



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:00 PM UTC

PDB ID : 1GK9 / pdb_00001gk9
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 : 2001-08-10
Resolution : 1.30 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
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

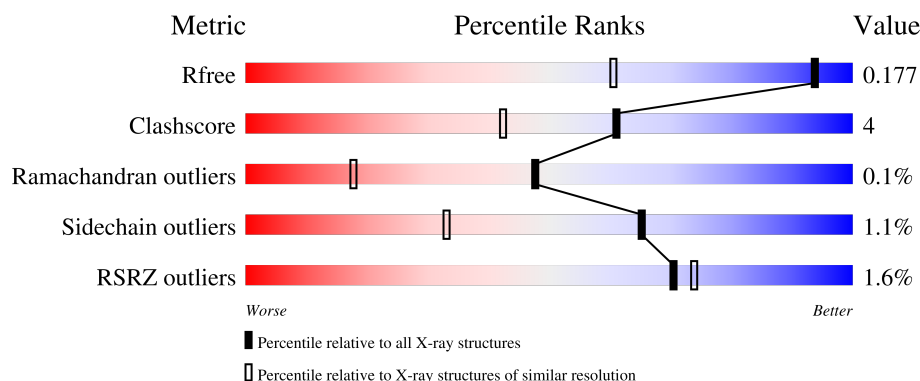
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	260	 68% 11% 20%
2	B	557	 2% 86% 13%

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	B	1578[B]	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7533 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.

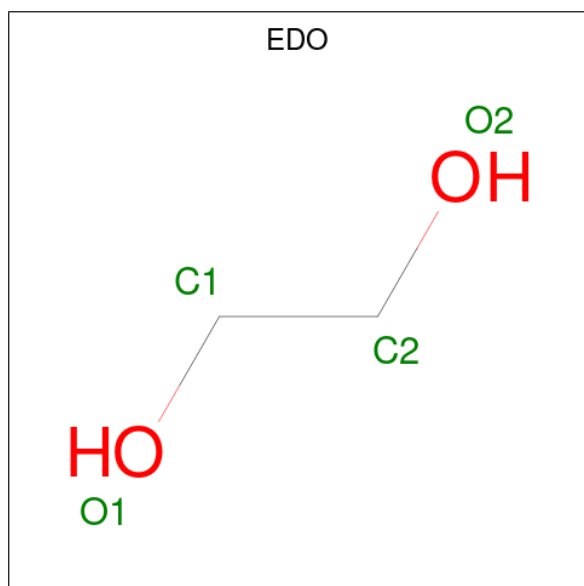
- Molecule 1 is a protein called PENICILLIN G ACYLASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	5	10	0
			1750	1114	293	334	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	8	40	0
			4751	3016	825	899	11			

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



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 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 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

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

- 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		

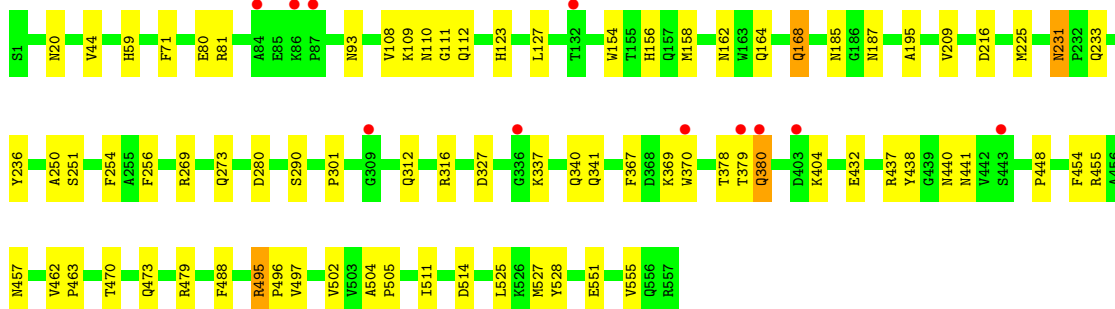
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	254	Total	O	0	5
			254	254		
5	B	669	Total	O	0	10
			669	669		

• Molecule 1: PENICILLIN G ACYLASE ALPHA SUBUNIT

TYR	GLU	Q2	S5	F23	D38	F41	G59	K60	D61	N72	D76	A102	K106	F119	N120	R128	I137	S149	I153	D164	K165	V168	S169	Q170	A173	L181	V182	M183	P184	S185	P198	L199	Q204	A209	ALA	LEU	LEU	PRO	ARG					
ASP	LEU	PRO	ALA	PRO	MET	ASP	ARG	PRO	ALA	LYS	GLY	ALA	LEU	ALA	LEU	ALA	LYS	ASN	ARG	GLY	THR	ILE	ALA	ALA	ALA	GLN	PHE	ALA	ALA	GLM	GLY	GLY	ALA	ASN	GLY	LEU	ALA	GLY	TYR					

Chain B:  2% 86% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.30Å 131.60Å 63.90Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	20.00 – 1.30 20.00 – 1.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-1.30) 94.0 (20.00-1.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 1.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.169 (Not available) , 0.177	Depositor DCC
R_{free} test set	5756 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	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	7533	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.26	1/1794 (0.1%)	1.66	26/2432 (1.1%)
2	B	1.16	7/4895 (0.1%)	1.56	48/6669 (0.7%)
All	All	1.19	8/6689 (0.1%)	1.59	74/9101 (0.8%)

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	6
All	All	0	7

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	LYS	CD-CE	-12.38	1.15	1.52
2	B	156	HIS	CE1-NE2	-7.24	1.25	1.32
2	B	231	ASN	CA-CB	7.19	1.57	1.52
2	B	231	ASN	CA-C	-6.34	1.48	1.53
2	B	231	ASN	C-O	5.87	1.26	1.23
2	B	111	GLY	N-CA	-5.66	1.39	1.45
2	B	448	PRO	C-N	-5.48	1.25	1.33
2	B	108	VAL	C-O	5.06	1.29	1.24

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	LYS	CG-CD-CE	12.94	141.05	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	ASN	OD1-CG-ND2	-9.26	113.34	122.60
2	B	369	LYS	CA-C-O	-9.20	109.70	120.10
2	B	164	GLN	CB-CG-CD	9.02	127.93	112.60
2	B	440	ASN	OD1-CG-ND2	-8.95	113.65	122.60
2	B	340	GLN	OE1-CD-NE2	8.76	131.36	122.60
2	B	20	ASN	CA-CB-CG	8.43	121.03	112.60
2	B	337	LYS	CA-CB-CG	8.21	130.52	114.10
2	B	369	LYS	O-C-N	-8.13	112.71	122.22
2	B	341	GLN	OE1-CD-NE2	8.06	130.66	122.60
2	B	455[A]	ARG	NE-CZ-NH2	7.90	126.31	119.20
2	B	455[B]	ARG	NE-CZ-NH2	7.90	126.31	119.20
1	A	38	ASP	CA-CB-CG	7.72	120.32	112.60
2	B	269	ARG	NE-CZ-NH2	-7.70	112.27	119.20
2	B	441	ASN	OD1-CG-ND2	7.68	130.28	122.60
2	B	156	HIS	CB-CG-CD2	-7.44	121.53	131.20
1	A	119	PHE	O-C-N	7.42	129.99	122.12
2	B	551	GLU	CA-CB-CG	7.16	128.43	114.10
1	A	168	VAL	O-C-N	-7.06	114.99	121.91
2	B	280	ASP	CA-C-O	-6.76	113.39	120.55
2	B	110	ASN	CA-CB-CG	6.57	119.17	112.60
1	A	128	ARG	NE-CZ-NH2	-6.41	113.43	119.20
2	B	312	GLN	OE1-CD-NE2	-6.25	116.35	122.60
1	A	59	GLY	CA-C-N	6.20	129.21	120.28
1	A	59	GLY	C-N-CA	6.20	129.21	120.28
2	B	59	HIS	ND1-CE1-NE2	6.08	114.48	108.40
2	B	112	GLN	OE1-CD-NE2	5.81	128.41	122.60
2	B	470	THR	O-C-N	-5.81	115.72	122.87
2	B	462	VAL	CA-C-O	5.79	122.95	119.19
2	B	273	GLN	CB-CG-CD	-5.78	102.78	112.60
1	A	165	LYS	CA-C-N	5.74	131.38	122.26
1	A	165	LYS	C-N-CA	5.74	131.38	122.26
2	B	316	ARG	O-C-N	-5.70	116.08	122.12
2	B	164	GLN	O-C-N	-5.55	116.35	122.07
1	A	170	GLN	CB-CG-CD	5.52	121.98	112.60
1	A	76	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	59	GLY	O-C-N	-5.49	116.88	122.98
1	A	60	LYS	CD-CE-NZ	-5.49	94.33	111.90
1	A	72	ASN	O-C-N	-5.49	115.76	122.34
1	A	173	ALA	CA-C-O	-5.47	114.62	120.42
2	B	236	TYR	CA-C-O	5.47	127.08	121.23
2	B	514	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	41	PHE	O-C-N	5.44	127.67	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LYS	CA-C-O	5.40	126.49	120.82
2	B	301	PRO	CA-C-N	5.38	127.43	120.44
2	B	301	PRO	C-N-CA	5.38	127.43	120.44
2	B	93	ASN	OD1-CG-ND2	5.37	127.97	122.60
2	B	108	VAL	CA-C-O	-5.36	114.86	120.27
2	B	525[A]	LEU	CA-C-O	-5.36	114.74	120.42
2	B	525[B]	LEU	CA-C-O	-5.36	114.74	120.42
2	B	195	ALA	O-C-N	-5.35	117.12	123.22
2	B	340	GLN	CG-CD-NE2	-5.32	108.42	116.40
2	B	462	VAL	O-C-N	-5.31	116.78	121.61
1	A	165	LYS	O-C-N	-5.29	115.35	122.23
2	B	511	ILE	O-C-N	5.28	128.90	123.20
2	B	231	ASN	CA-C-N	5.27	125.21	119.78
2	B	231	ASN	C-N-CA	5.27	125.21	119.78
1	A	61	ASP	OD1-CG-OD2	5.25	135.51	122.90
2	B	555	VAL	CB-CA-C	-5.24	101.64	110.71
2	B	20	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	102	ALA	O-C-N	-5.23	116.68	122.07
2	B	454	PHE	CA-CB-CG	5.20	119.00	113.80
2	B	127	LEU	CB-CA-C	-5.19	100.31	110.11
2	B	440	ASN	N-CA-C	5.15	119.54	113.16
2	B	93	ASN	CA-CB-CG	-5.14	107.46	112.60
1	A	28	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	137	ILE	N-CA-C	-5.11	105.52	110.42
1	A	60	LYS	N-CA-C	5.10	117.57	111.71
2	B	440	ASN	CB-CG-ND2	5.07	124.00	116.40
1	A	120	ASN	OD1-CG-ND2	5.04	127.64	122.60
2	B	337	LYS	CA-C-O	-5.03	113.31	120.51
2	B	185	ASN	OD1-CG-ND2	5.01	127.61	122.60
1	A	168	VAL	CA-C-N	5.01	127.25	120.44
1	A	168	VAL	C-N-CA	5.01	127.25	120.44

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5[B]	SER	Mainchain
2	B	109[B]	LYS	Mainchain
2	B	168[A]	GLN	Sidechain
2	B	168[B]	GLN	Mainchain
2	B	367[B]	PHE	Mainchain
2	B	380[B]	GLN	Mainchain

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Mol	Chain	Res	Type	Group
2	B	495[B]	ARG	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	1750	0	1679	19	0
2	B	4751	0	4546	41	0
3	A	16	0	24	3	0
3	B	92	0	136	8	0
4	B	1	0	0	0	0
5	A	254	0	0	4	0
5	B	669	0	0	6	0
All	All	7533	0	6385	55	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 (55) 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:149[A]:SER:HB2	5:B:2302[A]:HOH:O	1.48	1.14
1:A:199:LEU:HD11	2:B:225[B]:MET:HE1	1.30	1.10
2:B:168[A]:GLN:NE2	5:B:2215[A]:HOH:O	1.86	1.05
2:B:233[A]:GLN:NE2	5:B:2287[A]:HOH:O	1.76	0.98
2:B:488[B]:PHE:CE1	2:B:497:VAL:HG22	2.05	0.92
2:B:123[A]:HIS:HE1	2:B:216:ASP:OD1	1.56	0.89
2:B:168[B]:GLN:CB	2:B:168[B]:GLN:CD	2.53	0.82
2:B:380[B]:GLN:NE2	2:B:380[B]:GLN:H	1.79	0.79
1:A:204:GLN:HB3	5:A:2242:HOH:O	1.81	0.78
5:A:2171[A]:HOH:O	2:B:71[A]:PHE:HD1	1.68	0.77
5:A:2171[A]:HOH:O	2:B:71[A]:PHE:CD1	2.41	0.73
2:B:123[A]:HIS:CE1	2:B:216:ASP:OD1	2.44	0.70
2:B:488[B]:PHE:CD1	2:B:497:VAL:HG22	2.29	0.68
1:A:153:ILE:H	3:A:1210:EDO:H12	1.59	0.68
2:B:380[B]:GLN:H	2:B:380[B]:GLN:CD	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:ASN:HA	2:B:231:ASN:HD21	1.61	0.66
1:A:199:LEU:CD1	2:B:225[B]:MET:HE1	2.19	0.66
1:A:164:ASP:HB2	5:A:2189:HOH:O	1.96	0.65
2:B:168[B]:GLN:CD	2:B:168[B]:GLN:HB3	2.24	0.62
1:A:199:LEU:HD11	2:B:225[B]:MET:CE	2.20	0.62
1:A:149[A]:SER:CB	5:B:2302[A]:HOH:O	2.24	0.60
2:B:488[B]:PHE:CE1	2:B:497:VAL:CG2	2.84	0.59
1:A:183:ASN:C	1:A:183:ASN:HD22	2.11	0.59
2:B:502:VAL:HG23	2:B:527:MET:HE3	1.90	0.54
1:A:183:ASN:HD22	1:A:185[B]:SER:H	1.56	0.53
2:B:432:GLU:HG2	5:B:2489:HOH:O	2.07	0.53
2:B:488[B]:PHE:HE1	2:B:497:VAL:HG22	1.69	0.50
2:B:327:ASP:H	3:B:1578[B]:EDO:H11	1.76	0.50
1:A:182:VAL:HG22	3:A:1211[B]:EDO:H21	1.95	0.49
2:B:437[B]:ARG:HG2	2:B:438:TYR:CE2	2.48	0.49
1:A:198:PRO:HD2	2:B:225[A]:MET:HE1	1.93	0.48
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.95	0.48
1:A:183:ASN:HD22	1:A:185[A]:SER:H	1.60	0.47
3:B:1563:EDO:H22	5:B:2301:HOH:O	2.12	0.47
1:A:183:ASN:ND2	1:A:185[B]:SER:H	2.13	0.47
2:B:378[A]:THR:OG1	2:B:379[A]:THR:N	2.47	0.47
2:B:254:PHE:HE1	2:B:370[B]:TRP:CD2	2.32	0.46
2:B:457:ASN:HD22	2:B:463:PRO:HA	1.80	0.46
2:B:327:ASP:N	3:B:1578[B]:EDO:H11	2.30	0.46
2:B:80:GLU:OE2	2:B:123[A]:HIS:HD2	1.99	0.46
1:A:183:ASN:ND2	1:A:185[A]:SER:H	2.14	0.45
2:B:504:ALA:HA	2:B:505:PRO:C	2.42	0.45
1:A:183:ASN:HD21	1:A:185[B]:SER:HB2	1.83	0.44
2:B:250:ALA:O	3:B:1566[B]:EDO:H12	2.18	0.43
2:B:225[A]:MET:O	3:B:1575:EDO:H11	2.18	0.43
2:B:495[B]:ARG:HA	2:B:496:PRO:HD3	1.83	0.43
1:A:153:ILE:H	3:A:1210:EDO:C1	2.27	0.42
2:B:327:ASP:H	3:B:1578[B]:EDO:C1	2.31	0.42
2:B:327:ASP:CG	3:B:1578[B]:EDO:H12	2.46	0.41
2:B:290[A]:SER:OG	2:B:479:ARG:HB3	2.21	0.41
2:B:473:GLN:HE22	2:B:528:TYR:HD2	1.67	0.41
1:A:198:PRO:HG2	2:B:225[A]:MET:HE1	2.02	0.41
2:B:380[B]:GLN:NE2	2:B:380[B]:GLN:N	2.58	0.40
2:B:256:PHE:CD2	3:B:1559:EDO:H22	2.56	0.40
1:A:198:PRO:CG	2:B:225[A]:MET:HE1	2.52	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	216/260 (83%)	212 (98%)	4 (2%)	0	100	100
2	B	595/557 (107%)	582 (98%)	12 (2%)	1 (0%)	43	17
All	All	811/817 (99%)	794 (98%)	16 (2%)	1 (0%)	48	18

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

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	189/211 (90%)	185 (98%)	4 (2%)	47	11
2	B	500/460 (109%)	496 (99%)	4 (1%)	73	45
All	All	689/671 (103%)	681 (99%)	8 (1%)	65	29

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	181[A]	LEU
1	A	181[B]	LEU
1	A	183	ASN
2	B	81	ARG

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Mol	Chain	Res	Type
2	B	154	TRP
2	B	209	VAL
2	B	404	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	110	ASN
1	A	183	ASN
2	B	12	GLN
2	B	156	HIS
2	B	169	GLN
2	B	187	ASN
2	B	231	ASN
2	B	245	GLN
2	B	348	ASN
2	B	440	ASN
2	B	457	ASN
2	B	473	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	1572	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	B	1564	-	3,3,3	0.38	0	2,2,2	1.02	0
3	EDO	B	1571	-	3,3,3	0.55	0	2,2,2	0.40	0
3	EDO	B	1568	-	3,3,3	0.52	0	2,2,2	0.07	0
3	EDO	B	1567	-	3,3,3	0.38	0	2,2,2	0.43	0
3	EDO	A	1212	-	3,3,3	0.52	0	2,2,2	0.60	0
3	EDO	B	1578[B]	-	3,3,3	0.54	0	2,2,2	0.27	0
3	EDO	B	1573	-	3,3,3	0.49	0	2,2,2	0.74	0
3	EDO	B	1578[A]	-	3,3,3	0.65	0	2,2,2	0.57	0
3	EDO	B	1569	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	B	1566[B]	-	3,3,3	0.33	0	2,2,2	0.46	0
3	EDO	B	1570	-	3,3,3	0.48	0	2,2,2	0.62	0
3	EDO	B	1566[A]	-	3,3,3	0.39	0	2,2,2	0.67	0
3	EDO	B	1561	-	3,3,3	0.99	0	2,2,2	0.56	0
3	EDO	B	1563	-	3,3,3	0.97	0	2,2,2	1.02	0
3	EDO	B	1574	-	3,3,3	0.45	0	2,2,2	0.65	0
3	EDO	A	1211[B]	-	3,3,3	0.46	0	2,2,2	0.11	0
3	EDO	B	1560	-	3,3,3	0.78	0	2,2,2	0.27	0
3	EDO	A	1211[A]	-	3,3,3	0.47	0	2,2,2	0.30	0
3	EDO	B	1562	-	3,3,3	0.54	0	2,2,2	0.76	0
3	EDO	B	1575	-	3,3,3	1.12	0	2,2,2	1.03	0
3	EDO	B	1565	-	3,3,3	0.26	0	2,2,2	0.08	0
3	EDO	A	1210	-	3,3,3	0.53	0	2,2,2	0.29	0
3	EDO	B	1558	-	3,3,3	0.67	0	2,2,2	1.15	0
3	EDO	B	1559	-	3,3,3	0.52	0	2,2,2	0.27	0
3	EDO	B	1577	-	3,3,3	0.51	0	2,2,2	0.57	0
3	EDO	B	1576	-	3,3,3	0.40	0	2,2,2	0.21	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	1572	-	-	0/1/1/1	-
3	EDO	B	1564	-	-	0/1/1/1	-
3	EDO	B	1571	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1568	-	-	0/1/1/1	-
3	EDO	B	1567	-	-	1/1/1/1	-
3	EDO	A	1212	-	-	0/1/1/1	-
3	EDO	B	1578[B]	-	-	1/1/1/1	-
3	EDO	B	1573	-	-	0/1/1/1	-
3	EDO	B	1578[A]	-	-	0/1/1/1	-
3	EDO	B	1569	-	-	0/1/1/1	-
3	EDO	B	1566[B]	-	-	1/1/1/1	-
3	EDO	B	1570	-	-	0/1/1/1	-
3	EDO	B	1566[A]	-	-	0/1/1/1	-
3	EDO	B	1561	-	-	0/1/1/1	-
3	EDO	B	1563	-	-	0/1/1/1	-
3	EDO	B	1574	-	-	0/1/1/1	-
3	EDO	A	1211[B]	-	-	1/1/1/1	-
3	EDO	B	1560	-	-	0/1/1/1	-
3	EDO	A	1211[A]	-	-	0/1/1/1	-
3	EDO	B	1562	-	-	0/1/1/1	-
3	EDO	B	1575	-	-	0/1/1/1	-
3	EDO	B	1565	-	-	0/1/1/1	-
3	EDO	A	1210	-	-	1/1/1/1	-
3	EDO	B	1558	-	-	0/1/1/1	-
3	EDO	B	1559	-	-	0/1/1/1	-
3	EDO	B	1577	-	-	0/1/1/1	-
3	EDO	B	1576	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1566[B]	EDO	O1-C1-C2-O2
3	B	1578[B]	EDO	O1-C1-C2-O2
3	A	1210	EDO	O1-C1-C2-O2
3	A	1211[B]	EDO	O1-C1-C2-O2
3	B	1567	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1578[B]	EDO	4	0
3	B	1566[B]	EDO	1	0
3	B	1563	EDO	1	0
3	A	1211[B]	EDO	1	0
3	B	1575	EDO	1	0
3	A	1210	EDO	2	0
3	B	1559	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	208/260 (80%)	-0.15	1 (0%) 87 90	5, 12, 20, 68	12 (5%)
2	B	557/557 (100%)	-0.11	11 (1%) 65 69	4, 11, 25, 62	42 (7%)
All	All	765/817 (93%)	-0.12	12 (1%) 70 74	4, 11, 24, 68	54 (7%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	380[A]	GLN	5.1
1	A	2	GLN	3.8
2	B	132	THR	3.4
2	B	443[A]	SER	2.7
2	B	84	ALA	2.7
2	B	403	ASP	2.5
2	B	309	GLY	2.5
2	B	336	GLY	2.4
2	B	86[A]	LYS	2.4
2	B	379[A]	THR	2.2
2	B	87	PRO	2.1
2	B	370[A]	TRP	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	A	1210	4/4	0.85	0.13	20,26,30,33	0
3	EDO	B	1567	4/4	0.86	0.12	26,29,31,35	0
3	EDO	A	1212	4/4	0.87	0.12	22,25,27,28	0
3	EDO	A	1211[A]	4/4	0.90	0.10	14,17,19,22	4
3	EDO	A	1211[B]	4/4	0.90	0.10	12,16,18,20	4
3	EDO	B	1577	4/4	0.90	0.10	18,22,24,25	0
3	EDO	B	1578[A]	4/4	0.92	0.11	13,19,21,21	4
3	EDO	B	1578[B]	4/4	0.92	0.11	20,21,25,29	4
3	EDO	B	1565	4/4	0.94	0.07	18,19,24,25	0
3	EDO	B	1558	4/4	0.94	0.08	12,14,15,18	0
3	EDO	B	1575	4/4	0.94	0.11	15,20,21,23	0
3	EDO	B	1576	4/4	0.95	0.08	16,21,28,29	0
3	EDO	B	1573	4/4	0.95	0.14	19,21,21,22	0
3	EDO	B	1574	4/4	0.95	0.09	10,15,19,21	0
3	EDO	B	1564	4/4	0.95	0.07	15,16,17,18	0
3	EDO	B	1570	4/4	0.96	0.09	17,23,23,23	0
3	EDO	B	1563	4/4	0.96	0.08	12,12,16,16	0
3	EDO	B	1561	4/4	0.96	0.08	16,18,20,23	0
3	EDO	B	1569	4/4	0.96	0.06	13,15,17,18	0
3	EDO	B	1572	4/4	0.97	0.12	10,22,24,29	0
3	EDO	B	1562	4/4	0.97	0.06	11,11,13,16	0
3	EDO	B	1566[A]	4/4	0.97	0.05	8,10,10,10	4
3	EDO	B	1566[B]	4/4	0.97	0.05	13,13,16,17	4
3	EDO	B	1559	4/4	0.98	0.04	9,10,11,13	0
3	EDO	B	1571	4/4	0.98	0.05	11,12,13,13	0
3	EDO	B	1568	4/4	0.99	0.04	13,13,14,14	0
3	EDO	B	1560	4/4	0.99	0.03	8,8,9,9	0
4	CA	B	1579	1/1	1.00	0.02	7,7,7,7	0

6.5 Other polymers ⓘ

There are no such residues in this entry.