



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:57 PM GMT

PDB ID : 1DE0
Title : MODULATING THE MIDPOINT POTENTIAL OF THE [4FE-4S] CLUSTER OF THE NITROGENASE FE PROTEIN
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Deposited on : 1999-11-12
Resolution : 2.40 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

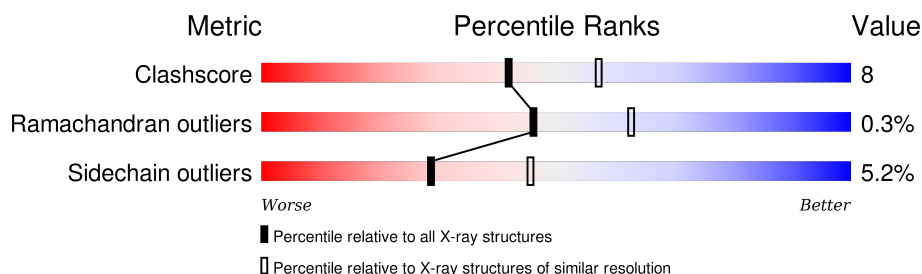
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	289	 78% 20% •
1	B	289	 77% 19% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4612 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.

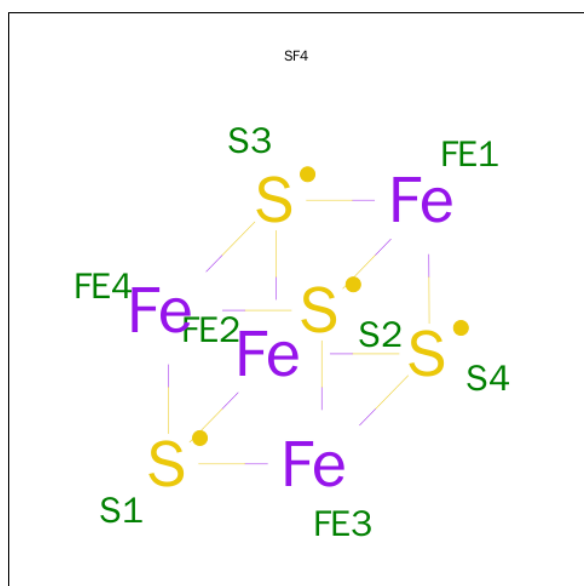
- Molecule 1 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2190	1366	370	433	21			
1	B	289	Total	C	N	O	S	0	0	0
			2190	1366	370	433	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	TRP	PHE	ENGINEERED	UNP P00459
B	135	TRP	PHE	ENGINEERED	UNP P00459

- 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		

- Molecule 3 is water.

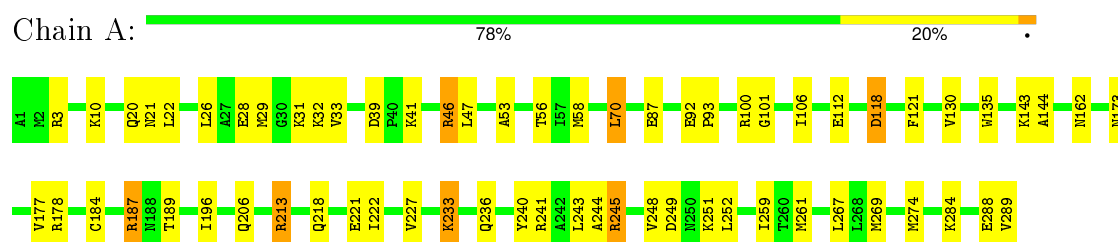
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total 122	O 122	0	0
3	B	102	Total 102	O 102	0	0

3 Residue-property plots

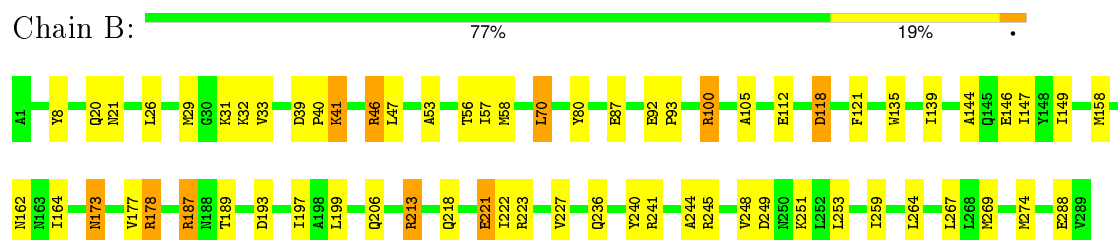
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: NITROGENASE IRON PROTEIN



• Molecule 1: NITROGENASE IRON PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.54Å 91.05Å 63.35Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4612	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/2215	1.54	21/2984 (0.7%)
1	B	0.66	0/2215	1.52	19/2984 (0.6%)
All	All	0.66	0/4430	1.53	40/5968 (0.7%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	ARG	NE-CZ-NH2	-22.28	109.16	120.30
1	B	245	ARG	CD-NE-CZ	21.79	154.10	123.60
1	A	245	ARG	CD-NE-CZ	21.70	153.97	123.60
1	A	100	ARG	CD-NE-CZ	21.66	153.93	123.60
1	B	100	ARG	CD-NE-CZ	21.66	153.93	123.60
1	B	100	ARG	NE-CZ-NH1	-21.41	109.59	120.30
1	B	245	ARG	NE-CZ-NH1	-20.85	109.88	120.30
1	B	245	ARG	NE-CZ-NH2	19.97	130.28	120.30
1	A	245	ARG	NE-CZ-NH2	-19.91	110.35	120.30
1	A	245	ARG	NE-CZ-NH1	19.90	130.25	120.30
1	A	100	ARG	NE-CZ-NH1	19.53	130.07	120.30
1	B	100	ARG	NE-CZ-NH2	18.90	129.75	120.30
1	A	135	TRP	CD1-CG-CD2	8.62	113.19	106.30
1	A	249	ASP	N-CA-CB	-8.32	95.63	110.60
1	B	135	TRP	CD1-CG-CD2	8.32	112.95	106.30
1	A	135	TRP	CE2-CD2-CG	-7.85	101.02	107.30
1	A	70	LEU	CA-CB-CG	7.67	132.94	115.30
1	B	70	LEU	CA-CB-CG	7.46	132.47	115.30
1	B	135	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B	178	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	46	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	187	ARG	NE-CZ-NH1	6.64	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	178	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	241	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	B	249	ASP	N-CA-CB	-6.25	99.35	110.60
1	B	241	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	46	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	241	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	29	MET	CA-CB-CG	5.64	122.89	113.30
1	A	3	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	135	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	A	241	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	B	135	TRP	CG-CD2-CE3	5.12	138.51	133.90
1	B	249	ASP	CA-CB-CG	5.10	124.63	113.40
1	B	29	MET	CA-CB-CG	5.08	121.94	113.30
1	A	252	LEU	CA-CB-CG	5.05	126.93	115.30
1	A	135	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	B	221	GLU	CA-CB-CG	5.01	124.43	113.40
1	A	249	ASP	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

There are no planarity outliers.

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	2190	0	2198	36	0
1	B	2190	0	2198	41	0
2	A	8	0	0	0	0
3	A	122	0	0	7	0
3	B	102	0	0	6	0
All	All	4612	0	4396	74	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 8.

All (74) 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:193:ASP:O	1:B:197:ILE:HG12	1.91	0.71
1:B:21:ASN:HD21	1:B:227:VAL:H	1.39	0.69
1:B:162:ASN:HD21	1:B:259:ILE:H	1.42	0.67
1:B:26:LEU:HD13	1:B:244:ALA:HB1	1.77	0.65
1:A:92:GLU:HG3	3:A:349:HOH:O	1.97	0.64
1:A:20:GLN:HE22	1:A:47:LEU:H	1.46	0.63
1:A:187:ARG:HA	1:A:213:ARG:NH1	2.14	0.63
1:A:21:ASN:HD21	1:A:227:VAL:H	1.45	0.62
1:B:20:GLN:HE22	1:B:47:LEU:H	1.48	0.61
1:A:10:LYS:HE3	3:A:385:HOH:O	2.00	0.61
1:B:187:ARG:HG3	1:B:189:THR:HG23	1.82	0.60
1:A:187:ARG:HG3	1:A:189:THR:HG23	1.83	0.59
1:B:146:GLU:HG2	1:B:253:LEU:HD11	1.85	0.58
1:A:162:ASN:HD21	1:A:259:ILE:H	1.52	0.57
1:A:26:LEU:HD13	1:A:244:ALA:HB1	1.86	0.57
1:B:187:ARG:HA	1:B:213:ARG:NH1	2.19	0.57
1:A:251:LYS:HE3	3:A:403:HOH:O	2.05	0.56
1:A:46:ARG:HD2	1:A:53:ALA:HA	1.87	0.56
1:B:46:ARG:HD2	1:B:53:ALA:HA	1.88	0.55
1:A:101:GLY:HA3	3:A:404:HOH:O	2.06	0.54
1:B:21:ASN:HD21	1:B:227:VAL:N	2.05	0.53
1:A:269:MET:HG3	1:A:274:MET:HB3	1.90	0.53
1:B:173:ASN:HB2	3:B:363:HOH:O	2.09	0.53
1:B:269:MET:HG3	1:B:274:MET:HB3	1.90	0.52
1:B:213:ARG:HG2	3:B:338:HOH:O	2.09	0.52
1:A:33:VAL:HG22	1:A:121:PHE:HB2	1.92	0.52
1:B:162:ASN:HD21	1:B:259:ILE:N	2.09	0.51
1:B:139:ILE:HG12	1:B:147:ILE:HD11	1.92	0.51
1:B:178:ARG:HB2	1:B:253:LEU:HD12	1.93	0.50
1:B:32:LYS:HG2	1:B:118:ASP:O	2.12	0.49
1:A:118:ASP:HA	3:A:294:HOH:O	2.12	0.49
1:A:21:ASN:HD21	1:A:227:VAL:N	2.10	0.49
1:A:233:LYS:HE2	3:B:345:HOH:O	2.11	0.49
1:A:106:ILE:HG21	1:A:143:LYS:HD2	1.95	0.48
1:B:33:VAL:HG22	1:B:121:PHE:HB2	1.95	0.48
1:A:32:LYS:HG2	1:A:118:ASP:O	2.12	0.48
1:B:269:MET:HE1	3:B:344:HOH:O	2.13	0.48
1:B:144:ALA:O	1:B:177:VAL:HG12	2.14	0.48
1:A:28:GLU:HA	3:A:405:HOH:O	2.13	0.48
1:B:187:ARG:HA	1:B:213:ARG:HH12	1.79	0.47
1:B:100:ARG:HB2	3:B:347:HOH:O	2.13	0.47
1:A:22:LEU:HD13	1:A:243:LEU:HG	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:MET:HG2	1:B:199:LEU:HD22	1.96	0.46
1:A:244:ALA:O	1:A:248:VAL:HG23	2.16	0.46
1:A:144:ALA:O	1:A:177:VAL:HG12	2.15	0.46
1:B:92:GLU:HA	1:B:93:PRO:HD3	1.87	0.46
1:A:130:VAL:HG22	1:B:40:PRO:HG2	1.97	0.46
1:B:57:ILE:HD12	1:B:105:ALA:HB1	1.97	0.45
1:A:92:GLU:HA	1:A:93:PRO:HD3	1.87	0.45
1:B:236:GLN:HG3	1:B:240:TYR:CE2	2.52	0.45
1:B:244:ALA:O	1:B:248:VAL:HG23	2.17	0.44
1:A:10:LYS:HB2	1:A:10:LYS:HE2	1.85	0.44
1:A:261:MET:HG2	3:A:400:HOH:O	2.17	0.44
1:B:80:TYR:HA	3:B:300:HOH:O	2.18	0.43
1:A:187:ARG:HA	1:A:213:ARG:HH12	1.84	0.43
1:A:289:VAL:HB	1:B:223:ARG:HH12	1.84	0.43
1:A:236:GLN:HG3	1:A:240:TYR:CE2	2.54	0.42
1:B:56:THR:HA	1:B:87:GLU:O	2.19	0.42
1:A:56:THR:HA	1:A:87:GLU:O	2.18	0.42
1:B:8:TYR:O	1:B:149:ILE:HA	2.19	0.42
1:A:218:GLN:HA	1:A:221:GLU:HG2	2.01	0.42
1:B:218:GLN:HA	1:B:221:GLU:HG2	2.02	0.42
1:A:162:ASN:HD21	1:A:259:ILE:N	2.18	0.42
1:A:184:CYS:HB2	1:A:196:ILE:HG21	2.01	0.42
1:B:26:LEU:O	1:B:31:LYS:HB2	2.20	0.41
1:B:253:LEU:HA	1:B:253:LEU:HD13	1.95	0.41
1:A:26:LEU:O	1:A:31:LYS:HB2	2.20	0.41
1:B:173:ASN:HD22	1:B:173:ASN:H	1.69	0.41
1:A:284:LYS:O	1:B:223:ARG:HD3	2.21	0.40
1:B:158:MET:HB3	1:B:264:LEU:HD11	2.03	0.40
1:B:8:TYR:HB3	1:B:164:ILE:HD13	2.03	0.40
1:B:41:LYS:HD3	1:B:41:LYS:H	1.87	0.40
1:A:20:GLN:HE22	1:A:47:LEU:N	2.17	0.40
1:B:251:LYS:HD3	1:B:251:LYS:HA	1.94	0.40

There are no symmetry-related clashes.

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	287/289 (99%)	276 (96%)	10 (4%)	1 (0%)	46	63
1	B	287/289 (99%)	278 (97%)	8 (3%)	1 (0%)	46	63
All	All	574/578 (99%)	554 (96%)	18 (3%)	2 (0%)	46	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ASP
1	B	118	ASP

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	233/233 (100%)	220 (94%)	13 (6%)	26	41
1	B	233/233 (100%)	222 (95%)	11 (5%)	32	50
All	All	466/466 (100%)	442 (95%)	24 (5%)	29	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	41	LYS
1	A	58	MET
1	A	70	LEU
1	A	112	GLU
1	A	173	ASN
1	A	206	GLN
1	A	213	ARG
1	A	222	ILE
1	A	233	LYS

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Mol	Chain	Res	Type
1	A	245	ARG
1	A	267	LEU
1	A	288	GLU
1	B	39	ASP
1	B	41	LYS
1	B	58	MET
1	B	70	LEU
1	B	112	GLU
1	B	173	ASN
1	B	206	GLN
1	B	213	ARG
1	B	222	ILE
1	B	267	LEU
1	B	288	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	ASN
1	A	142	ASN
1	A	145	GLN
1	A	162	ASN
1	A	173	ASN
1	A	188	ASN
1	A	218	GLN
1	B	20	GLN
1	B	21	ASN
1	B	142	ASN
1	B	145	GLN
1	B	162	ASN
1	B	173	ASN
1	B	188	ASN
1	B	206	GLN
1	B	218	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	290	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	290	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.