Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 07:11 AM EST

PDB ID	:	4ENL
Title	:	CRYSTAL STRUCTURE OF HOLOENZYME REFINED AT 1.9 ANGSTROMS RESOLUTION: TRIGONAL-BIPYRAMIDAL GEOMETRY OF THE CATION BINDING SITE
Authors	:	Lebioda, L.; Stec, B.
Deposited on	:	1990-11-13
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

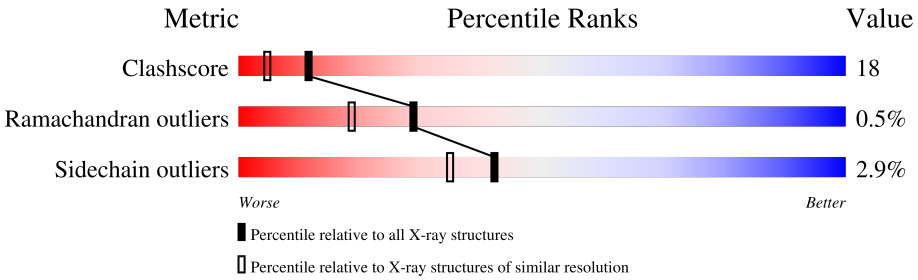
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	69% 25% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3643 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 ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3289	2076	569	638	6	0	0	0

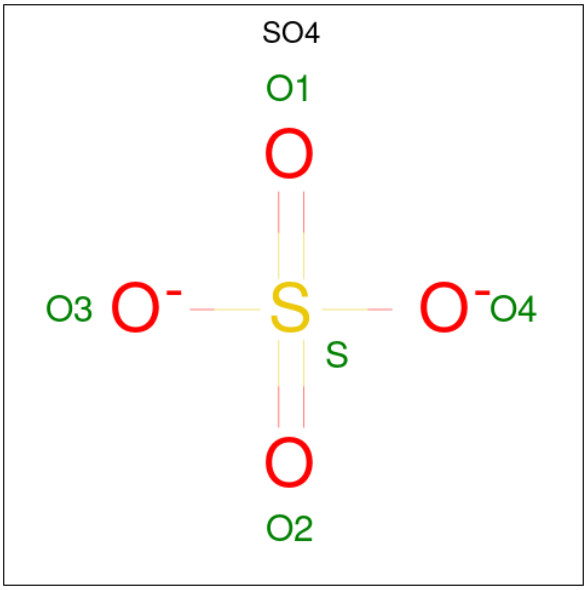
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	SER	LYS	conflict	UNP P00924

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	348	Total O 348 348	0	0

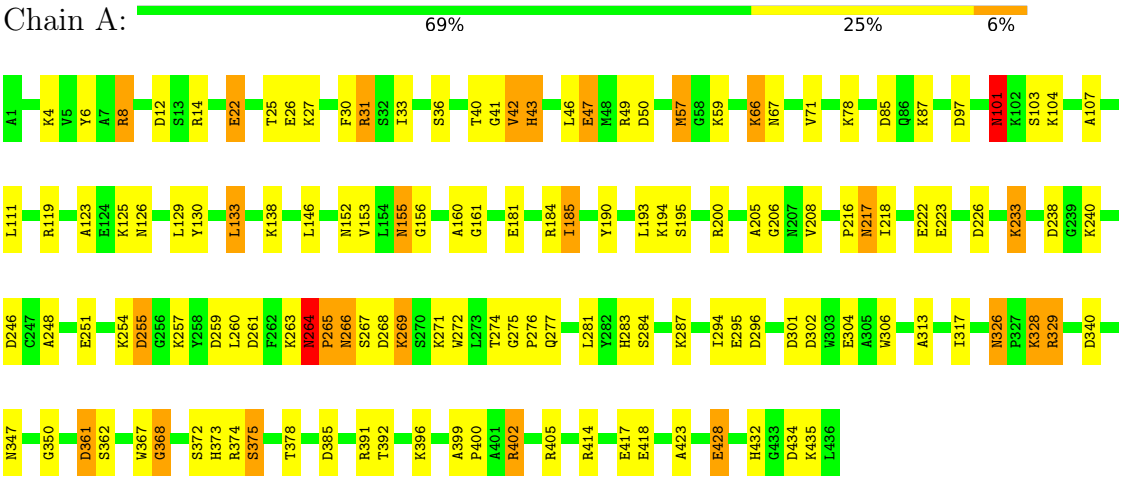
3 Residue-property plots (i)

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. 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: ENOLASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	124.10Å 124.10Å 66.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3643	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: SO4, 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	0.97	1/3349 (0.0%)	1.88	80/4531 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	SER	CB-OG	5.18	1.49	1.42

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184	ARG	CD-NE-CZ	32.70	169.38	123.60
1	A	14	ARG	NE-CZ-NH2	-15.62	112.49	120.30
1	A	8	ARG	NE-CZ-NH1	14.69	127.64	120.30
1	A	14	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	A	49	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	A	184	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	119	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	A	329	ARG	NE-CZ-NH2	9.87	125.23	120.30
1	A	181	GLU	OE1-CD-OE2	-8.40	113.22	123.30
1	A	22	GLU	OE1-CD-OE2	8.31	133.27	123.30
1	A	263	LYS	C-N-CA	8.19	142.18	121.70
1	A	414	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	340	ASP	CB-CG-OD1	8.01	125.51	118.30
1	A	402	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	119	ARG	NH1-CZ-NH2	7.87	128.06	119.40
1	A	414	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	36	SER	CB-CA-C	7.62	124.58	110.10
1	A	85	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	31	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	269	LYS	N-CA-CB	7.43	123.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	GLU	OE1-CD-OE2	7.42	132.20	123.30
1	A	329	ARG	CG-CD-NE	7.35	127.23	111.80
1	A	264	ASN	CA-CB-CG	-7.27	97.41	113.40
1	A	217	ASN	CB-CA-C	7.19	124.78	110.40
1	A	119	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	A	226	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	374	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	222	GLU	OE1-CD-OE2	-6.73	115.23	123.30
1	A	434	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	350	GLY	CA-C-O	-6.59	108.75	120.60
1	A	184	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	A	31	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	130	TYR	CB-CG-CD1	-6.16	117.31	121.00
1	A	66	LYS	CA-CB-CG	-6.15	99.86	113.40
1	A	374	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	251	GLU	OE1-CD-OE2	6.10	130.62	123.30
1	A	329	ARG	CD-NE-CZ	6.09	132.12	123.60
1	A	42	VAL	CB-CA-C	5.87	122.56	111.40
1	A	119	ARG	CD-NE-CZ	-5.82	115.45	123.60
1	A	195	SER	N-CA-CB	5.82	119.23	110.50
1	A	372	SER	N-CA-CB	-5.81	101.79	110.50
1	A	200	ARG	CD-NE-CZ	5.80	131.72	123.60
1	A	195	SER	CB-CA-C	-5.77	99.14	110.10
1	A	391	ARG	CD-NE-CZ	-5.74	115.57	123.60
1	A	43	HIS	N-CA-CB	5.71	120.88	110.60
1	A	8	ARG	CD-NE-CZ	5.70	131.58	123.60
1	A	87	LYS	N-CA-CB	5.66	120.78	110.60
1	A	251	GLU	CG-CD-OE1	-5.62	107.05	118.30
1	A	385	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	A	40	THR	C-N-CA	-5.60	110.53	122.30
1	A	233	LYS	CB-CG-CD	5.59	126.13	111.60
1	A	6	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	A	12	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	42	VAL	C-N-CA	5.48	135.39	121.70
1	A	417	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	A	361	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	A	190	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	296	ASP	CB-CG-OD2	5.38	123.15	118.30
1	A	328	LYS	CB-CG-CD	5.37	125.55	111.60
1	A	375	SER	CB-CA-C	-5.33	99.97	110.10
1	A	49	ARG	NH1-CZ-NH2	5.33	125.26	119.40
1	A	283	HIS	CA-CB-CG	-5.32	104.56	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	418	GLU	CA-CB-CG	5.26	124.98	113.40
1	A	405	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	161	GLY	N-CA-C	-5.25	99.97	113.10
1	A	200	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	368	GLY	N-CA-C	-5.24	100.01	113.10
1	A	428	GLU	CB-CG-CD	5.21	128.28	114.20
1	A	101	ASN	O-C-N	5.21	131.03	122.70
1	A	12	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	8	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	A	155	ASN	CB-CG-OD1	-5.17	111.27	121.60
1	A	50	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	A	185	ILE	CB-CG1-CD1	-5.13	99.53	113.90
1	A	375	SER	N-CA-CB	-5.09	102.86	110.50
1	A	264	ASN	N-CA-CB	5.09	119.77	110.60
1	A	85	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	248	ALA	N-CA-CB	5.03	117.14	110.10
1	A	25	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	284	SER	N-CA-CB	-5.01	102.99	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3289	0	3293	116	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	348	0	0	51	0
All	All	3643	0	3293	116	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 18.

All (116) 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:138:LYS:HE3	4:A:776:HOH:O	1.50	1.11
1:A:264:ASN:ND2	1:A:267:SER:HA	1.65	1.10
1:A:42:VAL:HG22	4:A:529:HOH:O	1.55	1.04
1:A:59:LYS:HE3	4:A:472:HOH:O	1.60	1.02
1:A:435:LYS:HE3	4:A:698:HOH:O	1.60	1.01
1:A:217:ASN:HB3	4:A:621:HOH:O	1.63	0.99
1:A:269:LYS:O	1:A:269:LYS:HG2	1.61	0.98
1:A:78:LYS:HE3	4:A:677:HOH:O	1.64	0.96
1:A:160:ALA:HB3	4:A:763:HOH:O	1.64	0.96
1:A:152:ASN:HB2	4:A:758:HOH:O	1.67	0.94
1:A:326:ASN:HD21	1:A:328:LYS:HG2	1.30	0.94
1:A:326:ASN:ND2	1:A:328:LYS:HG2	1.80	0.94
1:A:268:ASP:HB3	1:A:271:LYS:HD2	1.47	0.94
1:A:42:VAL:CG2	4:A:529:HOH:O	2.13	0.91
1:A:264:ASN:HD22	1:A:267:SER:HA	1.30	0.88
1:A:41:GLY:O	4:A:650:HOH:O	1.92	0.87
1:A:261:ASP:OD2	1:A:264:ASN:ND2	2.07	0.87
1:A:264:ASN:HB2	1:A:267:SER:HB2	1.54	0.87
1:A:205:ALA:O	4:A:513:HOH:O	1.93	0.86
1:A:287:LYS:HE2	4:A:752:HOH:O	1.76	0.85
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.07	0.84
1:A:41:GLY:CA	1:A:46:LEU:HD21	2.10	0.81
1:A:432:HIS:HD2	4:A:675:HOH:O	1.64	0.81
1:A:269:LYS:O	1:A:269:LYS:CG	2.29	0.80
1:A:208:VAL:HG11	4:A:781:HOH:O	1.83	0.79
1:A:42:VAL:HG13	4:A:529:HOH:O	1.85	0.77
1:A:42:VAL:CG1	4:A:529:HOH:O	2.34	0.76
1:A:432:HIS:CD2	4:A:675:HOH:O	2.40	0.73
1:A:257:LYS:HE3	1:A:269:LYS:HE2	1.71	0.72
1:A:78:LYS:HG3	4:A:677:HOH:O	1.89	0.72
1:A:41:GLY:N	1:A:46:LEU:HD21	2.04	0.71
1:A:326:ASN:C	1:A:326:ASN:HD22	1.94	0.70
1:A:194:LYS:HE3	1:A:206:GLY:O	1.92	0.70
1:A:66:LYS:CE	4:A:574:HOH:O	2.39	0.69
1:A:156:GLY:HA2	4:A:763:HOH:O	1.92	0.69
1:A:57:MET:SD	4:A:696:HOH:O	2.50	0.69
1:A:361:ASP:OD1	4:A:739:HOH:O	2.10	0.69
1:A:66:LYS:HG3	4:A:574:HOH:O	1.94	0.67
1:A:264:ASN:OD1	1:A:264:ASN:C	2.34	0.66
1:A:233:LYS:HE2	1:A:238:ASP:OD2	1.95	0.66
1:A:368:GLY:HA2	4:A:675:HOH:O	1.95	0.64
1:A:41:GLY:HA3	1:A:46:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:ND2	1:A:267:SER:CA	2.53	0.64
1:A:255:ASP:HB3	4:A:712:HOH:O	1.98	0.62
1:A:208:VAL:HG21	4:A:781:HOH:O	1.99	0.62
1:A:328:LYS:HG3	1:A:329:ARG:N	2.15	0.60
1:A:43:HIS:N	4:A:731:HOH:O	2.21	0.60
1:A:428:GLU:OE1	4:A:629:HOH:O	2.17	0.60
1:A:57:MET:CG	4:A:696:HOH:O	2.50	0.59
1:A:126:ASN:ND2	4:A:668:HOH:O	2.34	0.59
1:A:47:GLU:OE1	4:A:612:HOH:O	2.17	0.58
1:A:41:GLY:N	1:A:46:LEU:CD2	2.66	0.58
1:A:26:GLU:HG2	1:A:27:LYS:HG2	1.86	0.58
1:A:152:ASN:HD21	1:A:155:ASN:ND2	2.03	0.57
1:A:42:VAL:HG22	4:A:731:HOH:O	2.02	0.57
1:A:313:ALA:HB3	1:A:317:ILE:HD11	1.87	0.57
1:A:264:ASN:HD22	1:A:267:SER:CA	2.11	0.56
1:A:257:LYS:HG3	4:A:618:HOH:O	2.04	0.56
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.90	0.53
1:A:31:ARG:NH1	4:A:487:HOH:O	2.41	0.53
1:A:138:LYS:HG3	4:A:776:HOH:O	2.08	0.53
1:A:97:ASP:OD1	1:A:104:LYS:HB3	2.09	0.53
1:A:264:ASN:OD1	1:A:264:ASN:O	2.26	0.52
1:A:264:ASN:CB	1:A:267:SER:HB2	2.35	0.52
1:A:269:LYS:NZ	4:A:712:HOH:O	2.38	0.51
1:A:260:LEU:HD11	1:A:281:LEU:HD23	1.93	0.51
1:A:268:ASP:CB	1:A:271:LYS:HD2	2.33	0.50
1:A:125:LYS:O	1:A:126:ASN:HB2	2.12	0.49
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.93	0.49
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.94	0.49
1:A:217:ASN:OD1	4:A:448:HOH:O	2.19	0.48
1:A:111:LEU:HD22	1:A:347:ASN:HA	1.95	0.48
1:A:261:ASP:O	1:A:264:ASN:HB2	2.14	0.48
1:A:41:GLY:HA3	1:A:46:LEU:CD2	2.43	0.48
1:A:125:LYS:O	1:A:126:ASN:CB	2.61	0.48
1:A:264:ASN:HB3	1:A:267:SER:N	2.29	0.47
1:A:275:GLY:N	1:A:276:PRO:CD	2.76	0.47
1:A:216:PRO:C	1:A:217:ASN:HD22	2.18	0.47
1:A:66:LYS:CB	4:A:505:HOH:O	2.62	0.47
1:A:362:SER:O	1:A:367:TRP:HB2	2.15	0.47
1:A:138:LYS:HE3	4:A:777:HOH:O	2.14	0.47
1:A:399:ALA:HB1	1:A:400:PRO:HD2	1.97	0.46
1:A:26:GLU:HG2	1:A:27:LYS:N	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:ASP:OD1	4:A:511:HOH:O	2.21	0.46
1:A:264:ASN:CB	1:A:267:SER:N	2.78	0.46
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.97	0.46
1:A:129:LEU:HG	1:A:133:LEU:HD22	1.97	0.46
1:A:264:ASN:HB3	1:A:266:ASN:N	2.30	0.46
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.67	0.45
1:A:66:LYS:HB2	4:A:505:HOH:O	2.17	0.45
1:A:78:LYS:CE	4:A:677:HOH:O	2.43	0.45
1:A:255:ASP:HB3	1:A:269:LYS:HZ1	1.81	0.45
1:A:240:LYS:NZ	4:A:784:HOH:O	2.43	0.45
1:A:255:ASP:CB	1:A:269:LYS:NZ	2.80	0.45
1:A:4:LYS:HE3	4:A:770:HOH:O	2.16	0.44
1:A:26:GLU:HG2	1:A:27:LYS:CG	2.46	0.44
1:A:216:PRO:HG2	1:A:218:ILE:CD1	2.48	0.44
1:A:269:LYS:HA	1:A:272:TRP:CD1	2.53	0.44
1:A:30:PHE:CE1	1:A:123:ALA:HB2	2.53	0.44
1:A:4:LYS:HD2	4:A:769:HOH:O	2.17	0.44
1:A:264:ASN:HB3	1:A:265:PRO:CA	2.48	0.43
1:A:254:LYS:NZ	1:A:259:ASP:OD2	2.39	0.43
1:A:101:ASN:ND2	1:A:103:SER:OG	2.46	0.43
1:A:8:ARG:HH12	1:A:22:GLU:CD	2.23	0.43
1:A:67:ASN:O	1:A:71:VAL:HB	2.20	0.42
1:A:294:ILE:HD13	1:A:294:ILE:HG21	1.70	0.42
1:A:396:LYS:HE2	4:A:528:HOH:O	2.20	0.42
1:A:302:ASP:O	1:A:306:TRP:HD1	2.03	0.42
1:A:66:LYS:HB3	4:A:505:HOH:O	2.20	0.41
1:A:107:ALA:HB1	4:A:759:HOH:O	2.20	0.41
1:A:46:LEU:HD11	4:A:568:HOH:O	2.20	0.41
1:A:42:VAL:HA	4:A:731:HOH:O	2.20	0.41
1:A:274:THR:OG1	1:A:277:GLN:HG3	2.21	0.41
1:A:218:ILE:HG23	1:A:223:GLU:HB3	2.02	0.40
1:A:304:GLU:HG2	4:A:478:HOH:O	2.22	0.40
1:A:326:ASN:ND2	1:A:326:ASN:C	2.69	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	434/436 (100%)	418 (96%)	14 (3%)	2 (0%)	29 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	402	ARG

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	344/344 (100%)	334 (97%)	10 (3%)	42 35

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	MET
1	A	101	ASN
1	A	133	LEU
1	A	255	ASP
1	A	265	PRO
1	A	266	ASN
1	A	326	ASN
1	A	373	HIS
1	A	375	SER

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Mol	Chain	Res	Type
1	A	392	THR

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	101	ASN
1	A	155	ASN
1	A	207	ASN
1	A	217	ASN
1	A	326	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	SO4	A	444	-	4,4,4	0.70	0	6,6,6	0.32	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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.