYS
VAL
ASN
LEU
LYS
GLY
SER
GLY
PHE
VAL
SER
HIS
GLN
SER
ILE
SER
LYS
GLY
GLN
LYS
LEU
THR
GLU
LYS
ASP
LYS
ILE
ASP
VAL
GLU
PHE
SER
SER

4 Data and refinement statistics (i)

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) 67.5 (47.51-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.13%)	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)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, PNM, 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	0.69	0/4043	0.85	0/5436
1	C	0.69	0/3829	0.85	0/5151
All	All	0.69	0/7872	0.85	0/10587

There are no bond length outliers.

There are no bond angle outliers.

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	40	0
1	C	3750	0	3708	41	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	82	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 (82) 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:410:ILE:HA	1:A:427:THR:HG22	1.65	0.77
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:167:THR:O	1:C:186:LYS:NZ	2.20	0.68
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:C:273:MET:HE2	1:C:450:PRO:HB3	1.90	0.51
1:C:273:MET:HE1	1:C:450:PRO:HB3	1.92	0.51
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
1:C:303:ASN:H	1:C:307:GLN:HE21	1.58	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:539:MET:HE2	1:C:550:ILE:HG23	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:259:MET:HE1	1:C:555:MET:CE	2.46	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:C:372:LEU:HG	1:C:373:MET:HE2	2.00	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
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:326:GLN:NE2	1:A:478:THR:HG23	2.35	0.42
1:C:502:ASN:ND2	1:C:502:ASN:H	2.18	0.42
1:C:259:MET:CE	1:C:555:MET:HE2	2.50	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:C:539:MET:HE1	1:C:550:ILE:CG2	2.50	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:317:LYS:HG2	1:A:373:MET:HG3	2.03	0.41
1:C:248:ILE:HA	1:C:251:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:MET:CE	1:C:552:TYR:HB2	2.50	0.41
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:C:269:PHE:CD1	1:C:269:PHE:C	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	499/650 (77%)	458 (92%)	39 (8%)	2 (0%)	34	57
1	C	471/650 (72%)	425 (90%)	43 (9%)	3 (1%)	25	47
All	All	970/1300 (75%)	883 (91%)	82 (8%)	5 (0%)	29	52

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 (i)

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%)	399 (94%)	24 (6%)	20	41
1	C	399/552 (72%)	375 (94%)	24 (6%)	19	39
All	All	822/1104 (74%)	774 (94%)	48 (6%)	20	40

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
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	129	SER
1	A	131	LYS
1	A	132	LYS
1	A	146	THR
1	A	157	ASN
1	A	173	ASN
1	A	179	HIS
1	A	186	LYS
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	C	70	ASP
1	C	71	ARG
1	C	86	VAL
1	C	90	ASP
1	C	91	LYS
1	C	108	GLU
1	C	111	LYS
1	C	135	GLN
1	C	136	ILE
1	C	137	GLU
1	C	140	ARG

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Mol	Chain	Res	Type
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	236	ARG
1	C	262	ARG
1	C	326	GLN
1	C	349	SER
1	C	413	SER
1	C	502	ASN
1	C	523	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	A	425	GLN
1	A	502	ASN
1	C	307	GLN
1	C	326	GLN
1	C	377	GLN
1	C	425	GLN
1	C	502	ASN
1	C	563	GLN

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 monosaccharides 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	$\#\|Z\| > 2$
3	SO4	C	803	-	4,4,4	0.36	0	6,6,6	0.12	0
3	SO4	A	805	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	A	802	-	4,4,4	0.30	0	6,6,6	0.18	0
2	CIT	C	804	-	3,12,12	0.59	0	3,17,17	0.20	0
3	SO4	C	806	-	4,4,4	0.33	0	6,6,6	0.08	0
4	PNM	C	808	1	17,24,24	0.75	1 (5%)	22,34,34	0.92	2 (9%)
3	SO4	C	807	-	4,4,4	0.39	0	6,6,6	0.29	0
3	SO4	A	806	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	C	802	-	4,4,4	0.32	0	6,6,6	0.08	0
2	CIT	A	801	-	3,12,12	1.79	1 (33%)	3,17,17	1.80	1 (33%)
3	SO4	C	805	-	4,4,4	0.31	0	6,6,6	0.08	0
4	PNM	A	808	1	17,24,24	0.61	1 (5%)	22,34,34	0.87	2 (9%)
3	SO4	A	804	-	4,4,4	0.29	0	6,6,6	0.08	0
3	SO4	A	807	-	4,4,4	0.28	0	6,6,6	0.06	0
3	SO4	C	801	-	4,4,4	0.27	0	6,6,6	0.24	0
2	CIT	A	803	-	3,12,12	0.46	0	3,17,17	1.69	1 (33%)

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	C	804	-	-	3/6/16/16	-
4	PNM	C	808	1	-	0/8/33/33	0/2/2/2
4	PNM	A	808	1	-	0/8/33/33	0/2/2/2
2	CIT	A	801	-	-	3/6/16/16	-
2	CIT	A	803	-	-	4/6/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CIT	C2-C3	-2.60	1.51	1.54
4	C	808	PNM	C3-N4	2.59	1.50	1.46
4	A	808	PNM	C3-N4	2.12	1.49	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	CIT	C3-C2-C1	-2.99	110.19	114.98
2	A	803	CIT	C3-C4-C5	2.52	119.01	114.98
4	C	808	PNM	C6-N14-C15	-2.31	120.66	123.13
4	C	808	PNM	C3-C2-S1	2.06	107.89	103.81
4	A	808	PNM	C9-C2-S1	-2.05	105.78	109.21
4	A	808	PNM	C6-N14-C15	-2.01	120.97	123.13

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CIT	C1-C2-C3-O7
2	A	801	CIT	C1-C2-C3-C4
2	A	801	CIT	C1-C2-C3-C6
2	A	803	CIT	C1-C2-C3-C4
2	A	803	CIT	C1-C2-C3-C6
2	C	804	CIT	C1-C2-C3-O7
2	A	803	CIT	C1-C2-C3-O7
2	C	804	CIT	C1-C2-C3-C4
2	A	803	CIT	C6-C3-C4-C5
2	C	804	CIT	C1-C2-C3-C6

There are no ring outliers.

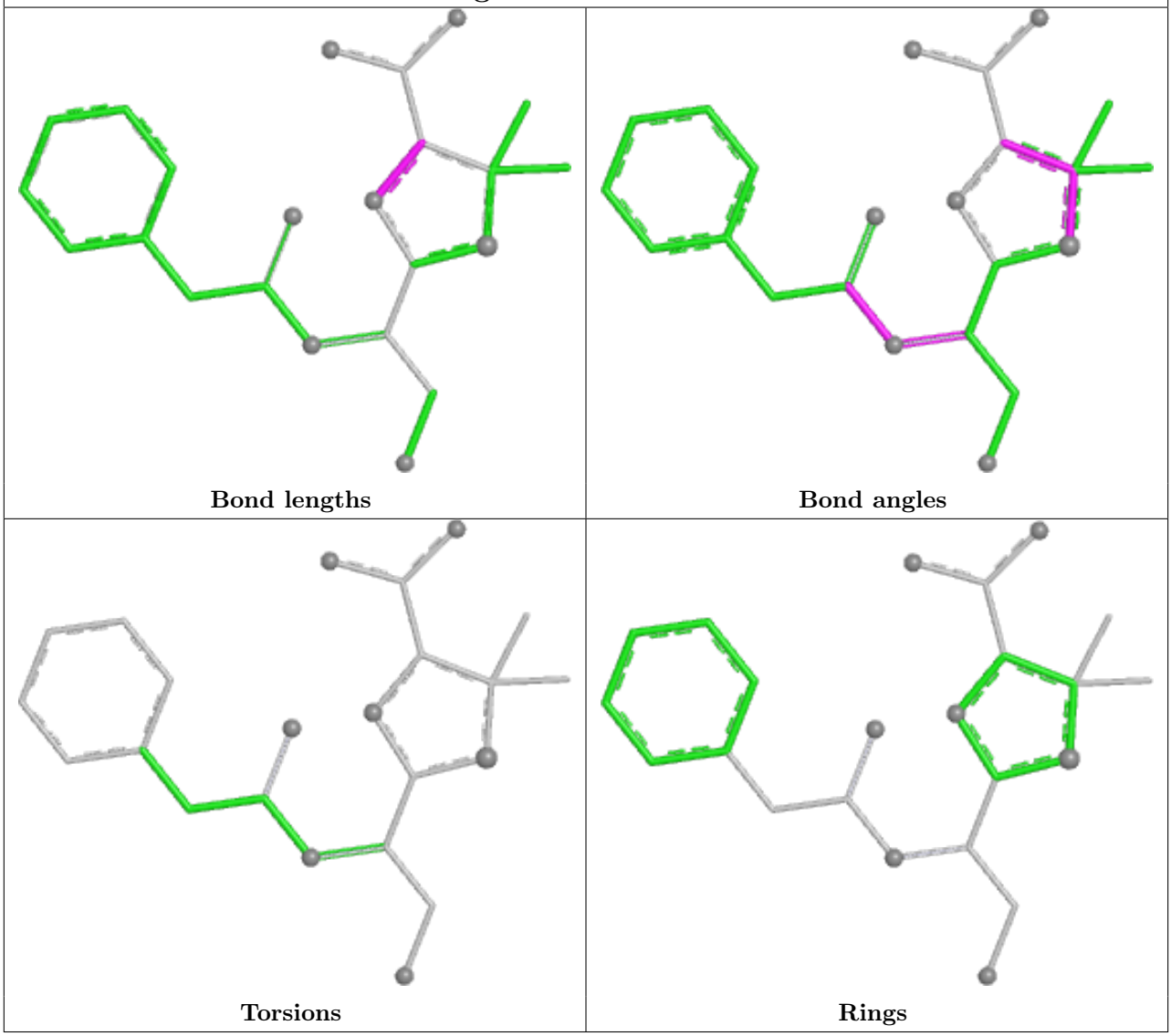
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	804	CIT	1	0
4	C	808	PNM	1	0
2	A	803	CIT	1	0

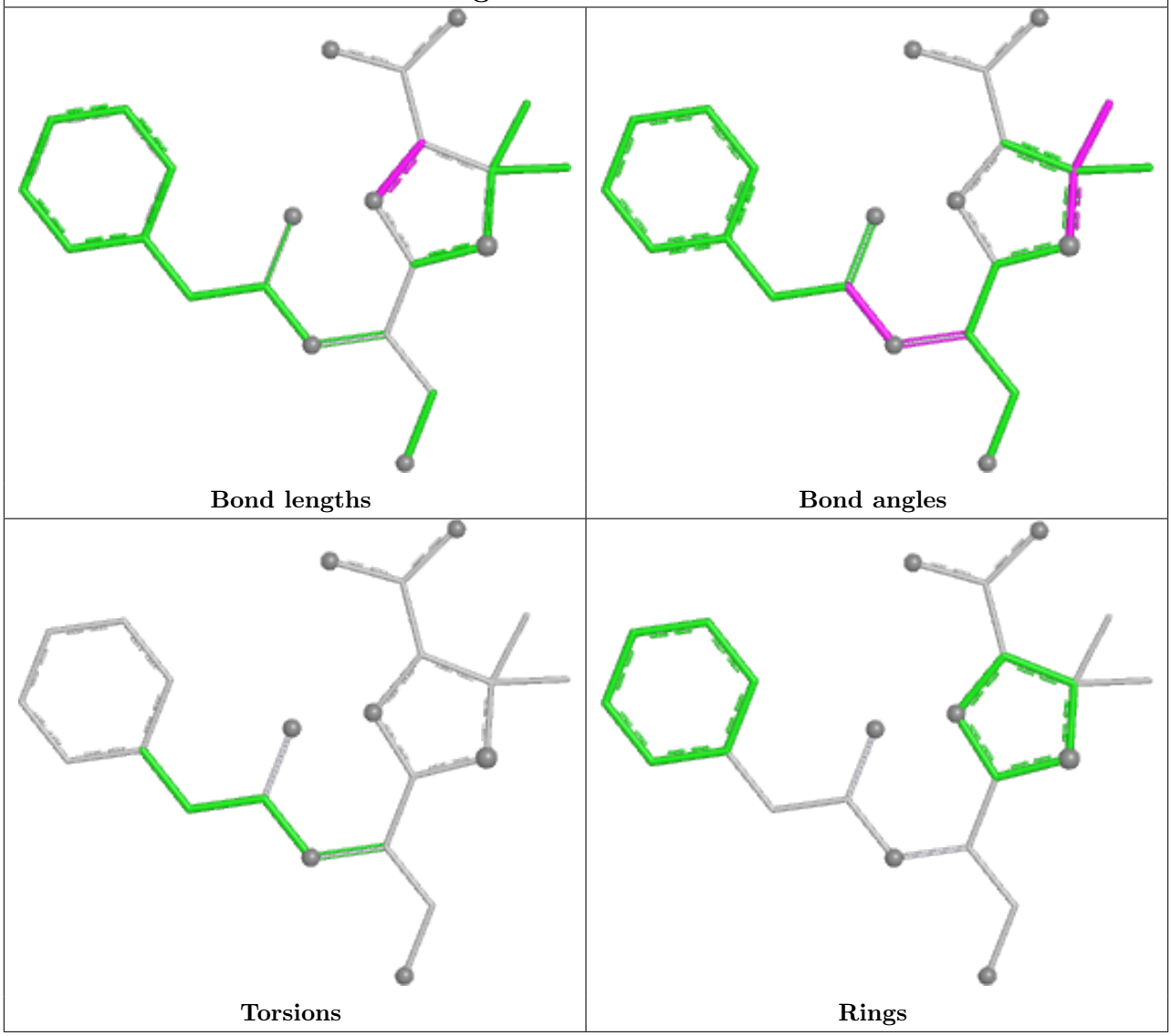
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand PNM C 808



Ligand PNM A 808



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.29	25 (4%)	28	23	34, 55, 117, 174	0
1	C	479/650 (73%)	0.43	45 (9%)	8	5	40, 63, 122, 148	0
All	All	982/1300 (75%)	0.36	70 (7%)	16	11	34, 59, 120, 174	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	ILE	11.8
1	C	88	VAL	7.3
1	C	138	PHE	6.9
1	C	87	ALA	6.6
1	C	134	PHE	6.5
1	C	90	ASP	6.5
1	A	119	MET	6.5
1	C	91	LYS	6.3
1	C	133	ALA	6.2
1	A	151	LEU	5.9
1	C	161	ILE	5.7
1	C	163	LEU	5.4
1	C	136	ILE	5.4
1	C	117	ILE	5.3
1	C	160	GLY	5.3
1	C	135	GLN	5.3
1	C	85	LEU	5.3
1	C	113	LEU	4.9
1	A	118	ASN	4.8
1	C	109	THR	4.3
1	A	120	LYS	4.2
1	C	154	GLU	4.0
1	C	108	GLU	3.9
1	A	116	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	147	TYR	3.9
1	A	124	ILE	3.8
1	C	96	ASN	3.8
1	A	233	GLN	3.7
1	C	94	SER	3.7
1	C	156	MET	3.7
1	A	122	GLU	3.6
1	A	148	GLN	3.6
1	A	113	LEU	3.6
1	C	162	SER	3.6
1	C	137	GLU	3.6
1	C	151	LEU	3.4
1	A	147	TYR	3.4
1	C	86	VAL	3.4
1	A	117	ILE	3.3
1	A	138	PHE	3.3
1	C	158	LEU	3.3
1	A	140	ARG	3.3
1	C	210	SER	3.2
1	C	95	ALA	3.2
1	A	132	LYS	3.2
1	C	153	ILE	3.0
1	C	141	LYS	3.0
1	C	523	ASN	2.8
1	A	128	LEU	2.8
1	C	589	LYS	2.7
1	C	92	LYS	2.7
1	C	164	LEU	2.7
1	A	115	THR	2.6
1	A	123	GLU	2.6
1	A	155	LYS	2.6
1	C	403	ASP	2.5
1	C	209	GLY	2.5
1	C	118	ASN	2.4
1	C	159	PRO	2.4
1	C	93	ALA	2.4
1	A	588	GLY	2.3
1	C	84	LYS	2.3
1	A	121	PRO	2.3
1	A	508	TYR	2.2
1	A	81	GLU	2.2
1	A	152	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	150	LYS	2.1
1	C	152	LYS	2.1
1	C	157	ASN	2.1
1	A	344	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

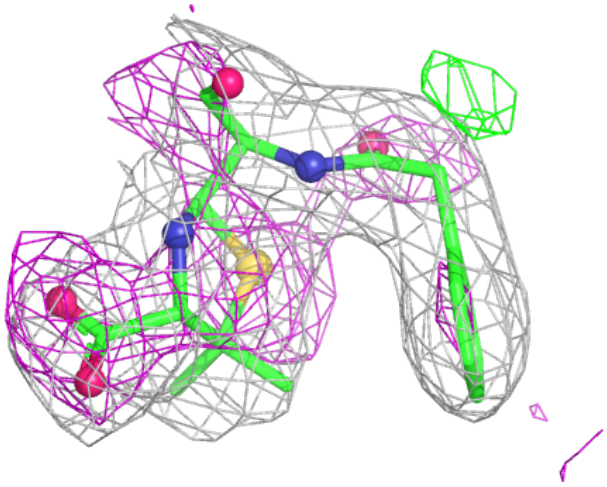
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	806	5/5	0.76	0.36	140,140,147,152	0
3	SO4	C	806	5/5	0.81	0.20	127,128,147,149	0
2	CIT	C	804	13/13	0.82	0.37	97,121,154,168	0
3	SO4	C	803	5/5	0.83	0.39	134,136,151,155	0
3	SO4	C	805	5/5	0.86	0.15	106,118,128,129	0
2	CIT	A	803	13/13	0.86	0.33	63,80,103,108	0
3	SO4	A	807	5/5	0.89	0.25	114,118,130,137	0
2	CIT	A	801	13/13	0.91	0.37	62,87,128,133	0
3	SO4	A	805	5/5	0.92	0.36	122,123,129,133	0
3	SO4	C	801	5/5	0.94	0.17	85,90,105,119	0
3	SO4	A	802	5/5	0.94	0.12	78,96,106,108	0
3	SO4	C	802	5/5	0.95	0.12	101,101,113,124	0
3	SO4	A	804	5/5	0.95	0.19	95,112,124,127	0
4	PNM	C	808	23/23	0.95	0.15	34,42,52,52	0
4	PNM	A	808	23/23	0.97	0.12	33,39,49,51	0
3	SO4	C	807	5/5	0.97	0.12	61,64,74,86	0

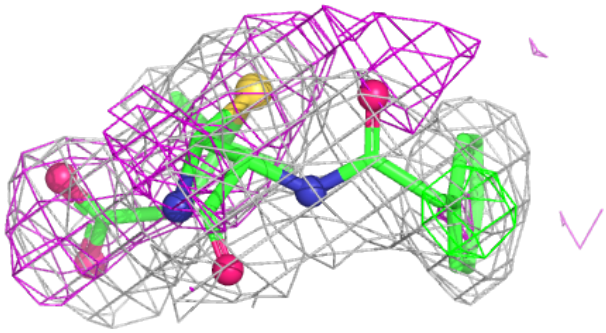
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

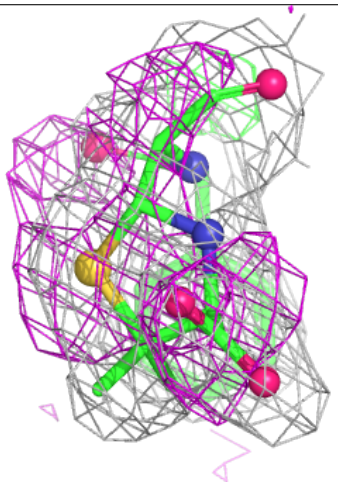
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

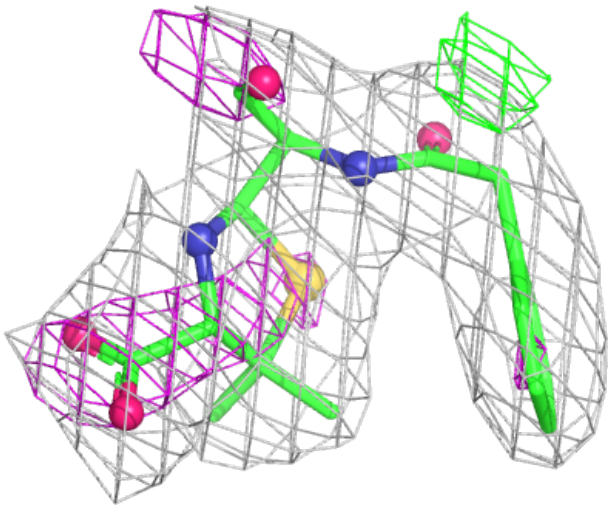
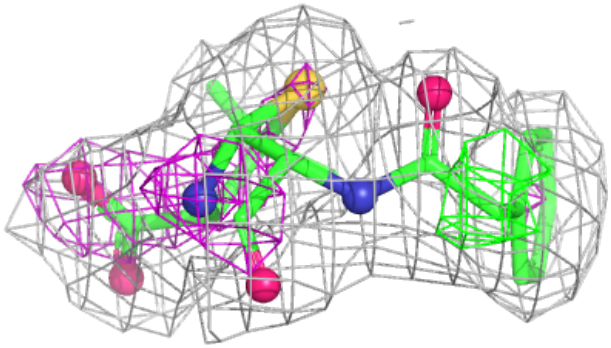
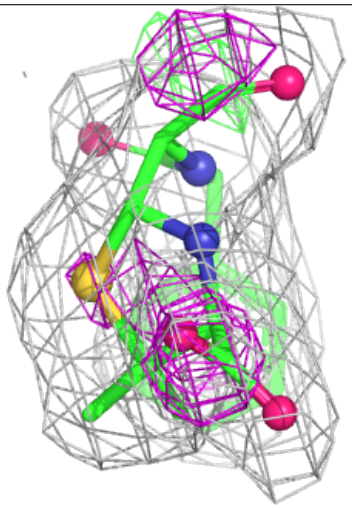
Electron density around PNM C 808:

$2mF_o$-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.