



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:33 AM UTC

PDB ID : 4YIP / pdb_00004yip
Title : X-ray structure of the iron/manganese cambialistic superoxide dismutase from *Streptococcus mutans*
Authors : Russo Krauss, I.; Merlino, A.; Pica, A.; Sica, F.
Deposited on : 2015-03-02
Resolution : 2.15 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
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

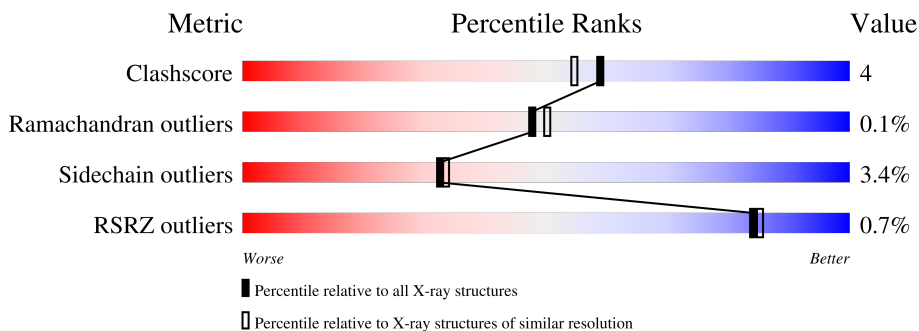
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	210	 82% 13% . .
1	B	210	 86% 10% .
1	C	210	 84% 10% . .
1	D	210	 83% 13% .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6699 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 Superoxide dismutase [Mn/Fe].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	203	Total 1615	C 1042	N 266	O 306	S 1	0	2	0
1	B	203	Total 1607	C 1036	N 265	O 305	S 1	0	1	0
1	C	201	Total 1586	C 1022	N 263	O 300	S 1	0	0	0
1	D	203	Total 1609	C 1037	N 265	O 306	S 1	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	LEU	-	expression tag	UNP P09738
A	203	GLU	-	expression tag	UNP P09738
A	204	HIS	-	expression tag	UNP P09738
A	205	HIS	-	expression tag	UNP P09738
A	206	HIS	-	expression tag	UNP P09738
A	207	HIS	-	expression tag	UNP P09738
A	208	HIS	-	expression tag	UNP P09738
A	209	HIS	-	expression tag	UNP P09738
B	202	LEU	-	expression tag	UNP P09738
B	203	GLU	-	expression tag	UNP P09738
B	204	HIS	-	expression tag	UNP P09738
B	205	HIS	-	expression tag	UNP P09738
B	206	HIS	-	expression tag	UNP P09738
B	207	HIS	-	expression tag	UNP P09738
B	208	HIS	-	expression tag	UNP P09738
B	209	HIS	-	expression tag	UNP P09738
C	202	LEU	-	expression tag	UNP P09738
C	203	GLU	-	expression tag	UNP P09738
C	204	HIS	-	expression tag	UNP P09738
C	205	HIS	-	expression tag	UNP P09738
C	206	HIS	-	expression tag	UNP P09738

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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	HIS	-	expression tag	UNP P09738
C	208	HIS	-	expression tag	UNP P09738
C	209	HIS	-	expression tag	UNP P09738
D	202	LEU	-	expression tag	UNP P09738
D	203	GLU	-	expression tag	UNP P09738
D	204	HIS	-	expression tag	UNP P09738
D	205	HIS	-	expression tag	UNP P09738
D	206	HIS	-	expression tag	UNP P09738
D	207	HIS	-	expression tag	UNP P09738
D	208	HIS	-	expression tag	UNP P09738
D	209	HIS	-	expression tag	UNP P09738

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

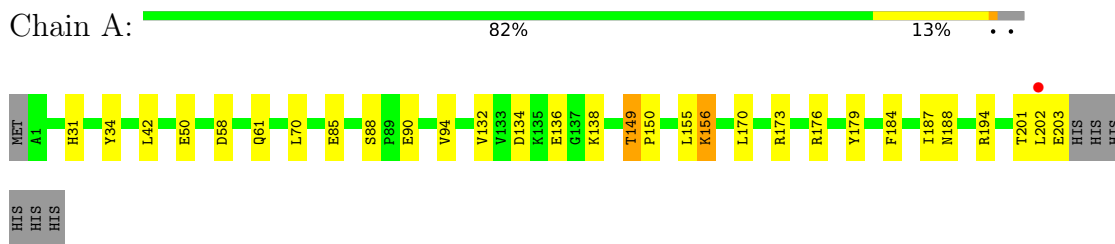
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	71	Total O 72 72	0	1
3	B	70	Total O 70 70	0	0
3	C	65	Total O 65 65	0	0
3	D	71	Total O 71 71	0	0

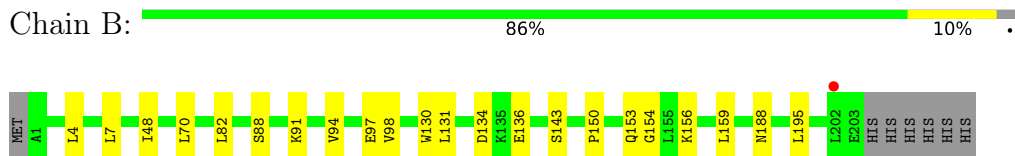
3 Residue-property plots [i](#)

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 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.

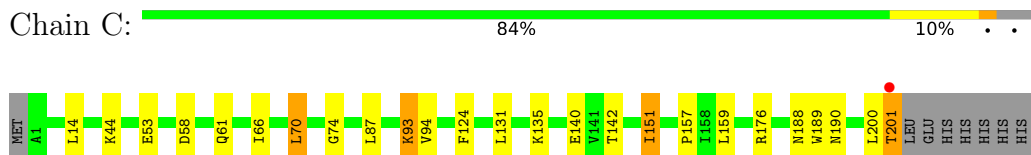
- Molecule 1: Superoxide dismutase [Mn/Fe]



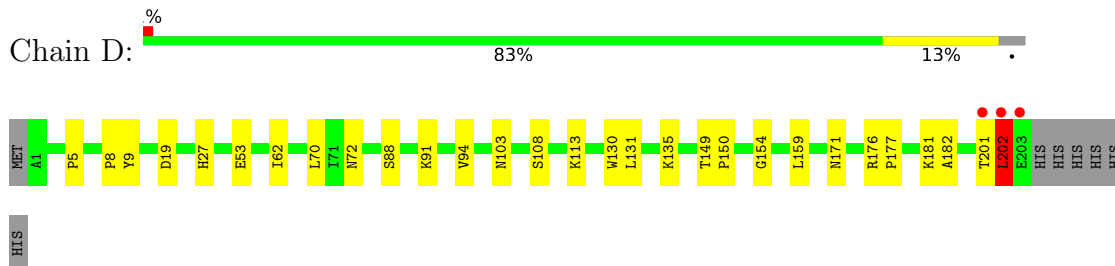
- Molecule 1: Superoxide dismutase [Mn/Fe]



- Molecule 1: Superoxide dismutase [Mn/Fe]



- Molecule 1: Superoxide dismutase [Mn/Fe]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.96Å 82.88Å 72.78Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	31.39 – 2.15 31.39 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (31.39-2.15) 92.3 (31.39-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.193 , 0.259 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6699	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	2/1664 (0.1%)	1.11	0/2275
1	B	1.02	0/1653	1.14	3/2262 (0.1%)
1	C	1.02	1/1629 (0.1%)	1.11	3/2229 (0.1%)
1	D	1.05	1/1655 (0.1%)	1.11	2/2264 (0.1%)
All	All	1.02	4/6601 (0.1%)	1.12	8/9030 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	HIS	CA-C	6.47	1.61	1.52
1	A	173	ARG	CA-C	-5.13	1.48	1.53
1	D	182	ALA	CA-C	5.11	1.59	1.52
1	C	140	GLU	N-CA	5.08	1.52	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	LEU	CA-C-N	-6.44	113.35	119.85
1	B	4	LEU	C-N-CA	-6.44	113.35	119.85
1	B	7	LEU	N-CA-C	-6.44	101.66	109.83
1	C	176	ARG	CA-C-N	-6.31	112.33	119.28
1	C	176	ARG	C-N-CA	-6.31	112.33	119.28
1	C	74	GLY	N-CA-C	-6.25	104.99	113.37
1	D	88	SER	CA-C-N	-5.29	114.37	119.87
1	D	88	SER	C-N-CA	-5.29	114.37	119.87

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	1615	0	1570	16	0
1	B	1607	0	1558	9	0
1	C	1586	0	1534	20	0
1	D	1609	0	1557	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	72	0	0	2	0
3	B	70	0	0	3	0
3	C	65	0	0	4	0
3	D	71	0	0	0	0
All	All	6699	0	6219	55	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 4.

All (55) 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:200:LEU:O	1:C:201:THR:HB	1.79	0.80
1:C:142:THR:HG22	3:C:426:HOH:O	1.90	0.71
1:B:88:SER:HB2	1:B:188:ASN:HB2	1.71	0.71
1:A:88:SER:HB2	1:A:188:ASN:HB2	1.73	0.70
1:A:134:ASP:HB2	1:A:138:LYS:H	1.58	0.67
1:B:154:GLY:HA2	3:B:421:HOH:O	1.96	0.65
1:C:53:GLU:HG3	3:C:427:HOH:O	1.96	0.64
1:C:93:LYS:HG3	1:C:94:VAL:O	1.97	0.64
1:A:94:VAL:HG23	3:A:423:HOH:O	1.97	0.64
1:C:93:LYS:HE2	1:C:94:VAL:H	1.63	0.64
1:B:134:ASP:HB3	1:B:136:GLU:H	1.66	0.60
1:C:58:ASP:OD2	1:C:61:GLN:HG2	2.02	0.60
1:A:58:ASP:O	1:A:61:GLN:HG2	2.02	0.59
1:A:85[A]:GLU:OE1	1:A:194:ARG:NH2	2.37	0.58
1:C:66:ILE:HD12	1:C:70:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:HE2	3:A:470:HOH:O	1.89	0.56
1:C:93:LYS:HB2	3:C:448:HOH:O	2.06	0.56
1:B:82:LEU:HD11	1:B:195:LEU:HD11	1.86	0.56
1:D:62:ILE:HD13	1:D:70:LEU:HD23	1.86	0.56
1:C:93:LYS:HE2	1:C:94:VAL:N	2.20	0.55
1:D:135:LYS:HE2	1:D:154:GLY:O	2.07	0.54
1:D:201:THR:O	1:D:202:LEU:HB2	2.08	0.54
1:C:188:ASN:OD1	1:C:190:ASN:HB2	2.08	0.53
1:B:156:LYS:NZ	3:B:438:HOH:O	2.38	0.53
1:D:176:ARG:N	1:D:177:PRO:CD	2.72	0.52
1:D:8:PRO:HD2	1:D:9:TYR:CE2	2.44	0.52
1:A:156:LYS:N	1:A:156:LYS:HD2	2.25	0.52
1:D:131:LEU:HB3	1:D:159:LEU:HB3	1.92	0.51
1:C:151:ILE:HD12	1:C:157:PRO:CD	2.41	0.51
1:C:14:LEU:HD11	1:C:87:LEU:HB3	1.93	0.51
1:D:103:ASN:OD1	1:D:108:SER:HA	2.10	0.51
1:A:202:LEU:O	1:A:203:GLU:HG2	2.10	0.50
1:C:200:LEU:O	1:C:201:THR:CB	2.55	0.49
1:C:44:LYS:HD3	3:C:440:HOH:O	2.13	0.48
1:A:132:VAL:HG21	1:A:155:LEU:HD13	1.97	0.46
1:C:70:LEU:HD12	1:C:70:LEU:HA	1.79	0.46
1:C:151:ILE:HD12	1:C:157:PRO:HD2	1.98	0.46
1:C:151:ILE:CD1	1:C:157:PRO:HD2	2.46	0.45
1:A:184:PHE:HA	1:A:187:ILE:HD12	1.98	0.44
1:D:19:ASP:OD1	1:D:171:ASN:HB2	2.18	0.44
1:A:149:THR:HA	1:A:150:PRO:HD3	1.88	0.43
1:A:201:THR:C	1:A:202:LEU:HD22	2.43	0.43
1:C:94:VAL:HG22	1:C:189:TRP:CD2	2.54	0.43
1:B:131:LEU:HB3	1:B:159:LEU:HB3	2.00	0.42
1:D:5:PRO:O	1:D:27:HIS:NE2	2.52	0.41
1:C:131:LEU:HB3	1:C:159:LEU:HB3	2.01	0.41
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.36	0.41
1:A:42:LEU:HD13	1:A:50:GLU:HG2	2.03	0.41
1:D:130:TRP:CE2	1:D:150:PRO:HD3	2.56	0.41
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.82	0.41
1:B:97:GLU:HG2	1:B:98:VAL:N	2.36	0.41
1:B:130:TRP:CZ2	1:B:150:PRO:HD3	2.56	0.40
1:C:124:PHE:CZ	1:D:72:ASN:HB3	2.57	0.40
1:A:176:ARG:O	1:A:179:TYR:HB3	2.21	0.40
1:B:94:VAL:HG23	3:B:408:HOH:O	2.21	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	203/210 (97%)	190 (94%)	13 (6%)	0	100	100
1	B	202/210 (96%)	194 (96%)	8 (4%)	0	100	100
1	C	199/210 (95%)	192 (96%)	7 (4%)	0	100	100
1	D	202/210 (96%)	192 (95%)	9 (4%)	1 (0%)	24	20
All	All	806/840 (96%)	768 (95%)	37 (5%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	202	LEU

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	126/171 (74%)	122 (97%)	4 (3%)	34	36
1	B	165/171 (96%)	160 (97%)	5 (3%)	36	38
1	C	162/171 (95%)	157 (97%)	5 (3%)	35	37
1	D	165/171 (96%)	158 (96%)	7 (4%)	26	25
All	All	618/684 (90%)	597 (97%)	21 (3%)	32	33

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	136	GLU
1	A	149	THR
1	A	156	LYS
1	B	48	ILE
1	B	70	LEU
1	B	91	LYS
1	B	143	SER
1	B	153	GLN
1	C	70	LEU
1	C	93	LYS
1	C	135	LYS
1	C	151	ILE
1	C	201	THR
1	D	53	GLU
1	D	91	LYS
1	D	94	VAL
1	D	113	LYS
1	D	149	THR
1	D	181	LYS
1	D	202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	B	68	GLN
1	B	153	GLN
1	C	68	GLN
1	C	146	ASN
1	D	68	GLN
1	D	72	ASN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	203/210 (96%)	-0.26	1 (0%) 87 89	19, 29, 47, 76	2 (0%)
1	B	203/210 (96%)	-0.14	1 (0%) 87 89	18, 30, 49, 66	1 (0%)
1	C	201/210 (95%)	-0.07	1 (0%) 87 89	21, 33, 50, 78	0
1	D	203/210 (96%)	-0.26	3 (1%) 72 76	20, 28, 45, 105	1 (0%)
All	All	810/840 (96%)	-0.18	6 (0%) 84 85	18, 30, 49, 105	4 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	202	LEU	3.8
1	A	202	LEU	3.8
1	B	202	LEU	2.9
1	D	203	GLU	2.6
1	D	201	THR	2.6
1	C	201	THR	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
2	FE	B	301	1/1	0.99	0.04	35,35,35,35	0
2	FE	A	301	1/1	1.00	0.02	34,34,34,34	0
2	FE	C	301	1/1	1.00	0.05	33,33,33,33	0
2	FE	D	301	1/1	1.00	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.