



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2016 – 11:39 AM EST

PDB ID : 1GM7
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

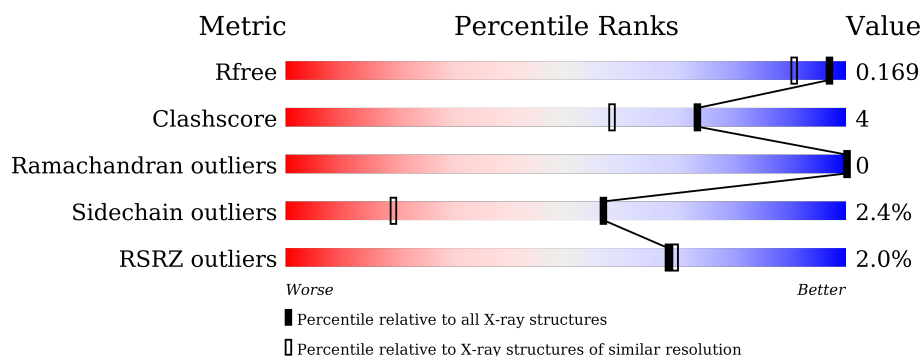
1 Overall quality at a glance ⓘ

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}	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 1% 88% 10% .. </div> </div>
2	B	557	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 2% 87% 11% . </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1210	-	-	-	X
3	EDO	A	1211	-	-	-	X
3	EDO	B	1563	-	-	-	X
3	EDO	B	1566	-	-	-	X
3	EDO	B	1568	-	-	-	X
3	EDO	B	1570[A]	-	-	-	X
3	EDO	B	1572	-	-	-	X
3	EDO	B	1574[A]	-	-	-	X
3	EDO	B	1574[B]	-	-	-	X
3	EDO	B	1575[B]	-	-	-	X
5	PNN	B	1577	-	-	-	X

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			

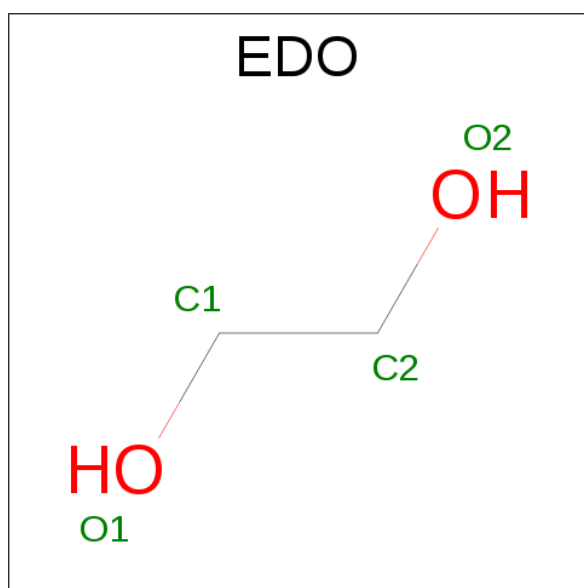
- Molecule 2 is a protein called PENICILLIN G ACYLASE BETA SUBUNIT.

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 (three-letter code: EDO) (formula: C₂H₆O₂).

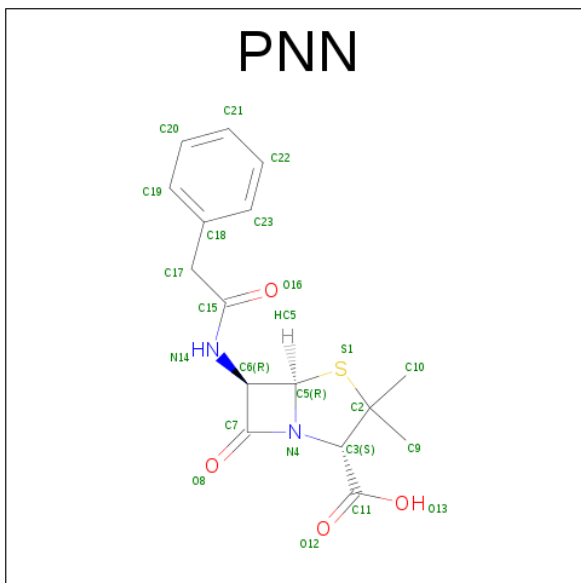


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
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 (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is PENICILLIN G (three-letter code: 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		

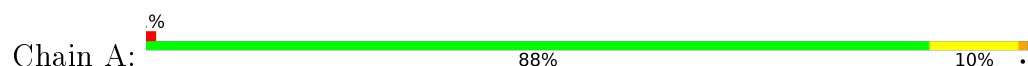
- Molecule 6 is water.

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

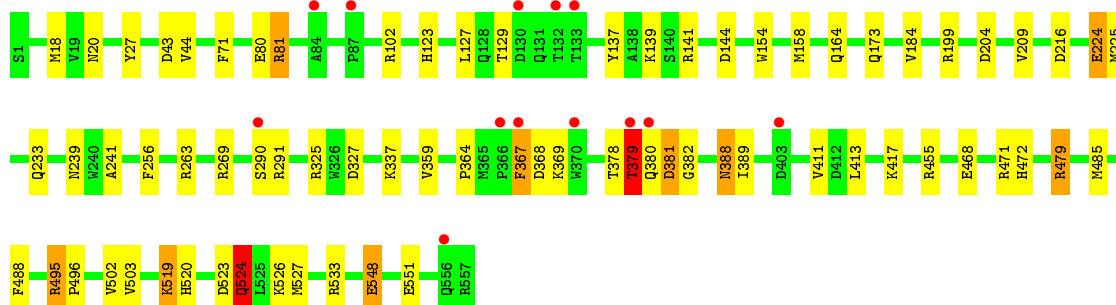
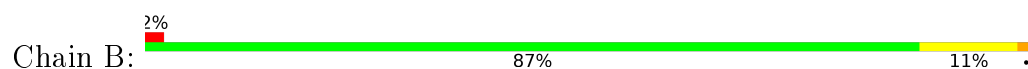
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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



• Molecule 2: PENICILLIN G ACYLASE BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.60 Å 131.80 Å 63.90 Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	30.00 – 1.45 29.97 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.45) 98.6 (29.97-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 1.44 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.173 0.155 , 0.169	Depositor DCC
R_{free} test set	4323 reflections (3.10%)	DCC
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.4	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: CA, EDO, SME, PNN

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	0.65	0/1759	1.31	17/2381 (0.7%)
2	B	0.67	2/4736 (0.0%)	1.28	40/6458 (0.6%)
All	All	0.66	2/6495 (0.0%)	1.29	57/8839 (0.6%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	526	LYS	CG-CD	-8.54	1.23	1.52
2	B	224	GLU	CA-CB	8.06	1.71	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	A	145	ARG	NE-CZ-NH2	-13.25	113.68	120.30
1	A	47	ARG	NE-CZ-NH2	-12.24	114.18	120.30
2	B	379[A]	THR	N-CA-CB	11.54	132.22	110.30
2	B	379[B]	THR	N-CA-CB	11.54	132.22	110.30
1	A	128	ARG	NE-CZ-NH2	-11.04	114.78	120.30
2	B	533	ARG	NE-CZ-NH1	10.42	125.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	455	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	B	379[A]	THR	CB-CA-C	-10.08	84.39	111.60
2	B	379[B]	THR	CB-CA-C	-10.08	84.39	111.60
2	B	81	ARG	CD-NE-CZ	9.13	136.38	123.60
2	B	81	ARG	NE-CZ-NH1	8.72	124.66	120.30
2	B	524	GLN	CG-CD-OE1	8.67	138.94	121.60
2	B	455	ARG	NE-CZ-NH1	8.30	124.45	120.30
2	B	369	LYS	O-C-N	7.99	135.48	122.70
2	B	524	GLN	CG-CD-NE2	-7.98	97.55	116.70
2	B	269	ARG	NE-CZ-NH2	-7.77	116.42	120.30
2	B	291	ARG	NE-CZ-NH2	-7.45	116.58	120.30
2	B	27	TYR	CB-CG-CD2	-7.32	116.61	121.00
2	B	479	ARG	NE-CZ-NH2	-7.25	116.67	120.30
2	B	199	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	B	102	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	194	GLU	OE1-CD-OE2	6.74	131.39	123.30
2	B	367	PHE	CB-CG-CD2	6.72	125.51	120.80
2	B	381	ASP	CB-CG-OD2	-6.71	112.27	118.30
2	B	141	ARG	NE-CZ-NH1	-6.63	116.98	120.30
2	B	127	LEU	CB-CA-C	-6.59	97.67	110.20
2	B	367	PHE	CB-CG-CD1	-6.55	116.22	120.80
2	B	137	TYR	CB-CG-CD2	-6.35	117.19	121.00
2	B	548	GLU	OE1-CD-OE2	6.25	130.80	123.30
2	B	224	GLU	CB-CA-C	6.20	122.80	110.40
2	B	368	ASP	CB-CG-OD2	-6.17	112.74	118.30
2	B	144[A]	ASP	CB-CG-OD2	-6.16	112.76	118.30
2	B	144[B]	ASP	CB-CG-OD2	-6.16	112.76	118.30
2	B	551	GLU	CA-CB-CG	5.98	126.56	113.40
1	A	29	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	A	152	GLU	OE1-CD-OE2	-5.80	116.34	123.30
2	B	43	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	39	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	B	495[A]	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	B	495[B]	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	89	ASP	CB-CG-OD2	-5.44	113.41	118.30
2	B	325	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	B	519	LYS	CB-CG-CD	-5.41	97.53	111.60
1	A	23	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	12	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	71	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	193[A]	GLN	CG-CD-OE1	5.23	132.05	121.60
1	A	193[B]	GLN	CG-CD-OE1	5.23	132.05	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	327	ASP	CB-CG-OD1	5.20	122.98	118.30
2	B	263	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	29	TYR	CB-CG-CD1	5.13	124.08	121.00
2	B	137	TYR	CB-CG-CD1	5.13	124.08	121.00
2	B	369	LYS	CG-CD-CE	-5.10	96.61	111.90
1	A	68	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	A	128	ARG	NH1-CZ-NH2	5.02	124.92	119.40
2	B	524	GLN	CB-CG-CD	5.01	124.64	111.60

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 ⓘ

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	14	0
2	B	4606	0	4405	43	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	52	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 (52) 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:HE21	1:A:207:GLN:H	1.19	0.90
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:524:GLN:HG2	2:B:527:MET:HE2	1.70	0.72
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
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:198:PRO:HG2	2:B:225:MET:HE1	1.88	0.56
2:B:379[A]:THR:HG23	2:B:382:GLY:N	2.22	0.55
1:A:183:ASN:HD22	1:A:183:ASN:C	2.11	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:524:GLN:HG2	2:B:527:MET:HE1	1.90	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:503:VAL:H	2:B:524:GLN:CD	2.13	0.51
3:B:1563:EDO:H22	6:B:2312:HOH:O	2.10	0.50
2:B:378[A]:THR:HG23	2:B:379[A]:THR:N	2.26	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:468[B]:GLU:H	2:B:468[B]:GLU:CD	2.24	0.40
2:B:239:ASN:ND2	2:B:241:ALA:H	2.19	0.40
2:B:18:MET:O	2:B:485:MET:HA	2.20	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%)	180 (97%)	5 (3%)	52	15
2	B	482/459 (105%)	471 (98%)	11 (2%)	58	21
All	All	667/638 (104%)	651 (98%)	16 (2%)	57	19

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	TYR
1	A	181	LEU
1	A	183	ASN
1	A	204	GLN
1	A	207	GLN
2	B	20	ASN
2	B	81	ARG
2	B	154	TRP
2	B	173	GLN
2	B	209	VAL
2	B	337	LYS
2	B	379[A]	THR
2	B	379[B]	THR
2	B	388	ASN
2	B	519	LYS
2	B	524	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	93	ASN
2	B	239	ASN
2	B	245	GLN
2	B	312	GLN
2	B	348	ASN
2	B	380	GLN
2	B	388	ASN
2	B	401	GLN

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Mol	Chain	Res	Type
2	B	472	HIS
2	B	520	HIS
2	B	546	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.79	0	6,9,11	0.88	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	-	0/5/7/9	0/0/0/0

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1210	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	A	1211	-	3,3,3	0.56	0	2,2,2	0.72	0
3	EDO	B	1558	-	3,3,3	0.28	0	2,2,2	0.16	0
3	EDO	B	1559	-	3,3,3	0.52	0	2,2,2	0.37	0
3	EDO	B	1560	-	3,3,3	0.54	0	2,2,2	0.41	0
3	EDO	B	1561	-	3,3,3	0.36	0	2,2,2	0.08	0
3	EDO	B	1562	-	3,3,3	0.45	0	2,2,2	0.27	0
3	EDO	B	1563	-	3,3,3	0.82	0	2,2,2	0.95	0
3	EDO	B	1564	-	3,3,3	0.44	0	2,2,2	0.23	0
3	EDO	B	1565	-	3,3,3	0.52	0	2,2,2	0.29	0
3	EDO	B	1566	-	3,3,3	0.46	0	2,2,2	0.23	0
3	EDO	B	1567	-	3,3,3	0.70	0	2,2,2	0.74	0
3	EDO	B	1568	-	3,3,3	0.44	0	2,2,2	0.45	0
3	EDO	B	1569	-	3,3,3	0.57	0	2,2,2	0.90	0
3	EDO	B	1570[A]	-	3,3,3	0.60	0	2,2,2	0.41	0
3	EDO	B	1570[B]	-	3,3,3	0.51	0	2,2,2	0.62	0
3	EDO	B	1571	-	3,3,3	0.53	0	2,2,2	0.56	0
3	EDO	B	1572	-	3,3,3	0.60	0	2,2,2	0.64	0
3	EDO	B	1573	-	3,3,3	0.64	0	2,2,2	1.72	1 (50%)
3	EDO	B	1574[A]	-	3,3,3	0.64	0	2,2,2	0.73	0
3	EDO	B	1574[B]	-	3,3,3	0.47	0	2,2,2	0.41	0
3	EDO	B	1575[A]	-	3,3,3	0.38	0	2,2,2	0.34	0
3	EDO	B	1575[B]	-	3,3,3	0.38	0	2,2,2	0.38	0
5	PNN	B	1577	-	22,25,25	0.92	1 (4%)	33,38,38	2.01	10 (30%)

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	A	1210	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1211	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1558	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1559	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1560	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1561	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1562	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1563	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1564	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1565	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1566	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1567	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1568	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1569	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1570[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1570[B]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1571	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1572	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1573	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1574[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1574[B]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1575[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1575[B]	-	-	0/1/1/1	0/0/0/0
5	PNN	B	1577	-	-	0/8/43/43	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1577	PNN	C17-C18	2.16	1.55	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1577	PNN	C21-C20-C19	-5.76	112.20	120.20
5	B	1577	PNN	C22-C23-C18	-2.89	116.26	120.65
5	B	1577	PNN	O8-C7-N4	-2.73	127.63	131.62
5	B	1577	PNN	C17-C15-N14	-2.20	112.63	115.88
5	B	1577	PNN	S1-C5-N4	-2.12	101.85	104.97
5	B	1577	PNN	O16-C15-C17	-2.07	116.03	121.89
3	B	1573	EDO	O1-C1-C2	2.34	128.23	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1577	PNN	C23-C18-C19	2.50	122.27	118.15
5	B	1577	PNN	C9-C2-C10	2.64	114.88	110.77
5	B	1577	PNN	C22-C21-C20	3.42	125.70	119.88
5	B	1577	PNN	O16-C15-N14	4.94	131.26	122.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

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	206/209 (98%)	-0.26	2 (0%) 84 85	8, 12, 21, 43	0
2	B	557/557 (100%)	-0.13	13 (2%) 64 65	7, 12, 29, 55	2 (0%)
All	All	763/766 (99%)	-0.16	15 (1%) 68 69	7, 12, 27, 55	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	132	THR	7.7
2	B	133	THR	5.1
2	B	370[A]	TRP	4.2
2	B	367	PHE	4.1
2	B	380	GLN	4.0
1	A	3	SER	3.9
2	B	379[A]	THR	3.3
1	A	4	SER	3.0
2	B	403	ASP	2.9
2	B	87	PRO	2.6
2	B	290[A]	SER	2.5
2	B	84	ALA	2.5
2	B	130	ASP	2.3
2	B	556	GLN	2.3
2	B	366	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
1	SME	A	16	9/10	0.98	0.07	-	8,9,11,12	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	EDO	B	1566	4/4	0.96	0.12	14.11	12,15,15,17	0
3	EDO	B	1575[B]	4/4	0.87	0.20	12.44	8,21,22,26	4
3	EDO	A	1211	4/4	0.89	0.15	7.55	26,30,30,32	0
3	EDO	B	1563	4/4	0.94	0.11	7.53	14,16,18,22	0
3	EDO	B	1570[A]	4/4	0.95	0.15	6.13	10,14,20,22	4
3	EDO	B	1568	4/4	0.91	0.19	5.86	19,23,24,27	0
5	PNN	B	1577	23/23	0.94	0.13	3.94	9,14,19,19	0
3	EDO	B	1574[B]	4/4	0.86	0.17	3.94	23,23,24,25	4
3	EDO	B	1574[A]	4/4	0.86	0.17	3.64	14,16,16,17	4
3	EDO	B	1572	4/4	0.95	0.16	3.07	20,22,22,23	0
3	EDO	A	1210	4/4	0.94	0.14	2.30	19,31,32,35	0
3	EDO	B	1573	4/4	0.93	0.13	1.53	18,24,28,28	0
3	EDO	B	1571	4/4	0.95	0.16	1.06	17,23,25,27	0
3	EDO	B	1567	4/4	0.96	0.09	0.47	14,16,16,18	0
3	EDO	B	1565	4/4	0.97	0.07	0.17	13,16,17,17	0
3	EDO	B	1560	4/4	0.97	0.08	0.07	12,12,13,13	0
3	EDO	B	1558	4/4	0.98	0.06	-0.02	11,14,14,16	0
3	EDO	B	1561	4/4	0.93	0.08	-0.22	19,22,25,26	0
3	EDO	B	1559	4/4	0.98	0.06	-1.11	9,10,14,14	0
4	CA	B	1576	1/1	1.00	0.05	-2.82	8,8,8,8	0
3	EDO	B	1564	4/4	0.99	0.05	-	15,15,16,17	0
3	EDO	B	1562	4/4	0.88	0.12	-	23,24,25,26	0
3	EDO	B	1569	4/4	0.89	0.16	-	26,27,28,31	0
3	EDO	B	1570[B]	4/4	0.95	0.15	-	13,16,18,19	4
3	EDO	B	1575[A]	4/4	0.87	0.20	-	11,14,15,15	4

6.5 Other polymers ⓘ

There are no such residues in this entry.