



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:56 AM UTC

PDB ID : 5NCD / pdb_00005ncd
Title : Crystal structure of the polysaccharide deacetylase Bc1974 from *Bacillus cereus* in complex with (2S)-2-amino-5-(diaminomethylideneamino)-N-hydroxypentamide
Authors : Giastas, P.; Andreou, A.; Eliopoulos, E.E.
Deposited on : 2017-03-03
Resolution : 2.45 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

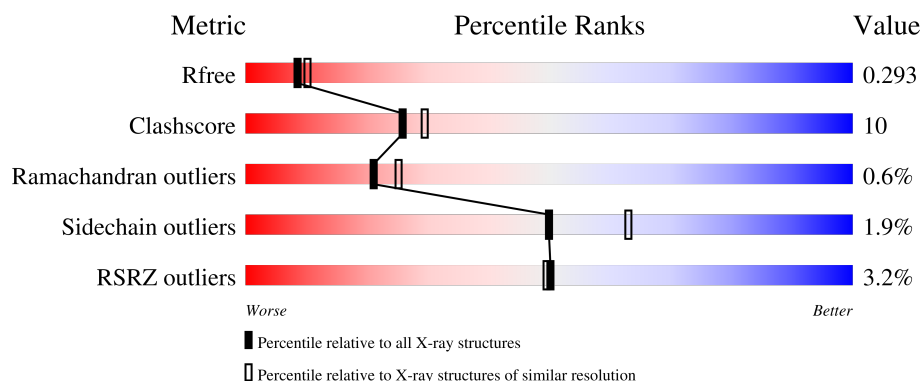
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	247	4% 65% 16% • 17%
1	B	247	% 66% 17% 17%
1	C	247	4% 64% 19% • 17%
1	D	247	2% 66% 17% • 17%

2 Entry composition [i](#)

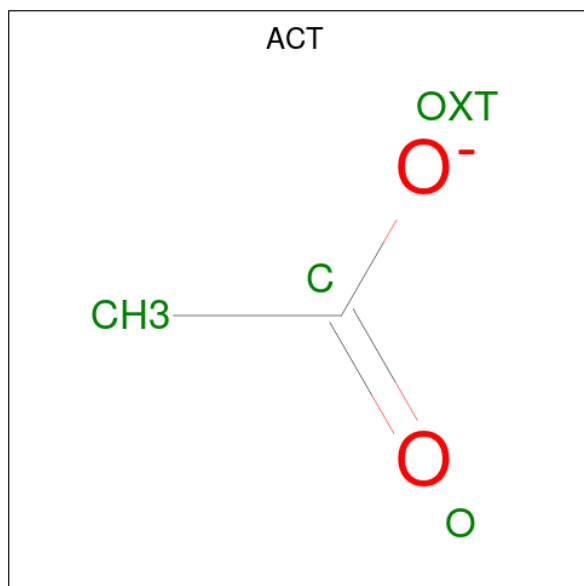
There are 6 unique types of molecules in this entry. The entry contains 6798 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Peptidoglycan N-acetylglucosamine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1651	1057	284	303	7			
1	B	206	Total	C	N	O	S	0	0	0
			1651	1057	284	303	7			
1	C	206	Total	C	N	O	S	0	0	0
			1645	1054	281	303	7			
1	D	206	Total	C	N	O	S	0	2	0
			1664	1066	286	305	7			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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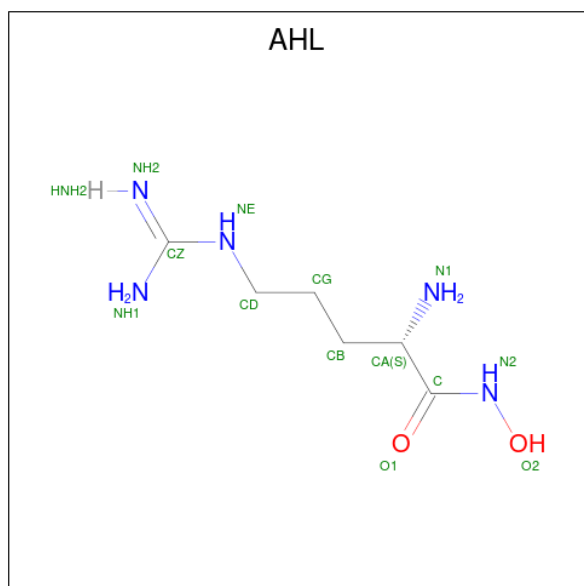
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-HYDROXY-L-ARGININAMIDE (CCD ID: AHL) (formula: C₆H₁₅N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			13	6	5	2		

- Molecule 5 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	6	7		

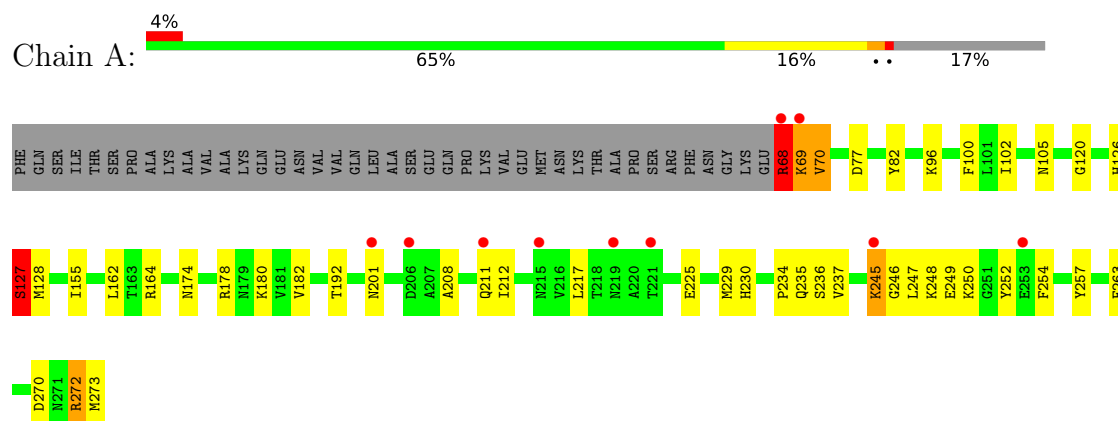
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	45	Total	O	0	0
			45	45		
6	C	30	Total	O	0	0
			30	30		
6	D	31	Total	O	0	0
			31	31		

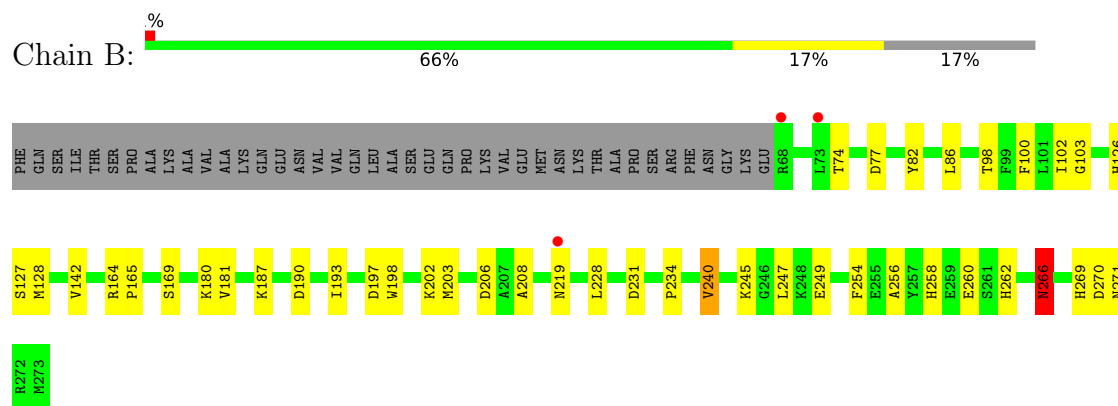
3 Residue-property plots [i](#)

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.

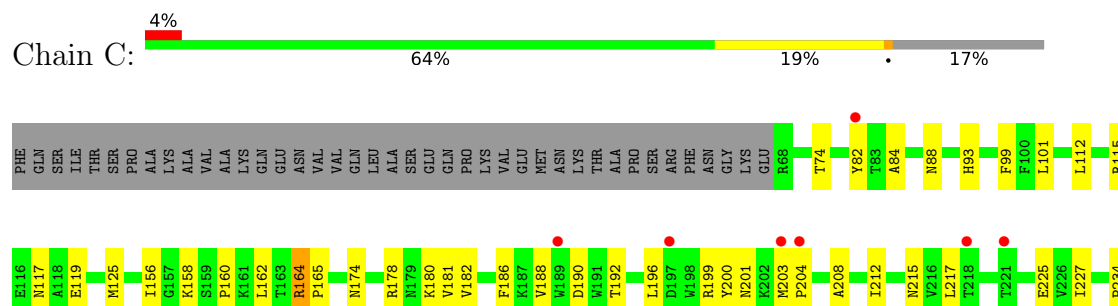
- Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase

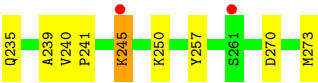


- Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase

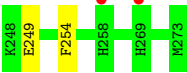


- Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase





● Molecule 1: Peptidoglycan N-acetylglucosamine deacetylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.65Å 117.44Å 99.49Å 90.00° 102.92° 90.00°	Depositor
Resolution (Å)	48.48 – 2.45 48.48 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.48-2.45) 98.3 (48.48-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.226 , 0.292 0.228 , 0.293	Depositor DCC
R_{free} test set	2081 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6798	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.13% 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: AHL, ACT, CIT, ZN

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	0.57	0/1696	0.96	7/2295 (0.3%)
1	B	0.59	0/1696	0.88	3/2295 (0.1%)
1	C	0.54	0/1690	0.91	5/2288 (0.2%)
1	D	0.56	0/1716	0.91	5/2322 (0.2%)
All	All	0.56	0/6798	0.92	20/9200 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	GLY	N-CA-C	-7.67	102.95	112.77
1	C	239	ALA	CA-C-N	6.16	124.12	120.24
1	C	239	ALA	C-N-CA	6.16	124.12	120.24
1	A	272	ARG	N-CA-C	-6.15	105.78	113.28
1	D	240	VAL	CA-C-N	-6.06	112.67	118.97
1	D	240	VAL	C-N-CA	-6.06	112.67	118.97
1	C	164	ARG	CA-C-N	-5.65	114.56	120.38
1	C	164	ARG	C-N-CA	-5.65	114.56	120.38
1	D	222	LYS	CA-C-N	5.64	126.89	119.84
1	D	222	LYS	C-N-CA	5.64	126.89	119.84
1	D	199	ARG	N-CA-C	-5.60	106.29	113.23
1	C	240	VAL	CB-CA-C	-5.18	108.86	114.35
1	B	266	ASN	N-CA-C	5.16	116.51	109.18
1	A	70	VAL	N-CA-C	5.08	115.59	108.17
1	B	240	VAL	CA-C-N	-5.07	113.33	118.85
1	B	240	VAL	C-N-CA	-5.07	113.33	118.85
1	A	263	PHE	CA-C-N	5.04	125.27	119.83
1	A	263	PHE	C-N-CA	5.04	125.27	119.83
1	A	68	ARG	CA-C-N	5.04	131.16	121.54
1	A	68	ARG	C-N-CA	5.04	131.16	121.54

There are no chirality outliers.

There are no planarity outliers.

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	1651	0	1611	33	0
1	B	1651	0	1611	33	0
1	C	1645	0	1600	29	0
1	D	1664	0	1624	29	0
2	A	4	0	3	0	0
2	C	4	0	3	1	0
2	D	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	13	0	14	4	0
5	B	13	0	5	2	0
6	A	39	0	0	2	0
6	B	45	0	0	8	0
6	C	30	0	0	1	0
6	D	31	0	0	2	0
All	All	6798	0	6474	125	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 10.

All (125) 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:B:128:MET:SD	6:B:408:HOH:O	2.14	1.05
1:C:117:ASN:HD22	1:C:156:ILE:HB	1.32	0.91
1:A:69:LYS:HB2	1:A:252:TYR:HA	1.66	0.76
1:B:228:LEU:HD21	4:B:301:AHL:N1	2.02	0.74
1:C:88:ASN:OD1	1:C:115:ARG:NH2	2.20	0.74
1:A:201:ASN:OD1	1:A:235:GLN:NE2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ASN:ND2	1:C:156:ILE:HB	2.01	0.73
1:B:202:LYS:NZ	6:B:404:HOH:O	2.22	0.71
1:C:74:THR:OG1	1:C:164:ARG:NH2	2.26	0.69
1:B:219:ASN:ND2	5:B:303:CIT:O2	2.26	0.68
4:B:301:AHL:HH11	4:B:301:AHL:HB2	1.57	0.68
1:C:93:HIS:NE2	1:C:245:LYS:NZ	2.40	0.68
1:B:228:LEU:HD21	4:B:301:AHL:HN12	1.58	0.67
1:A:245:LYS:O	1:A:245:LYS:HG3	1.95	0.66
1:D:231:ASP:OD1	6:D:401:HOH:O	2.14	0.66
1:D:91:LYS:NZ	6:D:402:HOH:O	2.30	0.65
1:C:180:LYS:NZ	6:C:402:HOH:O	2.29	0.65
1:D:88:ASN:OD1	1:D:115:ARG:NH2	2.30	0.62
1:B:193:ILE:HA	5:B:303:CIT:H22	1.81	0.61
1:C:245:LYS:HD2	1:C:245:LYS:N	2.17	0.60
1:B:256:ALA:O	6:B:401:HOH:O	2.15	0.60
1:C:196:LEU:HB2	1:C:215:ASN:HD22	1.66	0.59
1:B:262:HIS:O	6:B:402:HOH:O	2.16	0.59
1:D:233:HIS:HB2	1:D:236:SER:OG	2.03	0.58
1:A:247:LEU:HB2	1:A:254:PHE:HZ	1.67	0.58
1:D:245:LYS:NZ	1:D:249:GLU:OE2	2.38	0.57
1:D:169:SER:OG	1:D:190:ASP:OD2	2.23	0.57
1:B:126:HIS:O	1:B:127:SER:OG	2.21	0.56
1:D:179:ASN:O	1:D:183:GLU:HG3	2.06	0.55
1:C:165:PRO:HD3	1:C:188:VAL:HG13	1.88	0.55
1:A:180:LYS:NZ	6:A:402:HOH:O	2.40	0.54
1:C:174:ASN:O	1:C:178:ARG:HG3	2.08	0.54
1:C:178:ARG:O	1:C:182:VAL:HG23	2.08	0.54
1:B:203:MET:HG3	1:B:208:ALA:HB2	1.90	0.53
1:B:197:ASP:OD1	1:B:198:TRP:N	2.41	0.52
1:A:126:HIS:O	1:A:127:SER:HB3	2.08	0.52
1:B:74:THR:HG22	1:B:98:THR:HB	1.91	0.52
1:A:100:PHE:CG	1:A:164:ARG:HB3	2.45	0.52
1:A:229:MET:HE2	1:A:236:SER:OG	2.09	0.52
1:C:192:THR:OG1	1:C:225:GLU:OE1	2.24	0.51
1:D:130:HIS:CE1	1:D:166:PRO:HB3	2.46	0.51
1:D:200:TYR:HB3	1:D:208:ALA:HB1	1.92	0.51
1:B:82:TYR:CZ	1:B:234:PRO:HD3	2.45	0.51
1:D:115:ARG:HG2	1:D:119:GLU:OE2	2.10	0.51
1:A:100:PHE:CD1	1:A:164:ARG:HB3	2.46	0.51
1:D:100:PHE:CG	1:D:164:ARG:HB3	2.46	0.50
1:D:99:PHE:HB3	1:D:101:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:OD2	1:A:230:HIS:HD2	1.95	0.49
1:B:269:HIS:NE2	2:C:301:ACT:H3	2.27	0.49
1:D:203:MET:HG3	1:D:208:ALA:HB2	1.94	0.49
1:B:100:PHE:CG	1:B:164:ARG:HB3	2.47	0.49
1:D:100:PHE:HB3	1:D:126:HIS:HB2	1.95	0.49
1:C:245:LYS:HD2	1:C:245:LYS:H	1.76	0.49
1:C:74:THR:OG1	1:C:227:ILE:O	2.28	0.49
1:A:247:LEU:HB2	1:A:254:PHE:CZ	2.46	0.49
1:C:200:TYR:O	1:C:203:MET:HB2	2.13	0.49
1:D:245:LYS:O	1:D:249:GLU:HG2	2.14	0.48
1:A:208:ALA:O	1:A:212:ILE:HG13	2.13	0.48
1:C:270:ASP:HB3	1:C:273:MET:HE2	1.94	0.48
1:C:208:ALA:O	1:C:212:ILE:HG13	2.14	0.48
1:A:127:SER:OG	1:A:128:MET:N	2.48	0.47
1:C:99:PHE:HB3	1:C:101:LEU:HD21	1.95	0.47
1:D:158:LYS:O	1:D:160:PRO:HD3	2.15	0.46
1:C:82:TYR:CE2	1:C:234:PRO:HD3	2.50	0.46
1:A:82:TYR:CE2	1:A:234:PRO:HD3	2.50	0.46
1:C:217:LEU:O	1:C:250:LYS:NZ	2.47	0.46
1:A:100:PHE:HB3	1:A:126:HIS:HB2	1.98	0.46
1:B:103:GLY:HA3	6:B:408:HOH:O	2.15	0.46
1:B:247:LEU:HB2	1:B:254:PHE:CZ	2.51	0.45
1:A:162:LEU:HD22	1:A:257:TYR:CD2	2.52	0.45
4:B:301:AHB:HH11	4:B:301:AHB:CB	2.26	0.45
1:B:266:ASN:ND2	1:B:270:ASP:H	2.15	0.45
1:C:84:ALA:HB2	1:C:112:LEU:HD21	1.97	0.45
1:A:77:ASP:HA	1:A:102:ILE:HG13	1.98	0.45
1:B:86:LEU:HD13	1:B:240:VAL:HG21	1.97	0.45
1:D:83:THR:HB	1:D:112:LEU:HD13	1.99	0.45
1:B:169:SER:OG	1:B:190:ASP:OD2	2.32	0.44
1:A:174:ASN:O	1:A:178:ARG:HG3	2.17	0.44
1:D:200:TYR:HB2	1:D:212:ILE:HD11	1.99	0.44
1:C:158:LYS:O	1:C:160:PRO:HD3	2.17	0.44
1:D:111:ASP:O	1:D:114:LYS:HE3	2.18	0.44
1:A:77:ASP:O	1:A:105:ASN:ND2	2.50	0.44
1:B:258:HIS:HB3	1:B:260:GLU:OE1	2.18	0.44
1:A:96:LYS:HD2	1:A:120:GLY:O	2.17	0.44
1:B:245:LYS:O	1:B:249:GLU:HG3	2.18	0.44
1:D:100:PHE:CD1	1:D:164:ARG:HB3	2.53	0.43
1:B:100:PHE:CD1	1:B:164:ARG:HB3	2.53	0.43
1:A:192:THR:OG1	1:A:225:GLU:OE1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:OD2	1:A:272:ARG:NH2	2.34	0.43
1:A:217:LEU:O	1:A:250:LYS:NZ	2.45	0.43
1:B:187:LYS:NZ	6:B:413:HOH:O	2.51	0.43
1:B:271:ASN:ND2	1:C:199:ARG:O	2.36	0.43
1:C:201:ASN:OD1	1:C:235:GLN:NE2	2.52	0.43
1:D:206:ASP:N	1:D:206:ASP:OD1	2.52	0.43
1:A:68:ARG:HE	1:A:70:VAL:HG23	1.84	0.43
1:B:247:LEU:HB2	1:B:254:PHE:HZ	1.84	0.43
1:D:112:LEU:HD23	1:D:112:LEU:HA	1.90	0.43
1:A:68:ARG:HH21	1:A:70:VAL:HG21	1.84	0.42
1:D:173:LEU:HD12	1:D:173:LEU:HA	1.68	0.42
1:C:162:LEU:HD22	1:C:257:TYR:CD1	2.54	0.42
1:D:149:GLN:NE2	1:D:160:PRO:O	2.42	0.42
1:D:247:LEU:HB2	1:D:254:PHE:HZ	1.83	0.42
1:C:181:VAL:HG13	1:C:186:PHE:HB2	2.02	0.42
1:D:247:LEU:HB2	1:D:254:PHE:CZ	2.55	0.42
1:B:206:ASP:OD1	1:B:206:ASP:N	2.53	0.42
1:A:270:ASP:HB3	1:A:273:MET:HE2	2.02	0.42
1:B:77:ASP:HA	1:B:102:ILE:HG13	2.02	0.42
1:B:164:ARG:HA	1:B:165:PRO:HD3	1.86	0.42
1:A:162:LEU:HD22	1:A:257:TYR:CE2	2.55	0.42
1:D:125:MET:HE3	1:D:149:GLN:HB2	2.02	0.42
1:B:256:ALA:HA	6:B:416:HOH:O	2.20	0.42
1:A:245:LYS:CD	1:A:248:LYS:HE3	2.50	0.41
1:C:125:MET:HE2	1:C:125:MET:HB2	1.75	0.41
1:A:178:ARG:O	1:A:182:VAL:HG23	2.20	0.41
1:A:245:LYS:HD3	1:A:248:LYS:HE3	2.02	0.41
1:C:115:ARG:O	1:C:119:GLU:HG3	2.21	0.41
1:D:170:MET:HA	1:D:171:PRO:HA	1.84	0.41
1:A:82:TYR:CB	1:A:237:VAL:HG21	2.52	0.40
1:B:142:VAL:HG21	1:B:180:LYS:HB3	2.03	0.40
1:C:181:VAL:HG11	1:C:188:VAL:HG23	2.02	0.40
1:A:82:TYR:HB2	1:A:237:VAL:HG21	2.03	0.40
1:A:155:ILE:HD11	6:A:420:HOH:O	2.21	0.40
1:B:100:PHE:HB3	1:B:126:HIS:HB2	2.04	0.40
1:D:197:ASP:HA	1:D:212:ILE:HD13	2.04	0.40
1:B:231:ASP:OD1	6:B:403:HOH:O	2.22	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	204/247 (83%)	193 (95%)	9 (4%)	2 (1%)	12	13
1	B	204/247 (83%)	194 (95%)	10 (5%)	0	100	100
1	C	204/247 (83%)	193 (95%)	8 (4%)	3 (2%)	8	7
1	D	206/247 (83%)	194 (94%)	12 (6%)	0	100	100
All	All	818/988 (83%)	774 (95%)	39 (5%)	5 (1%)	21	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	127	SER
1	C	190	ASP
1	C	241	PRO
1	C	204	PRO

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	173/208 (83%)	168 (97%)	5 (3%)	37	49
1	B	173/208 (83%)	171 (99%)	2 (1%)	63	74
1	C	172/208 (83%)	171 (99%)	1 (1%)	78	85
1	D	175/208 (84%)	170 (97%)	5 (3%)	37	49
All	All	693/832 (83%)	680 (98%)	13 (2%)	50	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	127	SER
1	A	211	GLN
1	A	245	LYS
1	A	249	GLU
1	B	181	VAL
1	B	266	ASN
1	C	245	LYS
1	D	69	LYS
1	D	91	LYS
1	D	114	LYS
1	D	180	LYS
1	D	236	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	B	93	HIS
1	B	219	ASN
1	B	266	ASN
1	C	117	ASN
1	D	269	HIS

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

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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
2	ACT	D	301	3	3,3,3	0.94	0	3,3,3	1.80	1 (33%)
4	AHL	B	301	3	11,12,12	1.12	2 (18%)	11,14,14	0.51	0
2	ACT	A	301	3	3,3,3	1.07	0	3,3,3	0.96	0
5	CIT	B	303	-	12,12,12	1.06	0	17,17,17	1.50	1 (5%)
2	ACT	C	301	3	3,3,3	0.70	0	3,3,3	1.46	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
4	AHL	B	301	3	-	4/13/13/13	-
5	CIT	B	303	-	-	9/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	AHL	CZ-NH2	2.81	1.42	1.32
4	B	301	AHL	CZ-NH1	-2.18	1.26	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	303	CIT	O6-C6-C3	3.43	119.71	113.14
2	D	301	ACT	OXT-C-O	-2.49	112.78	122.03

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	AHL	NH1-CZ-NE-CD
4	B	301	AHL	NH2-CZ-NE-CD
5	B	303	CIT	O7-C3-C6-O5
5	B	303	CIT	O7-C3-C6-O6
5	B	303	CIT	C4-C3-C6-O5
5	B	303	CIT	C4-C3-C6-O6
5	B	303	CIT	C6-C3-C4-C5
5	B	303	CIT	C2-C3-C4-C5
5	B	303	CIT	O7-C3-C4-C5
4	B	301	AHL	NE-CD-CG-CB
5	B	303	CIT	C2-C3-C6-O5
5	B	303	CIT	C2-C3-C6-O6
4	B	301	AHL	N2-C-CA-N1

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	AHL	4	0
5	B	303	CIT	2	0
2	C	301	ACT	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	206/247 (83%)	0.54	10 (4%) 35 32	37, 58, 93, 140	0
1	B	206/247 (83%)	0.39	3 (1%) 72 73	34, 55, 74, 112	0
1	C	206/247 (83%)	0.57	9 (4%) 39 36	39, 60, 96, 113	0
1	D	206/247 (83%)	0.37	4 (1%) 66 67	32, 54, 72, 104	2 (0%)
All	All	824/988 (83%)	0.47	26 (3%) 50 49	32, 57, 92, 140	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ARG	3.8
1	C	245	LYS	3.4
1	C	261	SER	3.0
1	A	69	LYS	3.0
1	C	197	ASP	2.7
1	B	68	ARG	2.6
1	A	221	THR	2.4
1	C	204	PRO	2.4
1	C	189	TRP	2.4
1	D	258[A]	HIS	2.4
1	C	218	THR	2.4
1	A	215	ASN	2.4
1	A	206	ASP	2.3
1	C	203	MET	2.3
1	A	219	ASN	2.2
1	A	245	LYS	2.2
1	C	82	TYR	2.2
1	B	73	LEU	2.1
1	A	211	GLN	2.1
1	C	221	THR	2.1
1	A	253	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	94	ASP	2.1
1	D	269	HIS	2.1
1	A	201	ASN	2.0
1	B	219	ASN	2.0
1	D	187	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	ACT	D	301	4/4	0.56	0.22	52,54,60,63	0
2	ACT	A	301	4/4	0.71	0.25	50,56,63,65	0
2	ACT	C	301	4/4	0.77	0.17	44,55,59,60	0
4	AHL	B	301	13/13	0.79	0.20	53,65,80,82	0
5	CIT	B	303	13/13	0.81	0.17	74,85,93,96	0
3	ZN	A	302	1/1	0.98	0.04	49,49,49,49	0
3	ZN	C	302	1/1	0.98	0.11	79,79,79,79	0
3	ZN	B	302	1/1	0.99	0.10	79,79,79,79	0
3	ZN	D	302	1/1	0.99	0.06	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.