



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:18 PM UTC

PDB ID : 2MIN / pdb_00002min
Title : NITROGENASE MOFE PROTEIN FROM AZOTOBACTER VINELANDII,
OXIDIZED STATE
Authors : Peters, J.W.; Stowell, M.H.B.; Soltis, S.M.; Day, M.W.; Kim, J.; Rees, D.C.
Deposited on : 1996-12-20
Resolution : 2.03 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

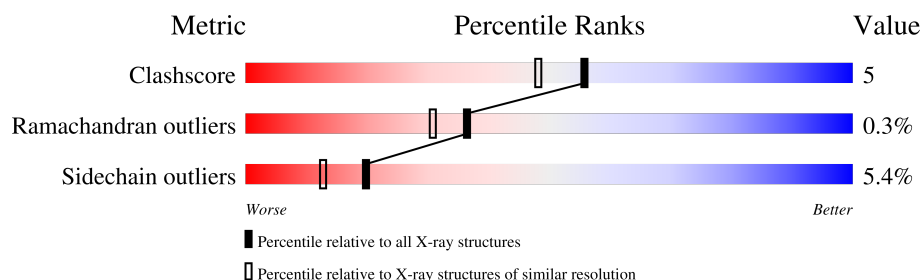
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)

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	491	70% 21% • 5%
1	C	491	71% 20% • 5%
2	B	522	77% 20% •
2	D	522	79% 17% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CFM	C	496	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16491 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.

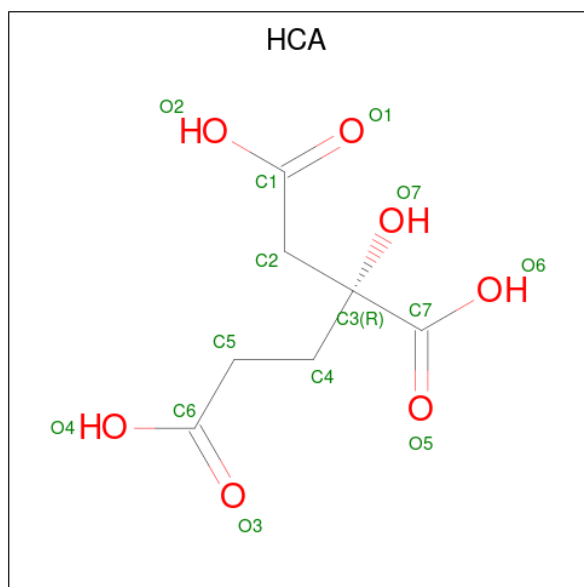
- Molecule 1 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3709	2361	630	694	24			
1	C	468	Total	C	N	O	S	0	0	0
			3713	2364	631	694	24			

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN.

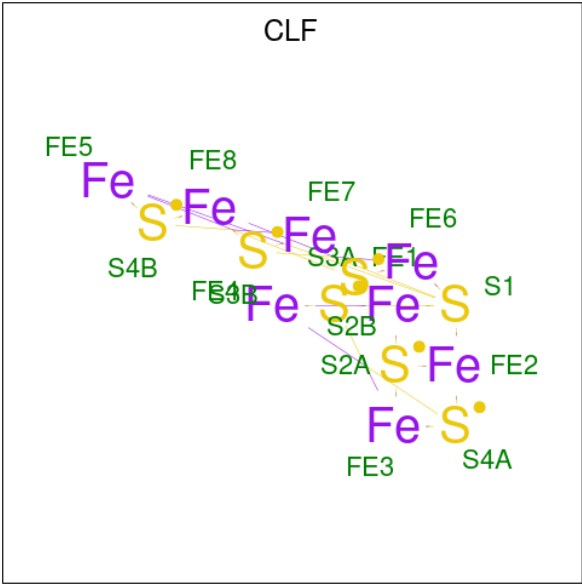
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



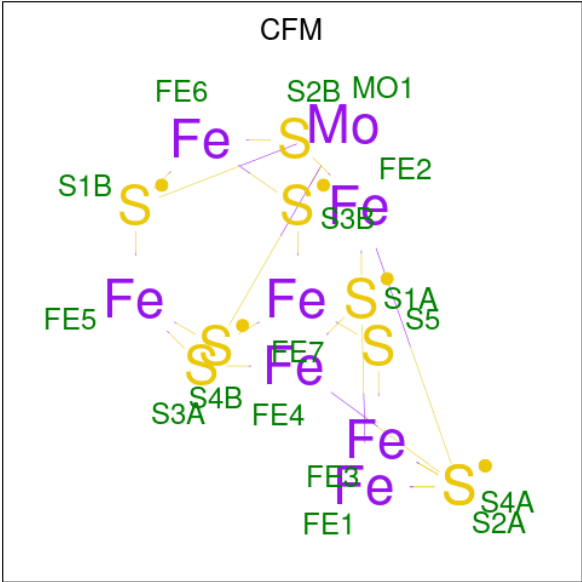
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			15	8	7		
4	C	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe₇MoS₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	132	Total	O	0	0
			132	132		
7	B	186	Total	O	0	0
			186	186		
7	C	126	Total	O	0	0
			126	126		
7	D	183	Total	O	0	0
			183	183		

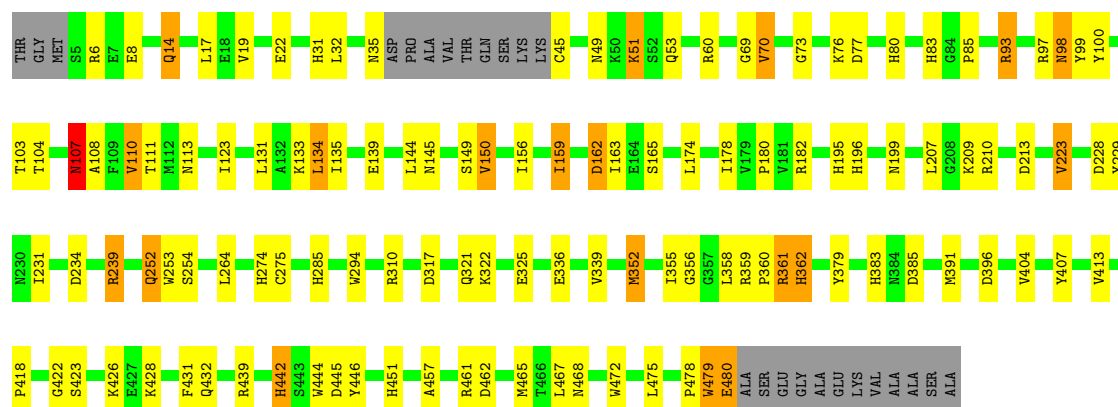
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

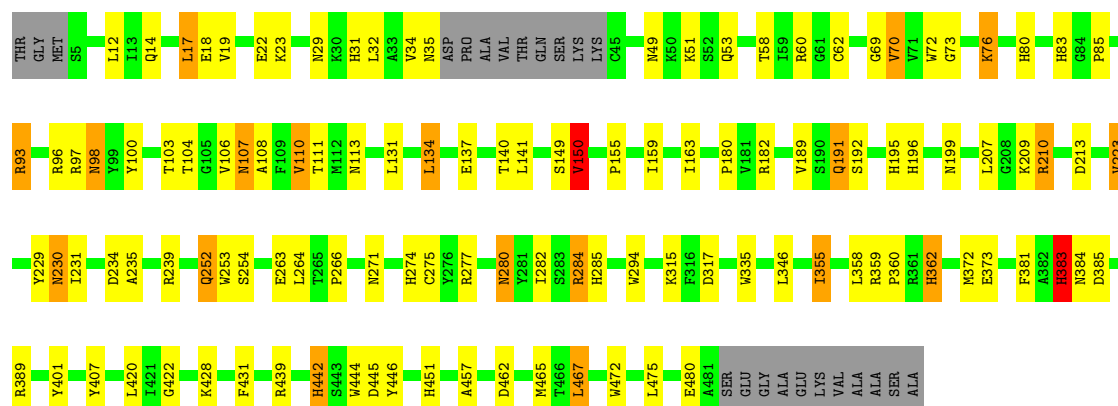
• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN

Chain A: 



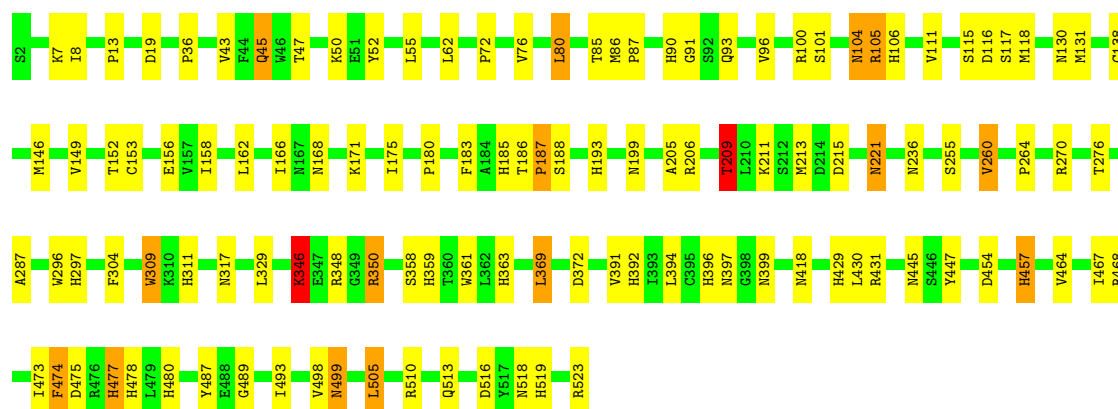
• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN

Chain C: 



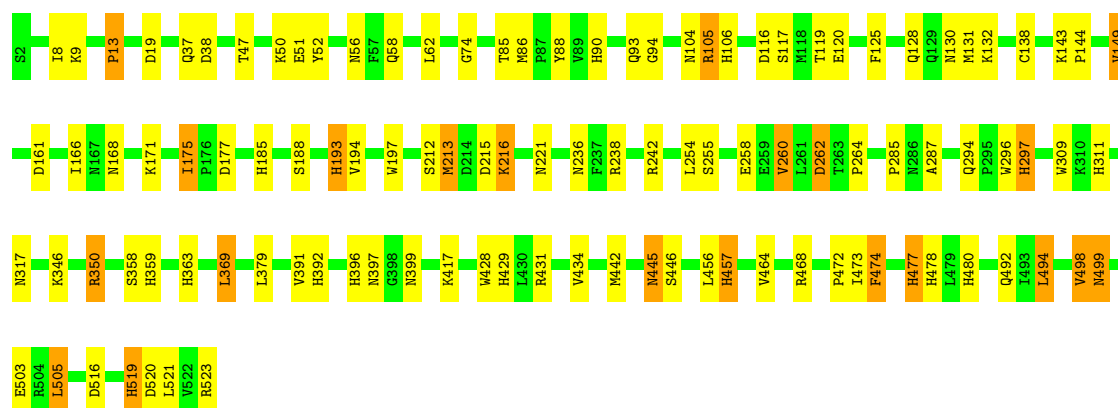
• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN

Chain B: 



• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN

Chain D: 79% 17% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.70Å 130.20Å 81.30Å 90.00° 110.80° 90.00°	Depositor
Resolution (Å)	30.00 – 2.03	Depositor
% Data completeness (in resolution range)	91.6 (30.00-2.03)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.0	Depositor
R, R_{free}	0.212 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16491	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: CLF, CA, CFM, HCA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.88	17/3795 (0.4%)	1.60	65/5117 (1.3%)
1	C	0.92	20/3799 (0.5%)	1.58	58/5123 (1.1%)
2	B	0.90	19/4280 (0.4%)	1.57	63/5786 (1.1%)
2	D	0.89	20/4280 (0.5%)	1.55	65/5786 (1.1%)
All	All	0.90	76/16154 (0.5%)	1.57	251/21812 (1.2%)

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	0	1
1	C	0	1
All	All	0	2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	HIS	CG-ND1	-12.33	1.24	1.38
2	D	188	SER	CB-OG	-9.19	1.23	1.42
1	C	195	HIS	CG-ND1	-8.28	1.29	1.38
1	C	442	HIS	ND1-CE1	8.10	1.40	1.32
1	C	70	VAL	CA-CB	7.96	1.63	1.55
2	B	396	HIS	CD2-NE2	-7.69	1.29	1.37
2	D	297	HIS	CD2-NE2	-7.46	1.29	1.37
2	D	396	HIS	CD2-NE2	-7.44	1.29	1.37
2	D	480	HIS	CD2-NE2	-7.44	1.29	1.37
2	B	480	HIS	CD2-NE2	-7.33	1.29	1.37
1	A	451	HIS	CD2-NE2	-7.27	1.29	1.37
2	B	297	HIS	CD2-NE2	-7.26	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	HIS	CD2-NE2	-7.16	1.29	1.37
2	B	193	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	442	HIS	CD2-NE2	-7.14	1.30	1.37
1	A	383	HIS	CD2-NE2	-7.09	1.30	1.37
1	C	195	HIS	ND1-CE1	-6.98	1.25	1.32
2	B	188	SER	CB-OG	-6.88	1.28	1.42
1	C	83	HIS	CD2-NE2	-6.86	1.30	1.37
2	D	311	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	83	HIS	CD2-NE2	-6.83	1.30	1.37
1	C	383	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	70	VAL	CA-CB	6.74	1.63	1.54
2	B	185	HIS	CD2-NE2	-6.66	1.30	1.37
1	A	442	HIS	ND1-CE1	6.64	1.39	1.32
2	B	457	HIS	CD2-NE2	-6.63	1.30	1.37
2	D	519	HIS	CD2-NE2	-6.59	1.30	1.37
2	B	477	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	31	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	451	HIS	CD2-NE2	-6.56	1.30	1.37
2	D	193	HIS	CD2-NE2	-6.56	1.30	1.37
1	C	80	HIS	CD2-NE2	-6.55	1.30	1.37
2	B	311	HIS	CD2-NE2	-6.51	1.30	1.37
2	D	185	HIS	CD2-NE2	-6.47	1.30	1.37
1	C	196	HIS	CD2-NE2	-6.43	1.30	1.37
2	B	90	HIS	CD2-NE2	-6.42	1.30	1.37
2	D	477	HIS	CD2-NE2	-6.40	1.30	1.37
2	D	90	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	80	HIS	CD2-NE2	-6.37	1.30	1.37
2	B	392	HIS	CD2-NE2	-6.36	1.30	1.37
1	A	196	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	31	HIS	CD2-NE2	-6.32	1.30	1.37
2	D	359	HIS	CD2-NE2	-6.29	1.30	1.37
1	C	362	HIS	CD2-NE2	-6.27	1.30	1.37
2	B	359	HIS	CD2-NE2	-6.22	1.31	1.37
2	B	519	HIS	CD2-NE2	-6.20	1.31	1.37
1	A	195	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	362	HIS	CD2-NE2	-6.10	1.31	1.37
2	D	457	HIS	CD2-NE2	-6.10	1.31	1.37
2	B	429	HIS	CD2-NE2	-6.09	1.31	1.37
2	D	106	HIS	CD2-NE2	-6.08	1.31	1.37
2	D	363	HIS	CD2-NE2	-6.08	1.31	1.37
2	D	392	HIS	CD2-NE2	-6.00	1.31	1.37
1	C	285	HIS	CD2-NE2	-5.98	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	HIS	CD2-NE2	-5.96	1.31	1.37
2	B	478	HIS	CD2-NE2	-5.85	1.31	1.37
2	D	478	HIS	CD2-NE2	-5.82	1.31	1.37
1	C	195	HIS	CD2-NE2	-5.81	1.31	1.37
2	B	106	HIS	CD2-NE2	-5.79	1.31	1.37
2	D	429	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	442	HIS	CG-ND1	-5.75	1.31	1.38
1	C	150	VAL	CA-CB	5.71	1.61	1.53
1	A	274	HIS	CD2-NE2	-5.55	1.31	1.37
1	C	196	HIS	CG-ND1	-5.39	1.32	1.38
2	D	311	HIS	CG-ND1	-5.31	1.32	1.38
1	C	274	HIS	CG-ND1	-5.30	1.32	1.38
1	C	274	HIS	CD2-NE2	-5.25	1.32	1.37
1	A	404	VAL	CA-CB	5.24	1.59	1.54
1	A	274	HIS	CG-ND1	-5.20	1.32	1.38
1	A	451	HIS	CG-ND1	-5.20	1.32	1.38
2	B	392	HIS	CG-ND1	-5.13	1.32	1.38
1	C	80	HIS	CG-ND1	-5.12	1.32	1.38
2	D	185	HIS	CG-ND1	-5.08	1.32	1.38
2	B	106	HIS	CG-ND1	-5.07	1.32	1.38
2	B	359	HIS	CG-ND1	-5.07	1.32	1.38
2	D	359	HIS	CG-ND1	-5.04	1.32	1.38

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	TRP	O-C-N	9.93	135.29	122.68
2	D	116	ASP	CA-CB-CG	9.77	122.37	112.60
2	D	516	ASP	CA-CB-CG	9.23	121.83	112.60
2	D	499	ASN	OD1-CG-ND2	-9.23	113.37	122.60
2	B	93	GLN	N-CA-C	8.59	121.79	111.82
1	C	49	ASN	OD1-CG-ND2	-8.58	114.02	122.60
1	C	253	TRP	O-C-N	8.54	133.52	122.68
2	B	19	ASP	CA-CB-CG	8.53	121.13	112.60
1	A	383	HIS	CB-CG-CD2	-8.51	120.14	131.20
2	B	499	ASN	OD1-CG-ND2	-8.28	114.33	122.60
1	A	223	VAL	N-CA-CB	-8.19	100.15	112.35
2	B	186	THR	CA-C-N	8.18	129.47	119.98
2	B	186	THR	C-N-CA	8.18	129.47	119.98
2	B	116	ASP	CA-CB-CG	8.15	120.75	112.60
1	C	76	LYS	N-CA-C	8.04	121.14	111.82
2	B	297	HIS	CA-CB-CG	8.00	121.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	PRO	N-CA-CB	7.94	110.23	103.17
1	A	31	HIS	CB-CG-CD2	-7.88	120.95	131.20
1	C	35	ASN	CA-CB-CG	7.82	120.42	112.60
1	C	383	HIS	CB-CG-CD2	-7.67	121.22	131.20
2	D	19	ASP	CA-CB-CG	7.60	120.20	112.60
2	B	213	MET	N-CA-C	7.58	121.45	111.75
1	A	22	GLU	N-CA-C	7.50	119.45	111.28
1	A	49	ASN	OD1-CG-ND2	-7.44	115.16	122.60
2	B	474	PHE	CA-CB-CG	7.38	121.18	113.80
1	A	70	VAL	N-CA-C	7.34	117.84	111.90
2	B	516	ASP	CA-CB-CG	7.26	119.86	112.60
1	C	31	HIS	CB-CG-CD2	-7.20	121.84	131.20
2	D	297	HIS	CA-CB-CG	7.14	120.94	113.80
2	B	260	VAL	CB-CA-C	-7.11	101.13	112.16
1	C	70	VAL	N-CA-C	7.10	117.67	111.56
2	B	391	VAL	N-CA-C	6.99	117.75	110.62
2	D	317	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	C	431	PHE	CA-CB-CG	-6.94	106.86	113.80
2	B	104	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	362	HIS	N-CA-C	6.83	119.74	111.82
1	A	60	ARG	N-CA-C	6.82	119.11	110.24
1	A	213	ASP	CA-CB-CG	6.82	119.42	112.60
2	D	492	GLN	OE1-CD-NE2	-6.78	115.82	122.60
2	D	93	GLN	N-CA-C	6.76	120.78	112.54
2	D	397	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	C	335	TRP	CG-CD2-CE3	6.71	140.61	133.90
2	D	474	PHE	CA-CB-CG	6.69	120.49	113.80
2	B	215	ASP	CA-CB-CG	6.67	119.27	112.60
1	C	384	ASN	OD1-CG-ND2	-6.65	115.95	122.60
2	B	199	ASN	OD1-CG-ND2	-6.65	115.95	122.60
1	C	60	ARG	N-CA-C	6.55	118.75	110.24
2	B	399	ASN	CA-CB-CG	6.55	119.15	112.60
2	B	117	SER	N-CA-C	6.54	120.40	111.17
1	A	162	ASP	CA-CB-CG	-6.51	106.09	112.60
1	C	69	GLY	CA-C-N	-6.50	116.52	123.08
1	C	69	GLY	C-N-CA	-6.50	116.52	123.08
1	A	110	VAL	N-CA-C	6.48	117.17	110.36
1	C	72	TRP	N-CA-C	6.45	119.27	111.40
1	C	317	ASP	CA-CB-CG	6.43	119.03	112.60
1	C	271	ASN	OD1-CG-ND2	-6.40	116.20	122.60
1	C	110	VAL	N-CA-C	6.38	117.13	110.62
1	C	70	VAL	O-C-N	-6.34	116.34	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	C	442	HIS	CB-CG-CD2	-6.31	122.99	131.20
1	A	145	ASN	CA-CB-CG	6.31	118.91	112.60
2	B	236	ASN	OD1-CG-ND2	-6.29	116.31	122.60
2	B	478	HIS	CA-CB-CG	-6.28	107.52	113.80
2	D	236	ASN	OD1-CG-ND2	-6.27	116.33	122.60
2	D	168	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	31	HIS	CB-CG-ND1	6.25	132.07	122.70
1	A	149	SER	CA-CB-OG	6.20	123.49	111.10
2	D	254	LEU	CA-C-N	6.17	133.33	121.54
2	D	254	LEU	C-N-CA	6.17	133.33	121.54
1	A	234	ASP	N-CA-C	6.17	118.80	111.33
1	A	479	TRP	CA-C-N	6.17	132.81	121.70
1	A	479	TRP	C-N-CA	6.17	132.81	121.70
1	A	396	ASP	CA-CB-CG	6.16	118.76	112.60
1	C	199	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	199	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	C	428	LYS	N-CA-C	6.14	118.52	111.02
2	D	58	GLN	OE1-CD-NE2	-6.12	116.48	122.60
2	B	317	ASN	OD1-CG-ND2	-6.11	116.49	122.60
2	D	104	ASN	OD1-CG-ND2	-6.10	116.50	122.60
2	B	518	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	442	HIS	CB-CG-CD2	-6.10	123.28	131.20
1	C	385	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	253	TRP	CA-C-N	6.09	133.16	121.54
1	A	253	TRP	C-N-CA	6.09	133.16	121.54
1	C	223	VAL	N-CA-CB	-6.07	101.13	112.36
2	B	45	GLN	OE1-CD-NE2	-6.07	116.53	122.60
2	D	478	HIS	CB-CG-CD2	-6.06	123.32	131.20
2	B	392	HIS	CB-CG-CD2	-6.03	123.36	131.20
1	A	385	ASP	CA-CB-CG	6.03	118.63	112.60
2	B	429	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	C	480	GLU	CA-CB-CG	6.01	126.11	114.10
2	D	130	ASN	OD1-CG-ND2	-6.00	116.60	122.60
2	D	262	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	83	HIS	CB-CG-CD2	-5.96	123.45	131.20
2	D	392	HIS	CB-CG-CD2	-5.96	123.46	131.20
2	D	445	ASN	CA-CB-CG	5.95	118.55	112.60
2	D	117	SER	N-CA-C	5.93	119.53	111.17
2	D	445	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	C	83	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	253	TRP	CA-C-O	5.89	127.05	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	SER	CA-CB-OG	5.89	122.88	111.10
1	A	76	LYS	N-CA-C	5.88	119.64	112.23
1	A	234	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	317	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	51	LYS	CA-CB-CG	5.83	125.77	114.10
1	C	335	TRP	CB-CG-CD1	-5.81	118.18	126.90
2	B	90	HIS	CB-CG-CD2	-5.80	123.66	131.20
2	D	359	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	A	207	LEU	N-CA-C	5.78	118.36	111.71
2	D	125	PHE	CA-CB-CG	-5.77	108.03	113.80
1	C	335	TRP	CG-CD1-NE1	-5.76	102.72	110.20
1	A	223	VAL	CB-CA-C	5.74	119.54	110.52
2	B	467	ILE	N-CA-C	-5.73	99.49	107.80
2	B	464	VAL	CA-C-N	5.73	125.66	119.76
2	B	464	VAL	C-N-CA	5.73	125.66	119.76
2	D	417	LYS	N-CA-C	5.72	118.29	111.71
1	C	253	TRP	CA-C-N	5.69	132.41	121.54
1	C	253	TRP	C-N-CA	5.69	132.41	121.54
1	C	53	GLN	OE1-CD-NE2	-5.68	116.92	122.60
2	B	130	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	C	230	ASN	OD1-CG-ND2	-5.67	116.93	122.60
2	B	149	VAL	N-CA-C	5.65	116.72	108.58
2	B	445	ASN	CA-CB-CG	5.64	118.24	112.60
1	C	98	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	A	98	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	C	230	ASN	CA-CB-CG	5.64	118.24	112.60
2	B	187	PRO	CA-N-CD	-5.63	104.12	112.00
2	D	480	HIS	CB-CG-CD2	-5.63	123.88	131.20
1	C	373	GLU	CA-CB-CG	5.62	125.33	114.10
1	C	444	TRP	CB-CG-CD1	-5.60	118.51	126.90
2	D	464	VAL	CA-C-N	5.59	125.52	119.76
2	D	464	VAL	C-N-CA	5.59	125.52	119.76
1	A	99	TYR	N-CA-C	5.59	118.38	110.50
2	B	221	ASN	CA-CB-CG	5.58	118.18	112.60
1	C	191	GLN	OE1-CD-NE2	-5.58	117.02	122.60
2	D	468	ARG	N-CA-C	5.58	117.55	108.63
1	A	444	TRP	CG-CD2-CE3	5.57	139.47	133.90
2	B	518	ASN	O-C-N	-5.55	115.52	122.35
1	C	472	TRP	CE2-CD2-CG	-5.55	100.53	107.20
2	D	216	LYS	CA-CB-CG	-5.54	103.02	114.10
2	B	168	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	A	423	SER	O-C-N	-5.54	118.96	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	ASP	CA-CB-CG	5.53	118.13	112.60
2	B	369	LEU	CA-CB-CG	5.52	135.63	116.30
2	B	429	HIS	CB-CG-ND1	5.51	130.96	122.70
2	D	520	ASP	N-CA-C	5.49	118.40	110.28
1	A	442	HIS	CA-CB-CG	5.47	119.27	113.80
2	D	363	HIS	CB-CG-CD2	-5.47	124.08	131.20
1	C	49	ASN	CA-CB-CG	5.47	118.07	112.60
2	B	480	HIS	CB-CG-CD2	-5.47	124.09	131.20
2	B	363	HIS	CB-CG-CD2	-5.46	124.10	131.20
2	D	478	HIS	N-CA-C	5.46	119.77	113.38
1	A	428	LYS	N-CA-C	5.46	117.68	111.02
2	B	397	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	A	321	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	B	276	THR	CA-CB-OG1	-5.44	101.44	109.60
1	C	444	TRP	CG-CD2-CE3	5.44	139.34	133.90
1	A	383	HIS	CB-CG-ND1	5.41	130.81	122.70
1	A	479	TRP	CG-CD2-CE3	5.39	139.29	133.90
2	B	418	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	C	234	ASP	CA-CB-CG	5.38	117.98	112.60
2	D	431	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	69	GLY	CA-C-N	-5.38	117.44	122.66
1	A	69	GLY	C-N-CA	-5.38	117.44	122.66
1	C	22	GLU	N-CA-C	5.37	117.83	111.33
2	B	101	SER	CA-CB-OG	-5.36	100.39	111.10
1	C	31	HIS	CB-CG-ND1	5.35	130.73	122.70
2	B	397	ASN	CA-CB-CG	5.35	117.95	112.60
2	D	58	GLN	CG-CD-NE2	5.35	124.42	116.40
2	D	104	ASN	CA-CB-CG	5.34	117.94	112.60
2	D	215	ASP	CA-CB-CG	5.33	117.93	112.60
2	B	209	THR	N-CA-CB	-5.33	101.49	110.49
2	D	175	ILE	CA-C-N	5.32	125.24	119.76
2	D	175	ILE	C-N-CA	5.32	125.24	119.76
1	A	73	GLY	CA-C-N	5.32	125.13	119.28
1	A	73	GLY	C-N-CA	5.32	125.13	119.28
1	C	253	TRP	CA-C-O	5.32	126.45	120.92
2	D	359	HIS	N-CA-C	5.31	117.82	111.71
2	D	369	LEU	CA-CB-CG	5.31	134.90	116.30
2	D	260	VAL	CB-CA-C	-5.30	101.67	111.79
2	D	90	HIS	CB-CG-CD2	-5.30	124.31	131.20
1	A	468	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	73	GLY	CA-C-N	5.29	125.09	119.28
1	C	73	GLY	C-N-CA	5.29	125.09	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	VAL	CB-CA-C	5.28	119.22	110.30
1	C	80	HIS	CB-CG-CD2	-5.27	124.34	131.20
1	A	444	TRP	CE2-CD2-CG	-5.27	100.88	107.20
2	B	346	LYS	CG-CD-CE	5.26	123.41	111.30
2	D	85	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	444	TRP	CB-CG-CD1	-5.25	119.02	126.90
2	B	309	TRP	CG-CD2-CE3	5.25	139.15	133.90
2	D	197	TRP	CG-CD2-CE3	5.24	139.14	133.90
1	A	80	HIS	CB-CG-CD2	-5.23	124.40	131.20
2	D	350	ARG	CA-CB-CG	-5.21	103.67	114.10
2	B	359	HIS	N-CA-C	5.20	117.85	111.82
1	A	472	TRP	CE2-CD2-CG	-5.20	100.97	107.20
2	D	359	HIS	CB-CG-ND1	5.19	130.48	122.70
2	D	120	GLU	CB-CA-C	-5.18	102.52	110.81
2	B	478	HIS	CB-CG-CD2	-5.17	124.47	131.20
2	D	56	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	431	PHE	CA-CB-CG	-5.16	108.64	113.80
1	C	442	HIS	CA-CB-CG	5.16	118.96	113.80
2	D	399	ASN	CA-CB-CG	5.16	117.76	112.60
2	B	372	ASP	CA-C-N	5.15	124.60	119.24
2	B	372	ASP	C-N-CA	5.15	124.60	119.24
2	D	294	GLN	CA-C-N	5.15	124.77	119.05
2	D	294	GLN	C-N-CA	5.15	124.77	119.05
1	A	107	ASN	OD1-CG-ND2	-5.15	117.45	122.60
2	D	498	VAL	CB-CA-C	-5.15	105.18	112.14
1	C	444	TRP	CE2-CD2-CG	-5.15	101.02	107.20
2	D	429	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	C	98	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	239	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	A	254	SER	CA-C-O	-5.12	113.18	120.51
1	A	53	GLN	CA-C-N	5.12	125.03	119.76
1	A	53	GLN	C-N-CA	5.12	125.03	119.76
2	B	117	SER	N-CA-CB	-5.11	103.94	111.71
1	C	72	TRP	CE2-CD2-CG	-5.11	101.06	107.20
2	D	161	ASP	CA-CB-CG	5.11	117.71	112.60
2	D	391	VAL	N-CA-C	5.11	115.83	110.62
2	B	193	HIS	CB-CG-CD2	-5.10	124.57	131.20
2	D	213	MET	N-CA-C	5.10	118.28	111.75
2	B	391	VAL	N-CA-CB	-5.10	103.61	110.54
1	A	432	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	C	29	ASN	OD1-CG-ND2	-5.09	117.50	122.60
2	D	197	TRP	N-CA-C	-5.09	105.65	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	A	228	ASP	N-CA-C	-5.08	99.83	108.26
1	A	14	GLN	OE1-CD-NE2	-5.08	117.53	122.60
1	C	280	ASN	CA-CB-CG	5.08	117.67	112.60
1	C	362	HIS	N-CA-C	5.08	118.73	112.54
2	D	149	VAL	N-CA-C	5.07	115.60	108.36
2	B	359	HIS	CB-CG-CD2	-5.06	124.63	131.20
2	D	494	LEU	CA-CB-CG	5.06	134.00	116.30
2	B	153	CYS	CA-CB-SG	5.05	126.00	114.40
2	B	260	VAL	N-CA-CB	5.04	119.27	110.65
2	D	185	HIS	CB-CG-CD2	-5.04	124.64	131.20
2	D	309	TRP	CG-CD1-NE1	-5.04	103.65	110.20
2	B	475	ASP	CA-CB-CG	5.04	117.64	112.60
2	B	296	TRP	CE2-CD2-CG	-5.03	101.16	107.20
2	D	428	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	294	TRP	CE2-CD2-CG	-5.03	101.16	107.20
2	B	350	ARG	CA-CB-CG	-5.03	104.04	114.10
1	C	34	VAL	N-CA-C	-5.02	101.19	108.36
1	A	35	ASN	CA-CB-CG	5.01	117.61	112.60
2	D	296	TRP	CE2-CD2-CG	-5.01	101.18	107.20
2	B	361	TRP	CE2-CD2-CG	-5.01	101.19	107.20
2	B	429	HIS	CA-CB-CG	5.01	118.81	113.80
1	A	77	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	362	HIS	CB-CG-CD2	-5.00	124.69	131.20
1	A	294	TRP	CG-CD2-CE3	5.00	138.90	133.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	TYR	Sidechain
1	C	446	TYR	Sidechain

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	3709	0	3636	40	0
1	C	3713	0	3638	44	0
2	B	4174	0	4087	43	0
2	D	4174	0	4087	36	0
3	A	14	0	6	0	0
3	C	14	0	6	1	0
4	A	15	0	0	1	0
4	C	15	0	0	1	0
5	A	17	0	0	1	0
5	C	17	0	0	5	0
6	B	2	0	0	0	0
7	A	132	0	0	2	0
7	B	186	0	0	3	0
7	C	126	0	0	3	0
7	D	183	0	0	1	0
All	All	16491	0	15460	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (147) 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)
2:B:209:THR:HG21	2:B:309:TRP:HE1	1.37	0.87
2:B:85:THR:HG22	2:B:146:MET:HB3	1.63	0.80
2:B:346:LYS:HE3	2:D:264:PRO:HG3	1.67	0.75
2:B:499:ASN:HD21	2:D:477:HIS:H	1.38	0.72
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.03	0.72
1:C:210:ARG:HD3	1:C:263:GLU:HB3	1.72	0.71
1:C:93:ARG:HD3	1:C:111:THR:O	1.93	0.69
1:C:93:ARG:HG3	1:C:113:ASN:HB2	1.75	0.69
2:B:477:HIS:H	2:D:499:ASN:HD21	1.38	0.68
2:B:468:ARG:HB3	2:B:473:ILE:HD12	1.78	0.66
1:C:457:ALA:HB1	2:D:8:ILE:HD12	1.78	0.66
1:A:93:ARG:HD2	1:A:111:THR:O	1.96	0.65
1:C:239:ARG:HE	1:C:252:GLN:HE21	1.45	0.65
1:A:239:ARG:HE	1:A:252:GLN:HE21	1.44	0.64
2:B:457:HIS:HE1	7:B:621:HOH:O	1.80	0.64
1:A:457:ALA:HB1	2:B:8:ILE:HD12	1.81	0.63
1:C:134:LEU:HD13	2:D:62:LEU:HD13	1.82	0.62
5:C:496:CFM:MO1	5:C:496:CFM:S3B	2.11	0.61
2:D:457:HIS:HE1	7:D:677:HOH:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASN:HD22	1:C:235:ALA:H	1.49	0.61
1:C:134:LEU:HB2	2:D:62:LEU:HB2	1.83	0.61
2:B:80:LEU:HD13	2:B:87:PRO:HG3	1.83	0.60
2:B:85:THR:HG21	2:B:146:MET:HE2	1.82	0.60
1:C:239:ARG:HE	1:C:252:GLN:NE2	1.98	0.60
1:C:442:HIS:HB2	7:C:514:HOH:O	2.00	0.60
1:A:135:ILE:HD13	1:A:178:ILE:HD13	1.85	0.59
2:B:100:ARG:HD2	2:B:111:VAL:O	2.03	0.59
1:C:85:PRO:HB2	4:C:498:CLF:S2B	2.43	0.58
1:A:239:ARG:HE	1:A:252:GLN:NE2	2.01	0.58
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.85	0.58
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.84	0.58
2:B:131:MET:HE2	2:B:166:ILE:HG12	1.86	0.57
2:B:264:PRO:HG2	2:B:270:ARG:NH2	2.19	0.57
3:C:494:HCA:O5	5:C:496:CFM:S3B	2.63	0.57
1:A:104:THR:HA	1:A:108:ALA:O	2.04	0.56
1:C:104:THR:HA	1:C:108:ALA:O	2.06	0.56
2:B:358:SER:HB3	2:B:498:VAL:HG21	1.88	0.56
1:C:137:GLU:HA	1:C:140:THR:HG22	1.88	0.56
1:A:85:PRO:HB2	4:A:498:CLF:S2B	2.46	0.55
1:C:150:VAL:HG13	1:C:180:PRO:HA	1.89	0.55
1:C:207:LEU:HD22	1:C:282:ILE:HD11	1.89	0.55
2:B:513:GLN:HE22	2:D:37:GLN:HE22	1.56	0.54
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.44	0.53
1:A:103:THR:H	1:A:107:ASN:ND2	2.07	0.53
2:B:510:ARG:HG2	2:D:456:LEU:HD23	1.90	0.53
2:D:434:VAL:HG11	2:D:442:MET:HE3	1.90	0.53
2:D:86:MET:HG2	2:D:138:CYS:SG	2.48	0.53
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.90	0.53
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.91	0.53
1:A:352:MET:HE3	1:A:418:PRO:HG3	1.91	0.53
2:B:205:ALA:O	2:B:209:THR:HB	2.09	0.52
1:C:280:ASN:O	1:C:284:ARG:HD3	2.09	0.52
2:B:489:GLY:O	2:B:493:ILE:HG12	2.09	0.52
1:C:462:ASP:HA	1:C:465:MET:HG2	1.90	0.51
2:D:358:SER:HB3	2:D:498:VAL:HG21	1.93	0.51
1:C:51:LYS:HD3	1:C:189:VAL:HG12	1.94	0.50
1:A:134:LEU:HD13	2:B:62:LEU:HD13	1.93	0.50
1:A:134:LEU:HB2	2:B:62:LEU:HB2	1.93	0.50
1:C:192:SER:OG	1:C:383:HIS:HE1	1.93	0.50
1:A:139:GLU:HG3	1:A:174:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:O	1:A:159:ILE:HG22	2.12	0.49
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.12	0.49
1:C:97:ARG:O	1:C:231:ILE:HA	2.12	0.49
1:A:229:TYR:CE2	5:A:496:CFM:S2A	3.05	0.49
1:A:45:CYS:N	7:A:623:HOH:O	2.45	0.48
2:D:242:ARG:HG3	2:D:242:ARG:HH11	1.78	0.48
1:A:123:ILE:HA	1:A:159:ILE:HD11	1.94	0.48
1:A:93:ARG:HD3	1:A:113:ASN:HB2	1.96	0.48
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.96	0.48
2:B:348:ARG:HG3	2:B:487:TYR:CE1	2.48	0.48
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.49	0.48
1:C:163:ILE:HG12	1:C:182:ARG:NH1	2.29	0.48
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.12	0.47
1:A:462:ASP:HA	1:A:465:MET:HG2	1.96	0.47
2:B:86:MET:HG2	2:B:138:CYS:SG	2.54	0.47
1:A:163:ILE:HD11	1:A:182:ARG:HD2	1.97	0.46
2:D:74:GLY:HA3	2:D:193:HIS:O	2.15	0.46
1:C:346:LEU:HD13	1:C:372:MET:HE2	1.96	0.46
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.16	0.46
2:B:105:ARG:HB3	2:B:474:PHE:CD1	2.51	0.46
1:A:426:LYS:HA	2:B:104:ASN:ND2	2.31	0.46
1:A:150:VAL:HG13	1:A:180:PRO:HA	1.97	0.46
1:A:479:TRP:O	1:A:480:GLU:HB2	2.16	0.45
1:C:19:VAL:HG11	1:C:407:TYR:CE2	2.51	0.45
1:A:442:HIS:HB2	7:A:544:HOH:O	2.16	0.45
2:B:505:LEU:HD13	2:B:523:ARG:CZ	2.47	0.45
2:B:447:TYR:CE1	2:D:521:LEU:HD21	2.50	0.45
1:C:140:THR:HG23	1:C:141:LEU:HG	1.98	0.45
2:D:131:MET:HE1	2:D:149:VAL:HG21	1.99	0.45
1:A:422:GLY:HA2	1:A:439:ARG:O	2.17	0.45
1:C:284:ARG:HD2	1:C:294:TRP:CZ2	2.52	0.45
1:A:352:MET:HE1	1:A:413:VAL:HA	1.97	0.44
1:C:239:ARG:NH2	7:C:539:HOH:O	2.50	0.44
1:C:422:GLY:HA2	1:C:439:ARG:O	2.17	0.44
1:A:163:ILE:HG12	1:A:182:ARG:NH1	2.32	0.44
2:D:194:VAL:HB	2:D:297:HIS:CG	2.53	0.44
2:D:213:MET:HA	2:D:216:LYS:HD2	1.99	0.44
1:C:103:THR:H	1:C:107:ASN:ND2	2.15	0.44
1:C:277:ARG:HD3	7:C:597:HOH:O	2.18	0.44
1:C:96:ARG:NH1	5:C:496:CFM:S5	2.91	0.44
2:B:91:GLY:HA3	2:B:152:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LYS:N	1:C:315:LYS:HD2	2.33	0.43
1:C:275:CYS:HA	1:C:358:LEU:HD22	2.00	0.43
2:D:9:LYS:HD3	2:D:13:PRO:HG2	2.00	0.43
2:B:394:LEU:HD13	2:B:430:LEU:HB2	2.00	0.43
2:D:88:TYR:O	2:D:149:VAL:HA	2.18	0.43
1:A:19:VAL:HG11	1:A:407:TYR:CE2	2.54	0.43
1:C:155:PRO:O	1:C:159:ILE:HG12	2.18	0.43
1:C:381:PHE:HZ	5:C:496:CFM:S2B	2.41	0.43
2:D:128:GLN:HG3	2:D:132:LYS:HE2	1.99	0.43
1:A:310:ARG:HD3	1:A:325:GLU:OE2	2.18	0.43
2:B:431:ARG:HD2	2:B:454:ASP:OD2	2.17	0.43
2:B:72:PRO:O	2:B:76:VAL:HG23	2.19	0.42
7:B:545:HOH:O	2:D:519:HIS:HE1	2.01	0.42
1:C:51:LYS:HD2	2:D:119:THR:HG21	2.01	0.42
1:A:159:ILE:HD13	1:A:159:ILE:HG21	1.79	0.42
2:B:156:GLU:HG3	2:B:187:PRO:HA	2.01	0.42
1:C:420:LEU:HB2	1:C:467:LEU:HD22	2.01	0.42
1:C:62:CYS:HB3	2:D:94:GLY:HA3	2.01	0.42
1:A:17:LEU:HD21	1:A:32:LEU:CD1	2.50	0.42
1:A:239:ARG:NE	1:A:252:GLN:NE2	2.68	0.42
2:B:118:MET:HE1	2:B:158:ILE:HD11	2.01	0.42
2:B:206:ARG:HG2	2:B:304:PHE:CE1	2.55	0.42
2:D:505:LEU:HD13	2:D:523:ARG:CZ	2.50	0.42
2:B:146:MET:HG3	2:B:180:PRO:HB2	2.01	0.41
2:D:216:LYS:HD3	2:D:285:PRO:HB2	2.01	0.41
2:D:346:LYS:O	2:D:350:ARG:HG3	2.20	0.41
1:A:17:LEU:HD21	1:A:32:LEU:HD11	2.02	0.41
1:C:76:LYS:HD3	1:C:100:TYR:HB2	2.01	0.41
2:D:446:SER:OG	2:D:473:ILE:HA	2.20	0.41
1:C:230:ASN:HD22	1:C:235:ALA:N	2.15	0.41
1:C:229:TYR:CE2	5:C:496:CFM:S2A	3.12	0.41
2:B:36:PRO:HD3	7:B:632:HOH:O	2.21	0.41
1:A:97:ARG:O	1:A:231:ILE:HA	2.21	0.41
1:C:17:LEU:HD21	1:C:32:LEU:CD1	2.50	0.41
1:A:356:GLY:O	1:A:379:TYR:HB3	2.21	0.41
1:C:62:CYS:O	1:C:191:GLN:HA	2.21	0.41
2:D:105:ARG:HB3	2:D:474:PHE:CD1	2.56	0.41
2:B:47:THR:HA	2:B:52:TYR:CG	2.55	0.41
2:B:350:ARG:HD3	2:D:262:ASP:O	2.21	0.41
2:D:47:THR:HA	2:D:52:TYR:CG	2.56	0.41
2:B:162:LEU:HD13	2:B:183:PHE:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:HA	1:A:339:VAL:HG12	2.02	0.40
2:B:513:GLN:HE22	2:D:37:GLN:NE2	2.17	0.40
2:D:143:LYS:N	2:D:144:PRO:HD3	2.37	0.40
2:D:445:ASN:HB2	2:D:472:PRO:O	2.20	0.40
2:D:131:MET:HE2	2:D:166:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/491 (94%)	439 (95%)	22 (5%)	2 (0%)	30	22
1	C	464/491 (94%)	441 (95%)	21 (4%)	2 (0%)	30	22
2	B	520/522 (100%)	508 (98%)	11 (2%)	1 (0%)	43	40
2	D	520/522 (100%)	507 (98%)	12 (2%)	1 (0%)	43	40
All	All	1967/2026 (97%)	1895 (96%)	66 (3%)	6 (0%)	36	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
2	D	255	SER
2	B	255	SER
1	C	254	SER
1	A	478	PRO
1	C	355	ILE

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	397/414 (96%)	367 (92%)	30 (8%)	12	6
1	C	396/414 (96%)	367 (93%)	29 (7%)	13	7
2	B	454/454 (100%)	438 (96%)	16 (4%)	32	27
2	D	454/454 (100%)	437 (96%)	17 (4%)	30	24
All	All	1701/1736 (98%)	1609 (95%)	92 (5%)	20	13

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	14	GLN
1	A	51	LYS
1	A	70	VAL
1	A	93	ARG
1	A	98	ASN
1	A	107	ASN
1	A	131	LEU
1	A	133	LYS
1	A	134	LEU
1	A	150	VAL
1	A	159	ILE
1	A	162	ASP
1	A	165	SER
1	A	209	LYS
1	A	210	ARG
1	A	223	VAL
1	A	252	GLN
1	A	264	LEU
1	A	322	LYS
1	A	352	MET
1	A	359	ARG
1	A	361	ARG
1	A	362	HIS

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Mol	Chain	Res	Type
1	A	391	MET
1	A	445	ASP
1	A	461	ARG
1	A	467	LEU
1	A	475	LEU
1	A	480	GLU
2	B	7	LYS
2	B	13	PRO
2	B	45	GLN
2	B	50	LYS
2	B	55	LEU
2	B	80	LEU
2	B	105	ARG
2	B	171	LYS
2	B	175	ILE
2	B	209	THR
2	B	211	LYS
2	B	260	VAL
2	B	329	LEU
2	B	346	LYS
2	B	369	LEU
2	B	505	LEU
1	C	12	LEU
1	C	14	GLN
1	C	17	LEU
1	C	18	GLU
1	C	23	LYS
1	C	58	THR
1	C	70	VAL
1	C	93	ARG
1	C	98	ASN
1	C	106	VAL
1	C	107	ASN
1	C	131	LEU
1	C	134	LEU
1	C	150	VAL
1	C	209	LYS
1	C	210	ARG
1	C	223	VAL
1	C	252	GLN
1	C	264	LEU
1	C	266	PRO

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Mol	Chain	Res	Type
1	C	284	ARG
1	C	359	ARG
1	C	362	HIS
1	C	383	HIS
1	C	389	ARG
1	C	401	TYR
1	C	445	ASP
1	C	467	LEU
1	C	475	LEU
2	D	13	PRO
2	D	38	ASP
2	D	50	LYS
2	D	51	GLU
2	D	105	ARG
2	D	171	LYS
2	D	175	ILE
2	D	177	ASP
2	D	212	SER
2	D	238	ARG
2	D	258	GLU
2	D	260	VAL
2	D	369	LEU
2	D	379	LEU
2	D	494	LEU
2	D	503	GLU
2	D	505	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	53	GLN
1	A	107	ASN
1	A	252	GLN
1	A	383	HIS
2	B	37	GLN
2	B	58	GLN
2	B	104	ASN
2	B	130	ASN
2	B	338	GLN
2	B	457	HIS
2	B	499	ASN

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Mol	Chain	Res	Type
2	B	518	ASN
1	C	35	ASN
1	C	107	ASN
1	C	230	ASN
1	C	252	GLN
1	C	271	ASN
1	C	362	HIS
1	C	383	HIS
2	D	37	GLN
2	D	53	GLN
2	D	104	ASN
2	D	128	GLN
2	D	130	ASN
2	D	136	GLN
2	D	163	ASN
2	D	167	ASN
2	D	168	ASN
2	D	286	ASN
2	D	338	GLN
2	D	457	HIS
2	D	499	ASN
2	D	513	GLN
2	D	519	HIS

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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	CLF	A	498	2,1	0,24,24	-	-	-		
4	CLF	C	498	2,1	0,24,24	-	-	-		
5	CFM	A	496	3,1	0,24,24	-	-	-		
5	CFM	C	496	3,1	0,24,24	-	-	-		
3	HCA	C	494	5	13,13,13	3.00	7 (53%)	15,18,18	2.43	7 (46%)
3	HCA	A	494	5	13,13,13	3.25	5 (38%)	15,18,18	2.29	6 (40%)

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
4	CLF	A	498	2,1	-	-	0/12/10/10
3	HCA	C	494	5	-	3/17/17/17	-
3	HCA	A	494	5	-	6/17/17/17	-
4	CLF	C	498	2,1	-	-	0/12/10/10

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	494	HCA	C3-C7	-7.86	1.45	1.53
3	A	494	HCA	C3-C7	-7.69	1.45	1.53
3	A	494	HCA	O5-C7	5.63	1.39	1.22
3	A	494	HCA	O4-C6	-5.22	1.13	1.30
3	C	494	HCA	O5-C7	4.77	1.37	1.22
3	A	494	HCA	C2-C3	-3.25	1.49	1.54
3	C	494	HCA	O6-C7	-2.59	1.21	1.30
3	C	494	HCA	O1-C1	2.55	1.30	1.22
3	C	494	HCA	O2-C1	-2.36	1.23	1.30
3	C	494	HCA	O7-C3	2.28	1.47	1.43
3	C	494	HCA	O4-C6	-2.24	1.23	1.30
3	A	494	HCA	O6-C7	-2.11	1.22	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	494	HCA	O6-C7-C3	5.27	123.26	113.14
3	A	494	HCA	O6-C7-C3	4.74	122.23	113.14
3	C	494	HCA	O5-C7-C3	-4.68	113.02	122.09
3	A	494	HCA	O5-C7-C3	-4.25	113.85	122.09
3	A	494	HCA	O4-C6-O3	-2.89	115.91	123.33
3	C	494	HCA	C3-C2-C1	2.82	121.63	113.92
3	C	494	HCA	O4-C6-C5	2.79	122.82	114.00
3	C	494	HCA	O4-C6-O3	-2.53	116.82	123.33
3	A	494	HCA	O2-C1-C2	2.40	121.94	114.35
3	A	494	HCA	C4-C5-C6	2.26	118.01	112.77
3	A	494	HCA	O1-C1-C2	-2.21	116.69	122.95
3	C	494	HCA	O2-C1-O1	-2.18	117.73	123.33
3	C	494	HCA	C4-C5-C6	2.14	117.73	112.77

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C2-C3-C4-C5
3	A	494	HCA	O7-C3-C4-C5
3	C	494	HCA	C2-C3-C4-C5
3	C	494	HCA	C7-C3-C4-C5
3	C	494	HCA	O7-C3-C4-C5
3	A	494	HCA	C7-C3-C4-C5
3	A	494	HCA	O2-C1-C2-C3
3	A	494	HCA	C4-C5-C6-O3
3	A	494	HCA	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	498	CLF	1	0
4	C	498	CLF	1	0
5	A	496	CFM	1	0
5	C	496	CFM	5	0
3	C	494	HCA	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

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.