



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:21 AM UTC

PDB ID : 5FRT / pdb_00005frt
Title : Structure of the FeSII (shethna) protein of Azotobacter vinelandii
Authors : Kabasakal, B.V.; Cotton, C.A.R.; Lieber, L.; Murray, J.W.
Deposited on : 2015-12-22
Resolution : 2.34 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	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

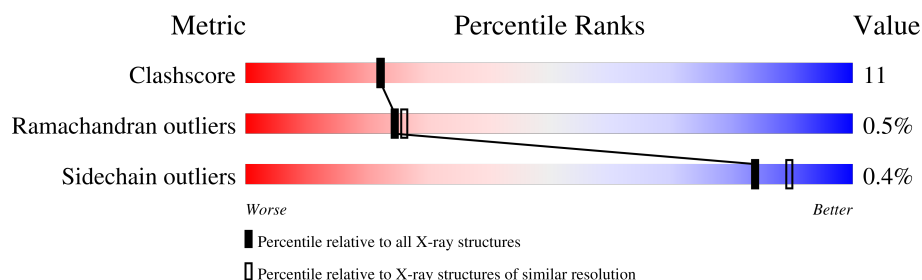
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	122	 80% 17% .
1	B	122	 80% 16% ..
1	C	122	 66% 31% ..
1	D	122	 75% 20% ..
1	E	122	 71% 14% . 14%

2 Entry composition [i](#)

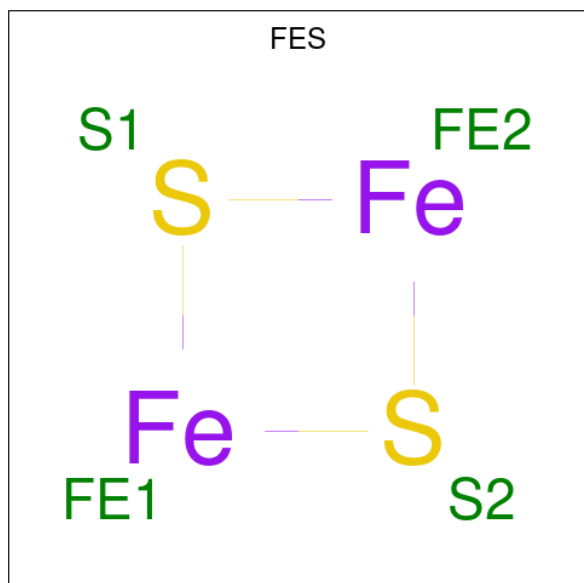
There are 3 unique types of molecules in this entry. The entry contains 4425 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DIMERIC (2FE-2S) PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			893	560	152	175	6			
1	B	119	Total	C	N	O	S	0	0	0
			901	563	157	175	6			
1	C	119	Total	C	N	O	S	0	0	0
			895	560	154	175	6			
1	D	119	Total	C	N	O	S	0	0	0
			884	556	149	173	6			
1	E	105	Total	C	N	O	S	0	0	0
			780	489	133	152	6			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total 18	O 18	0	0
3	B	12	Total 12	O 12	0	0
3	C	5	Total 5	O 5	0	0
3	D	10	Total 10	O 10	0	0
3	E	7	Total 7	O 7	0	0

3 Residue-property plots [i](#)

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. 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 failed to run properly.

• Molecule 1: DIMERIC (2FE-2S) PROTEIN

Chain A: 



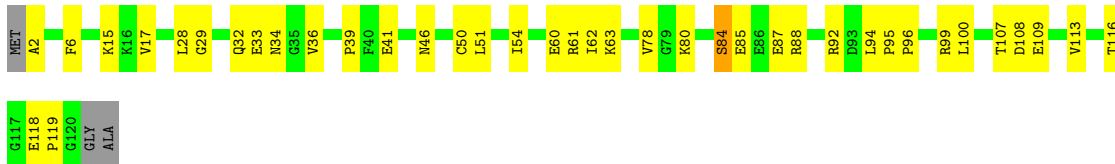
• Molecule 1: DIMERIC (2FE-2S) PROTEIN

Chain B: 



• Molecule 1: DIMERIC (2FE-2S) PROTEIN

Chain C: 



• Molecule 1: DIMERIC (2FE-2S) PROTEIN

Chain D: 



• Molecule 1: DIMERIC (2FE-2S) PROTEIN

Chain E: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.56Å 134.53Å 36.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.27 – 2.34	Depositor
% Data completeness (in resolution range)	99.8 (67.27-2.34)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.252	Depositor
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.363	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
Total number of atoms	4425	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

5.1 Standard geometry

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

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	0.26	0/906	0.53	0/1226
1	B	0.22	0/914	0.54	0/1236
1	C	0.36	0/908	0.84	3/1229 (0.2%)
1	D	0.41	1/897 (0.1%)	0.67	1/1215 (0.1%)
1	E	0.26	0/791	0.65	0/1069
All	All	0.31	1/4416 (0.0%)	0.65	4/5975 (0.1%)

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	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	GLU	CD-OE1	-5.51	1.14	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ARG	CG-CD-NE	-12.21	85.13	112.00
1	D	81	LEU	CA-CB-CG	6.92	140.53	116.30
1	C	92	ARG	N-CA-CB	-6.07	101.15	110.13
1	C	92	ARG	CD-NE-CZ	5.29	131.81	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	64	GLY	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	893	0	895	12	0
1	B	901	0	906	16	0
1	C	895	0	895	32	0
1	D	884	0	882	28	0
1	E	780	0	772	12	0
2	A	4	0	0	1	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
3	A	18	0	0	0	0
3	B	12	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
3	E	7	0	0	0	0
All	All	4425	0	4350	92	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 11.

All (92) 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:C:15:LYS:HZ1	1:C:34:ASN:HB2	1.49	0.78
1:C:2:ALA:N	1:C:108:ASP:O	2.19	0.76
1:B:85:GLU:OE2	1:B:88:ARG:NH1	2.18	0.75
1:C:15:LYS:HE3	1:C:17:VAL:CG2	2.18	0.74
1:A:94:LEU:HD12	1:A:95:PRO:HD2	1.70	0.73
1:D:76:LYS:HA	1:D:76:LYS:HE2	1.71	0.73
1:C:15:LYS:NZ	1:C:34:ASN:HB2	2.05	0.71
1:C:29:GLY:O	1:C:33:GLU:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:LEU:HD12	1:D:95:PRO:HD2	1.79	0.65
1:C:15:LYS:HE3	1:C:17:VAL:HG21	1.77	0.64
1:E:65:MET:O	1:E:66:LEU:HB2	1.96	0.63
1:B:94:LEU:HD12	1:B:95:PRO:HD2	1.82	0.62
1:C:61:ARG:HG2	1:C:62:ILE:HD12	1.82	0.62
1:C:100:LEU:HD12	1:D:71:GLU:HG3	1.83	0.60
1:C:15:LYS:HE3	1:C:17:VAL:HG23	1.82	0.60
1:D:10:LEU:HD12	1:D:11:MET:HG3	1.85	0.59
1:D:28:LEU:O	1:D:32:GLN:HG2	2.01	0.59
1:D:41:GLU:OE2	1:D:49:SER:CB	2.51	0.59
1:D:54:ILE:HD12	1:D:99:ARG:HG3	1.86	0.57
1:C:87:GLU:HG3	1:C:88:ARG:N	2.20	0.57
1:D:76:LYS:HE3	1:D:81:LEU:HB3	1.86	0.56
1:D:78:VAL:HG12	1:D:80:LYS:HG2	1.87	0.56
1:C:54:ILE:HD12	1:C:99:ARG:HG3	1.88	0.56
1:A:58:ASP:CG	1:A:110:ASP:H	2.14	0.55
1:C:15:LYS:NZ	1:C:36:VAL:HG23	2.22	0.54
1:C:94:LEU:HD12	1:C:95:PRO:HD2	1.90	0.54
1:C:54:ILE:HG12	1:C:113:VAL:HG12	1.90	0.54
1:B:41:GLU:OE2	1:B:119:PRO:HB3	2.08	0.53
1:C:15:LYS:HZ1	1:C:34:ASN:CB	2.17	0.53
1:D:65:MET:HE2	1:D:67:LEU:HB2	1.91	0.53
1:C:84:SER:HA	1:C:87:GLU:HG2	1.89	0.53
1:D:65:MET:CE	1:D:67:LEU:HB2	2.39	0.52
1:B:78:VAL:HG23	1:B:80:LYS:HB2	1.91	0.52
1:E:73:ASN:HA	1:E:76:LYS:HG2	1.90	0.52
1:B:75:LEU:HA	1:B:78:VAL:HG22	1.91	0.52
1:C:60:GLU:HG3	1:C:63:LYS:HA	1.93	0.51
1:D:41:GLU:CD	1:D:49:SER:CB	2.83	0.51
1:A:69:ASP:OD1	1:A:72:ARG:NH2	2.44	0.50
1:B:43:GLN:NE2	1:E:66:LEU:O	2.44	0.50
1:A:20:VAL:C	1:A:22:GLY:H	2.19	0.49
1:C:85:GLU:OE2	1:C:88:ARG:NH1	2.45	0.49
1:D:76:LYS:HE3	1:D:81:LEU:CB	2.41	0.49
1:D:71:GLU:O	1:D:75:LEU:HG	2.12	0.49
1:E:26:THR:HG22	1:E:29:GLY:H	1.79	0.48
1:C:28:LEU:O	1:C:32:GLN:HG2	2.14	0.47
1:E:47:CYS:SG	1:E:48:GLY:N	2.87	0.47
1:C:6:PHE:CG	1:C:36:VAL:HG21	2.50	0.47
1:C:51:LEU:HD21	1:D:80:LYS:HD2	1.96	0.47
1:D:41:GLU:HG2	1:D:47:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLU:OE2	1:D:49:SER:HB3	2.13	0.47
1:D:50:CYS:SG	1:D:100:LEU:HB3	2.55	0.47
1:A:8:SER:HB3	1:A:11:MET:HE2	1.97	0.47
1:C:78:VAL:HG23	1:C:80:LYS:HB2	1.97	0.47
1:D:41:GLU:OE2	1:D:49:SER:HB2	2.14	0.46
1:A:78:VAL:HG23	1:A:80:LYS:HB2	1.98	0.46
1:B:26:THR:HG22	1:B:29:GLY:H	1.81	0.46
1:B:40:PHE:CE2	1:E:66:LEU:HB3	2.51	0.46
1:D:61:ARG:HG3	1:D:94:LEU:HD13	1.97	0.46
1:D:8:SER:HB3	1:D:11:MET:HE2	1.98	0.46
1:C:116:THR:HG21	1:C:118:GLU:OE2	2.15	0.45
1:D:70:LYS:HD3	1:D:70:LYS:HA	1.70	0.45
1:A:41:GLU:HB2	1:A:47:CYS:SG	2.56	0.45
1:A:118:GLU:O	1:A:120:GLY:N	2.50	0.44
1:C:15:LYS:NZ	1:C:34:ASN:CB	2.77	0.44
1:D:85:GLU:OE1	1:D:85:GLU:HA	2.16	0.44
1:C:107:THR:OG1	1:C:109:GLU:HG2	2.16	0.44
1:B:50:CYS:SG	1:B:100:LEU:HB3	2.58	0.44
1:A:41:GLU:HG2	1:A:49:SER:CB	2.48	0.44
1:C:46:ASN:HA	1:D:74:VAL:HG21	2.00	0.43
1:B:41:GLU:HG2	1:E:70:LYS:HE3	1.99	0.43
1:E:8:SER:HB3	1:E:11:MET:HE2	2.00	0.43
1:B:8:SER:HB3	1:B:11:MET:HE2	2.01	0.43
1:C:41:GLU:OE2	1:C:119:PRO:CB	2.67	0.43
1:C:99:ARG:HD2	1:D:67:LEU:HD21	2.01	0.43
1:E:40:PHE:CD1	1:E:40:PHE:O	2.72	0.43
1:E:40:PHE:O	1:E:41:GLU:C	2.61	0.42
1:C:50:CYS:SG	1:C:100:LEU:HB3	2.59	0.42
1:C:39:PRO:HB3	1:C:119:PRO:HA	2.02	0.42
1:D:70:LYS:O	1:D:74:VAL:HG23	2.20	0.42
1:A:58:ASP:OD1	1:A:109:GLU:HB2	2.20	0.42
1:D:42:CYS:HB3	1:D:47:CYS:HB3	2.01	0.42
1:B:26:THR:HG22	1:B:28:LEU:N	2.34	0.42
1:B:28:LEU:HD21	1:B:40:PHE:CD1	2.55	0.42
1:B:54:ILE:HD12	1:B:99:ARG:HG3	2.00	0.41
1:B:24:ARG:H	1:B:24:ARG:HG2	1.64	0.41
1:E:50:CYS:O	1:E:52:VAL:HG13	2.21	0.41
1:C:95:PRO:HA	1:C:96:PRO:HD3	2.00	0.41
1:C:99:ARG:NE	1:D:67:LEU:HD21	2.35	0.41
1:A:47:CYS:O	2:A:5000:FES:S1	2.79	0.40
1:B:26:THR:HG22	1:B:28:LEU:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HD12	1:A:99:ARG:HG3	2.03	0.40
1:E:50:CYS:HB2	1:E:101:ALA:HB3	2.04	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	117/122 (96%)	114 (97%)	2 (2%)	1 (1%)	14	13
1	B	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
1	C	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
1	D	117/122 (96%)	115 (98%)	2 (2%)	0	100	100
1	E	101/122 (83%)	88 (87%)	11 (11%)	2 (2%)	6	3
All	All	569/610 (93%)	544 (96%)	22 (4%)	3 (0%)	24	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	42	CYS
1	E	65	MET
1	A	119	PRO

5.3.2 Protein sidechains [i](#)

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	99/103 (96%)	99 (100%)	0	100	100
1	B	100/103 (97%)	99 (99%)	1 (1%)	68	79
1	C	99/103 (96%)	98 (99%)	1 (1%)	68	79
1	D	97/103 (94%)	97 (100%)	0	100	100
1	E	86/103 (84%)	86 (100%)	0	100	100
All	All	481/515 (93%)	479 (100%)	2 (0%)	84	89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	26	THR
1	C	84	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	56	HIS
1	D	56	HIS

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](#)

5 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	FES	E	5000	1	0,4,4	-	-	-		
2	FES	B	5000	1	0,4,4	-	-	-		
2	FES	D	5000	1	0,4,4	-	-	-		
2	FES	C	5000	1	0,4,4	-	-	-		
2	FES	A	5000	1	0,4,4	-	-	-		

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	FES	E	5000	1	-	-	0/1/1/1
2	FES	B	5000	1	-	-	0/1/1/1
2	FES	D	5000	1	-	-	0/1/1/1
2	FES	C	5000	1	-	-	0/1/1/1
2	FES	A	5000	1	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5000	FES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.