



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:54 AM GMT

PDB ID : 2XSJ
Title : STRUCTURE OF DESULFORUBIDIN FROM DESULFOMICROBIUM
NORVEGICUM
Authors : Oliveira, T.F.; Khan, A.R.; Pereira, I.A.C.; Archer, M.
Deposited on : 2010-09-29
Resolution : 2.50 Å(reported)

This is a wwPDB validation summary 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>

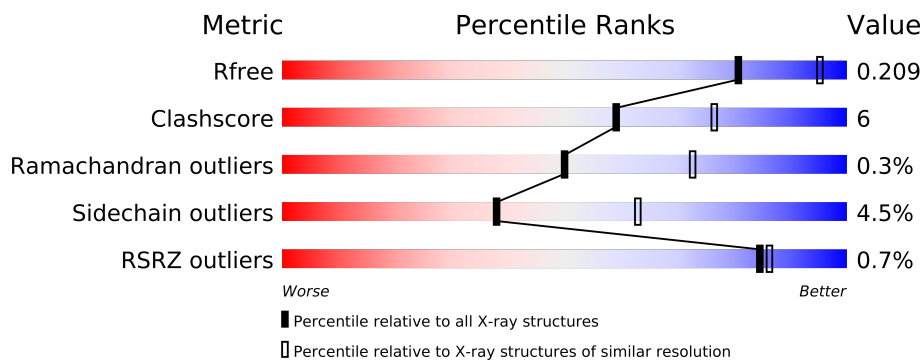
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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	437	
1	D	437	
2	B	386	
2	E	386	
3	C	105	
3	F	105	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15979 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 SULFITE REDUCTASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3456	2179	603	646	28			
1	D	436	Total	C	N	O	S	0	0	0
			3456	2179	603	646	28			

- Molecule 2 is a protein called SULFITE REDUCTASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	385	Total	C	N	O	S	0	0	0
			3026	1921	530	547	28			
2	E	385	Total	C	N	O	S	0	0	0
			3026	1921	530	547	28			

- Molecule 3 is a protein called SULFUR RELAY PROTEIN, TUSE/DSRC/DSVC FAMILY.

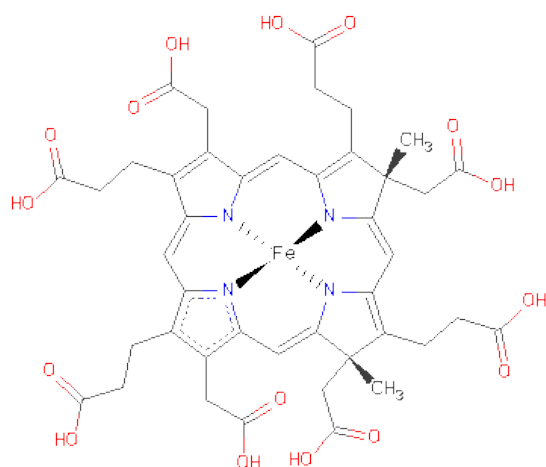
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	104	Total	C	N	O	S	0	0	0
			825	536	128	156	5			
3	F	104	Total	C	N	O	S	0	0	0
			825	536	128	156	5			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



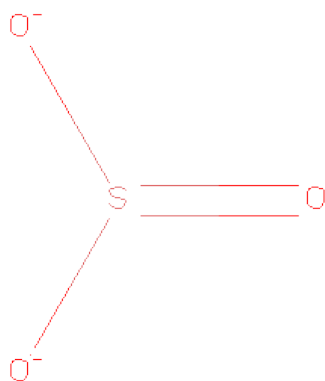
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		
4	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is SIROHEME (three-letter code: SRM) (formula: $C_{42}H_{42}FeN_4O_{16}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	B	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	D	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	E	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

- Molecule 6 is SULFITE ION (three-letter code: SO₃) (formula: O₃S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			4	3	1		
6	E	1	Total	O	S	0	0
			4	3	1		

- Molecule 7 is water.

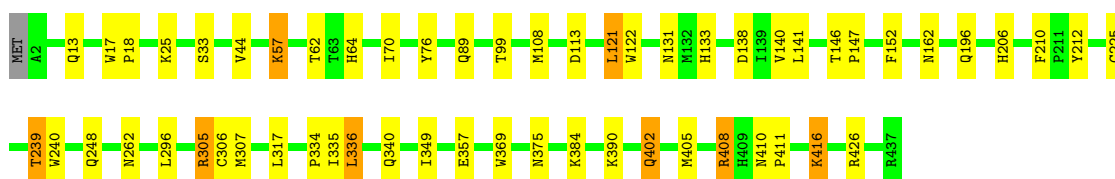
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	316	Total	O	0	0
			316	316		
7	B	215	Total	O	0	0
			215	215		
7	C	23	Total	O	0	0
			23	23		
7	D	281	Total	O	0	0
			281	281		
7	E	179	Total	O	0	0
			179	179		
7	F	27	Total	O	0	0
			27	27		

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.

• Molecule 1: SULFITE REDUCTASE ALPHA SUBUNIT

Chain A:



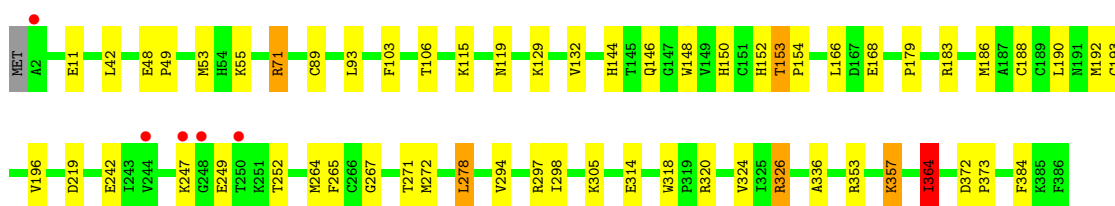
• Molecule 1: SULFITE REDUCTASE ALPHA SUBUNIT

Chain D:



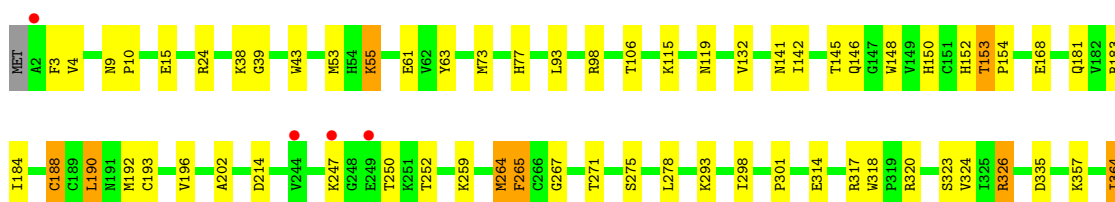
• Molecule 2: SULFITE REDUCTASE BETA SUBUNIT

Chain B:



• Molecule 2: SULFITE REDUCTASE BETA SUBUNIT

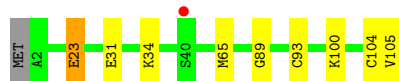
Chain E:





- Molecule 3: SULFUR RELAY PROTEIN, TUSE/DSRC/DSVC FAMILY

Chain C: 



- Molecule 3: SULFUR RELAY PROTEIN, TUSE/DSRC/DSVC FAMILY

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.34Å 135.09Å 178.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.51 – 2.50 45.10 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.51-2.50) 99.2 (45.10-2.53)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.156 , 0.208 0.161 , 0.209	Depositor DCC
R_{free} test set	4013 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 9.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	10 of 79871 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15979	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 50.17 % 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 6.7167e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, SO3, SRM

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	0.69	0/3546	0.66	2/4801 (0.0%)
1	D	0.70	0/3546	0.68	2/4801 (0.0%)
2	B	0.71	0/3104	0.68	3/4202 (0.1%)
2	E	0.73	0/3104	0.70	1/4202 (0.0%)
3	C	0.72	0/846	0.59	0/1135
3	F	0.71	0/846	0.57	0/1135
All	All	0.71	0/14992	0.67	8/20276 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	LEU	CA-CB-CG	7.09	131.60	115.30
1	D	305	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	31	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	B	297	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	305	ARG	NE-CZ-NH2	-5.68	117.46	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3456	0	3301	57	0
1	D	3456	0	3301	48	0
2	B	3026	0	2965	40	0
2	E	3026	0	2965	43	0
3	C	825	0	813	8	0
3	F	825	0	813	5	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	D	16	0	0	0	0
4	E	16	0	0	0	0
5	A	63	0	34	2	0
5	B	63	0	33	4	0
5	D	63	0	34	3	0
5	E	63	0	33	7	0
6	B	4	0	0	0	0
6	E	4	0	0	0	0
7	A	316	0	0	7	0
7	B	215	0	0	8	0
7	C	23	0	0	0	0
7	D	281	0	0	3	0
7	E	179	0	0	1	0
7	F	27	0	0	0	0
All	All	15979	0	14292	178	0

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 6.

The worst 5 of 178 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:57:LYS:NZ	1:D:64:HIS:H	1.29	1.31
1:A:57:LYS:HE2	1:A:64:HIS:N	1.60	1.16
1:D:57:LYS:HZ2	1:D:64:HIS:N	1.47	1.13
1:A:57:LYS:HE2	1:A:64:HIS:H	0.95	1.08
1:A:57:LYS:CE	1:A:64:HIS:H	1.73	1.01

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	434/437 (99%)	427 (98%)	7 (2%)	0	100	100
1	D	434/437 (99%)	421 (97%)	13 (3%)	0	100	100
2	B	383/386 (99%)	362 (94%)	18 (5%)	3 (1%)	27	46
2	E	383/386 (99%)	364 (95%)	16 (4%)	3 (1%)	27	46
3	C	102/105 (97%)	97 (95%)	5 (5%)	0	100	100
3	F	102/105 (97%)	99 (97%)	3 (3%)	0	100	100
All	All	1838/1856 (99%)	1770 (96%)	62 (3%)	6 (0%)	50	73

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	364	ILE
2	B	298	ILE
2	B	364	ILE
2	E	153	THR
2	B	153	THR

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	364/365 (100%)	349 (96%)	15 (4%)	41	67
1	D	364/365 (100%)	349 (96%)	15 (4%)	41	67
2	B	325/326 (100%)	307 (94%)	18 (6%)	30	52
2	E	325/326 (100%)	310 (95%)	15 (5%)	37	62
3	C	87/88 (99%)	85 (98%)	2 (2%)	63	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	87/88 (99%)	82 (94%)	5 (6%)	29	50
All	All	1552/1558 (100%)	1482 (96%)	70 (4%)	38	63

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	357	LYS
1	D	212	TYR
2	E	364	ILE
2	B	364	ILE
1	D	57	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	ASN
1	D	41	GLN
2	E	220	ASN
1	D	13	GLN
1	D	131	ASN

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 ⓘ

14 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$
4	SF4	A	501	1	12,12,12	5.84	11 (91%)	0,24,24	0.00	-
4	SF4	A	502	1	12,12,12	7.72	12 (100%)	0,24,24	0.00	-
5	SRM	A	503	1	70,70,70	1.86	20 (28%)	94,112,112	3.23	26 (27%)
4	SF4	B	501	2	12,12,12	93.80	12 (100%)	0,24,24	0.00	-
4	SF4	B	502	2	12,12,12	93.69	11 (91%)	0,24,24	0.00	-
5	SRM	B	503	3,2,6	70,70,70	1.91	20 (28%)	94,112,112	3.24	25 (26%)
6	SO3	B	504	5	3,3,3	1.19	0	2,3,3	0.61	0
4	SF4	D	501	1	12,12,12	6.37	10 (83%)	0,24,24	0.00	-
4	SF4	D	502	1	12,12,12	7.58	12 (100%)	0,24,24	0.00	-
5	SRM	D	503	1	70,70,70	1.86	19 (27%)	94,112,112	3.14	25 (26%)
4	SF4	E	501	2	12,12,12	7.50	11 (91%)	0,24,24	0.00	-
4	SF4	E	502	2	12,12,12	6.75	10 (83%)	0,24,24	0.00	-
5	SRM	E	503	3,2,6	70,70,70	1.92	22 (31%)	94,112,112	2.98	26 (27%)
6	SO3	E	504	5	3,3,3	1.27	0	2,3,3	0.59	0

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
4	SF4	A	501	1	-	0/0/48/48	0/0/5/5
4	SF4	A	502	1	-	0/0/48/48	0/0/5/5
5	SRM	A	503	1	-	0/38/126/126	0/0/8/8
4	SF4	B	501	2	-	0/0/48/48	0/0/5/5
4	SF4	B	502	2	-	0/0/48/48	0/0/5/5
5	SRM	B	503	3,2,6	-	0/38/126/126	0/0/8/8
6	SO3	B	504	5	-	0/0/0/0	0/0/0/0
4	SF4	D	501	1	-	0/0/48/48	0/0/5/5
4	SF4	D	502	1	-	0/0/48/48	0/0/5/5
5	SRM	D	503	1	-	0/38/126/126	0/0/8/8
4	SF4	E	501	2	-	0/0/48/48	0/0/5/5
4	SF4	E	502	2	-	0/0/48/48	0/0/5/5
5	SRM	E	503	3,2,6	-	0/38/126/126	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO3	E	504	5	-	0/0/0/0	0/0/0/0

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	SF4	S4-FE2	230.24	3.88	2.33
4	B	502	SF4	S4-FE1	229.43	3.87	2.33
4	B	502	SF4	S1-FE4	228.82	3.87	2.33
4	B	501	SF4	S2-FE4	228.20	3.86	2.33
4	D	502	SF4	S1-FE4	-13.74	2.24	2.33

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	503	SRM	C4A-NA-C1A	12.58	112.43	106.86
5	D	503	SRM	CAB-C3B-C2B	-12.35	110.90	123.49
5	B	503	SRM	CAA-C3A-C2A	-11.84	111.42	123.49
5	A	503	SRM	CAB-C3B-C2B	-11.83	111.43	123.49
5	B	503	SRM	C4A-NA-C1A	11.82	112.09	106.86

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	436/437 (99%)	-0.56	0 100 100	6, 15, 28, 37	0
1	D	436/437 (99%)	-0.52	1 (0%) 93 94	6, 15, 29, 36	0
2	B	385/386 (99%)	-0.53	5 (1%) 74 76	7, 15, 32, 59	0
2	E	385/386 (99%)	-0.55	4 (1%) 79 81	7, 15, 31, 59	0
3	C	104/105 (99%)	-0.25	1 (0%) 79 81	21, 29, 48, 54	1 (0%)
3	F	104/105 (99%)	-0.13	2 (1%) 64 66	19, 27, 48, 54	0
All	All	1850/1856 (99%)	-0.50	13 (0%) 84 86	6, 16, 34, 59	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	244	VAL	3.2
2	B	247	LYS	2.9
2	B	250	THR	2.7
2	E	247	LYS	2.7
2	E	2	ALA	2.5

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
5	SRM	B	503	63/63	0.16	0.33	8,12,20,22	0
5	SRM	D	503	63/63	0.12	0.09	4,9,16,22	0
5	SRM	A	503	63/63	0.12	0.04	7,11,18,24	0
5	SRM	E	503	63/63	0.14	-0.13	7,12,16,21	0
6	SO3	B	504	4/4	0.13	-1.24	17,17,18,18	0
6	SO3	E	504	4/4	0.11	-1.69	17,17,18,20	0
4	SF4	E	501	8/8	0.04	-1.76	10,13,14,14	0
4	SF4	A	502	8/8	0.08	-1.84	5,6,8,8	0
4	SF4	B	501	8/8	0.03	-1.88	13,14,16,16	0
4	SF4	D	502	8/8	0.08	-2.01	6,7,8,9	0
4	SF4	B	502	8/8	0.08	-2.31	11,12,15,25	0
4	SF4	A	501	8/8	0.04	-2.53	9,11,12,14	0
4	SF4	E	502	8/8	0.07	-2.79	11,12,16,23	0
4	SF4	D	501	8/8	0.04	-3.36	9,10,13,13	0

6.5 Other polymers ⓘ

There are no such residues in this entry.