



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:46 PM UTC

PDB ID : 3ENL / pdb_00003enl
Title : REFINED STRUCTURE OF YEAST APO-ENOLASE AT 2.25
ANGSTROMS RESOLUTION
Authors : Lebioda, L.; Stec, B.
Deposited on : 1990-11-13
Resolution : 2.25 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

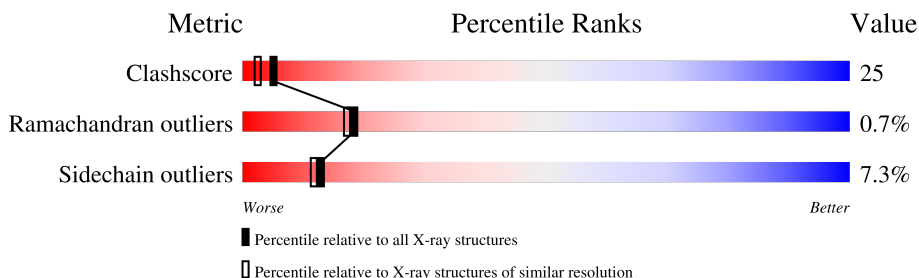
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

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	35% 44% 18% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3647 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.

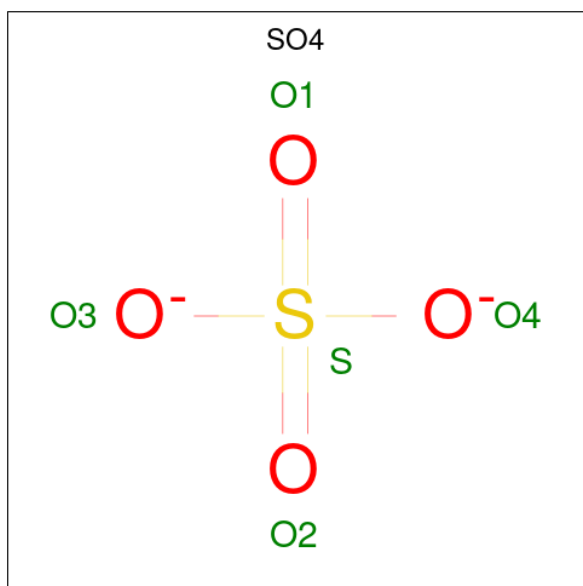
- Molecule 1 is a protein called ENOLASE.

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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

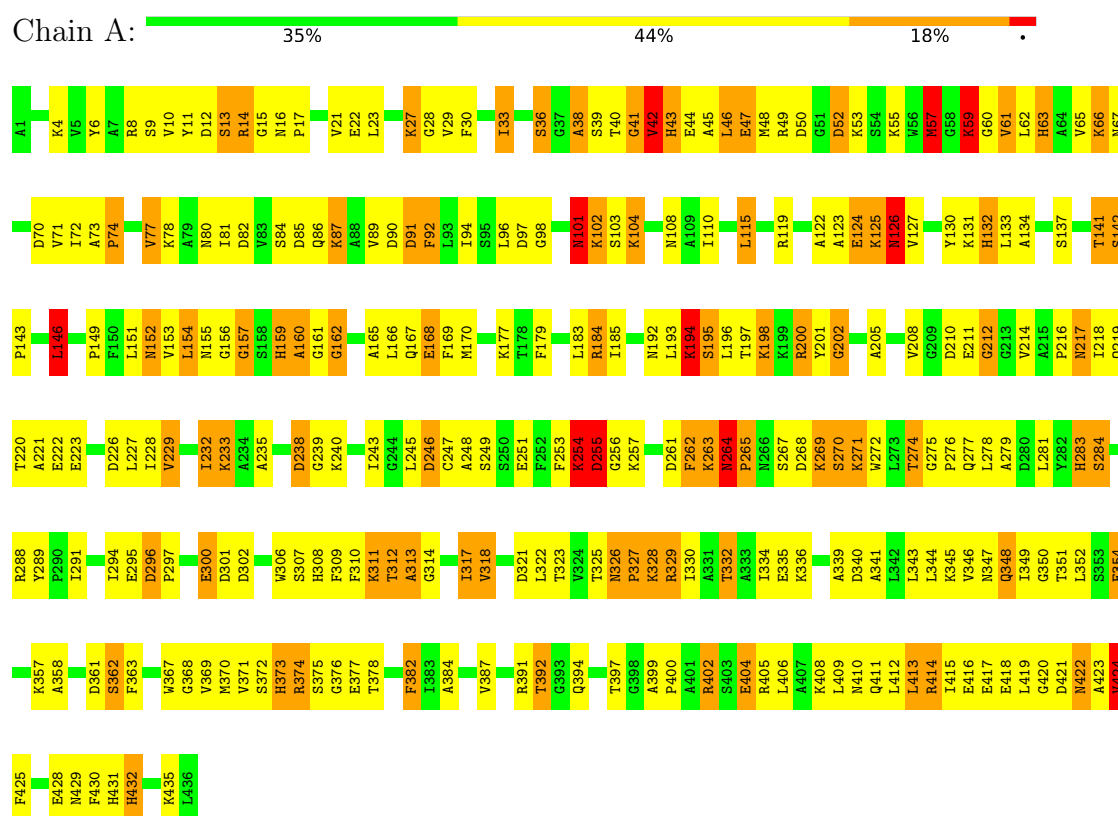
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	353	Total 353	O 353	0	0

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: ENOLASE



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) – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3647	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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

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	1.32	5/3349 (0.1%)	2.87	376/4531 (8.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	ARG	CD-NE	6.33	1.55	1.46
1	A	72	ILE	CA-CB	5.56	1.60	1.54
1	A	311	LYS	C-N	-5.24	1.26	1.33
1	A	283	HIS	C-N	-5.23	1.27	1.33
1	A	184	ARG	CZ-NH2	-5.22	1.26	1.33

All (376) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	CD-NE-CZ	20.40	152.96	124.40
1	A	329	ARG	NE-CZ-NH2	19.21	136.49	119.20
1	A	329	ARG	CD-NE-CZ	18.07	149.70	124.40
1	A	421	ASP	CA-CB-CG	12.81	125.41	112.60
1	A	184	ARG	CD-NE-CZ	-11.96	107.66	124.40
1	A	283	HIS	CA-C-N	11.84	135.83	120.44
1	A	283	HIS	C-N-CA	11.84	135.83	120.44
1	A	49	ARG	NE-CZ-NH1	11.70	133.20	121.50
1	A	428	GLU	CB-CG-CD	11.44	132.04	112.60
1	A	146	LEU	CB-CA-C	11.19	123.07	109.31
1	A	243	ILE	CA-C-N	10.80	130.21	122.33
1	A	243	ILE	C-N-CA	10.80	130.21	122.33
1	A	108	ASN	CA-CB-CG	10.79	123.39	112.60
1	A	362	SER	O-C-N	10.59	132.98	122.07
1	A	397	THR	CA-C-O	-10.30	109.82	120.32
1	A	110	ILE	N-CA-C	10.26	120.17	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ASN	CA-CB-CG	-10.23	102.37	112.60
1	A	340	ASP	CA-C-O	-10.05	108.52	119.08
1	A	126	ASN	OD1-CG-ND2	10.03	132.63	122.60
1	A	169	PHE	CA-C-O	-9.80	110.11	120.40
1	A	328	LYS	N-CA-C	-9.63	100.77	111.07
1	A	328	LYS	N-CA-CB	9.47	123.75	110.01
1	A	414	ARG	NE-CZ-NH2	-9.45	110.70	119.20
1	A	340	ASP	O-C-N	9.36	132.82	122.05
1	A	160	ALA	O-C-N	9.35	132.05	123.26
1	A	159	HIS	CA-CB-CG	-9.22	104.58	113.80
1	A	142	SER	O-C-N	9.12	126.74	121.27
1	A	184	ARG	NE-CZ-NH1	-8.93	112.57	121.50
1	A	41	GLY	N-CA-C	8.88	134.22	113.18
1	A	411	GLN	OE1-CD-NE2	-8.83	113.77	122.60
1	A	30	PHE	CA-CB-CG	-8.75	105.05	113.80
1	A	264	ASN	CA-CB-CG	8.68	121.28	112.60
1	A	263	LYS	CB-CA-C	8.67	124.82	110.17
1	A	86	GLN	OE1-CD-NE2	-8.58	114.02	122.60
1	A	10	VAL	CA-C-O	-8.54	112.47	121.44
1	A	192	ASN	OD1-CG-ND2	8.51	131.11	122.60
1	A	119	ARG	N-CA-C	-8.45	101.76	110.97
1	A	265	PRO	CA-C-N	8.43	137.64	121.54
1	A	265	PRO	C-N-CA	8.43	137.64	121.54
1	A	294	ILE	N-CA-CB	8.40	123.24	111.82
1	A	269	LYS	N-CA-CB	8.39	125.07	110.39
1	A	255	ASP	O-C-N	8.33	133.46	122.47
1	A	67	ASN	CA-CB-CG	-8.19	104.41	112.60
1	A	52	ASP	CA-CB-CG	-8.17	104.43	112.60
1	A	119	ARG	NE-CZ-NH2	8.14	126.53	119.20
1	A	98	GLY	N-CA-C	8.14	127.02	115.30
1	A	328	LYS	CB-CG-CD	8.02	129.75	111.30
1	A	43	HIS	N-CA-C	-7.97	98.66	110.06
1	A	307	SER	CA-CB-OG	-7.95	95.21	111.10
1	A	125	LYS	N-CA-C	-7.92	103.59	113.18
1	A	255	ASP	CA-C-O	-7.88	111.21	120.98
1	A	329	ARG	NH1-CZ-NH2	-7.85	109.10	119.30
1	A	288	ARG	NE-CZ-NH2	7.85	126.26	119.20
1	A	348	GLN	N-CA-CB	7.82	123.15	110.40
1	A	161	GLY	N-CA-C	-7.80	100.72	112.41
1	A	223	GLU	CG-CD-OE2	-7.79	100.49	118.40
1	A	195	SER	CB-CA-C	-7.78	98.67	110.88
1	A	132	HIS	CA-C-N	7.75	131.43	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	HIS	C-N-CA	7.75	131.43	120.28
1	A	134	ALA	CA-C-O	-7.75	112.21	120.42
1	A	43	HIS	CA-CB-CG	-7.72	106.08	113.80
1	A	348	GLN	N-CA-C	-7.65	103.40	112.89
1	A	115	LEU	CA-C-N	7.57	130.42	120.28
1	A	115	LEU	C-N-CA	7.57	130.42	120.28
1	A	192	ASN	CA-CB-CG	-7.56	105.04	112.60
1	A	17	PRO	CA-C-O	7.55	130.32	121.56
1	A	412	LEU	CA-C-N	7.55	130.26	120.44
1	A	412	LEU	C-N-CA	7.55	130.26	120.44
1	A	340	ASP	CB-CG-OD1	7.55	135.76	118.40
1	A	141	THR	CA-CB-OG1	-7.53	98.30	109.60
1	A	210	ASP	N-CA-C	7.53	120.44	111.33
1	A	167	GLN	CA-C-O	-7.49	112.54	120.55
1	A	200	ARG	CD-NE-CZ	7.47	134.86	124.40
1	A	246	ASP	N-CA-CB	7.46	123.01	110.69
1	A	263	LYS	N-CA-C	-7.44	103.32	113.30
1	A	372	SER	CA-C-O	7.37	129.61	121.06
1	A	368	GLY	N-CA-C	-7.36	99.93	112.51
1	A	278	LEU	CA-C-N	7.34	130.44	120.38
1	A	278	LEU	C-N-CA	7.34	130.44	120.38
1	A	284	SER	CB-CA-C	-7.34	99.36	110.88
1	A	310	PHE	CA-CB-CG	-7.34	106.46	113.80
1	A	36	SER	CA-C-N	7.33	131.70	122.83
1	A	36	SER	C-N-CA	7.33	131.70	122.83
1	A	233	LYS	CA-C-O	-7.27	113.19	120.82
1	A	85	ASP	CA-CB-CG	-7.25	105.35	112.60
1	A	279	ALA	O-C-N	7.24	129.80	122.12
1	A	325	THR	CA-CB-CG2	7.23	122.79	110.50
1	A	59	LYS	N-CA-CB	7.23	122.67	111.39
1	A	311	LYS	O-C-N	-7.23	114.46	122.12
1	A	59	LYS	CA-C-O	-7.21	111.78	120.65
1	A	168	GLU	CB-CG-CD	7.18	124.81	112.60
1	A	352	LEU	CB-CA-C	7.18	122.15	110.88
1	A	134	ALA	N-CA-C	-7.17	103.54	111.36
1	A	141	THR	CA-C-N	-7.17	114.37	122.26
1	A	141	THR	C-N-CA	-7.17	114.37	122.26
1	A	332	THR	O-C-N	7.13	129.41	122.07
1	A	329	ARG	NE-CZ-NH1	-7.11	114.39	121.50
1	A	418	GLU	CA-CB-CG	7.11	128.32	114.10
1	A	48	MET	N-CA-C	7.08	120.31	108.20
1	A	232	ILE	N-CA-C	-7.07	103.88	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLU	O-C-N	7.07	131.72	123.30
1	A	276	PRO	CA-C-O	-7.00	108.57	119.64
1	A	312	THR	N-CA-CB	-6.99	99.44	110.98
1	A	84	SER	O-C-N	6.98	130.85	122.27
1	A	167	GLN	OE1-CD-NE2	-6.97	115.62	122.60
1	A	184	ARG	CG-CD-NE	-6.96	96.68	112.00
1	A	262	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	214	VAL	N-CA-C	-6.94	102.49	110.05
1	A	67	ASN	CA-C-O	-6.92	113.21	120.55
1	A	184	ARG	CA-C-N	6.92	129.28	120.56
1	A	184	ARG	C-N-CA	6.92	129.28	120.56
1	A	108	ASN	CA-C-O	-6.91	113.10	120.42
1	A	125	LYS	CA-CB-CG	6.91	127.92	114.10
1	A	123	ALA	CA-C-N	6.89	129.51	120.28
1	A	123	ALA	C-N-CA	6.89	129.51	120.28
1	A	149	PRO	CA-C-N	6.88	132.41	122.85
1	A	149	PRO	C-N-CA	6.88	132.41	122.85
1	A	162	GLY	N-CA-C	-6.88	101.61	112.61
1	A	80	ASN	CA-CB-CG	-6.87	105.73	112.60
1	A	36	SER	CB-CA-C	6.86	121.54	110.29
1	A	89	VAL	CA-C-N	6.83	129.32	120.44
1	A	89	VAL	C-N-CA	6.83	129.32	120.44
1	A	45	ALA	N-CA-C	-6.81	100.36	110.23
1	A	217	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	411	GLN	CG-CD-OE1	6.79	134.38	120.80
1	A	77	VAL	CA-C-O	6.77	128.35	121.17
1	A	119	ARG	N-CA-CB	6.77	119.79	109.91
1	A	414	ARG	NE-CZ-NH1	6.77	128.27	121.50
1	A	402	ARG	CD-NE-CZ	-6.76	114.94	124.40
1	A	124	GLU	CG-CD-OE1	-6.75	102.87	118.40
1	A	126	ASN	CB-CA-C	-6.72	102.18	111.73
1	A	212	GLY	CA-C-O	-6.70	111.57	119.01
1	A	12	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	238	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	63	HIS	O-C-N	6.63	129.19	122.03
1	A	196	LEU	CA-C-O	-6.63	113.52	120.55
1	A	8	ARG	NH1-CZ-NH2	-6.63	110.69	119.30
1	A	372	SER	N-CA-CB	-6.62	99.22	111.53
1	A	126	ASN	CB-CG-ND2	-6.60	106.50	116.40
1	A	229	VAL	CB-CA-C	6.60	121.33	112.22
1	A	67	ASN	O-C-N	6.59	129.11	122.12
1	A	425	PHE	CA-C-O	-6.57	113.36	120.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	LEU	CA-C-N	6.55	129.59	120.29
1	A	409	LEU	C-N-CA	6.55	129.59	120.29
1	A	334	ILE	CB-CG1-CD1	6.54	127.53	113.80
1	A	417	GLU	CA-C-N	6.50	130.20	120.31
1	A	417	GLU	C-N-CA	6.50	130.20	120.31
1	A	119	ARG	CD-NE-CZ	6.47	133.46	124.40
1	A	170	MET	CA-C-O	-6.46	113.85	121.16
1	A	235	ALA	N-CA-C	-6.46	105.36	113.18
1	A	350	GLY	CA-C-O	-6.46	111.86	119.02
1	A	413	LEU	N-CA-C	-6.44	104.18	111.07
1	A	354	GLU	CA-C-N	6.44	128.90	120.28
1	A	354	GLU	C-N-CA	6.44	128.90	120.28
1	A	275	GLY	O-C-N	6.40	128.17	121.77
1	A	179	PHE	N-CA-C	-6.39	104.39	111.36
1	A	344	LEU	CD1-CG-CD2	-6.39	96.74	110.80
1	A	8	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	A	296	ASP	O-C-N	6.38	124.46	121.53
1	A	78	LYS	CA-C-O	-6.37	113.79	120.55
1	A	227	LEU	CA-C-N	6.36	129.45	120.42
1	A	227	LEU	C-N-CA	6.36	129.45	120.42
1	A	221	ALA	CA-C-O	-6.35	114.16	120.82
1	A	108	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	A	154	LEU	CA-CB-CG	6.33	138.45	116.30
1	A	78	LYS	CA-C-N	6.28	129.32	120.28
1	A	78	LYS	C-N-CA	6.28	129.32	120.28
1	A	102	LYS	N-CA-CB	-6.27	102.62	112.08
1	A	6	TYR	CA-C-O	-6.23	113.82	121.11
1	A	279	ALA	N-CA-CB	6.23	119.41	110.06
1	A	137	SER	O-C-N	6.22	130.12	122.34
1	A	328	LYS	CG-CD-CE	6.18	125.52	111.30
1	A	15	GLY	N-CA-C	-6.17	106.19	115.32
1	A	311	LYS	CA-CB-CG	-6.16	101.79	114.10
1	A	274	THR	CA-C-N	6.15	131.53	121.87
1	A	274	THR	C-N-CA	6.15	131.53	121.87
1	A	361	ASP	CB-CG-OD2	-6.14	104.28	118.40
1	A	119	ARG	CA-C-O	-6.13	114.56	121.00
1	A	60	GLY	N-CA-C	-6.11	102.04	112.30
1	A	309	PHE	CA-C-N	6.11	129.30	120.38
1	A	309	PHE	C-N-CA	6.11	129.30	120.38
1	A	155	ASN	OD1-CG-ND2	6.09	128.69	122.60
1	A	167	GLN	N-CA-C	6.09	118.83	111.40
1	A	149	PRO	O-C-N	-6.08	115.40	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	ILE	O-C-N	6.07	129.29	122.98
1	A	184	ARG	O-C-N	-6.07	115.54	122.09
1	A	289	TYR	O-C-N	6.04	126.26	121.55
1	A	104	LYS	CA-C-N	6.03	131.69	121.14
1	A	104	LYS	C-N-CA	6.03	131.69	121.14
1	A	227	LEU	CB-CA-C	6.02	121.08	110.85
1	A	363	PHE	CA-C-O	-6.01	114.18	120.55
1	A	264	ASN	CA-C-O	-6.01	111.93	120.16
1	A	28	GLY	CA-C-N	6.00	130.58	122.90
1	A	28	GLY	C-N-CA	6.00	130.58	122.90
1	A	55	LYS	O-C-N	6.00	131.56	123.34
1	A	420	GLY	CA-C-O	-5.96	113.65	121.51
1	A	239	GLY	CA-C-O	5.95	125.46	119.27
1	A	123	ALA	CA-C-O	5.95	127.27	120.90
1	A	74	PRO	CA-C-N	5.93	128.16	120.44
1	A	74	PRO	C-N-CA	5.93	128.16	120.44
1	A	352	LEU	CA-C-O	-5.93	114.59	120.82
1	A	141	THR	CA-C-O	5.91	126.63	119.78
1	A	294	ILE	CA-C-N	5.90	130.86	122.72
1	A	294	ILE	C-N-CA	5.90	130.86	122.72
1	A	131	LYS	CA-C-N	5.89	128.66	120.29
1	A	131	LYS	C-N-CA	5.89	128.66	120.29
1	A	358	ALA	CA-C-O	-5.89	113.45	120.10
1	A	30	PHE	CA-C-O	-5.86	113.99	120.38
1	A	404	GLU	N-CA-C	-5.86	105.63	112.89
1	A	382	PHE	CA-CB-CG	-5.86	107.94	113.80
1	A	208	VAL	CA-C-N	5.85	128.73	121.83
1	A	208	VAL	C-N-CA	5.85	128.73	121.83
1	A	415	ILE	CA-C-N	5.85	128.43	120.54
1	A	415	ILE	C-N-CA	5.85	128.43	120.54
1	A	169	PHE	O-C-N	5.84	130.83	123.12
1	A	161	GLY	O-C-N	5.84	128.43	122.88
1	A	42	VAL	CA-C-N	5.81	132.10	122.62
1	A	42	VAL	C-N-CA	5.81	132.10	122.62
1	A	368	GLY	CA-C-N	5.81	131.23	122.98
1	A	368	GLY	C-N-CA	5.81	131.23	122.98
1	A	101	ASN	CB-CG-ND2	5.81	125.11	116.40
1	A	387	VAL	CA-C-O	-5.81	114.91	120.95
1	A	428	GLU	CA-CB-CG	5.80	125.70	114.10
1	A	247	CYS	CA-C-O	-5.78	112.14	119.31
1	A	36	SER	CA-C-O	5.78	127.19	120.49
1	A	195	SER	O-C-N	5.75	128.00	122.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ARG	NH1-CZ-NH2	-5.75	111.83	119.30
1	A	349	ILE	CB-CA-C	5.75	117.15	110.88
1	A	384	ALA	CA-C-O	-5.75	114.78	120.70
1	A	254	LYS	CB-CA-C	-5.71	101.90	110.24
1	A	373	HIS	CA-CB-CG	5.70	119.50	113.80
1	A	108	ASN	N-CA-CB	5.70	118.59	110.16
1	A	156	GLY	N-CA-C	-5.69	99.69	113.18
1	A	245	LEU	O-C-N	5.67	130.60	123.23
1	A	92	PHE	CA-CB-CG	-5.67	108.13	113.80
1	A	13	SER	CA-CB-OG	5.66	122.42	111.10
1	A	157	GLY	O-C-N	5.66	128.90	122.62
1	A	226	ASP	O-C-N	5.66	128.12	122.12
1	A	243	ILE	CA-C-O	5.65	127.28	120.67
1	A	46	LEU	CA-C-O	5.64	127.06	120.80
1	A	223	GLU	CB-CA-C	-5.63	102.03	110.88
1	A	328	LYS	CA-C-O	-5.63	114.91	120.82
1	A	311	LYS	CA-C-N	5.63	131.04	122.37
1	A	311	LYS	C-N-CA	5.63	131.04	122.37
1	A	406	LEU	CA-C-O	-5.63	113.74	120.10
1	A	326	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	A	424	VAL	CA-C-O	-5.62	114.76	121.28
1	A	351	THR	N-CA-CB	5.62	121.97	111.52
1	A	70	ASP	N-CA-C	5.62	118.60	111.69
1	A	422	ASN	CA-CB-CG	-5.61	106.99	112.60
1	A	271	LYS	N-CA-C	5.61	120.12	113.28
1	A	284	SER	CA-CB-OG	-5.60	99.89	111.10
1	A	394	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	332	THR	CA-CB-CG2	5.60	120.02	110.50
1	A	232	ILE	O-C-N	5.59	127.72	121.90
1	A	91	ASP	N-CA-C	-5.59	105.19	111.28
1	A	141	THR	CA-CB-CG2	5.59	120.00	110.50
1	A	404	GLU	CG-CD-OE2	-5.58	105.57	118.40
1	A	311	LYS	CA-C-O	5.57	126.46	120.55
1	A	168	GLU	CG-CD-OE2	5.57	131.22	118.40
1	A	233	LYS	CA-CB-CG	-5.57	102.96	114.10
1	A	194	LYS	CA-CB-CG	-5.57	102.97	114.10
1	A	108	ASN	O-C-N	5.55	128.47	122.15
1	A	130	TYR	O-C-N	5.55	128.00	122.12
1	A	6	TYR	N-CA-CB	-5.54	101.28	111.37
1	A	391	ARG	NH1-CZ-NH2	-5.53	112.11	119.30
1	A	375	SER	O-C-N	5.53	127.77	122.07
1	A	310	PHE	O-C-N	5.53	128.50	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LEU	CB-CA-C	5.52	119.62	110.90
1	A	38	ALA	CA-C-O	-5.51	114.68	120.80
1	A	179	PHE	CA-CB-CG	-5.51	108.29	113.80
1	A	372	SER	CA-C-N	5.50	132.22	121.66
1	A	372	SER	C-N-CA	5.50	132.22	121.66
1	A	323	THR	O-C-N	5.50	129.13	122.48
1	A	248	ALA	CA-C-O	-5.48	115.48	121.84
1	A	432	HIS	CA-C-O	-5.48	112.67	120.51
1	A	222	GLU	CB-CG-CD	5.47	121.91	112.60
1	A	202	GLY	CA-C-N	5.47	128.37	120.38
1	A	202	GLY	C-N-CA	5.47	128.37	120.38
1	A	11	TYR	CA-C-N	5.46	133.05	122.07
1	A	11	TYR	C-N-CA	5.46	133.05	122.07
1	A	334	ILE	CA-C-N	5.46	127.91	120.54
1	A	334	ILE	C-N-CA	5.46	127.91	120.54
1	A	47	GLU	CG-CD-OE1	-5.46	105.85	118.40
1	A	223	GLU	OE1-CD-OE2	5.45	135.97	122.90
1	A	328	LYS	O-C-N	5.43	127.67	122.07
1	A	15	GLY	CA-C-O	-5.43	112.57	119.19
1	A	400	PRO	N-CA-C	-5.43	104.44	112.26
1	A	211	GLU	N-CA-C	5.42	120.00	113.17
1	A	227	LEU	N-CA-CB	-5.42	102.14	110.16
1	A	223	GLU	O-C-N	5.42	127.65	122.07
1	A	327	PRO	CB-CA-C	5.40	120.63	112.21
1	A	409	LEU	CA-C-O	-5.39	114.70	120.42
1	A	122	ALA	CA-C-O	-5.38	115.16	120.70
1	A	132	HIS	CA-C-O	5.38	126.12	120.42
1	A	312	THR	CA-C-O	-5.37	113.14	119.48
1	A	55	LYS	CG-CD-CE	-5.36	98.98	111.30
1	A	357	LYS	CA-CB-CG	-5.35	103.40	114.10
1	A	6	TYR	CA-CB-CG	-5.35	104.27	113.90
1	A	82	ASP	O-C-N	5.34	129.34	122.93
1	A	169	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	270	SER	CB-CA-C	5.32	120.89	110.67
1	A	160	ALA	CA-C-N	-5.31	117.01	122.27
1	A	160	ALA	C-N-CA	-5.31	117.01	122.27
1	A	44	GLU	O-C-N	5.31	129.43	123.27
1	A	57	MET	CA-C-O	5.31	126.22	120.12
1	A	415	ILE	O-C-N	-5.30	116.73	121.87
1	A	363	PHE	N-CA-CB	5.30	117.91	110.12
1	A	263	LYS	CA-C-N	5.30	134.73	121.80
1	A	263	LYS	C-N-CA	5.30	134.73	121.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	HIS	CA-CB-CG	-5.29	108.51	113.80
1	A	67	ASN	N-CA-CB	5.29	117.90	110.12
1	A	9	SER	CA-C-O	-5.29	114.67	120.43
1	A	318	VAL	CA-C-N	-5.27	115.44	122.72
1	A	318	VAL	C-N-CA	-5.27	115.44	122.72
1	A	391	ARG	CA-C-O	-5.27	115.01	121.28
1	A	40	THR	CB-CA-C	5.26	118.56	110.14
1	A	313	ALA	CA-C-O	-5.26	115.49	120.90
1	A	411	GLN	O-C-N	-5.26	116.16	122.15
1	A	40	THR	N-CA-CB	5.25	119.02	110.77
1	A	166	LEU	CA-C-O	-5.25	115.28	121.16
1	A	429	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	412	LEU	N-CA-CB	-5.24	102.15	110.28
1	A	17	PRO	O-C-N	-5.24	116.51	123.01
1	A	374	ARG	N-CA-C	-5.24	101.57	109.85
1	A	429	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	A	21	VAL	CA-C-N	5.23	130.36	122.99
1	A	21	VAL	C-N-CA	5.23	130.36	122.99
1	A	161	GLY	CA-C-N	-5.22	115.37	121.85
1	A	161	GLY	C-N-CA	-5.22	115.37	121.85
1	A	251	GLU	CG-CD-OE1	-5.22	106.39	118.40
1	A	211	GLU	CB-CG-CD	5.22	121.47	112.60
1	A	89	VAL	CA-CB-CG2	5.22	119.27	110.40
1	A	288	ARG	CA-C-O	-5.20	113.65	119.79
1	A	318	VAL	O-C-N	5.20	128.80	123.03
1	A	220	THR	CA-C-N	5.19	127.19	120.44
1	A	220	THR	C-N-CA	5.19	127.19	120.44
1	A	61	VAL	CB-CA-C	5.19	119.81	111.29
1	A	394	GLN	CG-CD-NE2	5.19	124.18	116.40
1	A	371	VAL	N-CA-C	-5.17	102.90	109.58
1	A	232	ILE	N-CA-CB	5.17	117.18	110.57
1	A	321	ASP	N-CA-CB	5.17	118.28	110.28
1	A	45	ALA	CB-CA-C	5.16	118.29	109.72
1	A	302	ASP	CA-C-N	5.16	127.50	120.54
1	A	302	ASP	C-N-CA	5.16	127.50	120.54
1	A	194	LYS	CA-C-O	5.16	126.02	120.55
1	A	127	VAL	CA-CB-CG2	5.15	119.16	110.40
1	A	119	ARG	O-C-N	5.15	127.39	122.03
1	A	159	HIS	CA-C-N	-5.13	111.68	122.41
1	A	159	HIS	C-N-CA	-5.13	111.68	122.41
1	A	223	GLU	CB-CG-CD	-5.13	103.88	112.60
1	A	291	ILE	N-CA-CB	-5.12	105.21	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	314	GLY	CA-C-N	5.11	130.28	122.92
1	A	314	GLY	C-N-CA	5.11	130.28	122.92
1	A	240	LYS	CA-C-N	5.11	129.90	123.10
1	A	240	LYS	C-N-CA	5.11	129.90	123.10
1	A	47	GLU	OE1-CD-OE2	5.11	135.16	122.90
1	A	33	ILE	N-CA-C	-5.11	100.77	108.12
1	A	27	LYS	CA-C-O	-5.10	113.53	119.14
1	A	126	ASN	CA-CB-CG	-5.09	107.51	112.60
1	A	301	ASP	CA-CB-CG	-5.09	107.50	112.60
1	A	59	LYS	O-C-N	5.08	129.01	122.20
1	A	152	ASN	CA-CB-CG	-5.08	107.53	112.60
1	A	49	ARG	CA-CB-CG	-5.07	103.95	114.10
1	A	198	LYS	N-CA-C	-5.07	105.75	111.28
1	A	373	HIS	CB-CG-CD2	5.05	137.77	131.20
1	A	132	HIS	O-C-N	-5.05	116.39	122.15
1	A	416	GLU	CB-CA-C	-5.03	102.76	110.81
1	A	408	LYS	CA-C-N	5.02	127.42	120.29
1	A	408	LYS	C-N-CA	5.02	127.42	120.29
1	A	346	VAL	N-CA-CB	5.02	116.74	110.47
1	A	249	SER	CA-C-N	5.01	127.49	120.28
1	A	249	SER	C-N-CA	5.01	127.49	120.28
1	A	264	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	377	GLU	CA-C-N	5.00	131.91	123.01
1	A	377	GLU	C-N-CA	5.00	131.91	123.01

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	163	0
2	A	5	0	0	0	0
3	A	353	0	0	43	1
All	All	3647	0	3293	163	1

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 25.

All (163) 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:264:ASN:ND2	1:A:265:PRO:HA	1.20	1.41
1:A:264:ASN:HB3	1:A:267:SER:HB2	1.27	1.15
1:A:36:SER:O	3:A:617:HOH:O	1.71	1.08
1:A:264:ASN:ND2	1:A:265:PRO:CA	2.17	1.07
1:A:66:LYS:HE3	3:A:574:HOH:O	1.52	1.06
1:A:41:GLY:CA	1:A:46:LEU:HD21	1.87	1.05
1:A:269:LYS:HB2	3:A:709:HOH:O	1.58	1.03
1:A:268:ASP:HB3	1:A:271:LYS:HD2	1.37	1.02
1:A:264:ASN:CG	1:A:265:PRO:HA	1.86	0.99
1:A:264:ASN:HD22	1:A:265:PRO:HA	1.28	0.96
1:A:27:LYS:HE3	1:A:124:GLU:HA	1.45	0.95
1:A:38:ALA:O	1:A:47:GLU:HB3	1.65	0.95
1:A:327:PRO:HB3	3:A:653:HOH:O	1.66	0.94
1:A:4:LYS:HE2	3:A:604:HOH:O	1.73	0.88
1:A:41:GLY:N	1:A:46:LEU:HD21	1.88	0.87
1:A:152:ASN:HB2	3:A:797:HOH:O	1.74	0.86
1:A:66:LYS:HE2	3:A:505:HOH:O	1.76	0.85
1:A:264:ASN:CB	1:A:267:SER:HB2	2.06	0.83
1:A:73:ALA:HB3	1:A:74:PRO:HD3	1.60	0.81
1:A:233:LYS:HE3	1:A:238:ASP:OD2	1.81	0.80
1:A:432:HIS:CD2	3:A:676:HOH:O	2.34	0.80
1:A:74:PRO:HA	3:A:678:HOH:O	1.82	0.80
1:A:432:HIS:HD2	3:A:676:HOH:O	1.64	0.80
1:A:126:ASN:ND2	3:A:669:HOH:O	2.14	0.79
1:A:269:LYS:O	1:A:269:LYS:HG2	1.85	0.76
1:A:27:LYS:CE	1:A:124:GLU:HA	2.15	0.76
1:A:257:LYS:HG3	3:A:619:HOH:O	1.84	0.76
1:A:41:GLY:HA2	1:A:46:LEU:HD21	1.67	0.75
1:A:313:ALA:HB1	1:A:317:ILE:HD11	1.67	0.75
1:A:268:ASP:CB	1:A:271:LYS:HD2	2.15	0.74
1:A:264:ASN:CG	1:A:265:PRO:CA	2.58	0.74
1:A:268:ASP:HB3	1:A:271:LYS:CD	2.18	0.73
1:A:265:PRO:HB2	3:A:745:HOH:O	1.90	0.72
1:A:327:PRO:CB	3:A:653:HOH:O	2.28	0.71
1:A:53:LYS:HG2	3:A:472:HOH:O	1.91	0.70
1:A:52:ASP:OD1	1:A:52:ASP:C	2.33	0.69
1:A:271:LYS:HB2	3:A:751:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:O	3:A:678:HOH:O	2.10	0.68
1:A:255:ASP:N	3:A:711:HOH:O	2.26	0.68
1:A:327:PRO:CG	3:A:653:HOH:O	2.42	0.67
1:A:41:GLY:HA3	1:A:46:LEU:HD21	1.73	0.66
1:A:228:ILE:O	1:A:232:ILE:HG13	1.96	0.66
1:A:33:ILE:HG22	1:A:378:THR:HG21	1.76	0.66
1:A:328:LYS:HG2	1:A:329:ARG:N	2.12	0.65
1:A:217:ASN:HD22	1:A:217:ASN:N	1.94	0.65
1:A:332:THR:HG22	1:A:336:LYS:HD2	1.77	0.64
1:A:347:ASN:OD1	1:A:374:ARG:NH1	2.29	0.63
1:A:125:LYS:HE3	1:A:132:HIS:CE1	2.34	0.63
1:A:50:ASP:OD2	1:A:62:LEU:HB2	1.99	0.63
1:A:264:ASN:HB2	1:A:267:SER:N	2.13	0.63
1:A:39:SER:HA	1:A:47:GLU:O	2.00	0.62
1:A:194:LYS:O	1:A:198:LYS:HG3	2.00	0.61
1:A:41:GLY:N	1:A:46:LEU:CD2	2.63	0.61
1:A:345:LYS:HB2	1:A:348:GLN:HG3	1.83	0.61
1:A:77:VAL:HB	3:A:678:HOH:O	2.02	0.60
1:A:326:ASN:HB3	1:A:329:ARG:HB2	1.84	0.60
1:A:332:THR:O	1:A:336:LYS:HG3	2.03	0.58
1:A:27:LYS:HE3	1:A:124:GLU:CA	2.27	0.58
1:A:300:GLU:O	1:A:322:LEU:HD12	2.05	0.57
1:A:313:ALA:CB	1:A:317:ILE:CD1	2.83	0.57
1:A:281:LEU:C	1:A:281:LEU:HD23	2.29	0.57
1:A:313:ALA:HB1	1:A:317:ILE:CD1	2.34	0.57
1:A:373:HIS:ND1	1:A:405:ARG:NH1	2.52	0.56
1:A:33:ILE:HD11	3:A:508:HOH:O	2.03	0.56
1:A:71:VAL:HG21	3:A:655:HOH:O	2.04	0.56
1:A:146:LEU:HD12	1:A:423:ALA:HB1	1.87	0.56
1:A:261:ASP:HA	3:A:734:HOH:O	2.04	0.56
1:A:312:THR:CG2	3:A:628:HOH:O	2.54	0.56
1:A:197:THR:HG22	1:A:205:ALA:HB1	1.86	0.56
1:A:435:LYS:HD2	3:A:699:HOH:O	2.05	0.56
1:A:143:PRO:HG2	1:A:424:VAL:HG13	1.88	0.55
1:A:87:LYS:HE2	1:A:91:ASP:OD2	2.07	0.54
1:A:328:LYS:HD2	3:A:529:HOH:O	2.07	0.54
1:A:308:HIS:O	1:A:311:LYS:HB2	2.08	0.53
1:A:216:PRO:C	1:A:217:ASN:HD22	2.16	0.53
1:A:264:ASN:CG	1:A:265:PRO:C	2.76	0.53
1:A:217:ASN:N	1:A:217:ASN:ND2	2.55	0.53
1:A:73:ALA:HB3	1:A:74:PRO:CD	2.36	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLN:HG2	3:A:591:HOH:O	2.07	0.53
1:A:4:LYS:HE2	3:A:471:HOH:O	2.09	0.52
1:A:212:GLY:HA3	1:A:399:ALA:HB3	1.91	0.52
1:A:313:ALA:CB	1:A:317:ILE:HD11	2.36	0.52
1:A:39:SER:CB	1:A:47:GLU:O	2.58	0.51
1:A:264:ASN:CB	1:A:267:SER:CB	2.85	0.51
1:A:38:ALA:C	1:A:47:GLU:HB3	2.35	0.51
1:A:97:ASP:C	3:A:764:HOH:O	2.54	0.51
1:A:317:ILE:O	1:A:339:ALA:HB1	2.10	0.51
1:A:59:LYS:HE3	3:A:558:HOH:O	2.12	0.50
1:A:253:PHE:CZ	1:A:256:GLY:HA2	2.45	0.50
1:A:274:THR:OG1	1:A:277:GLN:HG3	2.10	0.50
1:A:281:LEU:HD23	1:A:281:LEU:O	2.12	0.50
1:A:125:LYS:HE3	1:A:132:HIS:ND1	2.27	0.50
1:A:200:ARG:HB3	3:A:763:HOH:O	2.11	0.50
1:A:162:GLY:HA2	1:A:219:GLN:HE22	1.77	0.49
1:A:61:VAL:O	1:A:65:VAL:HG23	2.12	0.49
1:A:63:HIS:CD2	3:A:679:HOH:O	2.66	0.49
1:A:165:ALA:HA	1:A:262:PHE:HE1	1.78	0.49
1:A:143:PRO:CG	1:A:424:VAL:HG13	2.44	0.48
1:A:246:ASP:HA	1:A:295:GLU:HB3	1.96	0.48
1:A:101:ASN:ND2	1:A:103:SER:OG	2.46	0.48
1:A:143:PRO:HB2	1:A:422:ASN:O	2.13	0.48
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.48	0.48
1:A:152:ASN:O	1:A:399:ALA:HB2	2.14	0.48
1:A:42:VAL:HG11	3:A:618:HOH:O	2.13	0.48
1:A:42:VAL:HG12	1:A:43:HIS:N	2.29	0.48
1:A:63:HIS:HD2	3:A:679:HOH:O	1.97	0.47
1:A:269:LYS:O	1:A:269:LYS:CG	2.55	0.47
1:A:369:VAL:O	1:A:392:THR:HB	2.14	0.47
1:A:42:VAL:HG12	1:A:43:HIS:H	1.79	0.47
1:A:152:ASN:ND2	1:A:168:GLU:HB3	2.29	0.47
1:A:162:GLY:O	1:A:263:LYS:HE3	2.14	0.47
1:A:157:GLY:C	1:A:159:HIS:H	2.23	0.47
1:A:410:ASN:O	1:A:414:ARG:HG3	2.14	0.46
1:A:268:ASP:OD1	1:A:270:SER:HB2	2.16	0.46
1:A:261:ASP:O	1:A:264:ASN:HB3	2.16	0.46
1:A:272:TRP:N	1:A:272:TRP:CD1	2.81	0.46
1:A:362:SER:O	1:A:367:TRP:HB2	2.15	0.46
1:A:153:VAL:HB	1:A:193:LEU:HD23	1.98	0.45
1:A:159:HIS:O	1:A:160:ALA:HB2	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASN:HA	1:A:327:PRO:HD3	1.81	0.45
1:A:201:TYR:HB2	1:A:205:ALA:CB	2.46	0.45
1:A:254:LYS:O	1:A:255:ASP:HB2	2.15	0.45
1:A:73:ALA:N	1:A:74:PRO:HD2	2.32	0.45
1:A:268:ASP:C	1:A:270:SER:N	2.75	0.44
1:A:413:LEU:HD23	1:A:413:LEU:HA	1.85	0.44
1:A:269:LYS:HG3	1:A:272:TRP:CD2	2.52	0.44
1:A:318:VAL:HG22	1:A:341:ALA:HB3	1.98	0.44
1:A:115:LEU:HD22	1:A:382:PHE:CZ	2.52	0.44
1:A:125:LYS:O	1:A:126:ASN:CB	2.65	0.44
1:A:102:LYS:NZ	1:A:354:GLU:OE1	2.44	0.44
1:A:141:THR:O	3:A:589:HOH:O	2.21	0.44
1:A:312:THR:HG21	3:A:628:HOH:O	2.15	0.44
1:A:81:ILE:HD11	1:A:92:PHE:CG	2.53	0.43
1:A:184:ARG:HH11	1:A:184:ARG:HD3	1.09	0.43
1:A:90:ASP:O	1:A:94:ILE:HG13	2.19	0.43
1:A:14:ARG:HD2	1:A:376:GLY:HA2	1.99	0.43
1:A:326:ASN:HD22	1:A:327:PRO:CD	2.32	0.43
1:A:39:SER:HB2	1:A:47:GLU:O	2.18	0.43
1:A:185:ILE:HG21	1:A:185:ILE:HD13	1.69	0.43
1:A:57:MET:HE2	3:A:551:HOH:O	2.18	0.42
1:A:74:PRO:C	3:A:678:HOH:O	2.60	0.42
1:A:142:SER:HA	1:A:143:PRO:HA	1.64	0.42
1:A:257:LYS:HE3	1:A:269:LYS:HE2	2.02	0.42
1:A:343:LEU:HD12	1:A:370:MET:HB3	2.00	0.42
1:A:23:LEU:O	1:A:29:VAL:HA	2.20	0.42
1:A:152:ASN:ND2	3:A:797:HOH:O	2.52	0.42
1:A:50:ASP:N	1:A:50:ASP:OD1	2.52	0.41
1:A:313:ALA:CB	1:A:317:ILE:HD13	2.50	0.41
1:A:202:GLY:O	1:A:205:ALA:HB3	2.20	0.41
1:A:283:HIS:HE1	1:A:312:THR:O	2.04	0.41
1:A:152:ASN:CB	3:A:797:HOH:O	2.50	0.41
1:A:73:ALA:N	1:A:74:PRO:CD	2.83	0.41
1:A:332:THR:O	1:A:335:GLU:HB3	2.21	0.41
1:A:326:ASN:OD1	1:A:328:LYS:HE3	2.20	0.41
1:A:327:PRO:HA	1:A:330:ILE:HB	2.03	0.41
1:A:16:ASN:ND2	3:A:558:HOH:O	2.48	0.41
1:A:184:ARG:NH1	3:A:540:HOH:O	2.53	0.41
1:A:430:PHE:CD1	1:A:431:HIS:N	2.89	0.41
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.84	0.41
1:A:296:ASP:HA	1:A:306:TRP:CH2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:CB	1:A:404:GLU:HG3	2.51	0.40
1:A:66:LYS:HG3	3:A:680:HOH:O	2.21	0.40
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.90	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:474:HOH:O	3:A:665:HOH:O[4_564]	2.09	0.11

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%)	414 (95%)	17 (4%)	3 (1%)	18 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
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%)	319 (93%)	25 (7%)	13	12

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	57	MET
1	A	59	LYS
1	A	66	LYS
1	A	87	LYS
1	A	96	LEU
1	A	101	ASN
1	A	104	LYS
1	A	126	ASN
1	A	133	LEU
1	A	146	LEU
1	A	151	LEU
1	A	154	LEU
1	A	177	LYS
1	A	194	LYS
1	A	195	SER
1	A	229	VAL
1	A	254	LYS
1	A	255	ASP
1	A	264	ASN
1	A	284	SER
1	A	300	GLU
1	A	317	ILE
1	A	392	THR
1	A	424	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	43	HIS
1	A	63	HIS
1	A	101	ASN
1	A	126	ASN
1	A	152	ASN
1	A	155	ASN
1	A	217	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	219	GLN
1	A	266	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 ⓘ

1 ligand is 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	$\# Z > 2$
2	SO4	A	444	-	4,4,4	0.71	0	6,6,6	1.23	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	444	SO4	O4-S-O2	-2.05	98.83	109.56

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.