



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:43 PM UTC

PDB ID : 4MDH / pdb_00004mdh
Title : REFINED CRYSTAL STRUCTURE OF CYTOPLASMIC MALATE DEHYDROGENASE AT 2.5-ANGSTROMS RESOLUTION
Authors : Birktoft, J.J.; Banaszak, L.J.
Deposited on : 1989-04-12
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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

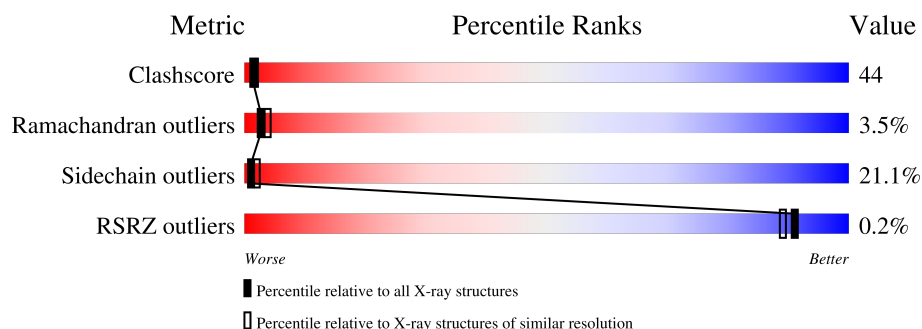
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	
1	B	334	

2 Entry composition [i](#)

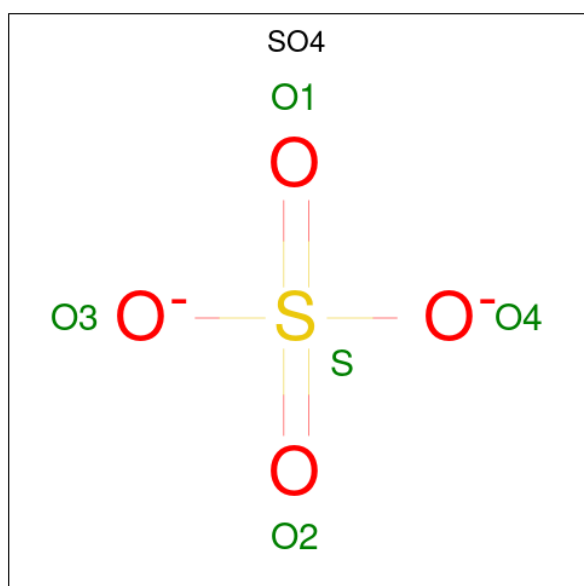
There are 4 unique types of molecules in this entry. The entry contains 5675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CYTOPLASMIC MALATE DEHYDROGENASE.

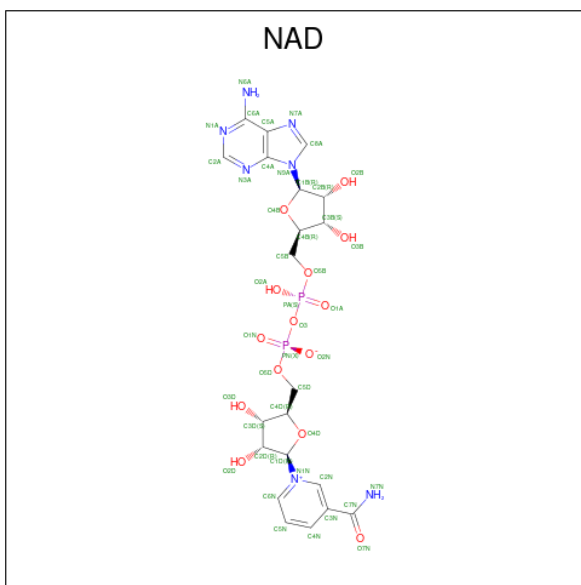
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2553	1625	427	488	13			
1	B	334	Total	C	N	O	S	0	0	0
			2553	1625	427	488	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
3	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

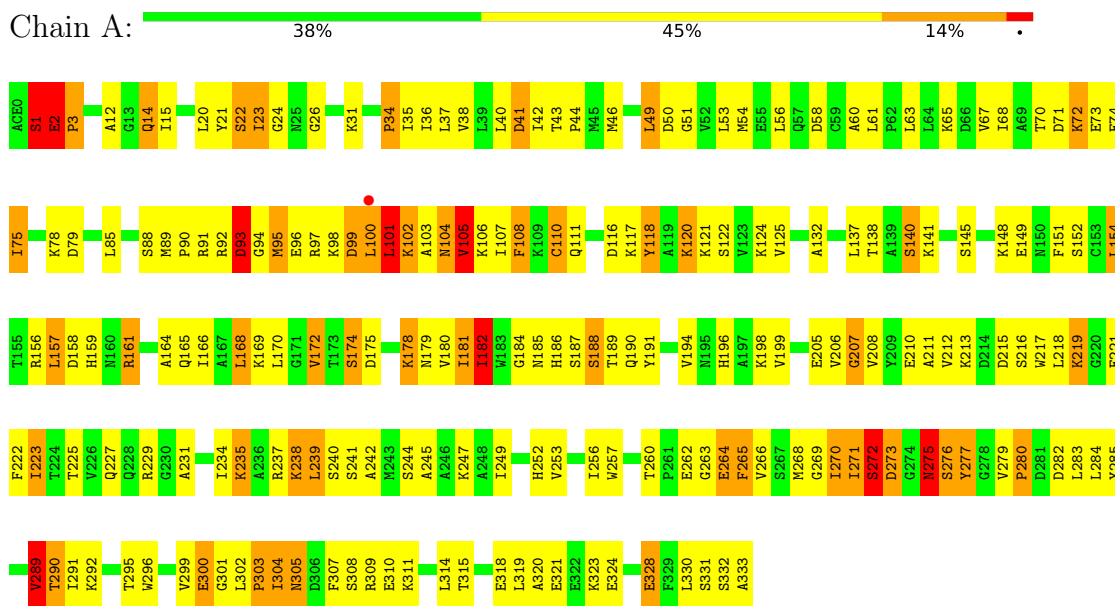
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	226	Total O 226 226	0	0
4	B	245	Total O 245 245	0	0

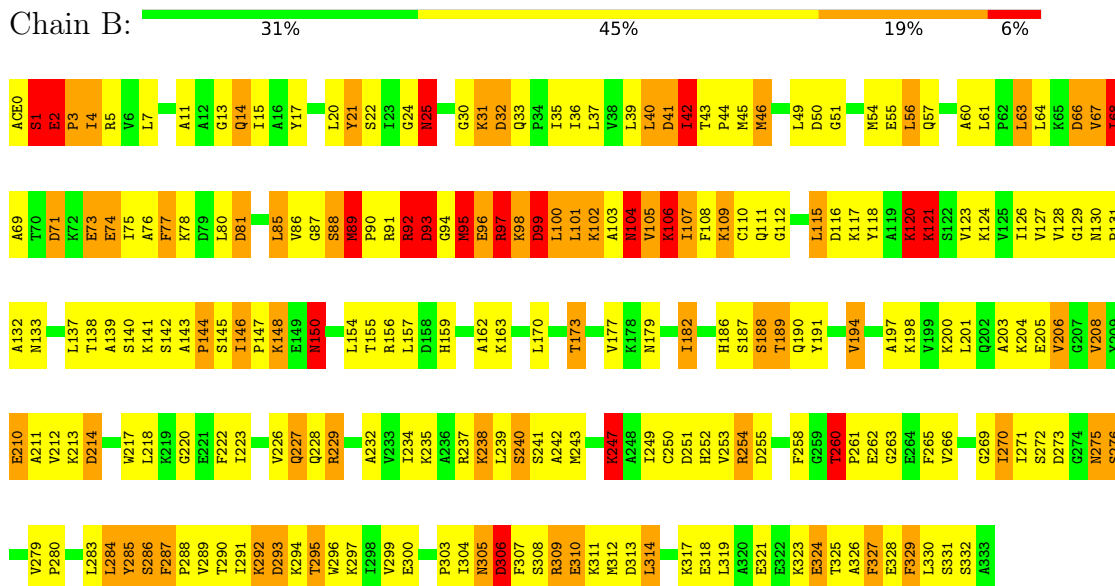
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CYTOPLASMIC MALATE DEHYDROGENASE



• Molecule 1: CYTOPLASMIC MALATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.20Å 86.60Å 58.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.50 6.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.50) 90.4 (6.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.167 , (Not available) 0.176 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 161.4	EDS
L-test for twinning ¹	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5675	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, SO4, NAD

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	1.30	3/2593 (0.1%)	1.86	65/3505 (1.9%)
1	B	1.36	11/2593 (0.4%)	1.94	91/3505 (2.6%)
All	All	1.33	14/5186 (0.3%)	1.90	156/7010 (2.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	LYS	CA-C	8.13	1.63	1.52
1	B	186	HIS	C-N	-6.32	1.27	1.33
1	B	324	GLU	CD-OE2	5.59	1.35	1.25
1	B	148	LYS	C-N	-5.57	1.26	1.34
1	B	210	GLU	CD-OE2	5.47	1.35	1.25
1	B	24	GLY	C-N	5.45	1.41	1.34
1	B	107	ILE	N-CA	5.28	1.52	1.46
1	B	306	ASP	CG-OD2	5.27	1.35	1.25
1	B	205	GLU	CD-OE2	5.18	1.35	1.25
1	A	14	GLN	CD-OE1	5.14	1.33	1.23
1	A	262	GLU	CD-OE2	5.13	1.35	1.25
1	A	215	ASP	CG-OD2	5.08	1.35	1.25
1	B	310	GLU	CD-OE2	5.04	1.34	1.25
1	B	25	ASN	N-CA	5.01	1.52	1.46

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	ASN	CB-CA-C	-9.61	94.23	109.70
1	A	95	MET	N-CA-C	-9.52	100.89	114.12
1	B	242	ALA	N-CA-C	9.51	121.25	111.07
1	B	214	ASP	CA-C-N	8.96	132.65	120.38
1	B	214	ASP	C-N-CA	8.96	132.65	120.38
1	A	93	ASP	CB-CA-C	8.61	124.01	109.72
1	A	101	LEU	CA-C-N	8.20	135.29	122.26
1	A	101	LEU	C-N-CA	8.20	135.29	122.26
1	B	99	ASP	N-CA-CB	8.07	124.13	110.49
1	B	327	PHE	N-CA-C	7.96	122.09	112.38
1	A	102	LYS	N-CA-C	-7.93	103.42	113.72
1	B	90	PRO	N-CA-CB	7.76	111.40	103.25
1	B	206	VAL	N-CA-C	7.71	117.76	110.74
1	A	118	TYR	N-CA-C	7.60	123.23	113.88
1	A	94	GLY	N-CA-C	-7.54	95.30	113.18
1	A	273	ASP	CA-CB-CG	-7.33	105.27	112.60
1	B	258	PHE	CA-CB-CG	-7.22	106.58	113.80
1	A	14	GLN	N-CA-C	7.17	118.74	111.07
1	A	50	ASP	N-CA-C	-7.06	103.58	111.28
1	B	331	SER	N-CA-C	7.04	121.31	113.21
1	A	50	ASP	CA-CB-CG	7.03	119.63	112.60
1	B	260	THR	N-CA-CB	6.96	117.82	109.74
1	A	74	GLU	N-CA-C	-6.90	104.83	113.18
1	A	132	ALA	CB-CA-C	6.89	121.87	110.92
1	A	207	GLY	N-CA-C	-6.87	103.28	112.14
1	B	21	TYR	CA-C-N	6.86	130.15	120.28
1	B	21	TYR	C-N-CA	6.86	130.15	120.28
1	B	73	GLU	N-CA-C	6.78	119.51	111.71
1	B	208	VAL	N-CA-C	6.75	117.44	110.36
1	A	289	VAL	N-CA-C	6.72	119.20	108.85
1	B	25	ASN	CB-CA-C	-6.61	97.64	110.46
1	A	24	GLY	CA-C-N	6.60	131.74	120.72
1	A	24	GLY	C-N-CA	6.60	131.74	120.72
1	B	99	ASP	CA-C-N	-6.60	112.00	122.76
1	B	99	ASP	C-N-CA	-6.60	112.00	122.76
1	A	102	LYS	CB-CA-C	-6.54	98.56	109.55
1	B	97	ARG	N-CA-CB	6.51	121.49	110.49
1	B	173	THR	CB-CA-C	6.50	121.27	109.37
1	A	2	GLU	CA-C-N	6.46	127.92	119.84
1	A	2	GLU	C-N-CA	6.46	127.92	119.84
1	A	110	CYS	N-CA-CB	6.45	119.61	110.12
1	A	132	ALA	N-CA-CB	6.42	119.58	109.82
1	A	154	LEU	N-CA-C	6.39	119.12	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	LYS	O-C-N	-6.28	115.88	123.16
1	B	14	GLN	N-CA-C	6.22	117.86	111.14
1	B	210	GLU	CA-C-N	6.21	128.51	120.44
1	B	210	GLU	C-N-CA	6.21	128.51	120.44
1	B	77	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	24	GLY	CA-C-N	6.19	129.42	120.38
1	B	24	GLY	C-N-CA	6.19	129.42	120.38
1	B	93	ASP	CA-CB-CG	-6.19	106.41	112.60
1	A	100	LEU	CB-CA-C	6.18	122.73	110.42
1	A	182	ILE	N-CA-CB	6.18	118.44	111.21
1	B	299	VAL	CA-C-N	-6.18	113.11	122.81
1	B	299	VAL	C-N-CA	-6.18	113.11	122.81
1	B	81	ASP	CA-CB-CG	-6.17	106.43	112.60
1	A	72	LYS	CA-C-N	-6.12	113.06	122.60
1	A	72	LYS	C-N-CA	-6.12	113.06	122.60
1	A	181	ILE	CA-C-N	-6.12	115.07	122.90
1	A	181	ILE	C-N-CA	-6.12	115.07	122.90
1	A	79	ASP	N-CA-C	6.08	119.92	111.90
1	B	90	PRO	CA-C-N	6.06	129.44	120.95
1	B	90	PRO	C-N-CA	6.06	129.44	120.95
1	B	328	GLU	N-CA-CB	6.05	119.42	110.53
1	A	105	VAL	CB-CA-C	6.00	120.24	112.14
1	A	328	GLU	N-CA-C	-5.99	106.10	113.41
1	A	175	ASP	CA-CB-CG	5.98	118.58	112.60
1	A	321	GLU	CA-C-N	5.97	128.28	120.28
1	A	321	GLU	C-N-CA	5.97	128.28	120.28
1	B	155	THR	N-CA-CB	5.93	118.81	110.98
1	B	89	MET	CA-C-N	5.92	127.24	119.84
1	B	89	MET	C-N-CA	5.92	127.24	119.84
1	B	226	VAL	CA-C-N	-5.91	111.90	120.29
1	B	226	VAL	C-N-CA	-5.91	111.90	120.29
1	A	23	ILE	N-CA-C	-5.91	105.09	110.82
1	B	24	GLY	CA-C-O	-5.89	114.63	121.00
1	A	277	TYR	N-CA-C	5.85	119.72	112.59
1	B	285	TYR	N-CA-CB	-5.80	101.57	110.85
1	B	24	GLY	O-C-N	5.78	127.73	122.18
1	A	280	PRO	N-CA-CB	5.74	108.78	103.39
1	B	162	ALA	CA-C-N	5.73	127.95	120.28
1	B	162	ALA	C-N-CA	5.73	127.95	120.28
1	B	71	ASP	N-CA-CB	-5.70	103.01	110.88
1	A	85	LEU	N-CA-C	5.68	118.53	108.24
1	A	272	SER	N-CA-C	5.61	117.84	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	TRP	N-CA-C	5.59	117.38	111.28
1	B	74	GLU	N-CA-CB	5.58	118.10	110.01
1	A	93	ASP	CA-CB-CG	-5.58	107.02	112.60
1	B	211	ALA	N-CA-C	5.57	117.03	111.07
1	B	263	GLY	CA-C-N	-5.57	113.19	122.21
1	B	263	GLY	C-N-CA	-5.57	113.19	122.21
1	B	41	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	108	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	215	ASP	N-CA-C	5.55	118.04	111.33
1	B	127	VAL	N-CA-C	5.54	116.37	107.73
1	B	93	ASP	N-CA-C	5.52	122.55	110.80
1	B	284	LEU	N-CA-CB	5.51	120.81	110.56
1	A	303	PRO	N-CA-CB	5.50	108.14	103.19
1	B	300	GLU	N-CA-C	5.47	118.47	109.72
1	B	31	LYS	N-CA-C	-5.47	106.45	113.01
1	A	36	ILE	N-CA-C	-5.45	98.61	107.28
1	A	104	ASN	N-CA-C	5.45	118.40	111.69
1	A	34	PRO	N-CA-CB	5.43	108.42	103.15
1	A	168	LEU	CA-C-N	5.43	127.50	120.44
1	A	168	LEU	C-N-CA	5.43	127.50	120.44
1	B	104	ASN	N-CA-C	-5.43	106.73	113.19
1	B	92	ARG	N-CA-CB	5.42	119.65	110.49
1	B	287	PHE	CA-CB-CG	5.41	119.21	113.80
1	B	150	ASN	CB-CA-C	5.39	121.15	110.42
1	A	101	LEU	N-CA-C	-5.39	99.32	110.80
1	B	251	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	89	MET	O-C-N	5.37	126.29	121.35
1	B	66	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	103	ALA	CA-C-N	5.35	129.72	120.58
1	A	103	ALA	C-N-CA	5.35	129.72	120.58
1	B	189	THR	CB-CA-C	5.35	119.21	110.17
1	A	132	ALA	N-CA-C	5.33	117.53	111.02
1	A	270	ILE	N-CA-CB	-5.33	105.72	112.60
1	B	120	LYS	CB-CA-C	-5.32	101.61	109.90
1	B	90	PRO	O-C-N	5.31	129.81	122.64
1	B	227	GLN	N-CA-CB	5.30	118.00	110.16
1	A	105	VAL	N-CA-C	5.30	116.03	110.62
1	B	286	SER	O-C-N	-5.29	117.19	123.22
1	A	92	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	B	150	ASN	CA-CB-CG	5.27	117.87	112.60
1	B	36	ILE	N-CA-C	-5.26	100.08	107.75
1	B	74	GLU	CB-CA-C	-5.26	102.63	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ILE	CB-CA-C	-5.24	105.23	112.24
1	B	42	ILE	N-CA-CB	-5.20	101.28	110.95
1	A	161	ARG	CA-C-N	5.16	127.15	120.44
1	A	161	ARG	C-N-CA	5.16	127.15	120.44
1	B	203	ALA	N-CA-C	-5.16	105.45	112.26
1	B	148	LYS	CA-C-N	5.13	127.67	120.28
1	B	148	LYS	C-N-CA	5.13	127.67	120.28
1	B	247	LYS	CA-C-N	5.13	127.58	120.29
1	B	247	LYS	C-N-CA	5.13	127.58	120.29
1	B	313	ASP	CA-C-N	5.13	127.15	120.28
1	B	313	ASP	C-N-CA	5.13	127.15	120.28
1	B	68	ILE	N-CA-C	5.12	116.03	108.45
1	B	137	LEU	N-CA-CB	5.11	117.42	110.01
1	B	144	PRO	CA-C-N	-5.09	112.23	121.14
1	B	144	PRO	C-N-CA	-5.09	112.23	121.14
1	B	173	THR	N-CA-CB	5.09	118.99	110.85
1	B	186	HIS	CA-C-N	-5.08	112.73	122.08
1	B	186	HIS	C-N-CA	-5.08	112.73	122.08
1	A	265	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	22	SER	CA-C-N	-5.05	113.52	120.74
1	A	22	SER	C-N-CA	-5.05	113.52	120.74
1	B	309	ARG	N-CA-CB	5.05	117.64	110.06
1	B	250	CYS	CA-C-N	5.04	127.44	120.29
1	B	250	CYS	C-N-CA	5.04	127.44	120.29
1	A	93	ASP	O-C-N	5.03	129.06	122.87
1	B	222	PHE	N-CA-C	-5.02	105.69	111.07
1	B	303	PRO	N-CA-CB	5.02	107.79	103.27
1	B	2	GLU	CA-C-N	5.02	126.12	119.84
1	B	2	GLU	C-N-CA	5.02	126.12	119.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	132	ALA	CA

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	2553	0	2618	232	1
1	B	2553	0	2618	233	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	44	0	26	4	0
3	B	44	0	26	5	0
4	A	226	0	0	29	0
4	B	245	0	0	27	0
All	All	5675	0	5288	461	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 44.

All (461) 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:101:LEU:HD21	1:A:104:ASN:ND2	1.29	1.42
1:B:204:LYS:HE3	1:B:206:VAL:HB	1.20	1.13
1:B:105:VAL:HG12	1:B:138:THR:HG21	1.28	1.12
1:B:98:LYS:HE2	1:B:101:LEU:HD13	1.33	1.10
1:A:178:LYS:HE3	1:A:264:GLU:HG2	1.34	1.10
1:A:101:LEU:CD2	1:A:104:ASN:ND2	2.15	1.09
1:B:100:LEU:HD11	1:B:102:LYS:HD2	1.35	1.09
1:A:12:ALA:HB2	1:A:49:LEU:HD21	1.33	1.05
1:A:159:HIS:HA	1:A:182:ILE:HD13	1.40	1.03
1:A:99:ASP:OD1	1:A:99:ASP:N	1.98	0.96
1:A:289:VAL:HG11	1:A:296:TRP:HB2	1.48	0.94
1:A:101:LEU:HD21	1:A:104:ASN:CG	1.93	0.92
1:A:91:ARG:HE	1:A:95:MET:HA	1.34	0.91
1:B:323:LYS:HG3	1:B:327:PHE:CE2	2.07	0.89
1:B:100:LEU:HD12	1:B:102:LYS:HB2	1.53	0.89
1:A:2:GLU:CG	1:A:3:PRO:HD2	2.05	0.85
1:A:223:ILE:HD12	1:A:311:LYS:NZ	1.92	0.84
1:B:98:LYS:HE2	1:B:101:LEU:CD1	2.07	0.84
1:A:304:ILE:CG2	1:A:309:ARG:HG2	2.09	0.83
1:B:126:ILE:HD13	1:B:253:VAL:HG22	1.58	0.83
1:A:289:VAL:CG1	1:A:296:TRP:HB2	2.07	0.83
1:B:49:LEU:HD23	1:B:69:ALA:HB1	1.60	0.82
1:B:304:ILE:HD12	1:B:312:MET:HE1	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:CE	1:B:206:VAL:HB	2.06	0.82
1:A:159:HIS:HA	1:A:182:ILE:CD1	2.11	0.81
1:A:12:ALA:HB2	1:A:49:LEU:CD2	2.09	0.81
1:A:223:ILE:HD12	1:A:311:LYS:HZ1	1.45	0.80
1:A:101:LEU:HD21	1:A:104:ASN:HD22	1.42	0.79
1:B:100:LEU:CD1	1:B:102:LYS:HD2	2.13	0.79
1:B:330:LEU:HD23	4:B:424:HOH:O	1.83	0.78
1:A:40:LEU:HD12	1:A:70:THR:O	1.83	0.78
1:A:304:ILE:HG22	1:A:309:ARG:HG2	1.66	0.78
1:B:102:LYS:O	1:B:105:VAL:HG23	1.84	0.78
1:A:319:LEU:HD22	4:A:534:HOH:O	1.84	0.78
1:A:72:LYS:HB2	1:A:75:ILE:HG13	1.65	0.78
1:B:105:VAL:CG1	1:B:138:THR:HG21	2.12	0.77
1:B:324:GLU:HG3	4:B:495:HOH:O	1.84	0.77
1:A:97:ARG:O	1:A:98:LYS:HG2	1.85	0.77
1:B:40:LEU:HD23	1:B:41:ASP:N	2.00	0.77
1:B:94:GLY:HA2	1:B:99:ASP:O	1.85	0.77
1:B:159:HIS:HA	1:B:182:ILE:HD13	1.65	0.77
1:A:206:VAL:HG22	1:A:207:GLY:H	1.49	0.76
1:B:100:LEU:CD1	1:B:102:LYS:HB2	2.16	0.76
1:B:40:LEU:HD12	1:B:76:ALA:CB	2.15	0.75
1:A:20:LEU:HD22	1:A:37:LEU:HD21	1.66	0.75
1:A:256:ILE:HG21	4:A:417:HOH:O	1.87	0.75
1:A:302:LEU:O	1:A:304:ILE:HD12	1.85	0.75
1:B:110:CYS:HB2	4:B:413:HOH:O	1.87	0.75
1:B:187:SER:O	1:B:190:GLN:HG2	1.86	0.75
1:B:260:THR:HG22	1:B:261:PRO:HD2	1.66	0.75
1:B:100:LEU:HD11	1:B:102:LYS:CD	2.15	0.75
1:A:1:SER:HB2	4:A:338:HOH:O	1.86	0.75
1:A:3:PRO:HA	1:A:34:PRO:O	1.87	0.74
1:B:101:LEU:HD23	4:B:367:HOH:O	1.85	0.74
1:B:106:LYS:O	1:B:109:LYS:HE2	1.87	0.74
1:B:107:ILE:O	1:B:111:GLN:HG3	1.88	0.74
1:A:101:LEU:CD2	1:A:104:ASN:HD22	1.97	0.74
1:A:285:TYR:HD2	1:A:319:LEU:HD12	1.52	0.74
1:B:179:ASN:HB3	1:B:265:PHE:CZ	2.21	0.74
1:A:93:ASP:HA	1:A:95:MET:HG3	1.69	0.74
1:A:31:LYS:HE3	4:A:372:HOH:O	1.87	0.74
1:B:121:LYS:HD2	1:B:145:SER:O	1.87	0.74
1:A:241:SER:HB2	3:A:335:NAD:H5N	1.69	0.73
1:A:182:ILE:HG12	4:A:518:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLY:HA2	1:B:286:SER:HA	1.71	0.73
1:B:280:PRO:HA	4:B:485:HOH:O	1.88	0.73
1:B:14:GLN:HG3	3:B:335:NAD:O2A	1.88	0.73
1:B:262:GLU:HG2	4:B:473:HOH:O	1.89	0.73
1:A:275:ASN:ND2	1:A:279:VAL:HB	2.04	0.72
1:A:159:HIS:CA	1:A:182:ILE:HD13	2.18	0.72
1:B:20:LEU:HD13	1:B:56:LEU:HD11	1.71	0.72
1:A:72:LYS:HD3	1:A:75:ILE:HG13	1.73	0.71
1:B:170:LEU:HD21	1:B:212:VAL:HG22	1.71	0.71
1:B:91:ARG:O	1:B:92:ARG:HG3	1.90	0.71
1:A:247:LYS:HD2	1:A:247:LYS:O	1.90	0.71
1:A:95:MET:HA	4:A:492:HOH:O	1.91	0.71
1:B:102:LYS:HB3	1:B:329:PHE:CE2	2.25	0.71
1:A:206:VAL:HG13	1:A:207:GLY:O	1.91	0.70
1:B:159:HIS:CA	1:B:182:ILE:HD13	2.21	0.70
1:A:149:GLU:HB3	4:A:352:HOH:O	1.90	0.70
1:A:275:ASN:ND2	1:A:279:VAL:O	2.24	0.70
1:A:72:LYS:CD	1:A:75:ILE:HG13	2.21	0.70
1:A:91:ARG:NH2	1:A:95:MET:O	2.25	0.70
1:A:63:LEU:HD13	4:A:342:HOH:O	1.91	0.70
1:B:271:ILE:HD12	1:B:283:LEU:O	1.90	0.70
1:A:307:PHE:CZ	1:A:311:LYS:HE3	2.27	0.69
1:A:305:ASN:O	1:A:309:ARG:HG3	1.93	0.69
1:B:103:ALA:HB2	1:B:329:PHE:CZ	2.27	0.69
1:A:96:GLU:N	4:A:491:HOH:O	2.26	0.69
1:A:206:VAL:HG21	1:A:210:GLU:OE2	1.90	0.69
1:B:94:GLY:O	1:B:99:ASP:HA	1.91	0.69
1:B:130:ASN:HA	1:B:132:ALA:N	2.08	0.68
1:A:49:LEU:N	1:A:49:LEU:HD23	2.07	0.68
1:B:159:HIS:HA	1:B:182:ILE:CD1	2.22	0.68
1:A:46:MET:HE3	1:A:71:ASP:HB3	1.76	0.68
1:A:91:ARG:HE	1:A:95:MET:CA	2.05	0.68
1:B:124:LYS:HG3	4:B:431:HOH:O	1.94	0.68
1:B:179:ASN:HB3	1:B:265:PHE:CE1	2.29	0.68
1:B:108:PHE:HB3	1:B:139:ALA:HB2	1.76	0.68
1:B:100:LEU:O	1:B:102:LYS:N	2.27	0.67
1:B:91:ARG:HD2	1:B:130:ASN:CB	2.24	0.67
1:B:237:ARG:NH1	1:B:240:SER:O	2.27	0.67
1:B:21:TYR:O	1:B:25:ASN:ND2	2.27	0.67
1:A:2:GLU:HG3	1:A:3:PRO:HD2	1.76	0.67
1:B:96:GLU:O	1:B:97:ARG:NE	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:HB2	1:A:319:LEU:HD21	1.77	0.67
1:B:40:LEU:HD12	1:B:76:ALA:HB1	1.75	0.67
1:A:101:LEU:CD2	1:A:104:ASN:CG	2.64	0.66
1:A:206:VAL:HG22	1:A:207:GLY:N	2.09	0.66
1:B:40:LEU:HD23	1:B:41:ASP:H	1.61	0.66
1:A:97:ARG:C	1:A:98:LYS:HG2	2.20	0.66
1:A:185:ASN:ND2	1:A:318:GLU:OE2	2.28	0.66
1:A:268:MET:HB3	1:A:289:VAL:HG21	1.75	0.66
1:B:109:LYS:HD3	4:B:424:HOH:O	1.95	0.66
1:B:272:SER:O	1:B:275:ASN:HB3	1.95	0.66
1:A:95:MET:HE1	1:A:231:ALA:HB1	1.78	0.66
1:B:43:THR:HB	1:B:44:PRO:HD3	1.76	0.66
1:B:304:ILE:HD12	1:B:312:MET:CE	2.24	0.66
1:A:174:SER:OG	1:B:60:ALA:HB1	1.96	0.65
1:A:99:ASP:HB2	4:A:442:HOH:O	1.95	0.65
1:A:218:LEU:HA	1:A:222:PHE:HB3	1.78	0.65
1:B:39:LEU:HB2	1:B:68:ILE:O	1.97	0.65
1:A:91:ARG:HG3	1:A:95:MET:HB3	1.77	0.65
1:A:137:LEU:HD21	1:A:323:LYS:HE3	1.78	0.65
1:B:91:ARG:HD2	1:B:130:ASN:HD22	1.61	0.65
1:A:272:SER:HB2	1:A:283:LEU:H	1.60	0.65
1:B:93:ASP:OD2	1:B:97:ARG:HB2	1.97	0.64
1:A:185:ASN:HB3	1:A:187:SER:HB2	1.78	0.64
1:B:170:LEU:HD21	1:B:212:VAL:CG2	2.28	0.64
1:A:185:ASN:CB	1:A:319:LEU:HD21	2.26	0.64
1:B:297:LYS:HE3	4:B:490:HOH:O	1.96	0.64
1:A:315:THR:O	1:A:319:LEU:HG	1.96	0.64
1:B:102:LYS:HB3	1:B:329:PHE:CD2	2.33	0.64
1:A:199:VAL:O	1:A:205:GLU:HA	1.97	0.64
1:B:74:GLU:O	1:B:74:GLU:HG3	1.95	0.64
1:B:232:ALA:O	1:B:235:LYS:HB3	1.98	0.64
1:A:71:ASP:HB2	4:A:526:HOH:O	1.98	0.63
1:B:98:LYS:HB2	4:B:570:HOH:O	1.98	0.63
1:B:51:GLY:HA2	1:B:54:MET:HE3	1.79	0.63
1:B:89:MET:O	1:B:101:LEU:HD21	1.98	0.63
1:A:26:GLY:HA2	4:A:342:HOH:O	1.98	0.63
1:A:101:LEU:HD23	1:A:104:ASN:HB2	1.79	0.63
1:A:96:GLU:OE1	1:A:235:LYS:NZ	2.30	0.63
1:B:1:SER:O	1:B:2:GLU:HB3	1.97	0.62
1:B:42:ILE:HG22	1:B:45:MET:HG2	1.81	0.62
1:B:111:GLN:O	1:B:115:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TYR:CE1	1:A:61:LEU:HD21	2.35	0.62
1:B:275:ASN:HD21	1:B:279:VAL:H	1.47	0.62
1:B:276:SER:HB3	4:B:482:HOH:O	1.98	0.62
1:B:94:GLY:N	1:B:98:LYS:O	2.32	0.62
1:A:187:SER:O	1:A:190:GLN:HG2	2.00	0.62
1:B:85:LEU:HB2	1:B:108:PHE:HE1	1.65	0.62
1:A:110:CYS:HB2	4:A:535:HOH:O	1.98	0.61
1:A:268:MET:HE2	1:A:270:ILE:CG2	2.30	0.61
1:A:320:ALA:O	1:A:324:GLU:HG3	2.01	0.61
1:B:287:PHE:HB3	1:B:288:PRO:HD2	1.82	0.61
1:B:156:ARG:O	1:B:156:ARG:HG3	2.00	0.61
1:B:270:ILE:HD13	1:B:296:TRP:CZ3	2.36	0.61
1:A:152:SER:HB3	1:A:268:MET:HE3	1.83	0.61
1:A:268:MET:HE1	1:A:296:TRP:CD1	2.36	0.61
1:B:80:LEU:O	1:B:120:LYS:HB2	2.01	0.61
1:B:217:TRP:CZ3	1:B:218:LEU:HD23	2.36	0.61
1:A:280:PRO:HB3	4:A:478:HOH:O	2.00	0.60
1:B:254:ARG:NH1	4:B:374:HOH:O	2.33	0.60
1:B:33:GLN:O	1:B:63:LEU:HD13	2.00	0.60
1:A:208:VAL:O	1:A:212:VAL:HG23	2.01	0.60
1:A:275:ASN:HD22	1:A:279:VAL:H	1.50	0.59
1:B:235:LYS:HG3	4:B:564:HOH:O	2.02	0.59
1:B:42:ILE:HG22	1:B:45:MET:CG	2.31	0.59
1:A:307:PHE:CE1	1:A:311:LYS:HE3	2.37	0.59
1:A:221:GLU:HG2	1:A:221:GLU:O	2.02	0.59
1:B:194:VAL:HG21	1:B:208:VAL:CG1	2.33	0.59
1:A:276:SER:OG	1:A:300:GLU:HG2	2.03	0.59
1:B:326:ALA:O	1:B:330:LEU:HD12	2.03	0.59
1:A:157:LEU:HD12	1:A:157:LEU:O	2.03	0.59
1:A:184:GLY:HA3	1:A:315:THR:HG21	1.84	0.58
1:B:304:ILE:HG21	1:B:312:MET:CE	2.33	0.58
1:A:217:TRP:CZ3	1:A:218:LEU:HD23	2.38	0.58
1:B:2:GLU:OE2	1:B:3:PRO:HD2	2.03	0.58
1:A:95:MET:HG3	4:A:491:HOH:O	2.03	0.58
1:A:309:ARG:HB3	4:A:359:HOH:O	2.02	0.58
1:B:91:ARG:HD2	1:B:130:ASN:HB2	1.84	0.58
1:B:77:PHE:HA	1:B:80:LEU:HD11	1.85	0.58
1:A:96:GLU:CD	1:A:235:LYS:HZ3	2.11	0.58
1:A:285:TYR:CD2	1:A:319:LEU:HD12	2.36	0.58
1:B:304:ILE:HG21	1:B:312:MET:HE1	1.85	0.58
1:B:124:LYS:HD3	1:B:150:ASN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ASN:ND2	1:B:279:VAL:O	2.37	0.57
1:B:237:ARG:CZ	1:B:239:LEU:HB2	2.35	0.57
1:B:305:ASN:C	1:B:305:ASN:HD22	2.12	0.57
1:B:309:ARG:HG3	4:B:343:HOH:O	2.04	0.57
1:B:14:GLN:NE2	4:B:475:HOH:O	2.37	0.57
1:B:4:ILE:HD12	1:B:33:GLN:CD	2.30	0.57
1:B:37:LEU:HB3	1:B:67:VAL:HG13	1.86	0.57
1:A:184:GLY:HA3	1:A:315:THR:CG2	2.34	0.57
1:A:242:ALA:HB3	1:B:17:TYR:OH	2.05	0.57
1:A:95:MET:CE	1:A:231:ALA:HB1	2.36	0.56
1:A:90:PRO:HG3	3:A:335:NAD:O1A	2.05	0.56
1:A:165:GLN:OE1	1:A:165:GLN:HA	2.05	0.56
1:A:186:HIS:HB3	4:A:441:HOH:O	2.05	0.56
1:B:317:LYS:O	1:B:321:GLU:HG3	2.06	0.56
1:B:121:LYS:HE3	1:B:147:PRO:CD	2.36	0.56
1:B:212:VAL:HG12	1:B:214:ASP:H	1.71	0.56
1:A:152:SER:HA	1:A:269:GLY:O	2.05	0.55
1:A:282:ASP:OD1	1:A:323:LYS:NZ	2.28	0.55
1:A:187:SER:HB3	1:A:189:THR:H	1.71	0.55
1:A:277:TYR:HD1	1:A:304:ILE:HD13	1.72	0.55
1:A:2:GLU:HG2	1:A:3:PRO:HD2	1.88	0.55
1:B:138:THR:HG21	1:B:330:LEU:HD21	1.89	0.55
3:A:335:NAD:H6N	4:A:552:HOH:O	2.05	0.55
1:A:137:LEU:HD21	1:A:323:LYS:CE	2.37	0.54
1:A:223:ILE:HG21	1:A:311:LYS:HZ2	1.72	0.54
1:A:51:GLY:O	1:A:54:MET:HB2	2.07	0.54
1:B:129:GLY:HA2	3:B:335:NAD:O3D	2.07	0.54
1:A:161:ARG:O	1:A:164:ALA:HB3	2.07	0.54
1:B:109:LYS:HG3	1:B:110:CYS:H	1.73	0.54
1:B:304:ILE:HB	4:B:384:HOH:O	2.08	0.54
1:A:245:ALA:O	1:A:249:ILE:HG13	2.08	0.54
1:A:185:ASN:O	1:A:190:GLN:HB3	2.08	0.54
1:B:98:LYS:CE	1:B:101:LEU:HD13	2.22	0.54
1:A:227:GLN:OE1	4:A:522:HOH:O	2.19	0.53
1:A:91:ARG:NE	1:A:95:MET:HB2	2.24	0.53
1:A:305:ASN:OD1	1:A:305:ASN:N	2.29	0.53
1:B:306:ASP:CG	1:B:307:PHE:N	2.65	0.53
1:A:196:HIS:HA	4:A:447:HOH:O	2.08	0.53
1:B:66:ASP:OD1	1:B:68:ILE:HD11	2.09	0.53
1:B:91:ARG:C	1:B:92:ARG:HG3	2.33	0.53
1:B:76:ALA:O	1:B:80:LEU:HD21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD13	1:B:100:LEU:C	2.33	0.53
1:B:142:SER:C	1:B:144:PRO:HD3	2.33	0.53
1:A:285:TYR:CD2	1:A:319:LEU:CD1	2.92	0.53
1:B:91:ARG:HD2	1:B:130:ASN:ND2	2.22	0.53
1:A:289:VAL:HG11	1:A:296:TRP:CB	2.31	0.53
1:A:275:ASN:HD22	1:A:279:VAL:N	2.07	0.53
1:B:102:LYS:HB3	1:B:329:PHE:HE2	1.72	0.53
1:B:323:LYS:HG3	1:B:327:PHE:HE2	1.69	0.52
1:B:13:GLY:HA3	3:B:335:NAD:O5B	2.10	0.52
1:B:93:ASP:HB2	1:B:98:LYS:N	2.24	0.52
1:A:93:ASP:OD2	4:A:504:HOH:O	2.19	0.52
1:A:170:LEU:HD13	1:A:199:VAL:HG11	1.91	0.52
1:B:91:ARG:HG3	4:B:367:HOH:O	2.10	0.52
1:B:247:LYS:HD2	1:B:247:LYS:C	2.34	0.52
1:B:326:ALA:C	1:B:330:LEU:HD12	2.34	0.52
1:A:304:ILE:HG22	1:A:309:ARG:CG	2.38	0.52
1:A:219:LYS:HD2	1:A:307:PHE:CE2	2.44	0.51
1:B:25:ASN:N	1:B:25:ASN:HD22	2.08	0.51
1:B:121:LYS:HE3	1:B:147:PRO:HD3	1.90	0.51
1:B:123:VAL:O	1:B:150:ASN:ND2	2.43	0.51
1:A:247:LYS:HD2	1:A:247:LYS:C	2.35	0.51
1:A:15:ILE:HG12	1:A:242:ALA:HA	1.93	0.51
1:A:117:LYS:HD2	1:A:118:TYR:CZ	2.46	0.51
1:A:148:LYS:HE2	1:A:271:ILE:HG21	1.91	0.51
1:A:158:ASP:HB3	4:A:518:HOH:O	2.10	0.51
1:A:244:SER:OG	1:B:55:GLU:OE1	2.26	0.51
1:A:72:LYS:HD3	1:A:75:ILE:CG1	2.39	0.51
1:A:165:GLN:HB2	1:A:222:PHE:HE2	1.76	0.51
1:B:93:ASP:HB3	1:B:97:ARG:H	1.75	0.51
1:B:290:THR:O	1:B:296:TRP:HA	2.10	0.50
1:B:124:LYS:HE3	1:B:294:LYS:HB3	1.93	0.50
1:B:159:HIS:N	1:B:182:ILE:HD13	2.26	0.50
1:B:194:VAL:HG21	1:B:208:VAL:HG11	1.94	0.50
1:A:206:VAL:HG21	1:A:210:GLU:CD	2.36	0.50
1:B:46:MET:O	1:B:50:ASP:OD2	2.30	0.50
1:B:93:ASP:HB3	1:B:97:ARG:N	2.27	0.50
1:A:188:SER:O	1:A:227:GLN:OE1	2.29	0.50
1:A:91:ARG:CZ	1:A:99:ASP:HB3	2.41	0.50
1:A:98:LYS:C	1:A:99:ASP:OD1	2.53	0.50
1:A:217:TRP:CZ3	1:A:218:LEU:CD2	2.95	0.50
1:B:141:LYS:HE3	1:B:327:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:HB2	1:B:104:ASN:OD1	2.12	0.49
1:B:237:ARG:O	1:B:238:LYS:HB3	2.11	0.49
1:B:308:SER:O	1:B:312:MET:HG3	2.11	0.49
1:B:39:LEU:HD13	1:B:67:VAL:HG12	1.93	0.49
1:B:89:MET:HB3	4:B:512:HOH:O	2.10	0.49
1:B:305:ASN:ND2	1:B:308:SER:H	2.10	0.49
1:B:194:VAL:HG21	1:B:208:VAL:HG12	1.95	0.49
1:A:91:ARG:NE	1:A:95:MET:HA	2.16	0.49
1:A:223:ILE:HG21	1:A:311:LYS:NZ	2.28	0.49
1:A:249:ILE:O	1:A:253:VAL:HG23	2.13	0.49
1:A:206:VAL:CG1	1:A:211:ALA:HB2	2.43	0.49
1:B:148:LYS:HD2	1:B:271:ILE:HG12	1.95	0.49
1:B:260:THR:HG21	1:B:266:VAL:HG13	1.94	0.49
1:A:156:ARG:HH12	1:A:266:VAL:HG11	1.78	0.49
1:B:106:LYS:O	1:B:109:LYS:HG3	2.13	0.49
1:B:146:ILE:HG22	1:B:150:ASN:HD21	1.78	0.49
1:B:210:GLU:HG3	4:B:395:HOH:O	2.13	0.49
1:A:169:LYS:HD3	1:A:217:TRP:CZ2	2.47	0.49
1:A:184:GLY:HA2	1:A:285:TYR:CE2	2.48	0.49
1:A:179:ASN:OD1	1:A:264:GLU:HA	2.13	0.48
1:A:275:ASN:ND2	1:A:279:VAL:CB	2.76	0.48
1:B:86:VAL:O	3:B:335:NAD:H4D	2.13	0.48
1:B:103:ALA:C	1:B:105:VAL:H	2.20	0.48
1:A:277:TYR:CD1	1:A:304:ILE:HD13	2.48	0.48
1:B:194:VAL:HG23	1:B:194:VAL:O	2.12	0.48
1:B:106:LYS:HA	4:B:424:HOH:O	2.13	0.48
1:A:165:GLN:NE2	1:A:225:THR:HG21	2.28	0.48
1:B:220:GLY:O	1:B:223:ILE:HB	2.13	0.48
1:B:141:LYS:CE	1:B:327:PHE:CZ	2.97	0.48
1:B:287:PHE:HB3	1:B:288:PRO:CD	2.44	0.48
1:A:72:LYS:HD3	1:A:75:ILE:CD1	2.44	0.48
1:B:25:ASN:ND2	1:B:25:ASN:H	2.12	0.48
1:A:107:ILE:O	1:A:111:GLN:HG3	2.14	0.47
1:A:235:LYS:HB2	1:A:235:LYS:HE3	1.33	0.47
1:B:91:ARG:NE	1:B:130:ASN:HB3	2.29	0.47
1:B:154:LEU:HD12	1:B:252:HIS:CD2	2.49	0.47
1:B:291:ILE:HA	1:B:295:THR:O	2.15	0.47
1:A:14:GLN:CD	1:A:242:ALA:HB2	2.40	0.47
1:A:238:LYS:O	1:A:239:LEU:HD13	2.15	0.47
1:B:189:THR:OG1	1:B:318:GLU:OE2	2.29	0.47
1:B:42:ILE:CG2	1:B:45:MET:HG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA2	1:A:54:MET:HE3	1.97	0.47
1:A:56:LEU:HD23	1:B:243:MET:SD	2.54	0.47
1:A:289:VAL:HG12	1:A:290:THR:N	2.30	0.47
1:B:77:PHE:CD2	1:B:115:LEU:HG	2.50	0.47
1:A:307:PHE:CZ	1:A:311:LYS:CE	2.98	0.47
1:A:206:VAL:CG2	1:A:207:GLY:H	2.23	0.47
1:B:102:LYS:C	1:B:329:PHE:CE2	2.93	0.47
1:B:130:ASN:ND2	2:B:334:SO4:O1	2.40	0.47
1:B:228:GLN:O	1:B:228:GLN:HG2	2.13	0.47
1:B:275:ASN:HD21	1:B:279:VAL:N	2.12	0.47
1:A:38:VAL:HG22	1:A:68:ILE:HD13	1.97	0.46
1:B:30:GLY:C	1:B:32:ASP:H	2.20	0.46
1:B:43:THR:OG1	1:B:71:ASP:OD2	2.28	0.46
1:A:40:LEU:HG	1:A:41:ASP:N	2.29	0.46
1:B:130:ASN:HA	1:B:131:PRO:C	2.39	0.46
1:B:201:LEU:HD12	1:B:206:VAL:HG11	1.98	0.46
1:A:275:ASN:ND2	1:A:279:VAL:CA	2.79	0.46
1:A:140:SER:HB2	1:A:151:PHE:CD1	2.50	0.46
1:A:179:ASN:ND2	1:A:263:GLY:O	2.41	0.46
1:A:277:TYR:CD1	1:A:304:ILE:CD1	2.98	0.46
1:B:163:LYS:HE3	1:B:177:VAL:O	2.16	0.46
1:A:188:SER:HA	1:A:227:GLN:HB2	1.96	0.46
1:A:72:LYS:CB	1:A:75:ILE:HG13	2.42	0.46
1:A:98:LYS:HA	1:A:99:ASP:OD1	2.16	0.46
1:A:108:PHE:N	1:A:108:PHE:CD2	2.81	0.46
1:A:268:MET:CE	1:A:296:TRP:CD1	2.98	0.46
1:B:133:ASN:HB2	4:B:362:HOH:O	2.15	0.46
1:B:327:PHE:HD1	1:B:330:LEU:HD12	1.81	0.46
1:B:43:THR:N	1:B:44:PRO:CD	2.79	0.46
1:B:102:LYS:CB	1:B:329:PHE:HE2	2.29	0.46
1:A:95:MET:SD	1:A:96:GLU:HG3	2.56	0.45
1:A:223:ILE:HD12	1:A:311:LYS:CE	2.45	0.45
1:B:86:VAL:O	1:B:86:VAL:HG12	2.15	0.45
1:B:307:PHE:CZ	1:B:311:LYS:HE2	2.51	0.45
1:A:165:GLN:NE2	1:A:225:THR:CG2	2.80	0.45
1:A:178:LYS:CG	1:A:179:ASN:N	2.79	0.45
1:B:156:ARG:NH1	1:B:255:ASP:OD1	2.30	0.45
1:A:91:ARG:NH2	1:A:99:ASP:OD2	2.49	0.45
1:B:43:THR:N	1:B:44:PRO:HD2	2.32	0.45
1:B:94:GLY:C	1:B:99:ASP:HA	2.41	0.45
1:B:156:ARG:HA	1:B:159:HIS:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:O	1:A:102:LYS:N	2.50	0.45
1:B:143:ALA:HB1	1:B:146:ILE:HG13	1.98	0.45
1:A:154:LEU:HD12	1:A:252:HIS:CD2	2.52	0.45
1:B:95:MET:C	1:B:97:ARG:N	2.72	0.45
1:B:293:ASP:N	4:B:519:HOH:O	2.22	0.45
1:B:220:GLY:O	1:B:223:ILE:N	2.50	0.45
1:A:125:VAL:HG21	1:A:151:PHE:CE2	2.52	0.44
1:B:0:ACE:O	1:B:1:SER:OG	2.35	0.44
1:B:295:THR:HB	4:B:519:HOH:O	2.17	0.44
1:A:282:ASP:HB2	4:A:473:HOH:O	2.17	0.44
1:B:130:ASN:HA	1:B:132:ALA:H	1.80	0.44
1:B:201:LEU:O	1:B:204:LYS:HG3	2.18	0.44
1:A:157:LEU:O	1:A:161:ARG:HG3	2.17	0.44
1:A:91:ARG:NE	1:A:95:MET:CB	2.81	0.44
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.95	0.44
1:B:5:ARG:NH2	1:B:78:LYS:O	2.50	0.44
1:A:156:ARG:NH1	1:A:266:VAL:HG11	2.33	0.44
1:B:112:GLY:O	1:B:116:ASP:N	2.39	0.44
1:B:61:LEU:HB2	1:B:64:LEU:HD12	1.99	0.44
1:B:138:THR:CG2	1:B:330:LEU:HD21	2.47	0.44
1:A:93:ASP:OD2	1:A:95:MET:HE3	2.18	0.44
1:A:185:ASN:CG	1:A:319:LEU:CD2	2.91	0.44
1:A:234:ILE:HA	1:A:239:LEU:O	2.18	0.44
1:A:277:TYR:OH	1:A:299:VAL:O	2.28	0.44
1:A:172:VAL:HG12	4:A:435:HOH:O	2.18	0.43
1:A:212:VAL:O	1:A:213:LYS:HB2	2.16	0.43
1:B:130:ASN:HB3	1:B:131:PRO:HA	1.99	0.43
1:A:41:ASP:OD2	1:A:42:ILE:HG12	2.18	0.43
1:A:91:ARG:CG	1:A:95:MET:CB	2.96	0.43
1:A:237:ARG:NH1	1:A:239:LEU:HD23	2.32	0.43
1:A:2:GLU:CB	1:A:3:PRO:HD2	2.47	0.43
1:A:181:ILE:CG1	1:A:265:PHE:HE1	2.31	0.43
1:A:328:GLU:O	1:A:332:SER:HB2	2.19	0.43
1:A:105:VAL:HG13	1:A:330:LEU:HD21	2.00	0.43
1:B:105:VAL:HG12	1:B:138:THR:CG2	2.21	0.43
1:A:120:LYS:C	1:A:122:SER:N	2.77	0.43
1:B:20:LEU:HA	1:B:20:LEU:HD23	1.71	0.43
1:B:21:TYR:CZ	1:B:25:ASN:ND2	2.87	0.43
1:B:102:LYS:HD3	1:B:325:THR:HG22	2.01	0.43
1:B:187:SER:OG	1:B:188:SER:N	2.49	0.43
1:B:197:ALA:HB3	1:B:208:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:53:LEU:HA	1.86	0.43
1:A:120:LYS:C	1:A:122:SER:H	2.26	0.43
1:A:229:ARG:NH2	1:B:57:GLN:OE1	2.41	0.43
1:A:332:SER:OG	1:A:333:ALA:N	2.51	0.43
1:A:270:ILE:HD12	1:A:296:TRP:CZ3	2.54	0.42
1:A:101:LEU:CD2	1:A:104:ASN:HB2	2.48	0.42
3:A:335:NAD:H8A	4:A:503:HOH:O	2.20	0.42
1:B:157:LEU:HB3	4:B:358:HOH:O	2.20	0.42
1:A:116:ASP:OD1	1:A:145:SER:OG	2.28	0.42
1:A:124:LYS:HB3	4:A:417:HOH:O	2.18	0.42
1:A:271:ILE:HD12	1:A:272:SER:H	1.83	0.42
1:A:271:ILE:HD12	1:A:283:LEU:O	2.19	0.42
1:A:277:TYR:OH	1:A:300:GLU:HA	2.18	0.42
1:B:109:LYS:HG3	1:B:110:CYS:N	2.33	0.42
1:B:307:PHE:CZ	1:B:311:LYS:CE	3.02	0.42
1:B:292:LYS:HB3	4:B:519:HOH:O	2.19	0.42
1:B:304:ILE:CG2	1:B:312:MET:CE	2.97	0.42
1:A:43:THR:HB	1:A:44:PRO:HD3	2.02	0.42
1:B:81:ASP:C	1:B:123:VAL:HG23	2.45	0.42
1:A:91:ARG:NE	1:A:95:MET:CA	2.79	0.42
1:A:260:THR:HG23	1:A:291:ILE:HD12	2.01	0.42
1:B:64:LEU:HD22	1:B:67:VAL:HG22	2.01	0.42
1:B:293:ASP:C	1:B:294:LYS:CG	2.93	0.42
1:A:180:VAL:HG23	4:A:514:HOH:O	2.19	0.42
1:A:301:GLY:O	1:A:303:PRO:HD3	2.19	0.42
1:B:37:LEU:HD12	1:B:64:LEU:HD21	2.01	0.42
1:B:327:PHE:HD1	1:B:330:LEU:CD1	2.32	0.42
1:B:327:PHE:CD1	1:B:330:LEU:CD1	3.03	0.42
1:A:95:MET:HE3	1:A:235:LYS:HE2	2.01	0.42
1:B:191:TYR:HE1	1:B:308:SER:HG	1.62	0.42
1:B:285:TYR:HB3	1:B:287:PHE:CE1	2.54	0.42
1:A:34:PRO:HG3	1:A:65:LYS:NZ	2.35	0.41
1:A:157:LEU:HD22	1:A:245:ALA:HA	2.02	0.41
1:A:166:ILE:O	1:A:169:LYS:HB3	2.19	0.41
1:B:21:TYR:HE1	1:B:61:LEU:HD21	1.85	0.41
1:A:96:GLU:CD	1:A:235:LYS:NZ	2.76	0.41
1:A:276:SER:CB	1:A:300:GLU:HG2	2.49	0.41
1:B:46:MET:HE2	1:B:46:MET:HB3	1.91	0.41
1:B:314:LEU:HB3	4:B:359:HOH:O	2.19	0.41
1:A:34:PRO:CG	1:A:65:LYS:HZ2	2.34	0.41
1:A:58:ASP:OD2	1:B:229:ARG:NE	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HG3	1:A:95:MET:CB	2.45	0.41
1:B:100:LEU:CD1	1:B:100:LEU:C	2.93	0.41
1:A:178:LYS:HG3	1:A:179:ASN:N	2.35	0.41
1:B:103:ALA:C	1:B:105:VAL:N	2.79	0.41
1:B:197:ALA:O	1:B:198:LYS:HD3	2.20	0.41
1:A:138:THR:HG21	1:A:330:LEU:HD11	2.03	0.41
1:A:234:ILE:HG12	1:A:240:SER:HB3	2.03	0.41
1:A:290:THR:O	1:A:296:TRP:HA	2.21	0.41
1:A:275:ASN:HD21	1:A:279:VAL:C	2.28	0.41
1:B:293:ASP:O	1:B:294:LYS:HG3	2.20	0.41
1:A:91:ARG:CG	1:A:95:MET:HB2	2.51	0.41
1:A:191:TYR:CD2	1:A:311:LYS:HD2	2.56	0.41
1:A:206:VAL:CG2	1:A:207:GLY:N	2.77	0.41
1:B:87:GLY:O	1:B:88:SER:HB3	2.21	0.41
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.95	0.41
1:B:128:VAL:O	3:B:335:NAD:H2N	2.21	0.41
1:A:21:TYR:HE1	1:A:61:LEU:HD21	1.85	0.40
1:A:157:LEU:HB3	4:A:424:HOH:O	2.20	0.40
1:A:299:VAL:HG22	4:A:484:HOH:O	2.20	0.40
1:B:110:CYS:O	1:B:110:CYS:SG	2.79	0.40
1:B:138:THR:HG23	1:B:330:LEU:HD22	2.03	0.40
1:B:190:GLN:CG	1:B:227:GLN:HG2	2.51	0.40
1:A:101:LEU:HD23	1:A:104:ASN:CB	2.50	0.40
1:B:194:VAL:CG2	1:B:208:VAL:CG1	2.98	0.40
1:B:30:GLY:C	1:B:32:ASP:N	2.78	0.40
1:B:210:GLU:HB2	4:B:395:HOH:O	2.21	0.40
1:A:152:SER:CB	1:A:268:MET:HE3	2.51	0.40
1:B:96:GLU:CD	1:B:97:ARG:HH21	2.29	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)
1:A:324:GLU:OE2	1:A:324:GLU:OE2[2_565]	1.48	0.72

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	305 (92%)	20 (6%)	7 (2%)	5	9
1	B	332/334 (99%)	290 (87%)	26 (8%)	16 (5%)	2	2
All	All	664/668 (99%)	595 (90%)	46 (7%)	23 (4%)	3	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1	SER
1	B	93	ASP
1	B	101	LEU
1	A	1	SER
1	A	3	PRO
1	A	101	LEU
1	A	273	ASP
1	B	11	ALA
1	B	97	ARG
1	B	106	LYS
1	A	88	SER
1	B	98	LYS
1	B	99	ASP
1	B	229	ARG
1	B	273	ASP
1	B	2	GLU
1	B	3	PRO
1	B	88	SER
1	B	121	LYS
1	A	60	ALA
1	B	95	MET
1	B	240	SER
1	A	172	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/280 (100%)	229 (82%)	51 (18%)	2	3
1	B	280/280 (100%)	213 (76%)	67 (24%)	1	1
All	All	560/560 (100%)	442 (79%)	118 (21%)	1	2

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	GLU
1	A	22	SER
1	A	23	ILE
1	A	35	ILE
1	A	41	ASP
1	A	49	LEU
1	A	67	VAL
1	A	73	GLU
1	A	75	ILE
1	A	78	LYS
1	A	89	MET
1	A	93	ASP
1	A	99	ASP
1	A	105	VAL
1	A	106	LYS
1	A	120	LYS
1	A	121	LYS
1	A	140	SER
1	A	141	LYS
1	A	157	LEU
1	A	168	LEU
1	A	174	SER
1	A	178	LYS
1	A	182	ILE
1	A	188	SER
1	A	194	VAL

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Mol	Chain	Res	Type
1	A	198	LYS
1	A	216	SER
1	A	219	LYS
1	A	223	ILE
1	A	235	LYS
1	A	238	LYS
1	A	239	LEU
1	A	264	GLU
1	A	271	ILE
1	A	272	SER
1	A	275	ASN
1	A	276	SER
1	A	284	LEU
1	A	289	VAL
1	A	290	THR
1	A	292	LYS
1	A	295	THR
1	A	300	GLU
1	A	304	ILE
1	A	305	ASN
1	A	308	SER
1	A	310	GLU
1	A	314	LEU
1	A	331	SER
1	B	1	SER
1	B	2	GLU
1	B	4	ILE
1	B	7	LEU
1	B	15	ILE
1	B	22	SER
1	B	25	ASN
1	B	31	LYS
1	B	32	ASP
1	B	35	ILE
1	B	40	LEU
1	B	42	ILE
1	B	46	MET
1	B	56	LEU
1	B	63	LEU
1	B	67	VAL
1	B	68	ILE
1	B	73	GLU

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Mol	Chain	Res	Type
1	B	75	ILE
1	B	85	LEU
1	B	89	MET
1	B	92	ARG
1	B	95	MET
1	B	96	GLU
1	B	97	ARG
1	B	99	ASP
1	B	100	LEU
1	B	102	LYS
1	B	104	ASN
1	B	105	VAL
1	B	109	LYS
1	B	115	LEU
1	B	117	LYS
1	B	118	TYR
1	B	120	LYS
1	B	121	LYS
1	B	140	SER
1	B	146	ILE
1	B	150	ASN
1	B	173	THR
1	B	182	ILE
1	B	188	SER
1	B	194	VAL
1	B	200	LYS
1	B	213	LYS
1	B	234	ILE
1	B	238	LYS
1	B	241	SER
1	B	247	LYS
1	B	249	ILE
1	B	254	ARG
1	B	260	THR
1	B	270	ILE
1	B	275	ASN
1	B	276	SER
1	B	284	LEU
1	B	289	VAL
1	B	292	LYS
1	B	293	ASP
1	B	295	THR

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Mol	Chain	Res	Type
1	B	305	ASN
1	B	306	ASP
1	B	310	GLU
1	B	314	LEU
1	B	319	LEU
1	B	329	PHE
1	B	332	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	252	HIS
1	A	275	ASN
1	B	25	ASN
1	B	111	GLN
1	B	135	ASN
1	B	150	ASN
1	B	165	GLN
1	B	228	GLN
1	B	275	ASN
1	B	305	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](#)

4 ligands are 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$
3	NAD	A	335	-	46,48,48	1.10	3 (6%)	64,73,73	1.45	6 (9%)
3	NAD	B	335	-	46,48,48	1.18	3 (6%)	64,73,73	1.08	5 (7%)
2	SO4	B	334	-	4,4,4	1.41	0	6,6,6	0.40	0
2	SO4	A	334	-	4,4,4	0.80	0	6,6,6	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	B	335	-	-	8/30/62/62	0/5/5/5
3	NAD	A	335	-	-	12/30/62/62	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	335	NAD	PA-O3	4.83	1.64	1.59
3	A	335	NAD	C4A-N9A	4.53	1.47	1.37
3	B	335	NAD	C4A-N9A	3.69	1.45	1.37
3	A	335	NAD	PA-O3	3.14	1.62	1.59
3	A	335	NAD	O4D-C1D	2.07	1.43	1.40
3	B	335	NAD	C2A-N3A	-2.03	1.30	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	335	NAD	O2N-PN-O3	-7.91	85.90	107.27
3	A	335	NAD	O4B-C1B-N9A	3.18	114.20	108.09
3	B	335	NAD	O2N-PN-O5D	-2.88	94.52	107.57
3	A	335	NAD	C4B-O4B-C1B	-2.73	103.43	109.47
3	B	335	NAD	O2A-PA-O3	2.64	114.41	107.27
3	B	335	NAD	C2B-C1B-N9A	2.27	118.94	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	335	NAD	C3B-C2B-C1B	-2.22	97.26	101.46
3	A	335	NAD	O5D-PN-O1N	2.11	117.30	108.94
3	A	335	NAD	C4D-O4D-C1D	-2.10	108.00	109.92
3	A	335	NAD	O3-PN-O1N	2.09	116.98	110.70
3	B	335	NAD	C4B-O4B-C1B	-2.01	105.02	109.47

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	335	NAD	C5D-O5D-PN-O2N
3	A	335	NAD	O4D-C1D-N1N-C2N
3	A	335	NAD	O4D-C1D-N1N-C6N
3	A	335	NAD	C2D-C1D-N1N-C2N
3	A	335	NAD	C2D-C1D-N1N-C6N
3	B	335	NAD	O4D-C1D-N1N-C2N
3	B	335	NAD	O4D-C1D-N1N-C6N
3	B	335	NAD	C2D-C1D-N1N-C2N
3	B	335	NAD	C2D-C1D-N1N-C6N
3	A	335	NAD	O4B-C4B-C5B-O5B
3	A	335	NAD	O4D-C4D-C5D-O5D
3	A	335	NAD	C3D-C4D-C5D-O5D
3	A	335	NAD	C3B-C4B-C5B-O5B
3	A	335	NAD	C5B-O5B-PA-O1A
3	A	335	NAD	C5D-O5D-PN-O1N
3	B	335	NAD	PN-O3-PA-O2A
3	B	335	NAD	C2B-C1B-N9A-C8A
3	B	335	NAD	O4B-C1B-N9A-C8A
3	A	335	NAD	C2B-C1B-N9A-C8A
3	B	335	NAD	O4B-C4B-C5B-O5B

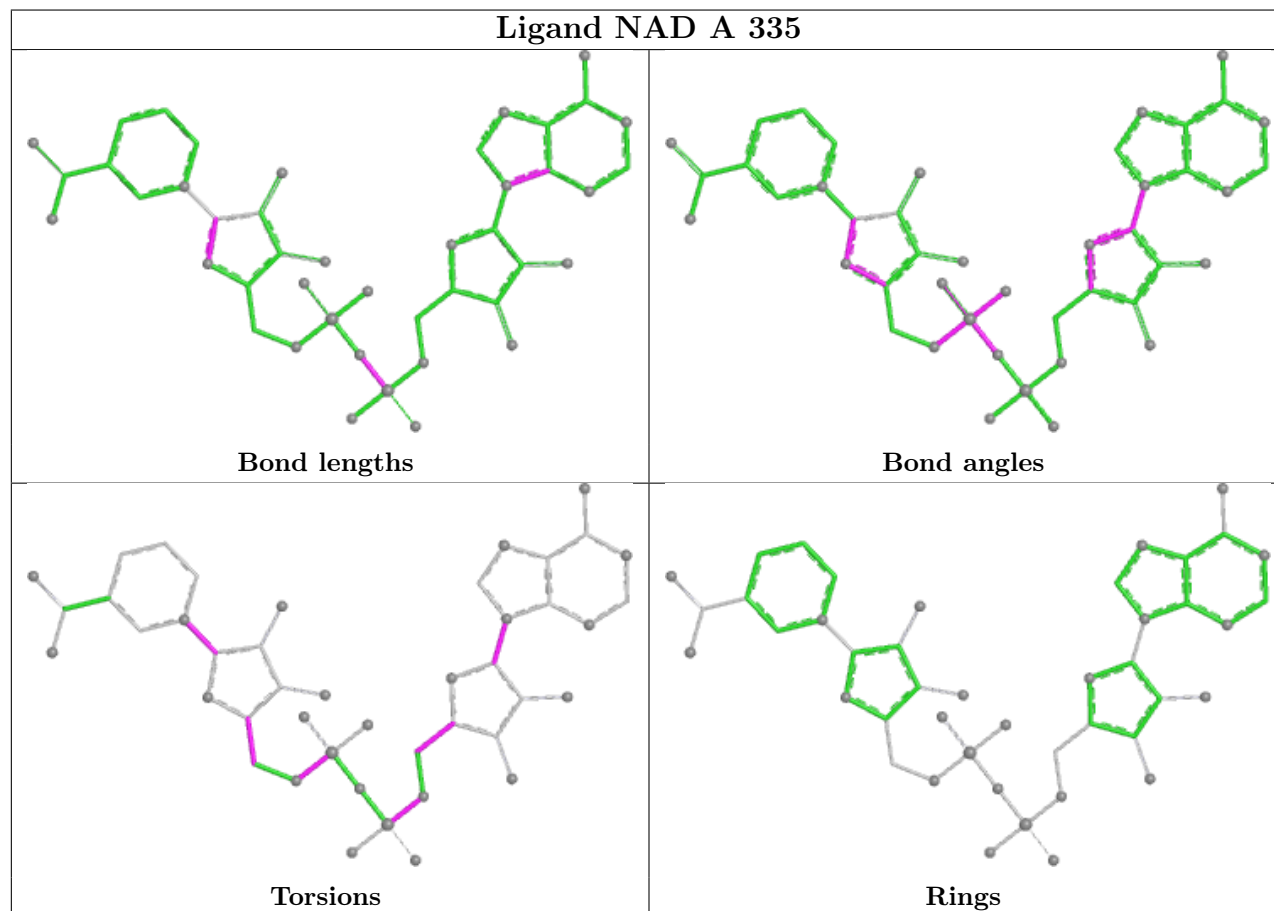
There are no ring outliers.

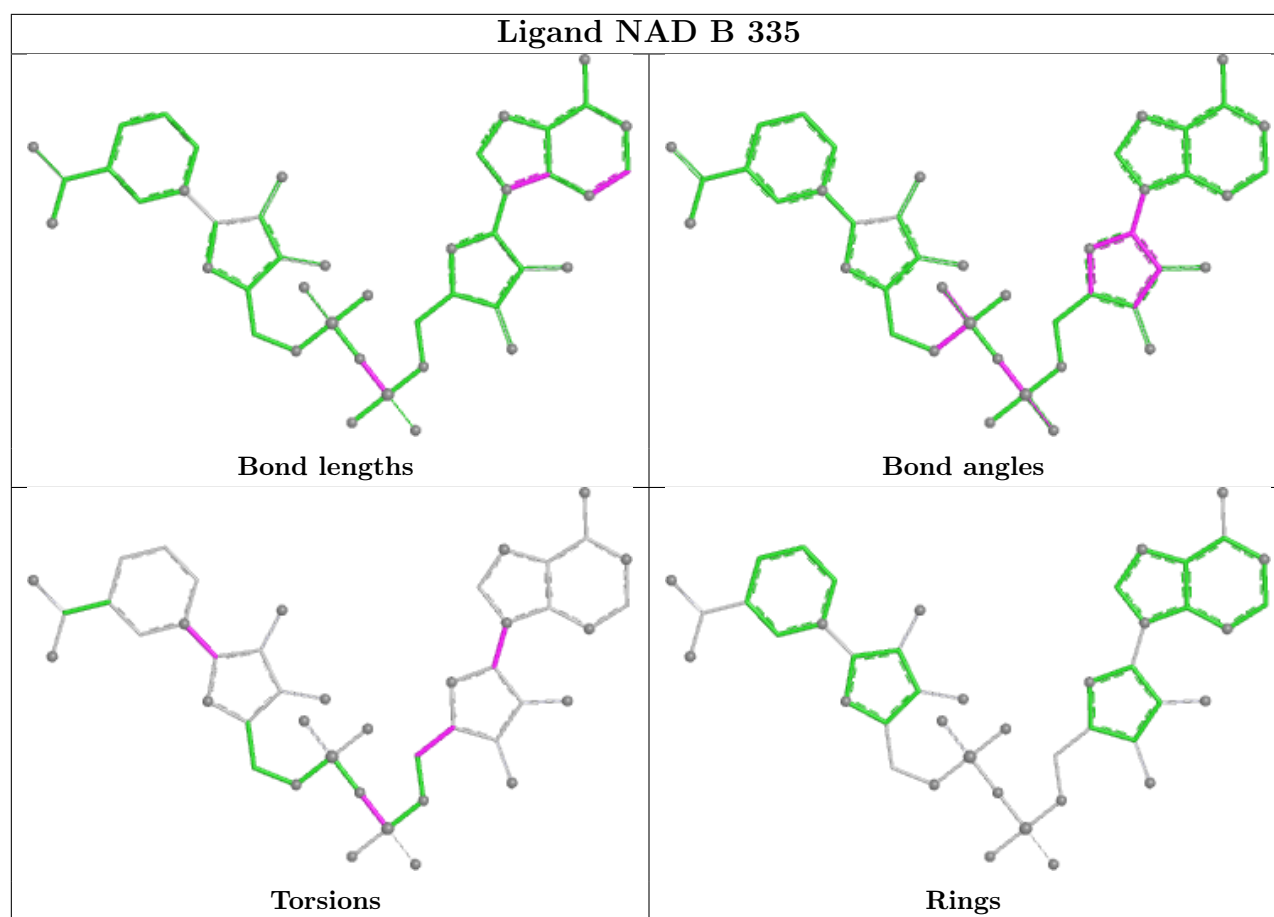
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	335	NAD	4	0
3	B	335	NAD	5	0
2	B	334	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/334 (99%)	-1.14	1 (0%) 90 87	2, 15, 34, 49	0
1	B	333/334 (99%)	-1.05	0 100 100	5, 18, 40, 50	0
All	All	666/668 (99%)	-1.10	1 (0%) 91 89	2, 17, 38, 50	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	LEU	2.4

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

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

6.3 Carbohydrates [i](#)

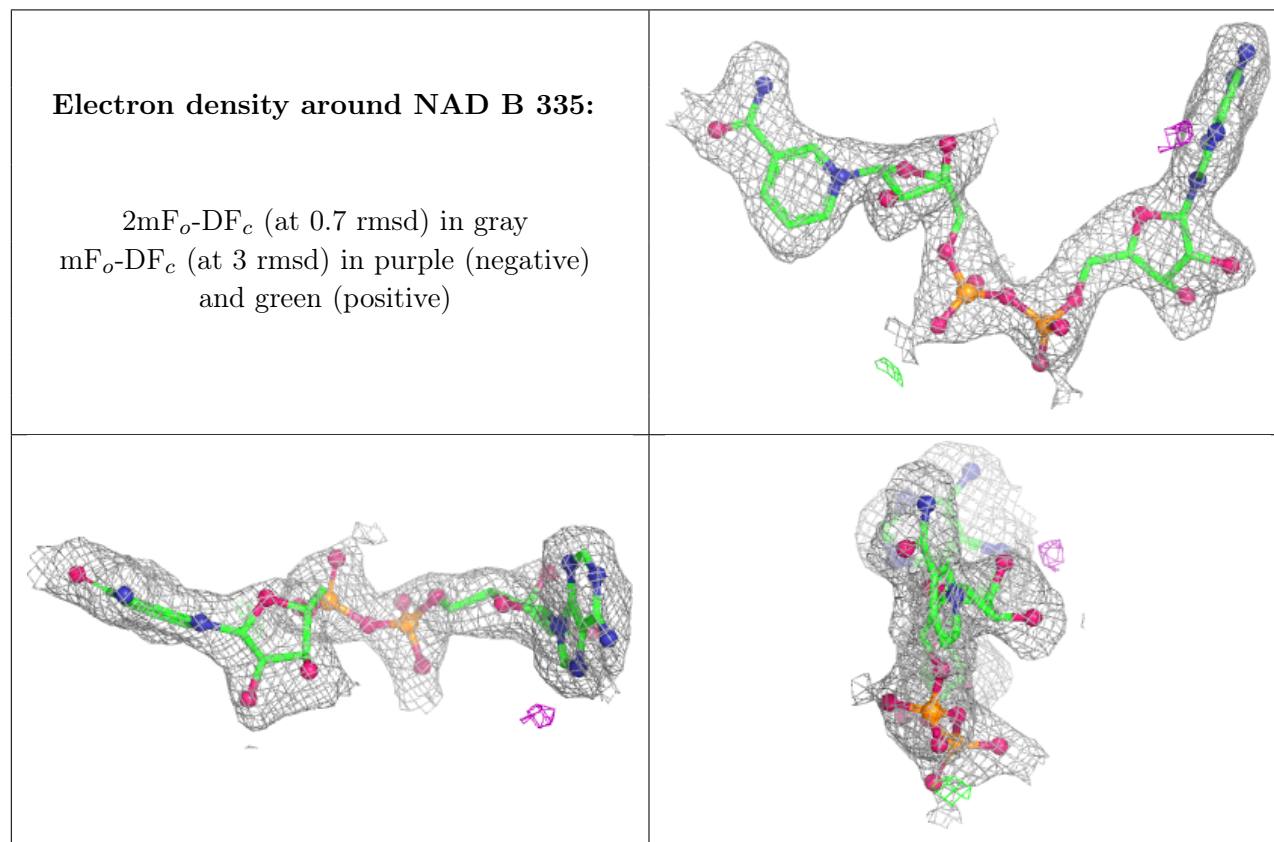
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

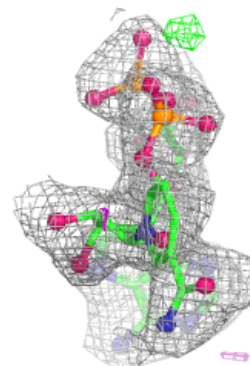
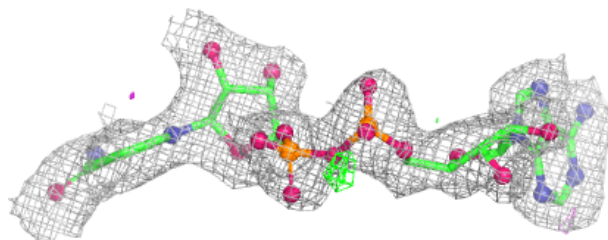
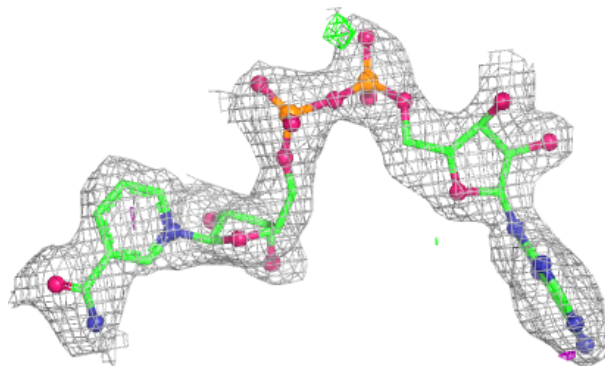
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	334	5/5	0.94	0.07	26,31,52,72	0
3	NAD	B	335	44/44	0.97	0.05	10,24,38,57	0
3	NAD	A	335	44/44	0.98	0.04	1,16,26,37	0
2	SO4	A	334	5/5	0.99	0.03	22,30,32,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around NAD A 335:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.