



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:20 PM UTC

PDB ID : 2NAC / pdb_00002nac
Title : HIGH RESOLUTION STRUCTURES OF HOLO AND APO FORMATE DE-HYDROGENASE
Authors : Lamzin, V.S.; Dauter, Z.; Popov, V.O.; Harutyunyan, E.H.; Wilson, K.S.
Deposited on : 1994-07-06
Resolution : 1.80 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
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

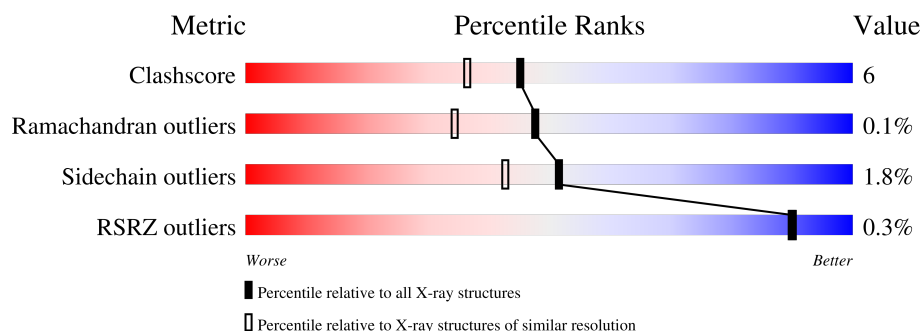
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	393	
1	B	393	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6713 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 NAD-DEPENDENT FORMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2920	1850	512	544	14			
1	B	374	Total	C	N	O	S	0	0	0
			2920	1850	512	544	14			

- 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		

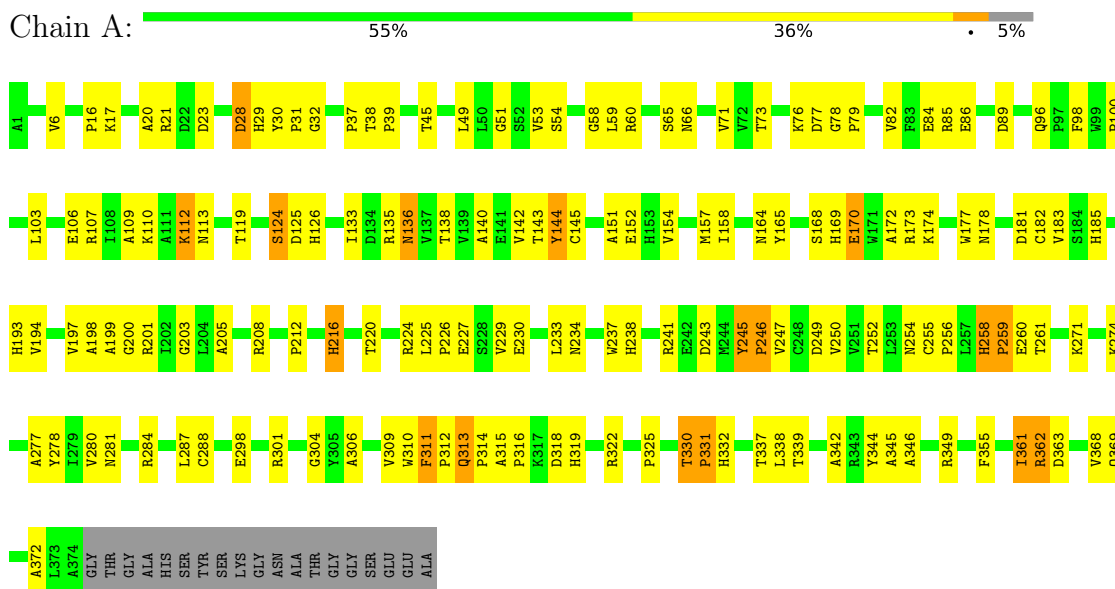
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	476	Total 476	O 476	0	0
3	B	387	Total 387	O 387	0	0

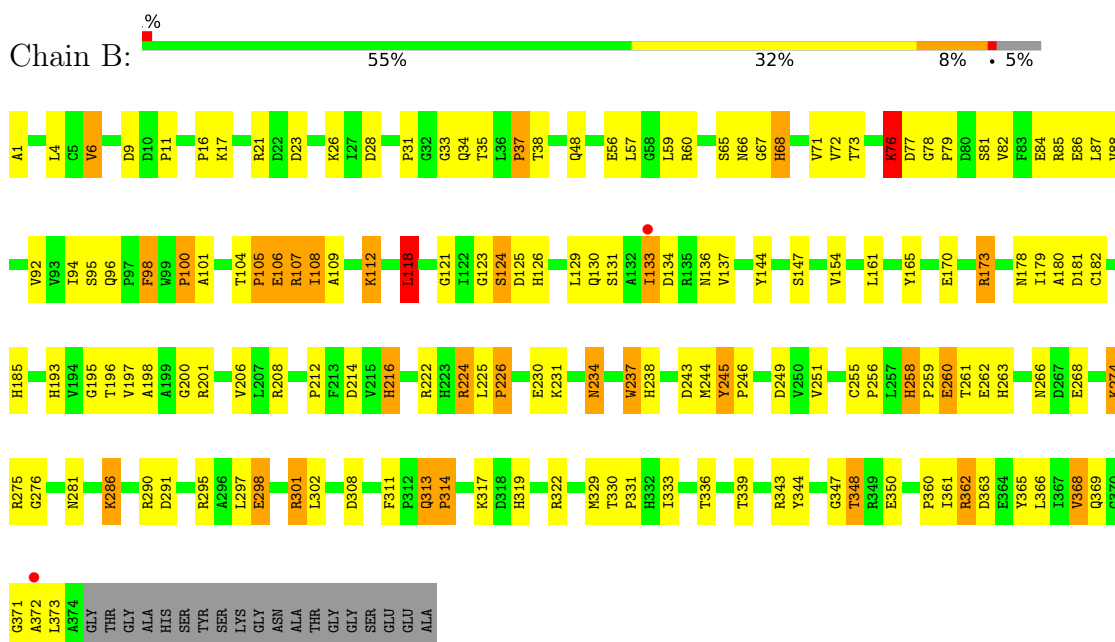
3 Residue-property plots

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: NAD-DEPENDENT FORMATE DEHYDROGENASE



• Molecule 1: NAD-DEPENDENT FORMATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.46Å 54.47Å 70.29Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 96.6 (10.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.84 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.146 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6713	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	1.47	11/2994 (0.4%)	2.38	209/4083 (5.1%)
1	B	1.44	11/2994 (0.4%)	2.43	196/4083 (4.8%)
All	All	1.45	22/5988 (0.4%)	2.41	405/8166 (5.0%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	330	THR	CA-C	8.79	1.60	1.52
1	B	245	TYR	N-CA	-6.86	1.40	1.46
1	B	330	THR	CA-C	6.31	1.58	1.52
1	A	280	VAL	CA-C	6.00	1.60	1.52
1	B	193	HIS	CA-C	5.91	1.59	1.52
1	A	58	GLY	CA-C	5.78	1.58	1.51
1	A	311	PHE	C-O	-5.77	1.20	1.25
1	B	154	VAL	CA-C	5.74	1.59	1.52
1	B	95	SER	CA-C	5.71	1.59	1.52
1	A	154	VAL	CA-C	5.58	1.59	1.52
1	B	181	ASP	N-CA	5.47	1.53	1.46
1	A	140	ALA	CA-C	5.47	1.59	1.52
1	A	151	ALA	CA-C	5.34	1.59	1.52
1	A	278	TYR	CA-C	5.26	1.59	1.52
1	B	249	ASP	CA-C	5.23	1.59	1.52
1	B	4	LEU	CA-C	5.23	1.59	1.52
1	A	306	ALA	CA-C	5.23	1.58	1.52
1	B	38	THR	CA-CB	5.16	1.58	1.53
1	A	158	ILE	CA-C	5.12	1.59	1.52
1	A	45	THR	C-N	-5.10	1.27	1.33
1	B	216	HIS	C-N	-5.09	1.26	1.33
1	B	147	SER	CA-C	5.00	1.59	1.52

All (405) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	CD-NE-CZ	19.69	151.96	124.40
1	A	274	LYS	CA-CB-CG	12.59	139.28	114.10
1	B	363	ASP	CA-CB-CG	11.20	123.80	112.60
1	B	208	ARG	CD-NE-CZ	11.17	140.04	124.40
1	A	284	ARG	CD-NE-CZ	10.89	139.65	124.40
1	A	311	PHE	CA-CB-CG	-10.29	103.51	113.80
1	B	28	ASP	CB-CA-C	-10.16	91.47	109.24
1	A	66	ASN	CA-CB-CG	-9.90	102.70	112.60
1	B	21	ARG	NE-CZ-NH2	-9.66	110.51	119.20
1	B	136	ASN	CA-CB-CG	9.62	122.22	112.60
1	A	243	ASP	CA-CB-CG	9.51	122.11	112.60
1	B	234	ASN	CA-CB-CG	9.39	121.99	112.60
1	A	136	ASN	OD1-CG-ND2	9.35	131.95	122.60
1	B	94	ILE	O-C-N	-9.32	113.13	123.20
1	A	136	ASN	CA-CB-CG	-9.14	103.46	112.60
1	B	268	GLU	CA-C-O	-9.13	111.30	120.70
1	B	60	ARG	NE-CZ-NH2	9.02	127.32	119.20
1	B	100	PRO	O-C-N	9.01	134.41	123.06
1	B	275	ARG	NE-CZ-NH2	-8.93	111.16	119.20
1	B	195	GLY	O-C-N	8.93	130.63	123.49
1	A	28	ASP	N-CA-CB	8.80	123.32	110.47
1	B	84	GLU	CA-CB-CG	-8.47	97.15	114.10
1	B	147	SER	O-C-N	8.46	131.09	122.12
1	B	311	PHE	CA-CB-CG	-8.46	105.33	113.80
1	A	78	GLY	CA-C-N	8.34	127.98	119.56
1	A	78	GLY	C-N-CA	8.34	127.98	119.56
1	B	201	ARG	NE-CZ-NH2	-8.31	111.72	119.20
1	B	16	PRO	CA-C-O	8.26	131.22	121.31
1	B	48	GLN	CG-CD-NE2	-8.26	104.02	116.40
1	A	193	HIS	CA-CB-CG	-8.22	105.58	113.80
1	B	301	ARG	CD-NE-CZ	8.21	135.90	124.40
1	B	173	ARG	NE-CZ-NH1	8.21	129.71	121.50
1	A	372	ALA	O-C-N	8.16	132.15	123.42
1	B	173	ARG	CD-NE-CZ	8.13	135.79	124.40
1	B	201	ARG	NH1-CZ-NH2	8.13	129.87	119.30
1	B	369	GLN	OE1-CD-NE2	8.07	130.67	122.60
1	B	98	PHE	CA-CB-CG	-8.05	105.75	113.80
1	B	21	ARG	NH1-CZ-NH2	8.03	129.74	119.30
1	A	37	PRO	N-CA-CB	8.02	110.31	103.25
1	B	173	ARG	NH1-CZ-NH2	-7.94	108.98	119.30
1	A	16	PRO	N-CA-CB	7.90	110.34	103.31
1	B	59	LEU	N-CA-C	7.87	123.18	113.50
1	B	206	VAL	CA-C-O	-7.87	112.83	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	31	PRO	CA-C-O	7.85	129.88	121.32
1	A	32	GLY	CA-C-O	-7.79	110.93	119.27
1	B	319	HIS	CA-C-N	7.79	127.50	119.56
1	B	319	HIS	C-N-CA	7.79	127.50	119.56
1	A	112	LYS	N-CA-C	7.78	120.66	111.71
1	A	306	ALA	O-C-N	7.71	132.04	123.25
1	B	68	HIS	N-CA-C	-7.62	98.16	109.81
1	A	124	SER	N-CA-CB	-7.58	100.18	111.25
1	B	100	PRO	CA-C-O	-7.53	112.45	121.48
1	B	78	GLY	CA-C-N	7.46	127.10	119.56
1	B	78	GLY	C-N-CA	7.46	127.10	119.56
1	A	260	GLU	N-CA-CB	-7.43	99.20	110.12
1	B	266	ASN	OD1-CG-ND2	-7.41	115.19	122.60
1	A	54	SER	CA-C-N	7.37	128.11	120.00
1	A	54	SER	C-N-CA	7.37	128.11	120.00
1	B	369	GLN	CA-CB-CG	-7.34	99.42	114.10
1	B	11	PRO	CA-C-N	7.33	130.86	120.53
1	B	11	PRO	C-N-CA	7.33	130.86	120.53
1	B	112	LYS	N-CA-C	7.33	119.35	111.36
1	B	108	ILE	O-C-N	7.29	129.34	121.83
1	B	343	ARG	NE-CZ-NH1	-7.29	114.22	121.50
1	A	216	HIS	CA-CB-CG	-7.22	106.58	113.80
1	A	173	ARG	CD-NE-CZ	7.18	134.45	124.40
1	A	32	GLY	N-CA-C	-7.15	106.18	114.69
1	A	143	THR	CA-CB-OG1	-7.13	98.90	109.60
1	A	28	ASP	CB-CA-C	-7.12	96.78	109.24
1	A	194	VAL	CA-C-O	-7.12	112.92	120.39
1	B	60	ARG	CD-NE-CZ	7.12	134.36	124.40
1	B	96	GLN	O-C-N	-7.11	114.80	121.20
1	A	178	ASN	N-CA-CB	-7.09	100.92	111.71
1	A	107	ARG	NH1-CZ-NH2	7.08	128.50	119.30
1	A	316	PRO	N-CA-CB	7.07	109.50	103.35
1	A	60	ARG	N-CA-C	7.06	118.63	111.07
1	A	172	ALA	CA-C-O	7.06	128.23	120.82
1	B	222	ARG	CG-CD-NE	7.06	127.53	112.00
1	A	337	THR	O-C-N	-7.05	114.76	122.79
1	A	124	SER	CA-C-O	7.02	129.88	121.17
1	A	339	THR	CA-C-O	-7.01	113.46	120.82
1	B	291	ASP	O-C-N	7.00	131.71	122.33
1	B	84	GLU	CA-C-O	7.00	127.97	120.55
1	A	201	ARG	NE-CZ-NH1	6.98	128.48	121.50
1	B	275	ARG	NH1-CZ-NH2	6.97	128.37	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ARG	NH1-CZ-NH2	6.97	128.36	119.30
1	A	233	LEU	CA-C-O	6.96	127.49	119.35
1	B	66	ASN	CA-C-O	6.96	128.16	119.95
1	A	306	ALA	CA-C-O	-6.95	113.82	121.33
1	B	295	ARG	O-C-N	6.90	129.44	122.12
1	A	288	CYS	CA-C-O	6.90	128.15	120.70
1	A	332	HIS	ND1-CE1-NE2	6.86	115.25	108.40
1	B	161	LEU	O-C-N	6.83	129.47	122.09
1	B	123	GLY	O-C-N	6.83	131.57	122.70
1	B	137	VAL	CB-CA-C	-6.80	102.73	110.96
1	A	368	VAL	CA-C-O	6.80	127.57	120.36
1	A	201	ARG	O-C-N	6.78	129.30	122.12
1	A	31	PRO	N-CA-CB	6.77	109.36	103.27
1	B	107	ARG	NE-CZ-NH1	-6.77	114.73	121.50
1	A	125	ASP	CB-CA-C	6.76	122.96	110.11
1	B	178	ASN	N-CA-CB	-6.76	101.43	111.71
1	B	182	CYS	CA-C-O	6.76	127.58	120.42
1	B	9	ASP	CB-CG-OD2	-6.75	102.86	118.40
1	B	137	VAL	O-C-N	6.74	131.16	122.94
1	A	201	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	A	145	CYS	O-C-N	6.70	130.05	122.22
1	B	179	ILE	CA-C-O	-6.70	114.31	121.27
1	A	17	LYS	N-CA-C	-6.69	105.25	113.41
1	A	113	ASN	OD1-CG-ND2	-6.66	115.94	122.60
1	A	178	ASN	N-CA-C	6.61	120.48	111.17
1	B	197	VAL	CA-C-N	6.59	134.12	121.54
1	B	197	VAL	C-N-CA	6.59	134.12	121.54
1	A	21	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	A	38	THR	CA-C-N	6.57	126.53	120.03
1	A	38	THR	C-N-CA	6.57	126.53	120.03
1	B	118	LEU	O-C-N	-6.57	115.85	123.27
1	A	238	HIS	CA-CB-CG	-6.56	107.24	113.80
1	B	368	VAL	N-CA-C	-6.55	98.69	108.12
1	B	368	VAL	N-CA-CB	6.54	121.06	111.52
1	A	301	ARG	CD-NE-CZ	6.53	133.54	124.40
1	A	89	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	349	ARG	NE-CZ-NH1	-6.51	114.99	121.50
1	A	96	GLN	OE1-CD-NE2	6.50	129.10	122.60
1	A	330	THR	O-C-N	6.50	125.87	121.71
1	B	268	GLU	N-CA-CB	6.47	119.45	110.07
1	B	136	ASN	CA-C-O	6.47	128.98	121.28
1	B	343	ARG	NH1-CZ-NH2	6.47	127.71	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	THR	CA-C-N	6.44	128.91	120.28
1	A	337	THR	C-N-CA	6.44	128.91	120.28
1	B	68	HIS	N-CA-CB	6.44	120.71	111.05
1	B	71	VAL	N-CA-CB	6.44	119.57	111.46
1	B	298	GLU	CA-CB-CG	6.42	126.93	114.10
1	B	238	HIS	ND1-CE1-NE2	6.41	114.81	108.40
1	B	33	GLY	O-C-N	6.41	130.23	122.60
1	A	30	TYR	CA-C-O	6.40	127.94	120.96
1	A	85	ARG	NE-CZ-NH1	-6.39	115.11	121.50
1	A	85	ARG	NH1-CZ-NH2	6.39	127.61	119.30
1	B	178	ASN	N-CA-C	6.39	120.18	111.17
1	A	164	ASN	O-C-N	-6.38	114.92	122.58
1	A	362	ARG	NE-CZ-NH2	-6.37	113.46	119.20
1	B	344	TYR	CA-CB-CG	6.37	125.36	113.90
1	A	200	GLY	O-C-N	-6.36	117.13	122.92
1	A	227	GLU	CA-C-N	6.36	128.80	120.28
1	A	227	GLU	C-N-CA	6.36	128.80	120.28
1	B	336	THR	CA-C-O	6.35	128.03	120.53
1	A	203	GLY	O-C-N	-6.35	115.84	122.13
1	A	142	VAL	CA-C-N	6.35	130.12	121.05
1	A	142	VAL	C-N-CA	6.35	130.12	121.05
1	A	278	TYR	CA-C-O	-6.31	113.98	121.11
1	A	234	ASN	CA-CB-CG	-6.29	106.31	112.60
1	B	48	GLN	OE1-CD-NE2	6.28	128.88	122.60
1	B	35	THR	CA-CB-OG1	-6.27	100.20	109.60
1	A	82	VAL	N-CA-CB	6.26	119.05	110.54
1	B	78	GLY	CA-C-O	6.25	130.47	121.52
1	A	338	LEU	CA-C-N	6.25	128.57	120.44
1	A	338	LEU	C-N-CA	6.25	128.57	120.44
1	B	313	GLN	CB-CA-C	6.25	118.47	110.16
1	B	72	VAL	O-C-N	-6.24	116.62	123.18
1	A	224	ARG	CG-CD-NE	-6.23	98.29	112.00
1	A	369	GLN	OE1-CD-NE2	6.23	128.83	122.60
1	A	194	VAL	O-C-N	6.22	129.97	123.26
1	A	103	LEU	CA-C-O	6.20	129.27	121.58
1	B	95	SER	N-CA-CB	6.18	121.33	111.56
1	B	226	PRO	N-CA-CB	6.18	108.81	103.31
1	A	319	HIS	CA-C-N	6.18	126.08	119.28
1	A	319	HIS	C-N-CA	6.18	126.08	119.28
1	B	76	LYS	CB-CG-CD	6.17	125.50	111.30
1	B	301	ARG	CB-CA-C	-6.16	100.56	110.79
1	B	260	GLU	CB-CG-CD	6.16	123.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ALA	N-CA-C	6.15	118.95	111.82
1	B	298	GLU	O-C-N	6.15	128.64	122.12
1	B	251	VAL	O-C-N	6.14	129.84	123.20
1	A	246	PRO	N-CA-CB	6.14	109.62	103.48
1	B	339	THR	CA-C-N	6.14	128.50	120.28
1	B	339	THR	C-N-CA	6.14	128.50	120.28
1	B	129	LEU	CA-C-N	-6.11	112.50	120.44
1	B	129	LEU	C-N-CA	-6.11	112.50	120.44
1	B	101	ALA	O-C-N	6.10	130.37	122.87
1	A	258	HIS	CA-C-N	6.09	125.81	119.05
1	A	258	HIS	C-N-CA	6.09	125.81	119.05
1	A	284	ARG	NE-CZ-NH2	6.08	124.67	119.20
1	A	28	ASP	O-C-N	6.07	130.98	122.36
1	A	157	MET	O-C-N	-6.07	115.23	122.15
1	B	11	PRO	O-C-N	-6.06	115.58	122.91
1	B	216	HIS	CA-C-O	-6.06	113.88	120.36
1	A	322	ARG	NE-CZ-NH2	6.05	124.65	119.20
1	B	165	TYR	N-CA-C	6.05	117.54	111.07
1	B	56	GLU	CA-C-O	6.04	127.45	120.32
1	A	113	ASN	O-C-N	6.04	129.88	122.34
1	A	21	ARG	O-C-N	6.03	130.56	122.96
1	A	372	ALA	CA-C-O	-6.03	114.78	121.23
1	B	368	VAL	CA-C-N	-6.00	113.50	122.39
1	B	368	VAL	C-N-CA	-6.00	113.50	122.39
1	B	81	SER	O-C-N	-5.99	116.02	122.85
1	B	154	VAL	O-C-N	5.99	127.78	121.91
1	B	9	ASP	OD1-CG-OD2	5.97	137.24	122.90
1	B	286	LYS	CA-CB-CG	-5.97	102.16	114.10
1	A	53	VAL	N-CA-C	5.95	117.40	110.62
1	B	230	GLU	O-C-N	-5.95	115.81	122.12
1	A	199	ALA	O-C-N	5.93	129.72	121.83
1	A	304	GLY	O-C-N	5.93	129.86	123.87
1	A	157	MET	CA-C-N	5.92	128.01	120.56
1	A	157	MET	C-N-CA	5.92	128.01	120.56
1	A	84	GLU	CA-C-N	5.91	128.20	120.28
1	A	84	GLU	C-N-CA	5.91	128.20	120.28
1	B	301	ARG	NH1-CZ-NH2	5.90	126.97	119.30
1	B	237	TRP	CA-C-N	5.90	131.09	122.77
1	B	237	TRP	C-N-CA	5.90	131.09	122.77
1	A	145	CYS	CA-C-O	-5.89	113.44	120.10
1	B	84	GLU	CG-CD-OE2	-5.88	104.89	118.40
1	A	363	ASP	CA-CB-CG	-5.87	106.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASN	CA-C-O	5.86	128.38	120.47
1	B	290	ARG	O-C-N	-5.86	115.37	122.11
1	A	254	ASN	O-C-N	5.86	130.04	122.19
1	A	182	CYS	O-C-N	-5.85	115.77	122.09
1	A	243	ASP	CB-CG-OD2	5.85	131.85	118.40
1	B	331	PRO	O-C-N	-5.84	115.61	122.86
1	A	237	TRP	CA-C-N	5.84	131.73	122.74
1	A	237	TRP	C-N-CA	5.84	131.73	122.74
1	A	344	TYR	CA-CB-CG	5.84	124.41	113.90
1	A	345	ALA	CA-C-N	5.82	128.56	120.29
1	A	345	ALA	C-N-CA	5.82	128.56	120.29
1	B	94	ILE	CA-C-O	5.82	126.53	120.36
1	B	262	GLU	CA-C-O	5.82	127.50	120.81
1	B	281	ASN	O-C-N	5.82	130.59	123.14
1	A	86	GLU	CB-CG-CD	5.77	122.41	112.60
1	A	85	ARG	CA-C-O	5.77	126.66	120.55
1	B	214	ASP	CA-C-O	5.77	128.14	121.28
1	B	37	PRO	CA-C-O	5.76	127.88	121.36
1	A	256	PRO	N-CA-CB	5.74	109.71	103.23
1	B	180	ALA	O-C-N	5.73	128.93	122.22
1	B	322	ARG	NE-CZ-NH2	5.73	124.35	119.20
1	A	259	PRO	CA-C-N	5.73	127.95	120.28
1	A	259	PRO	C-N-CA	5.73	127.95	120.28
1	A	144	TYR	CA-C-N	5.72	128.52	120.28
1	A	144	TYR	C-N-CA	5.72	128.52	120.28
1	A	249	ASP	CA-C-O	5.72	126.59	120.24
1	A	260	GLU	N-CA-C	5.71	117.50	111.28
1	A	71	VAL	N-CA-CB	5.71	118.65	111.46
1	A	298	GLU	O-C-N	-5.70	116.07	122.12
1	B	112	LYS	CA-C-O	-5.70	114.38	120.42
1	B	365	TYR	CA-C-O	5.70	126.37	119.31
1	B	100	PRO	N-CA-C	5.69	121.06	111.32
1	A	310	TRP	O-C-N	5.68	130.04	123.17
1	A	112	LYS	CG-CD-CE	5.67	124.34	111.30
1	A	168	SER	O-C-N	-5.67	116.11	122.12
1	B	297	LEU	CA-C-O	5.67	126.43	120.42
1	B	372	ALA	N-CA-C	5.66	117.45	108.79
1	A	30	TYR	CA-C-N	5.66	125.94	119.83
1	A	30	TYR	C-N-CA	5.66	125.94	119.83
1	B	333	ILE	N-CA-C	5.66	121.11	109.34
1	A	185	HIS	CA-C-N	5.64	130.95	123.00
1	A	185	HIS	C-N-CA	5.64	130.95	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	O-C-N	5.64	129.21	122.27
1	A	205	ALA	N-CA-C	-5.63	105.22	111.36
1	A	59	LEU	N-CA-C	5.62	120.42	113.50
1	B	68	HIS	O-C-N	5.62	130.98	122.94
1	A	100	PRO	N-CA-C	5.62	119.71	110.55
1	A	331	PRO	N-CA-C	-5.62	103.29	111.33
1	B	34	GLN	CG-CD-NE2	-5.62	107.97	116.40
1	B	137	VAL	N-CA-CB	5.62	117.40	111.00
1	A	76	LYS	N-CA-CB	-5.61	102.88	110.95
1	A	261	THR	O-C-N	-5.61	115.07	122.42
1	B	105	PRO	N-CA-C	-5.61	105.89	113.40
1	A	361	ILE	O-C-N	-5.60	116.11	122.72
1	A	277	ALA	N-CA-CB	-5.60	102.71	110.38
1	A	23	ASP	CA-C-O	-5.59	115.43	121.36
1	A	170	GLU	CA-C-O	-5.59	114.63	120.55
1	B	208	ARG	N-CA-CB	5.59	118.33	110.12
1	B	329	MET	N-CA-C	5.58	117.90	110.53
1	A	281	ASN	OD1-CG-ND2	5.57	128.17	122.60
1	A	113	ASN	CB-CG-ND2	5.56	124.74	116.40
1	B	360	PRO	N-CA-CB	5.55	108.54	103.15
1	B	134	ASP	CB-CA-C	-5.55	102.17	110.88
1	A	250	VAL	O-C-N	5.54	129.19	123.20
1	B	350	GLU	O-C-N	-5.54	116.25	122.12
1	A	337	THR	N-CA-C	-5.53	103.22	110.53
1	A	344	TYR	O-C-N	-5.53	115.46	122.27
1	A	181	ASP	CA-CB-CG	-5.53	107.07	112.60
1	B	65	SER	O-C-N	-5.53	115.20	122.39
1	B	238	HIS	ND1-CG-CD2	5.52	111.62	106.10
1	B	366	LEU	N-CA-C	5.52	118.24	109.96
1	A	355	PHE	CA-C-N	5.51	128.69	120.31
1	A	355	PHE	C-N-CA	5.51	128.69	120.31
1	B	84	GLU	CG-CD-OE1	5.50	131.05	118.40
1	B	85	ARG	NH1-CZ-NH2	5.50	126.45	119.30
1	A	174	LYS	CA-CB-CG	-5.49	103.11	114.10
1	A	234	ASN	N-CA-CB	-5.49	103.58	111.70
1	B	106	GLU	CB-CG-CD	5.48	121.92	112.60
1	B	298	GLU	CA-C-O	-5.48	114.75	120.55
1	B	258	HIS	CB-CA-C	-5.47	99.40	110.17
1	B	88	VAL	O-C-N	5.46	127.24	121.89
1	B	37	PRO	N-CA-CB	5.46	108.06	103.25
1	A	39	PRO	N-CA-C	-5.46	103.23	111.41
1	B	86	GLU	N-CA-C	5.45	119.78	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	PRO	N-CA-CB	5.45	108.59	102.60
1	B	196	THR	CA-CB-CG2	5.45	119.76	110.50
1	B	297	LEU	O-C-N	-5.45	115.94	122.15
1	B	268	GLU	CB-CG-CD	5.44	121.85	112.60
1	A	49	LEU	CA-C-O	5.43	126.74	120.60
1	B	33	GLY	CA-C-O	-5.43	112.99	119.07
1	A	245	TYR	CA-C-N	5.43	125.10	119.56
1	A	245	TYR	C-N-CA	5.43	125.10	119.56
1	B	261	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	133	ILE	O-C-N	5.41	127.21	121.91
1	A	229	VAL	N-CA-C	-5.41	105.45	110.53
1	A	277	ALA	O-C-N	-5.40	116.06	122.65
1	A	174	LYS	CA-C-O	-5.40	112.04	119.12
1	B	244	MET	O-C-N	-5.40	115.21	122.23
1	A	183	VAL	N-CA-C	5.39	120.46	113.07
1	B	302	LEU	N-CA-CB	5.38	119.46	110.85
1	A	177	TRP	CB-CA-C	5.38	121.13	110.42
1	A	346	ALA	N-CA-C	-5.38	105.50	111.36
1	B	71	VAL	CB-CA-C	-5.37	103.11	110.96
1	B	362	ARG	CA-C-O	5.37	126.87	121.07
1	B	251	VAL	CA-C-O	-5.37	114.67	120.36
1	B	6	VAL	O-C-N	5.36	130.05	122.97
1	A	85	ARG	O-C-N	-5.36	116.44	122.12
1	A	77	ASP	CA-C-O	5.34	126.25	120.43
1	A	325	PRO	CB-CA-C	-5.34	104.39	111.23
1	B	249	ASP	N-CA-C	-5.34	105.50	112.23
1	A	98	PHE	CA-CB-CG	-5.33	108.47	113.80
1	A	258	HIS	CA-CB-CG	-5.33	108.47	113.80
1	B	85	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	A	107	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	B	121	GLY	N-CA-C	-5.32	103.48	110.29
1	B	222	ARG	CB-CG-CD	5.31	123.51	111.30
1	B	372	ALA	CA-C-O	5.31	126.91	121.23
1	A	197	VAL	CA-C-N	5.30	131.67	121.54
1	A	197	VAL	C-N-CA	5.30	131.67	121.54
1	B	362	ARG	O-C-N	-5.30	116.75	123.12
1	B	195	GLY	CA-C-O	-5.29	116.82	120.94
1	A	79	PRO	N-CA-C	5.28	120.46	113.86
1	B	60	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	B	234	ASN	CB-CA-C	-5.28	104.40	111.89
1	B	198	ALA	N-CA-CB	5.27	119.40	110.49
1	A	246	PRO	CA-C-O	-5.26	111.66	119.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	A	112	LYS	N-CA-CB	-5.24	102.15	110.22
1	A	342	ALA	CA-C-O	-5.24	115.00	120.55
1	A	230	GLU	O-C-N	-5.23	116.57	122.12
1	A	362	ARG	NH1-CZ-NH2	5.23	126.10	119.30
1	B	333	ILE	CB-CA-C	-5.22	102.72	111.29
1	A	53	VAL	O-C-N	-5.22	116.77	121.89
1	A	287	LEU	CA-C-O	5.22	125.81	119.49
1	A	237	TRP	O-C-N	-5.21	117.11	123.16
1	B	216	HIS	O-C-N	5.21	129.16	123.22
1	A	252	THR	CA-CB-CG2	5.21	119.35	110.50
1	B	82	VAL	CA-C-O	5.20	126.35	120.95
1	A	51	GLY	O-C-N	-5.19	115.36	122.68
1	B	238	HIS	N-CA-CB	5.19	118.92	110.77
1	B	81	SER	N-CA-CB	-5.19	102.56	110.45
1	B	124	SER	CB-CA-C	-5.19	104.84	111.22
1	B	274	LYS	CB-CA-C	-5.17	100.02	109.54
1	A	250	VAL	CA-C-O	-5.17	114.88	120.36
1	B	34	GLN	OE1-CD-NE2	5.17	127.77	122.60
1	B	276	GLY	O-C-N	-5.16	115.92	122.32
1	A	165	TYR	N-CA-C	5.16	116.91	111.28
1	A	346	ALA	CA-C-N	5.16	125.67	120.00
1	A	346	ALA	C-N-CA	5.16	125.67	120.00
1	A	29	HIS	ND1-CG-CD2	5.16	111.25	106.10
1	B	92	VAL	O-C-N	5.15	128.76	123.20
1	B	238	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	152	GLU	CA-C-N	5.15	127.18	120.28
1	A	152	GLU	C-N-CA	5.15	127.18	120.28
1	A	315	ALA	CA-C-N	5.15	125.08	119.78
1	A	315	ALA	C-N-CA	5.15	125.08	119.78
1	B	200	GLY	O-C-N	-5.15	116.67	122.85
1	A	30	TYR	O-C-N	-5.14	114.65	121.34
1	B	245	TYR	N-CA-C	5.14	119.93	113.25
1	A	82	VAL	CA-CB-CG1	5.14	119.14	110.40
1	A	318	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	295	ARG	CA-C-O	-5.14	115.11	120.55
1	A	65	SER	CA-C-N	5.12	130.59	122.60
1	A	65	SER	C-N-CA	5.12	130.59	122.60
1	A	309	VAL	CA-C-O	5.12	126.66	120.67
1	B	77	ASP	CA-C-O	5.12	126.16	120.43
1	B	193	HIS	CB-CG-CD2	-5.12	124.55	131.20
1	B	79	PRO	N-CA-CB	5.11	108.42	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	THR	CA-CB-OG1	-5.11	101.93	109.60
1	B	249	ASP	OD1-CG-OD2	5.11	135.16	122.90
1	B	266	ASN	O-C-N	-5.11	115.99	122.78
1	A	313	GLN	CG-CD-NE2	5.10	124.05	116.40
1	B	231	LYS	CB-CA-C	-5.10	102.18	110.85
1	B	308	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	45	THR	O-C-N	5.08	127.60	121.29
1	B	263	HIS	CA-CB-CG	5.08	118.88	113.80
1	A	28	ASP	CA-C-N	-5.08	114.24	122.36
1	A	28	ASP	C-N-CA	-5.08	114.24	122.36
1	B	237	TRP	O-C-N	-5.07	117.28	123.16
1	A	261	THR	CA-CB-CG2	5.07	119.11	110.50
1	B	348	THR	CA-C-N	5.07	127.02	120.44
1	B	348	THR	C-N-CA	5.07	127.02	120.44
1	A	362	ARG	CB-CA-C	-5.06	101.55	109.70
1	B	23	ASP	O-C-N	5.06	128.84	122.92
1	A	241	ARG	CG-CD-NE	5.05	123.10	112.00
1	A	119	THR	O-C-N	-5.04	117.48	123.22
1	A	368	VAL	O-C-N	-5.03	117.76	123.20
1	B	57	LEU	CA-C-N	5.03	129.51	120.77
1	B	57	LEU	C-N-CA	5.03	129.51	120.77
1	B	193	HIS	O-C-N	5.03	128.95	123.27
1	A	220	THR	N-CA-C	-5.02	101.44	109.23
1	A	255	CYS	CA-C-N	5.01	125.22	120.31
1	A	255	CYS	C-N-CA	5.01	125.22	120.31
1	A	169	HIS	O-C-N	-5.00	116.82	122.12

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	2920	0	2876	22	0
1	B	2920	0	2876	46	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	1	0
3	A	476	0	0	8	4
3	B	387	0	0	19	4
All	All	6713	0	5752	68	7

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 6.

All (68) 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:135:ARG:NH1	3:A:632:HOH:O	2.04	0.91
1:B:124:SER:HB3	3:B:594:HOH:O	1.78	0.83
1:B:301:ARG:HB2	3:B:525:HOH:O	1.80	0.81
1:A:258:HIS:HB3	1:A:259:PRO:HD2	1.68	0.75
1:B:243:ASP:OD2	3:B:568:HOH:O	2.06	0.72
1:A:106:GLU:O	1:A:110:LYS:HG3	1.90	0.72
1:B:234:ASN:HB3	3:B:647:HOH:O	1.90	0.71
1:B:67:GLY:O	3:B:684:HOH:O	2.14	0.65
2:B:402:SO4:O3	3:B:451:HOH:O	2.11	0.65
1:A:225:LEU:HB3	1:A:226:PRO:HD2	1.79	0.64
1:B:368:VAL:HG22	1:B:373:LEU:HD23	1.78	0.64
1:B:258:HIS:HB3	1:B:259:PRO:CD	2.28	0.63
1:B:87:LEU:HD21	1:B:107:ARG:HB3	1.79	0.62
1:B:313:GLN:HA	1:B:314:PRO:C	2.25	0.61
1:B:104:THR:O	1:B:108:ILE:HG13	2.01	0.61
1:A:170:GLU:HG3	3:B:750:HOH:O	2.00	0.59
1:B:124:SER:N	3:B:594:HOH:O	2.36	0.59
1:A:258:HIS:CB	1:A:259:PRO:HD2	2.31	0.57
1:A:245:TYR:HB2	1:A:246:PRO:HD3	1.88	0.56
1:A:109:ALA:O	1:A:112:LYS:HE3	2.06	0.56
1:B:98:PHE:HE2	3:B:735:HOH:O	1.88	0.56
1:B:225:LEU:HB3	1:B:226:PRO:HD2	1.88	0.54
1:A:124:SER:HB2	3:A:565:HOH:O	2.08	0.53
1:B:104:THR:HB	1:B:105:PRO:HD2	1.91	0.51
1:A:212:PRO:HG3	1:B:212:PRO:HG3	1.92	0.51
1:B:124:SER:CB	3:B:594:HOH:O	2.49	0.51
3:A:537:HOH:O	1:B:216:HIS:HE1	1.94	0.51
1:A:208:ARG:NE	3:A:534:HOH:O	2.43	0.51
1:B:170:GLU:CD	1:B:173:ARG:HH21	2.18	0.50
1:B:17:LYS:HE2	3:B:668:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:HIS:HB3	1:A:259:PRO:CD	2.40	0.50
1:B:126:HIS:H	1:B:126:HIS:CD2	2.29	0.49
1:B:255:CYS:HB2	1:B:256:PRO:HD2	1.95	0.49
1:A:126:HIS:H	1:A:126:HIS:CD2	2.31	0.49
1:A:271:LYS:NZ	3:A:557:HOH:O	2.16	0.48
1:B:361:ILE:O	1:B:362:ARG:C	2.55	0.48
1:A:216:HIS:HD2	3:A:601:HOH:O	1.96	0.48
1:B:298:GLU:HG3	3:B:780:HOH:O	2.13	0.48
1:B:124:SER:CA	3:B:594:HOH:O	2.61	0.47
1:B:258:HIS:HB3	1:B:259:PRO:HD2	1.94	0.46
1:B:234:ASN:ND2	3:B:647:HOH:O	2.48	0.46
1:B:105:PRO:HB3	1:B:131:SER:OG	2.15	0.46
1:B:118:LEU:HD13	1:B:348:THR:HG23	1.97	0.46
3:A:831:HOH:O	1:B:173:ARG:HG3	2.16	0.45
1:B:274:LYS:HE2	3:B:579:HOH:O	2.16	0.45
1:A:311:PHE:HA	1:A:312:PRO:HA	1.79	0.44
1:A:313:GLN:HA	1:A:314:PRO:C	2.42	0.44
1:B:1:ALA:O	1:B:68:HIS:HB3	2.18	0.44
1:B:17:LYS:H	1:B:17:LYS:HG2	1.47	0.44
1:B:133:ILE:O	1:B:371:GLY:HA2	2.18	0.43
1:B:245:TYR:HB2	1:B:246:PRO:HD3	2.00	0.43
1:A:216:HIS:HE1	3:B:502:HOH:O	2.02	0.43
1:B:224:ARG:HG2	1:B:237:TRP:CD2	2.53	0.43
1:B:6:VAL:HA	1:B:73:THR:O	2.19	0.43
1:B:106:GLU:O	1:B:109:ALA:HB3	2.18	0.43
1:B:112:LYS:HB2	3:B:703:HOH:O	2.19	0.43
1:A:6:VAL:HA	1:A:73:THR:O	2.19	0.42
1:B:76:LYS:HE2	1:B:100:PRO:O	2.19	0.42
1:B:216:HIS:HD2	3:B:569:HOH:O	2.01	0.42
1:A:361:ILE:O	1:A:362:ARG:C	2.62	0.42
1:B:185:HIS:HE1	3:B:450:HOH:O	2.03	0.42
1:B:26:LYS:HE2	1:B:26:LYS:HB3	1.93	0.41
1:B:6:VAL:HG11	1:B:76:LYS:HG3	2.02	0.41
1:A:247:VAL:HB	3:A:751:HOH:O	2.19	0.41
1:B:108:ILE:HD12	1:B:131:SER:HB2	2.03	0.41
1:B:130:GLN:O	1:B:133:ILE:HB	2.21	0.41
1:B:37:PRO:HB3	1:B:347:GLY:HA2	2.03	0.40
1:A:330:THR:HB	1:A:331:PRO:CD	2.52	0.40

All (7) 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:528:HOH:O	3:A:563:HOH:O[2_657]	2.04	0.16
3:B:479:HOH:O	3:B:528:HOH:O[2_556]	2.05	0.15
3:A:524:HOH:O	3:A:528:HOH:O[2_647]	2.06	0.14
3:A:599:HOH:O	3:B:581:HOH:O[1_565]	2.09	0.11
3:B:489:HOH:O	3:B:664:HOH:O[1_565]	2.13	0.07
3:B:523:HOH:O	3:B:528:HOH:O[2_556]	2.14	0.06
3:A:500:HOH:O	3:A:528:HOH:O[2_647]	2.16	0.04

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	364/393 (93%)	356 (98%)	7 (2%)	1 (0%)	36	25
1	B	372/393 (95%)	357 (96%)	15 (4%)	0	100	100
All	All	736/786 (94%)	713 (97%)	22 (3%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA

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	312/323 (97%)	309 (99%)	3 (1%)	68	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	312/323 (97%)	304 (97%)	8 (3%)	40	28
All	All	624/646 (97%)	613 (98%)	11 (2%)	51	43

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	136	ASN
1	A	144	TYR
1	B	76	LYS
1	B	118	LEU
1	B	125	ASP
1	B	133	ILE
1	B	144	TYR
1	B	260	GLU
1	B	286	LYS
1	B	317	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	126	HIS
1	A	185	HIS
1	A	216	HIS
1	A	234	ASN
1	A	258	HIS
1	A	263	HIS
1	B	126	HIS
1	B	185	HIS
1	B	216	HIS
1	B	263	HIS
1	B	369	GLN

5.3.3 RNA ⓘ

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](#)

2 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	$\# Z > 2$
2	SO4	B	402	-	4,4,4	0.88	0	6,6,6	1.79	1 (16%)
2	SO4	A	401	-	4,4,4	0.87	0	6,6,6	1.56	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	SO4	O4-S-O1	3.90	129.95	109.56
2	A	401	SO4	O4-S-O1	3.26	126.60	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	SO4	1	0

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	374/393 (95%)	-0.76	0	100 100	6, 15, 39, 69	0
1	B	374/393 (95%)	-0.45	2 (0%)	87 88	5, 16, 55, 85	0
All	All	748/786 (95%)	-0.60	2 (0%)	90 90	5, 15, 48, 85	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	ALA	2.2
1	B	133	ILE	2.0

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	402	5/5	0.85	0.12	37,39,48,52	0
2	SO4	A	401	5/5	0.89	0.10	40,43,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.