



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 2, 2025 – 12:44 am BST

PDB ID : 1GKF / pdb_00001gkf
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 : 2001-08-13
Resolution : 1.41 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

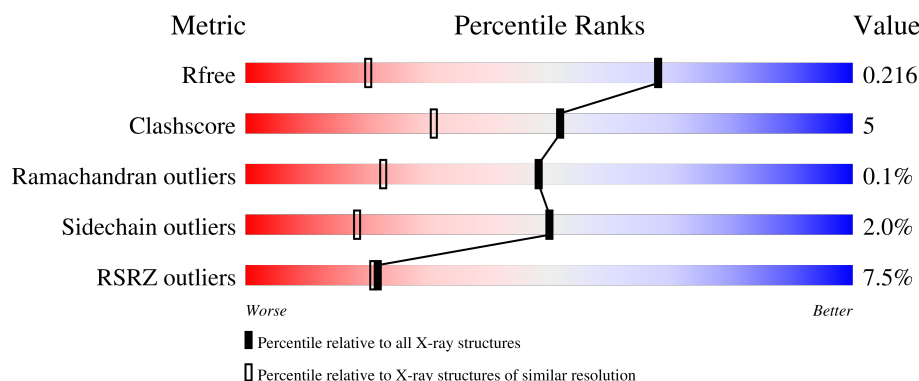
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3500 (1.44-1.40)
Clashscore	180529	3801 (1.44-1.40)
Ramachandran outliers	177936	3734 (1.44-1.40)
Sidechain outliers	177891	3733 (1.44-1.40)
RSRZ outliers	164620	3499 (1.44-1.40)

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	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>11%</div> <div>20%</div> </div> </div>
2	B	557	<div> <div>8%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7283 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	13	1
			1764	1121	300	333	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	SME	MET	modified residue	UNP P06875

- 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	15	18	0
			4562	2896	788	867	11			

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	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	1
			7	4	3		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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

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

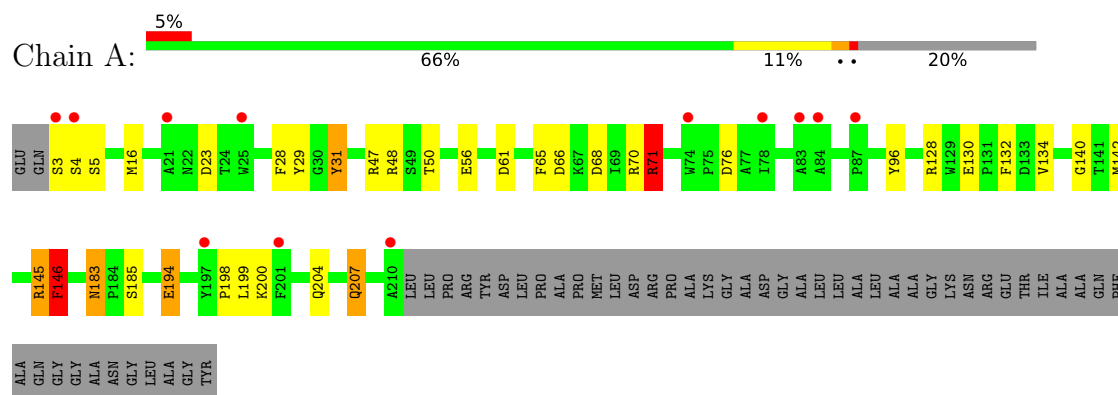
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	241	Total 241	O 241	2	5
5	B	660	Total 660	O 660	0	10

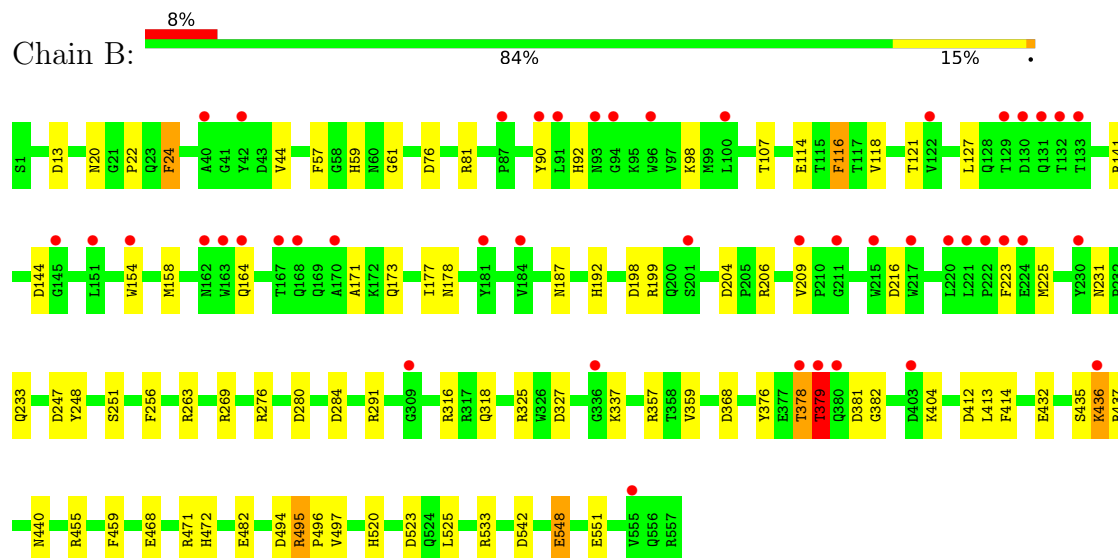
3 Residue-property plots [i](#)

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



• 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	51.20Å 131.70Å 63.90Å 90.00° 105.70° 90.00°	Depositor
Resolution (Å)	25.00 – 1.41 25.00 – 1.41	Depositor EDS
% Data completeness (in resolution range)	97.4 (25.00-1.41) 97.3 (25.00-1.41)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 1.41Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.168 0.204 , 0.216	Depositor DCC
R_{free} test set	4583 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	10.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	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	0.95	EDS
Total number of atoms	7283	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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, SME, 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	0.96	1/1797 (0.1%)	1.64	33/2435 (1.4%)
2	B	0.98	4/4691 (0.1%)	1.52	55/6396 (0.9%)
All	All	0.97	5/6488 (0.1%)	1.55	88/8831 (1.0%)

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	3
2	B	0	3
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	LYS	CD-CE	18.66	1.98	1.51
2	B	81	ARG	CD-NE	-11.34	1.27	1.46
1	A	200	LYS	CG-CD	-8.39	1.24	1.52
2	B	432	GLU	CG-CD	-6.50	1.42	1.51
2	B	482	GLU	CD-OE2	5.77	1.31	1.25

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	455	ARG	NE-CZ-NH2	-18.45	111.08	120.30
2	B	533	ARG	NE-CZ-NH1	17.12	128.86	120.30
2	B	471	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	A	48	ARG	NE-CZ-NH1	13.75	127.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	199	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	A	128	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	A	48	ARG	NE-CZ-NH2	-12.23	114.19	120.30
2	B	495[A]	ARG	NE-CZ-NH2	12.02	126.31	120.30
2	B	495[B]	ARG	NE-CZ-NH2	12.02	126.31	120.30
2	B	455	ARG	NE-CZ-NH1	11.96	126.28	120.30
2	B	533	ARG	NE-CZ-NH2	-11.26	114.67	120.30
1	A	200	LYS	CB-CG-CD	10.99	140.18	111.60
2	B	199	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	47	ARG	NE-CZ-NH2	-10.55	115.02	120.30
2	B	381	ASP	CB-CG-OD2	-10.21	109.11	118.30
2	B	269	ARG	NE-CZ-NH2	-9.74	115.43	120.30
2	B	357	ARG	NE-CZ-NH2	-9.63	115.49	120.30
2	B	291	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	145[A]	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	A	145[B]	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	A	76	ASP	CB-CG-OD2	-9.00	110.20	118.30
2	B	379[A]	THR	CA-C-N	8.69	136.31	117.20
2	B	379[B]	THR	CA-C-N	8.69	136.31	117.20
1	A	23	ASP	CB-CG-OD1	8.58	126.02	118.30
1	A	194	GLU	OE1-CD-OE2	8.43	133.42	123.30
2	B	280	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	70	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	A	128	ARG	NH1-CZ-NH2	7.66	127.82	119.40
2	B	198	ASP	CB-CG-OD2	-7.48	111.56	118.30
2	B	325	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	B	247	ASP	CB-CG-OD2	-7.28	111.75	118.30
2	B	13	ASP	CB-CG-OD2	-7.28	111.75	118.30
2	B	412	ASP	CB-CG-OD1	7.11	124.70	118.30
2	B	548	GLU	OE1-CD-OE2	6.93	131.62	123.30
2	B	206	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	B	280	ASP	CB-CG-OD1	6.74	124.37	118.30
2	B	81	ARG	CG-CD-NE	6.60	125.66	111.80
2	B	141	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	B	437	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	47	ARG	NH1-CZ-NH2	6.53	126.58	119.40
2	B	284	ASP	CB-CG-OD2	-6.29	112.64	118.30
2	B	127	LEU	CB-CA-C	-6.27	98.29	110.20
1	A	130	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	61	ASP	CB-CG-OD2	-6.18	112.73	118.30
2	B	495[A]	ARG	NH1-CZ-NH2	-6.18	112.60	119.40
2	B	495[B]	ARG	NH1-CZ-NH2	-6.18	112.60	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142[A]	MET	CG-SD-CE	6.04	109.86	100.20
1	A	142[B]	MET	CG-SD-CE	6.04	109.86	100.20
2	B	327	ASP	CB-CG-OD1	6.02	123.72	118.30
2	B	337	LYS	CA-CB-CG	5.95	126.48	113.40
1	A	66	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	29	TYR	CB-CG-CD2	-5.84	117.50	121.00
2	B	551	GLU	CA-CB-CG	5.82	126.21	113.40
2	B	76	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	96	TYR	CB-CG-CD2	-5.75	117.55	121.00
2	B	379[A]	THR	O-C-N	-5.75	113.50	122.70
2	B	379[B]	THR	O-C-N	-5.75	113.50	122.70
1	A	200	LYS	CG-CD-CE	5.67	128.92	111.90
1	A	28	PHE	CB-CG-CD2	5.66	124.76	120.80
2	B	414	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	A	96	TYR	CB-CG-CD1	5.54	124.32	121.00
1	A	31	TYR	CB-CG-CD1	5.51	124.31	121.00
2	B	468	GLU	CG-CD-OE2	-5.45	107.39	118.30
2	B	471	ARG	NE-CZ-NH2	-5.45	117.57	120.30
2	B	98	LYS	CD-CE-NZ	5.43	124.19	111.70
2	B	269	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	31	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	A	146[A]	PHE	C-N-CA	5.37	135.12	121.70
1	A	146[B]	PHE	C-N-CA	5.37	135.12	121.70
2	B	263	ARG	NE-CZ-NH1	-5.34	117.63	120.30
2	B	542	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	437	ARG	NE-CZ-NH2	5.32	122.96	120.30
2	B	368	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	134	VAL	O-C-N	-5.28	114.26	122.70
1	A	65	PHE	CB-CG-CD1	-5.25	117.13	120.80
2	B	316	ARG	NE-CZ-NH1	-5.23	117.68	120.30
2	B	276	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	71[A]	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	71[B]	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	B	24	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	B	164	GLN	O-C-N	-5.13	114.49	122.70
2	B	98	LYS	CG-CD-CE	-5.13	96.52	111.90
2	B	116	PHE	CB-CG-CD2	-5.12	117.22	120.80
2	B	144[A]	ASP	CB-CG-OD2	-5.11	113.70	118.30
2	B	144[B]	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	132	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	A	70	ARG	NH1-CZ-NH2	5.06	124.96	119.40
2	B	525	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146[B]	PHE	Mainchain
1	A	5[B]	SER	Mainchain
1	A	71[B]	ARG	Mainchain
2	B	318[B]	GLN	Mainchain
2	B	376	TYR	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	1764	0	1702	29	0
2	B	4562	0	4364	45	0
3	B	55	0	80	5	0
4	B	1	0	0	0	0
5	A	241	0	0	6	0
5	B	660	0	0	10	2
All	All	7283	0	6146	63	2

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 5.

All (63) 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:495[A]:ARG:NH2	5:B:2577[A]:HOH:O	1.70	1.24
2:B:114[A]:GLU:OE1	5:B:2154[A]:HOH:O	1.81	0.98
1:A:207:GLN:H	1:A:207:GLN:HE21	1.18	0.91
2:B:59:HIS:HD2	2:B:61:GLY:H	1.22	0.83
1:A:146[B]:PHE:HB2	5:A:2151:HOH:O	1.79	0.82
1:A:207:GLN:HE22	2:B:204:ASP:H	1.28	0.80
2:B:497:VAL:HG12	5:B:2581:HOH:O	1.83	0.77
1:A:199:LEU:HG	2:B:225[B]:MET:HE1	1.69	0.75
1:A:146[B]:PHE:HA	5:A:2157:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ALA:O	3:B:1562:EDO:H12	1.93	0.68
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.76	0.67
1:A:68:ASP:OD1	1:A:71[B]:ARG:NH2	2.28	0.67
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.77	0.66
3:B:1569:EDO:H22	5:B:2313:HOH:O	1.97	0.65
1:A:71[B]:ARG:HD3	2:B:116:PHE:CE2	2.32	0.64
1:A:207:GLN:NE2	2:B:204:ASP:H	1.94	0.64
2:B:187:ASN:HD22	2:B:231:ASN:HD21	1.46	0.63
2:B:223:PHE:HD1	3:B:1562:EDO:H21	1.63	0.63
2:B:378[A]:THR:OG1	2:B:379[A]:THR:N	2.28	0.62
2:B:92:HIS:HE1	2:B:216:ASP:OD2	1.84	0.61
1:A:71[B]:ARG:HG3	2:B:118:VAL:HG22	1.83	0.61
2:B:92:HIS:HD2	5:B:2107:HOH:O	1.86	0.58
2:B:59:HIS:CD2	2:B:61:GLY:H	2.13	0.58
1:A:145[B]:ARG:HD2	5:A:2153:HOH:O	2.05	0.57
5:A:2151:HOH:O	2:B:177:ILE:HD11	2.08	0.54
1:A:71[B]:ARG:HD3	2:B:116:PHE:HE2	1.73	0.54
2:B:494:ASP:OD1	2:B:495[B]:ARG:NH1	2.40	0.53
1:A:183:ASN:C	1:A:183:ASN:HD22	2.11	0.53
1:A:207:GLN:H	1:A:207:GLN:NE2	1.99	0.52
1:A:50:THR:HG22	1:A:140[B]:GLY:HA3	1.93	0.51
1:A:194:GLU:OE2	2:B:233:GLN:HG2	2.11	0.50
1:A:56[A]:GLU:HG2	2:B:107:THR:HB	1.94	0.50
1:A:183:ASN:HD22	1:A:185[B]:SER:H	1.58	0.50
1:A:145[B]:ARG:HD3	2:B:459:PHE:CE1	2.46	0.49
2:B:187:ASN:ND2	2:B:231:ASN:HD21	2.10	0.49
2:B:225[A]:MET:O	3:B:1568:EDO:H12	2.13	0.49
2:B:472:HIS:HD2	5:B:2526:HOH:O	1.97	0.48
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.96	0.47
1:A:183:ASN:HD22	1:A:185[A]:SER:H	1.61	0.47
2:B:192:HIS:CE1	2:B:248:TYR:OH	2.68	0.47
2:B:379[A]:THR:HG22	2:B:382:GLY:O	2.14	0.47
1:A:71[B]:ARG:HD2	5:B:2159:HOH:O	2.14	0.46
1:A:198:PRO:HG2	2:B:225[A]:MET:HE1	1.98	0.46
2:B:178:ASN:OD1	2:B:192:HIS:HD2	1.99	0.46
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.51	0.45
1:A:145[B]:ARG:NH1	5:A:2153:HOH:O	2.44	0.45
2:B:379[A]:THR:CG2	2:B:382:GLY:O	2.65	0.44
2:B:435:SER:HB2	2:B:440:ASN:HD22	1.82	0.44
1:A:183:ASN:ND2	1:A:185[B]:SER:H	2.15	0.44
1:A:183:ASN:ND2	1:A:185[A]:SER:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:HIS:HE1	5:B:2622:HOH:O	2.01	0.42
2:B:22:PRO:HG3	2:B:57:PHE:CZ	2.54	0.42
1:A:146[B]:PHE:HE2	5:B:2013:HOH:O	2.02	0.42
1:A:71[B]:ARG:HG3	2:B:116:PHE:HE2	1.85	0.42
2:B:90:TYR:CZ	2:B:121:THR:HB	2.55	0.41
2:B:436:LYS:HA	2:B:436:LYS:HD3	1.78	0.41
1:A:183:ASN:HD21	1:A:185[B]:SER:HB2	1.86	0.41
1:A:199:LEU:CG	2:B:225[B]:MET:HE1	2.42	0.41
2:B:192:HIS:HE1	2:B:248:TYR:OH	2.04	0.41
2:B:496:PRO:HD2	5:B:2581:HOH:O	2.21	0.41
1:A:146[B]:PHE:HD2	5:A:2157:HOH:O	2.03	0.41
2:B:359:VAL:HG22	2:B:413:LEU:HD13	2.02	0.41
2:B:256:PHE:CD2	3:B:1558:EDO:H22	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2126:HOH:O	5:B:2508:HOH:O[1_656]	2.04	0.16
5:B:2170:HOH:O	5:B:2378:HOH:O[1_656]	2.17	0.03

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	218/260 (84%)	213 (98%)	5 (2%)	0	100	100
2	B	573/557 (103%)	558 (97%)	14 (2%)	1 (0%)	44	21
All	All	791/817 (97%)	771 (98%)	19 (2%)	1 (0%)	48	23

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	188/210 (90%)	182 (97%)	6 (3%)	34	7
2	B	477/459 (104%)	469 (98%)	8 (2%)	56	25
All	All	665/669 (99%)	651 (98%)	14 (2%)	50	16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	SER
1	A	31	TYR
1	A	183	ASN
1	A	204	GLN
1	A	207	GLN
2	B	20	ASN
2	B	154	TRP
2	B	173	GLN
2	B	209	VAL
2	B	378[A]	THR
2	B	378[B]	THR
2	B	404	LYS
2	B	436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	170	GLN
1	A	183	ASN
1	A	203	GLN

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Mol	Chain	Res	Type
1	A	204	GLN
1	A	207	GLN
2	B	59	HIS
2	B	92	HIS
2	B	93	ASN
2	B	134	GLN
2	B	187	ASN
2	B	192	HIS
2	B	226	ASN
2	B	245	GLN
2	B	401	GLN
2	B	420	GLN
2	B	440	ASN
2	B	472	HIS
2	B	473	GLN
2	B	520	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	7,8,9	1.09	1 (14%)	4,9,11	0.60	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	-	1/6/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	SME	OE-S	-2.16	1.44	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	SME	C-CA-CB-CG

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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	1560	-	3,3,3	0.65	0	2,2,2	0.20	0
3	EDO	B	1559[B]	-	3,3,3	0.56	0	2,2,2	0.34	0
3	EDO	B	1563	-	3,3,3	0.58	0	2,2,2	1.33	0
3	EDO	B	1566	-	3,3,3	0.61	0	2,2,2	0.45	0
3	EDO	B	1567	-	3,3,3	0.54	0	2,2,2	0.82	0
3	EDO	B	1562	-	3,3,3	0.43	0	2,2,2	1.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	B	1569	-	3,3,3	1.42	0	2,2,2	0.71	0
3	EDO	B	1568	-	3,3,3	0.87	0	2,2,2	2.18	1 (50%)
3	EDO	B	1570	-	3,3,3	0.65	0	2,2,2	0.54	0
3	EDO	B	1564	-	3,3,3	0.27	0	2,2,2	0.40	0
3	EDO	B	1561	-	3,3,3	0.61	0	2,2,2	0.18	0
3	EDO	B	1558	-	3,3,3	0.58	0	2,2,2	0.21	0
3	EDO	B	1565	-	3,3,3	0.54	0	2,2,2	0.45	0
3	EDO	B	1559[A]	-	3,3,3	0.53	0	2,2,2	0.50	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	1560	-	-	0/1/1/1	-
3	EDO	B	1559[B]	-	-	1/1/1/1	-
3	EDO	B	1563	-	-	0/1/1/1	-
3	EDO	B	1566	-	-	0/1/1/1	-
3	EDO	B	1567	-	-	0/1/1/1	-
3	EDO	B	1562	-	-	1/1/1/1	-
3	EDO	B	1569	-	-	1/1/1/1	-
3	EDO	B	1568	-	-	1/1/1/1	-
3	EDO	B	1570	-	-	0/1/1/1	-
3	EDO	B	1564	-	-	0/1/1/1	-
3	EDO	B	1561	-	-	0/1/1/1	-
3	EDO	B	1558	-	-	0/1/1/1	-
3	EDO	B	1565	-	-	0/1/1/1	-
3	EDO	B	1559[A]	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1568	EDO	O1-C1-C2	2.58	130.47	111.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1562	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	1559[B]	EDO	O1-C1-C2-O2
3	B	1569	EDO	O1-C1-C2-O2
3	B	1568	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1562	EDO	2	0
3	B	1569	EDO	1	0
3	B	1568	EDO	1	0
3	B	1558	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	207/260 (79%)	0.76	12 (5%)	30 29	3, 11, 19, 44	15 (7%)
2	B	557/557 (100%)	0.62	45 (8%)	19 19	4, 11, 24, 60	23 (4%)
All	All	764/817 (93%)	0.66	57 (7%)	22 21	3, 11, 22, 60	38 (4%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	379[A]	THR	7.6
2	B	132	THR	4.0
1	A	3	SER	3.7
2	B	215	TRP	3.5
2	B	133	THR	3.4
2	B	94	GLY	3.4
2	B	378[A]	THR	3.4
2	B	223	PHE	3.3
2	B	42	TYR	3.3
1	A	201	PHE	3.1
2	B	403	ASP	3.1
2	B	380	GLN	2.9
2	B	100	LEU	2.9
1	A	84	ALA	2.9
2	B	168	GLN	2.9
2	B	131	GLN	2.8
1	A	4	SER	2.7
2	B	164	GLN	2.7
2	B	129	THR	2.7
2	B	436	LYS	2.7
2	B	224	GLU	2.7
2	B	222	PRO	2.7
1	A	25	TRP	2.7
1	A	210	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	211	GLY	2.5
2	B	93	ASN	2.4
2	B	220	LEU	2.4
2	B	170	ALA	2.4
2	B	91	LEU	2.4
2	B	130	ASP	2.4
2	B	122	VAL	2.3
2	B	201	SER	2.3
2	B	221	LEU	2.3
2	B	96	TRP	2.3
1	A	21	ALA	2.3
1	A	197	TYR	2.2
2	B	336	GLY	2.2
2	B	162	ASN	2.2
2	B	217	TRP	2.2
2	B	209	VAL	2.2
2	B	40	ALA	2.2
1	A	78	ILE	2.2
2	B	181	TYR	2.2
2	B	184[A]	VAL	2.1
2	B	309	GLY	2.1
1	A	74	TRP	2.1
2	B	154	TRP	2.1
2	B	151	LEU	2.1
2	B	555	VAL	2.1
1	A	87	PRO	2.1
2	B	90	TYR	2.1
2	B	145	GLY	2.1
2	B	230	TYR	2.1
1	A	83	ALA	2.0
2	B	167	THR	2.0
2	B	87	PRO	2.0
2	B	163	TRP	2.0

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

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(\AA^2)	Q<0.9
1	SME	A	16	9/10	0.95	0.09	9,9,11,11	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	EDO	B	1559[A]	4/4	0.74	0.16	18,19,20,26	3
3	EDO	B	1559[B]	4/4	0.74	0.16	20,21,22,26	3
3	EDO	B	1569	4/4	0.81	0.19	15,22,24,25	0
3	EDO	B	1562	4/4	0.83	0.19	20,21,21,23	0
3	EDO	B	1567	4/4	0.84	0.16	24,25,26,29	0
4	CA	B	1571	1/1	0.90	0.08	7,7,7,7	0
3	EDO	B	1568	4/4	0.91	0.14	14,24,24,27	0
3	EDO	B	1563	4/4	0.92	0.10	13,17,19,20	0
3	EDO	B	1564	4/4	0.92	0.10	12,16,16,17	0
3	EDO	B	1560	4/4	0.94	0.09	12,15,16,17	0
3	EDO	B	1566	4/4	0.94	0.13	18,20,22,23	0
3	EDO	B	1565	4/4	0.95	0.07	13,16,16,16	0
3	EDO	B	1570	4/4	0.95	0.11	11,16,24,26	0
3	EDO	B	1558	4/4	0.95	0.06	8,9,10,10	0
3	EDO	B	1561	4/4	0.96	0.07	17,17,17,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.