



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:38 PM GMT

PDB ID : 1GK9  
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](mailto: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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

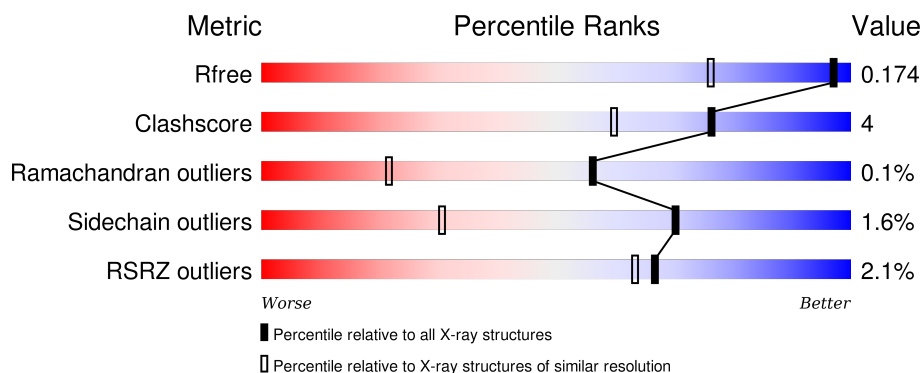
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1475 (1.34-1.26)
Clashscore	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)
RSRZ outliers	91569	1476 (1.34-1.26)

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  $\geq 3$ , 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	260	<div> <div></div> <div>69%</div> <div>11%</div> <div>20%</div> </div>
2	B	557	<div> <div>3%</div> <div>87%</div> <div>12%</div> <div></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[A]	-	-	-	X
3	EDO	A	1211[B]	-	-	-	X
3	EDO	A	1212	-	-	-	X
3	EDO	B	1561	-	-	-	X
3	EDO	B	1563	-	-	-	X
3	EDO	B	1569	-	-	-	X
3	EDO	B	1570	-	-	-	X
3	EDO	B	1571	-	-	-	X
3	EDO	B	1573	-	-	-	X
3	EDO	B	1574	-	-	-	X
3	EDO	B	1576	-	-	-	X
3	EDO	B	1577	-	-	-	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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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		

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

- 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		

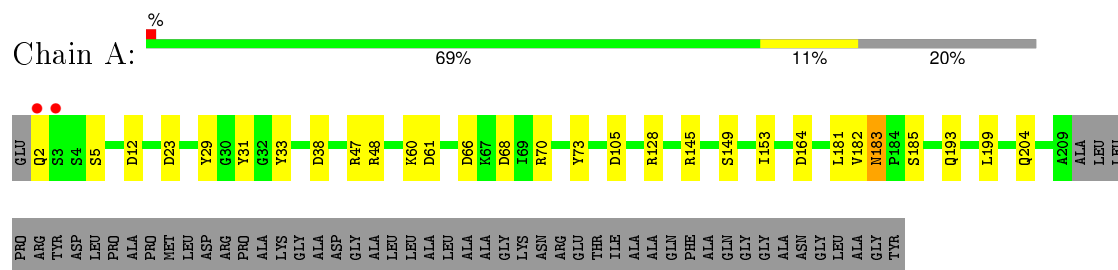
- Molecule 5 is water.

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

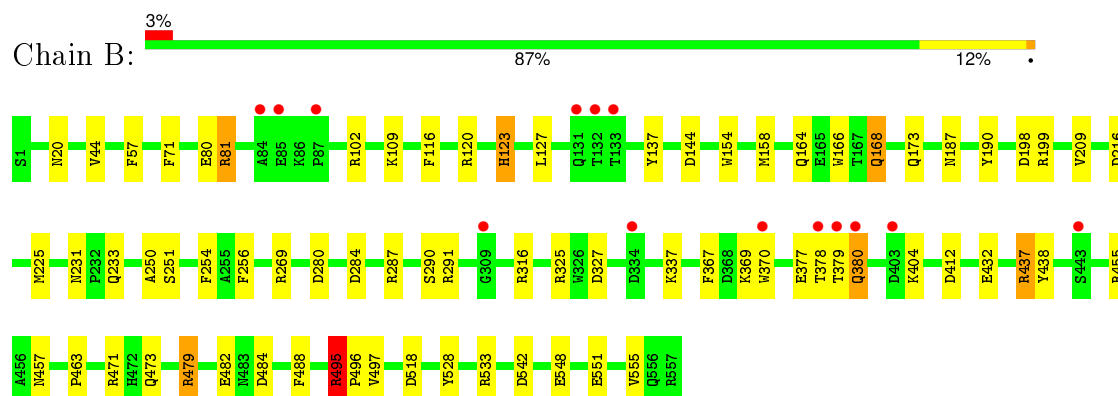
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	51.30 Å 131.60 Å 63.90 Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	20.00 – 1.30 19.99 – 1.30	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-1.30) 95.3 (19.99-1.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 1.30 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.148 , 0.169 0.154 , 0.174	Depositor DCC
$R_{free}$ test set	5756 reflections (3.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.8	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 190183 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.99	1/1794 (0.1%)	1.51	24/2432 (1.0%)
2	B	0.91	1/4895 (0.0%)	1.58	54/6669 (0.8%)
All	All	0.93	2/6689 (0.0%)	1.56	78/9101 (0.9%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	LYS	CD-CE	-14.38	1.15	1.51
2	B	482	GLU	CD-OE2	6.04	1.32	1.25

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	455[A]	ARG	NE-CZ-NH2	-24.69	107.95	120.30
2	B	455[B]	ARG	NE-CZ-NH2	-24.69	107.95	120.30
2	B	495[A]	ARG	NE-CZ-NH2	17.09	128.85	120.30
2	B	495[B]	ARG	NE-CZ-NH2	17.09	128.85	120.30
2	B	269	ARG	NE-CZ-NH2	-16.06	112.27	120.30
2	B	455[A]	ARG	NE-CZ-NH1	14.29	127.45	120.30
2	B	455[B]	ARG	NE-CZ-NH1	14.29	127.45	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH2	-13.74	113.43	120.30
2	B	437[A]	ARG	NE-CZ-NH2	12.54	126.57	120.30
2	B	437[B]	ARG	NE-CZ-NH2	12.54	126.57	120.30
1	A	23	ASP	CB-CG-OD1	11.63	128.77	118.30
2	B	471	ARG	NE-CZ-NH1	10.95	125.77	120.30
1	A	61	ASP	CB-CG-OD2	-10.24	109.08	118.30
2	B	316	ARG	NE-CZ-NH2	-10.02	115.29	120.30
2	B	369	LYS	O-C-N	9.88	138.51	122.70
2	B	102	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	60	LYS	CG-CD-CE	9.72	141.05	111.90
1	A	48	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	B	377[A]	GLU	OE1-CD-OE2	9.31	134.47	123.30
2	B	377[B]	GLU	OE1-CD-OE2	9.31	134.47	123.30
2	B	542	ASP	CB-CG-OD2	9.30	126.67	118.30
2	B	199	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	A	48	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	B	280	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	A	105	ASP	CB-CG-OD1	8.38	125.84	118.30
2	B	198	ASP	CB-CG-OD2	-8.16	110.96	118.30
2	B	337	LYS	CA-CB-CG	7.78	130.52	113.40
2	B	518	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	68	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	60	LYS	CD-CE-NZ	-7.55	94.33	111.70
2	B	484	ASP	CB-CG-OD1	7.52	125.06	118.30
2	B	144[A]	ASP	CB-CG-OD1	-7.47	111.58	118.30
2	B	144[B]	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	66	ASP	CB-CG-OD1	7.17	124.75	118.30
2	B	548	GLU	OE1-CD-OE2	7.05	131.76	123.30
2	B	412	ASP	CB-CG-OD2	-6.93	112.07	118.30
2	B	551	GLU	CA-CB-CG	6.83	128.43	113.40
2	B	280	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	533	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	B	291	ARG	NE-CZ-NH1	-6.60	117.00	120.30
2	B	116	PHE	CB-CG-CD2	-6.43	116.30	120.80
2	B	495[A]	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
2	B	495[B]	ARG	NH1-CZ-NH2	-6.43	112.33	119.40
1	A	61	ASP	OD1-CG-OD2	6.43	135.51	123.30
1	A	70	ARG	NE-CZ-NH2	-6.43	117.09	120.30
2	B	284	ASP	CB-CG-OD2	-6.35	112.59	118.30
2	B	164	GLN	CB-CG-CD	6.28	127.93	111.60
1	A	12	ASP	CB-CG-OD2	-6.19	112.73	118.30
2	B	412	ASP	CB-CG-OD1	6.17	123.85	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	O-C-N	6.16	132.56	122.70
1	A	33	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	A	38	ASP	CB-CG-OD2	6.01	123.71	118.30
2	B	287	ARG	NE-CZ-NH1	-5.98	117.31	120.30
2	B	316	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	479	ARG	NE-CZ-NH2	-5.93	117.34	120.30
2	B	437[A]	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
2	B	437[B]	ARG	NH1-CZ-NH2	-5.89	112.92	119.40
1	A	193[A]	GLN	CG-CD-OE1	5.85	133.29	121.60
1	A	193[B]	GLN	CG-CD-OE1	5.85	133.29	121.60
2	B	325	ARG	NE-CZ-NH1	-5.83	117.38	120.30
2	B	166	TRP	CD1-CG-CD2	5.77	110.92	106.30
1	A	29	TYR	CB-CG-CD2	-5.66	117.61	121.00
2	B	120	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	128	ARG	NH1-CZ-NH2	5.58	125.54	119.40
1	A	47	ARG	NE-CZ-NH2	-5.53	117.54	120.30
2	B	190	TYR	CG-CD2-CE2	5.50	125.70	121.30
2	B	269	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	B	123[A]	HIS	CA-CB-CG	5.31	122.63	113.60
2	B	123[B]	HIS	CA-CB-CG	5.31	122.63	113.60
2	B	81	ARG	CD-NE-CZ	5.25	130.94	123.60
2	B	190	TYR	CB-CG-CD2	5.24	124.14	121.00
1	A	73	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	B	127	LEU	CB-CA-C	-5.21	100.31	110.20
1	A	29	TYR	CB-CG-CD1	5.20	124.12	121.00
2	B	57	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	B	555	VAL	CB-CA-C	-5.14	101.64	111.40
1	A	73	TYR	CB-CG-CD1	5.08	124.05	121.00
2	B	137	TYR	CB-CG-CD1	-5.02	117.99	121.00

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
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	16	0
2	B	4751	0	4546	35	0
3	A	16	0	24	3	0
3	B	92	0	136	7	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	49	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 (49) 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	1.29	1.14
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:380[B]:GLN:H	2:B:380[B]:GLN:NE2	1.79	0.79
1:A:204:GLN:HB3	5:A:2242:HOH:O	1.81	0.78
2:B:168[B]:GLN:CB	2:B:168[B]:GLN:CD	2.53	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
1:A:199:LEU:CD1	2:B:225[B]:MET:HE1	2.17	0.68
2:B:187:ASN:HA	2:B:231:ASN:HD21	1.61	0.66
1:A:164:ASP:HB2	5:A:2189:HOH:O	1.96	0.65
2:B:380[B]:GLN:H	2:B:380[B]:GLN:CD	2.02	0.63
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168[B]:GLN:HB3	2:B:168[B]:GLN:CD	2.24	0.56
1:A:183:ASN:C	1:A:183:ASN:HD22	2.11	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
1:A:199:LEU:HD11	2:B:225[B]:MET:CE	2.20	0.51
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
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:457:ASN:HD22	2:B:463:PRO:HA	1.80	0.46
2:B:254:PHE:HE1	2:B:370[B]:TRP:CD2	2.32	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
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:473:GLN:HE22	2:B:528:TYR:HD2	1.67	0.41
2:B:290[A]:SER:OG	2:B:479:ARG:HB3	2.21	0.41
2:B:380[B]:GLN:N	2:B:380[B]:GLN:NE2	2.58	0.40
2:B:256:PHE:CD2	3:B:1559:EDO:H22	2.56	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	216/260 (83%)	212 (98%)	4 (2%)	0	100	100
2	B	595/557 (107%)	582 (98%)	12 (2%)	1 (0%)	52	20
All	All	811/817 (99%)	794 (98%)	16 (2%)	1 (0%)	56	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	251	SER

### 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	189/211 (90%)	184 (97%)	5 (3%)	54	12
2	B	500/460 (109%)	494 (99%)	6 (1%)	78	43
All	All	689/671 (103%)	678 (98%)	11 (2%)	70	30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	31	TYR
1	A	181[A]	LEU
1	A	181[B]	LEU
1	A	183	ASN
2	B	20	ASN
2	B	81	ARG
2	B	154	TRP
2	B	173	GLN
2	B	209	VAL
2	B	404	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	108	ASN
1	A	183	ASN
2	B	156	HIS
2	B	187	ASN
2	B	231	ASN
2	B	245	GLN
2	B	348	ASN
2	B	401	GLN
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 carbohydrates 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	A	1210	-	3,3,3	0.60	0	2,2,2	0.33	0
3	EDO	A	1211[A]	-	3,3,3	0.53	0	2,2,2	0.34	0
3	EDO	A	1211[B]	-	3,3,3	0.50	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	A	1212	-	3,3,3	0.57	0	2,2,2	0.65	0
3	EDO	B	1558	-	3,3,3	0.67	0	2,2,2	1.25	0
3	EDO	B	1559	-	3,3,3	0.54	0	2,2,2	0.30	0
3	EDO	B	1560	-	3,3,3	0.79	0	2,2,2	0.31	0
3	EDO	B	1561	-	3,3,3	0.94	0	2,2,2	0.60	0
3	EDO	B	1562	-	3,3,3	0.59	0	2,2,2	0.83	0
3	EDO	B	1563	-	3,3,3	1.03	0	2,2,2	1.10	0
3	EDO	B	1564	-	3,3,3	0.44	0	2,2,2	1.10	0
3	EDO	B	1565	-	3,3,3	0.29	0	2,2,2	0.08	0
3	EDO	B	1566[A]	-	3,3,3	0.44	0	2,2,2	0.71	0
3	EDO	B	1566[B]	-	3,3,3	0.37	0	2,2,2	0.47	0
3	EDO	B	1567	-	3,3,3	0.42	0	2,2,2	0.47	0
3	EDO	B	1568	-	3,3,3	0.57	0	2,2,2	0.10	0
3	EDO	B	1569	-	3,3,3	0.53	0	2,2,2	0.29	0
3	EDO	B	1570	-	3,3,3	0.55	0	2,2,2	0.68	0
3	EDO	B	1571	-	3,3,3	0.58	0	2,2,2	0.44	0
3	EDO	B	1572	-	3,3,3	0.43	0	2,2,2	0.40	0
3	EDO	B	1573	-	3,3,3	0.56	0	2,2,2	0.80	0
3	EDO	B	1574	-	3,3,3	0.43	0	2,2,2	0.68	0
3	EDO	B	1575	-	3,3,3	1.07	0	2,2,2	1.07	0
3	EDO	B	1576	-	3,3,3	0.45	0	2,2,2	0.25	0
3	EDO	B	1577	-	3,3,3	0.57	0	2,2,2	0.62	0
3	EDO	B	1578[A]	-	3,3,3	0.66	0	2,2,2	0.63	0
3	EDO	B	1578[B]	-	3,3,3	0.55	0	2,2,2	0.29	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	A	1210	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1211[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1211[B]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1212	-	-	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

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1566[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1566[B]	-	-	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	-	-	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	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1575	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1576	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1577	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1578[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1578[B]	-	-	0/1/1/1	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.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1210	EDO	2	0
3	A	1211[B]	EDO	1	0
3	B	1559	EDO	1	0
3	B	1563	EDO	1	0
3	B	1566[B]	EDO	1	0
3	B	1575	EDO	1	0
3	B	1578[B]	EDO	3	0

## 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, 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	208/260 (80%)	-0.24	2 (0%) 84 83	8, 12, 20, 68	2 (0%)
2	B	557/557 (100%)	-0.17	14 (2%) 61 57	6, 12, 26, 62	4 (0%)
All	All	765/817 (93%)	-0.19	16 (2%) 67 63	6, 12, 24, 68	6 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLN	9.9
2	B	132	THR	7.3
2	B	131	GLN	4.7
2	B	133	THR	4.0
2	B	380[A]	GLN	3.9
2	B	84	ALA	3.3
2	B	403	ASP	3.3
2	B	379[A]	THR	3.3
2	B	309	GLY	3.2
1	A	3	SER	2.7
2	B	87	PRO	2.6
2	B	443[A]	SER	2.5
2	B	370[A]	TRP	2.5
2	B	85[A]	GLU	2.4
2	B	378[A]	THR	2.3
2	B	334	ASP	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 ⓘ

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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EDO	B	1569	4/4	0.96	0.08	17.68	13,15,17,18	0
3	EDO	B	1576	4/4	0.96	0.19	7.26	16,21,28,29	0
3	EDO	A	1211[B]	4/4	0.96	0.13	5.12	12,16,18,20	4
3	EDO	A	1211[A]	4/4	0.96	0.13	5.12	14,17,19,22	4
3	EDO	B	1574	4/4	0.96	0.09	4.69	10,15,19,21	0
3	EDO	B	1573	4/4	0.94	0.19	4.65	19,21,21,22	0
3	EDO	B	1577	4/4	0.92	0.25	4.61	18,22,24,25	0
3	EDO	B	1570	4/4	0.95	0.12	4.13	17,23,23,23	0
3	EDO	A	1212	4/4	0.88	0.14	2.72	22,25,27,28	0
3	EDO	B	1571	4/4	0.98	0.08	2.65	11,12,13,13	0
3	EDO	B	1563	4/4	0.95	0.09	2.60	12,12,16,16	0
3	EDO	A	1210	4/4	0.81	0.11	2.31	20,26,30,33	0
3	EDO	B	1561	4/4	0.97	0.08	2.26	16,18,20,23	0
3	EDO	B	1572	4/4	0.97	0.16	1.84	10,22,24,29	0
3	EDO	B	1575	4/4	0.93	0.13	1.33	15,20,21,23	0
3	EDO	B	1558	4/4	0.95	0.09	1.26	12,14,15,18	0
3	EDO	B	1566[A]	4/4	0.98	0.07	1.02	8,10,10,10	4
3	EDO	B	1566[B]	4/4	0.98	0.07	0.77	13,13,16,17	4
3	EDO	B	1564	4/4	0.97	0.07	0.50	15,16,17,18	0
3	EDO	B	1559	4/4	0.98	0.06	0.48	9,10,11,13	0
3	EDO	B	1562	4/4	0.97	0.06	0.43	11,11,13,16	0
3	EDO	B	1565	4/4	0.93	0.07	0.37	18,19,24,25	0
3	EDO	B	1567	4/4	0.84	0.11	0.32	26,29,31,35	0
3	EDO	B	1560	4/4	0.99	0.05	-1.02	8,8,9,9	0
4	CA	B	1579	1/1	1.00	0.02	-2.97	7,7,7,7	0
3	EDO	B	1568	4/4	0.99	0.05	-	13,13,14,14	0
3	EDO	B	1578[B]	4/4	0.96	0.19	-	20,21,25,29	4
3	EDO	B	1578[A]	4/4	0.96	0.19	-	13,19,21,21	4

## 6.5 Other polymers

There are no such residues in this entry.