



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2024 – 11:14 PM EDT

PDB ID : 1MWT  
Title : Structure of penicillin G acyl-Penicillin binding protein 2a from methicillin resistant *Staphylococcus aureus* strain 27r at 2.45 Å resolution.  
Authors : Lim, D.C.; Strynadka, N.C.J.  
Deposited on : 2002-10-01  
Resolution : 2.45 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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

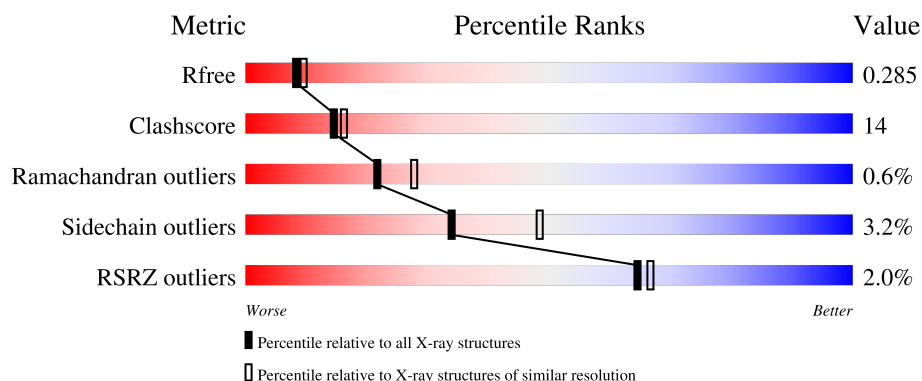
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.45 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))
$R_{free}$	164625	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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  $\geq 3$ , 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	646	
1	B	646	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10298 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 PBP2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	635	Total	C	N	O	S	0	0	0
			5101	3216	860	1010	15			
1	B	626	Total	C	N	O	S	0	0	0
			5036	3179	846	996	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP O54286
B	23	MET	-	initiating methionine	UNP O54286

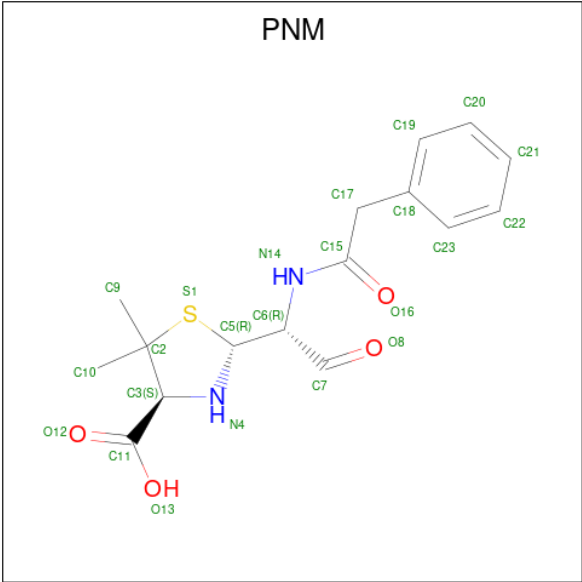
- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cd	0	0
			4	4		
2	B	5	Total	Cd	0	0
			5	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	2	Total	Cl	0	0
			2	2		

- Molecule 4 is OPEN FORM - PENICILLIN G (three-letter code: PNM) (formula: C<sub>16</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>S).



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

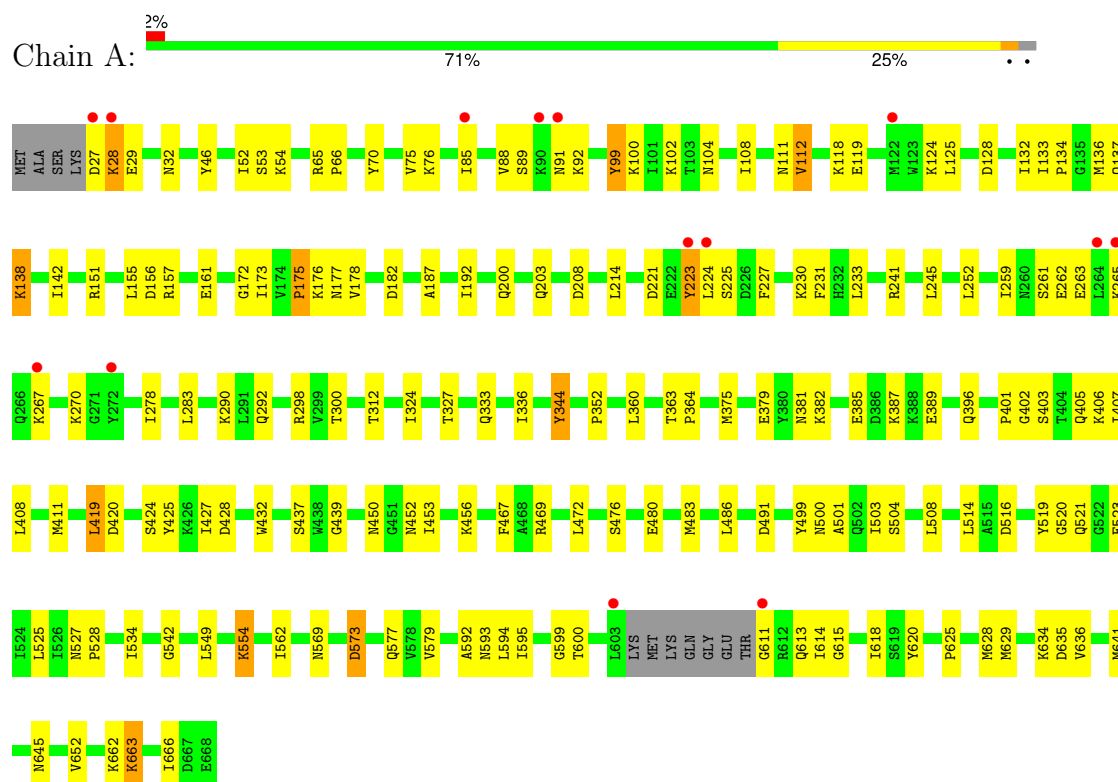
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	39	Total	O	0	0
			39	39		

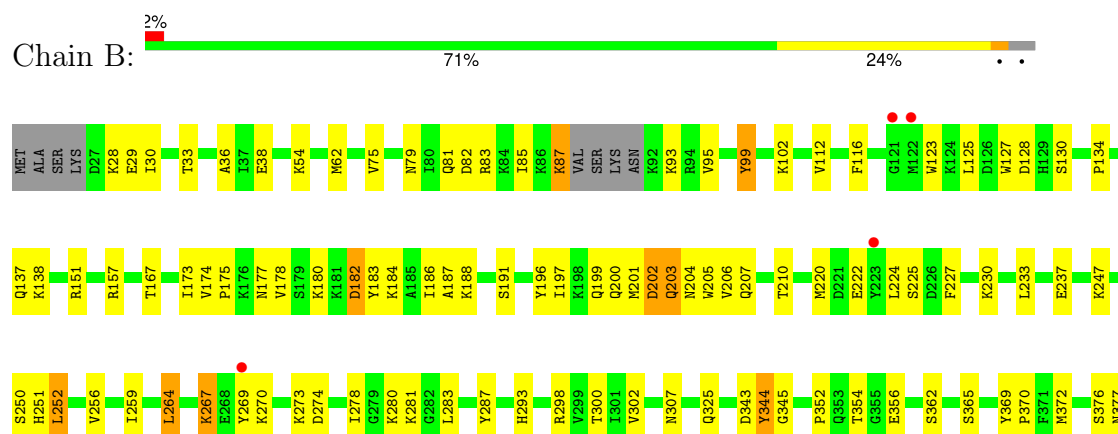
### 3 Residue-property plots

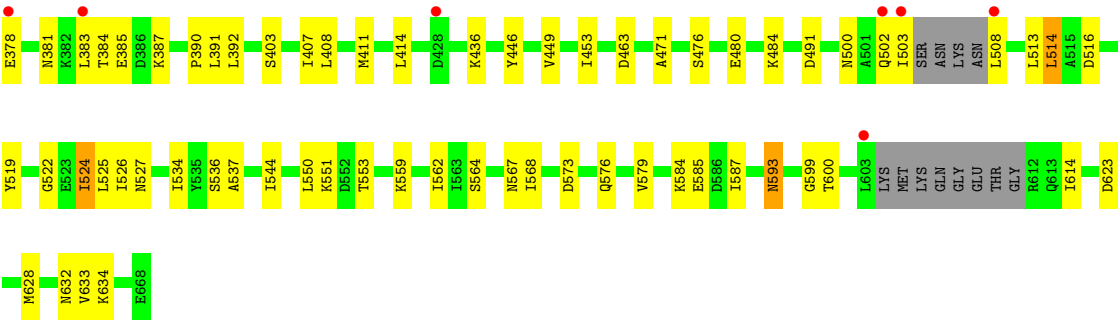
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PBP2a



#### • Molecule 1: PBP2a





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.55Å 103.27Å 186.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 2.45 24.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.89-2.45) 97.3 (24.89-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.44Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.295 0.225 , 0.285	Depositor DCC
$R_{free}$ test set	2863 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.3	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CD, PNM, CL

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	0.33	0/5186	0.58	0/6974
1	B	0.32	0/5119	0.58	0/6882
All	All	0.33	0/10305	0.58	0/13856

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

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	5101	0	5092	147	0
1	B	5036	0	5024	134	0
2	A	4	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	23	0	18	0	0
4	B	23	0	18	3	0
5	A	63	0	0	6	0
5	B	39	0	0	1	0
All	All	10298	0	10152	281	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 14.

All (281) 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:B:267:LYS:H	1:B:267:LYS:HD3	1.27	0.95
1:B:600:THR:HG22	4:B:708:PNM:HC3	1.56	0.88
1:B:414:LEU:HB3	1:B:567:ASN:HD22	1.35	0.87
1:B:381:ASN:HA	1:B:384:THR:HG22	1.57	0.87
1:B:403:SER:HB2	1:B:599:GLY:HA2	1.60	0.82
1:A:554:LYS:HD3	1:A:554:LYS:H	1.43	0.82
1:B:579:VAL:HG13	1:B:587:ILE:HG23	1.58	0.82
1:A:119:GLU:HG3	1:A:124:LYS:HG3	1.61	0.81
1:A:112:VAL:HG13	1:A:134:PRO:HB3	1.62	0.81
1:B:503:ILE:HD12	1:B:524:ILE:HA	1.61	0.81
1:A:491:ASP:HA	1:A:500:ASN:HD21	1.46	0.80
1:B:186:ILE:HD13	1:B:233:LEU:HD21	1.62	0.80
1:A:611:GLY:HA3	1:A:635:ASP:OD1	1.82	0.80
1:B:87:LYS:HE2	1:B:87:LYS:H	1.47	0.79
1:B:200:GLN:HA	1:B:203:GLN:HE21	1.46	0.79
1:B:576:GLN:HE22	1:B:593:ASN:HD21	1.30	0.79
1:A:138:LYS:H	1:A:138:LYS:HD2	1.47	0.78
1:A:89:SER:HB3	1:A:92:LYS:HB2	1.67	0.77
1:A:387:LYS:HG3	5:A:1110:HOH:O	1.86	0.76
1:B:414:LEU:HB3	1:B:567:ASN:ND2	2.02	0.75
1:B:503:ILE:CD1	1:B:525:LEU:H	1.99	0.75
1:A:352:PRO:HG3	1:A:628:MET:HG3	1.70	0.74
1:A:629:MET:CE	1:A:652:VAL:HG11	2.17	0.74
1:A:333:GLN:HE22	1:A:360:LEU:H	1.34	0.73
1:A:138:LYS:H	1:A:138:LYS:CD	2.01	0.73
1:A:136:MET:CE	1:A:142:ILE:HD11	2.20	0.72
1:A:28:LYS:HD2	1:A:28:LYS:N	2.06	0.71
1:B:503:ILE:HD11	1:B:525:LEU:H	1.54	0.71
1:A:491:ASP:HA	1:A:500:ASN:ND2	2.06	0.70
1:B:87:LYS:HE2	1:B:87:LYS:N	2.05	0.70
1:A:91:ASN:HD22	1:A:118:LYS:HB3	1.56	0.69
1:A:486:LEU:HD23	1:A:562:ILE:HD12	1.74	0.69
1:A:230:LYS:HD2	1:A:231:PHE:CE1	2.28	0.69
1:B:524:ILE:HD12	1:B:524:ILE:H	1.58	0.68
1:A:262:GLU:HA	1:A:265:LYS:HE3	1.75	0.67
1:B:247:LYS:HB3	1:B:365:SER:HB3	1.75	0.67
1:A:136:MET:HE2	1:A:142:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLU:HG3	1:A:508:LEU:HD12	1.78	0.65
1:B:269:TYR:CE2	1:B:278:ILE:HD12	2.33	0.64
1:B:408:LEU:CD2	1:B:534:ILE:HG21	2.28	0.64
1:A:267:LYS:HD3	1:A:270:LYS:HE3	1.80	0.64
1:B:267:LYS:O	1:B:270:LYS:HG3	1.98	0.64
1:B:502:GLN:O	1:B:503:ILE:HD13	1.98	0.64
1:A:187:ALA:HB1	1:A:192:ILE:O	1.97	0.63
1:A:336:ILE:HD11	1:A:629:MET:CE	2.29	0.63
1:A:76:LYS:HE3	1:A:104:ASN:OD1	1.99	0.63
1:A:403:SER:HB2	1:A:599:GLY:HA2	1.81	0.62
1:B:516:ASP:HA	1:B:519:TYR:CE2	2.34	0.62
1:B:79:ASN:HB3	1:B:81:GLN:NE2	2.14	0.62
1:B:251:HIS:CD2	1:B:362:SER:HB3	2.34	0.62
1:A:569:ASN:O	1:A:573:ASP:HB2	1.99	0.62
1:B:381:ASN:HA	1:B:384:THR:CG2	2.26	0.62
1:B:502:GLN:C	1:B:503:ILE:HD13	2.19	0.62
1:A:99:TYR:HD1	1:A:112:VAL:HG11	1.64	0.62
1:A:406:LYS:HE2	1:A:519:TYR:HB2	1.81	0.62
1:B:259:ILE:HG12	1:B:264:LEU:HG	1.82	0.62
1:B:471:ALA:HB1	1:B:514:LEU:HD22	1.81	0.62
1:A:408:LEU:HD11	1:A:534:ILE:HD13	1.82	0.61
1:A:112:VAL:CG1	1:A:134:PRO:HB3	2.30	0.61
1:B:354:THR:OG1	1:B:356:GLU:HG3	2.01	0.60
1:A:27:ASP:OD1	1:A:85:ILE:HG21	2.02	0.60
1:B:269:TYR:HE2	1:B:278:ILE:HD12	1.67	0.60
1:A:298:ARG:HG2	1:A:300:THR:HG23	1.83	0.60
1:B:54:LYS:HA	1:B:62:MET:SD	2.42	0.60
1:B:593:ASN:HB2	1:B:623:ASP:OD2	2.01	0.59
1:B:522:GLY:H	1:B:524:ILE:HD11	1.66	0.58
1:A:629:MET:HE3	1:A:652:VAL:HG11	1.83	0.58
1:B:138:LYS:H	1:B:138:LYS:HZ3	1.52	0.58
1:A:262:GLU:HA	1:A:265:LYS:HZ2	1.69	0.58
1:B:576:GLN:HE22	1:B:593:ASN:ND2	2.01	0.57
1:A:46:TYR:CE1	1:A:54:LYS:HG3	2.38	0.57
1:A:408:LEU:HD13	1:A:534:ILE:HG21	1.85	0.57
1:A:407:ILE:O	1:A:411:MET:HG3	2.05	0.57
1:A:408:LEU:CD1	1:A:534:ILE:HG21	2.34	0.57
1:A:381:ASN:HB3	1:A:385:GLU:OE2	2.05	0.57
1:A:182:ASP:HB3	1:A:231:PHE:CD2	2.40	0.56
1:A:252:LEU:O	1:A:283:LEU:HG	2.05	0.56
1:A:182:ASP:HB3	1:A:231:PHE:HD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HA	1:A:227:PHE:HB3	1.87	0.56
1:A:138:LYS:HD2	1:A:138:LYS:N	2.19	0.56
1:A:262:GLU:HA	1:A:265:LYS:CE	2.35	0.56
1:A:501:ALA:HB1	1:A:525:LEU:O	2.05	0.56
1:B:87:LYS:H	1:B:87:LYS:CE	2.19	0.56
1:B:186:ILE:HA	1:B:227:PHE:HZ	1.70	0.55
1:A:336:ILE:HD11	1:A:629:MET:HE2	1.87	0.55
1:A:136:MET:HE1	1:A:142:ILE:HD11	1.88	0.55
1:A:592:ALA:HA	5:A:1138:HOH:O	2.06	0.55
1:B:203:GLN:HB2	1:B:206:VAL:HG23	1.89	0.55
1:B:384:THR:HG23	1:B:385:GLU:HG3	1.88	0.55
1:A:176:LYS:HG3	1:A:208:ASP:O	2.06	0.55
1:A:200:GLN:O	1:A:203:GLN:HG3	2.07	0.55
1:B:352:PRO:HG3	1:B:628:MET:HG3	1.88	0.54
1:A:173:ILE:HG13	1:A:214:LEU:HD11	1.89	0.54
1:A:472:LEU:HD23	1:A:514:LEU:HD12	1.88	0.54
1:A:406:LYS:HD3	1:A:467:PHE:CD1	2.42	0.54
1:B:491:ASP:HA	1:B:500:ASN:OD1	2.07	0.54
1:B:600:THR:HA	1:B:614:ILE:O	2.07	0.54
1:B:524:ILE:H	1:B:524:ILE:CD1	2.17	0.54
1:A:29:GLU:HA	1:A:32:ASN:HD22	1.72	0.54
1:A:629:MET:HE1	1:A:652:VAL:HG11	1.88	0.54
1:A:290:LYS:HB2	1:A:324:ILE:HD11	1.90	0.53
1:B:99:TYR:CD1	1:B:134:PRO:HG3	2.43	0.53
1:B:180:LYS:HA	1:B:183:TYR:CD1	2.43	0.53
1:A:300:THR:HG22	1:A:312:THR:HA	1.89	0.53
1:B:247:LYS:HA	1:B:250:SER:OG	2.09	0.53
1:B:137:GLN:HB3	1:B:138:LYS:HZ1	1.74	0.53
1:B:298:ARG:HD3	5:B:804:HOH:O	2.08	0.53
1:B:600:THR:CG2	4:B:708:PNM:HC3	2.35	0.52
1:A:27:ASP:N	1:A:28:LYS:HD2	2.24	0.52
1:B:267:LYS:HD3	1:B:267:LYS:N	2.11	0.52
1:B:484:LYS:NZ	1:B:484:LYS:HB2	2.25	0.52
1:A:516:ASP:HA	1:A:519:TYR:CE2	2.45	0.52
1:B:137:GLN:HB3	1:B:138:LYS:NZ	2.26	0.52
1:A:151:ARG:HD3	1:A:241:ARG:CZ	2.40	0.51
1:A:456:LYS:HE3	1:A:577:GLN:HE21	1.74	0.51
1:B:446:TYR:HB3	4:B:708:PNM:H101	1.92	0.51
1:A:172:GLY:HA2	1:A:214:LEU:HG	1.92	0.51
1:B:584:LYS:HG3	1:B:585:GLU:H	1.76	0.51
1:B:259:ILE:HD13	1:B:264:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:TYR:HD1	1:B:112:VAL:HG11	1.76	0.51
1:B:403:SER:HB2	1:B:599:GLY:CA	2.37	0.51
1:B:449:VAL:HG23	1:B:449:VAL:O	2.11	0.51
1:A:519:TYR:HE1	1:A:521:GLN:NE2	2.08	0.51
1:A:133:ILE:HB	1:A:136:MET:HE3	1.93	0.51
1:A:75:VAL:HG23	1:A:75:VAL:O	2.10	0.51
1:B:449:VAL:O	1:B:453:ILE:HD11	2.10	0.50
1:A:344:TYR:CD1	1:A:344:TYR:C	2.85	0.50
1:A:363:THR:HA	1:A:364:PRO:C	2.30	0.50
1:A:425:TYR:HD2	1:A:469:ARG:NH1	2.09	0.50
1:A:262:GLU:HA	1:A:265:LYS:NZ	2.27	0.50
1:B:196:TYR:O	1:B:199:GLN:HB3	2.11	0.50
1:B:343:ASP:HB3	1:B:633:VAL:HG13	1.93	0.50
1:A:432:TRP:CZ2	1:A:469:ARG:NE	2.80	0.50
1:A:615:GLY:HA3	1:A:645:ASN:HD21	1.76	0.50
1:A:636:VAL:HG23	1:A:641:MET:HA	1.93	0.50
1:A:527:ASN:ND2	1:A:528:PRO:HD2	2.26	0.50
1:B:38:GLU:OE1	1:B:83:ARG:NH2	2.45	0.50
1:B:200:GLN:HA	1:B:203:GLN:NE2	2.22	0.49
1:A:155:LEU:CD2	1:A:161:GLU:HG2	2.42	0.49
1:B:79:ASN:HB3	1:B:81:GLN:HE21	1.76	0.49
1:B:200:GLN:CA	1:B:203:GLN:HE21	2.19	0.49
1:B:614:ILE:HD13	1:B:634:LYS:HA	1.93	0.49
1:A:91:ASN:ND2	1:A:118:LYS:HD3	2.28	0.49
1:A:336:ILE:HD11	1:A:629:MET:HE1	1.95	0.49
1:B:182:ASP:N	1:B:182:ASP:OD2	2.44	0.49
1:B:384:THR:HG23	1:B:385:GLU:N	2.28	0.49
1:B:471:ALA:HB1	1:B:514:LEU:CD2	2.42	0.49
1:B:550:LEU:HB2	1:B:553:THR:OG1	2.13	0.49
1:A:100:LYS:HA	1:A:108:ILE:O	2.13	0.49
1:B:503:ILE:HD12	1:B:524:ILE:CG2	2.43	0.49
1:A:66:PRO:HG3	1:A:132:ILE:HD13	1.95	0.49
1:B:174:VAL:HB	1:B:177:ASN:ND2	2.28	0.49
1:A:224:LEU:HD12	1:A:224:LEU:N	2.28	0.48
1:A:437:SER:C	1:A:439:GLY:H	2.15	0.48
1:A:554:LYS:H	1:A:554:LYS:CD	2.19	0.48
1:B:175:PRO:HG3	1:B:201:MET:HE3	1.94	0.48
1:A:476:SER:HB2	1:A:508:LEU:HB2	1.94	0.48
1:A:52:ILE:HG23	1:A:53:SER:H	1.79	0.47
1:A:336:ILE:CG1	1:A:629:MET:HE1	2.44	0.47
1:A:634:LYS:O	1:A:635:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:TYR:CG	1:B:134:PRO:HG3	2.50	0.47
1:B:325:GLN:OE1	1:B:551:LYS:HG2	2.15	0.47
1:B:573:ASP:O	1:B:576:GLN:HB3	2.14	0.47
1:A:344:TYR:HA	1:A:364:PRO:HD3	1.97	0.47
1:A:128:ASP:OD2	1:A:128:ASP:C	2.54	0.47
1:A:176:LYS:HB2	1:A:176:LYS:NZ	2.30	0.47
1:A:408:LEU:CD1	1:A:534:ILE:HD13	2.45	0.46
1:B:378:GLU:HA	1:B:378:GLU:OE2	2.14	0.46
1:B:252:LEU:HD22	1:B:283:LEU:HG	1.98	0.46
1:A:428:ASP:HA	1:A:450:ASN:OD1	2.15	0.46
1:A:595:ILE:HD11	1:A:620:TYR:CZ	2.50	0.46
1:B:157:ARG:HB2	1:B:551:LYS:HE2	1.96	0.46
1:A:66:PRO:HG3	1:A:132:ILE:CD1	2.46	0.46
1:A:173:ILE:HG23	1:A:178:VAL:HB	1.97	0.46
1:B:536:SER:HA	1:B:628:MET:SD	2.55	0.46
1:B:587:ILE:HG12	1:B:587:ILE:O	2.15	0.46
1:B:302:VAL:CG1	1:B:307:ASN:HA	2.46	0.46
1:A:327:THR:OG1	1:A:549:LEU:HA	2.16	0.46
1:B:138:LYS:H	1:B:138:LYS:NZ	2.12	0.46
1:A:138:LYS:H	1:A:138:LYS:CE	2.28	0.45
1:A:192:ILE:HA	5:A:1136:HOH:O	2.15	0.45
1:B:584:LYS:HG3	1:B:585:GLU:N	2.31	0.45
1:A:259:ILE:HA	1:A:263:GLU:OE2	2.16	0.45
1:A:615:GLY:HA3	1:A:645:ASN:ND2	2.30	0.45
1:A:613:GLN:HE22	1:A:641:MET:HG2	1.82	0.45
1:B:256:VAL:HG22	1:B:372:MET:CE	2.47	0.45
1:B:436:LYS:O	1:B:436:LYS:HG2	2.17	0.45
1:B:544:ILE:HD11	1:B:562:ILE:HD13	1.97	0.45
1:A:396:GLN:HG2	1:A:499:TYR:CD1	2.52	0.45
1:A:424:SER:HA	1:A:453:ILE:O	2.17	0.45
1:A:133:ILE:HB	1:A:136:MET:CE	2.47	0.45
1:A:382:LYS:HD3	1:A:382:LYS:C	2.37	0.45
1:B:544:ILE:HB	1:B:559:LYS:HB2	1.99	0.45
1:A:173:ILE:CG2	1:A:178:VAL:HB	2.46	0.45
1:A:504:SER:HA	1:A:523:GLU:HB2	1.99	0.45
1:B:222:GLU:HA	1:B:225:SER:HB3	1.99	0.45
1:B:564:SER:O	1:B:568:ILE:HG13	2.17	0.45
1:A:231:PHE:HB2	1:A:233:LEU:HG	1.99	0.44
1:B:220:MET:HE2	1:B:220:MET:HA	1.99	0.44
1:A:292:GLN:OE1	1:A:292:GLN:HA	2.17	0.44
1:A:452:ASN:O	1:A:453:ILE:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLY:HA3	1:B:632:ASN:O	2.16	0.44
1:A:46:TYR:O	1:A:54:LYS:HE2	2.17	0.44
1:B:503:ILE:CD1	1:B:524:ILE:HA	2.41	0.44
1:B:526:ILE:HG22	1:B:527:ASN:N	2.31	0.44
1:B:287:TYR:CZ	1:B:550:LEU:HD11	2.52	0.44
1:A:223:TYR:N	1:A:223:TYR:CD2	2.85	0.44
1:A:662:LYS:C	1:A:663:LYS:HD2	2.38	0.44
1:B:220:MET:HE2	1:B:224:LEU:HD23	2.00	0.44
1:B:503:ILE:CD1	1:B:524:ILE:HG22	2.48	0.44
1:B:537:ALA:CB	1:B:562:ILE:HD11	2.48	0.44
1:A:52:ILE:HG23	1:A:53:SER:N	2.33	0.44
1:B:352:PRO:HA	1:B:536:SER:HB2	2.00	0.44
1:A:265:LYS:NZ	1:A:265:LYS:HB2	2.33	0.43
1:A:375:MET:HB2	1:A:379:GLU:OE2	2.18	0.43
1:A:396:GLN:HG2	1:A:499:TYR:CE1	2.52	0.43
1:A:562:ILE:HD13	1:A:562:ILE:HA	1.90	0.43
1:B:407:ILE:O	1:B:411:MET:HG3	2.17	0.43
1:B:476:SER:HB2	1:B:508:LEU:O	2.19	0.43
1:A:70:TYR:HB3	1:A:75:VAL:CG2	2.48	0.43
1:B:138:LYS:H	1:B:138:LYS:CE	2.32	0.43
1:B:344:TYR:CD2	1:B:344:TYR:C	2.91	0.43
1:B:600:THR:HG23	1:B:600:THR:O	2.18	0.43
1:A:261:SER:O	1:A:265:LYS:HG3	2.18	0.43
1:A:221:ASP:O	1:A:225:SER:HB2	2.18	0.43
1:A:425:TYR:CE2	1:A:469:ARG:HB3	2.53	0.43
1:B:30:ILE:HG23	1:B:116:PHE:CZ	2.54	0.43
1:B:93:LYS:HG3	1:B:123:TRP:CH2	2.53	0.43
1:B:125:LEU:HD13	1:B:127:TRP:N	2.34	0.43
1:A:408:LEU:CD1	1:A:486:LEU:HD13	2.49	0.43
1:B:82:ASP:OD1	1:B:82:ASP:O	2.37	0.43
1:B:387:LYS:HA	1:B:387:LYS:HE2	2.01	0.43
1:B:280:LYS:O	1:B:281:LYS:HG3	2.19	0.43
1:A:157:ARG:HD3	1:A:666:ILE:O	2.18	0.43
1:A:600:THR:HA	1:A:614:ILE:O	2.19	0.43
1:A:405:GLN:O	1:A:408:LEU:HB2	2.19	0.42
1:B:383:LEU:HB3	1:B:391:LEU:CD1	2.49	0.42
1:A:65:ARG:N	1:A:66:PRO:CD	2.82	0.42
1:B:33:THR:O	1:B:36:ALA:HB3	2.19	0.42
1:A:437:SER:C	1:A:439:GLY:N	2.72	0.42
1:B:414:LEU:HD22	1:B:567:ASN:ND2	2.35	0.42
1:B:536:SER:HA	1:B:628:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HA	1:A:629:MET:O	2.19	0.42
1:B:187:ALA:HB2	1:B:197:ILE:HD12	2.01	0.42
1:B:369:TYR:HB2	1:B:370:PRO:HD3	2.00	0.42
1:B:167:THR:CG2	1:B:237:GLU:HG3	2.50	0.42
1:B:191:SER:HB3	1:B:376:SER:HB3	2.01	0.42
1:A:252:LEU:O	1:A:252:LEU:HD12	2.19	0.42
1:A:427:ILE:HA	5:A:1140:HOH:O	2.18	0.42
1:B:138:LYS:HZ3	1:B:138:LYS:N	2.18	0.42
1:B:251:HIS:HE1	1:B:390:PRO:O	2.02	0.42
1:A:137:GLN:HB3	1:A:138:LYS:HD2	2.00	0.42
1:A:419:LEU:HD23	1:A:420:ASP:N	2.34	0.42
1:B:85:ILE:HG12	1:B:95:VAL:HG22	2.02	0.42
1:B:174:VAL:HB	1:B:177:ASN:HD22	1.85	0.42
1:B:536:SER:HA	1:B:628:MET:HE3	2.01	0.42
1:B:173:ILE:HG23	1:B:178:VAL:HB	2.02	0.41
1:B:202:ASP:O	1:B:203:GLN:C	2.57	0.41
1:B:524:ILE:HD12	1:B:524:ILE:N	2.30	0.41
1:B:29:GLU:HG3	1:B:30:ILE:N	2.36	0.41
1:A:88:VAL:O	1:A:88:VAL:HG12	2.19	0.41
1:A:389:GLU:HA	5:A:1115:HOH:O	2.20	0.41
1:A:542:GLY:O	1:A:562:ILE:HB	2.20	0.41
1:B:207:GLN:HB2	1:B:210:THR:OG1	2.20	0.41
1:B:151:ARG:HA	1:B:293:HIS:CD2	2.55	0.41
1:A:223:TYR:N	1:A:223:TYR:HD2	2.19	0.41
1:A:521:GLN:HG3	5:A:1133:HOH:O	2.20	0.41
1:A:425:TYR:CD2	1:A:469:ARG:NH1	2.89	0.41
1:B:128:ASP:C	1:B:128:ASP:OD2	2.59	0.41
1:A:75:VAL:HA	1:A:102:LYS:O	2.21	0.41
1:A:263:GLU:OE2	1:A:278:ILE:HD11	2.21	0.41
1:A:402:GLY:O	1:A:520:GLY:HA3	2.20	0.41
1:A:579:VAL:HG11	1:A:594:LEU:O	2.20	0.41
1:B:75:VAL:HA	1:B:102:LYS:O	2.21	0.41
1:A:483:MET:HB2	1:A:503:ILE:HD13	2.02	0.40
1:B:180:LYS:HA	1:B:183:TYR:CE1	2.56	0.40
1:B:204:ASN:OD1	1:B:205:TRP:N	2.54	0.40
1:A:401:PRO:O	1:A:402:GLY:C	2.58	0.40
1:A:223:TYR:HB2	1:A:224:LEU:HD12	2.01	0.40
1:B:298:ARG:HG2	1:B:300:THR:HG23	2.03	0.40
1:A:173:ILE:HG23	1:A:178:VAL:CG2	2.52	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	631/646 (98%)	593 (94%)	36 (6%)	2 (0%)	37	45
1	B	618/646 (96%)	574 (93%)	39 (6%)	5 (1%)	16	21
All	All	1249/1292 (97%)	1167 (93%)	75 (6%)	7 (1%)	22	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	203	GLN
1	B	273	LYS
1	A	175	PRO
1	B	28	LYS
1	B	264	LEU
1	B	188	LYS
1	A	625	PRO

### 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	567/576 (98%)	550 (97%)	17 (3%)	36	51
1	B	559/576 (97%)	540 (97%)	19 (3%)	32	46
All	All	1126/1152 (98%)	1090 (97%)	36 (3%)	34	48

All (36) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	28	LYS
1	A	99	TYR
1	A	111	ASN
1	A	112	VAL
1	A	125	LEU
1	A	138	LYS
1	A	156	ASP
1	A	175	PRO
1	A	177	ASN
1	A	223	TYR
1	A	245	LEU
1	A	344	TYR
1	A	419	LEU
1	A	554	LYS
1	A	573	ASP
1	A	593	ASN
1	A	663	LYS
1	B	87	LYS
1	B	99	TYR
1	B	130	SER
1	B	182	ASP
1	B	184	LYS
1	B	202	ASP
1	B	230	LYS
1	B	252	LEU
1	B	267	LYS
1	B	274	ASP
1	B	344	TYR
1	B	377	ASN
1	B	392	LEU
1	B	463	ASP
1	B	480	GLU
1	B	513	LEU
1	B	514	LEU
1	B	524	ILE
1	B	593	ASN

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

Mol	Chain	Res	Type
1	A	32	ASN
1	A	81	GLN
1	A	91	ASN

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Mol	Chain	Res	Type
1	A	137	GLN
1	A	207	GLN
1	A	305	ASN
1	A	333	GLN
1	A	377	ASN
1	A	433	GLN
1	A	500	ASN
1	A	521	GLN
1	A	540	ASN
1	A	593	ASN
1	A	613	GLN
1	A	645	ASN
1	B	32	ASN
1	B	81	GLN
1	B	115	ASN
1	B	177	ASN
1	B	251	HIS
1	B	266	GLN
1	B	305	ASN
1	B	377	ASN
1	B	396	GLN
1	B	433	GLN
1	B	502	GLN
1	B	567	ASN
1	B	577	GLN
1	B	593	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 13 are monoatomic - leaving 2 for Mogul analysis.

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
4	PNM	B	708	1	19,24,24	1.54	4 (21%)	25,34,34	2.08	3 (12%)
4	PNM	A	1007	1	19,24,24	1.49	3 (15%)	25,34,34	2.00	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
4	PNM	B	708	1	-	2/12/33/33	0/2/2/2
4	PNM	A	1007	1	-	1/12/33/33	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	PNM	C21-C20	3.88	1.46	1.38
4	B	708	PNM	C21-C20	3.83	1.46	1.38
4	B	708	PNM	C15-N14	2.88	1.40	1.34
4	A	1007	PNM	C15-N14	2.68	1.39	1.34
4	B	708	PNM	O13-C11	-2.39	1.23	1.30
4	A	1007	PNM	O13-C11	-2.17	1.23	1.30
4	B	708	PNM	C6-N14	2.06	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	708	PNM	C7-C6-N14	-7.79	97.52	109.80
4	A	1007	PNM	C7-C6-N14	-7.48	98.00	109.80
4	B	708	PNM	C5-C6-N14	4.83	120.17	109.93
4	A	1007	PNM	C5-C6-N14	4.48	119.42	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	708	PNM	C2-C3-C11	2.17	116.48	112.37

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	708	PNM	O13-C11-C3-N4
4	B	708	PNM	O12-C11-C3-N4
4	A	1007	PNM	C7-C6-N14-C15

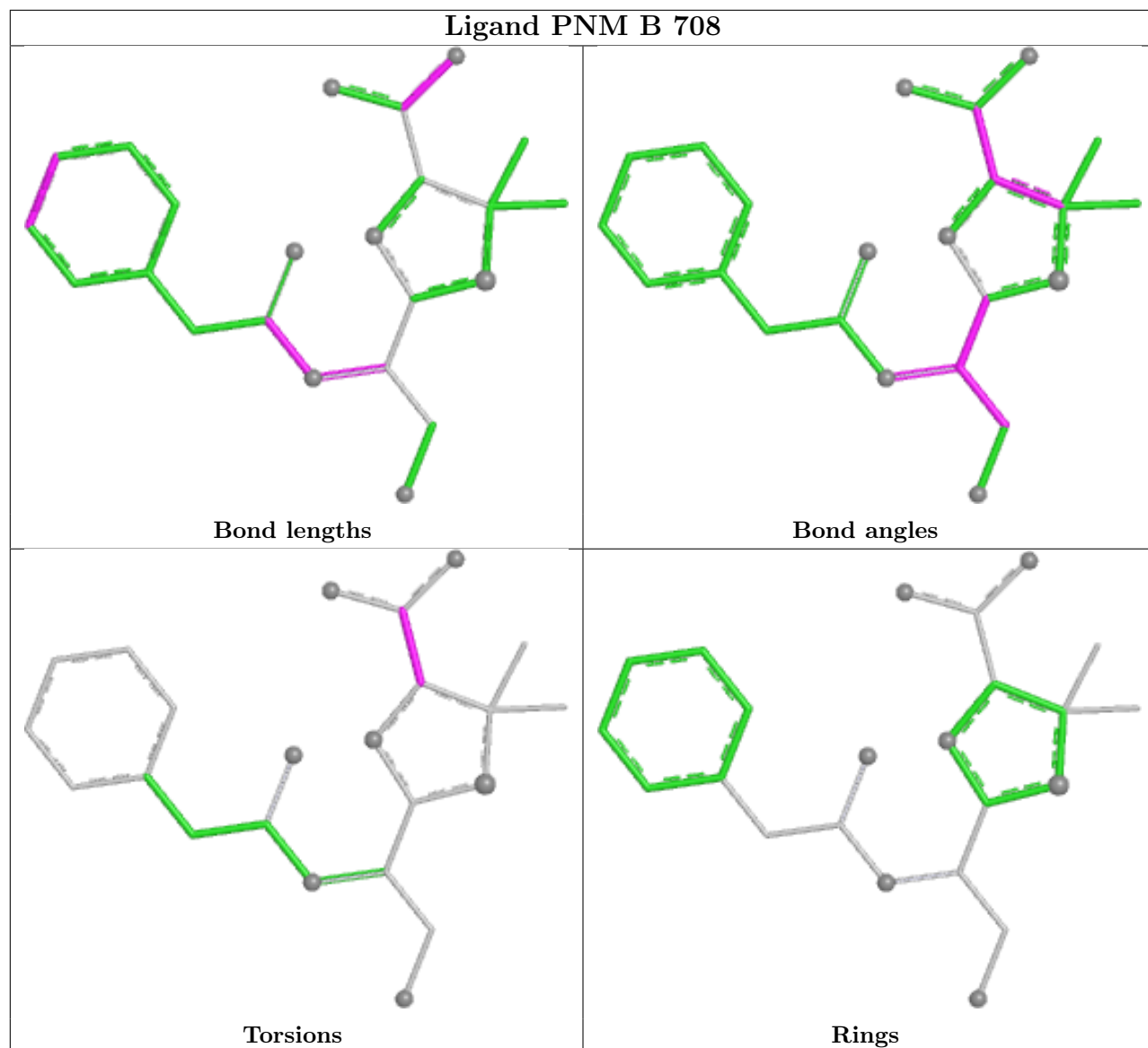
There are no ring outliers.

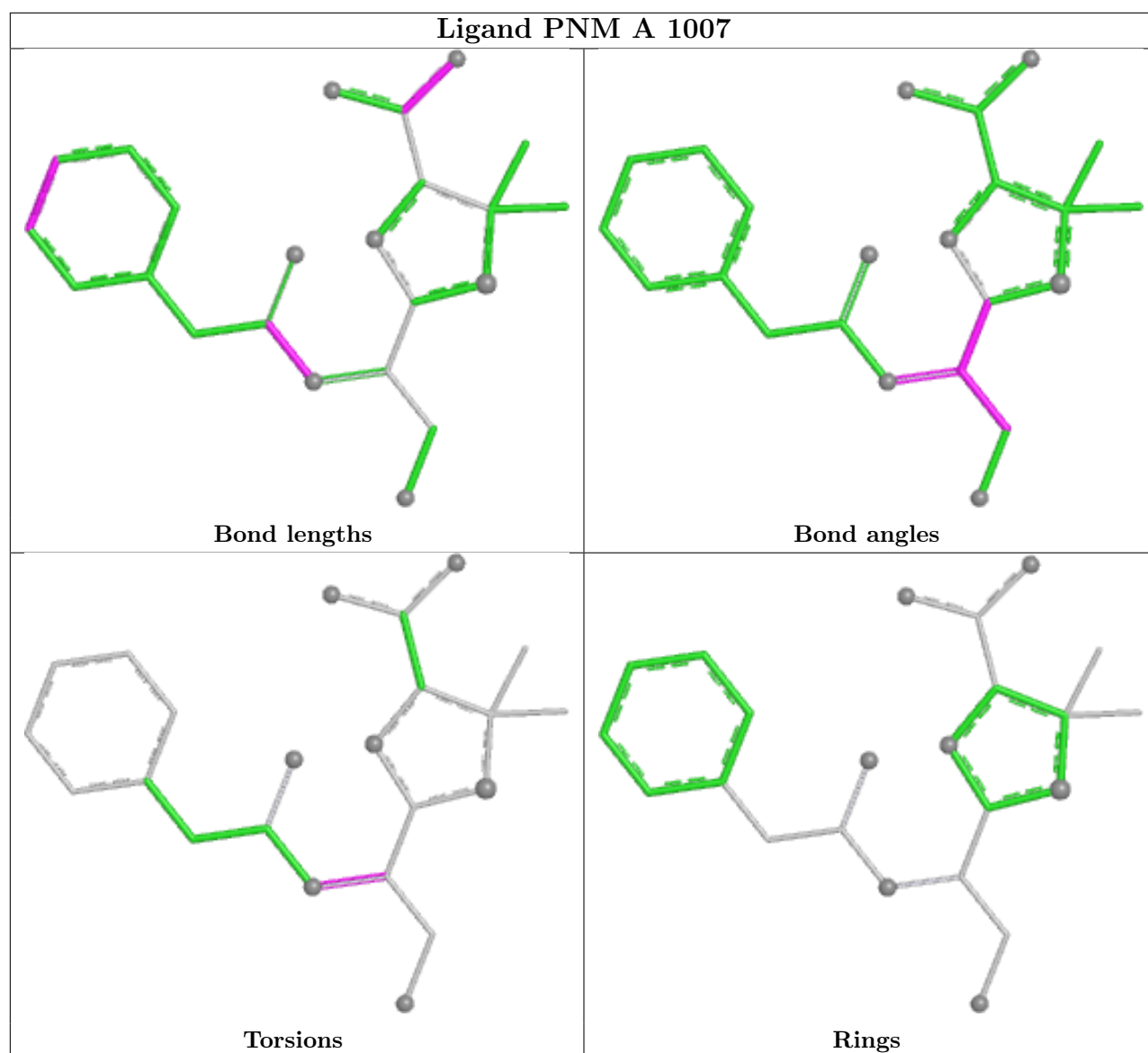
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	708	PNM	3	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.

## Ligand PNM B 708





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	635/646 (98%)	-0.13	14 (2%) 62 65	21, 45, 83, 101	0
1	B	626/646 (96%)	0.05	11 (1%) 67 69	27, 50, 82, 102	0
All	All	1261/1292 (97%)	-0.04	25 (1%) 64 67	21, 48, 83, 102	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	503	ILE	4.1
1	A	28	LYS	3.6
1	B	603	LEU	3.3
1	B	502	GLN	3.2
1	A	264	LEU	3.1
1	B	269	TYR	3.0
1	A	223	TYR	2.9
1	A	272	TYR	2.9
1	B	122	MET	2.7
1	A	265	LYS	2.7
1	B	223	TYR	2.6
1	A	611	GLY	2.6
1	B	383	LEU	2.6
1	A	267	LYS	2.4
1	A	27	ASP	2.4
1	B	508	LEU	2.3
1	A	90	LYS	2.2
1	A	603	LEU	2.2
1	B	121	GLY	2.2
1	B	428	ASP	2.2
1	A	122	MET	2.1
1	A	224	LEU	2.1
1	A	91	ASN	2.0
1	B	378	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	85	ILE	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, 95<sup>th</sup> 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.

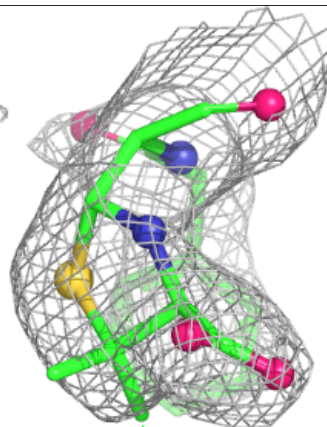
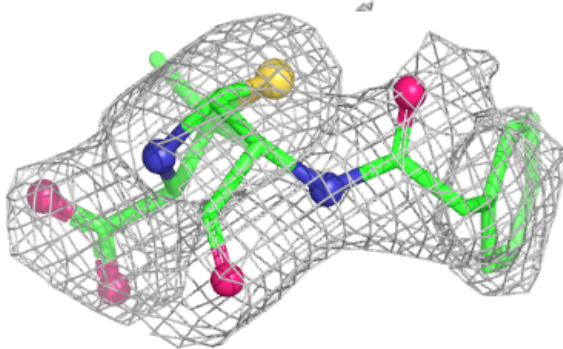
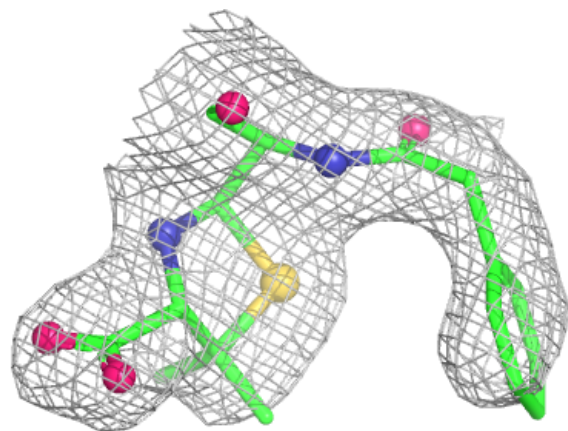
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CD	B	703	1/1	0.93	0.10	60,60,60,60	1
2	CD	B	705	1/1	0.93	0.09	60,60,60,60	1
2	CD	A	1003	1/1	0.94	0.11	67,67,67,67	1
2	CD	A	1004	1/1	0.94	0.07	61,61,61,61	1
4	PNM	B	708	23/23	0.94	0.10	48,53,66,69	0
4	PNM	A	1007	23/23	0.96	0.08	31,40,60,62	0
3	CL	A	1006	1/1	0.98	0.06	38,38,38,38	0
2	CD	B	704	1/1	0.99	0.07	57,57,57,57	1
3	CL	B	706	1/1	0.99	0.04	30,30,30,30	0
3	CL	B	707	1/1	0.99	0.03	32,32,32,32	0
2	CD	B	702	1/1	0.99	0.03	35,35,35,35	0
3	CL	A	1005	1/1	0.99	0.03	36,36,36,36	0
2	CD	A	1002	1/1	1.00	0.03	42,42,42,42	0
2	CD	B	701	1/1	1.00	0.01	34,34,34,34	0
2	CD	A	1001	1/1	1.00	0.02	35,35,35,35	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.



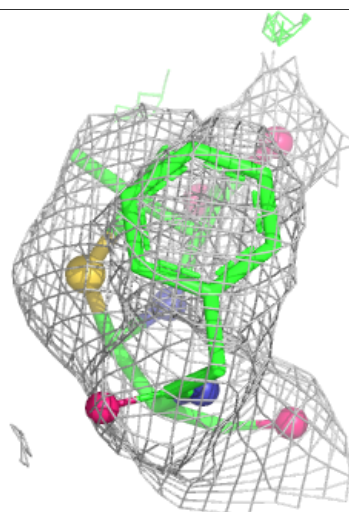
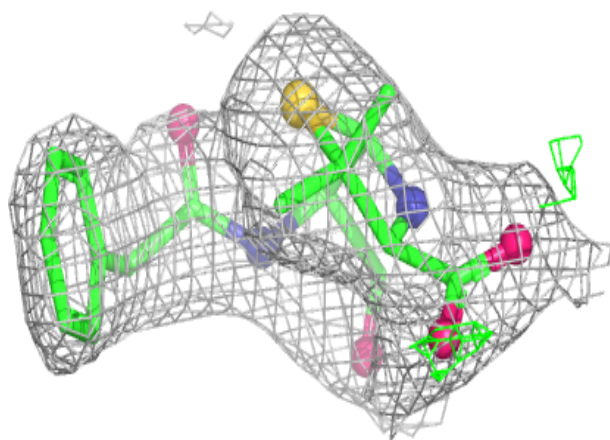
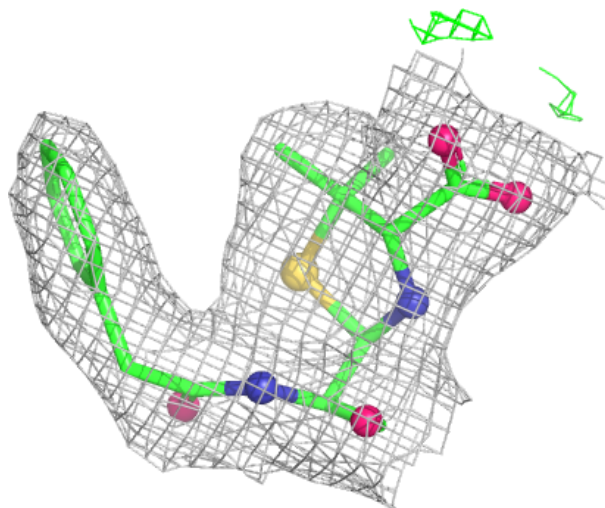
**Electron density around PNM B 708:**

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



**Electron density around PNM A 1007:**

$2mF_o-DF_c$  (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.