



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:03 PM GMT

PDB ID : 2ZVS
Title : Crystal structure of the 2[4FE-4S] ferredoxin from escherichia coli
Authors : Giastas, P.; Mavridis, M.I.
Deposited on : 2008-11-18
Resolution : 1.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

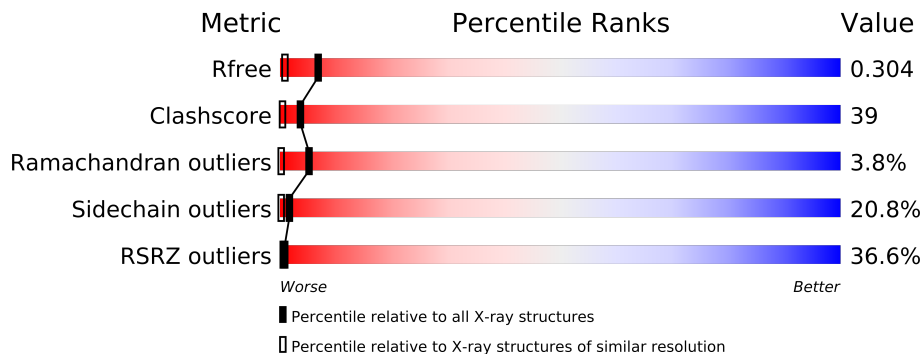
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.65 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))
R_{free}	66092	1404 (1.68-1.64)
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	85	
1	B	85	
1	C	85	

2 Entry composition i

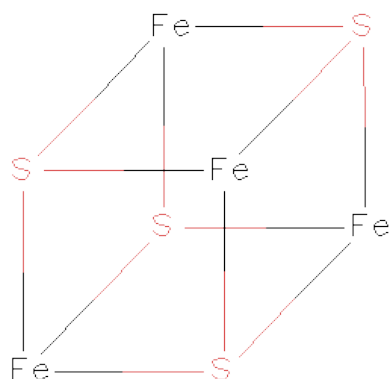
There are 3 unique types of molecules in this entry. The entry contains 2121 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Uncharacterized ferredoxin-like protein yfhL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	81	Total	C	N	O	S	10	0	0
			638	398	104	125	11			
1	B	80	Total	C	N	O	S	13	0	0
			628	392	101	124	11			
1	C	80	Total	C	N	O	S	26	0	0
			628	392	101	124	11			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		

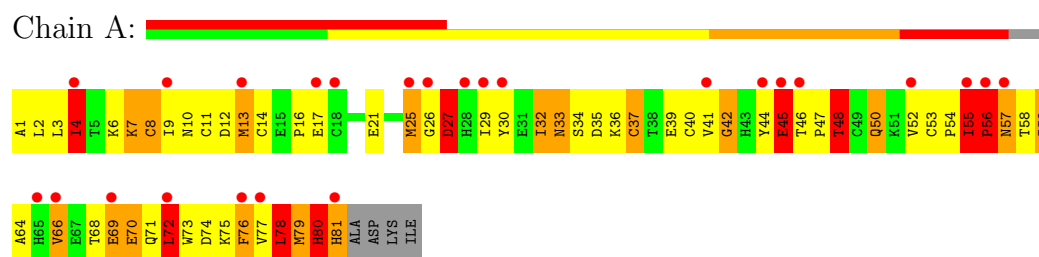
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	56	Total	O	0	0
			56	56		
3	C	58	Total	O	0	0
			58	58		

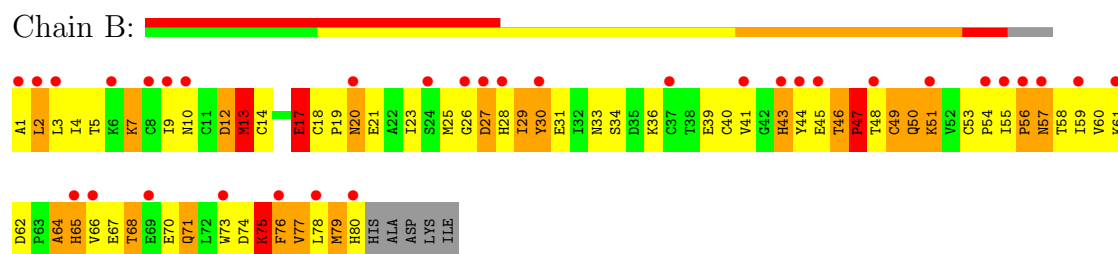
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

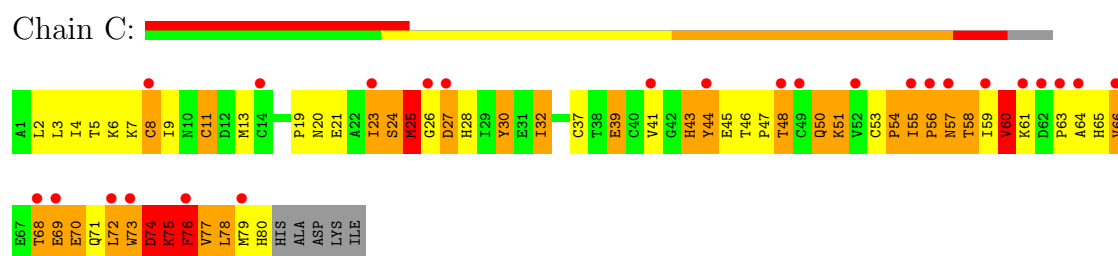
- Molecule 1: Uncharacterized ferredoxin-like protein yfhL



- Molecule 1: Uncharacterized ferredoxin-like protein yfhL



- Molecule 1: Uncharacterized ferredoxin-like protein yfhL



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	65.54Å 65.54Å 132.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.65 56.76 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.65) 99.1 (56.76-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 1.60Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.203 , 0.273 0.225 , 0.304	Depositor DCC
R_{free} test set	1266 reflections (3.03%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 53.8	EDS
Estimated twinning fraction	0.377 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 82935 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2121	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 67.72 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9129e-06.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

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	0.99	1/653 (0.2%)	2.97	77/888 (8.7%)
1	B	0.92	0/642	2.46	41/873 (4.7%)
1	C	0.87	0/642	2.50	51/873 (5.8%)
All	All	0.93	1/1937 (0.1%)	2.66	169/2634 (6.4%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	N-CD	5.43	1.55	1.47

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	VAL	CA-CB-CG1	18.69	138.94	110.90
1	A	35	ASP	CB-CG-OD1	16.46	133.12	118.30
1	A	79	MET	C-N-CA	15.84	161.29	121.70
1	A	81	HIS	CA-C-O	14.94	151.48	120.10
1	B	27	ASP	CA-CB-CG	14.55	145.41	113.40
1	C	27	ASP	CB-CG-OD2	12.09	129.18	118.30
1	B	71	GLN	CA-CB-CG	12.04	139.89	113.40
1	A	44	TYR	CB-CG-CD2	11.41	127.85	121.00
1	A	61	LYS	CA-C-O	11.40	144.04	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	76	PHE	CB-CG-CD2	-10.95	113.13	120.80
1	C	74	ASP	CB-CG-OD1	10.95	128.15	118.30
1	A	76	PHE	CB-CG-CD1	10.94	128.46	120.80
1	A	56	PRO	CA-N-CD	-10.73	96.48	111.50
1	B	64	ALA	CB-CA-C	-10.67	94.10	110.10
1	C	6	LYS	O-C-N	-10.58	105.77	122.70
1	B	79	MET	CA-CB-CG	10.44	131.04	113.30
1	A	44	TYR	CA-CB-CG	10.13	132.64	113.40
1	A	77	VAL	CG1-CB-CG2	-10.10	94.74	110.90
1	C	78	LEU	CB-CG-CD2	9.90	127.83	111.00
1	A	4	ILE	CB-CG1-CD1	9.74	141.19	113.90
1	B	39	GLU	C-N-CA	9.57	145.62	121.70
1	C	25	MET	C-N-CA	9.37	141.98	122.30
1	B	64	ALA	N-CA-CB	9.33	123.16	110.10
1	A	77	VAL	CA-CB-CG2	-9.02	97.37	110.90
1	A	48	THR	CA-CB-CG2	-8.84	100.03	112.40
1	B	13	MET	CA-CB-CG	8.82	128.30	113.30
1	A	33	ASN	O-C-N	8.75	136.69	122.70
1	C	76	PHE	O-C-N	8.69	136.61	122.70
1	A	55	ILE	C-N-CA	8.68	158.47	122.00
1	A	80	HIS	CA-C-N	8.61	136.15	117.20
1	C	30	TYR	CG-CD1-CE1	-8.46	114.53	121.30
1	A	25	MET	O-C-N	-8.35	109.00	123.20
1	A	79	MET	CA-C-N	8.20	135.23	117.20
1	A	4	ILE	C-N-CA	8.12	141.99	121.70
1	B	58	THR	CA-CB-CG2	-8.06	101.11	112.40
1	C	76	PHE	CA-C-N	-8.00	99.61	117.20
1	A	40	CYS	O-C-N	7.92	135.37	122.70
1	A	44	TYR	CB-CG-CD1	-7.83	116.30	121.00
1	C	58	THR	C-N-CA	7.83	141.26	121.70
1	A	79	MET	CA-C-O	-7.66	104.02	120.10
1	C	77	VAL	CA-CB-CG1	-7.58	99.54	110.90
1	A	62	ASP	CB-CG-OD2	7.54	125.09	118.30
1	C	39	GLU	C-N-CA	7.51	140.48	121.70
1	A	27	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	55	ILE	C-N-CD	-7.50	104.09	120.60
1	C	56	PRO	CA-N-CD	-7.39	101.16	111.50
1	A	45	GLU	OE1-CD-OE2	-7.33	114.50	123.30
1	A	72	LEU	O-C-N	7.33	134.42	122.70
1	A	78	LEU	CB-CG-CD2	7.31	123.43	111.00
1	A	68	THR	C-N-CA	-7.31	103.44	121.70
1	C	11	CYS	C-N-CA	7.30	139.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	THR	C-N-CA	7.28	139.90	121.70
1	A	77	VAL	CB-CA-C	7.28	125.23	111.40
1	A	68	THR	O-C-N	-7.17	111.23	122.70
1	A	37	CYS	CA-CB-SG	7.14	126.85	114.00
1	B	30	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	B	25	MET	C-N-CA	-7.07	107.45	122.30
1	C	56	PRO	N-CD-CG	-7.03	92.65	103.20
1	B	56	PRO	N-CA-CB	-7.00	94.90	102.60
1	C	50	GLN	O-C-N	6.99	133.88	122.70
1	A	80	HIS	CA-C-O	-6.98	105.45	120.10
1	C	27	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	C	75	LYS	CB-CG-CD	6.95	129.67	111.60
1	B	18	CYS	CA-C-O	6.92	134.64	120.10
1	A	77	VAL	N-CA-CB	-6.76	96.63	111.50
1	B	43	HIS	CA-CB-CG	6.68	124.95	113.60
1	B	76	PHE	CB-CG-CD1	-6.66	116.14	120.80
1	A	60	VAL	C-N-CA	-6.61	105.17	121.70
1	C	43	HIS	CA-CB-CG	-6.60	102.38	113.60
1	C	54	PRO	CB-CA-C	-6.56	95.60	112.00
1	C	70	GLU	OE1-CD-OE2	6.53	131.14	123.30
1	B	50	GLN	C-N-CA	6.53	138.01	121.70
1	A	32	ILE	CA-C-O	6.52	133.80	120.10
1	A	78	LEU	CA-C-O	6.52	133.79	120.10
1	A	69	GLU	CB-CA-C	6.51	123.42	110.40
1	A	58	THR	O-C-N	6.50	133.11	122.70
1	C	78	LEU	CD1-CG-CD2	-6.48	91.06	110.50
1	A	61	LYS	O-C-N	-6.43	112.41	122.70
1	C	30	TYR	CZ-CE2-CD2	-6.42	114.02	119.80
1	A	26	GLY	O-C-N	6.41	132.95	122.70
1	C	78	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	B	47	PRO	O-C-N	-6.38	112.48	122.70
1	A	48	THR	CA-CB-OG1	6.34	122.31	109.00
1	A	78	LEU	O-C-N	-6.32	112.59	122.70
1	A	32	ILE	O-C-N	-6.32	112.59	122.70
1	A	61	LYS	CA-C-N	-6.32	103.31	117.20
1	A	61	LYS	C-N-CA	6.31	137.48	121.70
1	C	54	PRO	C-N-CA	6.28	137.39	121.70
1	A	2	LEU	O-C-N	6.23	132.67	122.70
1	A	52	VAL	O-C-N	-6.21	112.77	122.70
1	B	56	PRO	CA-N-CD	-6.17	102.87	111.50
1	B	76	PHE	CG-CD2-CE2	-6.16	114.02	120.80
1	A	72	LEU	CA-CB-CG	6.14	129.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	PRO	N-CA-CB	-6.10	95.89	102.60
1	C	27	ASP	C-N-CA	6.09	136.92	121.70
1	A	25	MET	C-N-CA	-6.08	109.53	122.30
1	C	19	PRO	O-C-N	6.08	132.42	122.70
1	B	56	PRO	N-CD-CG	-6.06	94.12	103.20
1	A	61	LYS	CA-CB-CG	-5.95	100.32	113.40
1	C	30	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	B	62	ASP	CB-CA-C	5.92	122.23	110.40
1	A	34	SER	N-CA-CB	-5.88	101.68	110.50
1	C	73	TRP	O-C-N	-5.87	113.31	122.70
1	C	30	TYR	O-C-N	5.85	132.06	122.70
1	A	76	PHE	CZ-CE2-CD2	5.85	127.12	120.10
1	C	56	PRO	N-CA-CB	-5.84	96.17	102.60
1	C	32	ILE	O-C-N	-5.83	113.37	122.70
1	A	70	GLU	O-C-N	-5.78	113.45	122.70
1	C	37	CYS	O-C-N	5.74	131.88	122.70
1	C	60	VAL	O-C-N	5.73	131.87	122.70
1	C	48	THR	CA-C-O	5.70	132.08	120.10
1	B	76	PHE	CD1-CE1-CZ	-5.65	113.32	120.10
1	B	75	LYS	O-C-N	-5.63	113.70	122.70
1	A	78	LEU	CD1-CG-CD2	-5.62	93.64	110.50
1	A	57	ASN	CB-CG-OD1	-5.60	110.40	121.60
1	A	35	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	45	GLU	C-N-CA	5.59	135.66	121.70
1	A	80	HIS	N-CA-C	5.58	126.07	111.00
1	B	59	ILE	O-C-N	-5.57	113.79	122.70
1	A	7	LYS	CB-CA-C	-5.54	99.32	110.40
1	C	76	PHE	CB-CA-C	-5.53	99.35	110.40
1	C	8	CYS	O-C-N	5.50	131.50	122.70
1	B	30	TYR	C-N-CA	-5.49	107.99	121.70
1	B	51	LYS	C-N-CA	5.47	135.39	121.70
1	C	48	THR	CB-CA-C	-5.47	96.83	111.60
1	B	23	ILE	CB-CA-C	-5.45	100.70	111.60
1	C	2	LEU	N-CA-CB	5.44	121.27	110.40
1	A	45	GLU	CB-CG-CD	5.42	128.84	114.20
1	B	17	GLU	CA-CB-CG	5.40	125.28	113.40
1	B	7	LYS	CA-CB-CG	-5.38	101.57	113.40
1	C	57	ASN	O-C-N	5.38	131.30	122.70
1	C	44	TYR	CA-C-O	-5.36	108.84	120.10
1	C	77	VAL	CA-CB-CG2	5.35	118.92	110.90
1	A	14	CYS	O-C-N	-5.35	114.14	122.70
1	A	41	VAL	C-N-CA	5.34	133.52	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	LYS	O-C-N	5.33	131.23	122.70
1	A	53	CYS	CA-CB-SG	-5.33	104.41	114.00
1	C	70	GLU	CB-CA-C	5.33	121.05	110.40
1	A	45	GLU	CG-CD-OE1	5.30	128.90	118.30
1	C	69	GLU	CA-C-N	-5.29	105.56	117.20
1	A	25	MET	CA-C-O	5.29	131.21	120.10
1	B	30	TYR	CG-CD1-CE1	-5.29	117.07	121.30
1	A	71	GLN	CA-C-O	5.29	131.20	120.10
1	C	30	TYR	CD1-CG-CD2	5.28	123.71	117.90
1	B	58	THR	CA-C-O	5.28	131.18	120.10
1	C	6	LYS	CA-C-O	5.26	131.15	120.10
1	B	49	CYS	CA-CB-SG	5.26	123.46	114.00
1	A	50	GLN	OE1-CD-NE2	5.25	133.96	121.90
1	B	2	LEU	C-N-CA	5.24	134.81	121.70
1	C	76	PHE	C-N-CA	-5.22	108.65	121.70
1	A	37	CYS	N-CA-CB	5.22	119.99	110.60
1	A	55	ILE	CA-C-O	-5.22	109.15	120.10
1	B	71	GLN	O-C-N	-5.21	114.37	122.70
1	A	57	ASN	CB-CG-ND2	5.18	129.13	116.70
1	B	74	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	13	MET	CG-SD-CE	5.16	108.46	100.20
1	A	16	PRO	O-C-N	-5.16	114.45	122.70
1	B	62	ASP	O-C-N	-5.15	111.32	121.10
1	C	20	ASN	CA-C-O	-5.11	109.36	120.10
1	A	66	VAL	O-C-N	5.10	130.86	122.70
1	A	35	ASP	OD1-CG-OD2	-5.09	113.62	123.30
1	C	20	ASN	O-C-N	5.09	130.85	122.70
1	C	24	SER	CB-CA-C	5.09	119.78	110.10
1	C	76	PHE	CB-CG-CD1	-5.09	117.24	120.80
1	B	56	PRO	N-CA-C	5.08	125.32	112.10
1	B	26	GLY	C-N-CA	-5.05	109.07	121.70
1	C	68	THR	O-C-N	-5.05	114.62	122.70
1	B	40	CYS	CB-CA-C	-5.04	100.31	110.40
1	A	42	GLY	O-C-N	5.01	130.71	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ILE	Peptide
1	A	79	MET	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	638	0	605	43	0
1	B	628	0	598	52	3
1	C	628	0	598	47	3
2	A	16	0	0	1	0
2	B	16	0	0	2	0
2	C	16	0	0	4	0
3	A	65	0	0	8	0
3	B	56	0	0	4	0
3	C	58	0	0	2	0
All	All	2121	0	1801	142	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

All (142) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:55:ILE:HD12	1:B:57:ASN:HD21	1.36	0.91
1:C:41:VAL:HG11	1:C:68:THR:HG23	1.62	0.82
1:C:66:VAL:HG22	1:C:70:GLU:HB3	1.63	0.80
1:B:47:PRO:O	1:B:51:LYS:HG3	1.81	0.80
1:C:7:LYS:HB2	1:C:57:ASN:OD1	1.83	0.77
1:B:41:VAL:HG21	1:B:71:GLN:HG3	1.67	0.76
1:B:68:THR:HA	1:B:71:GLN:HG2	1.66	0.74
1:B:7:LYS:HB2	1:B:57:ASN:HD22	1.50	0.74
1:B:12:ASP:HB3	1:B:30:TYR:OH	1.88	0.74
1:B:73:TRP:O	1:B:77:VAL:HG22	1.88	0.73
1:A:59:ILE:HG23	1:A:60:VAL:O	1.89	0.72
1:B:3:LEU:HB2	1:B:61:LYS:HG3	1.72	0.71
1:A:4:ILE:HD11	1:A:32:ILE:HG13	1.76	0.68
1:B:9:ILE:HG23	1:B:55:ILE:HD11	1.74	0.68
1:C:66:VAL:HG11	3:C:108:HOH:O	1.94	0.68
1:B:33:ASN:HD22	1:B:36:LYS:HE3	1.59	0.67
1:B:66:VAL:HG13	1:B:70:GLU:HB2	1.75	0.67
1:C:39:GLU:HB2	1:C:71:GLN:HE21	1.61	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:LEU:HD22	1:A:61:LYS:HD2	1.78	0.66
1:A:29:ILE:HG22	1:A:30:TYR:O	1.96	0.65
1:A:50:GLN:HB3	3:A:123:HOH:O	1.97	0.65
1:C:71:GLN:HA	1:C:74:ASP:OD1	1.97	0.64
1:C:65:HIS:O	1:C:66:VAL:HB	1.97	0.64
1:A:54:PRO:HG2	1:A:55:ILE:HG12	1.80	0.63
1:B:12:ASP:HB3	1:B:30:TYR:CZ	2.35	0.62
1:C:5:THR:HG23	1:C:57:ASN:O	2.00	0.61
1:C:11:CYS:HA	3:C:122:HOH:O	2.00	0.61
1:B:55:ILE:CD1	1:B:57:ASN:HD21	2.12	0.61
1:B:66:VAL:HG22	1:B:70:GLU:OE1	2.01	0.61
1:C:61:LYS:HB3	1:C:64:ALA:HB3	1.83	0.60
1:B:66:VAL:HG13	1:B:70:GLU:OE1	2.01	0.60
1:C:75:LYS:HE2	1:C:76:PHE:CD1	2.37	0.60
1:A:33:ASN:HB3	3:A:110:HOH:O	2.02	0.59
1:B:19:PRO:HB2	1:B:43:HIS:CE1	2.37	0.59
1:C:3:LEU:HD13	1:C:61:LYS:HD2	1.85	0.59
1:B:66:VAL:CG1	1:B:70:GLU:HB2	2.32	0.58
1:A:66:VAL:CG1	1:A:70:GLU:HB2	2.34	0.58
1:C:43:HIS:HB3	1:C:44:TYR:CD2	2.39	0.58
1:C:8:CYS:HA	1:C:57:ASN:ND2	2.18	0.57
1:A:72:LEU:HG	1:A:76:PHE:CE2	2.40	0.56
1:A:42:GLY:HA3	1:A:75:LYS:HE3	1.85	0.56
1:B:46:THR:O	1:B:51:LYS:HE3	2.06	0.56
1:A:8:CYS:HA	1:A:57:ASN:HD22	1.71	0.56
1:A:61:LYS:HB3	3:A:98:HOH:O	2.05	0.55
1:B:55:ILE:HD12	1:B:55:ILE:O	2.06	0.55
1:A:76:PHE:O	1:A:80:HIS:HA	2.06	0.55
1:B:41:VAL:CG2	1:B:71:GLN:HE21	2.21	0.54
1:A:74:ASP:O	1:A:78:LEU:HD12	2.06	0.54
1:C:32:ILE:HD13	2:C:506:SF4:S2	2.48	0.54
1:C:9:ILE:HD13	1:C:55:ILE:HD11	1.90	0.53
1:C:4:ILE:HG12	2:C:405:SF4:S2	2.48	0.53
1:B:4:ILE:HD13	1:B:30:TYR:HB3	1.90	0.53
1:B:41:VAL:HG23	1:B:71:GLN:HE21	1.73	0.53
1:B:78:LEU:HD23	3:B:89:HOH:O	2.09	0.53
1:C:71:GLN:HA	1:C:71:GLN:OE1	2.08	0.53
1:A:9:ILE:HG12	1:A:55:ILE:HD11	1.89	0.52
1:B:44:TYR:HB3	1:B:51:LYS:NZ	2.25	0.52
1:A:66:VAL:HG13	1:A:70:GLU:HB2	1.92	0.52
1:B:80:HIS:HA	3:B:90:HOH:O	2.09	0.52
1:B:65:HIS:O	1:B:66:VAL:HG23	2.09	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:67:GLU:HB3	3:B:87:HOH:O	2.09	0.51
1:A:11:CYS:SG	1:A:13:MET:HB2	2.51	0.51
1:A:6:LYS:HG3	3:A:96:HOH:O	2.11	0.51
1:C:70:GLU:O	1:C:74:ASP:OD2	2.29	0.51
1:C:54:PRO:HB2	1:C:55:ILE:HG13	1.92	0.50
1:B:44:TYR:HB3	1:B:51:LYS:HZ3	1.76	0.50
1:C:55:ILE:O	1:C:57:ASN:OD1	2.29	0.50
1:A:3:LEU:HD23	1:A:61:LYS:NZ	2.26	0.50
1:C:73:TRP:O	1:C:77:VAL:HG23	2.12	0.50
1:B:33:ASN:ND2	1:B:36:LYS:HE3	2.26	0.49
1:C:68:THR:HA	1:C:71:GLN:HB2	1.95	0.49
1:A:73:TRP:HA	1:A:76:PHE:HD2	1.77	0.49
1:B:55:ILE:O	1:B:57:ASN:ND2	2.46	0.49
1:C:41:VAL:CG1	1:C:68:THR:HG23	2.40	0.49
1:B:13:MET:CE	1:B:54:PRO:HD3	2.43	0.49
1:A:3:LEU:HB3	1:A:61:LYS:HG3	1.96	0.48
1:B:61:LYS:HB3	1:B:64:ALA:HB3	1.96	0.48
1:B:27:ASP:HB2	1:B:28:HIS:H	1.64	0.48
1:A:8:CYS:HB3	1:A:29:ILE:HG23	1.96	0.47
1:C:55:ILE:O	1:C:57:ASN:N	2.48	0.47
1:C:8:CYS:HA	1:C:57:ASN:HD22	1.80	0.47
1:C:66:VAL:CG2	1:C:70:GLU:HB3	2.40	0.47
1:A:17:GLU:OE2	1:A:48:THR:HG21	2.15	0.47
1:A:46:THR:HA	1:A:47:PRO:HD3	1.81	0.47
1:C:25:MET:HG2	1:C:30:TYR:CE1	2.49	0.47
1:A:55:ILE:HB	1:A:57:ASN:ND2	2.30	0.47
1:B:75:LYS:HD3	3:B:179:HOH:O	2.14	0.47
1:A:6:LYS:HA	1:A:29:ILE:CD1	2.45	0.46
1:B:20:ASN:HD22	1:B:79:MET:CE	2.29	0.46
1:C:23:ILE:O	1:C:24:SER:HB3	2.15	0.46
1:B:19:PRO:HB2	1:B:43:HIS:ND1	2.30	0.46
1:A:39:GLU:HA	2:A:102:SF4:S4	2.55	0.46
1:B:29:ILE:N	1:B:29:ILE:HD13	2.30	0.46
1:A:6:LYS:HE3	3:A:138:HOH:O	2.15	0.46
1:A:36:LYS:HE2	3:A:109:HOH:O	2.15	0.46
1:C:47:PRO:HB3	2:C:506:SF4:S4	2.56	0.45
1:B:2:LEU:HD22	1:B:60:VAL:HA	1.98	0.45
1:C:61:LYS:HG2	1:C:63:PRO:HG2	1.98	0.45
1:A:45:GLU:OE1	1:A:46:THR:N	2.49	0.45
1:A:7:LYS:O	1:A:57:ASN:ND2	2.50	0.45
1:A:81:HIS:N	3:A:86:HOH:O	2.48	0.45
1:B:46:THR:HG22	1:B:47:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:61:LYS:HB3	1:B:64:ALA:CB	2.46	0.45
1:C:45:GLU:OE1	1:C:45:GLU:HA	2.17	0.45
1:B:53:CYS:HA	2:B:203:SF4:S1	2.57	0.45
1:C:39:GLU:CB	1:C:71:GLN:HE21	2.27	0.44
1:A:57:ASN:OD1	1:A:57:ASN:N	2.47	0.44
1:C:59:ILE:HG22	1:C:60:VAL:O	2.18	0.44
1:B:47:PRO:HB2	1:B:50:GLN:HB2	2.00	0.44
1:A:60:VAL:O	1:A:61:LYS:HG2	2.16	0.44
1:B:5:THR:OG1	1:B:57:ASN:O	2.29	0.44
1:C:61:LYS:HG3	1:C:63:PRO:HD2	1.99	0.44
1:C:75:LYS:HE2	1:C:76:PHE:CE1	2.53	0.43
1:B:13:MET:HE2	1:B:54:PRO:HD3	2.00	0.43
1:B:1:ALA:HB3	1:B:64:ALA:CB	2.47	0.43
1:C:53:CYS:HA	1:C:54:PRO:HD2	1.69	0.43
1:B:20:ASN:HD22	1:B:79:MET:HE2	1.84	0.43
1:A:9:ILE:HG12	1:A:55:ILE:CD1	2.49	0.43
1:A:1:ALA:HB1	1:A:37:CYS:HB3	2.00	0.43
1:C:48:THR:O	1:C:48:THR:HG22	2.18	0.42
1:C:74:ASP:OD2	1:C:74:ASP:N	2.49	0.42
1:A:8:CYS:HB3	1:A:29:ILE:CG2	2.50	0.42
1:C:41:VAL:HG12	1:C:72:LEU:HD12	2.02	0.42
1:A:80:HIS:O	1:A:81:HIS:HB2	2.20	0.42
1:A:80:HIS:ND1	1:A:80:HIS:O	2.53	0.41
1:B:17:GLU:HB3	1:B:48:THR:CG2	2.49	0.41
1:C:9:ILE:CD1	1:C:55:ILE:HD11	2.49	0.41
1:A:10:ASN:OD1	1:A:29:ILE:HA	2.20	0.41
1:A:4:ILE:HD11	1:A:32:ILE:CG1	2.48	0.41
1:B:14:CYS:HB3	2:B:203:SF4:S1	2.60	0.41
1:C:47:PRO:O	1:C:50:GLN:HB2	2.21	0.41
1:C:48:THR:HB	2:C:506:SF4:S1	2.61	0.41
1:C:74:ASP:O	1:C:78:LEU:HD12	2.20	0.40
1:A:61:LYS:O	1:A:64:ALA:N	2.50	0.40
1:B:77:VAL:H	1:B:77:VAL:HG22	1.60	0.40
1:B:75:LYS:HG3	1:B:76:PHE:N	2.30	0.40
1:A:56:PRO:HD3	3:A:114:HOH:O	2.20	0.40
1:C:46:THR:OG1	1:C:51:LYS:HD2	2.22	0.40
1:B:2:LEU:O	1:B:61:LYS:HE2	2.22	0.40
1:B:29:ILE:HD13	1:B:29:ILE:H	1.86	0.40
1:C:26:GLY:O	1:C:28:HIS:N	2.55	0.40
1:C:74:ASP:O	1:C:78:LEU:CD1	2.70	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:VAL:CG1	1:C:80:HIS:CE1[4.545]	1.50	0.70
1:B:41:VAL:CG1	1:C:80:HIS:ND1[4.545]	1.84	0.36
1:B:41:VAL:CG1	1:C:80:HIS:NE2[4.545]	2.00	0.20

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	79/85 (93%)	67 (85%)	8 (10%)	4 (5%)	3	0
1	B	78/85 (92%)	64 (82%)	12 (15%)	2 (3%)	8	0
1	C	78/85 (92%)	67 (86%)	8 (10%)	3 (4%)	5	0
All	All	235/255 (92%)	198 (84%)	28 (12%)	9 (4%)	5	0

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	PRO
1	B	56	PRO
1	C	27	ASP
1	C	56	PRO
1	A	80	HIS
1	A	27	ASP
1	C	66	VAL
1	B	47	PRO
1	A	55	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	76/79 (96%)	60 (79%)	16 (21%)	1	0
1	B	75/79 (95%)	58 (77%)	17 (23%)	1	0
1	C	75/79 (95%)	61 (81%)	14 (19%)	2	0
All	All	226/237 (95%)	179 (79%)	47 (21%)	2	0

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	8	CYS
1	A	12	ASP
1	A	13	MET
1	A	21	GLU
1	A	25	MET
1	A	27	ASP
1	A	45	GLU
1	A	48	THR
1	A	55	ILE
1	A	56	PRO
1	A	59	ILE
1	A	60	VAL
1	A	69	GLU
1	A	72	LEU
1	A	78	LEU
1	B	10	ASN
1	B	12	ASP
1	B	13	MET
1	B	17	GLU
1	B	20	ASN
1	B	21	GLU
1	B	29	ILE
1	B	31	GLU
1	B	34	SER
1	B	46	THR
1	B	47	PRO
1	B	49	CYS
1	B	57	ASN
1	B	65	HIS
1	B	68	THR
1	B	75	LYS
1	B	77	VAL
1	C	13	MET

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Mol	Chain	Res	Type
1	C	21	GLU
1	C	23	ILE
1	C	25	MET
1	C	51	LYS
1	C	55	ILE
1	C	58	THR
1	C	60	VAL
1	C	69	GLU
1	C	72	LEU
1	C	74	ASP
1	C	75	LYS
1	C	76	PHE
1	C	79	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	ASN
1	B	20	ASN
1	B	57	ASN
1	B	71	GLN
1	B	80	HIS
1	C	71	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	SF4	A	101	1	12,12,12	7.91	12 (100%)	0,24,24	0.00	-
2	SF4	A	102	1	12,12,12	7.51	12 (100%)	0,24,24	0.00	-
2	SF4	B	203	1	12,12,12	7.50	12 (100%)	0,24,24	0.00	-
2	SF4	B	304	1	12,12,12	7.69	12 (100%)	0,24,24	0.00	-
2	SF4	C	405	1	12,12,12	7.98	12 (100%)	0,24,24	0.00	-
2	SF4	C	506	1	12,12,12	7.86	12 (100%)	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
2	SF4	A	101	1	-	0/0/48/48	0/0/5/5
2	SF4	A	102	1	-	0/0/48/48	0/0/5/5
2	SF4	B	203	1	-	0/0/48/48	0/0/5/5
2	SF4	B	304	1	-	0/0/48/48	0/0/5/5
2	SF4	C	405	1	-	0/0/48/48	0/0/5/5
2	SF4	C	506	1	-	0/0/48/48	0/0/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	405	SF4	S2-FE1	-12.23	2.25	2.33
2	C	506	SF4	S4-FE2	-10.84	2.26	2.33
2	B	203	SF4	S2-FE3	-10.69	2.26	2.33
2	C	405	SF4	S1-FE4	-10.09	2.26	2.33
2	A	101	SF4	S2-FE4	-9.93	2.26	2.33
2	C	506	SF4	S1-FE2	-9.82	2.26	2.33
2	A	101	SF4	S4-FE1	-9.72	2.26	2.33
2	B	304	SF4	S2-FE3	-9.67	2.26	2.33
2	B	203	SF4	S4-FE2	-9.59	2.26	2.33
2	A	101	SF4	S1-FE3	-9.42	2.26	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	102	SF4	S3-FE2	-9.35	2.27	2.33
2	A	102	SF4	S2-FE4	-9.26	2.27	2.33
2	A	101	SF4	S1-FE4	-9.19	2.27	2.33
2	B	203	SF4	S4-FE1	-8.91	2.27	2.33
2	C	506	SF4	S3-FE4	-8.90	2.27	2.33
2	B	304	SF4	S4-FE3	-8.87	2.27	2.33
2	A	101	SF4	S4-FE2	-8.55	2.27	2.33
2	B	304	SF4	S3-FE1	-8.32	2.27	2.33
2	A	101	SF4	S3-FE1	-8.20	2.27	2.33
2	B	203	SF4	S2-FE4	-8.16	2.27	2.33
2	B	304	SF4	S1-FE3	-8.07	2.27	2.33
2	A	102	SF4	S1-FE3	-8.06	2.27	2.33
2	C	506	SF4	S1-FE3	-7.96	2.27	2.33
2	C	405	SF4	S4-FE2	-7.93	2.27	2.33
2	B	203	SF4	S3-FE1	-7.87	2.28	2.33
2	B	304	SF4	S3-FE2	-7.87	2.28	2.33
2	C	405	SF4	S3-FE2	-7.84	2.28	2.33
2	C	506	SF4	S4-FE3	-7.75	2.28	2.33
2	C	506	SF4	S4-FE1	-7.74	2.28	2.33
2	A	101	SF4	S3-FE4	-7.68	2.28	2.33
2	C	405	SF4	S4-FE3	-7.66	2.28	2.33
2	B	304	SF4	S4-FE1	-7.60	2.28	2.33
2	C	506	SF4	S3-FE2	-7.58	2.28	2.33
2	A	101	SF4	S4-FE3	-7.56	2.28	2.33
2	A	102	SF4	S4-FE2	-7.55	2.28	2.33
2	C	405	SF4	S2-FE3	-7.46	2.28	2.33
2	A	102	SF4	S4-FE3	-7.45	2.28	2.33
2	A	102	SF4	S1-FE2	-7.43	2.28	2.33
2	A	102	SF4	S4-FE1	-7.41	2.28	2.33
2	A	101	SF4	S2-FE1	-7.40	2.28	2.33
2	A	102	SF4	S2-FE3	-7.38	2.28	2.33
2	B	304	SF4	S2-FE1	-7.37	2.28	2.33
2	B	203	SF4	S3-FE2	-7.29	2.28	2.33
2	C	506	SF4	S2-FE4	-7.26	2.28	2.33
2	B	203	SF4	S1-FE4	-7.22	2.28	2.33
2	C	405	SF4	S1-FE2	-7.21	2.28	2.33
2	B	304	SF4	S2-FE4	-7.20	2.28	2.33
2	C	405	SF4	S2-FE4	-7.18	2.28	2.33
2	C	405	SF4	S4-FE1	-7.15	2.28	2.33
2	B	304	SF4	S4-FE2	-7.12	2.28	2.33
2	A	102	SF4	S2-FE1	-7.04	2.28	2.33
2	B	304	SF4	S1-FE2	-7.01	2.28	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	102	SF4	S3-FE1	-7.00	2.28	2.33
2	C	405	SF4	S1-FE3	-6.86	2.28	2.33
2	B	203	SF4	S4-FE3	-6.83	2.28	2.33
2	A	102	SF4	S1-FE4	-6.82	2.28	2.33
2	C	506	SF4	S3-FE1	-6.74	2.28	2.33
2	C	405	SF4	S3-FE1	-6.61	2.28	2.33
2	C	506	SF4	S2-FE1	-6.56	2.28	2.33
2	B	304	SF4	S1-FE4	-6.39	2.29	2.33
2	B	203	SF4	S1-FE3	-6.34	2.29	2.33
2	A	101	SF4	S3-FE2	-6.26	2.29	2.33
2	B	304	SF4	S3-FE4	-6.07	2.29	2.33
2	C	506	SF4	S2-FE3	-5.99	2.29	2.33
2	C	506	SF4	S1-FE4	-5.47	2.29	2.33
2	C	405	SF4	S3-FE4	-5.28	2.29	2.33
2	B	203	SF4	S1-FE2	-5.27	2.29	2.33
2	B	203	SF4	S3-FE4	-4.87	2.30	2.33
2	A	101	SF4	S2-FE3	-4.85	2.30	2.33
2	B	203	SF4	S2-FE1	-4.21	2.30	2.33
2	A	102	SF4	S3-FE4	-3.97	2.30	2.33
2	A	101	SF4	S1-FE2	-3.29	2.31	2.33

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

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	81/85 (95%)	1.76	28 (34%) 1 0	15, 26, 37, 49	1 (1%)
1	B	80/85 (94%)	1.95	33 (41%) 1 0	15, 29, 40, 55	3 (3%)
1	C	79/85 (92%)	1.70	25 (31%) 1 0	16, 26, 38, 48	3 (3%)
All	All	240/255 (94%)	1.80	86 (35%) 1 0	15, 27, 39, 55	7 (2%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	ASN	6.5
1	C	73	TRP	5.7
1	C	57	ASN	5.5
1	B	30	TYR	5.4
1	A	56	PRO	5.3
1	A	57	ASN	5.1
1	B	80	HIS	5.1
1	B	55	ILE	5.0
1	B	44	TYR	5.0
1	C	48	THR	4.8
1	B	73	TRP	4.2
1	B	56	PRO	4.2
1	C	59	ILE	4.2
1	A	30	TYR	4.1
1	A	81	HIS	4.1
1	C	8	CYS	4.0
1	A	76	PHE	3.9
1	B	45	GLU	3.9
1	A	41	VAL	3.8
1	C	68	THR	3.8
1	A	44	TYR	3.8
1	A	26	GLY	3.8
1	C	26	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	76	PHE	3.7
1	C	27	ASP	3.7
1	A	17	GLU	3.5
1	C	72	LEU	3.5
1	A	25	MET	3.4
1	B	26	GLY	3.4
1	A	4	ILE	3.3
1	B	59	ILE	3.3
1	B	10	ASN	3.2
1	C	55	ILE	3.2
1	C	44	TYR	3.1
1	C	56	PRO	3.0
1	C	69	GLU	3.0
1	A	66	VAL	3.0
1	C	79	MET	3.0
1	A	28	HIS	2.9
1	A	45	GLU	2.9
1	A	72	LEU	2.9
1	A	61	LYS	2.9
1	A	46	THR	2.8
1	B	78	LEU	2.8
1	A	29	ILE	2.8
1	B	9	ILE	2.8
1	C	52	VAL	2.8
1	A	65	HIS	2.8
1	B	28	HIS	2.7
1	B	3	LEU	2.7
1	C	23	ILE	2.7
1	C	63	PRO	2.7
1	B	69	GLU	2.6
1	B	51	LYS	2.6
1	B	24	SER	2.6
1	B	27	ASP	2.6
1	A	9	ILE	2.5
1	C	62	ASP	2.5
1	B	61	LYS	2.5
1	A	77	VAL	2.4
1	A	69	GLU	2.4
1	C	64	ALA	2.4
1	B	54	PRO	2.4
1	B	2	LEU	2.4
1	B	8	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	2.3
1	B	6	LYS	2.3
1	C	61	LYS	2.3
1	B	20	ASN	2.3
1	A	13	MET	2.3
1	B	66	VAL	2.2
1	C	49	CYS	2.2
1	C	76	PHE	2.2
1	B	65	HIS	2.2
1	A	52	VAL	2.2
1	A	18	CYS	2.2
1	B	43	HIS	2.1
1	A	60	VAL	2.1
1	A	55	ILE	2.1
1	B	37	CYS	2.1
1	C	14	CYS	2.1
1	C	41	VAL	2.1
1	C	66	VAL	2.1
1	A	63	PRO	2.1
1	B	41	VAL	2.0
1	B	48	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SF4	A	101	8/8	0.12	-0.76	21,22,25,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SF4	B	203	8/8	0.12	-0.90	28,31,35,37	0
2	SF4	C	405	8/8	0.09	-1.12	17,19,23,23	0
2	SF4	C	506	8/8	0.09	-1.13	17,19,23,24	0
2	SF4	A	102	8/8	0.11	-1.30	15,20,27,27	0
2	SF4	B	304	8/8	0.11	-1.45	20,24,26,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.