



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 02:38 pm BST

PDB ID : 2MIN
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

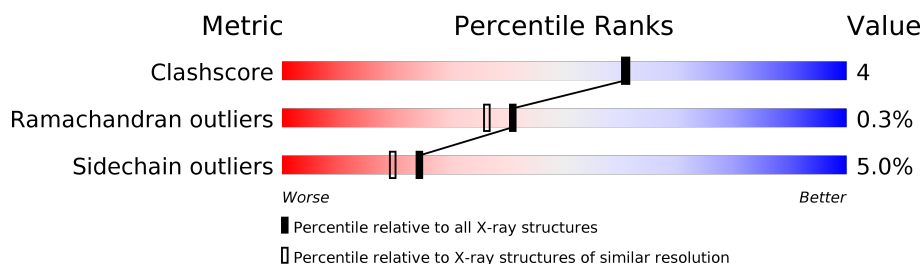
1 Overall quality at a glance

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	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)

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 on 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	
1	C	491	
2	B	522	
2	D	522	

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.

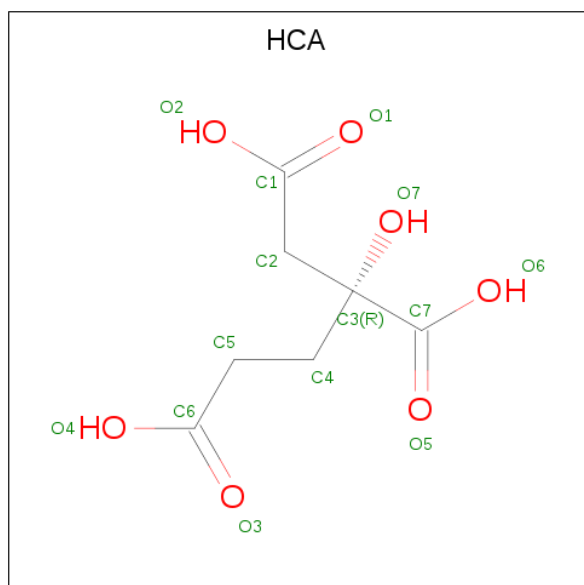
- Molecule 1 is a protein called NITROGENASE MOLYBDENUM IRON PROTEIN.

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.

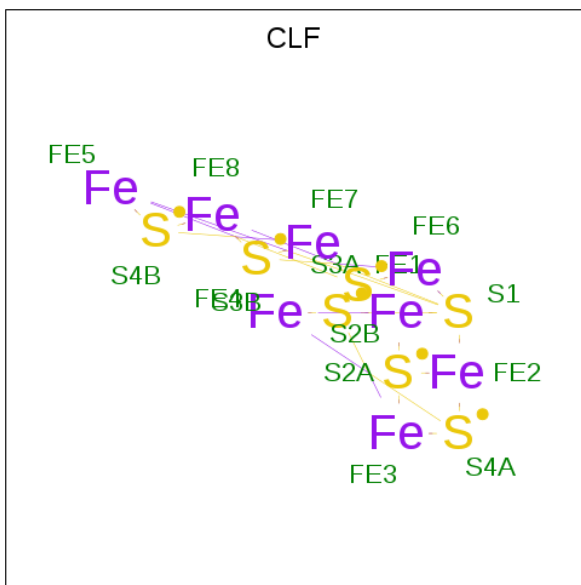
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (three-letter code: HCA) (formula: C₇H₁₀O₇).



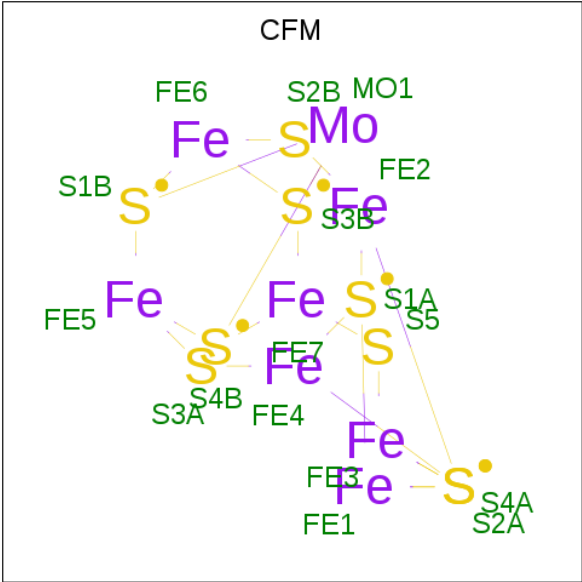
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	7	7		
3	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 4 is FE(8)-S(7) CLUSTER (three-letter code: CLF) (formula: Fe_8S_7).



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 (three-letter code: CFM) (formula: Fe_7MoS_9).



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 (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is water.

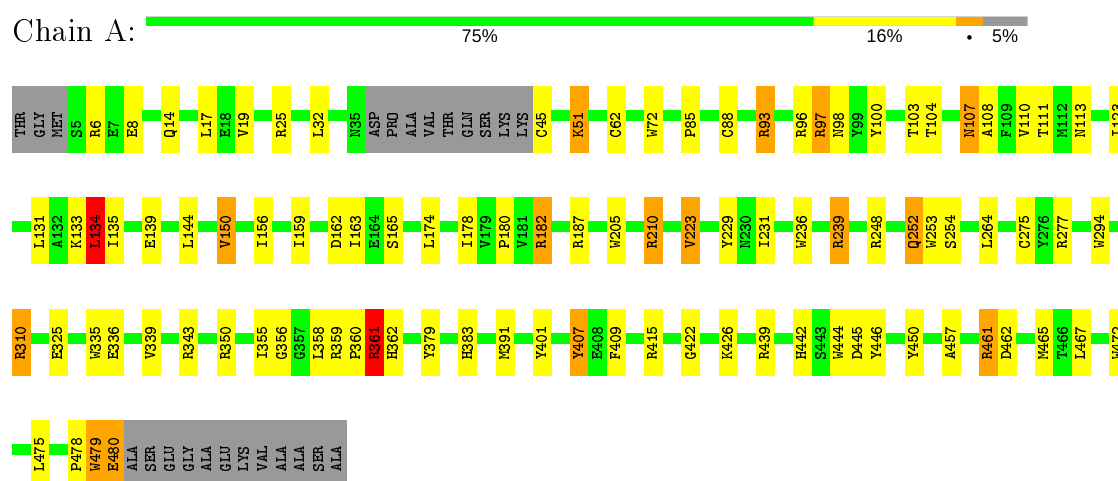
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	132	Total	O	0	0
			132	132		
7	B	186	Total	O	0	0
			186	186		
7	C	126	Total	O	0	0
			126	126		
7	D	183	Total	O	0	0
			183	183		

3 Residue-property plots [i](#)

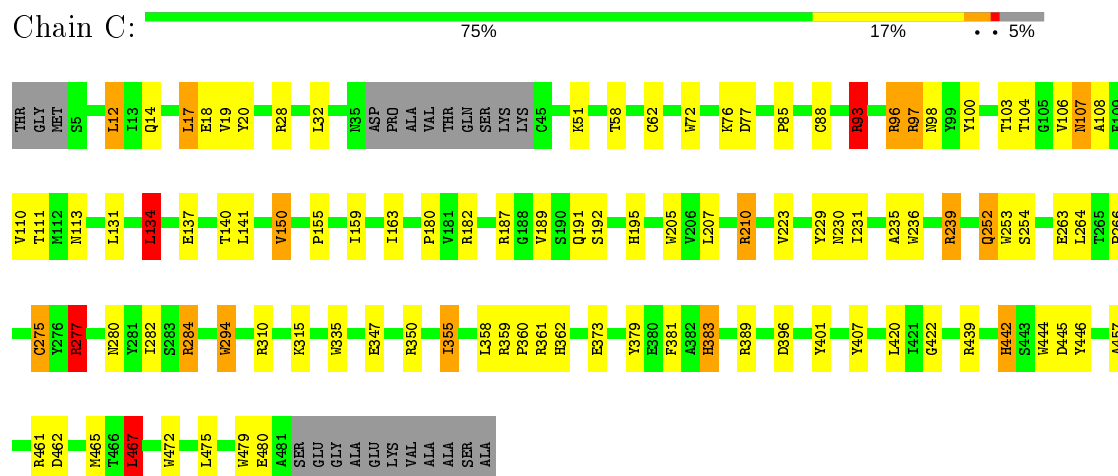
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

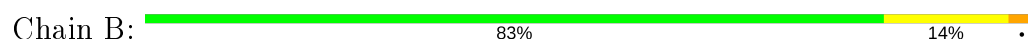
• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN

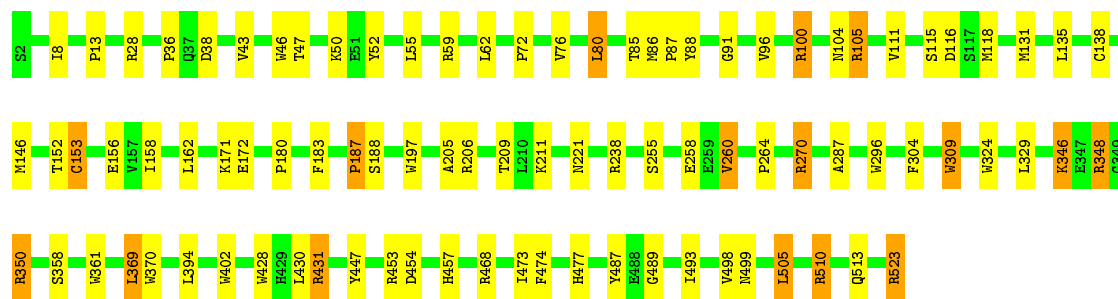


• Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN



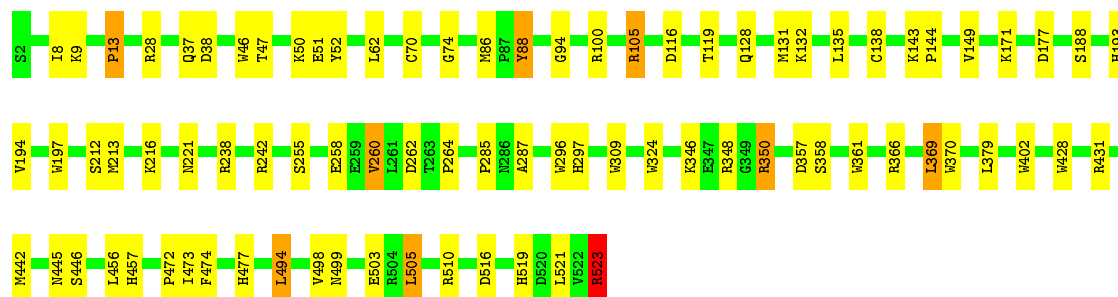
• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN





• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN

Chain D: 84% 14%



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	107.70 Å 130.20 Å 81.30 Å 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLF, HCA, CA, CFM

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	0.75	2/3795 (0.1%)	1.46	61/5117 (1.2%)
1	C	0.76	3/3799 (0.1%)	1.43	61/5123 (1.2%)
2	B	0.76	2/4280 (0.0%)	1.35	56/5786 (1.0%)
2	D	0.76	2/4280 (0.0%)	1.33	51/5786 (0.9%)
All	All	0.76	9/16154 (0.1%)	1.39	229/21812 (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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	188	SER	CB-OG	-14.21	1.23	1.42
2	B	188	SER	CB-OG	-10.66	1.28	1.42
1	A	88	CYS	CB-SG	-7.35	1.69	1.82
2	D	70	CYS	CB-SG	-6.43	1.71	1.82
2	B	153	CYS	CB-SG	-6.40	1.71	1.82
1	C	275	CYS	CB-SG	6.40	1.93	1.82
1	C	442	HIS	CG-ND1	-6.39	1.24	1.38
1	C	88	CYS	CB-SG	-5.43	1.73	1.81
1	A	62	CYS	CB-SG	-5.11	1.73	1.81

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	ARG	NE-CZ-NH1	11.93	126.26	120.30
2	D	431	ARG	NE-CZ-NH2	-11.88	114.36	120.30
2	B	523	ARG	NE-CZ-NH1	11.68	126.14	120.30
2	B	431	ARG	NE-CZ-NH1	11.64	126.12	120.30
2	D	431	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	239	ARG	NE-CZ-NH2	-11.44	114.58	120.30
1	C	97	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	A	361	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	A	97	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	C	239	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	C	210	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	C	239	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	A	96	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	A	239	ARG	NE-CZ-NH1	10.44	125.52	120.30
2	D	523	ARG	NE-CZ-NH2	-10.33	115.14	120.30
2	D	348	ARG	NE-CZ-NH1	10.20	125.40	120.30
2	D	523	ARG	NE-CZ-NH1	10.15	125.37	120.30
2	B	431	ARG	NE-CZ-NH2	-10.09	115.25	120.30
2	B	105	ARG	NE-CZ-NH1	9.85	125.22	120.30
2	D	105	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	A	361	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	97	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	C	335	TRP	CD1-CG-CD2	9.45	113.86	106.30
1	A	96	ARG	NE-CZ-NH1	9.29	124.95	120.30
2	D	309	TRP	CD1-CG-CD2	9.21	113.67	106.30
2	B	523	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	C	253	TRP	CD1-CG-CD2	9.13	113.61	106.30
1	A	253	TRP	CA-C-N	-9.05	97.29	117.20
2	B	59	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	B	270	ARG	NE-CZ-NH1	8.94	124.77	120.30
2	B	369	LEU	CA-CB-CG	8.84	135.63	115.30
1	C	472	TRP	CD1-CG-CD2	8.79	113.33	106.30
1	C	93	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	253	TRP	CD1-CG-CD2	8.72	113.28	106.30
1	C	72	TRP	CD1-CG-CD2	8.65	113.22	106.30
2	B	402	TRP	CD1-CG-CD2	8.57	113.16	106.30
2	D	510	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	359	ARG	NE-CZ-NH1	8.53	124.56	120.30
2	D	369	LEU	CA-CB-CG	8.52	134.90	115.30
1	C	472	TRP	CE2-CD2-CG	-8.46	100.53	107.30
2	B	348	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	B	296	TRP	CD1-CG-CD2	8.39	113.01	106.30
2	B	348	ARG	NE-CZ-NH2	-8.28	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	ARG	NE-CZ-NH1	8.26	124.43	120.30
2	D	361	TRP	CD1-CG-CD2	8.26	112.91	106.30
2	B	309	TRP	CD1-CG-CD2	8.25	112.90	106.30
2	D	46	TRP	CD1-CG-CD2	8.24	112.89	106.30
2	B	197	TRP	CD1-CG-CD2	8.19	112.85	106.30
2	B	361	TRP	CD1-CG-CD2	8.19	112.85	106.30
1	C	96	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	D	296	TRP	CD1-CG-CD2	8.14	112.81	106.30
2	D	494	LEU	CA-CB-CG	8.13	134.00	115.30
1	A	472	TRP	CD1-CG-CD2	8.12	112.79	106.30
2	B	46	TRP	CD1-CG-CD2	8.12	112.79	106.30
1	C	277	ARG	NE-CZ-NH1	8.09	124.35	120.30
2	B	428	TRP	CD1-CG-CD2	8.04	112.73	106.30
1	A	444	TRP	CE2-CD2-CG	-8.02	100.88	107.30
2	B	270	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	72	TRP	CD1-CG-CD2	7.95	112.66	106.30
1	A	444	TRP	CD1-CG-CD2	7.95	112.66	106.30
2	B	59	ARG	NE-CZ-NH2	-7.93	116.33	120.30
2	D	428	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	A	335	TRP	CD1-CG-CD2	7.92	112.64	106.30
1	A	472	TRP	CE2-CD2-CG	-7.92	100.97	107.30
1	A	294	TRP	CD1-CG-CD2	7.89	112.61	106.30
1	A	253	TRP	O-C-N	7.87	135.29	122.70
1	C	444	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	93	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	C	253	TRP	CA-C-N	-7.82	100.00	117.20
2	D	402	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	C	72	TRP	CE2-CD2-CG	-7.79	101.06	107.30
2	D	357	ASP	CB-CG-OD2	-7.77	111.31	118.30
2	D	197	TRP	CD1-CG-CD2	7.76	112.51	106.30
1	A	479	TRP	CD1-CG-CD2	7.74	112.49	106.30
2	B	238	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	461	ARG	NE-CZ-NH1	7.69	124.14	120.30
2	B	296	TRP	CE2-CD2-CG	-7.68	101.16	107.30
2	D	428	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	A	294	TRP	CE2-CD2-CG	-7.67	101.16	107.30
2	D	350	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	A	134	LEU	CA-CB-CG	7.65	132.89	115.30
2	D	296	TRP	CE2-CD2-CG	-7.65	101.18	107.30
1	C	294	TRP	CD1-CG-CD2	7.64	112.42	106.30
2	B	361	TRP	CE2-CD2-CG	-7.64	101.19	107.30
2	B	100	ARG	NE-CZ-NH2	-7.63	116.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	46	TRP	CE2-CD2-CG	-7.60	101.22	107.30
2	D	370	TRP	CD1-CG-CD2	7.60	112.38	106.30
2	B	350	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	C	134	LEU	CA-CB-CG	7.59	132.75	115.30
2	D	197	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	A	277	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	335	TRP	CE2-CD2-CG	-7.53	101.27	107.30
2	B	370	TRP	CD1-CG-CD2	7.52	112.31	106.30
1	C	444	TRP	CD1-CG-CD2	7.50	112.30	106.30
2	D	361	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	C	479	TRP	CD1-CG-CD2	7.48	112.29	106.30
2	B	428	TRP	CE2-CD2-CG	-7.47	101.33	107.30
1	C	335	TRP	CG-CD2-CE3	7.45	140.61	133.90
2	B	402	TRP	CE2-CD2-CG	-7.44	101.34	107.30
1	A	205	TRP	CD1-CG-CD2	7.43	112.24	106.30
1	C	236	TRP	CD1-CG-CD2	7.42	112.24	106.30
1	C	277	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	C	205	TRP	CE2-CD2-CG	-7.40	101.38	107.30
2	B	46	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	A	236	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	C	205	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	C	335	TRP	CG-CD1-NE1	-7.38	102.72	110.10
2	B	197	TRP	CE2-CD2-CG	-7.38	101.39	107.30
2	B	309	TRP	CE2-CD2-CG	-7.37	101.41	107.30
1	A	479	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	C	97	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	D	348	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	72	TRP	CE2-CD2-CG	-7.29	101.46	107.30
1	C	294	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	A	210	ARG	NE-CZ-NH2	-7.25	116.68	120.30
2	D	402	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	B	324	TRP	CD1-CG-CD2	7.18	112.05	106.30
2	D	238	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	205	TRP	CE2-CD2-CG	-7.15	101.58	107.30
2	B	453	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	B	100	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	335	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	236	TRP	CE2-CD2-CG	-7.02	101.68	107.30
1	A	93	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	479	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	A	277	ARG	NE-CZ-NH1	6.97	123.78	120.30
2	B	350	ARG	NE-CZ-NH1	6.97	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	TRP	CE2-CD2-CG	-6.95	101.74	107.30
2	B	324	TRP	CE2-CD2-CG	-6.90	101.78	107.30
2	D	324	TRP	CE2-CD2-CG	-6.87	101.80	107.30
1	C	310	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	D	370	TRP	CE2-CD2-CG	-6.86	101.81	107.30
2	B	370	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	C	335	TRP	CB-CG-CD1	-6.78	118.18	127.00
2	B	28	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	253	TRP	O-C-N	6.76	133.52	122.70
2	B	153	CYS	CA-CB-SG	6.67	126.00	114.00
2	D	28	ARG	NE-CZ-NH2	-6.61	117.00	120.30
2	D	324	TRP	CD1-CG-CD2	6.59	111.57	106.30
2	B	510	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	343	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	444	TRP	CB-CG-CD1	-6.53	118.51	127.00
1	A	253	TRP	CE2-CD2-CG	-6.53	102.08	107.30
1	C	187	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	25	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	310	ARG	NE-CZ-NH1	6.49	123.54	120.30
2	D	309	TRP	CG-CD1-NE1	-6.45	103.65	110.10
2	D	309	TRP	CE2-CD2-CG	-6.42	102.16	107.30
2	D	100	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	A	450	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	A	461	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	C	253	TRP	CE2-CD2-CG	-6.23	102.31	107.30
2	D	510	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	444	TRP	CG-CD2-CE3	6.19	139.47	133.90
1	A	350	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	444	TRP	CB-CG-CD1	-6.14	119.02	127.00
1	C	444	TRP	CG-CD2-CE3	6.05	139.34	133.90
1	A	479	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	C	359	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	B	309	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	A	253	TRP	CG-CD1-NE1	-5.89	104.21	110.10
1	C	253	TRP	CG-CD1-NE1	-5.84	104.26	110.10
2	B	309	TRP	CG-CD2-CE3	5.83	139.15	133.90
1	C	210	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	D	197	TRP	CG-CD2-CE3	5.82	139.14	133.90
2	D	100	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	461	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	B	510	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	C	480	GLU	CA-CB-CG	5.78	126.11	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	PRO	N-CA-CB	5.78	110.23	103.30
2	D	105	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	D	357	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	28	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	467	LEU	CA-CB-CG	5.71	128.42	115.30
1	A	415	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	253	TRP	CB-CG-CD1	-5.63	119.67	127.00
1	A	51	LYS	CA-CB-CG	5.62	125.77	113.40
1	A	187	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	D	516	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	88	CYS	CA-CB-SG	5.56	124.02	114.00
1	A	294	TRP	CG-CD2-CE3	5.56	138.90	133.90
1	C	361	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	D	197	TRP	CB-CG-CD1	-5.52	119.82	127.00
2	B	361	TRP	CG-CD2-CE3	5.49	138.84	133.90
2	D	296	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	C	93	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	236	TRP	CG-CD2-CE3	5.45	138.81	133.90
1	C	373	GLU	CA-CB-CG	5.42	125.33	113.40
2	B	238	ARG	NE-CZ-NH2	-5.41	117.59	120.30
2	B	260	VAL	CB-CA-C	-5.40	101.13	111.40
1	C	28	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	72	TRP	CG-CD1-NE1	-5.40	104.70	110.10
1	C	472	TRP	CG-CD2-CE3	5.39	138.75	133.90
2	B	402	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	C	77	ASP	CB-CG-OD1	5.35	123.11	118.30
2	D	442	MET	CG-SD-CE	-5.34	91.65	100.20
2	B	361	TRP	CB-CG-CD1	-5.34	120.06	127.00
2	B	361	TRP	CG-CD1-NE1	-5.34	104.76	110.10
2	D	350	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	182	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	253	TRP	CB-CG-CD1	-5.30	120.11	127.00
2	D	361	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	A	407	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	D	366	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	B	187	PRO	CA-N-CD	-5.27	104.12	111.50
2	D	46	TRP	CG-CD1-NE1	-5.27	104.83	110.10
2	B	197	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	C	205	TRP	CG-CD2-CE3	5.23	138.61	133.90
1	A	254	SER	CA-C-N	5.22	126.64	116.20
2	B	197	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	C	195	HIS	CG-ND1-CE1	5.18	115.45	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	379	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	C	12	LEU	CA-CB-CG	5.17	127.20	115.30
2	B	296	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	223	VAL	N-CA-CB	-5.16	100.15	111.50
1	C	20	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	D	260	VAL	CB-CA-C	-5.12	101.67	111.40
1	C	72	TRP	CG-CD2-CE3	5.11	138.50	133.90
2	D	28	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	236	TRP	CG-CD2-CE3	5.09	138.48	133.90
2	B	116	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	248	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	197	TRP	CB-CG-CD1	-5.05	120.43	127.00
2	B	296	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	C	350	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	D	402	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	294	TRP	CB-CG-CD1	-5.01	120.48	127.00
1	A	479	TRP	CB-CG-CD1	-5.00	120.50	127.00
2	D	116	ASP	CB-CG-OD1	5.00	122.80	118.30

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	38	0
1	C	3713	0	3638	43	0
2	B	4174	0	4087	42	0
2	D	4174	0	4087	34	0
3	A	14	0	6	0	0
3	C	14	0	6	1	0
4	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	141	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 4.

All (141) 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:S3B	5:C:496:CFM:MO1	2.11	0.61
2:D:457:HIS:HE1	7:D:677:HOH:O	1.83	0.61
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:MET:HE2	2:B:135:LEU:HD11	1.83	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: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:D:131:MET:HE2	2:D:135:LEU:HD11	1.87	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: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
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
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:HH11	2:D:242:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:118:MET:HE1	2:B:158:ILE:HD11	1.97	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
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
1:C:140:THR:HG23	1:C:141:LEU:HG	1.98	0.45
2:B:447:TYR:CE1	2:D:521:LEU:HD21	2.50	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:51:LYS:HD2	2:D:119:THR:HG21	2.01	0.42
7:B:545:HOH:O	2:D:519:HIS:HE1	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: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:C:62:CYS:O	1:C:191:GLN:HA	2.21	0.41
1:A:356:GLY:O	1:A:379:TYR:HB3	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
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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	463/491 (94%)	439 (95%)	22 (5%)	2 (0%)	34	28
1	C	464/491 (94%)	441 (95%)	21 (4%)	2 (0%)	34	28
2	B	520/522 (100%)	508 (98%)	11 (2%)	1 (0%)	47	43
2	D	520/522 (100%)	507 (98%)	12 (2%)	1 (0%)	47	43
All	All	1967/2026 (97%)	1895 (96%)	66 (3%)	6 (0%)	41	36

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%)	371 (94%)	26 (6%)	17	11
1	C	396/414 (96%)	369 (93%)	27 (7%)	16	10
2	B	454/454 (100%)	438 (96%)	16 (4%)	36	34
2	D	454/454 (100%)	438 (96%)	16 (4%)	36	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1701/1736 (98%)	1616 (95%)	85 (5%)	24	19

All (85) 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	98	ASN
1	A	107	ASN
1	A	131	LEU
1	A	133	LYS
1	A	134	LEU
1	A	150	VAL
1	A	162	ASP
1	A	165	SER
1	A	210	ARG
1	A	223	VAL
1	A	252	GLN
1	A	264	LEU
1	A	361	ARG
1	A	362	HIS
1	A	383	HIS
1	A	391	MET
1	A	401	TYR
1	A	409	PHE
1	A	445	ASP
1	A	461	ARG
1	A	467	LEU
1	A	475	LEU
1	A	480	GLU
2	B	13	PRO
2	B	38	ASP
2	B	50	LYS
2	B	55	LEU
2	B	80	LEU
2	B	88	TYR
2	B	153	CYS
2	B	171	LYS
2	B	172	GLU
2	B	211	LYS
2	B	258	GLU

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Mol	Chain	Res	Type
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	58	THR
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	223	VAL
1	C	252	GLN
1	C	264	LEU
1	C	266	PRO
1	C	277	ARG
1	C	284	ARG
1	C	347	GLU
1	C	362	HIS
1	C	383	HIS
1	C	389	ARG
1	C	396	ASP
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	88	TYR
2	D	171	LYS
2	D	177	ASP
2	D	212	SER
2	D	258	GLU
2	D	260	VAL

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Mol	Chain	Res	Type
2	D	369	LEU
2	D	379	LEU
2	D	494	LEU
2	D	503	GLU
2	D	505	LEU
2	D	523	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	252	GLN
1	A	383	HIS
2	B	37	GLN
2	B	104	ASN
2	B	130	ASN
2	B	286	ASN
2	B	457	HIS
2	B	499	ASN
2	B	518	ASN
2	B	519	HIS
1	C	49	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	104	ASN
2	D	128	GLN
2	D	130	ASN
2	D	163	ASN
2	D	167	ASN
2	D	168	ASN
2	D	286	ASN
2	D	457	HIS
2	D	499	ASN
2	D	513	GLN
2	D	518	ASN
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 carbohydrates 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	1,2	0,24,24	0.00	-	-		
3	HCA	A	494	5	4,13,13	2.38	2 (50%)	4,18,18	2.86	3 (75%)
4	CLF	C	498	1,2	0,24,24	0.00	-	-		
5	CFM	C	496	1,3	0,24,24	0.00	-	-		
3	HCA	C	494	5	4,13,13	1.69	1 (25%)	4,18,18	3.05	2 (50%)
5	CFM	A	496	1,3	0,24,24	0.00	-	-		

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	1,2	-	-	0/12/10/10
4	CLF	C	498	1,2	-	-	0/12/10/10
3	HCA	A	494	5	-	3/7/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HCA	C	494	5	-	4/7/17/17	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	494	HCA	C2-C3	-3.52	1.49	1.54
3	C	494	HCA	O7-C3	2.85	1.47	1.43
3	A	494	HCA	C4-C3	2.76	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	494	HCA	C4-C5-C6	4.37	118.01	111.39
3	C	494	HCA	C4-C5-C6	4.19	117.73	111.39
3	C	494	HCA	C3-C2-C1	4.15	121.63	114.98
3	A	494	HCA	C4-C3-C7	2.68	116.25	111.52
3	A	494	HCA	C3-C2-C1	2.54	119.04	114.98

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	C	494	HCA	C7-C3-C4-C5
3	C	494	HCA	O7-C3-C4-C5
3	C	494	HCA	C3-C4-C5-C6

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	C	496	CFM	5	0
3	C	494	HCA	1	0
5	A	496	CFM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.