



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:22 AM UTC

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	:	4-5-2 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

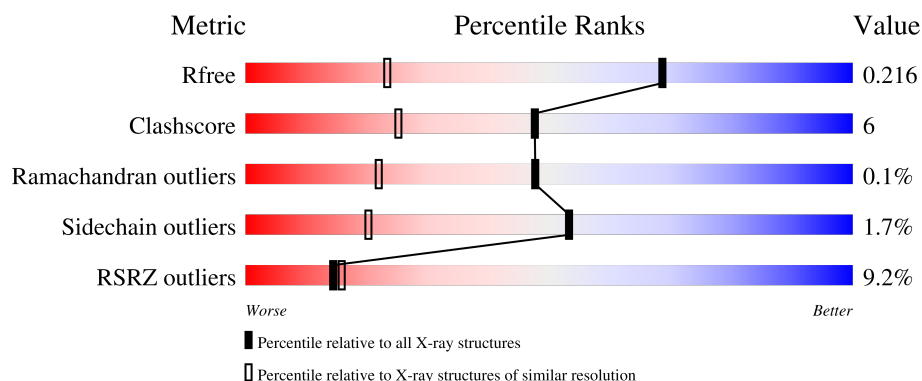
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.41 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}	180053	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (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	6% 64% 14% 20%
2	B	557	10% 83% 15%

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

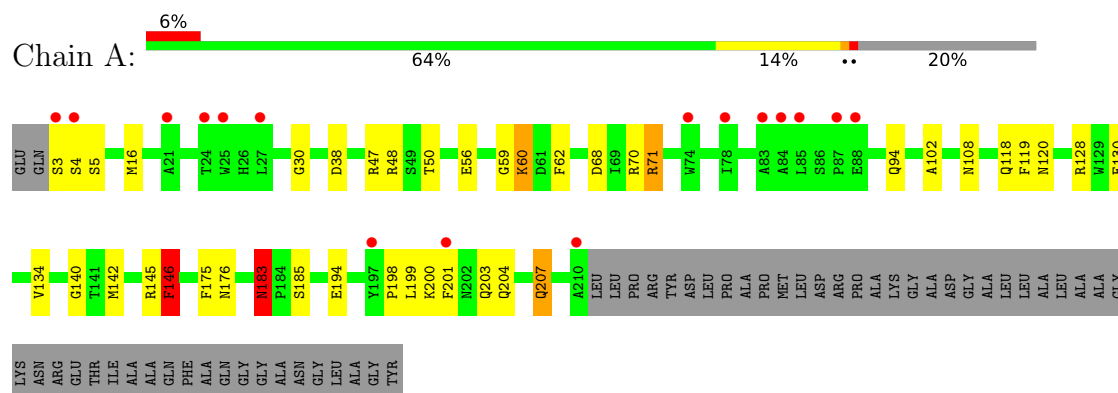
- Molecule 5 is water.

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

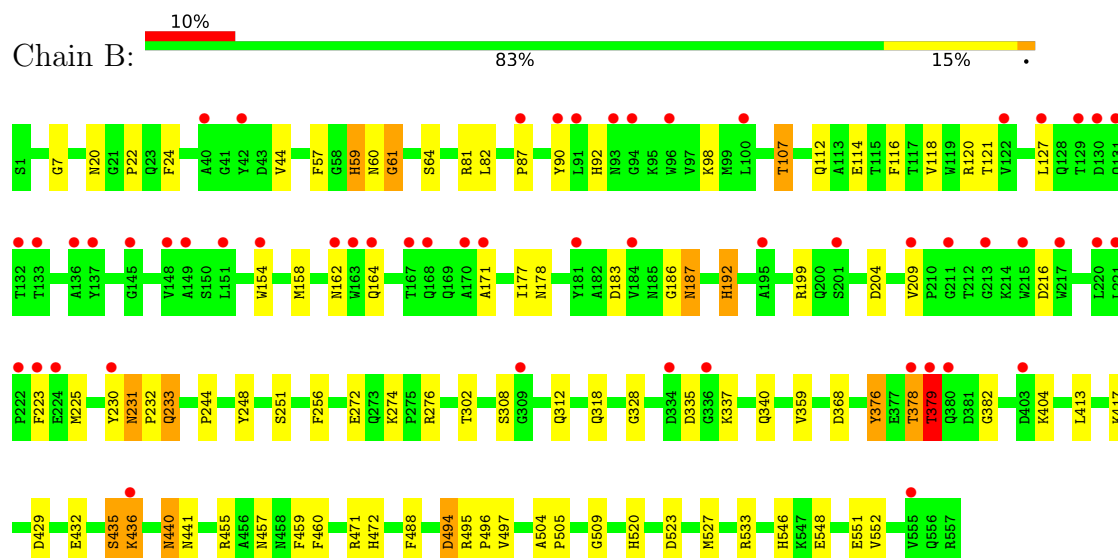
3 Residue-property plots [i](#)

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	4584 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	1.21	1/1797 (0.1%)	1.80	37/2435 (1.5%)
2	B	1.21	8/4691 (0.2%)	1.62	68/6396 (1.1%)
All	All	1.21	9/6488 (0.1%)	1.68	105/8831 (1.2%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	LYS	CD-CE	15.15	1.98	1.52
2	B	81	ARG	CD-NE	-13.62	1.27	1.46
1	A	200	LYS	CG-CD	-9.50	1.24	1.52
2	B	231	ASN	C-O	7.49	1.27	1.23
2	B	231	ASN	CA-C	-6.02	1.49	1.53
2	B	192	HIS	ND1-CE1	5.63	1.38	1.32
2	B	527	MET	SD-CE	-5.52	1.65	1.79
2	B	509	GLY	CA-C	5.28	1.56	1.51
2	B	230	TYR	C-O	5.23	1.29	1.24

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	LYS	CB-CG-CD	12.56	140.18	111.30
1	A	94	GLN	OE1-CD-NE2	10.78	133.38	122.60
2	B	20	ASN	CA-CB-CG	10.41	123.01	112.60
1	A	176	ASN	OD1-CG-ND2	-10.28	112.32	122.60
1	A	203	GLN	OE1-CD-NE2	10.17	132.77	122.60
2	B	455	ARG	NE-CZ-NH2	-9.03	111.08	119.20
2	B	312	GLN	OE1-CD-NE2	-8.65	113.95	122.60
2	B	440	ASN	OD1-CG-ND2	-8.44	114.16	122.60
2	B	59	HIS	CB-CG-CD2	-8.44	120.23	131.20
2	B	187	ASN	OD1-CG-ND2	8.28	130.88	122.60
1	A	134	VAL	O-C-N	-7.81	114.26	121.91
1	A	200	LYS	CG-CD-CE	7.66	128.92	111.30
1	A	146[A]	PHE	CA-C-N	7.51	135.12	122.65
1	A	146[A]	PHE	C-N-CA	7.51	135.12	122.65
1	A	146[B]	PHE	CA-C-N	7.51	135.12	122.65
1	A	146[B]	PHE	C-N-CA	7.51	135.12	122.65
2	B	533	ARG	NE-CZ-NH1	7.36	128.86	121.50
2	B	164	GLN	O-C-N	-7.20	114.49	122.12
1	A	119	PHE	O-C-N	6.95	129.48	122.12
1	A	176	ASN	CB-CG-ND2	6.83	126.64	116.40
2	B	186	GLY	O-C-N	6.65	130.23	122.45
1	A	146[A]	PHE	O-C-N	-6.60	115.13	122.12
1	A	146[B]	PHE	O-C-N	-6.60	115.13	122.12
1	A	128	ARG	NH1-CZ-NH2	6.56	127.82	119.30
1	A	175	PHE	O-C-N	-6.55	115.18	122.12
1	A	102	ALA	O-C-N	-6.49	115.25	122.12
2	B	417	LYS	CA-C-N	6.45	126.40	119.76
2	B	417	LYS	C-N-CA	6.45	126.40	119.76
2	B	98	LYS	CG-CD-CE	-6.42	96.52	111.30
2	B	112	GLN	OE1-CD-NE2	6.32	128.92	122.60
2	B	127	LEU	CB-CA-C	-6.25	98.29	110.11
2	B	429	ASP	CA-C-O	6.23	127.15	120.55
2	B	81	ARG	CG-CD-NE	6.21	125.66	112.00
1	A	38	ASP	CA-CB-CG	6.20	118.80	112.60
2	B	337	LYS	CA-CB-CG	6.19	126.48	114.10
2	B	87	PRO	N-CA-CB	6.17	108.80	103.31
2	B	231	ASN	CA-C-N	6.15	126.16	119.89
2	B	231	ASN	C-N-CA	6.15	126.16	119.89
2	B	552	VAL	N-CA-CB	6.12	119.59	111.64
2	B	551	GLU	CA-CB-CG	6.05	126.21	114.10
1	A	59	GLY	CA-C-N	6.05	129.00	120.28
1	A	59	GLY	C-N-CA	6.05	129.00	120.28
2	B	429	ASP	O-C-N	-6.04	115.72	122.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	276	ARG	CA-C-O	5.97	128.15	121.40
1	A	201	PHE	CA-CB-CG	-5.97	107.83	113.80
2	B	509	GLY	O-C-N	5.95	127.62	121.97
2	B	274	LYS	O-C-N	-5.93	115.81	121.57
2	B	199	ARG	NE-CZ-NH2	-5.90	113.89	119.20
2	B	272	GLU	CB-CG-CD	5.90	122.62	112.60
1	A	128	ARG	NE-CZ-NH2	-5.87	113.92	119.20
2	B	441	ASN	OD1-CG-ND2	5.86	128.46	122.60
2	B	376	TYR	O-C-N	5.82	129.32	122.34
2	B	59	HIS	CB-CG-ND1	5.81	131.42	122.70
2	B	546	HIS	CB-CG-CD2	-5.73	123.75	131.20
2	B	60	ASN	CA-CB-CG	5.71	118.31	112.60
2	B	471	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	A	118	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	A	48	ARG	NE-CZ-NH1	5.68	127.18	121.50
2	B	460	PHE	CA-CB-CG	5.67	119.47	113.80
1	A	130	GLU	CA-C-N	5.66	125.77	119.32
1	A	130	GLU	C-N-CA	5.66	125.77	119.32
2	B	340	GLN	OE1-CD-NE2	5.65	128.25	122.60
2	B	368	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	47	ARG	NH1-CZ-NH2	5.60	126.58	119.30
2	B	164	GLN	CA-C-N	5.58	127.75	120.28
2	B	164	GLN	C-N-CA	5.58	127.75	120.28
2	B	494	ASP	CA-CB-CG	-5.57	107.03	112.60
1	A	48	ARG	NE-CZ-NH2	-5.57	114.19	119.20
2	B	164	GLN	CB-CG-CD	5.52	121.98	112.60
2	B	162	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	183	ASN	CA-CB-CG	5.40	118.00	112.60
2	B	183	ASP	CA-CB-CG	5.38	117.98	112.60
2	B	233	GLN	CG-CD-NE2	-5.37	108.34	116.40
1	A	59	GLY	O-C-N	-5.36	117.03	122.98
2	B	328	GLY	CA-C-O	-5.36	113.07	119.02
2	B	127	LEU	O-C-N	5.34	130.13	122.28
1	A	108	ASN	OD1-CG-ND2	5.33	127.93	122.60
2	B	82	LEU	O-C-N	5.31	129.12	122.43
1	A	60	LYS	CA-C-O	-5.28	114.13	120.10
1	A	30	GLY	O-C-N	5.27	127.25	122.19
1	A	60	LYS	O-C-N	5.25	128.37	122.22
2	B	340	GLN	CG-CD-NE2	-5.25	108.52	116.40
2	B	435	SER	CA-C-O	-5.25	113.93	119.97
2	B	457	ASN	OD1-CG-ND2	-5.21	117.39	122.60
2	B	432	GLU	CA-C-N	5.18	127.49	120.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	432	GLU	C-N-CA	5.18	127.49	120.65
2	B	120	ARG	O-C-N	-5.17	117.36	123.41
2	B	61	GLY	CA-C-N	5.17	128.64	123.16
2	B	61	GLY	C-N-CA	5.17	128.64	123.16
2	B	107	THR	O-C-N	-5.16	117.13	122.96
1	A	62	PHE	CA-CB-CG	-5.15	108.65	113.80
2	B	274	LYS	CA-C-O	5.15	126.53	120.41
2	B	308	SER	CA-C-N	-5.12	113.62	122.83
2	B	308	SER	C-N-CA	-5.12	113.62	122.83
2	B	244	PRO	CB-CA-C	-5.11	104.65	112.11
1	A	70	ARG	NE-CZ-NH1	-5.11	116.39	121.50
2	B	379[A]	THR	N-CA-C	-5.11	101.92	109.94
2	B	379[B]	THR	N-CA-C	-5.11	101.92	109.94
2	B	335	ASP	CA-C-N	5.11	130.01	120.87
2	B	335	ASP	C-N-CA	5.11	130.01	120.87
2	B	232	PRO	N-CA-CB	5.10	107.61	103.32
2	B	302	THR	O-C-N	-5.04	116.78	122.12
2	B	7	GLY	O-C-N	5.04	129.49	122.84
2	B	533	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	120	ASN	OD1-CG-ND2	5.02	127.62	122.60

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	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4562	0	4364	51	0
3	B	55	0	80	5	0
4	B	1	0	0	0	0
5	A	241	0	0	7	0
5	B	660	0	0	10	2
All	All	7283	0	6146	70	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 6.

All (70) 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:146[B]:PHE:HA	5:A:2157:HOH:O	1.93	0.69
2:B:171:ALA:O	3:B:1562:EDO:H12	1.93	0.68
1:A:199:LEU:HG	2:B:225[B]:MET:HE1	1.76	0.67
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
1:A:142[A]:MET:HE3	5:A:2151:HOH:O	1.98	0.63
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
1:A:199:LEU:CG	2:B:225[B]:MET:HE1	2.32	0.59
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:183:ASN:C	1:A:183:ASN:HD22	2.11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:GLN:H	1:A:207:GLN:NE2	1.99	0.52
1:A:198:PRO:CG	2:B:225[A]:MET:HE1	2.41	0.51
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:198:PRO:HG2	2:B:225[A]:MET:HE1	1.93	0.50
1:A:145[B]:ARG:HD3	2:B:459:PHE:CE1	2.46	0.49
1:A:199:LEU:CD1	2:B:225[B]:MET:HE1	2.42	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
1:A:198:PRO:HD2	2:B:225[A]:MET:HE1	1.95	0.48
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
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
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
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:504:ALA:HA	2:B:505:PRO:C	2.46	0.41
1:A:199:LEU:HD11	2:B:225[B]:MET:HE1	2.03	0.40
2:B:64:SER:HG	2:B:488[B]:PHE:HZ	1.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	218/260 (84%)	213 (98%)	5 (2%)	0	100	100
2	B	573/557 (103%)	558 (97%)	14 (2%)	1 (0%)	43	20
All	All	791/817 (97%)	771 (98%)	19 (2%)	1 (0%)	48	22

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 6
2	B	477/459 (104%)	471 (99%)	6 (1%)	61 29
All	All	665/669 (99%)	653 (98%)	12 (2%)	53 18

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	4	SER
1	A	60	LYS
1	A	183	ASN
1	A	204	GLN
1	A	207	GLN
2	B	154	TRP
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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	110	ASN
1	A	183	ASN
1	A	204	GLN
1	A	207	GLN
2	B	12	GLN
2	B	59	HIS
2	B	92	HIS
2	B	93	ASN
2	B	134	GLN
2	B	169	GLN
2	B	187	ASN
2	B	192	HIS
2	B	226	ASN
2	B	245	GLN
2	B	341	GLN
2	B	401	GLN
2	B	409	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	420	GLN
2	B	440	ASN
2	B	472	HIS
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	6,8,9	1.16	1 (16%)	3,9,11	0.59	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	-2.11	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	1567	-	3,3,3	0.49	0	2,2,2	0.84	0
3	EDO	B	1568	-	3,3,3	0.88	0	2,2,2	2.00	1 (50%)
3	EDO	B	1566	-	3,3,3	0.55	0	2,2,2	0.49	0
3	EDO	B	1563	-	3,3,3	0.54	0	2,2,2	1.32	0
3	EDO	B	1562	-	3,3,3	0.39	0	2,2,2	1.20	0
3	EDO	B	1559[A]	-	3,3,3	0.48	0	2,2,2	0.46	0
3	EDO	B	1561	-	3,3,3	0.56	0	2,2,2	0.23	0
3	EDO	B	1565	-	3,3,3	0.51	0	2,2,2	0.45	0
3	EDO	B	1559[B]	-	3,3,3	0.51	0	2,2,2	0.33	0
3	EDO	B	1569	-	3,3,3	1.37	0	2,2,2	0.73	0
3	EDO	B	1570	-	3,3,3	0.62	0	2,2,2	0.46	0
3	EDO	B	1558	-	3,3,3	0.58	0	2,2,2	0.21	0
3	EDO	B	1564	-	3,3,3	0.26	0	2,2,2	0.33	0
3	EDO	B	1560	-	3,3,3	0.61	0	2,2,2	0.13	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	1567	-	-	0/1/1/1	-
3	EDO	B	1568	-	-	1/1/1/1	-
3	EDO	B	1566	-	-	0/1/1/1	-
3	EDO	B	1563	-	-	0/1/1/1	-
3	EDO	B	1562	-	-	1/1/1/1	-
3	EDO	B	1559[A]	-	-	0/1/1/1	-
3	EDO	B	1561	-	-	0/1/1/1	-
3	EDO	B	1565	-	-	0/1/1/1	-
3	EDO	B	1559[B]	-	-	1/1/1/1	-
3	EDO	B	1569	-	-	1/1/1/1	-
3	EDO	B	1570	-	-	0/1/1/1	-
3	EDO	B	1558	-	-	0/1/1/1	-
3	EDO	B	1564	-	-	0/1/1/1	-
3	EDO	B	1560	-	-	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	2.37	130.47	112.39

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
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	1568	EDO	1	0
3	B	1562	EDO	2	0
3	B	1569	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%)	0.82	16 (7%)	19 21	3, 11, 19, 44	15 (7%)
2	B	557/557 (100%)	0.68	54 (9%)	13 14	4, 11, 24, 60	23 (4%)
All	All	764/817 (93%)	0.72	70 (9%)	14 16	3, 11, 22, 60	38 (4%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	379[A]	THR	7.8
2	B	132	THR	4.1
1	A	3	SER	3.9
2	B	215	TRP	3.6
2	B	133	THR	3.5
2	B	94	GLY	3.5
2	B	378[A]	THR	3.5
2	B	223	PHE	3.4
2	B	42	TYR	3.4
1	A	201	PHE	3.2
2	B	403	ASP	3.1
1	A	84	ALA	3.1
2	B	100	LEU	3.0
2	B	380	GLN	3.0
2	B	168	GLN	3.0
2	B	131	GLN	2.9
1	A	4	SER	2.9
2	B	129	THR	2.8
2	B	164	GLN	2.8
1	A	210	ALA	2.8
2	B	222	PRO	2.8
2	B	224	GLU	2.8
1	A	25	TRP	2.8
2	B	436	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	211	GLY	2.6
2	B	170	ALA	2.5
2	B	93	ASN	2.5
2	B	220	LEU	2.5
2	B	91	LEU	2.5
2	B	130	ASP	2.4
2	B	122	VAL	2.4
2	B	201	SER	2.4
2	B	221	LEU	2.4
2	B	96	TRP	2.4
1	A	21	ALA	2.4
1	A	197	TYR	2.3
2	B	336	GLY	2.3
2	B	217	TRP	2.3
2	B	162	ASN	2.3
2	B	40	ALA	2.3
2	B	209	VAL	2.3
1	A	78	ILE	2.3
2	B	181	TYR	2.3
2	B	309	GLY	2.2
2	B	184[A]	VAL	2.2
1	A	74	TRP	2.2
2	B	154	TRP	2.2
2	B	151	LEU	2.2
2	B	555	VAL	2.2
1	A	87	PRO	2.2
1	A	83	ALA	2.1
2	B	145	GLY	2.1
2	B	90	TYR	2.1
2	B	230	TYR	2.1
2	B	87	PRO	2.1
2	B	167	THR	2.1
2	B	163	TRP	2.1
1	A	24	THR	2.1
2	B	171	ALA	2.1
1	A	85	LEU	2.1
2	B	148	VAL	2.0
2	B	127	LEU	2.0
2	B	213	GLY	2.0
1	A	88	GLU	2.0
2	B	136	ALA	2.0
2	B	149	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	195	ALA	2.0
1	A	27	LEU	2.0
2	B	334	ASP	2.0
2	B	137[A]	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å 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	0.89	0.07	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.