



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:59 PM UTC

PDB ID : 4ENL / pdb_00004enl
Title : CRYSTAL STRUCTURE OF HOLOENZYME REFINED AT 1.9
ANGSTROMS RESOLUTION: TRIGONAL-BIPYRAMIDAL GEOME-
TRY 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	:	4-5-2 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

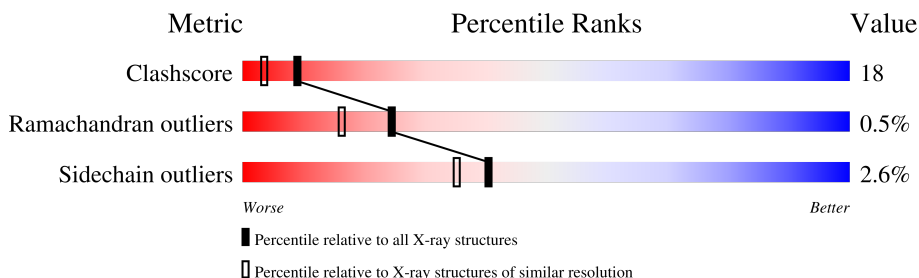
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	

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
1	A	436	Total	C	N	O	S	0	0	0
			3289	2076	569	638	6			

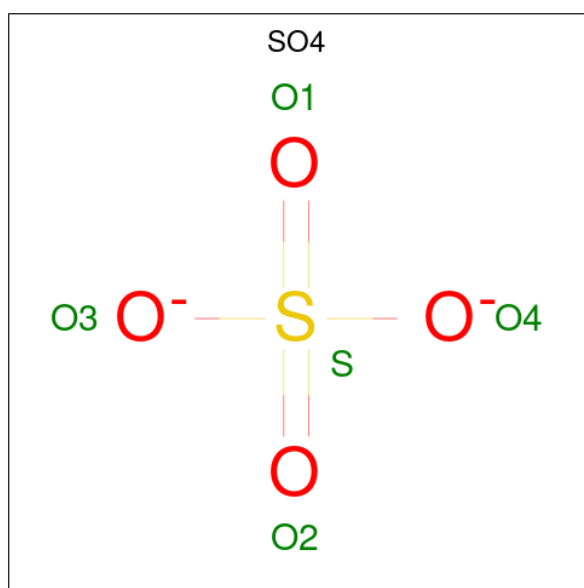
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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 water.

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

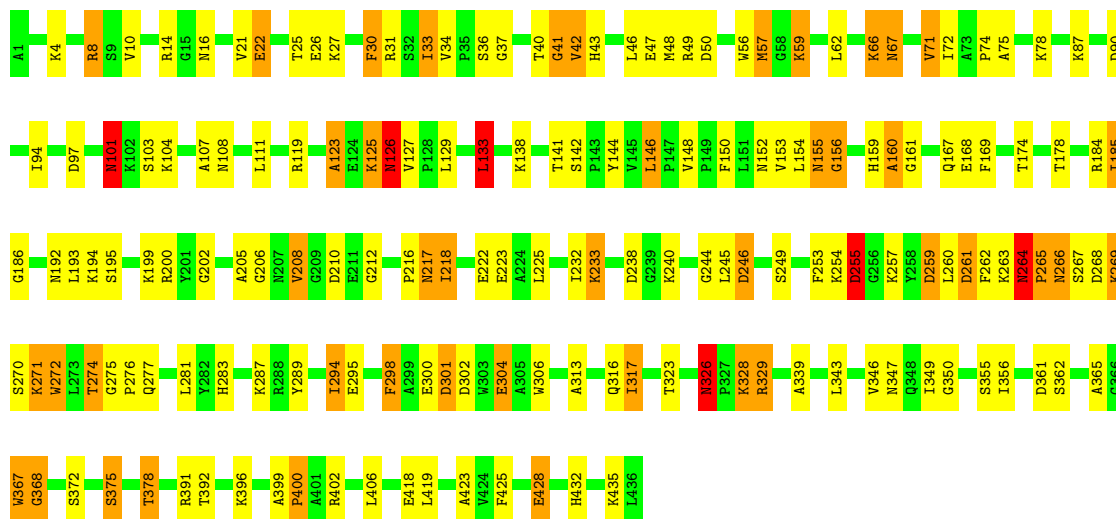
3 Residue-property plots

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: ENOLASE

Chain A: 



4 Data and refinement statistics

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: ZN, 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	1.22	2/3349 (0.1%)	2.32	164/4531 (3.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	GLY	N-CA	5.24	1.49	1.44
1	A	244	GLY	N-CA	5.09	1.50	1.45

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ARG	CD-NE-CZ	32.13	169.38	124.40
1	A	264	ASN	CA-CB-CG	-15.20	97.41	112.60
1	A	148	VAL	N-CA-C	-11.33	98.89	108.63
1	A	301	ASP	CA-CB-CG	-10.17	102.43	112.60
1	A	350	GLY	CA-C-O	-9.84	108.75	119.27
1	A	126	ASN	OD1-CG-ND2	9.55	132.15	122.60
1	A	283	HIS	CA-CB-CG	-9.24	104.56	113.80
1	A	428	GLU	CB-CG-CD	9.22	128.28	112.60
1	A	126	ASN	CA-CB-CG	-9.07	103.53	112.60
1	A	10	VAL	CA-C-O	-9.03	111.15	121.44
1	A	108	ASN	CA-CB-CG	8.79	121.39	112.60
1	A	263	LYS	CA-C-N	8.35	142.18	121.80
1	A	263	LYS	C-N-CA	8.35	142.18	121.80
1	A	323	THR	N-CA-C	8.33	123.75	113.50
1	A	161	GLY	N-CA-C	-8.29	99.97	112.41
1	A	42	VAL	CB-CA-C	8.28	122.56	111.21
1	A	36	SER	CB-CA-C	8.22	124.58	109.46
1	A	425	PHE	CA-C-O	-8.17	111.31	120.54
1	A	368	GLY	N-CA-C	-8.15	100.01	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	N-CA-C	8.12	122.47	112.23
1	A	50	ASP	CA-CB-CG	-8.01	104.59	112.60
1	A	202	GLY	CA-C-O	8.01	127.42	122.22
1	A	161	GLY	CA-C-O	-7.98	114.30	122.28
1	A	217	ASN	CB-CA-C	7.93	124.78	111.30
1	A	269	LYS	N-CA-CB	7.76	123.98	110.39
1	A	155	ASN	CA-C-O	-7.71	112.40	121.11
1	A	34	VAL	N-CA-CB	-7.64	100.52	111.21
1	A	255	ASP	CA-C-O	-7.62	112.71	121.54
1	A	266	ASN	N-CA-C	-7.55	101.38	110.44
1	A	217	ASN	CA-CB-CG	-7.51	105.09	112.60
1	A	266	ASN	CA-CB-CG	7.50	120.10	112.60
1	A	356	ILE	CA-C-O	-7.50	112.91	120.85
1	A	127	VAL	O-C-N	7.49	126.96	121.72
1	A	195	SER	CB-CA-C	-7.48	99.14	110.88
1	A	14	ARG	NE-CZ-NH2	-7.46	112.49	119.20
1	A	406	LEU	CA-C-O	-7.27	111.89	120.10
1	A	87	LYS	N-CA-CB	7.25	120.78	110.12
1	A	66	LYS	CA-CB-CG	-7.12	99.86	114.10
1	A	94	ILE	N-CA-CB	-7.08	102.26	110.55
1	A	218	ILE	O-C-N	7.02	130.30	123.14
1	A	329	ARG	CG-CD-NE	6.92	127.23	112.00
1	A	185	ILE	CB-CG1-CD1	-6.79	99.53	113.80
1	A	101	ASN	O-C-N	6.78	131.03	122.22
1	A	375	SER	CB-CA-C	-6.78	99.97	110.81
1	A	119	ARG	NH1-CZ-NH2	6.74	128.06	119.30
1	A	329	ARG	NE-CZ-NH2	6.71	125.23	119.20
1	A	123	ALA	CA-C-N	6.70	129.15	120.44
1	A	123	ALA	C-N-CA	6.70	129.15	120.44
1	A	160	ALA	CA-C-O	-6.64	114.13	121.23
1	A	167	GLN	N-CA-C	6.57	119.77	111.69
1	A	167	GLN	CA-C-O	-6.54	112.98	120.24
1	A	71	VAL	O-C-N	6.47	126.77	121.85
1	A	233	LYS	CB-CG-CD	6.45	126.13	111.30
1	A	160	ALA	O-C-N	6.41	130.27	123.42
1	A	289	TYR	O-C-N	6.40	127.78	121.57
1	A	119	ARG	CD-NE-CZ	-6.40	115.45	124.40
1	A	141	THR	CA-CB-OG1	-6.37	100.05	109.60
1	A	195	SER	N-CA-CB	6.36	119.23	110.01
1	A	155	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	A	146	LEU	CB-CA-C	6.35	117.82	108.87
1	A	40	THR	N-CA-C	-6.33	98.10	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	LYS	O-C-N	6.32	128.82	122.12
1	A	119	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	A	391	ARG	CD-NE-CZ	-6.31	115.57	124.40
1	A	37	GLY	CA-C-O	-6.29	116.05	121.78
1	A	328	LYS	CB-CG-CD	6.20	125.55	111.30
1	A	192	ASN	CA-CB-CG	-6.17	106.43	112.60
1	A	8	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	A	169	PHE	CA-C-O	-6.11	113.76	120.36
1	A	316	GLN	OE1-CD-NE2	6.11	128.71	122.60
1	A	159	HIS	CA-CB-CG	-6.11	107.69	113.80
1	A	87	LYS	CA-C-O	-6.11	114.08	120.55
1	A	133	LEU	CA-C-N	6.07	128.33	120.44
1	A	133	LEU	C-N-CA	6.07	128.33	120.44
1	A	266	ASN	O-C-N	6.04	129.86	121.83
1	A	50	ASP	CA-C-O	-6.03	114.16	120.55
1	A	210	ASP	CA-C-O	-6.01	113.31	120.10
1	A	71	VAL	CA-C-O	-6.00	115.60	120.70
1	A	199	LYS	CA-C-O	-5.99	114.53	120.82
1	A	150	PHE	CA-CB-CG	-5.98	107.82	113.80
1	A	41	GLY	CA-C-N	-5.98	112.94	122.50
1	A	41	GLY	C-N-CA	-5.98	112.94	122.50
1	A	244	GLY	CA-C-O	-5.97	116.28	120.94
1	A	72	ILE	N-CA-C	5.96	116.14	110.42
1	A	30	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	355	SER	CA-CB-OG	-5.91	99.29	111.10
1	A	419	LEU	CA-C-O	-5.91	111.98	119.31
1	A	349	ILE	CB-CA-C	5.89	116.24	111.06
1	A	343	LEU	N-CA-C	-5.77	100.42	109.25
1	A	42	VAL	N-CA-C	-5.77	100.11	108.87
1	A	232	ILE	O-C-N	5.76	127.56	121.91
1	A	208	VAL	N-CA-C	5.75	117.62	108.89
1	A	270	SER	N-CA-C	-5.73	105.55	112.54
1	A	372	SER	CA-C-O	5.72	127.80	121.11
1	A	274	THR	CA-C-O	-5.70	115.39	121.94
1	A	67	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	A	14	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	A	14	ARG	O-C-N	5.63	129.05	122.24
1	A	212	GLY	CA-C-O	-5.62	112.78	119.07
1	A	245	LEU	O-C-N	5.61	130.49	123.19
1	A	156	GLY	N-CA-C	-5.60	103.41	111.20
1	A	40	THR	CA-C-N	-5.55	110.53	121.41
1	A	40	THR	C-N-CA	-5.55	110.53	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	339	ALA	CA-C-O	-5.55	115.17	120.94
1	A	168	GLU	CB-CG-CD	5.52	121.99	112.60
1	A	329	ARG	CD-NE-CZ	5.52	132.12	124.40
1	A	367	TRP	CA-C-O	-5.51	115.31	121.81
1	A	300	GLU	CA-C-O	-5.50	113.12	119.61
1	A	304	GLU	CA-C-O	-5.48	114.74	120.55
1	A	365	ALA	N-CA-C	-5.48	106.44	113.02
1	A	33	ILE	CA-C-O	-5.47	114.70	120.39
1	A	418	GLU	CA-CB-CG	5.44	124.98	114.10
1	A	49	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	A	346	VAL	CA-C-O	-5.39	115.44	121.05
1	A	174	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	298	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	62	LEU	O-C-N	5.36	128.50	122.22
1	A	142	SER	CA-CB-OG	-5.35	100.40	111.10
1	A	90	ASP	CB-CA-C	5.34	119.66	110.79
1	A	125	LYS	N-CA-C	-5.33	106.74	113.18
1	A	133	LEU	N-CA-CB	-5.32	102.03	110.22
1	A	317	ILE	CB-CG1-CD1	-5.30	102.67	113.80
1	A	148	VAL	CA-C-O	5.29	123.81	119.47
1	A	75	ALA	CA-C-O	5.29	126.37	120.82
1	A	264	ASN	N-CA-CB	5.28	119.77	110.37
1	A	246	ASP	N-CA-CB	5.27	119.39	110.69
1	A	222	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	372	SER	N-CA-CB	-5.26	101.79	111.37
1	A	42	VAL	CA-C-N	5.26	135.39	125.66
1	A	42	VAL	C-N-CA	5.26	135.39	125.66
1	A	25	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	108	ASN	O-C-N	5.23	128.12	122.15
1	A	200	ARG	CD-NE-CZ	5.23	131.72	124.40
1	A	378	THR	CA-CB-CG2	5.21	119.35	110.50
1	A	150	PHE	O-C-N	5.20	129.28	122.68
1	A	274	THR	OG1-CB-CG2	5.19	119.68	109.30
1	A	294	ILE	N-CA-CB	5.17	118.86	111.82
1	A	261	ASP	O-C-N	5.17	129.13	122.20
1	A	271	LYS	CG-CD-CE	5.17	123.19	111.30
1	A	178	THR	O-C-N	5.16	129.41	123.17
1	A	16	ASN	N-CA-C	-5.16	103.03	110.40
1	A	21	VAL	CA-C-O	-5.15	114.64	120.67
1	A	225	LEU	CA-C-O	-5.15	114.05	119.97
1	A	22	GLU	O-C-N	5.15	129.43	123.30
1	A	419	LEU	O-C-N	5.14	129.56	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ARG	CD-NE-CZ	5.13	131.58	124.40
1	A	253	PHE	CA-C-O	-5.12	114.75	120.54
1	A	144	TYR	CA-C-N	-5.12	116.43	123.14
1	A	144	TYR	C-N-CA	-5.12	116.43	123.14
1	A	262	PHE	CA-C-N	-5.12	114.09	122.54
1	A	262	PHE	C-N-CA	-5.12	114.09	122.54
1	A	186	GLY	CA-C-O	-5.12	115.48	120.75
1	A	255	ASP	O-C-N	5.11	129.10	122.40
1	A	245	LEU	CA-C-O	-5.09	115.36	121.11
1	A	259	ASP	CA-CB-CG	-5.09	107.51	112.60
1	A	326	ASN	CB-CA-C	5.09	115.82	110.17
1	A	400	PRO	CA-C-O	-5.08	117.55	121.31
1	A	101	ASN	CA-C-O	-5.08	113.81	119.95
1	A	272	TRP	CA-C-O	-5.08	116.03	121.56
1	A	298	PHE	CA-C-N	5.07	128.40	120.75
1	A	298	PHE	C-N-CA	5.07	128.40	120.75
1	A	74	PRO	CB-CA-C	5.07	120.98	112.62
1	A	59	LYS	CA-CB-CG	-5.06	103.99	114.10
1	A	356	ILE	CB-CG1-CD1	-5.02	103.26	113.80

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	3289	0	3293	121	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	348	0	0	52	0
All	All	3643	0	3293	121	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 (121) 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:ND2	1:A:328:LYS:HG2	1.80	0.94
1:A:326:ASN:HD21	1:A:328:LYS:HG2	1.30	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:326:ASN:C	1:A:326:ASN:HD22	1.94	0.75
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:264:ASN:OD1	1:A:264:ASN:C	2.34	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: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:43:HIS:N	4:A:731:HOH:O	2.21	0.60
1:A:328:LYS:HG3	1:A:329:ARG:N	2.15	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:216:PRO:C	1:A:217:ASN:HD22	2.18	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:240:LYS:NZ	4:A:784:HOH:O	2.43	0.50
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:8:ARG:HH12	1:A:22:GLU:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:48:MET:HE3	1:A:48:MET:HB2	1.81	0.43
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:67:ASN:O	1:A:71:VAL:HB	2.20	0.42
1:A:154:LEU:C	1:A:154:LEU:HD23	2.44	0.42
1:A:56:TRP:C	1:A:57:MET:CG	2.92	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:249:SER:OG	1:A:298:PHE:C	2.63	0.41
1:A:326:ASN:ND2	1:A:326:ASN:C	2.69	0.41
1:A:42:VAL:HA	4:A:731:HOH:O	2.20	0.41
1:A:194:LYS:NZ	4:A:728:HOH:O	2.23	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

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%)	24	16

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%)	335 (97%)	9 (3%)	40	35

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	MET
1	A	101	ASN
1	A	126	ASN
1	A	133	LEU
1	A	255	ASP
1	A	265	PRO
1	A	326	ASN
1	A	375	SER
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 oligosaccharides 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	0.76	0	6,6,6	0.33	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.