



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 11:16 AM EDT

PDB ID : 3MIN / pdb_00003min
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)	:	2.50

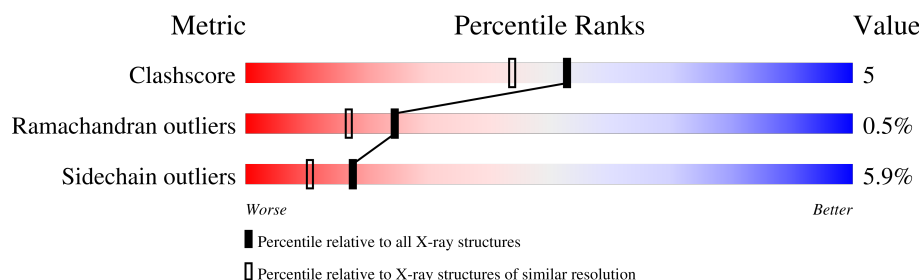
1 Overall quality at a glance

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	71% 19% • 5%
1	C	491	75% 15% • • 5%
2	B	522	77% 18% •
2	D	522	78% 18% •

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16490 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.

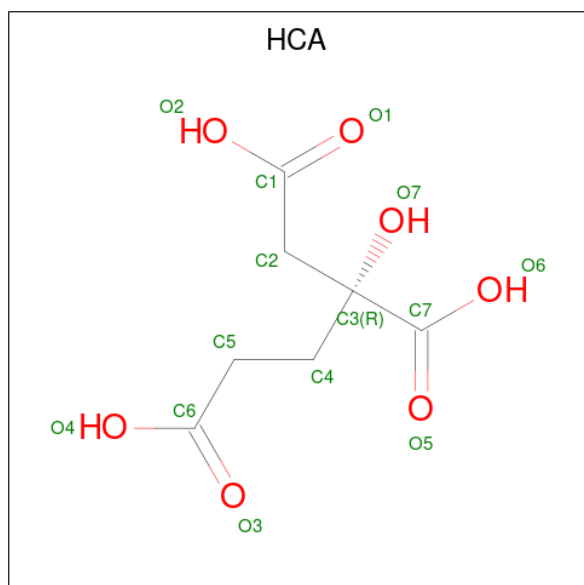
- Molecule 1 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN.

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.

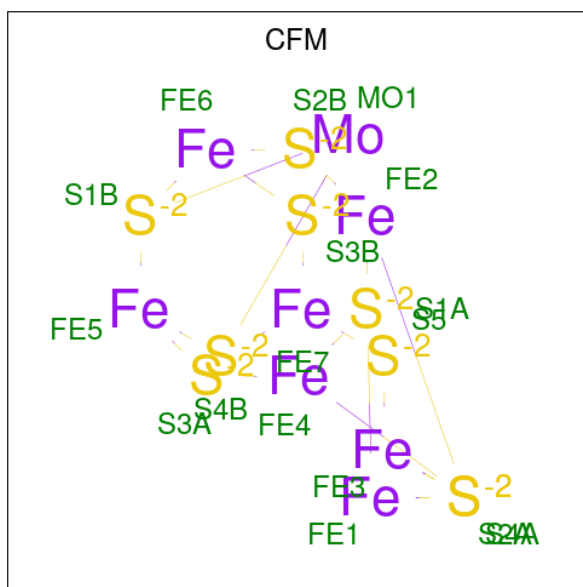
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4173	2666	705	774	28			

- 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-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).

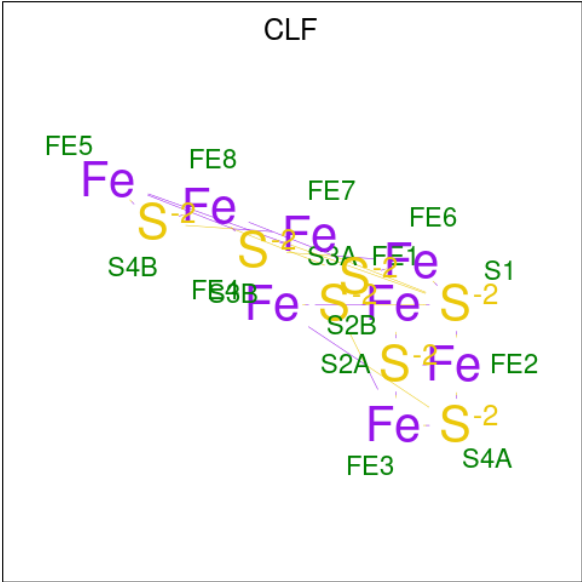


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
4	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		

- Molecule 6 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			15	8	7		
6	D	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 7 is water.

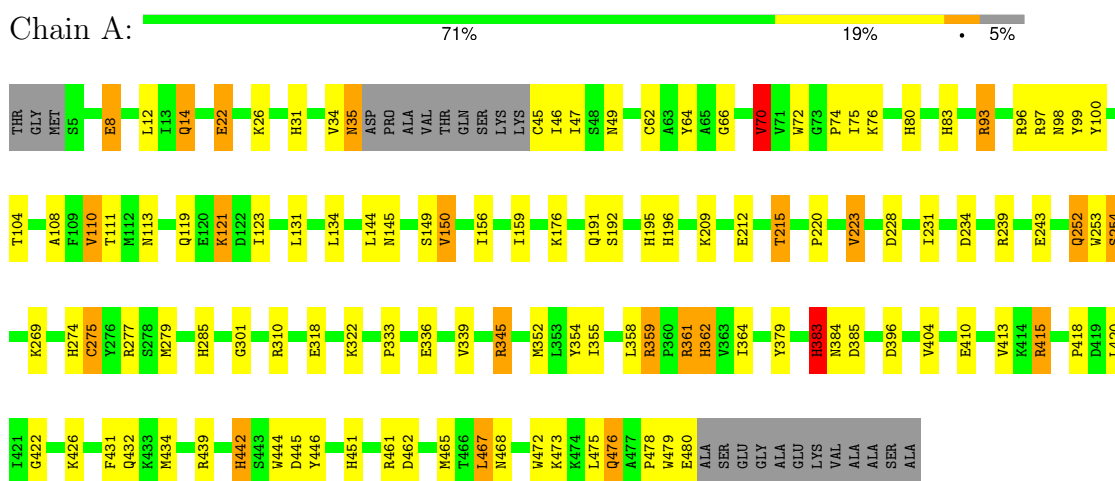
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total	O	0	0
			134	134		
7	B	185	Total	O	0	0
			185	185		
7	C	129	Total	O	0	0
			129	129		
7	D	179	Total	O	0	0
			179	179		

3 Residue-property plots

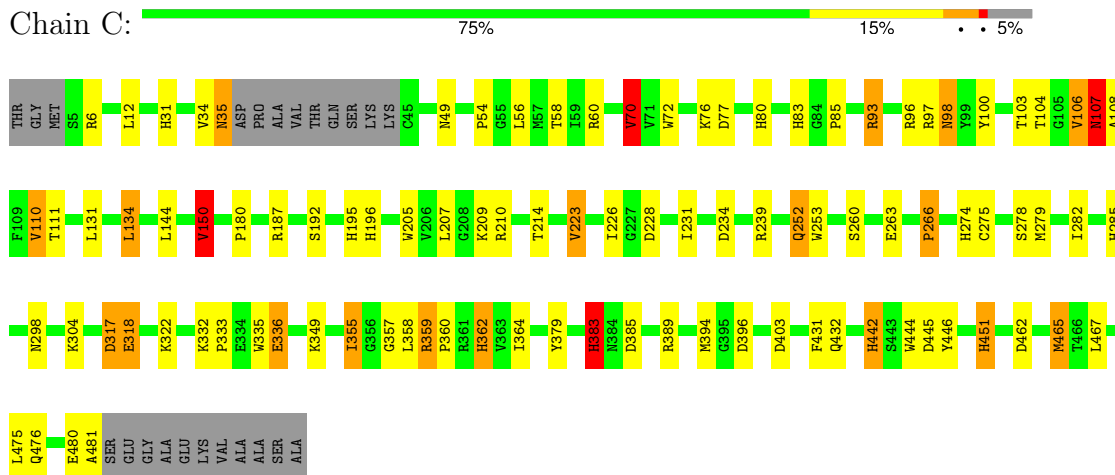
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

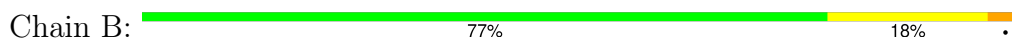
• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN

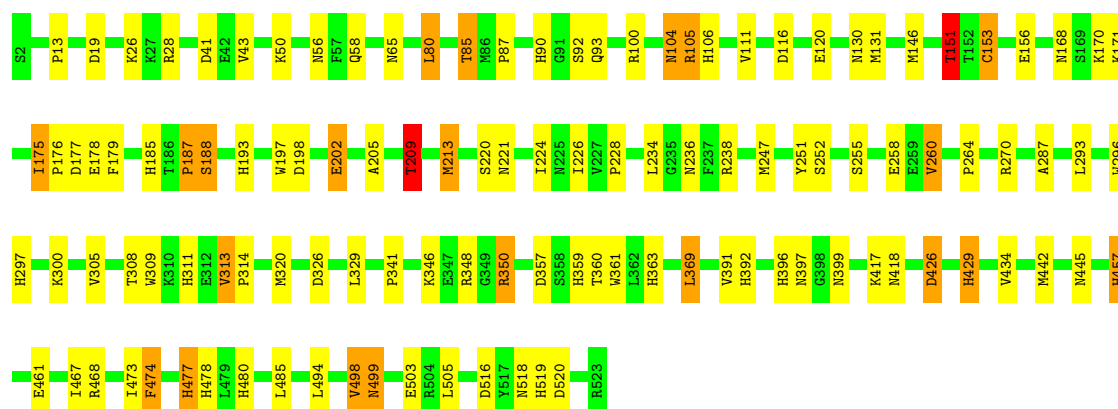


• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN



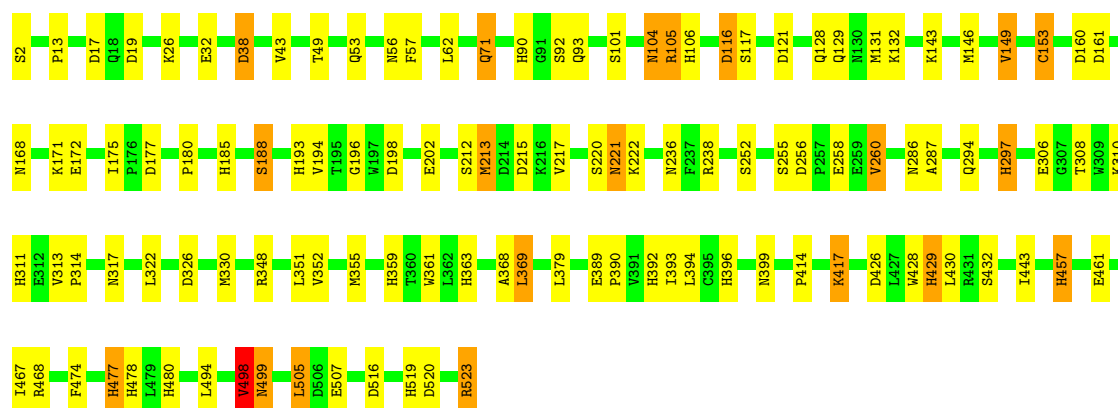
• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN





• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN

Chain D: 78% 18% •



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	108.00Å 131.30Å 81.00Å 90.00° 110.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.03	Depositor
% Data completeness (in resolution range)	89.6 (30.00-2.03)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.98	Depositor
R, R_{free}	0.206 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16490	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: CFM, CA, HCA, CLF

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	0.89	15/3795 (0.4%)	1.59	64/5117 (1.3%)
1	C	0.89	19/3799 (0.5%)	1.57	37/5123 (0.7%)
2	B	0.87	18/4280 (0.4%)	1.55	58/5786 (1.0%)
2	D	0.87	17/4279 (0.4%)	1.56	63/5785 (1.1%)
All	All	0.88	69/16153 (0.4%)	1.56	222/21811 (1.0%)

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 (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	HIS	CG-ND1	-10.38	1.26	1.38
1	A	442	HIS	ND1-CE1	8.87	1.41	1.32
1	C	70	VAL	CA-CB	7.80	1.63	1.55
2	B	396	HIS	CD2-NE2	-7.43	1.29	1.37
1	A	31	HIS	CD2-NE2	-7.34	1.29	1.37
1	A	150	VAL	CA-CB	7.31	1.62	1.54
2	D	297	HIS	CD2-NE2	-7.22	1.29	1.37
2	B	153	CYS	CB-SG	-7.19	1.57	1.81
1	C	442	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	83	HIS	CD2-NE2	-7.10	1.30	1.37
2	D	396	HIS	CD2-NE2	-7.06	1.30	1.37
2	B	457	HIS	CD2-NE2	-7.02	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	31	HIS	CD2-NE2	-7.01	1.30	1.37
1	C	383	HIS	CD2-NE2	-6.91	1.30	1.37
1	C	362	HIS	CD2-NE2	-6.84	1.30	1.37
2	B	429	HIS	CD2-NE2	-6.80	1.30	1.37
2	B	480	HIS	CD2-NE2	-6.79	1.30	1.37
2	D	193	HIS	CD2-NE2	-6.79	1.30	1.37
1	C	83	HIS	CD2-NE2	-6.78	1.30	1.37
2	D	457	HIS	CD2-NE2	-6.75	1.30	1.37
2	D	359	HIS	CD2-NE2	-6.74	1.30	1.37
2	D	429	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	442	HIS	CD2-NE2	-6.68	1.30	1.37
2	B	477	HIS	CD2-NE2	-6.67	1.30	1.37
2	B	185	HIS	CD2-NE2	-6.64	1.30	1.37
2	D	392	HIS	CD2-NE2	-6.62	1.30	1.37
2	D	311	HIS	CD2-NE2	-6.62	1.30	1.37
2	D	480	HIS	CD2-NE2	-6.60	1.30	1.37
2	B	392	HIS	CD2-NE2	-6.58	1.30	1.37
2	B	297	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	383	HIS	CD2-NE2	-6.57	1.30	1.37
1	C	274	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	451	HIS	CD2-NE2	-6.55	1.30	1.37
2	B	311	HIS	CD2-NE2	-6.55	1.30	1.37
1	C	196	HIS	CD2-NE2	-6.52	1.30	1.37
1	C	80	HIS	CD2-NE2	-6.52	1.30	1.37
2	B	90	HIS	CD2-NE2	-6.51	1.30	1.37
2	D	185	HIS	CD2-NE2	-6.47	1.30	1.37
2	D	90	HIS	CD2-NE2	-6.47	1.30	1.37
2	B	519	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	442	HIS	ND1-CE1	6.36	1.39	1.32
2	D	519	HIS	CD2-NE2	-6.35	1.30	1.37
1	A	196	HIS	CD2-NE2	-6.19	1.31	1.37
2	B	193	HIS	CD2-NE2	-6.15	1.31	1.37
2	D	477	HIS	CD2-NE2	-6.13	1.31	1.37
2	D	106	HIS	CD2-NE2	-6.11	1.31	1.37
2	B	363	HIS	CD2-NE2	-6.10	1.31	1.37
1	C	285	HIS	CD2-NE2	-6.07	1.31	1.37
1	C	451	HIS	CD2-NE2	-6.05	1.31	1.37
2	B	106	HIS	CD2-NE2	-6.04	1.31	1.37
2	B	359	HIS	CD2-NE2	-6.03	1.31	1.37
1	C	150	VAL	CA-CB	6.01	1.61	1.54
2	D	478	HIS	CD2-NE2	-5.96	1.31	1.37
2	D	363	HIS	CD2-NE2	-5.95	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	362	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	285	HIS	CD2-NE2	-5.77	1.31	1.37
1	C	106	VAL	CA-CB	5.65	1.62	1.54
1	C	196	HIS	CG-ND1	-5.64	1.32	1.38
1	A	275	CYS	CB-SG	5.63	1.99	1.81
1	C	195	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	274	HIS	CD2-NE2	-5.58	1.31	1.37
1	A	70	VAL	CA-CB	5.58	1.61	1.54
1	A	195	HIS	CD2-NE2	-5.51	1.31	1.37
2	B	478	HIS	CD2-NE2	-5.49	1.31	1.37
2	B	188	SER	CB-OG	5.36	1.52	1.42
2	D	153	CYS	CB-SG	-5.26	1.63	1.81
1	C	451	HIS	CG-ND1	-5.18	1.32	1.38
1	C	362	HIS	CG-ND1	-5.14	1.32	1.38

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	ASN	CA-CB-CG	11.00	123.60	112.60
1	A	253	TRP	O-C-N	9.48	134.73	122.68
2	D	499	ASN	OD1-CG-ND2	-9.23	113.37	122.60
2	B	116	ASP	CA-CB-CG	9.06	121.67	112.60
2	D	19	ASP	CA-CB-CG	8.98	121.58	112.60
2	B	19	ASP	CA-CB-CG	8.62	121.22	112.60
2	D	498	VAL	CB-CA-C	-8.55	101.02	111.97
2	B	297	HIS	CA-CB-CG	8.31	122.11	113.80
1	C	253	TRP	O-C-N	8.13	132.69	122.93
2	D	297	HIS	CA-CB-CG	8.12	121.92	113.80
1	C	76	LYS	N-CA-C	8.11	121.03	111.71
1	C	383	HIS	CB-CG-CD2	-7.97	120.84	131.20
1	A	432	GLN	OE1-CD-NE2	-7.92	114.68	122.60
1	A	431	PHE	CA-CB-CG	-7.86	105.94	113.80
2	B	499	ASN	OD1-CG-ND2	-7.76	114.84	122.60
1	C	317	ASP	CA-CB-CG	7.75	120.35	112.60
2	D	116	ASP	CA-CB-CG	7.72	120.32	112.60
2	B	104	ASN	CA-CB-CG	7.71	120.31	112.60
2	D	56	ASN	CA-CB-CG	7.67	120.28	112.60
1	C	480	GLU	N-CA-C	-7.63	101.28	110.44
1	A	31	HIS	CB-CG-CD2	-7.61	121.31	131.20
1	A	215	THR	N-CA-C	7.56	122.16	112.34
2	B	429	HIS	CB-CG-CD2	-7.49	121.47	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	HIS	CB-CG-CD2	-7.37	121.62	131.20
2	D	121	ASP	CA-CB-CG	7.29	119.89	112.60
1	C	431	PHE	CA-CB-CG	-7.25	106.55	113.80
2	D	188	SER	CA-CB-OG	7.24	125.57	111.10
1	C	223	VAL	N-CA-CB	-7.19	101.63	112.35
2	D	498	VAL	N-CA-CB	7.16	118.93	110.55
2	B	516	ASP	CA-CB-CG	7.13	119.73	112.60
2	B	474	PHE	CA-CB-CG	7.12	120.92	113.80
2	D	104	ASN	CA-CB-CG	7.10	119.70	112.60
1	A	70	VAL	N-CA-C	7.05	117.88	111.81
2	D	90	HIS	CB-CG-CD2	-7.04	122.04	131.20
1	C	31	HIS	CB-CG-CD2	-6.95	122.17	131.20
1	A	223	VAL	N-CA-CB	-6.91	99.58	112.36
2	B	518	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	35	ASN	OD1-CG-ND2	-6.89	115.71	122.60
2	B	58	GLN	OE1-CD-NE2	-6.87	115.73	122.60
2	D	260	VAL	CB-CA-C	-6.86	98.68	111.79
1	C	465	MET	CG-SD-CE	-6.84	85.85	100.90
1	C	442	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	A	253	TRP	CA-C-N	6.78	134.49	121.54
1	A	253	TRP	C-N-CA	6.78	134.49	121.54
1	A	83	HIS	CB-CG-CD2	-6.78	122.39	131.20
2	B	90	HIS	CB-CG-CD2	-6.73	122.45	131.20
1	C	432	GLN	OE1-CD-NE2	-6.68	115.92	122.60
2	B	56	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	149	SER	CA-CB-OG	6.66	124.41	111.10
1	C	83	HIS	CB-CG-CD2	-6.65	122.56	131.20
2	D	215	ASP	CA-CB-CG	6.64	119.24	112.60
2	D	317	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	234	ASP	CA-CB-CG	6.61	119.21	112.60
2	D	294	GLN	CA-C-N	6.59	126.36	119.05
2	D	294	GLN	C-N-CA	6.59	126.36	119.05
2	D	359	HIS	CB-CG-CD2	-6.43	122.84	131.20
1	C	77	ASP	CA-CB-CG	6.43	119.03	112.60
2	D	516	ASP	CA-CB-CG	6.43	119.03	112.60
2	B	429	HIS	CB-CG-ND1	6.41	132.31	122.70
1	A	191	GLN	CA-CB-CG	6.40	126.91	114.10
2	B	399	ASN	CA-CB-CG	6.40	119.00	112.60
2	B	391	VAL	N-CA-C	6.39	117.14	110.62
2	B	151	THR	N-CA-CB	-6.37	99.73	111.13
2	D	213	MET	N-CA-C	6.36	120.14	112.38
2	D	198	ASP	CA-CB-CG	6.33	118.93	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	168	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	C	107	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	D	161	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	8	GLU	CB-CG-CD	6.21	123.16	112.60
1	A	76	LYS	N-CA-C	6.21	118.59	111.02
1	A	191	GLN	OE1-CD-NE2	-6.21	116.39	122.60
2	B	392	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	C	110	VAL	N-CA-C	6.18	116.85	110.36
2	B	168	ASN	OD1-CG-ND2	-6.17	116.43	122.60
2	B	130	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	C	385	ASP	CA-CB-CG	6.15	118.75	112.60
2	D	477	HIS	CA-CB-CG	6.12	119.92	113.80
2	D	90	HIS	CB-CG-ND1	6.08	131.81	122.70
2	D	369	LEU	N-CA-CB	-6.08	100.75	111.39
1	A	442	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	A	22	GLU	N-CA-C	6.06	118.67	111.33
2	B	359	HIS	CB-CG-CD2	-6.03	123.36	131.20
2	B	213	MET	N-CA-C	6.02	119.45	111.75
2	B	399	ASN	OD1-CG-ND2	-5.97	116.62	122.60
1	C	80	HIS	CB-CG-CD2	-5.96	123.44	131.20
2	D	256	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	75	ILE	O-C-N	5.95	129.30	122.64
1	A	196	HIS	CB-CG-CD2	-5.93	123.48	131.20
1	A	110	VAL	N-CA-C	5.90	117.34	110.62
1	A	223	VAL	CB-CA-C	5.87	120.22	110.30
1	C	383	HIS	CB-CG-ND1	5.86	131.49	122.70
2	B	397	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	C	274	HIS	CA-CB-CG	-5.82	107.98	113.80
2	D	519	HIS	N-CA-C	-5.80	100.88	109.11
1	A	361	ARG	N-CA-C	-5.79	106.26	113.55
1	A	479	TRP	CA-C-N	5.78	132.11	121.70
1	A	479	TRP	C-N-CA	5.78	132.11	121.70
2	B	363	HIS	CB-CG-CD2	-5.76	123.71	131.20
1	A	383	HIS	CB-CG-ND1	5.75	131.32	122.70
2	B	153	CYS	CA-CB-SG	5.74	127.59	114.40
2	B	361	TRP	CG-CD2-CE3	5.73	139.63	133.90
1	A	31	HIS	CB-CG-ND1	5.72	131.29	122.70
2	D	443	ILE	N-CA-C	-5.71	99.42	107.75
2	B	220	SER	N-CA-C	5.70	119.34	112.38
2	D	392	HIS	CB-CG-CD2	-5.70	123.79	131.20
1	C	274	HIS	CB-CG-CD2	-5.70	123.79	131.20
2	B	426	ASP	CA-CB-CG	5.68	118.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	TRP	CG-CD2-CE3	5.67	139.56	133.90
2	D	32	GLU	N-CA-C	5.67	119.45	112.54
2	D	363	HIS	CB-CG-CD2	-5.66	123.84	131.20
2	B	90	HIS	CB-CG-ND1	5.65	131.18	122.70
2	D	417	LYS	N-CA-C	5.64	118.97	111.75
2	D	93	GLN	N-CA-C	5.64	119.27	112.38
2	D	117	SER	N-CA-C	5.64	119.02	111.24
1	A	228	ASP	N-CA-C	-5.63	99.10	108.34
1	C	70	VAL	N-CA-C	5.63	117.02	111.67
2	D	220	SER	N-CA-C	5.62	118.18	111.71
1	A	384	ASN	N-CA-C	5.62	118.17	111.71
1	A	34	VAL	N-CA-C	-5.60	100.41	108.53
1	A	362	HIS	N-CA-C	5.58	119.35	112.54
2	B	313	VAL	CA-C-N	5.57	125.51	119.78
2	B	313	VAL	C-N-CA	5.57	125.51	119.78
1	A	279	MET	CA-CB-CG	-5.56	102.99	114.10
1	A	468	ASN	CB-CG-ND2	5.55	124.73	116.40
1	A	384	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	C	228	ASP	N-CA-C	-5.53	99.28	108.34
2	B	197	TRP	N-CA-C	-5.51	105.19	111.14
1	C	335	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	385	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	253	TRP	CA-C-O	5.49	126.63	120.92
2	B	350	ARG	N-CA-C	-5.49	105.38	111.36
2	D	478	HIS	CB-CG-CD2	-5.47	124.08	131.20
2	D	17	ASP	CA-CB-CG	5.45	118.05	112.60
2	B	417	LYS	N-CA-C	5.45	119.03	112.38
1	C	444	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	C	83	HIS	CB-CG-ND1	5.41	130.81	122.70
2	B	188	SER	CA-CB-OG	5.40	121.91	111.10
2	D	369	LEU	CA-CB-CG	5.40	135.22	116.30
2	B	467	ILE	N-CA-C	-5.40	99.97	107.80
1	A	444	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	C	444	TRP	CB-CG-CD1	-5.39	118.81	126.90
2	D	399	ASN	CA-CB-CG	5.39	117.99	112.60
2	D	236	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	C	31	HIS	CB-CG-ND1	5.38	130.77	122.70
1	A	444	TRP	CB-CG-CD1	-5.37	118.84	126.90
2	D	480	HIS	CB-CG-CD2	-5.37	124.22	131.20
2	B	369	LEU	CA-CB-CG	5.37	135.09	116.30
2	D	71	GLN	N-CA-C	5.37	120.85	113.77
1	A	274	HIS	CB-CG-CD2	-5.36	124.23	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASN	CA-CB-CG	5.36	117.95	112.60
2	B	296	TRP	CE2-CD2-CG	-5.35	100.78	107.20
2	D	361	TRP	CG-CD2-CE3	5.35	139.25	133.90
2	B	357	ASP	CA-CB-CG	5.35	117.95	112.60
2	D	368	ALA	N-CA-C	-5.35	100.98	109.59
2	B	480	HIS	CB-CG-CD2	-5.34	124.25	131.20
2	D	38	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	8	GLU	CA-CB-CG	5.33	124.77	114.10
2	D	258	GLU	CA-CB-CG	5.33	124.77	114.10
1	A	279	MET	N-CA-C	5.33	120.96	113.02
2	B	93	GLN	N-CA-C	5.32	117.99	111.82
1	C	318	GLU	N-CA-C	5.32	117.07	111.28
2	D	185	HIS	CB-CG-CD2	-5.31	124.29	131.20
2	D	149	VAL	N-CA-C	5.31	115.95	108.36
2	B	65	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	C	72	TRP	N-CA-C	5.29	117.86	111.40
2	B	260	VAL	CB-CA-C	-5.28	101.70	111.79
1	C	442	HIS	CA-CB-CG	5.28	119.08	113.80
2	B	236	ASN	OD1-CG-ND2	-5.27	117.33	122.60
2	D	222	LYS	N-CA-C	5.27	118.47	111.30
2	B	41	ASP	CA-CB-CG	5.26	117.86	112.60
1	C	98	ASN	OD1-CG-ND2	-5.26	117.34	122.60
2	B	296	TRP	CG-CD2-CE3	5.26	139.16	133.90
2	B	197	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	C	49	ASN	OD1-CG-ND2	-5.25	117.35	122.60
2	D	49	THR	N-CA-C	5.24	117.62	110.55
2	B	457	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	C	205	TRP	CG-CD2-CE3	5.22	139.12	133.90
1	A	14	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	C	34	VAL	CA-C-O	-5.21	114.92	120.39
1	A	234	ASP	N-CA-C	5.21	117.63	111.33
2	B	187	PRO	N-CA-C	5.21	118.67	110.50
1	A	80	HIS	CB-CG-CD2	-5.20	124.44	131.20
1	A	99	TYR	N-CA-C	5.20	117.83	110.50
2	D	361	TRP	CE2-CD2-CG	-5.20	100.96	107.20
2	B	198	ASP	CA-CB-CG	5.19	117.79	112.60
2	B	498	VAL	CB-CA-C	-5.19	105.13	112.14
1	A	301	GLY	CA-C-N	5.18	124.36	118.97
1	A	301	GLY	C-N-CA	5.18	124.36	118.97
1	A	472	TRP	CE2-CD2-CG	-5.18	100.98	107.20
1	A	396	ASP	N-CA-C	-5.18	103.20	110.50
1	A	444	TRP	CG-CD2-CE3	5.16	139.06	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	NE-CZ-NH1	5.14	126.64	121.50
2	D	221	ASN	OD1-CG-ND2	-5.14	117.46	122.60
2	D	428	TRP	CE2-CD2-CG	-5.13	101.04	107.20
2	D	221	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	384	ASN	CA-CB-CG	-5.12	107.48	112.60
2	B	445	ASN	CA-CB-CG	5.12	117.72	112.60
2	B	58	GLN	CG-CD-NE2	5.11	124.07	116.40
1	C	253	TRP	CG-CD2-CE3	5.11	139.01	133.90
2	D	523	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	A	49	ASN	OD1-CG-ND2	-5.09	117.51	122.60
1	A	359	ARG	NE-CZ-NH1	5.09	126.59	121.50
2	B	361	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	A	72	TRP	CG-CD2-CE3	5.08	138.98	133.90
1	A	468	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	D	468	ARG	N-CA-C	5.08	116.96	108.23
1	C	335	TRP	CE2-CD2-CG	-5.08	101.11	107.20
1	A	83	HIS	CB-CG-ND1	5.07	130.31	122.70
2	D	160	ASP	CA-CB-CG	5.07	117.67	112.60
2	B	209	THR	N-CA-C	5.06	119.20	112.72
2	B	478	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	361	ARG	NE-CZ-NH1	5.05	126.55	121.50
2	B	520	ASP	N-CA-C	5.05	117.63	110.10
2	D	519	HIS	CB-CG-CD2	-5.05	124.63	131.20
2	D	129	GLN	OE1-CD-NE2	-5.03	117.57	122.60
2	D	260	VAL	N-CA-CB	5.03	120.74	110.78
2	D	467	ILE	N-CA-C	-5.02	99.94	107.37
1	A	345	ARG	CD-NE-CZ	5.02	131.42	124.40
2	D	520	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	75	ILE	CA-C-N	5.01	127.75	120.79
1	A	75	ILE	C-N-CA	5.01	127.75	120.79
2	D	428	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	3637	46	0
1	C	3713	0	3639	41	0
2	B	4174	0	4088	44	0
2	D	4173	0	4088	39	0
3	A	14	0	6	0	0
3	C	14	0	6	0	0
4	A	17	0	0	1	0
4	C	17	0	0	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	15	0	0	0	0
6	D	15	0	0	1	0
7	A	134	0	0	9	0
7	B	185	0	0	1	0
7	C	129	0	0	2	0
7	D	179	0	0	4	0
All	All	16490	0	15464	157	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 (157) 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:360:THR:HA	1:C:465:MET:HE1	1.52	0.91
2:B:499:ASN:HD21	2:D:477:HIS:H	1.19	0.86
1:A:93:ARG:HG3	1:A:113:ASN:HB2	1.60	0.84
2:D:351:LEU:HG	2:D:355:MET:HE2	1.61	0.81
2:B:209:THR:HG21	2:B:309:TRP:HE1	1.45	0.81
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.02	0.75
2:D:352:VAL:HA	2:D:355:MET:HE3	1.69	0.75
2:B:202:GLU:HG3	2:B:300:LYS:HG2	1.69	0.75
2:D:322:LEU:HD22	2:D:355:MET:HE1	1.67	0.75
2:B:477:HIS:H	2:D:499:ASN:HD21	1.37	0.72
1:A:93:ARG:HD3	1:A:111:THR:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:THR:HG22	1:C:60:ARG:H	1.62	0.65
1:A:12:LEU:HD13	1:A:415:ARG:HG3	1.79	0.65
1:C:93:ARG:HD2	1:C:111:THR:O	1.99	0.62
2:D:390:PRO:HB2	2:D:393:ILE:HD11	1.81	0.62
1:A:352:MET:HE1	1:A:413:VAL:HA	1.83	0.61
7:A:619:HOH:O	2:B:120:GLU:HG3	2.02	0.59
1:A:476:GLN:NE2	1:A:480:GLU:HA	2.17	0.59
1:C:239:ARG:HE	1:C:252:GLN:NE2	2.01	0.59
1:C:332:LYS:O	1:C:336:GLU:HB2	2.04	0.58
1:C:96:ARG:NH1	4:C:496:CFM:S5	2.77	0.58
2:B:205:ALA:O	2:B:209:THR:HB	2.05	0.56
1:C:239:ARG:HE	1:C:252:GLN:HE21	1.53	0.56
1:A:66:GLY:O	1:A:70:VAL:HG22	2.06	0.56
2:D:221:ASN:OD1	2:D:287:ALA:HA	2.06	0.56
2:D:128:GLN:HG3	2:D:132:LYS:HE2	1.88	0.55
2:B:100:ARG:HD2	2:B:111:VAL:O	2.06	0.55
1:A:410:GLU:HG3	1:A:434:MET:HE1	1.88	0.54
1:C:104:THR:HA	1:C:108:ALA:O	2.08	0.54
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.90	0.54
2:B:151:THR:HG21	2:B:156:GLU:OE2	2.07	0.53
1:A:239:ARG:HE	1:A:252:GLN:NE2	2.06	0.53
2:D:131:MET:HE1	2:D:149:VAL:HG21	1.91	0.53
7:A:559:HOH:O	2:B:26:LYS:HB3	2.08	0.53
2:B:176:PRO:HG2	2:B:179:PHE:HB2	1.91	0.53
2:D:457:HIS:HE1	7:D:676:HOH:O	1.92	0.52
1:A:156:ILE:O	1:A:159:ILE:HG22	2.09	0.52
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.44	0.52
1:A:461:ARG:HG2	1:A:461:ARG:HH11	1.74	0.52
1:C:226:ILE:HG22	1:C:279:MET:HB3	1.92	0.52
2:B:457:HIS:HE1	7:B:621:HOH:O	1.93	0.52
2:B:213:MET:HE2	2:B:308:THR:O	2.11	0.51
2:D:217:VAL:H	2:D:286:ASN:ND2	2.08	0.51
2:B:156:GLU:HG3	2:B:187:PRO:HB3	1.93	0.51
2:B:228:PRO:HA	2:B:293:LEU:HD12	1.93	0.51
2:D:53:GLN:HE21	2:D:432:SER:HB3	1.75	0.51
1:A:361:ARG:HD2	7:A:581:HOH:O	2.11	0.50
1:C:476:GLN:NE2	1:C:481:ALA:HA	2.26	0.50
1:A:121:LYS:H	1:A:121:LYS:HZ3	1.59	0.50
1:C:355:ILE:HD12	1:C:359:ARG:HB3	1.94	0.50
1:C:134:LEU:HD13	2:D:62:LEU:HD13	1.94	0.49
2:B:85:THR:HG21	2:B:146:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.46	0.49
1:A:277:ARG:HD3	7:A:562:HOH:O	2.11	0.49
1:A:361:ARG:O	1:A:364:ILE:HG12	2.13	0.49
2:B:105:ARG:HB3	2:B:474:PHE:CD1	2.47	0.49
1:C:192:SER:OG	1:C:383:HIS:HE1	1.95	0.49
2:B:305:VAL:O	2:B:309:TRP:HB2	2.13	0.49
2:B:426:ASP:O	2:B:429:HIS:HB2	2.13	0.49
2:B:221:ASN:OD1	2:B:287:ALA:HA	2.13	0.48
2:B:434:VAL:HG11	2:B:442:MET:HE3	1.95	0.48
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.96	0.48
2:D:494:LEU:O	2:D:498:VAL:HG23	2.13	0.48
1:A:144:LEU:CD1	2:B:43:VAL:HG21	2.43	0.48
1:A:119:GLN:HB2	1:A:121:LYS:HE2	1.95	0.47
2:B:477:HIS:N	2:D:499:ASN:HD21	2.09	0.47
2:B:151:THR:CG2	2:B:156:GLU:HG2	2.44	0.47
1:A:104:THR:HA	1:A:108:ALA:O	2.14	0.47
1:A:62:CYS:SG	1:A:64:TYR:HB3	2.55	0.47
1:A:336:GLU:HA	1:A:339:VAL:HG12	1.96	0.47
1:C:355:ILE:CD1	1:C:359:ARG:HB3	2.45	0.47
2:B:477:HIS:H	2:D:499:ASN:ND2	2.09	0.47
1:A:192:SER:OG	1:A:383:HIS:HE1	1.98	0.46
1:A:97:ARG:O	1:A:231:ILE:HA	2.14	0.46
2:B:320:MET:HG3	2:B:485:LEU:HD23	1.96	0.46
1:C:58:THR:HG23	1:C:403:ASP:OD1	2.15	0.46
2:D:105:ARG:HB3	2:D:474:PHE:CD1	2.50	0.46
1:C:103:THR:H	1:C:107:ASN:HD22	1.63	0.46
1:C:332:LYS:N	1:C:333:PRO:HD2	2.31	0.46
1:C:349:LYS:HD3	1:C:349:LYS:HA	1.76	0.46
2:D:101:SER:HA	2:D:104:ASN:HD22	1.80	0.46
1:C:318:GLU:HG3	1:C:322:LYS:HE3	1.98	0.46
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.96	0.46
2:D:2:SER:N	7:D:658:HOH:O	2.49	0.46
2:D:153:CYS:HB3	2:D:188:SER:OG	2.15	0.46
2:D:426:ASP:H	2:D:429:HIS:HD2	1.63	0.46
1:A:352:MET:HE3	1:A:418:PRO:HG3	1.97	0.46
2:B:234:LEU:HD23	2:B:238:ARG:NH2	2.30	0.46
1:A:476:GLN:HE22	1:A:480:GLU:HA	1.81	0.46
2:B:264:PRO:HG2	2:B:270:ARG:NH2	2.31	0.45
2:D:326:ASP:OD1	2:D:348:ARG:HD2	2.15	0.45
2:B:468:ARG:HB3	2:B:473:ILE:HD12	1.98	0.45
2:B:226:ILE:HD13	2:B:251:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:SER:HB3	7:D:656:HOH:O	2.16	0.45
2:B:346:LYS:O	2:B:350:ARG:HG3	2.18	0.44
2:D:194:VAL:HB	2:D:297:HIS:CG	2.52	0.44
1:A:361:ARG:HB3	1:A:379:TYR:OH	2.18	0.44
1:A:442:HIS:HB2	7:A:542:HOH:O	2.16	0.44
1:A:46:ILE:HG23	7:A:590:HOH:O	2.16	0.44
1:C:357:GLY:HA2	1:C:379:TYR:HD2	1.82	0.44
1:A:159:ILE:HG21	1:A:159:ILE:HD13	1.75	0.44
2:B:499:ASN:ND2	2:D:477:HIS:H	2.01	0.44
1:C:58:THR:HG22	1:C:60:ARG:N	2.31	0.44
2:D:414:PRO:HA	2:D:417:LYS:HD3	2.00	0.44
1:C:364:ILE:HD12	1:C:394:MET:SD	2.58	0.44
2:D:146:MET:HG3	2:D:180:PRO:HB2	1.99	0.43
2:D:394:LEU:HD13	2:D:430:LEU:HB2	2.00	0.43
1:A:123:ILE:HA	1:A:159:ILE:HD11	2.00	0.43
1:C:85:PRO:HB2	6:D:525:CLF:S2B	2.59	0.43
1:A:239:ARG:NH1	7:A:559:HOH:O	2.52	0.43
2:B:247:MET:HE2	2:B:247:MET:HB3	1.96	0.43
2:B:247:MET:HG2	2:B:341:PRO:HD2	2.01	0.43
1:A:22:GLU:HG3	1:A:26:LYS:HE3	2.00	0.42
1:A:45:CYS:N	7:A:622:HOH:O	2.53	0.42
2:B:153:CYS:HB3	2:B:188:SER:OG	2.18	0.42
1:C:298:ASN:ND2	1:C:304:LYS:HG2	2.33	0.42
2:D:71:GLN:O	2:D:196:GLY:HA3	2.19	0.42
1:C:462:ASP:HA	1:C:465:MET:HG2	2.00	0.42
1:A:121:LYS:H	1:A:121:LYS:NZ	2.18	0.42
1:A:333:PRO:HD3	7:A:627:HOH:O	2.20	0.42
1:A:422:GLY:HA2	1:A:439:ARG:O	2.19	0.42
2:B:234:LEU:HD23	2:B:238:ARG:HH22	1.85	0.42
2:B:494:LEU:O	2:B:498:VAL:HG23	2.19	0.42
1:C:144:LEU:HD21	2:D:43:VAL:HG21	2.02	0.42
1:C:442:HIS:HB2	7:C:513:HOH:O	2.19	0.42
2:D:2:SER:N	7:D:641:HOH:O	2.52	0.42
2:D:105:ARG:HB3	2:D:474:PHE:CE1	2.53	0.42
1:A:478:PRO:HB2	2:D:330:MET:SD	2.59	0.42
1:C:150:VAL:HG13	1:C:180:PRO:HA	2.01	0.42
2:B:80:LEU:HD13	2:B:87:PRO:HG3	2.02	0.42
2:D:313:VAL:HA	2:D:314:PRO:HD3	1.90	0.42
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.35	0.41
2:D:57:PHE:HA	2:D:429:HIS:CE1	2.55	0.41
1:C:56:LEU:HB2	7:C:579:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:VAL:HG11	4:C:496:CFM:S2B	2.59	0.41
1:C:207:LEU:HD22	1:C:282:ILE:HD11	2.01	0.41
1:A:96:ARG:NH1	4:A:496:CFM:S5	2.94	0.41
1:A:420:LEU:HB2	1:A:467:LEU:HD22	2.02	0.41
2:B:313:VAL:HA	2:B:314:PRO:HD3	1.87	0.41
1:A:74:PRO:HB2	1:A:254:SER:HB3	2.02	0.41
1:C:54:PRO:HB3	2:D:116:ASP:O	2.20	0.41
2:D:389:GLU:HA	2:D:390:PRO:HD3	1.88	0.41
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.56	0.41
2:B:326:ASP:OD1	2:B:348:ARG:HD2	2.21	0.41
2:D:213:MET:HE2	2:D:308:THR:O	2.21	0.41
1:A:144:LEU:HD11	2:B:43:VAL:HG21	2.03	0.41
1:A:220:PRO:HA	1:A:269:LYS:HE2	2.03	0.41
2:B:170:LYS:HG3	2:B:175:ILE:CD1	2.51	0.41
2:D:505:LEU:HD13	2:D:523:ARG:CZ	2.51	0.41
1:A:462:ASP:HA	1:A:465:MET:HG2	2.03	0.41
1:A:426:LYS:HA	2:B:104:ASN:ND2	2.36	0.40
1:C:209:LYS:HB2	1:C:209:LYS:HE3	1.85	0.40
2:D:306:GLU:O	2:D:310:LYS:HA	2.21	0.40
1:C:275:CYS:SG	1:C:278:SER:OG	2.70	0.40
1:A:239:ARG:HE	1:A:252:GLN:HE21	1.67	0.40
1:C:97:ARG:O	1:C:231:ILE:HA	2.21	0.40
1:C:263:GLU:O	1:C:266:PRO:HD2	2.21	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%)	443 (96%)	17 (4%)	3 (1%)	21 12
1	C	464/491 (94%)	432 (93%)	28 (6%)	4 (1%)	14 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	520/522 (100%)	496 (95%)	23 (4%)	1 (0%)	43	40
2	D	520/522 (100%)	501 (96%)	18 (4%)	1 (0%)	43	40
All	All	1967/2026 (97%)	1872 (95%)	86 (4%)	9 (0%)	24	17

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	GLU
1	C	6	ARG
1	A	254	SER
2	B	255	SER
2	D	255	SER
1	C	266	PRO
1	C	317	ASP
1	C	355	ILE
1	A	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%)	372 (94%)	24 (6%)	17	10
2	B	454/454 (100%)	429 (94%)	25 (6%)	19	12
2	D	454/454 (100%)	433 (95%)	21 (5%)	24	17
All	All	1701/1736 (98%)	1601 (94%)	100 (6%)	18	10

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	14	GLN
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	47	ILE
1	A	70	VAL
1	A	93	ARG
1	A	98	ASN
1	A	121	LYS
1	A	131	LEU
1	A	134	LEU
1	A	150	VAL
1	A	176	LYS
1	A	209	LYS
1	A	212	GLU
1	A	215	THR
1	A	223	VAL
1	A	243	GLU
1	A	252	GLN
1	A	310	ARG
1	A	322	LYS
1	A	345	ARG
1	A	359	ARG
1	A	362	HIS
1	A	383	HIS
1	A	415	ARG
1	A	445	ASP
1	A	467	LEU
1	A	473	LYS
1	A	475	LEU
1	A	476	GLN
2	B	13	PRO
2	B	28	ARG
2	B	50	LYS
2	B	80	LEU
2	B	85	THR
2	B	92	SER
2	B	105	ARG
2	B	131	MET
2	B	151	THR
2	B	171	LYS
2	B	175	ILE
2	B	177	ASP
2	B	178	GLU
2	B	202	GLU
2	B	209	THR

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Mol	Chain	Res	Type
2	B	224	ILE
2	B	252	SER
2	B	258	GLU
2	B	260	VAL
2	B	329	LEU
2	B	369	LEU
2	B	418	ASN
2	B	461	GLU
2	B	503	GLU
2	B	505	LEU
1	C	12	LEU
1	C	35	ASN
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	187	ARG
1	C	210	ARG
1	C	214	THR
1	C	223	VAL
1	C	252	GLN
1	C	336	GLU
1	C	359	ARG
1	C	362	HIS
1	C	383	HIS
1	C	389	ARG
1	C	396	ASP
1	C	445	ASP
1	C	467	LEU
1	C	475	LEU
2	D	13	PRO
2	D	26	LYS
2	D	38	ASP
2	D	92	SER
2	D	105	ARG
2	D	143	LYS
2	D	171	LYS
2	D	172	GLU

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Mol	Chain	Res	Type
2	D	175	ILE
2	D	177	ASP
2	D	202	GLU
2	D	212	SER
2	D	238	ARG
2	D	252	SER
2	D	260	VAL
2	D	369	LEU
2	D	379	LEU
2	D	461	GLU
2	D	498	VAL
2	D	505	LEU
2	D	507	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	252	GLN
1	A	383	HIS
2	B	58	GLN
2	B	104	ASN
2	B	130	ASN
2	B	136	GLN
2	B	286	ASN
2	B	294	GLN
2	B	457	HIS
2	B	499	ASN
2	B	519	HIS
1	C	53	GLN
1	C	107	ASN
1	C	252	GLN
1	C	362	HIS
1	C	383	HIS
1	C	384	ASN
2	D	4	GLN
2	D	37	GLN
2	D	53	GLN
2	D	104	ASN
2	D	128	GLN
2	D	129	GLN
2	D	130	ASN

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Mol	Chain	Res	Type
2	D	163	ASN
2	D	167	ASN
2	D	168	ASN
2	D	286	ASN
2	D	429	HIS
2	D	457	HIS
2	D	499	ASN
2	D	519	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	CFM	C	496	1,3	0,24,24	-	-	-		
3	HCA	A	494	4	13,13,13	2.90	3 (23%)	15,18,18	2.51	6 (40%)
4	CFM	A	496	1,3	0,24,24	-	-	-		
6	CLF	B	525	1,2	0,24,24	-	-	-		
6	CLF	D	525	1,2	0,24,24	-	-	-		
3	HCA	C	494	4	13,13,13	2.97	4 (30%)	15,18,18	2.38	7 (46%)

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
6	CLF	D	525	1,2	-	-	0/12/10/10
3	HCA	A	494	4	-	5/17/17/17	-
6	CLF	B	525	1,2	-	-	0/12/10/10
3	HCA	C	494	4	-	2/17/17/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	494	HCA	C3-C7	-8.31	1.44	1.53
3	A	494	HCA	C3-C7	-7.97	1.45	1.53
3	A	494	HCA	O5-C7	5.68	1.39	1.22
3	C	494	HCA	O5-C7	5.31	1.38	1.22
3	A	494	HCA	O1-C1	2.42	1.30	1.22
3	C	494	HCA	C4-C3	2.15	1.59	1.53
3	C	494	HCA	O1-C1	2.08	1.28	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	494	HCA	O6-C7-C3	5.03	122.79	113.14
3	C	494	HCA	O6-C7-C3	4.92	122.58	113.14
3	A	494	HCA	O5-C7-C3	-4.53	113.32	122.09
3	C	494	HCA	O5-C7-C3	-4.48	113.42	122.09
3	A	494	HCA	O7-C3-C7	-3.20	104.42	108.96
3	A	494	HCA	O4-C6-O3	-3.03	115.53	123.33
3	A	494	HCA	C3-C2-C1	2.99	122.09	113.92
3	C	494	HCA	O4-C6-O3	-2.88	115.93	123.33
3	C	494	HCA	C3-C2-C1	2.75	121.43	113.92
3	A	494	HCA	O2-C1-O1	-2.71	116.37	123.33
3	C	494	HCA	C4-C5-C6	2.37	118.25	112.77
3	C	494	HCA	O4-C6-C5	2.25	121.12	114.00
3	C	494	HCA	O2-C1-O1	-2.12	117.89	123.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	494	HCA	C2-C3-C4-C5
3	A	494	HCA	C7-C3-C4-C5
3	A	494	HCA	O7-C3-C4-C5
3	C	494	HCA	C2-C3-C4-C5
3	A	494	HCA	C3-C4-C5-C6
3	A	494	HCA	C4-C5-C6-O4
3	C	494	HCA	C4-C5-C6-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	496	CFM	2	0
4	A	496	CFM	1	0
6	D	525	CLF	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.