



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:31 AM UTC

PDB ID : 1BLC / pdb_00001blc
Title : INHIBITION OF BETA-LACTAMASE BY CLAVULANATE: TRAPPED INTERMEDIATES IN CRYOCRYSTALLOGRAPHIC STUDIES
Authors : Chen, C.C.H.; Herzberg, O.
Deposited on : 1993-09-27
Resolution : 2.20 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

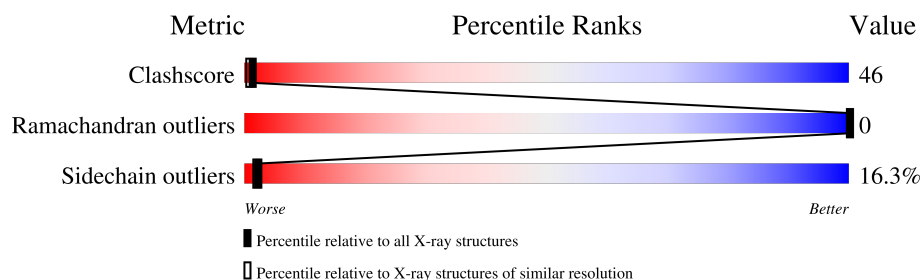
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

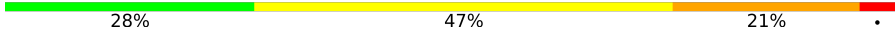
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	257	

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	CEM	A	301[A]	X	X	X	-
4	TEM	A	626[B]	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2384 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 BETA-LACTAMASE.

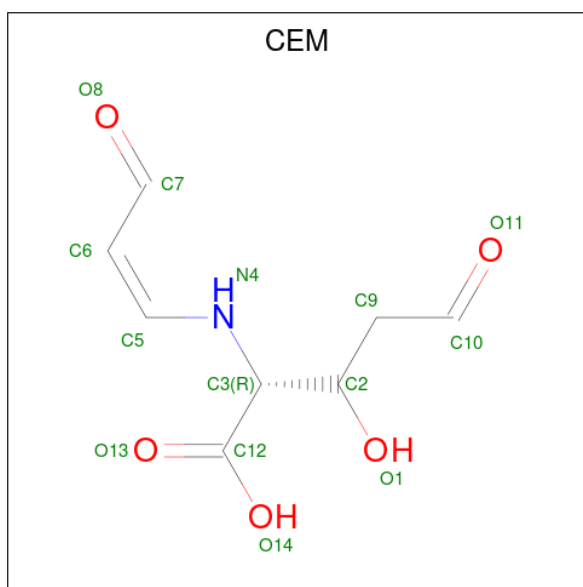
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			2030	1293	341	393	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



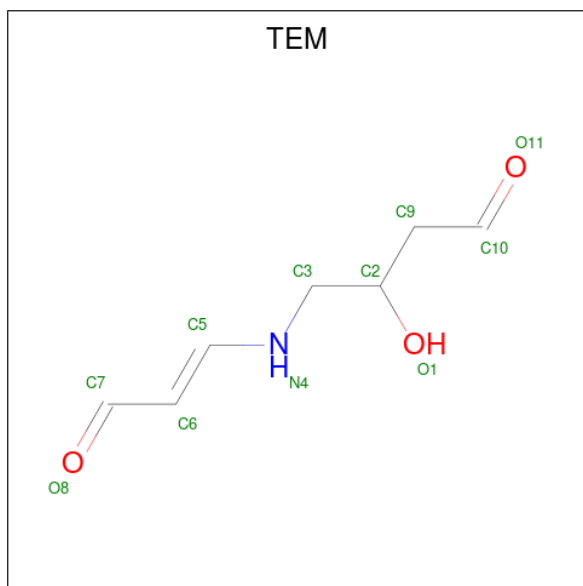
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is N-(1-CARBOXY-2-HYDROXY-4-OXO-BUTYL)-N-(3-OXO-CISPROPENYL)AMINE (CCD ID: CEM) (formula: C₈H₁₁NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			14	8	1	5		

- Molecule 4 is N-(2-HYDROXY-4-OXO-BUTYL)-N-(3-OXO-TRANSPROPENYL)AMINE (CCD ID: TEM) (formula: $C_7H_{11}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			11	7	1	3		

- Molecule 5 is water.

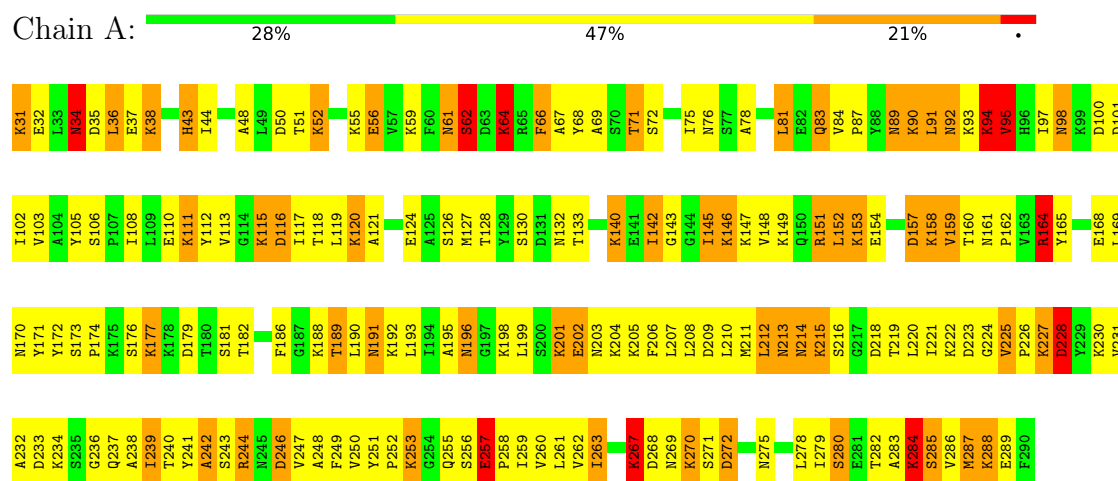
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	324	Total 324	O 324	0	0

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: BETA-LACTAMASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	54.10Å 88.00Å 141.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2384	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CEM, SO4, TEM

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	1.61	16/2065 (0.8%)	2.39	119/2772 (4.3%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	THR	N-CA	6.70	1.54	1.46
1	A	75	ILE	CA-CB	6.60	1.62	1.54
1	A	263	ILE	C-O	6.58	1.31	1.24
1	A	239	ILE	CA-CB	5.90	1.61	1.54
1	A	283	ALA	C-N	-5.70	1.26	1.33
1	A	67	ALA	C-O	5.64	1.30	1.24
1	A	133	THR	C-O	5.57	1.30	1.24
1	A	108	ILE	C-N	-5.40	1.26	1.33
1	A	282	THR	N-CA	5.34	1.52	1.46
1	A	118	THR	N-CA	5.33	1.53	1.45
1	A	221	ILE	CA-CB	5.30	1.60	1.54
1	A	142	ILE	CA-CB	5.21	1.62	1.54
1	A	244	ARG	C-O	5.10	1.29	1.24
1	A	94	LYS	CA-CB	-5.04	1.44	1.53
1	A	128	THR	CA-CB	5.00	1.61	1.53
1	A	89	ASN	CG-OD1	5.00	1.33	1.23

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	LYS	CA-CB-CG	11.62	137.34	114.10
1	A	186	PHE	CA-C-N	10.22	131.29	119.94
1	A	186	PHE	C-N-CA	10.22	131.29	119.94
1	A	34	ASN	CA-CB-CG	-9.96	102.64	112.60
1	A	269	ASN	CA-CB-CG	-8.54	104.06	112.60
1	A	116	ASP	O-C-N	8.42	132.78	123.10
1	A	102	ILE	N-CA-C	8.40	119.80	109.30
1	A	246	ASP	CB-CA-C	8.11	123.58	109.80
1	A	176	SER	CA-C-N	8.07	137.32	121.58
1	A	176	SER	C-N-CA	8.07	137.32	121.58
1	A	228	ASP	CA-CB-CG	-8.04	104.56	112.60
1	A	35	ASP	CB-CA-C	7.83	125.54	109.95
1	A	61	ASN	CA-C-N	7.80	131.51	120.28
1	A	61	ASN	C-N-CA	7.80	131.51	120.28
1	A	157	ASP	CA-C-O	7.65	129.42	120.70
1	A	189	THR	CA-CB-OG1	-7.56	98.26	109.60
1	A	34	ASN	OD1-CG-ND2	7.53	130.13	122.60
1	A	213	ASN	CA-CB-CG	-7.53	105.07	112.60
1	A	76	ASN	O-C-N	7.46	129.75	122.07
1	A	268	ASP	CA-CB-CG	-7.39	105.21	112.60
1	A	52	LYS	CA-C-O	7.35	128.72	121.00
1	A	93	LYS	CB-CA-C	-7.34	99.51	109.71
1	A	56	GLU	CG-CD-OE2	7.16	134.87	118.40
1	A	140	LYS	CA-C-O	-7.15	113.31	120.82
1	A	248	ALA	N-CA-C	7.04	119.77	109.07
1	A	127	MET	CA-C-O	-6.87	113.78	121.00
1	A	34	ASN	CA-C-O	-6.84	113.64	120.82
1	A	89	ASN	CB-CG-ND2	6.83	126.65	116.40
1	A	268	ASP	N-CA-C	6.58	118.11	111.07
1	A	84	VAL	O-C-N	6.55	128.57	121.10
1	A	288	LYS	N-CA-CB	6.50	119.68	110.12
1	A	64	LYS	CA-C-N	6.42	129.99	120.87
1	A	64	LYS	C-N-CA	6.42	129.99	120.87
1	A	283	ALA	CA-C-N	6.42	129.21	120.54
1	A	283	ALA	C-N-CA	6.42	129.21	120.54
1	A	151	ARG	CB-CA-C	6.39	120.92	110.88
1	A	202	GLU	CG-CD-OE1	6.39	133.10	118.40
1	A	249	PHE	CA-CB-CG	-6.29	107.51	113.80
1	A	248	ALA	CA-C-N	6.28	132.03	123.11
1	A	248	ALA	C-N-CA	6.28	132.03	123.11
1	A	66	PHE	O-C-N	6.21	130.33	123.25
1	A	90	LYS	CA-CB-CG	6.16	126.41	114.10
1	A	284	LYS	N-CA-CB	-6.14	100.80	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ASN	OD1-CG-ND2	6.13	128.73	122.60
1	A	284	LYS	CG-CD-CE	-6.10	97.28	111.30
1	A	140	LYS	O-C-N	6.07	128.32	122.07
1	A	196	ASN	N-CA-CB	-6.02	100.32	110.49
1	A	286	VAL	O-C-N	5.98	127.75	121.89
1	A	271	SER	CA-C-O	-5.96	112.22	119.43
1	A	75	ILE	O-C-N	5.94	128.08	121.90
1	A	280	SER	CA-C-O	5.94	126.85	120.55
1	A	242	ALA	N-CA-CB	-5.91	103.03	111.84
1	A	195	ALA	O-C-N	5.88	128.13	122.07
1	A	118	THR	N-CA-CB	-5.87	102.33	110.38
1	A	159	VAL	N-CA-CB	-5.87	102.40	110.68
1	A	240	THR	N-CA-CB	-5.84	101.85	110.85
1	A	145	ILE	CA-C-N	5.82	128.66	120.28
1	A	145	ILE	C-N-CA	5.82	128.66	120.28
1	A	262	VAL	O-C-N	5.78	129.86	123.10
1	A	225	VAL	O-C-N	5.75	127.66	121.10
1	A	94	LYS	N-CA-CB	5.75	119.95	110.69
1	A	93	LYS	CA-C-O	-5.74	115.21	120.95
1	A	62	SER	CA-CB-OG	-5.69	99.73	111.10
1	A	206	PHE	CA-CB-CG	5.58	119.38	113.80
1	A	140	LYS	N-CA-CB	5.57	118.08	110.01
1	A	284	LYS	CB-CG-CD	-5.57	98.50	111.30
1	A	159	VAL	N-CA-C	5.56	116.95	111.67
1	A	92	ASN	CB-CG-ND2	5.54	124.72	116.40
1	A	182	THR	CA-CB-OG1	-5.52	101.33	109.60
1	A	241	TYR	CA-CB-CG	-5.51	103.98	113.90
1	A	108	ILE	CA-C-N	5.50	129.91	120.72
1	A	108	ILE	C-N-CA	5.50	129.91	120.72
1	A	170	ASN	CA-CB-CG	5.49	118.09	112.60
1	A	91	LEU	CA-C-O	5.49	125.71	119.18
1	A	203	ASN	O-C-N	5.46	128.38	122.15
1	A	288	LYS	O-C-N	5.46	127.91	122.12
1	A	148	VAL	N-CA-C	-5.45	105.19	110.42
1	A	214	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	A	128	THR	CA-CB-CG2	5.44	119.75	110.50
1	A	219	THR	CA-CB-CG2	5.43	119.74	110.50
1	A	170	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	71	THR	CA-C-O	5.37	126.17	120.10
1	A	231	VAL	O-C-N	5.36	128.88	123.20
1	A	202	GLU	CG-CD-OE2	-5.35	106.10	118.40
1	A	285	SER	CA-C-N	5.33	128.05	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	SER	C-N-CA	5.33	128.05	120.53
1	A	212	LEU	N-CA-CB	-5.33	102.26	110.20
1	A	188	LYS	CA-C-N	5.30	127.39	120.28
1	A	188	LYS	C-N-CA	5.30	127.39	120.28
1	A	132	ASN	CA-C-O	-5.30	114.80	120.42
1	A	190	LEU	N-CA-CB	-5.30	102.33	110.12
1	A	119	LEU	CB-CA-C	5.28	119.56	110.79
1	A	288	LYS	CB-CA-C	-5.27	102.03	110.79
1	A	250	VAL	CA-C-O	-5.26	114.87	120.39
1	A	116	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	164	ARG	O-C-N	5.22	130.22	122.97
1	A	43	HIS	CA-CB-CG	-5.21	108.58	113.80
1	A	157	ASP	N-CA-CB	5.21	119.26	110.46
1	A	164	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	A	81	LEU	CA-C-N	5.21	128.22	120.31
1	A	81	LEU	C-N-CA	5.21	128.22	120.31
1	A	206	PHE	CA-C-N	5.19	127.66	120.29
1	A	206	PHE	C-N-CA	5.19	127.66	120.29
1	A	66	PHE	CA-CB-CG	5.18	118.98	113.80
1	A	95	VAL	N-CA-CB	-5.18	101.19	111.91
1	A	164	ARG	CD-NE-CZ	5.16	131.63	124.40
1	A	181	SER	O-C-N	5.16	128.68	123.26
1	A	267	LYS	CA-C-N	5.15	127.14	120.44
1	A	267	LYS	C-N-CA	5.15	127.14	120.44
1	A	288	LYS	CA-CB-CG	5.14	124.38	114.10
1	A	182	THR	CA-C-O	-5.13	115.35	120.63
1	A	117	ILE	N-CA-C	-5.12	100.52	108.81
1	A	257	GLU	O-C-N	5.11	127.15	121.43
1	A	50	ASP	N-CA-C	-5.09	100.86	108.96
1	A	152	LEU	CA-C-O	5.07	126.32	120.90
1	A	37	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	160	THR	OG1-CB-CG2	5.04	119.39	109.30
1	A	181	SER	CA-C-O	-5.02	116.06	121.38
1	A	272	ASP	CA-C-O	-5.01	115.67	121.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	244	ARG	Sidechain

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	2030	0	2114	182	0
2	A	5	0	0	0	0
3	A	14	0	7	16	0
4	A	11	0	8	3	0
5	A	324	0	0	55	0
All	All	2384	0	2129	191	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 46.

All (191) 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:158:LYS:H	1:A:158:LYS:HD2	0.98	1.07
1:A:214:ASN:HD21	1:A:216:SER:HB2	1.17	1.06
1:A:69:ALA:HB1	3:A:301[A]:CEM:O8	1.57	1.05
1:A:201:LYS:HD3	1:A:201:LYS:C	1.80	1.05
1:A:259:ILE:HD13	1:A:287:MET:CE	1.86	1.05
1:A:158:LYS:H	1:A:158:LYS:CD	1.67	1.04
1:A:227:LYS:HE2	1:A:227:LYS:H	1.28	0.99
1:A:288:LYS:HB2	5:A:473:HOH:O	1.60	0.99
1:A:168:GLU:HG2	1:A:171:TYR:CE2	1.98	0.99
1:A:199:LEU:HG	5:A:471:HOH:O	1.62	0.98
1:A:259:ILE:HD13	1:A:287:MET:HE1	1.44	0.97
1:A:34:ASN:O	1:A:38:LYS:HE2	1.69	0.93
1:A:158:LYS:HD2	1:A:158:LYS:N	1.83	0.92
3:A:301[A]:CEM:H3	5:A:356:HOH:O	1.70	0.90
1:A:31:LYS:HE2	5:A:352:HOH:O	1.71	0.89
1:A:31:LYS:HZ1	1:A:284:LYS:HE2	1.37	0.89
1:A:105:TYR:CE2	4:A:626[B]:TEM:H91	2.10	0.85
1:A:145:ILE:HD13	5:A:404:HOH:O	1.74	0.85
1:A:164:ARG:NH2	1:A:171:TYR:HB2	1.92	0.85
1:A:55:LYS:HE2	1:A:289:GLU:O	1.77	0.84
1:A:237:GLN:H	3:A:301[A]:CEM:H6	1.43	0.83
1:A:164:ARG:HH22	1:A:171:TYR:HB2	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LYS:O	1:A:153:LYS:HG2	1.80	0.81
4:A:626[B]:TEM:N4	5:A:367:HOH:O	2.13	0.80
1:A:31:LYS:HE2	1:A:31:LYS:N	1.97	0.80
1:A:201:LYS:C	1:A:201:LYS:CD	2.58	0.77
1:A:106:SER:O	1:A:110:GLU:HB3	1.87	0.75
1:A:149:LYS:HZ2	1:A:162:PRO:HD2	1.51	0.75
1:A:251:TYR:CE1	1:A:258:PRO:HB3	2.21	0.75
1:A:284:LYS:HD2	1:A:284:LYS:C	2.13	0.73
1:A:87:PRO:HB2	1:A:89:ASN:OD1	1.89	0.72
1:A:237:GLN:N	3:A:301[A]:CEM:H6	2.03	0.72
1:A:31:LYS:N	5:A:352:HOH:O	2.23	0.71
1:A:214:ASN:ND2	1:A:216:SER:HB2	2.00	0.71
1:A:224:GLY:O	1:A:284:LYS:HG2	1.90	0.71
1:A:227:LYS:H	1:A:227:LYS:CE	2.03	0.70
1:A:237:GLN:H	3:A:301[A]:CEM:C6	2.05	0.70
1:A:59:LYS:HE2	5:A:596:HOH:O	1.92	0.69
1:A:31:LYS:NZ	1:A:284:LYS:HE2	2.08	0.69
1:A:209:ASP:O	1:A:213:ASN:ND2	2.26	0.69
1:A:257:GLU:HB2	5:A:461:HOH:O	1.93	0.68
1:A:172:TYR:N	5:A:330:HOH:O	2.27	0.68
1:A:255:GLN:NE2	5:A:545:HOH:O	2.26	0.68
1:A:34:ASN:O	1:A:38:LYS:CE	2.41	0.68
1:A:69:ALA:CB	3:A:301[A]:CEM:O8	2.38	0.67
1:A:31:LYS:HE3	1:A:285:SER:HB2	1.75	0.67
1:A:201:LYS:HD3	1:A:202:GLU:N	2.08	0.67
3:A:301[A]:CEM:O13	5:A:433:HOH:O	2.12	0.67
1:A:201:LYS:NZ	1:A:205:LYS:HD3	2.10	0.67
1:A:171:TYR:C	5:A:330:HOH:O	2.37	0.67
1:A:230:LYS:HD2	5:A:575:HOH:O	1.95	0.66
1:A:31:LYS:CE	1:A:285:SER:HB2	2.26	0.66
3:A:301[A]:CEM:C5	5:A:356:HOH:O	2.44	0.65
1:A:38:LYS:HG2	5:A:491:HOH:O	1.96	0.65
1:A:94:LYS:HD3	5:A:375:HOH:O	1.97	0.64
1:A:64:LYS:HD3	5:A:347:HOH:O	1.97	0.64
1:A:111:LYS:HE3	1:A:111:LYS:HA	1.80	0.64
1:A:177:LYS:NZ	5:A:353:HOH:O	2.26	0.63
1:A:158:LYS:HD3	1:A:159:VAL:HG23	1.80	0.63
1:A:31:LYS:N	1:A:285:SER:HB2	2.14	0.62
1:A:145:ILE:CD1	5:A:404:HOH:O	2.41	0.62
1:A:48:ALA:HA	1:A:260:VAL:O	2.00	0.62
1:A:288:LYS:HG3	5:A:580:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:TYR:CD1	1:A:72:SER:HB2	2.35	0.61
1:A:153:LYS:HD2	5:A:587:HOH:O	2.00	0.61
1:A:62:SER:HB2	5:A:319:HOH:O	1.99	0.61
1:A:212:LEU:HD13	1:A:232:ALA:HB2	1.82	0.61
1:A:103:VAL:O	5:A:422:HOH:O	2.16	0.60
1:A:234:LYS:NZ	3:A:301[A]:CEM:O14	2.33	0.60
1:A:149:LYS:O	1:A:153:LYS:CG	2.49	0.60
1:A:43:HIS:CE1	5:A:398:HOH:O	2.55	0.59
1:A:34:ASN:HD22	1:A:38:LYS:NZ	2.01	0.59
1:A:164:ARG:HD3	1:A:179:ASP:OD2	2.01	0.59
1:A:113:VAL:HB	5:A:453:HOH:O	2.01	0.59
1:A:238:ALA:HB3	1:A:243:SER:HB2	1.84	0.59
1:A:149:LYS:NZ	1:A:162:PRO:HD2	2.18	0.58
1:A:230:LYS:HE2	5:A:563:HOH:O	2.01	0.58
1:A:171:TYR:CD1	1:A:239:ILE:HD12	2.38	0.58
1:A:201:LYS:CD	1:A:202:GLU:N	2.65	0.58
1:A:143:GLY:O	1:A:147:LYS:HG2	2.03	0.58
1:A:191:ASN:ND2	5:A:499:HOH:O	2.22	0.56
1:A:98:ASN:O	1:A:101:ASP:HB2	2.06	0.55
1:A:89:ASN:ND2	1:A:90:LYS:HD3	2.21	0.55
1:A:161:ASN:HB2	5:A:555:HOH:O	2.06	0.55
1:A:239:ILE:HD11	4:A:626[B]:TEM:O11	2.06	0.54
1:A:112:TYR:HA	1:A:115:LYS:HD2	1.89	0.54
1:A:171:TYR:CE1	1:A:239:ILE:HD12	2.43	0.54
1:A:233:ASP:HB2	1:A:247:VAL:O	2.07	0.54
1:A:236:GLY:HA2	3:A:301[A]:CEM:C6	2.38	0.53
1:A:227:LYS:HE2	1:A:227:LYS:N	2.10	0.53
1:A:165:TYR:C	1:A:169:LEU:HD23	2.33	0.53
1:A:207:LEU:O	1:A:211:MET:HG3	2.09	0.53
1:A:275:ASN:O	1:A:278:LEU:HB3	2.09	0.53
1:A:32:GLU:HG3	5:A:470:HOH:O	2.08	0.53
1:A:32:GLU:HG3	5:A:487:HOH:O	2.09	0.53
1:A:91:LEU:HB3	1:A:120:LYS:HB2	1.91	0.53
1:A:228:ASP:HB3	1:A:253:LYS:HD2	1.91	0.53
1:A:158:LYS:CD	1:A:158:LYS:N	2.48	0.52
1:A:38:LYS:CG	5:A:491:HOH:O	2.54	0.52
1:A:68:TYR:HB2	1:A:71:THR:OG1	2.10	0.52
1:A:196:ASN:HB2	5:A:561:HOH:O	2.08	0.52
1:A:168:GLU:HB2	5:A:528:HOH:O	2.10	0.52
1:A:252:PRO:HG2	1:A:255:GLN:OE1	2.10	0.51
1:A:228:ASP:CB	1:A:253:LYS:HD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:HD3	1:A:201:LYS:O	2.07	0.51
1:A:225:VAL:HG12	1:A:287:MET:HG2	1.93	0.51
1:A:201:LYS:HZ3	1:A:205:LYS:HD3	1.75	0.50
1:A:34:ASN:ND2	1:A:38:LYS:NZ	2.59	0.50
1:A:89:ASN:ND2	1:A:90:LYS:CD	2.75	0.50
3:A:301[A]:CEM:H5	5:A:356:HOH:O	2.07	0.50
1:A:204:LYS:HE2	5:A:373:HOH:O	2.11	0.50
1:A:228:ASP:O	5:A:477:HOH:O	2.19	0.49
1:A:143:GLY:HA3	1:A:147:LYS:HG3	1.94	0.49
1:A:126:SER:O	1:A:130:SER:HA	2.12	0.49
3:A:301[A]:CEM:O13	3:A:301[A]:CEM:O1	2.24	0.49
1:A:31:LYS:N	1:A:285:SER:CB	2.76	0.49
1:A:252:PRO:HB2	1:A:255:GLN:HB3	1.95	0.49
1:A:218:ASP:O	1:A:223:ASP:HB2	2.13	0.48
1:A:43:HIS:HB3	1:A:64:LYS:NZ	2.27	0.48
1:A:87:PRO:HG2	1:A:90:LYS:HD3	1.95	0.48
1:A:149:LYS:NZ	1:A:162:PRO:O	2.45	0.48
1:A:261:LEU:HD11	1:A:263:ILE:HG13	1.94	0.48
1:A:202:GLU:H	1:A:202:GLU:CD	2.22	0.48
1:A:115:LYS:HE3	5:A:362:HOH:O	2.14	0.48
1:A:233:ASP:HA	1:A:247:VAL:O	2.13	0.48
1:A:230:LYS:CE	5:A:563:HOH:O	2.58	0.48
1:A:237:GLN:N	3:A:301[A]:CEM:C6	2.71	0.48
1:A:64:LYS:HD2	1:A:66:PHE:CE1	2.48	0.47
1:A:44:ILE:HD11	1:A:278:LEU:HD11	1.96	0.47
1:A:227:LYS:HA	5:A:594:HOH:O	2.13	0.47
1:A:201:LYS:NZ	1:A:205:LYS:CD	2.76	0.47
1:A:270:LYS:HD2	5:A:548:HOH:O	2.14	0.47
1:A:121:ALA:O	5:A:344:HOH:O	2.21	0.47
1:A:31:LYS:N	1:A:31:LYS:CE	2.76	0.47
1:A:215:LYS:HA	1:A:215:LYS:HE3	1.97	0.47
1:A:242:ALA:HB3	1:A:267:LYS:HG3	1.97	0.47
1:A:89:ASN:OD1	1:A:89:ASN:N	2.31	0.47
1:A:124:GLU:HG2	1:A:210:LEU:HD21	1.97	0.46
1:A:157:ASP:HA	1:A:158:LYS:HD2	1.96	0.46
1:A:168:GLU:CG	5:A:528:HOH:O	2.63	0.46
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.68	0.46
1:A:242:ALA:HB2	1:A:272:ASP:O	2.16	0.46
3:A:301[A]:CEM:H5	5:A:553:HOH:O	2.15	0.46
1:A:120:LYS:NZ	1:A:124:GLU:OE2	2.45	0.45
1:A:110:GLU:HG3	1:A:111:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HE3	5:A:587:HOH:O	2.17	0.45
1:A:146:LYS:HB2	5:A:480:HOH:O	2.17	0.45
1:A:83:GLN:OE1	1:A:142:ILE:HA	2.16	0.44
1:A:31:LYS:HE2	1:A:285:SER:HB2	1.97	0.44
1:A:215:LYS:HG3	1:A:218:ASP:OD2	2.16	0.44
1:A:168:GLU:HG3	5:A:528:HOH:O	2.17	0.44
1:A:149:LYS:HE2	5:A:464:HOH:O	2.16	0.44
1:A:192:LYS:NZ	5:A:605:HOH:O	2.50	0.44
1:A:95:VAL:O	1:A:116:ASP:HA	2.18	0.44
1:A:98:ASN:C	1:A:98:ASN:HD22	2.26	0.44
1:A:151:ARG:HD2	1:A:154:GLU:OE1	2.18	0.44
1:A:199:LEU:N	5:A:471:HOH:O	2.51	0.43
1:A:140:LYS:HG3	5:A:552:HOH:O	2.18	0.43
1:A:153:LYS:HG2	1:A:153:LYS:H	1.45	0.43
1:A:196:ASN:CB	5:A:481:HOH:O	2.66	0.43
1:A:31:LYS:N	1:A:285:SER:HG	2.17	0.43
1:A:233:ASP:OD2	1:A:246:ASP:OD1	2.36	0.43
1:A:284:LYS:HZ3	1:A:284:LYS:HG3	1.65	0.43
1:A:48:ALA:O	1:A:56:GLU:HA	2.18	0.43
1:A:34:ASN:HD22	1:A:38:LYS:HZ3	1.66	0.43
1:A:220:LEU:HD22	1:A:279:ILE:HD12	2.01	0.43
1:A:98:ASN:HD22	1:A:100:ASP:H	1.66	0.42
1:A:201:LYS:HZ1	1:A:205:LYS:CD	2.31	0.42
1:A:259:ILE:CD1	1:A:287:MET:HE1	2.30	0.42
1:A:78:ALA:HB3	1:A:193:LEU:HD13	2.02	0.42
1:A:280:SER:O	1:A:284:LYS:HB2	2.19	0.42
1:A:261:LEU:HD11	1:A:263:ILE:CG1	2.50	0.42
1:A:208:LEU:O	1:A:212:LEU:HB2	2.20	0.42
1:A:34:ASN:ND2	1:A:38:LYS:HZ3	2.18	0.41
1:A:44:ILE:O	1:A:61:ASN:HB2	2.21	0.41
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.87	0.41
1:A:97:ILE:HA	1:A:101:ASP:OD2	2.20	0.41
1:A:161:ASN:CG	5:A:555:HOH:O	2.63	0.41
1:A:227:LYS:H	1:A:227:LYS:CD	2.33	0.41
1:A:68:TYR:HB2	1:A:71:THR:HG1	1.86	0.41
1:A:255:GLN:HG2	1:A:257:GLU:O	2.21	0.41
1:A:196:ASN:ND2	5:A:493:HOH:O	2.53	0.41
1:A:224:GLY:HA3	1:A:280:SER:O	2.21	0.41
1:A:225:VAL:HB	1:A:226:PRO:CD	2.51	0.41
1:A:51:THR:OG1	1:A:258:PRO:HD2	2.21	0.40
1:A:196:ASN:HB2	5:A:481:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:HG2	1:A:171:TYR:CD2	2.50	0.40
1:A:234:LYS:HA	1:A:234:LYS:HD2	1.92	0.40
1:A:201:LYS:HZ1	1:A:205:LYS:HD3	1.84	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	256/257 (100%)	245 (96%)	11 (4%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	228/227 (100%)	191 (84%)	37 (16%)	2 2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	34	ASN
1	A	36	LEU

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Mol	Chain	Res	Type
1	A	38	LYS
1	A	52	LYS
1	A	62	SER
1	A	64	LYS
1	A	83	GLN
1	A	92	ASN
1	A	94	LYS
1	A	95	VAL
1	A	98	ASN
1	A	111	LYS
1	A	115	LYS
1	A	120	LYS
1	A	146	LYS
1	A	152	LEU
1	A	153	LYS
1	A	158	LYS
1	A	164	ARG
1	A	173	SER
1	A	174	PRO
1	A	177	LYS
1	A	189	THR
1	A	198	LYS
1	A	201	LYS
1	A	215	LYS
1	A	222	LYS
1	A	227	LYS
1	A	228	ASP
1	A	253	LYS
1	A	256	SER
1	A	257	GLU
1	A	267	LYS
1	A	270	LYS
1	A	284	LYS
1	A	287	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	41	ASN
1	A	98	ASN
1	A	196	ASN

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Mol	Chain	Res	Type
1	A	214	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are 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$
3	CEM	A	301[A]	1	12,13,13	3.61	5 (41%)	12,15,15	3.33	7 (58%)
4	TEM	A	626[B]	1	8,10,10	2.97	2 (25%)	7,10,10	2.88	3 (42%)
2	SO4	A	300	-	4,4,4	0.77	0	6,6,6	0.80	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	CEM	A	301[A]	1	1/1/3/8	6/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TEM	A	626[B]	1	1/1/1/6	4/9/9/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301[A]	CEM	O1-C2	-9.65	1.23	1.43
4	A	626[B]	TEM	O1-C2	-6.86	1.23	1.43
3	A	301[A]	CEM	C5-N4	4.21	1.48	1.33
4	A	626[B]	TEM	O11-C10	4.11	1.43	1.20
3	A	301[A]	CEM	O11-C10	4.04	1.42	1.20
3	A	301[A]	CEM	C5-C6	-3.62	1.30	1.37
3	A	301[A]	CEM	O14-C12	-2.47	1.22	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301[A]	CEM	O1-C2-C9	5.90	122.83	109.24
4	A	626[B]	TEM	O1-C2-C9	5.14	123.13	109.45
3	A	301[A]	CEM	C12-C3-N4	5.08	121.25	110.05
3	A	301[A]	CEM	C9-C2-C3	4.72	121.45	112.28
3	A	301[A]	CEM	O11-C10-C9	-4.19	113.18	125.38
4	A	626[B]	TEM	O11-C10-C9	-3.96	113.87	125.38
3	A	301[A]	CEM	O13-C12-C3	-3.69	109.62	121.86
3	A	301[A]	CEM	O14-C12-C3	3.39	125.92	114.15
4	A	626[B]	TEM	O1-C2-C3	3.09	119.46	109.29
3	A	301[A]	CEM	O8-C7-C6	-2.15	118.74	125.61

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	301[A]	CEM	C2
4	A	626[B]	TEM	C2

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301[A]	CEM	C9-C2-C3-N4
3	A	301[A]	CEM	C9-C2-C3-C12
3	A	301[A]	CEM	C3-C2-C9-C10
4	A	626[B]	TEM	O1-C2-C3-N4
4	A	626[B]	TEM	C6-C5-N4-C3

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Mol	Chain	Res	Type	Atoms
3	A	301[A]	CEM	O13-C12-C3-C2
4	A	626[B]	TEM	C3-C2-C9-C10
4	A	626[B]	TEM	O11-C10-C9-C2
3	A	301[A]	CEM	O14-C12-C3-C2
3	A	301[A]	CEM	O1-C2-C9-C10

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301[A]	CEM	16	0
4	A	626[B]	TEM	3	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.