



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:30 AM UTC

PDB ID : 1B90 / pdb_00001b90
Title : BACILLUS CEREUS BETA-AMYLASE APO FORM
Authors : Mikami, B.; Adachi, M.; Kage, T.; Sarikaya, E.; Nanmori, T.; Shinke, R.;
Utsumi, S.
Deposited on : 1999-03-06
Resolution : 2.50 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

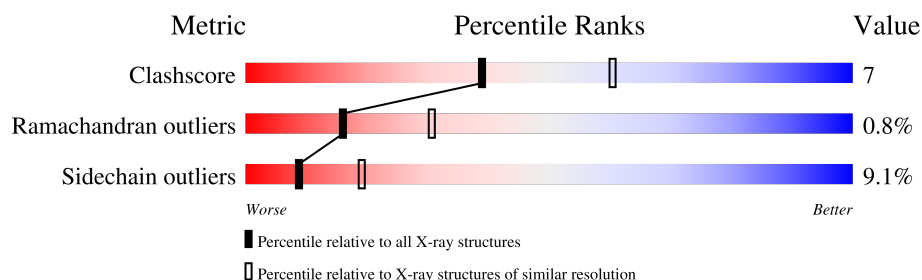
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	516	

2 Entry composition [i](#)

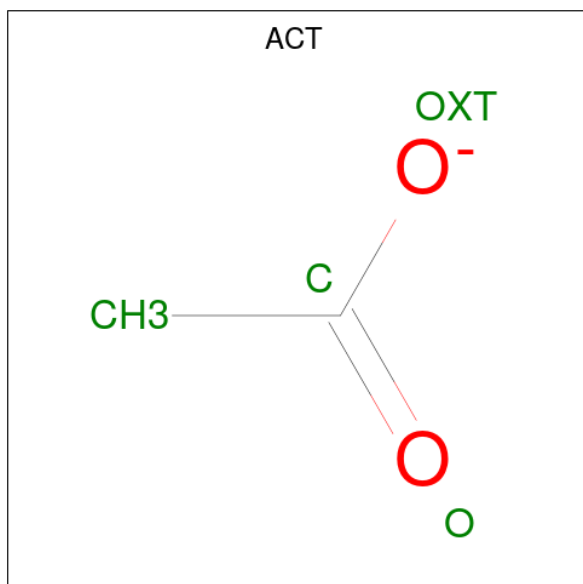
There are 5 unique types of molecules in this entry. The entry contains 4249 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (BETA-AMYLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4119	2645	676	781	17	0	0	0

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



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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

- Molecule 5 is water.

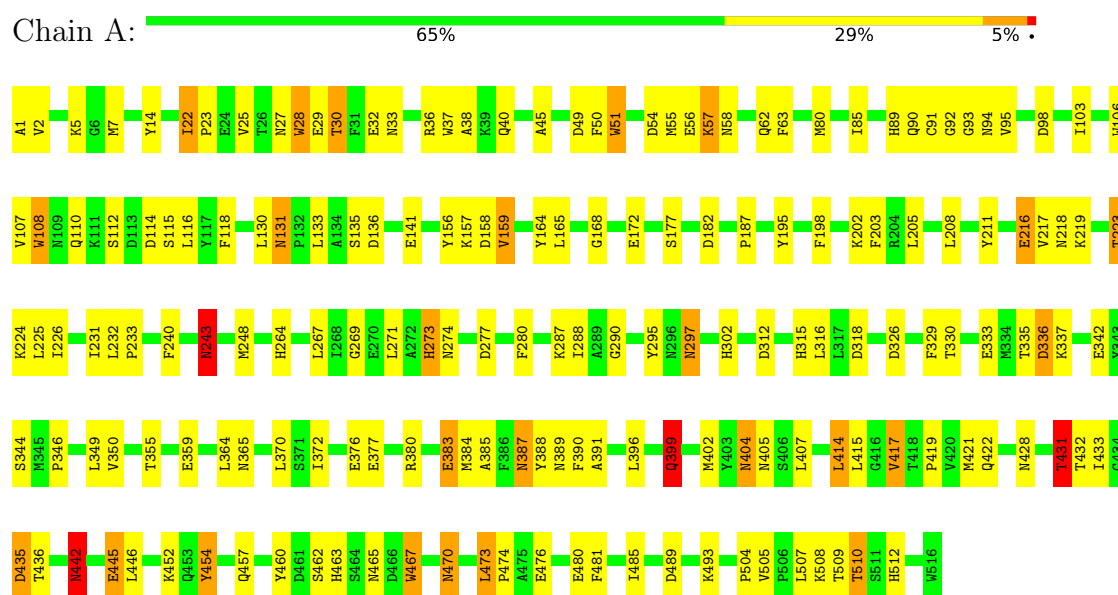
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		

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: PROTEIN (BETA-AMYLASE)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.08 Å 92.10 Å 65.67 Å 90.00° 101.81° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	84.7 (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.164 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4249	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: ACT, CA, SO4

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	1.06	9/4234 (0.2%)	1.84	108/5751 (1.9%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	HIS	CD2-NE2	-7.51	1.29	1.37
1	A	273	HIS	CD2-NE2	-7.11	1.30	1.37
1	A	512	HIS	CD2-NE2	-6.86	1.30	1.37
1	A	302	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	463	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	89	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	315	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	512	HIS	CG-ND1	-5.14	1.32	1.38
1	A	30	THR	CA-CB	5.08	1.61	1.53

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	THR	N-CA-C	13.68	130.91	112.30
1	A	116	LEU	N-CA-C	11.26	124.88	111.82
1	A	57	LYS	N-CA-C	10.78	123.00	111.03
1	A	136	ASP	CA-CB-CG	10.19	122.79	112.60
1	A	505	VAL	N-CA-C	-9.63	100.34	108.63
1	A	414	LEU	N-CA-C	9.51	123.38	111.69
1	A	243	ASN	CA-CB-CG	8.79	121.39	112.60
1	A	389	ASN	N-CA-C	8.22	122.83	111.74
1	A	182	ASP	CA-CB-CG	8.18	120.78	112.60
1	A	476	GLU	CA-CB-CG	7.99	130.07	114.10
1	A	277	ASP	N-CA-C	7.86	119.92	111.36
1	A	274	ASN	CA-CB-CG	7.77	120.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	TYR	N-CA-C	7.41	126.18	109.81
1	A	49	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	329	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	442	ASN	N-CA-C	7.06	120.01	111.82
1	A	330	THR	N-CA-CB	-6.97	99.91	111.49
1	A	58	ASN	N-CA-C	6.57	118.44	111.28
1	A	63	PHE	N-CA-C	6.48	120.85	109.96
1	A	28	TRP	CG-CD2-CE3	6.39	140.29	133.90
1	A	217	VAL	N-CA-C	-6.37	104.44	110.42
1	A	240	PHE	CA-CB-CG	-6.31	107.49	113.80
1	A	28	TRP	N-CA-C	6.30	120.07	112.38
1	A	428	ASN	N-CA-C	6.29	120.09	111.54
1	A	337	LYS	N-CA-C	-6.27	104.59	112.93
1	A	312	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	509	THR	N-CA-C	6.26	118.38	108.67
1	A	168	GLY	CA-C-N	6.18	126.13	119.76
1	A	168	GLY	C-N-CA	6.18	126.13	119.76
1	A	114	ASP	CA-CB-CG	6.18	118.78	112.60
1	A	264	HIS	CB-CG-CD2	-6.15	123.20	131.20
1	A	223	THR	N-CA-CB	-6.13	98.26	109.10
1	A	383	GLU	N-CA-C	6.12	117.95	111.28
1	A	344	SER	N-CA-C	6.12	118.25	108.41
1	A	203	PHE	N-CA-C	-6.04	104.32	111.03
1	A	273	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	25	VAL	N-CA-CB	-6.00	106.72	111.64
1	A	431	THR	N-CA-CB	-5.97	101.59	110.24
1	A	465	ASN	N-CA-C	5.91	119.70	111.90
1	A	231	ILE	N-CA-C	-5.90	99.07	107.98
1	A	106	TRP	CG-CD2-CE3	5.90	139.80	133.90
1	A	94	ASN	N-CA-C	5.89	118.81	109.50
1	A	135	SER	N-CA-C	5.86	119.91	112.87
1	A	399	GLN	N-CA-C	5.86	119.53	112.38
1	A	326	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	318	ASP	N-CA-C	-5.83	105.00	111.36
1	A	364	LEU	CA-C-O	5.83	127.63	120.92
1	A	435	ASP	N-CA-C	5.80	118.03	110.43
1	A	302	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	476	GLU	N-CA-C	5.72	119.13	111.24
1	A	493	LYS	CB-CG-CD	-5.71	98.17	111.30
1	A	280	PHE	N-CA-C	5.69	118.69	111.69
1	A	37	TRP	CE2-CD2-CG	-5.68	100.39	107.20
1	A	232	LEU	N-CA-C	5.68	117.41	108.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASN	CA-C-O	5.67	126.82	120.92
1	A	493	LYS	CB-CA-C	-5.66	101.96	110.90
1	A	94	ASN	O-C-N	5.65	130.19	123.24
1	A	108	TRP	CG-CD2-CE3	5.61	139.51	133.90
1	A	233	PRO	CA-C-N	5.61	125.62	119.90
1	A	233	PRO	C-N-CA	5.61	125.62	119.90
1	A	330	THR	O-C-N	-5.59	114.60	122.26
1	A	54	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	50	PHE	N-CA-C	-5.59	99.41	108.52
1	A	333	GLU	CB-CG-CD	5.57	122.06	112.60
1	A	391	ALA	N-CA-C	-5.53	106.49	113.18
1	A	432	THR	CA-CB-OG1	-5.53	101.30	109.60
1	A	315	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	A	141	GLU	N-CA-C	5.46	117.23	111.28
1	A	177	SER	N-CA-C	5.45	119.99	113.23
1	A	55	MET	N-CA-C	5.45	119.78	113.18
1	A	158	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	28	TRP	CB-CG-CD1	-5.44	118.74	126.90
1	A	22	ILE	CA-C-O	-5.43	114.58	118.71
1	A	62	GLN	N-CA-C	-5.43	97.96	107.73
1	A	387	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	106	TRP	CB-CG-CD1	-5.40	118.81	126.90
1	A	56	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	118	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	417	VAL	N-CA-CB	-5.35	100.04	111.37
1	A	195	TYR	N-CA-C	5.31	119.07	112.59
1	A	28	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	A	473	LEU	N-CA-C	5.27	118.26	109.09
1	A	131	ASN	CA-C-N	5.26	126.42	119.84
1	A	131	ASN	C-N-CA	5.26	126.42	119.84
1	A	226	ILE	CB-CA-C	-5.26	105.00	111.94
1	A	481	PHE	CA-CB-CG	5.25	119.06	113.80
1	A	106	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	A	396	LEU	O-C-N	-5.24	116.53	123.13
1	A	389	ASN	N-CA-CB	-5.23	104.24	112.13
1	A	467	TRP	O-C-N	-5.22	117.37	123.27
1	A	273	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	454	TYR	O-C-N	-5.21	115.33	121.32
1	A	89	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	457	GLN	N-CA-C	5.18	118.26	109.76
1	A	297	ASN	CA-C-N	5.17	124.78	119.05
1	A	297	ASN	C-N-CA	5.17	124.78	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	LEU	N-CA-C	5.13	118.58	109.96
1	A	108	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	51	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	326	ASP	N-CA-C	-5.08	103.69	110.55
1	A	405	ASN	N-CA-C	5.08	117.71	111.82
1	A	433	ILE	N-CA-CB	-5.07	103.35	110.05
1	A	115	SER	CA-C-N	5.06	128.00	120.31
1	A	115	SER	C-N-CA	5.06	128.00	120.31
1	A	98	ASP	N-CA-C	5.04	121.55	110.80
1	A	108	TRP	CB-CG-CD1	-5.04	119.34	126.90
1	A	290	GLY	N-CA-C	-5.01	101.30	113.18
1	A	336	ASP	CA-CB-CG	5.00	117.60	112.60

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	4119	0	3984	55	0
2	A	4	0	3	0	0
3	A	5	0	0	0	0
4	A	1	0	0	0	0
5	A	120	0	0	1	0
All	All	4249	0	3987	55	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 7.

All (55) 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:365:ASN:HB3	5:A:619:HOH:O	1.85	0.75
1:A:103:ILE:HD11	1:A:108:TRP:CZ2	2.24	0.72
1:A:1:ALA:HA	1:A:387:ASN:HD22	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLN:HE22	1:A:510:THR:H	1.40	0.70
1:A:198:PHE:O	1:A:202:LYS:HG2	1.92	0.68
1:A:218:ASN:OD1	1:A:223:THR:HG23	1.99	0.63
1:A:372:ILE:HG23	1:A:377:GLU:HB2	1.83	0.61
1:A:28:TRP:O	1:A:32:GLU:HG3	2.02	0.60
1:A:51:TRP:CZ2	1:A:91:CYS:SG	2.96	0.59
1:A:14:TYR:HD1	1:A:45:ALA:HB3	1.67	0.59
1:A:399:GLN:HE21	1:A:399:GLN:H	1.51	0.59
1:A:156:TYR:O	1:A:159:VAL:HG12	2.03	0.59
1:A:446:LEU:HD21	1:A:473:LEU:HD21	1.86	0.58
1:A:431:THR:HG21	1:A:467:TRP:HE1	1.67	0.58
1:A:295:TYR:HE2	1:A:349:LEU:HD13	1.68	0.57
1:A:172:GLU:HG2	1:A:287:LYS:HD2	1.87	0.55
1:A:90:GLN:HE21	1:A:93:GLY:HA3	1.71	0.55
1:A:27:ASN:ND2	1:A:29:GLU:HB3	2.22	0.55
1:A:27:ASN:HD22	1:A:29:GLU:H	1.56	0.54
1:A:33:ASN:HD22	1:A:36:ARG:HE	1.57	0.54
1:A:269:GLY:O	1:A:273:HIS:HD2	1.90	0.54
1:A:218:ASN:HA	1:A:223:THR:HG22	1.89	0.53
1:A:445:GLU:HG3	1:A:474:PRO:HD3	1.90	0.53
1:A:404:ASN:ND2	1:A:407:LEU:H	2.07	0.52
1:A:336:ASP:HA	1:A:346:PRO:HD2	1.92	0.52
1:A:399:GLN:H	1:A:399:GLN:NE2	2.07	0.51
1:A:442:ASN:ND2	1:A:480:GLU:H	2.08	0.51
1:A:355:THR:O	1:A:359:GLU:HG3	2.11	0.51
1:A:460:TYR:CE2	1:A:462:SER:HA	2.46	0.50
1:A:211:TYR:HB3	1:A:216:GLU:HB3	1.92	0.50
1:A:33:ASN:ND2	1:A:36:ARG:HH21	2.11	0.49
1:A:422:GLN:NE2	1:A:510:THR:H	2.07	0.49
1:A:90:GLN:NE2	1:A:93:GLY:HA3	2.28	0.48
1:A:7:MET:HE2	1:A:419:PRO:HB3	1.95	0.48
1:A:445:GLU:HG3	1:A:474:PRO:CD	2.44	0.47
1:A:335:THR:HG23	1:A:380:ARG:HD3	1.96	0.47
1:A:385:ALA:HA	1:A:390:PHE:CD1	2.50	0.47
1:A:383:GLU:O	1:A:387:ASN:HB2	2.17	0.45
1:A:107:VAL:O	1:A:110:GLN:HG2	2.17	0.45
1:A:267:LEU:O	1:A:271:LEU:HG	2.17	0.45
1:A:422:GLN:HB2	1:A:473:LEU:HD12	1.99	0.45
1:A:421:MET:HE2	1:A:421:MET:HB3	1.87	0.45
1:A:85:ILE:HG12	1:A:164:TYR:HB2	1.99	0.44
1:A:435:ASP:HB3	1:A:485:ILE:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLU:HG3	1:A:474:PRO:HG3	1.99	0.44
1:A:14:TYR:CD1	1:A:45:ALA:HB3	2.50	0.44
1:A:1:ALA:HB3	1:A:5:LYS:O	2.19	0.43
1:A:346:PRO:O	1:A:350:VAL:HG23	2.20	0.42
1:A:404:ASN:HD22	1:A:407:LEU:H	1.68	0.42
1:A:131:ASN:OD1	1:A:133:LEU:HB2	2.20	0.42
1:A:287:LYS:HG2	1:A:288:ILE:N	2.35	0.42
1:A:218:ASN:HA	1:A:223:THR:CG2	2.50	0.41
1:A:22:ILE:HB	1:A:23:PRO:HD3	2.03	0.41
1:A:38:ALA:HB2	1:A:402:MET:HE1	2.03	0.41
1:A:384:MET:O	1:A:388:TYR:HB2	2.21	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	514/516 (100%)	478 (93%)	32 (6%)	4 (1%)	16 31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	VAL
1	A	243	ASN
1	A	454	TYR
1	A	92	GLY

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	440/440 (100%)	400 (91%)	40 (9%)	9 19

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	30	THR
1	A	40	GLN
1	A	57	LYS
1	A	80	MET
1	A	112	SER
1	A	130	LEU
1	A	157	LYS
1	A	159	VAL
1	A	165	LEU
1	A	187	PRO
1	A	205	LEU
1	A	208	LEU
1	A	216	GLU
1	A	219	LYS
1	A	224	LYS
1	A	225	LEU
1	A	243	ASN
1	A	248	MET
1	A	297	ASN
1	A	316	LEU
1	A	342	GLU
1	A	370	LEU
1	A	376	GLU
1	A	399	GLN
1	A	404	ASN
1	A	414	LEU
1	A	415	LEU
1	A	417	VAL
1	A	431	THR
1	A	436	THR
1	A	442	ASN
1	A	445	GLU
1	A	452	LYS

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Mol	Chain	Res	Type
1	A	470	ASN
1	A	489	ASP
1	A	504	PRO
1	A	507	LEU
1	A	508	LYS
1	A	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	33	ASN
1	A	41	ASN
1	A	73	GLN
1	A	90	GLN
1	A	273	HIS
1	A	292	HIS
1	A	297	ASN
1	A	352	ASN
1	A	387	ASN
1	A	399	GLN
1	A	404	ASN
1	A	422	GLN
1	A	442	ASN
1	A	463	HIS
1	A	470	ASN
1	A	496	GLN
1	A	512	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 [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	A	920	-	3,3,3	1.08	0	3,3,3	0.94	0
3	SO4	A	921	-	4,4,4	0.26	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.