



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:37 PM UTC

PDB ID : 2HMQ / pdb_00002hmq
Title : THE STRUCTURES OF MET AND AZIDOMET HEMERYTHRIN AT 1.66
ANGSTROMS RESOLUTION
Authors : Holmes, M.A.; Stenkamp, R.E.
Deposited on : 1990-10-18
Resolution : 1.66 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

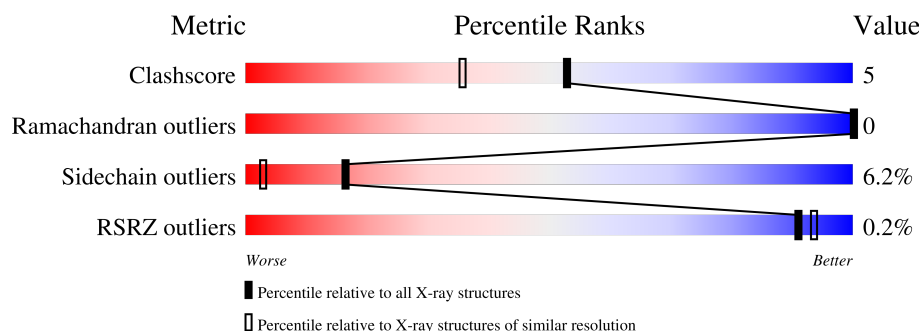
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	114	
1	B	114	
1	C	114	
1	D	114	

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
2	ACT	A	114	-	X	-	-
2	ACT	C	114	-	X	-	-
2	ACT	D	114	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4153 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 HEMERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	7	0
			965	619	166	177	3			
1	B	113	Total	C	N	O	S	0	3	0
			960	616	164	177	3			
1	C	113	Total	C	N	O	S	0	1	0
			952	612	163	174	3			
1	D	113	Total	C	N	O	S	0	2	0
			955	613	164	175	3			

There are 4 discrepancies between the modelled and reference sequences:

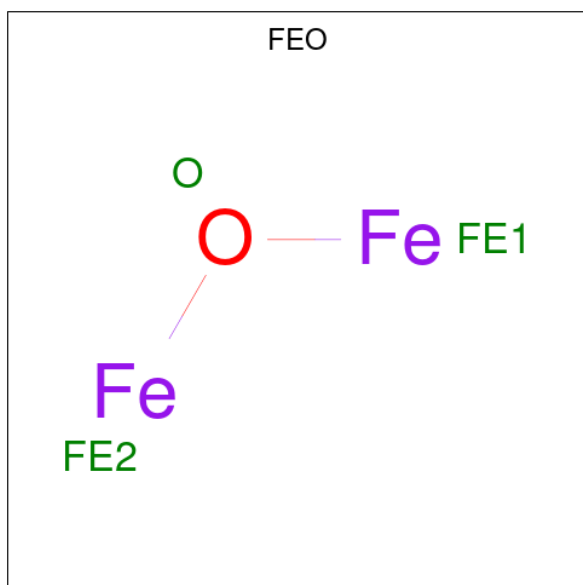
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	VAL	microheterogeneity	UNP P02246
B	21	ILE	VAL	microheterogeneity	UNP P02246
C	21	ILE	VAL	microheterogeneity	UNP P02246
D	21	ILE	VAL	microheterogeneity	UNP P02246

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	Fe 2	O 1	0	0
3	B	1	Total 3	Fe 2	O 1	0	0
3	C	1	Total 3	Fe 2	O 1	0	0
3	D	1	Total 3	Fe 2	O 1	0	0

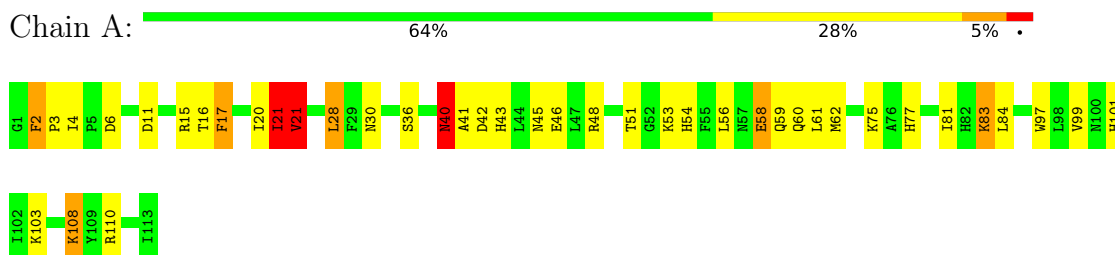
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	B	70	Total 70	O 70	0	0
4	C	66	Total 66	O 66	0	0
4	D	88	Total 88	O 88	0	0

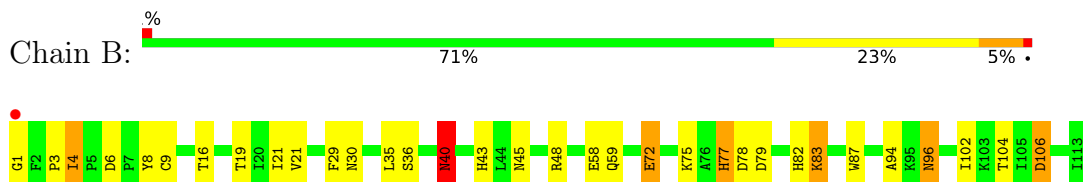
3 Residue-property plots

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

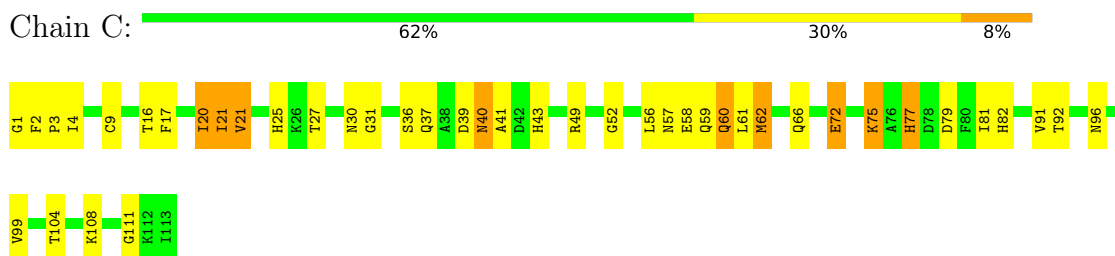
• Molecule 1: HEMERYTHRIN



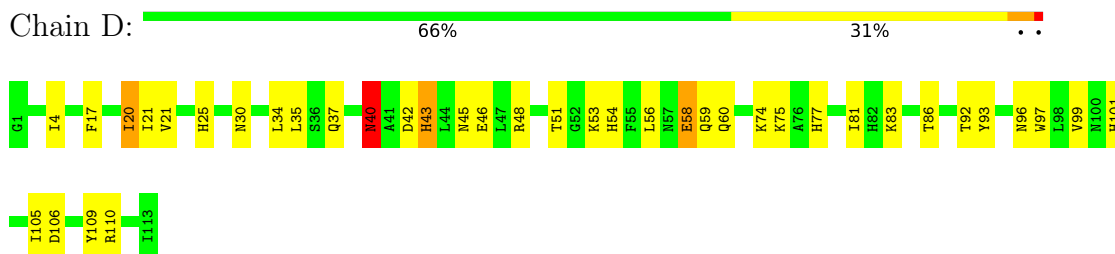
• Molecule 1: HEMERYTHRIN



• Molecule 1: HEMERYTHRIN



• Molecule 1: HEMERYTHRIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	86.60Å 86.60Å 80.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.66 10.00 – 1.66	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.66) 91.6 (10.00-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.66Å)	Xtriage
Refinement program	PROFFT	Depositor
R, R_{free}	0.189 , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4153	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FEO, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.65	2/1030 (0.2%)	2.12	44/1390 (3.2%)
1	B	1.57	2/996 (0.2%)	2.11	28/1346 (2.1%)
1	C	1.59	8/979 (0.8%)	2.10	41/1323 (3.1%)
1	D	1.62	3/987 (0.3%)	2.10	36/1334 (2.7%)
All	All	1.61	15/3992 (0.4%)	2.11	149/5393 (2.8%)

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	B	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	56	LEU	C-N	-6.26	1.25	1.33
1	C	92	THR	CB-OG1	6.10	1.53	1.43
1	C	1	GLY	N-CA	5.88	1.54	1.45
1	C	37	GLN	C-N	-5.87	1.26	1.33
1	C	77	HIS	ND1-CE1	-5.70	1.26	1.32
1	B	1	GLY	N-CA	5.63	1.54	1.45
1	B	104	THR	C-N	-5.57	1.26	1.33
1	C	20	ILE	C-N	-5.48	1.26	1.33
1	A	110	ARG	CD-NE	-5.39	1.38	1.46
1	D	97	TRP	C-N	-5.39	1.26	1.33
1	C	81	ILE	C-O	-5.30	1.18	1.24
1	D	74	LYS	C-N	-5.28	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	LEU	C-N	-5.21	1.26	1.33
1	C	16	THR	N-CA	-5.18	1.39	1.46
1	C	27	THR	CA-CB	5.17	1.61	1.53

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	ASN	CA-CB-CG	-12.19	100.41	112.60
1	A	17	PHE	CA-CB-CG	-11.63	102.17	113.80
1	B	96	ASN	OD1-CG-ND2	11.42	134.02	122.60
1	A	108[A]	LYS	CA-CB-CG	10.91	135.92	114.10
1	A	108[B]	LYS	CA-CB-CG	10.91	135.92	114.10
1	C	41	ALA	CA-C-O	-10.01	109.81	120.42
1	C	60	GLN	OE1-CD-NE2	9.91	132.51	122.60
1	A	110	ARG	NE-CZ-NH2	-9.39	110.75	119.20
1	C	99	VAL	O-C-N	-9.23	112.71	121.94
1	C	27	THR	CA-C-O	-8.10	110.65	119.97
1	A	83	LYS	CB-CG-CD	8.06	129.85	111.30
1	C	17	PHE	CA-CB-CG	-7.90	105.90	113.80
1	B	48	ARG	CD-NE-CZ	7.80	135.32	124.40
1	D	110	ARG	NE-CZ-NH2	-7.71	112.26	119.20
1	B	6	ASP	CA-C-O	-7.60	113.66	119.59
1	D	34	LEU	CA-C-O	-7.58	112.86	120.82
1	A	45	ASN	CB-CG-ND2	7.40	127.50	116.40
1	A	6	ASP	CA-CB-CG	-7.35	105.25	112.60
1	B	78	ASP	CA-C-O	-7.30	111.85	120.10
1	C	20	ILE	CA-C-O	-7.15	113.51	120.95
1	D	40	ASN	OD1-CG-ND2	-7.11	115.49	122.60
1	B	106	ASP	CB-CG-OD1	7.10	134.73	118.40
1	B	77	HIS	CE1-NE2-CD2	-7.09	101.91	109.00
1	D	37	GLN	O-C-N	-6.97	114.56	122.09
1	A	110	ARG	CD-NE-CZ	6.92	134.09	124.40
1	D	40	ASN	CA-CB-CG	6.90	119.50	112.60
1	C	91	VAL	CA-C-O	6.87	127.89	120.47
1	C	77	HIS	CA-C-N	6.82	129.42	120.28
1	C	77	HIS	C-N-CA	6.82	129.42	120.28
1	D	30	ASN	CA-C-N	6.79	127.48	119.94
1	D	30	ASN	C-N-CA	6.79	127.48	119.94
1	B	30	ASN	OD1-CG-ND2	6.75	129.35	122.60
1	A	40	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	A	48	ARG	NH1-CZ-NH2	6.69	128.00	119.30
1	B	4	ILE	CA-C-O	-6.67	114.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	THR	CA-C-N	6.57	128.97	120.56
1	B	104	THR	C-N-CA	6.57	128.97	120.56
1	B	4	ILE	CB-CG1-CD1	6.56	127.58	113.80
1	C	52	GLY	CA-C-O	-6.52	114.03	120.75
1	C	82	HIS	CA-CB-CG	-6.49	107.31	113.80
1	C	27	THR	CA-C-N	6.47	129.47	120.29
1	C	27	THR	C-N-CA	6.47	129.47	120.29
1	D	58	GLU	CA-C-N	6.45	128.93	120.28
1	D	58	GLU	C-N-CA	6.45	128.93	120.28
1	D	17	PHE	CA-CB-CG	-6.45	107.36	113.80
1	A	30	ASN	CA-C-N	6.37	127.05	119.98
1	A	30	ASN	C-N-CA	6.37	127.05	119.98
1	A	46	GLU	CB-CG-CD	6.37	123.42	112.60
1	B	77	HIS	CG-CD2-NE2	6.36	113.56	107.20
1	A	58	GLU	CA-C-N	6.34	128.77	120.28
1	A	58	GLU	C-N-CA	6.34	128.77	120.28
1	A	75	LYS	CB-CG-CD	6.32	125.84	111.30
1	D	25	HIS	CA-C-O	-6.31	113.86	120.55
1	B	75	LYS	O-C-N	-6.28	115.46	122.12
1	D	42	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	19	THR	CA-CB-OG1	-6.25	100.23	109.60
1	C	75	LYS	CA-CB-CG	6.24	126.58	114.10
1	D	56	LEU	CA-C-O	-6.22	114.29	120.82
1	D	48	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	A	30	ASN	CA-C-O	-6.18	114.33	120.82
1	D	54	HIS	CA-CB-CG	-6.15	107.65	113.80
1	A	41	ALA	CA-C-O	-6.15	113.90	120.42
1	D	4	ILE	CA-C-O	-6.13	115.53	119.15
1	B	45	ASN	O-C-N	6.12	129.13	122.15
1	D	97	TRP	CA-C-O	-6.12	114.07	120.55
1	C	60	GLN	CG-CD-NE2	-6.08	107.28	116.40
1	A	101	HIS	CA-CB-CG	-6.06	107.74	113.80
1	C	30	ASN	CA-C-N	6.05	126.70	119.98
1	C	30	ASN	C-N-CA	6.05	126.70	119.98
1	A	101	HIS	ND1-CG-CD2	6.05	112.15	106.10
1	D	45	ASN	CB-CG-ND2	6.02	125.43	116.40
1	C	39	ASP	CA-C-O	-5.98	114.66	121.66
1	D	99	VAL	O-C-N	-5.97	116.06	121.91
1	D	106	ASP	CB-CG-OD1	5.96	132.12	118.40
1	A	84	LEU	CA-C-O	-5.96	113.12	119.97
1	D	81	ILE	CB-CG1-CD1	5.95	126.30	113.80
1	C	92	THR	CA-C-N	5.93	128.54	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	THR	C-N-CA	5.93	128.54	120.54
1	A	99	VAL	CA-C-O	-5.89	114.93	121.17
1	B	3	PRO	CA-C-O	5.87	128.37	121.56
1	B	94	ALA	CA-C-O	-5.85	114.22	120.42
1	C	92	THR	CA-CB-OG1	-5.83	100.85	109.60
1	C	72	GLU	CB-CG-CD	5.83	122.51	112.60
1	A	42	ASP	CA-CB-CG	-5.81	106.79	112.60
1	D	46	GLU	CG-CD-OE1	5.81	131.76	118.40
1	A	97	TRP	CA-C-O	-5.78	114.72	120.90
1	C	56	LEU	CA-C-O	-5.78	114.30	120.42
1	C	36	SER	N-CA-C	-5.77	105.34	112.38
1	A	103	LYS	O-C-N	-5.77	114.70	122.43
1	A	60	GLN	CA-C-O	-5.75	114.33	120.42
1	C	108	LYS	CA-C-O	-5.71	113.65	120.10
1	C	49	ARG	CA-C-N	5.68	127.90	120.28
1	C	49	ARG	C-N-CA	5.68	127.90	120.28
1	B	16	THR	N-CA-C	-5.65	106.55	113.50
1	C	58	GLU	O-C-N	-5.65	116.13	122.12
1	C	111	GLY	CA-C-O	5.63	125.24	119.10
1	B	82	HIS	CA-C-O	-5.63	114.55	120.63
1	C	111	GLY	O-C-N	-5.63	115.04	122.42
1	A	4	ILE	CA-C-O	-5.60	115.11	119.20
1	A	60	GLN	CA-CB-CG	-5.50	103.10	114.10
1	B	79	ASP	CA-CB-CG	5.47	118.08	112.60
1	B	40	ASN	CA-CB-CG	5.47	118.07	112.60
1	D	43	HIS	CA-CB-CG	-5.45	108.35	113.80
1	D	93	TYR	O-C-N	5.43	127.74	122.09
1	C	21[A]	ILE	CA-C-O	-5.38	115.15	120.85
1	C	21[B]	VAL	CA-C-O	-5.38	115.15	120.85
1	A	46	GLU	CG-CD-OE1	5.38	130.76	118.40
1	A	21[A]	ILE	CA-C-O	-5.37	115.48	121.17
1	A	21[B]	VAL	CA-C-O	-5.37	115.48	121.17
1	C	79	ASP	CA-C-O	-5.37	114.73	120.42
1	A	48	ARG	CA-C-O	-5.36	114.87	120.55
1	A	83	LYS	CA-CB-CG	5.35	124.81	114.10
1	B	8	TYR	CA-C-N	5.35	131.12	122.29
1	B	8	TYR	C-N-CA	5.35	131.12	122.29
1	C	4	ILE	CA-C-O	-5.35	116.00	119.15
1	A	2	PHE	O-C-N	5.33	127.67	121.21
1	A	28[A]	LEU	CA-C-O	-5.32	114.33	120.24
1	A	28[B]	LEU	CA-C-O	-5.32	114.33	120.24
1	B	75	LYS	CB-CG-CD	5.32	123.54	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	HIS	CA-CB-CG	-5.30	108.50	113.80
1	C	31	GLY	O-C-N	5.24	127.22	122.19
1	C	62	MET	CA-C-O	-5.23	115.01	120.55
1	D	35	LEU	CA-C-O	-5.21	114.21	120.10
1	D	75	LYS	CA-CB-CG	5.20	124.50	114.10
1	A	36	SER	N-CA-C	-5.20	105.79	111.82
1	A	61	LEU	CA-C-N	5.20	127.20	120.44
1	A	61	LEU	C-N-CA	5.20	127.20	120.44
1	D	20	ILE	CB-CG1-CD1	5.19	124.70	113.80
1	A	11	ASP	CA-C-O	-5.19	115.70	121.51
1	C	58	GLU	CB-CG-CD	-5.17	103.81	112.60
1	D	92	THR	CA-CB-OG1	-5.16	101.86	109.60
1	C	25	HIS	CA-C-N	5.15	127.18	120.28
1	C	25	HIS	C-N-CA	5.15	127.18	120.28
1	D	48	ARG	CA-C-O	-5.15	115.09	120.55
1	D	51	THR	CA-C-N	5.15	125.81	119.99
1	D	51	THR	C-N-CA	5.15	125.81	119.99
1	A	48	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	2	PHE	N-CA-C	-5.13	103.68	110.40
1	B	29	PHE	N-CA-CB	5.12	117.57	109.94
1	C	104	THR	CA-C-O	-5.11	113.56	119.64
1	D	86	THR	CA-C-N	5.05	128.28	121.05
1	D	86	THR	C-N-CA	5.05	128.28	121.05
1	D	96	ASN	CA-C-O	-5.05	115.50	120.70
1	B	72[A]	GLU	CB-CG-CD	5.05	121.18	112.60
1	B	72[B]	GLU	CB-CG-CD	5.05	121.18	112.60
1	D	105	ILE	CA-C-O	-5.05	114.67	120.83
1	D	101	HIS	CA-CB-CG	-5.04	108.76	113.80
1	C	66	GLN	CG-CD-NE2	-5.03	108.85	116.40
1	A	110	ARG	NH1-CZ-NH2	5.02	125.83	119.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
1	B	9	CYS	Mainchain

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	965	0	910	12	0
1	B	960	0	910	8	0
1	C	952	0	906	9	0
1	D	955	0	908	7	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	0	0
3	A	3	0	0	1	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	69	0	0	0	0
4	B	70	0	0	0	0
4	C	66	0	0	2	0
4	D	88	0	0	1	0
All	All	4153	0	3646	37	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 (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLN:HE21	1:D:77:HIS:HD1	1.07	1.03
1:B:59:GLN:HE21	1:B:77:HIS:HD1	1.06	1.01
1:A:59:GLN:HE21	1:A:77:HIS:HD1	1.11	0.98
1:C:59:GLN:HE21	1:C:77:HIS:HD1	1.08	0.98
1:A:2:PHE:HB3	1:A:3:PRO:HD2	1.74	0.70
3:A:115:FEO:O	3:A:115:FEO:FE2	1.43	0.69
1:C:59:GLN:HA	1:C:62:MET:HE3	1.75	0.68
1:D:59:GLN:NE2	1:D:77:HIS:HD1	1.88	0.66
1:B:59:GLN:NE2	1:B:77:HIS:HD1	1.86	0.66
1:A:40:ASN:ND2	1:A:43:HIS:H	1.97	0.62
1:B:21[A]:ILE:HD12	1:B:58:GLU:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ASN:ND2	1:D:43:HIS:H	2.02	0.57
1:B:40:ASN:C	1:B:40:ASN:HD22	2.12	0.57
1:C:40:ASN:HD22	1:C:40:ASN:C	2.13	0.57
1:A:16:THR:O	1:A:17:PHE:HB2	2.06	0.56
1:A:21[A]:ILE:CD1	1:A:58:GLU:HG3	2.37	0.55
1:C:40:ASN:ND2	1:C:43:HIS:H	2.04	0.55
1:D:21[A]:ILE:HD12	1:D:58:GLU:HG3	1.88	0.55
1:C:21[A]:ILE:HD11	1:C:61:LEU:HD23	1.91	0.53
1:A:59:GLN:NE2	1:A:77:HIS:HD1	1.93	0.53
1:A:40:ASN:C	1:A:40:ASN:HD22	2.19	0.50
1:B:40:ASN:ND2	1:B:43:HIS:H	2.10	0.49
1:B:35:LEU:HD13	1:B:87:TRP:CZ2	2.49	0.47
1:B:83:LYS:HE3	1:B:83:LYS:HA	1.96	0.47
1:A:51:THR:HG22	1:A:81[B]:ILE:HD11	1.97	0.46
1:C:59:GLN:NE2	1:C:77:HIS:HD1	1.92	0.44
1:D:21[A]:ILE:CD1	1:D:58:GLU:HG3	2.47	0.44
1:C:20:ILE:HG13	4:C:146:HOH:O	2.16	0.44
1:D:40:ASN:HD22	1:D:43:HIS:H	1.66	0.42
1:A:21[A]:ILE:HD12	1:A:58:GLU:HG3	2.01	0.42
1:B:102:ILE:HA	1:B:106:ASP:HB2	2.00	0.42
1:A:28[A]:LEU:HD21	1:A:51:THR:HA	2.02	0.41
1:A:59:GLN:HA	1:A:62:MET:HE3	2.02	0.41
1:C:57:ASN:ND2	4:C:154:HOH:O	2.52	0.41
1:C:2:PHE:HB3	1:C:3:PRO:HD2	2.03	0.40
1:A:2:PHE:CB	1:A:3:PRO:HD2	2.44	0.40
1:D:21[A]:ILE:HD13	4:D:227:HOH:O	2.22	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	116/114 (102%)	114 (98%)	2 (2%)	0	100	100
1	B	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
1	C	110/114 (96%)	109 (99%)	1 (1%)	0	100	100
1	D	111/114 (97%)	111 (100%)	0	0	100	100
All	All	449/456 (98%)	443 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	107/101 (106%)	98 (92%)	9 (8%)	10	1
1	B	103/101 (102%)	96 (93%)	7 (7%)	14	2
1	C	101/101 (100%)	95 (94%)	6 (6%)	18	3
1	D	102/101 (101%)	96 (94%)	6 (6%)	18	3
All	All	413/404 (102%)	385 (93%)	28 (7%)	16	2

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	21[A]	ILE
1	A	21[B]	VAL
1	A	40	ASN
1	A	53[A]	LYS
1	A	53[B]	LYS
1	A	83	LYS
1	A	108[A]	LYS
1	A	108[B]	LYS
1	B	4	ILE
1	B	36	SER
1	B	40	ASN
1	B	72[A]	GLU

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Mol	Chain	Res	Type
1	B	72[B]	GLU
1	B	83	LYS
1	B	96	ASN
1	C	9	CYS
1	C	40	ASN
1	C	60	GLN
1	C	72	GLU
1	C	75	LYS
1	C	96	ASN
1	D	20	ILE
1	D	40	ASN
1	D	53	LYS
1	D	60	GLN
1	D	83	LYS
1	D	109	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	40	ASN
1	A	57	ASN
1	A	59	GLN
1	B	37	GLN
1	B	40	ASN
1	B	45	ASN
1	B	57	ASN
1	B	59	GLN
1	B	96	ASN
1	C	37	GLN
1	C	40	ASN
1	C	45	ASN
1	C	57	ASN
1	C	59	GLN
1	C	60	GLN
1	C	96	ASN
1	C	100	ASN
1	D	37	GLN
1	D	40	ASN
1	D	57	ASN
1	D	59	GLN
1	D	60	GLN

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Mol	Chain	Res	Type
1	D	63	GLN

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACT	A	114	1	3,3,3	3.03	2 (66%)	3,3,3	2.07	2 (66%)
3	FEO	B	115	1	0,2,2	-	-	-		
3	FEO	C	115	1,4	0,2,2	-	-	-		
2	ACT	D	114	1	3,3,3	2.70	2 (66%)	3,3,3	1.87	1 (33%)
3	FEO	D	115	1	0,2,2	-	-	-		
2	ACT	C	114	1	3,3,3	2.76	2 (66%)	3,3,3	1.50	1 (33%)
3	FEO	A	115	1,4	0,2,2	-	-	-		
2	ACT	B	114	1	3,3,3	2.82	1 (33%)	3,3,3	1.16	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	114	ACT	O-C	4.25	1.40	1.22
2	B	114	ACT	O-C	4.19	1.40	1.22
2	C	114	ACT	O-C	3.79	1.38	1.22
2	D	114	ACT	O-C	3.47	1.37	1.22
2	D	114	ACT	CH3-C	2.56	1.59	1.49
2	A	114	ACT	CH3-C	2.51	1.59	1.49
2	C	114	ACT	CH3-C	2.46	1.58	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	114	ACT	OXT-C-O	2.88	132.72	122.03
2	D	114	ACT	OXT-C-O	2.62	131.75	122.03
2	A	114	ACT	O-C-CH3	-2.07	114.03	122.53
2	C	114	ACT	OXT-C-O	2.01	129.49	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	115	FEO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	112/114 (98%)	-0.64	0 100 100	7, 14, 30, 49	5 (4%)
1	B	112/114 (98%)	-0.29	1 (0%) 81 86	11, 20, 35, 59	2 (1%)
1	C	112/114 (98%)	-0.53	0 100 100	10, 17, 35, 63	0
1	D	112/114 (98%)	-0.72	0 100 100	7, 14, 28, 37	1 (0%)
All	All	448/456 (98%)	-0.55	1 (0%) 91 93	7, 17, 34, 63	8 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACT	B	114	4/4	0.86	0.10	17,19,20,21	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	D	114	4/4	0.86	0.10	14,18,19,20	4
2	ACT	C	114	4/4	0.89	0.08	18,19,21,22	4
2	ACT	A	114	4/4	0.90	0.10	13,14,16,20	4
3	FEO	A	115	3/3	0.99	0.02	5,5,12,13	0
3	FEO	B	115	3/3	0.99	0.03	12,12,18,19	0
3	FEO	C	115	3/3	0.99	0.03	8,8,14,17	0
3	FEO	D	115	3/3	0.99	0.03	6,6,11,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.