



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:39 pm BST

PDB ID : 3MIN  
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](mailto: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.

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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

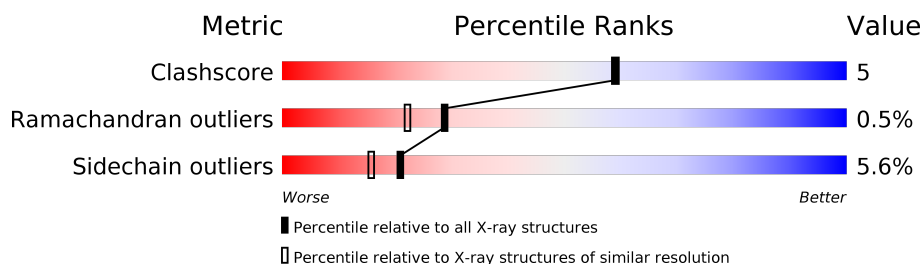
# 1 Overall quality at a glance

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  $\geq 3$ , 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	



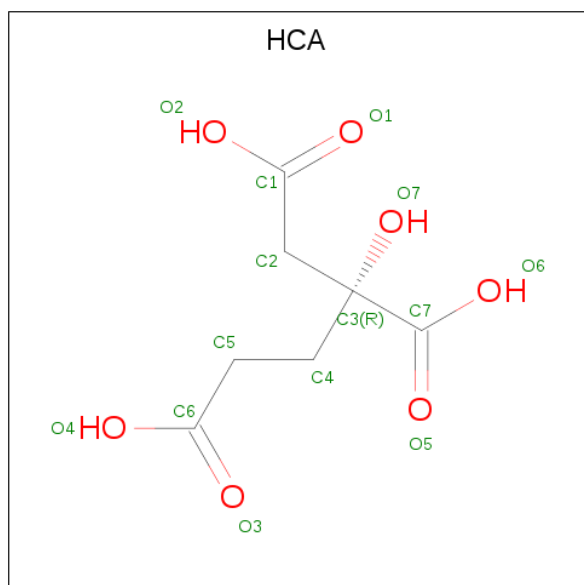
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

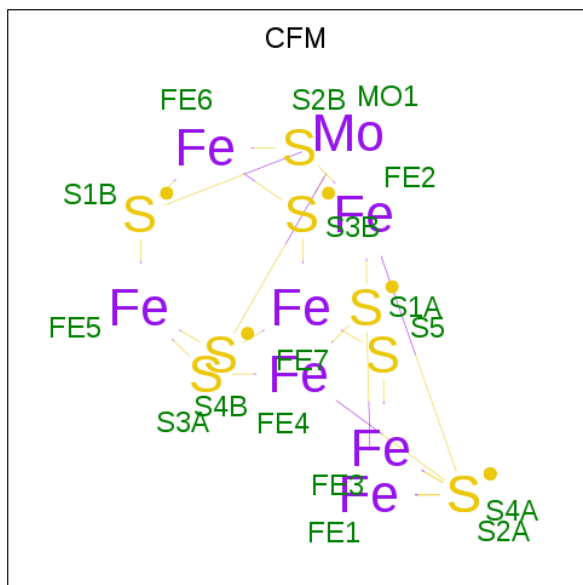
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total 4174	C 2666	N 705	O 775	S 28	0	0	0
2	D	522	Total 4173	C 2666	N 705	O 774	S 28	0	0	0

- Molecule 3 is 3-HYDROXY-3-CARBOXY-ADIPIIC ACID (three-letter code: 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 (three-letter code: CFM) (formula:  $\text{Fe}_7\text{MoS}_9$ ).

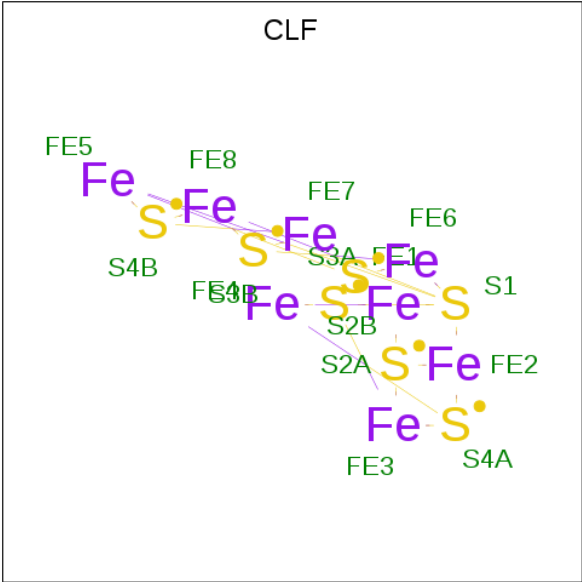


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
4	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 5 is CALCIUM ION (three-letter code: 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 (three-letter code: CLF) (formula:  $\text{Fe}_8\text{S}_7$ ).



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.

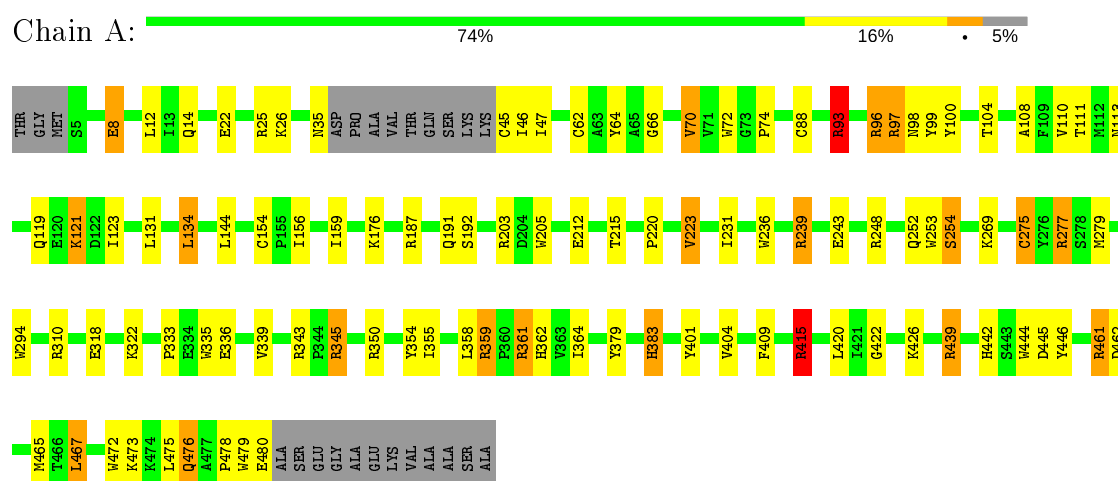
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total	O	0	0
			134	134		
7	B	185	Total	O	0	0
			185	185		
7	C	129	Total	O	0	0
			129	129		
7	D	179	Total	O	0	0
			179	179		

### 3 Residue-property plots

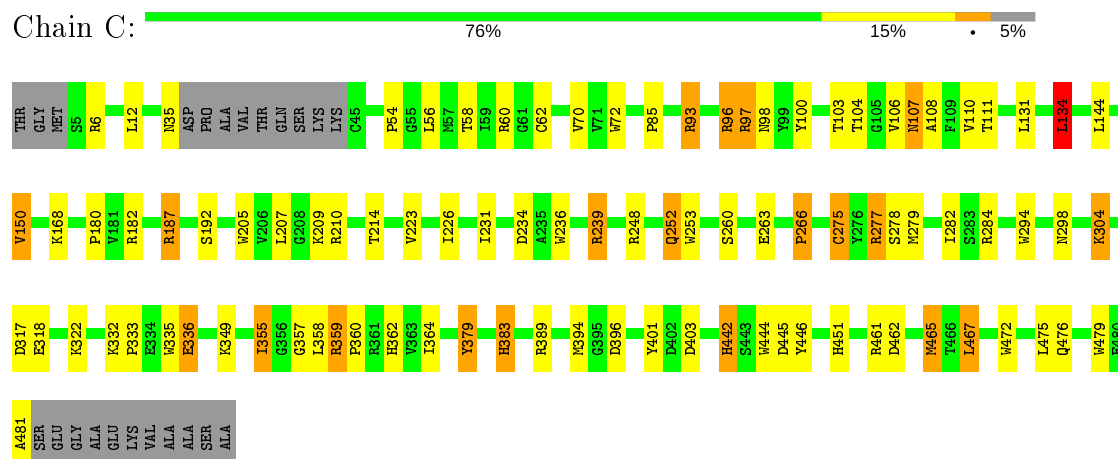
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

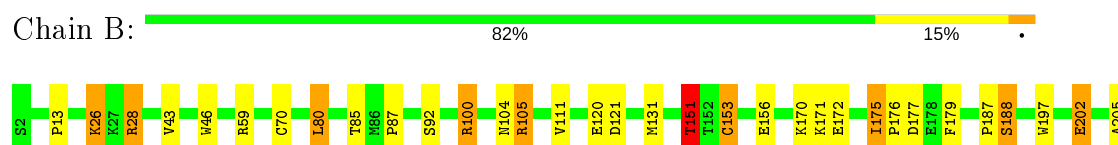
#### • Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN

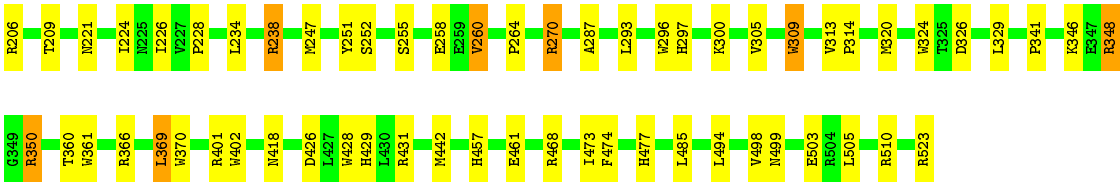


#### • Molecule 1: NITROGENASE MOLYBDENUM IRON PROTEIN

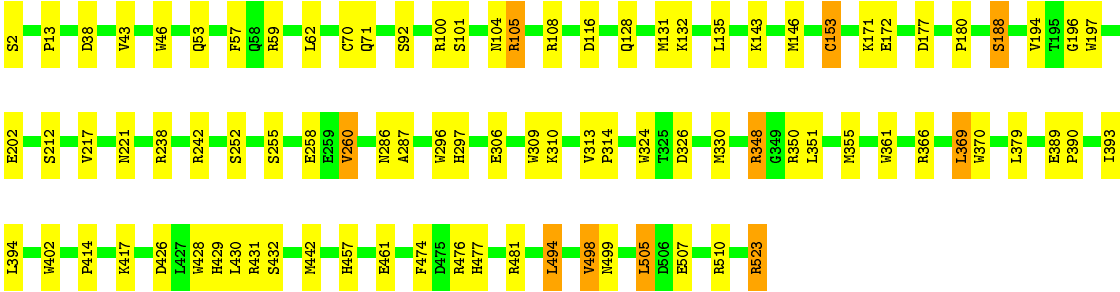
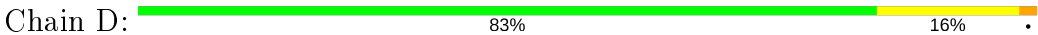


#### • Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN





• Molecule 2: NITROGENASE MOLYBDENUM IRON PROTEIN



## 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, $\alpha$ , $\beta$ , $\gamma$	108.00 Å   131.30 Å   81.00 Å 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 <sup>2</sup> )	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: 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	0.77	3/3795 (0.1%)	1.45	66/5117 (1.3%)
1	C	0.75	3/3799 (0.1%)	1.39	53/5123 (1.0%)
2	B	0.77	2/4280 (0.0%)	1.34	63/5786 (1.1%)
2	D	0.75	2/4279 (0.0%)	1.34	58/5785 (1.0%)
All	All	0.76	10/16153 (0.1%)	1.38	240/21811 (1.1%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	CYS	CB-SG	-14.54	1.57	1.82
2	D	153	CYS	CB-SG	-10.80	1.63	1.82
1	A	275	CYS	CB-SG	10.34	1.99	1.82
1	A	88	CYS	CB-SG	-9.51	1.66	1.82
1	C	275	CYS	CB-SG	8.26	1.96	1.82
2	B	188	SER	CB-OG	8.18	1.52	1.42
2	D	188	SER	CB-OG	7.07	1.51	1.42
1	C	62	CYS	CB-SG	-6.85	1.70	1.82
1	C	442	HIS	CG-ND1	-5.42	1.26	1.38
1	A	154	CYS	CB-SG	-5.25	1.73	1.81

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	A	359	ARG	NE-CZ-NH1	12.57	126.59	120.30
1	A	361	ARG	NE-CZ-NH1	12.51	126.55	120.30
2	D	523	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	96	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	A	96	ARG	NE-CZ-NH1	10.56	125.58	120.30
2	D	431	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	D	431	ARG	NE-CZ-NH2	-9.67	115.47	120.30
1	A	361	ARG	NE-CZ-NH2	-9.46	115.57	120.30
2	B	59	ARG	NE-CZ-NH2	-9.23	115.69	120.30
2	B	348	ARG	NE-CZ-NH1	9.19	124.89	120.30
2	B	59	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	B	402	TRP	CD1-CG-CD2	9.13	113.61	106.30
2	B	523	ARG	NE-CZ-NH1	9.05	124.82	120.30
1	A	277	ARG	NE-CZ-NH1	9.02	124.81	120.30
2	D	523	ARG	NE-CZ-NH1	9.01	124.80	120.30
2	B	100	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	C	465	MET	CG-SD-CE	-8.97	85.85	100.20
1	C	97	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	472	TRP	CD1-CG-CD2	8.88	113.41	106.30
2	D	402	TRP	CD1-CG-CD2	8.87	113.39	106.30
2	B	348	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	D	238	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	C	97	ARG	NE-CZ-NH1	8.80	124.70	120.30
2	D	428	TRP	CD1-CG-CD2	8.73	113.28	106.30
2	B	296	TRP	CD1-CG-CD2	8.69	113.25	106.30
2	D	369	LEU	CA-CB-CG	8.66	135.22	115.30
2	B	369	LEU	CA-CB-CG	8.61	135.09	115.30
1	C	444	TRP	CD1-CG-CD2	8.57	113.15	106.30
1	C	359	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	C	96	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	C	335	TRP	CD1-CG-CD2	8.52	113.11	106.30
1	A	253	TRP	CA-C-N	-8.45	98.61	117.20
1	C	294	TRP	CD1-CG-CD2	8.44	113.05	106.30
1	C	472	TRP	CD1-CG-CD2	8.39	113.02	106.30
2	B	510	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	444	TRP	CD1-CG-CD2	8.28	112.92	106.30
2	B	523	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	B	197	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	C	444	TRP	CE2-CD2-CG	-8.26	100.69	107.30
2	D	361	TRP	CD1-CG-CD2	8.26	112.91	106.30
2	B	46	TRP	CD1-CG-CD2	8.26	112.91	106.30
2	D	105	ARG	NE-CZ-NH1	8.26	124.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	479	TRP	CD1-CG-CD2	8.25	112.90	106.30
2	B	270	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	97	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	444	TRP	CE2-CD2-CG	-8.22	100.72	107.30
1	A	236	TRP	CD1-CG-CD2	8.17	112.83	106.30
2	B	296	TRP	CE2-CD2-CG	-8.16	100.78	107.30
2	B	105	ARG	NE-CZ-NH1	8.14	124.37	120.30
2	B	309	TRP	CD1-CG-CD2	8.10	112.78	106.30
1	A	72	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	294	TRP	CD1-CG-CD2	8.08	112.76	106.30
1	A	479	TRP	CD1-CG-CD2	8.06	112.75	106.30
2	B	370	TRP	CD1-CG-CD2	8.03	112.73	106.30
2	B	350	ARG	NE-CZ-NH1	8.02	124.31	120.30
2	B	197	TRP	CE2-CD2-CG	-8.00	100.90	107.30
2	D	46	TRP	CD1-CG-CD2	8.00	112.70	106.30
2	B	100	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	96	ARG	NE-CZ-NH2	-7.95	116.32	120.30
2	D	370	TRP	CD1-CG-CD2	7.95	112.66	106.30
2	B	428	TRP	CD1-CG-CD2	7.94	112.66	106.30
2	B	270	ARG	NE-CZ-NH2	-7.94	116.33	120.30
2	D	361	TRP	CE2-CD2-CG	-7.92	100.96	107.30
1	A	277	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	A	472	TRP	CE2-CD2-CG	-7.90	100.98	107.30
1	C	277	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	C	236	TRP	CD1-CG-CD2	7.85	112.58	106.30
2	B	361	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	C	205	TRP	CD1-CG-CD2	7.85	112.58	106.30
1	C	72	TRP	CD1-CG-CD2	7.82	112.56	106.30
2	D	428	TRP	CE2-CD2-CG	-7.82	101.04	107.30
2	B	238	ARG	NE-CZ-NH1	7.79	124.20	120.30
2	D	296	TRP	CD1-CG-CD2	7.77	112.52	106.30
2	B	361	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	A	205	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	C	335	TRP	CE2-CD2-CG	-7.74	101.11	107.30
2	D	510	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	335	TRP	CD1-CG-CD2	7.67	112.43	106.30
2	D	309	TRP	CD1-CG-CD2	7.66	112.43	106.30
1	A	72	TRP	CE2-CD2-CG	-7.61	101.21	107.30
1	C	205	TRP	CE2-CD2-CG	-7.56	101.25	107.30
1	A	294	TRP	CE2-CD2-CG	-7.56	101.25	107.30
2	B	153	CYS	CA-CB-SG	7.55	127.59	114.00
1	C	472	TRP	CE2-CD2-CG	-7.55	101.26	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	100	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	93	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	335	TRP	CE2-CD2-CG	-7.53	101.28	107.30
1	A	253	TRP	O-C-N	7.52	134.73	122.70
2	B	402	TRP	CE2-CD2-CG	-7.51	101.29	107.30
2	B	324	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	25	ARG	NE-CZ-NH1	7.51	124.05	120.30
2	B	324	TRP	CD1-CG-CD2	7.48	112.28	106.30
2	D	370	TRP	CE2-CD2-CG	-7.47	101.32	107.30
2	D	296	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	A	205	TRP	CE2-CD2-CG	-7.45	101.34	107.30
1	C	253	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	C	253	TRP	CD1-CG-CD2	7.39	112.22	106.30
2	B	428	TRP	CE2-CD2-CG	-7.39	101.39	107.30
2	B	370	TRP	CE2-CD2-CG	-7.38	101.40	107.30
2	D	197	TRP	CE2-CD2-CG	-7.37	101.41	107.30
2	D	46	TRP	CE2-CD2-CG	-7.36	101.41	107.30
2	B	46	TRP	CE2-CD2-CG	-7.33	101.44	107.30
2	D	309	TRP	CE2-CD2-CG	-7.33	101.44	107.30
1	A	97	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	C	253	TRP	CA-C-N	-7.31	101.12	117.20
2	D	197	TRP	CD1-CG-CD2	7.29	112.13	106.30
1	C	294	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	C	479	TRP	CE2-CD2-CG	-7.26	101.49	107.30
2	D	324	TRP	CE2-CD2-CG	-7.25	101.50	107.30
2	D	402	TRP	CE2-CD2-CG	-7.24	101.51	107.30
2	B	309	TRP	CE2-CD2-CG	-7.24	101.51	107.30
1	A	236	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	C	239	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	C	72	TRP	CE2-CD2-CG	-7.22	101.53	107.30
1	A	479	TRP	CE2-CD2-CG	-7.17	101.56	107.30
2	B	431	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	D	242	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	C	93	ARG	NE-CZ-NH1	7.07	123.84	120.30
2	D	100	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	C	236	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	C	93	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	D	324	TRP	CD1-CG-CD2	6.98	111.89	106.30
1	A	359	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	253	TRP	CE2-CD2-CG	-6.92	101.76	107.30
2	B	510	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	439	ARG	NE-CZ-NH1	6.84	123.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	TRP	CD1-CG-CD2	6.83	111.77	106.30
1	A	345	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	D	481	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	D	242	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	134	LEU	CA-CB-CG	6.74	130.80	115.30
1	C	187	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	D	260	VAL	CB-CA-C	-6.70	98.68	111.40
1	A	415	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	D	348	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	D	348	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	461	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	B	361	TRP	CG-CD2-CE3	6.37	139.63	133.90
1	C	134	LEU	CA-CB-CG	6.34	129.89	115.30
1	C	444	TRP	CB-CG-CD1	-6.30	118.81	127.00
2	B	197	TRP	CG-CD2-CE3	6.29	139.56	133.90
1	A	444	TRP	CB-CG-CD1	-6.28	118.84	127.00
1	C	253	TRP	O-C-N	6.24	132.69	122.70
2	B	431	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	B	28	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	28	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	D	350	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	C	359	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	D	481	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	191	GLN	CA-CB-CG	6.14	126.91	113.40
1	C	335	TRP	CG-CD2-CE3	6.12	139.41	133.90
1	A	99	TYR	CB-CG-CD2	-6.11	117.33	121.00
2	D	366	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	279	MET	CA-CB-CG	-6.07	102.99	113.30
1	A	343	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	D	510	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	B	402	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	C	461	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	D	59	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	B	442	MET	CG-SD-CE	-6.00	90.61	100.20
2	D	361	TRP	CG-CD2-CE3	5.95	139.25	133.90
2	B	366	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	B	296	TRP	CG-CD2-CE3	5.84	139.16	133.90
2	B	70	CYS	CA-CB-SG	5.84	124.52	114.00
1	C	379	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	C	205	TRP	CG-CD2-CE3	5.80	139.12	133.90
1	C	248	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	444	TRP	CG-CD2-CE3	5.73	139.06	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	239	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	335	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	C	253	TRP	CG-CD2-CE3	5.68	139.01	133.90
2	D	153	CYS	CA-CB-SG	5.67	124.21	114.00
1	A	72	TRP	CG-CD2-CE3	5.65	138.98	133.90
2	D	428	TRP	CG-CD1-NE1	-5.62	104.48	110.10
1	A	343	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	335	TRP	CB-CG-CD1	-5.61	119.71	127.00
1	A	345	ARG	CD-NE-CZ	5.59	131.42	123.60
2	B	151	THR	N-CA-CB	-5.56	99.73	110.30
2	D	428	TRP	CG-CD2-CE3	5.56	138.90	133.90
2	B	197	TRP	CB-CG-CD1	-5.55	119.78	127.00
1	C	284	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	B	206	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	275	CYS	CA-CB-SG	-5.51	104.07	114.00
2	D	366	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	B	238	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	D	402	TRP	CG-CD1-NE1	-5.49	104.61	110.10
2	D	498	VAL	CB-CA-C	-5.46	101.02	111.40
1	A	203	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	294	TRP	CG-CD2-CE3	5.44	138.80	133.90
2	B	361	TRP	CB-CG-CD1	-5.43	119.94	127.00
1	A	223	VAL	N-CA-CB	-5.42	99.58	111.50
1	C	182	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	309	TRP	CG-CD1-NE1	-5.42	104.68	110.10
1	C	444	TRP	CG-CD2-CE3	5.39	138.75	133.90
2	D	494	LEU	CA-CB-CG	5.38	127.66	115.30
2	B	428	TRP	CG-CD2-CE3	5.36	138.72	133.90
2	D	108	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	D	188	SER	CA-CB-OG	5.32	125.57	111.20
1	C	284	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	D	309	TRP	CG-CD2-CE3	5.31	138.68	133.90
2	B	309	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	A	205	TRP	CG-CD2-CE3	5.28	138.65	133.90
1	A	187	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	472	TRP	CG-CD1-NE1	-5.25	104.85	110.10
2	D	197	TRP	CG-CD2-CE3	5.25	138.62	133.90
1	A	479	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	D	70	CYS	CA-CB-SG	5.23	123.42	114.00
1	C	479	TRP	CG-CD1-NE1	-5.23	104.87	110.10
1	A	472	TRP	CB-CG-CD1	-5.19	120.25	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	324	TRP	CG-CD2-CE3	5.18	138.56	133.90
2	B	428	TRP	CG-CD1-NE1	-5.18	104.92	110.10
1	A	8	GLU	CA-CB-CG	5.17	124.77	113.40
1	A	93	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	D	258	GLU	CA-CB-CG	5.17	124.77	113.40
2	B	296	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	C	467	LEU	CA-CB-CG	5.16	127.16	115.30
2	B	350	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	350	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	D	476	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	294	TRP	CB-CG-CD1	-5.13	120.33	127.00
2	D	442	MET	CG-SD-CE	-5.13	91.99	100.20
1	A	335	TRP	CG-CD2-CE3	5.12	138.51	133.90
2	B	402	TRP	CG-CD2-CE3	5.12	138.51	133.90
2	D	197	TRP	CB-CG-CD1	-5.12	120.35	127.00
1	A	253	TRP	C-N-CA	5.12	134.49	121.70
2	B	260	VAL	CB-CA-C	-5.11	101.70	111.40
1	C	205	TRP	CB-CG-CD1	-5.11	120.36	127.00
2	B	296	TRP	CB-CG-CD1	-5.09	120.39	127.00
2	D	361	TRP	CG-CD1-NE1	-5.07	105.03	110.10
1	A	253	TRP	CG-CD2-CE3	5.05	138.45	133.90
1	C	472	TRP	CG-CD1-NE1	-5.04	105.06	110.10
1	A	335	TRP	CB-CG-CD1	-5.03	120.47	127.00
1	C	294	TRP	CG-CD1-NE1	-5.01	105.09	110.10
2	B	297	HIS	CA-CB-CG	5.01	122.11	113.60
2	B	324	TRP	CG-CD2-CE3	5.01	138.41	133.90
1	A	72	TRP	CB-CG-CD1	-5.00	120.49	127.00
1	A	236	TRP	CG-CD2-CE3	5.00	138.40	133.90
2	B	401	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	3637	43	0
1	C	3713	0	3639	42	0
2	B	4174	0	4088	41	0
2	D	4173	0	4088	36	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	148	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 (148) 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: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:B:209:THR:HG21	2:B:309:TRP:HE1	1.45	0.81
2:D:131:MET:HE2	2:D:135:LEU:HD11	1.67	0.77
2:B:209:THR:HG21	2:B:309:TRP:NE1	2.02	0.75
2:B:202:GLU:HG3	2:B:300:LYS:HG2	1.69	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
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
7:A:619:HOH:O	2:B:120:GLU:HG3	2.02	0.59
2:B:360:THR:HG22	1:C:465:MET:HE1	1.84	0.59
1:A:476:GLN:NE2	1:A:480:GLU:HA	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:351:LEU:HG	2:D:355:MET:HE2	1.89	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
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:HH11	1:A:461:ARG:HG2	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: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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:336:GLU:HA	1:A:339:VAL:HG12	1.96	0.47
1:A:62:CYS:SG	1:A:64:TYR:HB3	2.55	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:153:CYS:HB3	2:D:188:SER:OG	2.15	0.46
2:D:2:SER:N	7:D:658:HOH:O	2.49	0.46
2:D:426:ASP:H	2:D:429:HIS:HD2	1.63	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
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
2:B:360:THR:HA	1:C:465:MET:CE	2.47	0.44
1:A:159:ILE:HD13	1:A:159:ILE:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:121:LYS:H	1:A:121:LYS:HZ3	1.67	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:C:150:VAL:HG13	1:C:180:PRO:HA	2.01	0.42
1:A:478:PRO:HB2	2:D:330:MET:SD	2.59	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:207:LEU:HD22	1:C:282:ILE:HD11	2.01	0.41
1:C:56:LEU:HB2	7:C:579:HOH:O	2.20	0.41
1:C:70:VAL:HG11	4:C:496:CFM:S2B	2.59	0.41
1:A:420:LEU:HB2	1:A:467:LEU:HD22	2.02	0.41
1:A:96:ARG:NH1	4:A:496:CFM:S5	2.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:C:209:LYS:HB2	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:263:GLU:O	1:C:266:PRO:HD2	2.21	0.40
1:C:97:ARG:O	1:C:231:ILE:HA	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%)	25	18
1	C	464/491 (94%)	432 (93%)	28 (6%)	4 (1%)	17	10
2	B	520/522 (100%)	496 (95%)	23 (4%)	1 (0%)	47	43
2	D	520/522 (100%)	501 (96%)	18 (4%)	1 (0%)	47	43
All	All	1967/2026 (97%)	1872 (95%)	86 (4%)	9 (0%)	29	22

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

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Mol	Chain	Res	Type
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%)	13	8
1	C	396/414 (96%)	371 (94%)	25 (6%)	18	12
2	B	454/454 (100%)	430 (95%)	24 (5%)	22	17
2	D	454/454 (100%)	438 (96%)	16 (4%)	36	34
All	All	1701/1736 (98%)	1606 (94%)	95 (6%)	21	16

All (95) 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
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	176	LYS
1	A	212	GLU
1	A	215	THR
1	A	223	VAL
1	A	239	ARG
1	A	243	GLU
1	A	310	ARG

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Mol	Chain	Res	Type
1	A	322	LYS
1	A	345	ARG
1	A	359	ARG
1	A	362	HIS
1	A	383	HIS
1	A	401	TYR
1	A	409	PHE
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	26	LYS
2	B	28	ARG
2	B	80	LEU
2	B	85	THR
2	B	92	SER
2	B	121	ASP
2	B	131	MET
2	B	151	THR
2	B	171	LYS
2	B	172	GLU
2	B	175	ILE
2	B	177	ASP
2	B	202	GLU
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	98	ASN
1	C	106	VAL
1	C	107	ASN

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Mol	Chain	Res	Type
1	C	131	LEU
1	C	134	LEU
1	C	150	VAL
1	C	168	LYS
1	C	187	ARG
1	C	210	ARG
1	C	214	THR
1	C	223	VAL
1	C	252	GLN
1	C	277	ARG
1	C	304	LYS
1	C	336	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	92	SER
2	D	143	LYS
2	D	171	LYS
2	D	172	GLU
2	D	177	ASP
2	D	202	GLU
2	D	212	SER
2	D	252	SER
2	D	260	VAL
2	D	369	LEU
2	D	379	LEU
2	D	461	GLU
2	D	505	LEU
2	D	507	GLU

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	252	GLN
1	A	383	HIS

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Mol	Chain	Res	Type
1	A	476	GLN
2	B	37	GLN
2	B	58	GLN
2	B	104	ASN
2	B	128	GLN
2	B	130	ASN
2	B	168	ASN
2	B	457	HIS
2	B	499	ASN
2	B	518	ASN
2	B	519	HIS
1	C	107	ASN
1	C	252	GLN
1	C	271	ASN
1	C	362	HIS
1	C	383	HIS
1	C	476	GLN
2	D	53	GLN
2	D	104	ASN
2	D	128	GLN
2	D	129	GLN
2	D	130	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
3	HCA	A	494	4	4,13,13	0.56	0	4,18,18	2.62	1 (25%)
4	CFM	C	496	1,3	0,24,24	0.00	-	-		
6	CLF	D	525	1,2	0,24,24	0.00	-	-		
3	HCA	C	494	4	4,13,13	2.26	1 (25%)	4,18,18	3.11	2 (50%)
4	CFM	A	496	1,3	0,24,24	0.00	-	-		
6	CLF	B	525	1,2	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
3	HCA	A	494	4	-	4/7/17/17	-
6	CLF	D	525	1,2	-	-	0/12/10/10
3	HCA	C	494	4	-	3/7/17/17	-
6	CLF	B	525	1,2	-	-	0/12/10/10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	494	HCA	C4-C3	4.38	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	494	HCA	C4-C5-C6	4.53	118.25	111.39
3	A	494	HCA	C3-C2-C1	4.44	122.09	114.98
3	C	494	HCA	C3-C2-C1	4.02	121.43	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	A	494	HCA	C3-C4-C5-C6
3	C	494	HCA	C2-C3-C4-C5
3	C	494	HCA	O7-C3-C4-C5
3	C	494	HCA	C7-C3-C4-C5

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
6	D	525	CLF	1	0
4	A	496	CFM	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.