



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 10:05 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

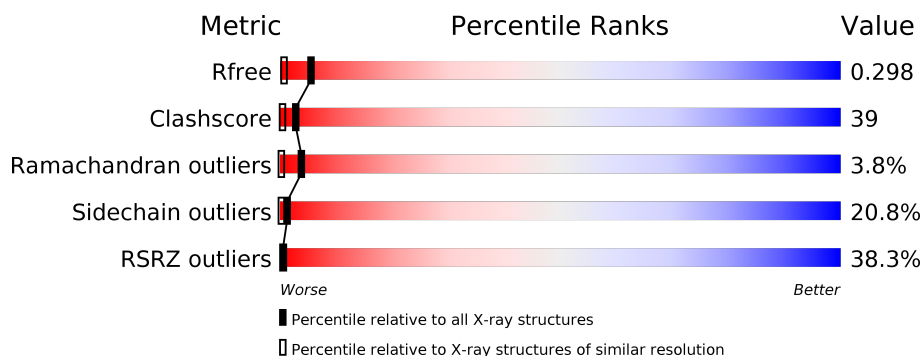
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	100719	1368 (1.66-1.66)
Clashscore	112137	1468 (1.66-1.66)
Ramachandran outliers	110173	1438 (1.66-1.66)
Sidechain outliers	110143	1438 (1.66-1.66)
RSRZ outliers	101464	1371 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	85	<div> <div>33%</div> <div>20% 42% 21% 12% 5%</div> </div>
1	B	85	<div> <div>42%</div> <div>19% 46% 25% 5% 6%</div> </div>
1	C	85	<div> <div>33%</div> <div>26% 32% 31% 6% 6%</div> </div>

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	SF4	B	203	-	-	X	-
2	SF4	C	506	-	-	X	-

2 Entry composition [i](#)

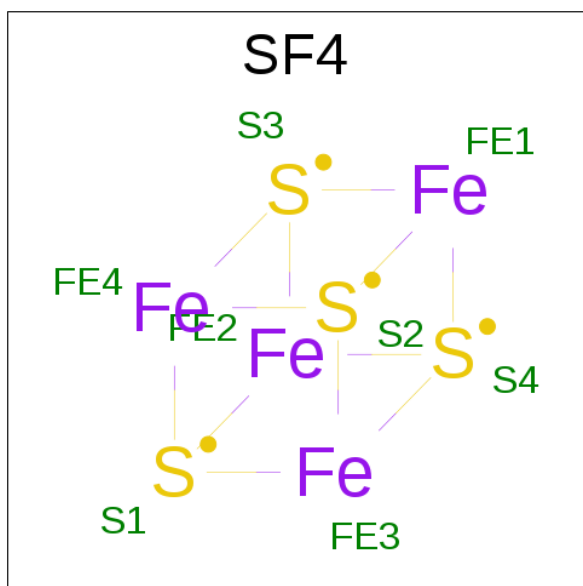
There are 3 unique types of molecules in this entry. The entry contains 2121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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		

Continued on next page...

Continued from previous page...

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		

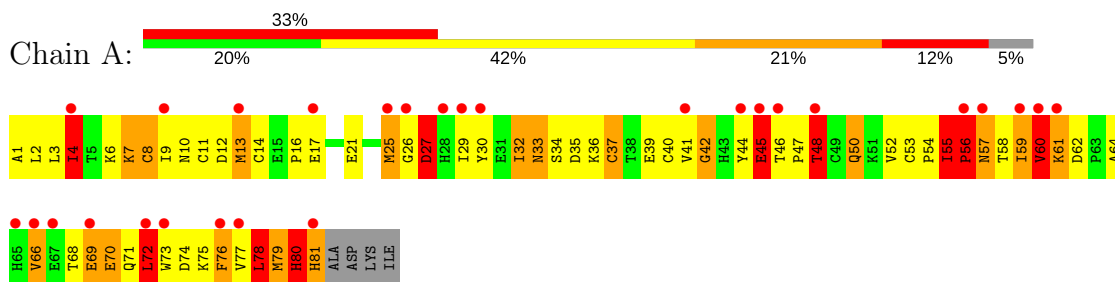
- Molecule 3 is water.

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		

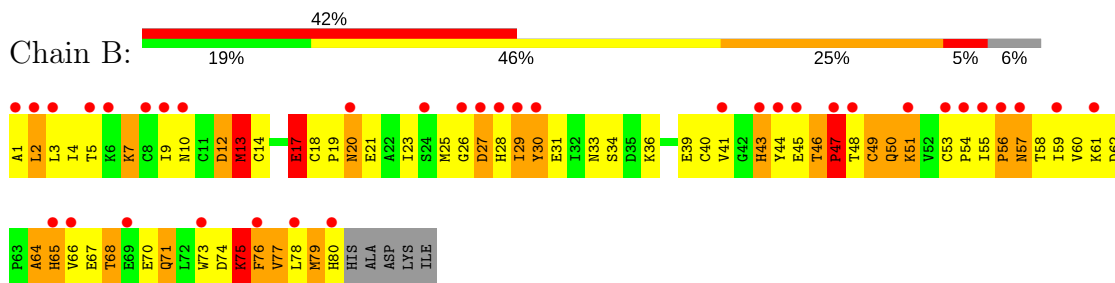
3 Residue-property plots [i](#)

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

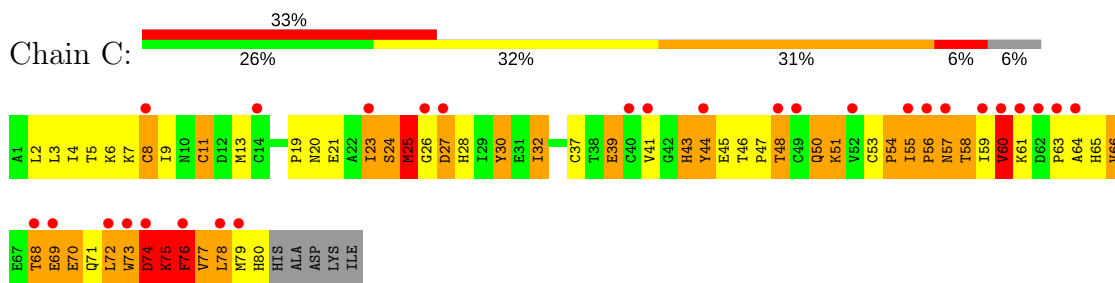
- Molecule 1: Uncharacterized ferredoxin-like protein yfhL



- 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) 99.0 (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 0.222 , 0.298	Depositor DCC
R_{free} test set	1074 reflections (2.90%)	DCC
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 70.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.377 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	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.

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 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	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

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 39.

All (142) 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: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:A:3:LEU:HD22	1:A:61:LYS:HD2	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLU:HB2	1:C:71:GLN:HE21	1.61	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:A:8:CYS:HA	1:A:57:ASN:HD22	1.71	0.56
1:B:46:THR:O	1:B:51:LYS:HE3	2.06	0.56
1:A:61:LYS:HB3	3:A:98:HOH:O	2.05	0.55
1:A:76:PHE:O	1:A:80:HIS:HA	2.06	0.55
1:B:55:ILE:HD12	1:B:55:ILE:O	2.06	0.55
1:A:74:ASP:O	1:A:78:LEU:HD12	2.06	0.54
1:B:41:VAL:CG2	1:B:71:GLN:HE21	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:O	1:B:66:VAL:HG23	2.09	0.51
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:A:3:LEU:HD23	1:A:61:LYS:NZ	2.26	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: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:A:73:TRP:HA	1:A:76:PHE:HD2	1.77	0.49
1:C:68:THR:HA	1:C:71:GLN:HB2	1.95	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:A:17:GLU:OE2	1:A:48:THR:HG21	2.15	0.47
1:C:66:VAL:CG2	1:C:70:GLU:HB3	2.40	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:A:39:GLU:HA	2:A:102:SF4:S4	2.55	0.46
1:B:19:PRO:HB2	1:B:43:HIS:ND1	2.30	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:A:45:GLU:OE1	1:A:46:THR:N	2.49	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:7:LYS:O	1:A:57:ASN:ND2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:A:57:ASN:OD1	2.47	0.44
1:C:59:ILE:HG22	1:C:60:VAL:O	2.18	0.44
1:A:60:VAL:O	1:A:61:LYS:HG2	2.16	0.44
1:B:47:PRO:HB2	1:B:50:GLN:HB2	2.00	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:B:20:ASN:HD22	1:B:79:MET:HE2	1.84	0.43
1:C:53:CYS:HA	1:C:54:PRO:HD2	1.69	0.43
1:A:1:ALA:HB1	1:A:37:CYS:HB3	2.00	0.43
1:A:9:ILE:HG12	1:A:55:ILE:CD1	2.49	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:A:10:ASN:OD1	1:A:29:ILE:HA	2.20	0.41
1:C:9:ILE:CD1	1:C:55:ILE:HD11	2.49	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:A:61:LYS:O	1:A:64:ALA:N	2.50	0.40
1:C:74:ASP:O	1:C:78:LEU:HD12	2.20	0.40
1:A:56:PRO:HD3	3:A:114:HOH:O	2.20	0.40
1:B:75:LYS:HG3	1:B:76:PHE:N	2.30	0.40
1:B:77:VAL:H	1:B:77:VAL:HG22	1.60	0.40
1:C:46:THR:OG1	1:C:51:LYS:HD2	2.22	0.40
1:B:29:ILE:HD13	1:B:29:ILE:H	1.86	0.40
1:B:2:LEU:O	1:B:61:LYS:HE2	2.22	0.40
1:C:26:GLY:O	1:C:28:HIS:N	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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 [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	79/85 (93%)	67 (85%)	8 (10%)	4 (5%)	2	0
1	B	78/85 (92%)	64 (82%)	12 (15%)	2 (3%)	6	0
1	C	78/85 (92%)	67 (86%)	8 (10%)	3 (4%)	4	0
All	All	235/255 (92%)	198 (84%)	28 (12%)	9 (4%)	4	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%)	1	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 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

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	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	A	102	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	203	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	B	304	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	405	1	0,12,12	0.00	-	0,24,24	0.00	-
2	SF4	C	506	1	0,12,12	0.00	-	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	0/6/5/5
2	SF4	A	102	1	-	0/0/48/48	0/6/5/5
2	SF4	B	203	1	-	0/0/48/48	0/6/5/5
2	SF4	B	304	1	-	0/0/48/48	0/6/5/5
2	SF4	C	405	1	-	0/0/48/48	0/6/5/5
2	SF4	C	506	1	-	0/0/48/48	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	102	SF4	1	0
2	B	203	SF4	2	0
2	C	405	SF4	1	0
2	C	506	SF4	3	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

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%)	1.78	28 (34%) 0 0	15, 26, 37, 49	1 (1%)
1	B	80/85 (94%)	1.97	36 (45%) 0 0	15, 29, 40, 55	3 (3%)
1	C	79/85 (92%)	1.71	28 (35%) 0 0	16, 26, 38, 48	3 (3%)
All	All	240/255 (94%)	1.82	92 (38%) 0 0	15, 27, 39, 55	7 (2%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	TRP	6.9
1	B	30	TYR	6.0
1	C	57	ASN	5.5
1	B	44	TYR	5.1
1	A	56	PRO	4.9
1	B	73	TRP	4.8
1	C	27	ASP	4.7
1	A	26	GLY	4.6
1	B	55	ILE	4.6
1	B	57	ASN	4.6
1	C	48	THR	4.6
1	A	57	ASN	4.4
1	A	76	PHE	4.4
1	B	80	HIS	4.3
1	A	30	TYR	4.3
1	A	41	VAL	4.2
1	A	44	TYR	4.1
1	A	81	HIS	4.1
1	C	72	LEU	4.0
1	C	26	GLY	3.9
1	B	56	PRO	3.9
1	C	8	CYS	3.9
1	C	59	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	10	ASN	3.9
1	B	26	GLY	3.7
1	C	69	GLU	3.6
1	A	28	HIS	3.6
1	C	68	THR	3.6
1	B	78	LEU	3.5
1	B	45	GLU	3.4
1	A	17	GLU	3.4
1	B	76	PHE	3.3
1	C	55	ILE	3.2
1	C	79	MET	3.2
1	A	25	MET	3.2
1	C	44	TYR	3.2
1	A	4	ILE	3.1
1	B	28	HIS	3.1
1	A	66	VAL	3.0
1	B	3	LEU	3.0
1	C	52	VAL	2.9
1	A	9	ILE	2.9
1	A	29	ILE	2.9
1	B	8	CYS	2.8
1	A	65	HIS	2.8
1	C	23	ILE	2.8
1	C	56	PRO	2.8
1	C	61	LYS	2.8
1	A	72	LEU	2.7
1	A	45	GLU	2.7
1	B	69	GLU	2.7
1	B	54	PRO	2.7
1	A	77	VAL	2.7
1	C	64	ALA	2.7
1	C	60	VAL	2.7
1	B	9	ILE	2.6
1	B	59	ILE	2.6
1	B	2	LEU	2.6
1	B	48	THR	2.6
1	B	41	VAL	2.6
1	A	61	LYS	2.6
1	B	27	ASP	2.6
1	A	13	MET	2.6
1	B	1	ALA	2.5
1	B	53	CYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	46	THR	2.5
1	B	61	LYS	2.5
1	B	65	HIS	2.4
1	A	59	ILE	2.4
1	B	66	VAL	2.4
1	A	73	TRP	2.3
1	A	69	GLU	2.3
1	C	49	CYS	2.3
1	B	47	PRO	2.3
1	B	51	LYS	2.3
1	C	14	CYS	2.3
1	B	6	LYS	2.2
1	C	76	PHE	2.2
1	A	60	VAL	2.1
1	B	5	THR	2.1
1	C	40	CYS	2.1
1	C	41	VAL	2.1
1	C	62	ASP	2.1
1	C	74	ASP	2.1
1	B	43	HIS	2.1
1	A	67	GLU	2.1
1	B	29	ILE	2.1
1	C	78	LEU	2.0
1	B	24	SER	2.0
1	A	48	THR	2.0
1	B	20	ASN	2.0
1	C	63	PRO	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SF4	A	101	8/8	0.97	0.12	-0.64	21,22,25,29	0
2	SF4	B	203	8/8	0.93	0.13	-0.95	28,31,35,37	0
2	SF4	B	304	8/8	0.97	0.11	-1.15	20,24,26,31	0
2	SF4	C	405	8/8	0.98	0.09	-1.16	17,19,23,23	0
2	SF4	A	102	8/8	0.98	0.11	-1.16	15,20,27,27	0
2	SF4	C	506	8/8	0.98	0.08	-1.28	17,19,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.