



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 1GM7 / pdb_00001gm7
Title : Crystal structures of penicillin acylase enzyme-substrate complexes: Structural insights into the catalytic mechanism
Authors : McVey, C.E.; Walsh, M.A.; Dodson, G.G.; Wilson, K.S.; Brannigan, J.A.
Deposited on : 2001-09-11
Resolution : 1.45 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

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

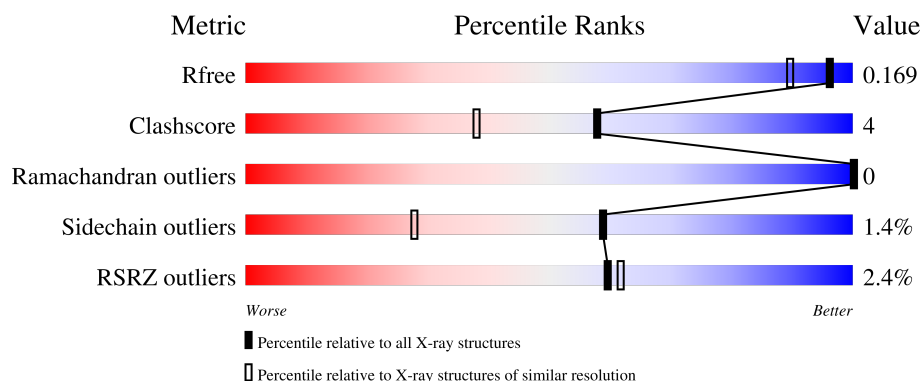
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

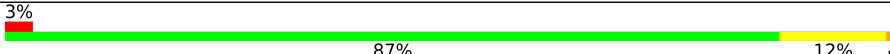
The reported resolution of this entry is 1.45 Å.

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}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 ≥ 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	209	 89% 9%
2	B	557	 3% 87% 12%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7378 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 G ACYLASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	8	0
			1726	1098	290	329	9			

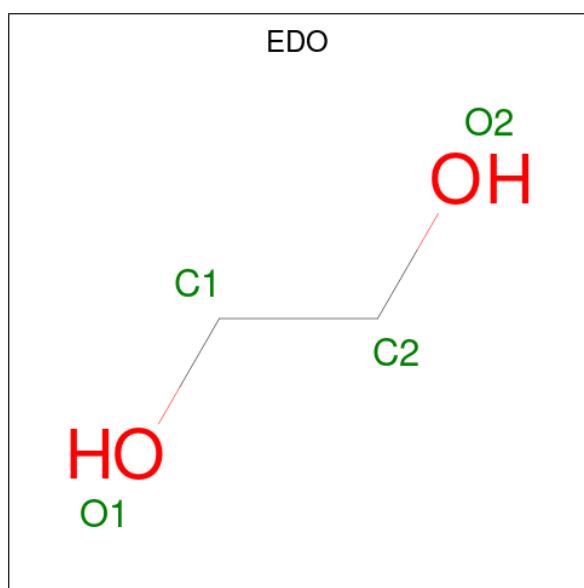
- Molecule 2 is a protein called PENICILLIN G ACYLASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	7	23	0
			4606	2924	800	872	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	241	ALA	ASN	engineered mutation	UNP P06875

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

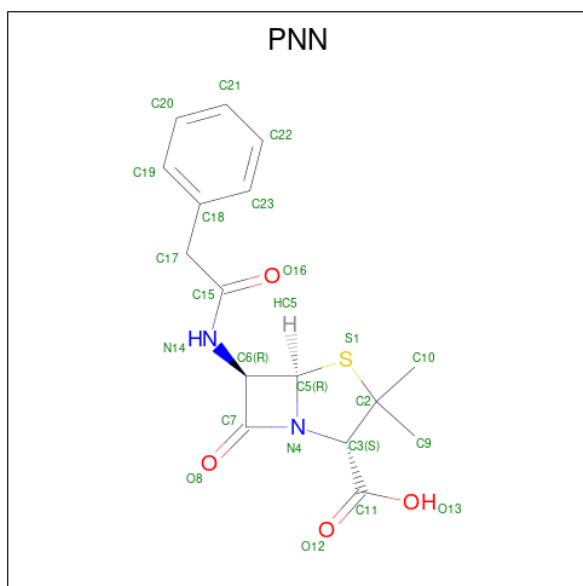


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 8 4 4	0	1
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 8 4 4	0	1
3	B	1	Total C O 8 4 4	0	1

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is PENICILLIN G (CCD ID: PNN) (formula: $C_{16}H_{18}N_2O_4S$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	252	Total	O	2	7
			252	252		
6	B	678	Total	O	0	14
			678	678		

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.

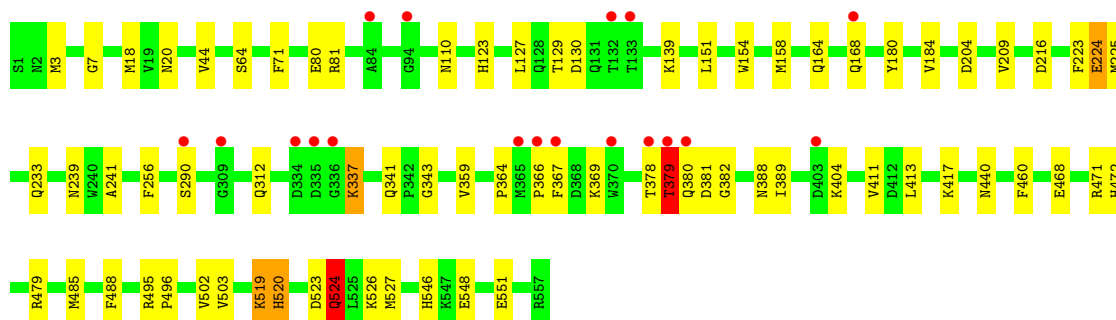
• Molecule 1: PENICILLIN G ACYLASE ALPHA SUBUNIT

Chain A:  89% 9%



• Molecule 2: PENICILLIN G ACYLASE BETA SUBUNIT

Chain B:  3% 87% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.60Å 131.80Å 63.90Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.45 30.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.45) 99.2 (30.00-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.44Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.173 0.155 , 0.169	Depositor DCC
R_{free} test set	4326 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.1	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	0.97	EDS
Total number of atoms	7378	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: SME, PNN, EDO, CA

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	0.79	0/1759	1.38	13/2381 (0.5%)
2	B	0.82	5/4736 (0.1%)	1.38	30/6458 (0.5%)
All	All	0.81	5/6495 (0.1%)	1.38	43/8839 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	224	GLU	CA-CB	11.59	1.71	1.53
2	B	526	LYS	CG-CD	-9.67	1.23	1.52
2	B	224	GLU	CA-C	7.14	1.62	1.52
2	B	223	PHE	C-N	6.92	1.43	1.33
2	B	224	GLU	C-N	5.60	1.42	1.33

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	524	GLN	CG-CD-NE2	-12.56	97.55	116.40
1	A	203	GLN	OE1-CD-NE2	-9.89	112.71	122.60
2	B	20	ASN	CA-CB-CG	9.23	121.83	112.60
2	B	524	GLN	CG-CD-OE1	9.07	138.94	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	81	ARG	CD-NE-CZ	8.56	136.38	124.40
2	B	168	GLN	CB-CG-CD	-7.54	99.78	112.60
2	B	520	HIS	CB-CG-CD2	-7.54	121.41	131.20
2	B	369	LYS	CA-C-O	-7.23	112.66	120.32
1	A	28	PHE	CA-CB-CG	-7.18	106.62	113.80
2	B	224	GLU	CB-CA-C	7.13	122.80	110.68
2	B	524	GLN	CB-CG-CD	7.08	124.64	112.60
1	A	76	ASP	CA-CB-CG	6.93	119.53	112.60
2	B	127	LEU	CB-CA-C	-6.58	97.67	110.11
2	B	369	LYS	O-C-N	-6.43	115.30	122.12
2	B	369	LYS	CG-CD-CE	-6.39	96.61	111.30
1	A	38	ASP	CA-CB-CG	6.28	118.88	112.60
2	B	551	GLU	CA-CB-CG	6.23	126.56	114.10
1	A	145	ARG	NE-CZ-NH1	6.17	127.67	121.50
2	B	460	PHE	CA-CB-CG	6.16	119.96	113.80
2	B	312	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	A	145	ARG	NE-CZ-NH2	-6.14	113.68	119.20
1	A	112	GLU	CB-CG-CD	6.10	122.97	112.60
2	B	110	ASN	CA-CB-CG	6.08	118.68	112.60
2	B	519	LYS	CB-CG-CD	-5.99	97.53	111.30
1	A	183	ASN	CA-CB-CG	5.74	118.34	112.60
2	B	520	HIS	CB-CG-ND1	5.73	131.30	122.70
2	B	546	HIS	CA-CB-CG	-5.66	108.14	113.80
2	B	312	GLN	CB-CG-CD	5.59	122.10	112.60
1	A	47	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	A	94	GLN	OE1-CD-NE2	5.43	128.03	122.60
2	B	343	GLY	N-CA-C	5.41	119.22	112.73
2	B	404	LYS	N-CA-C	-5.39	106.20	112.89
1	A	60	LYS	N-CA-C	5.33	118.89	112.38
2	B	366	PRO	CA-C-N	5.32	127.94	120.28
2	B	366	PRO	C-N-CA	5.32	127.94	120.28
2	B	341	GLN	OE1-CD-NE2	5.29	127.89	122.60
2	B	7	GLY	O-C-N	5.24	127.86	122.88
2	B	130	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	337	LYS	CB-CG-CD	5.17	123.20	111.30
2	B	224	GLU	N-CA-C	-5.17	105.08	111.33
1	A	184	PRO	N-CA-CB	5.14	108.45	103.51
2	B	440	ASN	N-CA-C	5.11	119.49	113.16
1	A	67	LYS	O-C-N	5.11	127.53	122.12

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5[B]	SER	Mainchain
2	B	129[B]	THR	Mainchain
2	B	224	GLU	Mainchain
2	B	379[B]	THR	Mainchain

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	1726	0	1662	17	0
2	B	4606	0	4405	48	0
3	A	8	0	12	1	0
3	B	84	0	125	2	0
4	B	1	0	0	0	0
5	B	23	0	17	0	0
6	A	252	0	0	0	0
6	B	678	0	0	6	0
All	All	7378	0	6221	57	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 4.

All (57) 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)
2:B:379[A]:THR:OG1	2:B:380:GLN:N	1.61	1.07
1:A:207:GLN:H	1:A:207:GLN:HE21	1.19	0.90
2:B:524:GLN:HG2	2:B:527:MET:HE2	1.54	0.88
2:B:524:GLN:HG2	2:B:527:MET:CE	2.13	0.78
1:A:207:GLN:HE22	2:B:204:ASP:H	1.30	0.78
1:A:177:GLN:HE22	2:B:411:VAL:H	1.34	0.74
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.73	0.71
2:B:80:GLU:OE2	2:B:123[B]:HIS:HD2	1.73	0.71
2:B:388:ASN:HD22	2:B:389:ILE:H	1.40	0.67
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.78	0.66
1:A:207:GLN:NE2	2:B:204:ASP:H	1.96	0.62
1:A:198:PRO:HG2	2:B:225:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495[A]:ARG:HG3	6:B:2562[A]:HOH:O	2.01	0.60
2:B:503:VAL:N	2:B:524:GLN:OE1	2.29	0.59
1:A:183:ASN:C	1:A:183:ASN:HD22	2.11	0.59
1:A:198:PRO:CG	2:B:225:MET:HE1	2.35	0.57
2:B:503:VAL:H	2:B:524:GLN:CD	2.13	0.56
2:B:379[A]:THR:HG23	2:B:382:GLY:N	2.22	0.55
1:A:198:PRO:HD2	2:B:225:MET:HE1	1.89	0.54
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.89	0.54
2:B:472:HIS:HD2	6:B:2520:HOH:O	1.92	0.53
2:B:502:VAL:HA	2:B:524:GLN:OE1	2.10	0.52
2:B:123[B]:HIS:HE1	2:B:216:ASP:OD1	1.92	0.52
2:B:378[A]:THR:HG23	2:B:379[A]:THR:N	2.26	0.50
3:B:1563:EDO:H22	6:B:2312:HOH:O	2.10	0.50
1:A:183:ASN:HD22	1:A:185[B]:SER:H	1.60	0.49
2:B:379[B]:THR:OG1	2:B:380:GLN:N	2.43	0.49
2:B:417:LYS:NZ	6:B:2482:HOH:O	2.46	0.49
2:B:256:PHE:CD2	3:B:1559:EDO:H11	2.48	0.49
2:B:471[A]:ARG:HD2	6:B:2545[A]:HOH:O	2.12	0.49
1:A:72:ASN:HD21	2:B:139:LYS:NZ	2.12	0.47
2:B:64:SER:HG	2:B:488[B]:PHE:HZ	1.62	0.47
1:A:198:PRO:CD	2:B:225:MET:HE1	2.46	0.46
2:B:364:PRO:O	2:B:367:PHE:HB2	2.16	0.46
2:B:388:ASN:ND2	2:B:389:ILE:H	2.11	0.46
1:A:207:GLN:HE21	1:A:207:GLN:N	2.00	0.45
1:A:183:ASN:ND2	1:A:185[B]:SER:H	2.14	0.45
2:B:468[B]:GLU:H	2:B:468[B]:GLU:CD	2.24	0.45
2:B:151:LEU:HD23	2:B:151:LEU:C	2.42	0.45
1:A:194:GLU:OE2	2:B:233[B]:GLN:HG3	2.17	0.44
1:A:183:ASN:HD22	1:A:185[A]:SER:H	1.64	0.43
2:B:359[B]:VAL:CG1	2:B:413:LEU:HD13	2.49	0.43
2:B:184[A]:VAL:HG12	2:B:488[A]:PHE:CD1	2.55	0.42
1:A:183:ASN:ND2	1:A:185[A]:SER:H	2.16	0.42
2:B:80:GLU:OE2	2:B:123[B]:HIS:CD2	2.60	0.42
2:B:3:MET:HE3	2:B:180:TYR:HB2	2.01	0.42
2:B:184[A]:VAL:HG12	2:B:488[A]:PHE:HD1	1.84	0.42
2:B:379[A]:THR:HG21	2:B:381:ASP:HB2	2.02	0.42
1:A:153:ILE:HD12	3:A:1211:EDO:H21	2.01	0.42
2:B:290[B]:SER:OG	2:B:479:ARG:HB3	2.19	0.42
2:B:164:GLN:NE2	6:B:2218[A]:HOH:O	2.53	0.41
2:B:471[A]:ARG:HD3	2:B:471[A]:ARG:HA	1.87	0.41
2:B:71:PHE:CD1	2:B:256:PHE:CE2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:MET:O	2:B:485:MET:HA	2.20	0.40
2:B:239:ASN:ND2	2:B:241:ALA:H	2.19	0.40
2:B:495[B]:ARG:HA	2:B:496:PRO:HD3	1.92	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	212/209 (101%)	209 (99%)	3 (1%)	0	100	100
2	B	578/557 (104%)	566 (98%)	12 (2%)	0	100	100
All	All	790/766 (103%)	775 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/179 (103%)	182 (98%)	3 (2%)	55	23
2	B	482/459 (105%)	475 (98%)	7 (2%)	57	25
All	All	667/638 (104%)	657 (98%)	10 (2%)	59	25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	LEU
1	A	183	ASN
1	A	207	GLN
2	B	154	TRP
2	B	209	VAL
2	B	337	LYS
2	B	379[A]	THR
2	B	379[B]	THR
2	B	519	LYS
2	B	524	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	120	ASN
1	A	177	GLN
1	A	183	ASN
1	A	204	GLN
1	A	207	GLN
2	B	12	GLN
2	B	93	ASN
2	B	239	ASN
2	B	245	GLN
2	B	273	GLN
2	B	348	ASN
2	B	380	GLN
2	B	388	ASN
2	B	401	GLN
2	B	409	GLN
2	B	472	HIS
2	B	520	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SME	A	16	1	6,8,9	0.75	0	3,9,11	0.52	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
1	SME	A	16	1	-	0/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 1 is monoatomic - leaving 24 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
3	EDO	B	1558	-	3,3,3	0.26	0	2,2,2	0.17	0
3	EDO	B	1570[B]	-	3,3,3	0.49	0	2,2,2	0.57	0
3	EDO	B	1575[A]	-	3,3,3	0.36	0	2,2,2	0.30	0
3	EDO	B	1567	-	3,3,3	0.67	0	2,2,2	0.68	0
3	EDO	B	1565	-	3,3,3	0.49	0	2,2,2	0.28	0
3	EDO	A	1210	-	3,3,3	0.42	0	2,2,2	0.40	0
3	EDO	B	1569	-	3,3,3	0.54	0	2,2,2	0.83	0
3	EDO	B	1575[B]	-	3,3,3	0.37	0	2,2,2	0.34	0
3	EDO	B	1574[A]	-	3,3,3	0.63	0	2,2,2	0.67	0
3	EDO	B	1574[B]	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	B	1566	-	3,3,3	0.44	0	2,2,2	0.22	0
3	EDO	B	1559	-	3,3,3	0.50	0	2,2,2	0.32	0
3	EDO	B	1560	-	3,3,3	0.51	0	2,2,2	0.38	0
3	EDO	B	1568	-	3,3,3	0.41	0	2,2,2	0.42	0
3	EDO	B	1573	-	3,3,3	0.68	0	2,2,2	1.53	1 (50%)
5	PNN	B	1577	-	25,25,25	1.44	4 (16%)	38,38,38	2.41	14 (36%)
3	EDO	B	1562	-	3,3,3	0.42	0	2,2,2	0.26	0
3	EDO	A	1211	-	3,3,3	0.55	0	2,2,2	0.66	0
3	EDO	B	1561	-	3,3,3	0.33	0	2,2,2	0.07	0
3	EDO	B	1564	-	3,3,3	0.42	0	2,2,2	0.21	0
3	EDO	B	1563	-	3,3,3	0.79	0	2,2,2	0.87	0
3	EDO	B	1571	-	3,3,3	0.51	0	2,2,2	0.53	0
3	EDO	B	1572	-	3,3,3	0.58	0	2,2,2	0.60	0
3	EDO	B	1570[A]	-	3,3,3	0.58	0	2,2,2	0.38	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
3	EDO	B	1558	-	-	0/1/1/1	-
3	EDO	B	1570[B]	-	-	1/1/1/1	-
3	EDO	B	1575[A]	-	-	0/1/1/1	-
3	EDO	B	1567	-	-	0/1/1/1	-
3	EDO	B	1565	-	-	0/1/1/1	-
3	EDO	A	1210	-	-	0/1/1/1	-
3	EDO	B	1569	-	-	0/1/1/1	-
3	EDO	B	1575[B]	-	-	1/1/1/1	-
3	EDO	B	1574[A]	-	-	1/1/1/1	-
3	EDO	B	1574[B]	-	-	1/1/1/1	-
3	EDO	B	1566	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1559	-	-	0/1/1/1	-
3	EDO	B	1560	-	-	0/1/1/1	-
3	EDO	B	1568	-	-	0/1/1/1	-
3	EDO	B	1573	-	-	0/1/1/1	-
5	PNN	B	1577	-	-	0/12/43/43	0/3/3/3
3	EDO	B	1562	-	-	0/1/1/1	-
3	EDO	A	1211	-	-	0/1/1/1	-
3	EDO	B	1561	-	-	0/1/1/1	-
3	EDO	B	1564	-	-	0/1/1/1	-
3	EDO	B	1563	-	-	0/1/1/1	-
3	EDO	B	1571	-	-	0/1/1/1	-
3	EDO	B	1572	-	-	0/1/1/1	-
3	EDO	B	1570[A]	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1577	PNN	O12-C11	4.28	1.34	1.22
5	B	1577	PNN	O13-C11	-3.14	1.20	1.30
5	B	1577	PNN	C17-C18	2.30	1.55	1.51
5	B	1577	PNN	C20-C19	2.00	1.42	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1577	PNN	C21-C20-C19	-6.52	112.20	120.24
5	B	1577	PNN	O13-C11-C3	5.99	129.68	112.47
5	B	1577	PNN	O16-C15-N14	4.91	131.26	122.95
5	B	1577	PNN	C22-C21-C20	4.26	125.70	119.87
5	B	1577	PNN	O12-C11-C3	-4.19	109.93	122.89
5	B	1577	PNN	C22-C23-C18	-3.09	116.26	120.61
5	B	1577	PNN	O8-C7-N4	-2.99	127.63	131.75
5	B	1577	PNN	O16-C15-C17	-2.75	116.03	121.99
5	B	1577	PNN	C23-C18-C19	2.72	122.27	118.23
5	B	1577	PNN	C9-C2-C10	2.57	114.88	110.70
5	B	1577	PNN	S1-C5-N4	-2.28	101.85	104.93
5	B	1577	PNN	C11-C3-N4	-2.25	108.38	112.10
5	B	1577	PNN	C17-C15-N14	-2.09	112.63	115.88
3	B	1573	EDO	O1-C1-C2	2.08	128.23	112.39
5	B	1577	PNN	C17-C18-C19	-2.01	117.94	120.89

There are no chirality outliers.

All (4) torsion outliers are listed below:

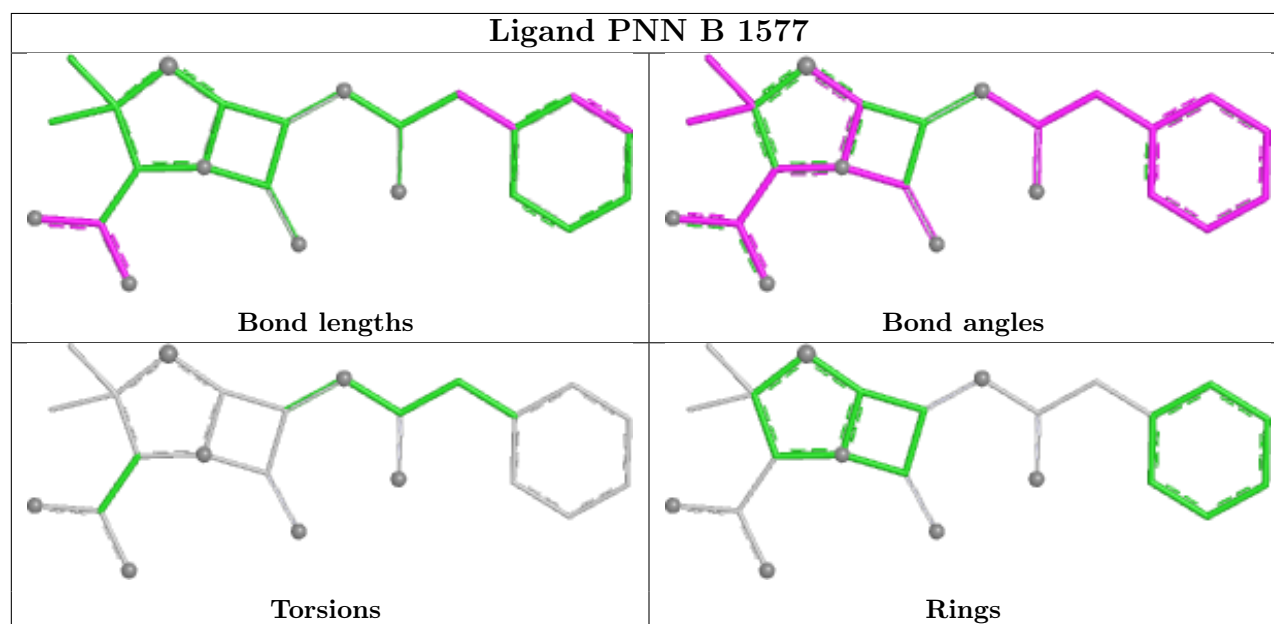
Mol	Chain	Res	Type	Atoms
3	B	1574[B]	EDO	O1-C1-C2-O2
3	B	1574[A]	EDO	O1-C1-C2-O2
3	B	1575[B]	EDO	O1-C1-C2-O2
3	B	1570[B]	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1559	EDO	1	0
3	A	1211	EDO	1	0
3	B	1563	EDO	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	206/209 (98%)	-0.34	0	100	100	5, 12, 21, 43	8 (3%)
2	B	557/557 (100%)	-0.16	18 (3%)	50	53	5, 12, 28, 55	25 (4%)
All	All	763/766 (99%)	-0.21	18 (2%)	59	62	5, 12, 27, 55	33 (4%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	367	PHE	7.3
2	B	132	THR	4.4
2	B	370[A]	TRP	4.3
2	B	379[A]	THR	3.9
2	B	336	GLY	3.2
2	B	380	GLN	2.9
2	B	84	ALA	2.9
2	B	94	GLY	2.9
2	B	290[A]	SER	2.9
2	B	403	ASP	2.7
2	B	334	ASP	2.7
2	B	309	GLY	2.6
2	B	366	PRO	2.6
2	B	133	THR	2.5
2	B	168	GLN	2.2
2	B	365	MET	2.2
2	B	335	ASP	2.1
2	B	378[A]	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SME	A	16	9/10	0.99	0.05	8,9,11,12	0

6.3 Carbohydrates [i](#)

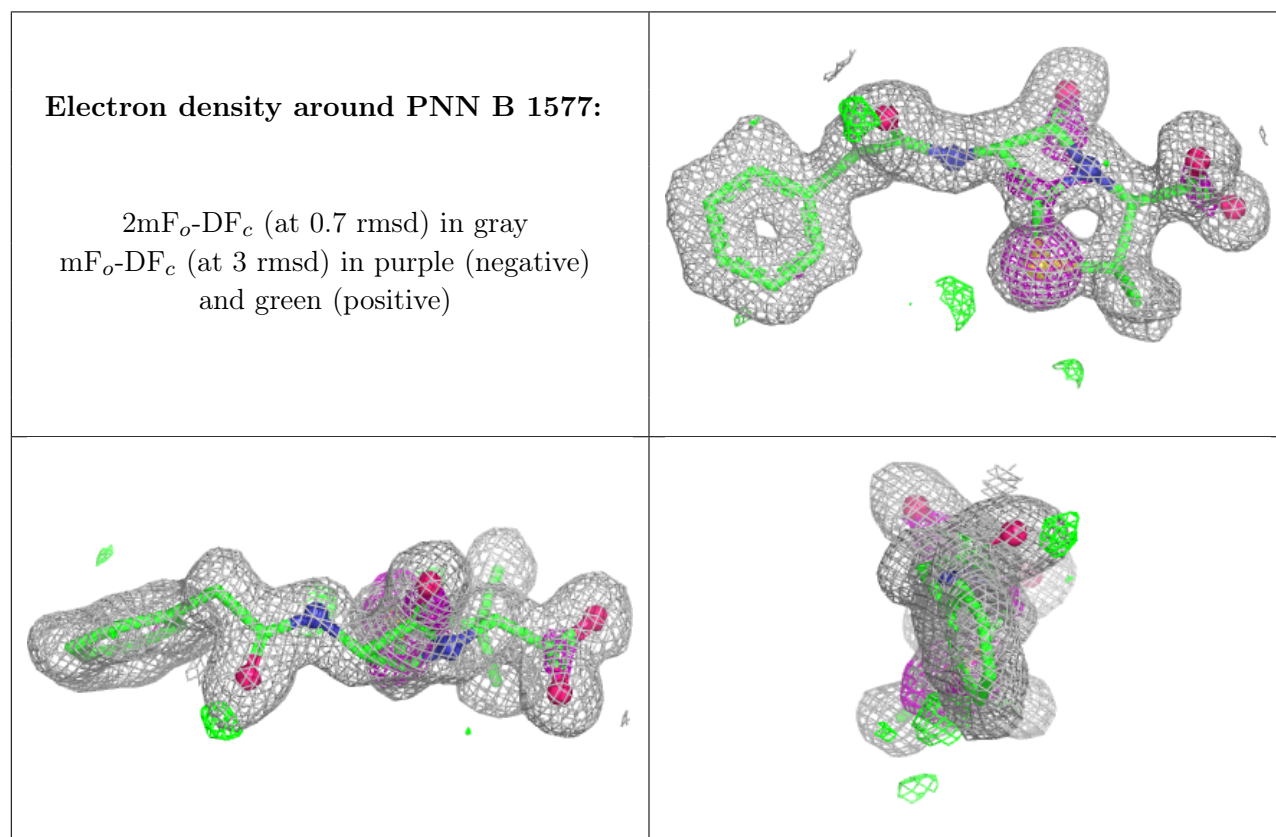
There are no oligosaccharides in this entry.

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
3	EDO	A	1211	4/4	0.86	0.14	26,30,30,32	0
3	EDO	B	1574[A]	4/4	0.89	0.12	14,16,16,17	4
3	EDO	B	1574[B]	4/4	0.89	0.12	23,23,24,25	4
3	EDO	B	1562	4/4	0.90	0.11	23,24,25,26	0
3	EDO	B	1568	4/4	0.90	0.14	19,23,24,27	0
3	EDO	B	1569	4/4	0.91	0.09	26,27,28,31	0
3	EDO	A	1210	4/4	0.93	0.11	19,31,32,35	0
3	EDO	B	1575[A]	4/4	0.93	0.10	11,14,15,15	4
3	EDO	B	1575[B]	4/4	0.93	0.10	8,21,22,26	4
3	EDO	B	1561	4/4	0.94	0.08	19,22,25,26	0
3	EDO	B	1563	4/4	0.94	0.09	14,16,18,22	0
3	EDO	B	1571	4/4	0.94	0.16	17,23,25,27	0
3	EDO	B	1573	4/4	0.94	0.12	18,24,28,28	0
3	EDO	B	1572	4/4	0.95	0.12	20,22,22,23	0
3	EDO	B	1567	4/4	0.96	0.09	14,16,16,18	0
3	EDO	B	1560	4/4	0.96	0.07	12,12,13,13	0
5	PNN	B	1577	23/23	0.96	0.07	9,14,19,19	0
3	EDO	B	1570[A]	4/4	0.97	0.09	10,14,20,22	4
3	EDO	B	1570[B]	4/4	0.97	0.09	13,16,18,19	4
3	EDO	B	1558	4/4	0.97	0.05	11,14,14,16	0
3	EDO	B	1565	4/4	0.97	0.06	13,16,17,17	0
3	EDO	B	1566	4/4	0.97	0.07	12,15,15,17	0
3	EDO	B	1564	4/4	0.99	0.05	15,15,16,17	0
3	EDO	B	1559	4/4	0.99	0.05	9,10,14,14	0
4	CA	B	1576	1/1	1.00	0.02	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.