



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:59 PM GMT

PDB ID : 2A9D
Title : Crystal structure of recombinant chicken sulfite oxidase with Arg at residue 161
Authors : Karakas, E.; Wilson, H.L.; Graf, T.N.; Xiang, S.; Jaramillo-Busquets, S.; Rajagopalan, K.V.; Kisker, C.
Deposited on : 2005-07-11
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

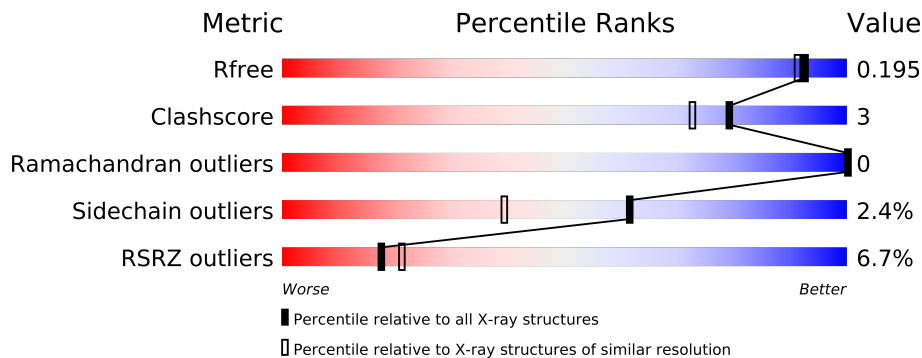
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **FAILED**
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 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	372	
1	B	372	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	7504	-	X
2	SO4	B	8504	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6539 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.

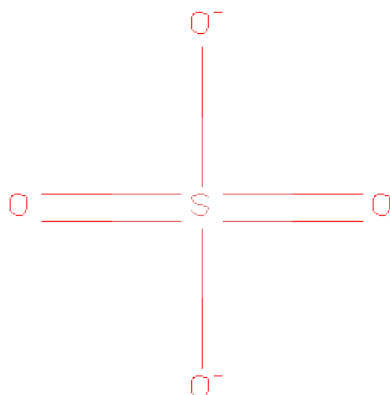
- Molecule 1 is a protein called Sulfite Oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2859	1813	519	520	7			
1	B	359	Total	C	N	O	S	0	2	0
			2786	1764	509	506	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	ARG	GLY	ENGINEERED	UNP P07850
B	161	ARG	GLY	ENGINEERED	UNP P07850

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



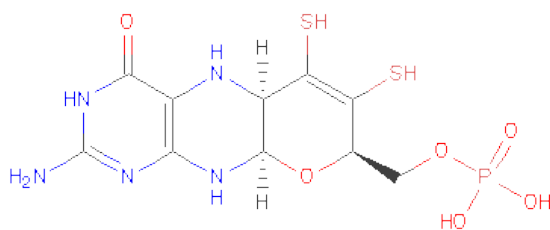
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
3	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 4 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mo	0	0
			1	1		
4	A	1	Total	Mo	0	0
			1	1		

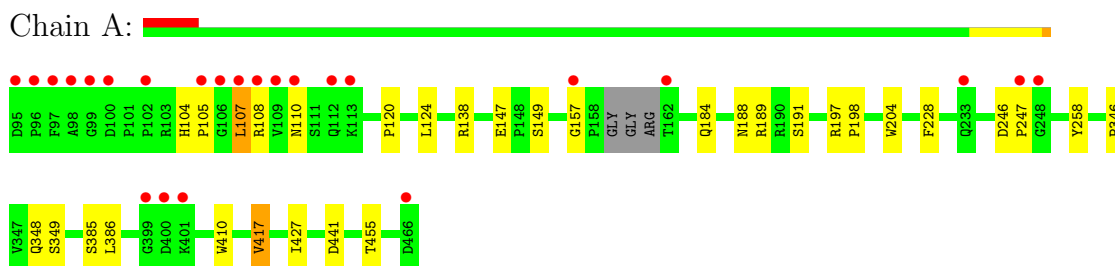
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	421	Total 421	O 421	0	0
5	B	403	Total 403	O 403	0	0

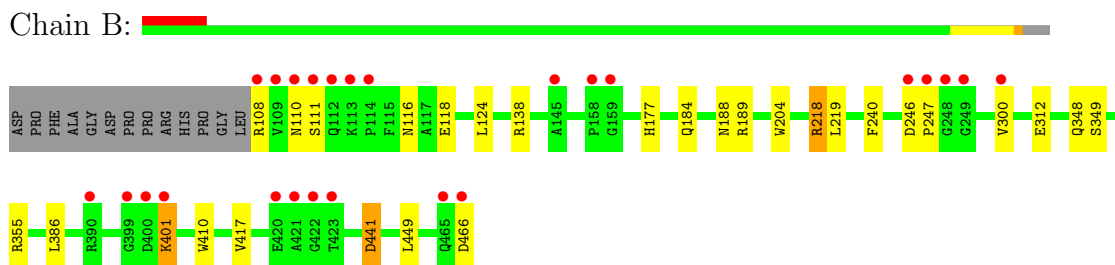
3 Residue-property plots

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.

• Molecule 1: Sulfite Oxidase



• Molecule 1: Sulfite Oxidase



4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.14Å 123.10Å 55.13Å 90.00° 94.31° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 28.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-1.70) 95.1 (28.93-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.155 , 0.187 0.165 , 0.195	Depositor DCC
R_{free} test set	3913 reflections (5.31%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: MO, SO4, MTE

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	0.56	0/2946	0.76	0/4031
1	B	0.59	1/2879 (0.0%)	0.80	3/3938 (0.1%)
All	All	0.58	1/5825 (0.0%)	0.78	3/7969 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	GLU	CB-CG	-5.25	1.42	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	B	218	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	441	ASP	CB-CG-OD1	5.41	123.17	118.30

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	2859	0	2796	23	0
1	B	2786	0	2733	15	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	24	0	10	0	0
3	B	24	0	10	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	421	0	0	1	0
5	B	403	0	0	1	0
All	All	6539	0	5549	38	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 3.

All (38) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:386:LEU:HD11	1:A:417:VAL:HG11	1.67	0.75
1:B:189:ARG:HH11	1:B:348:GLN:HE22	1.42	0.66
1:B:108:ARG:N	1:B:118:GLU:O	2.33	0.61
1:B:111:SER:HB3	1:B:116:ASN:HD22	1.64	0.61
1:B:184:GLN:HE21	1:B:188:ASN:HD22	1.50	0.60
1:A:386:LEU:HD11	1:A:417:VAL:CG1	2.35	0.57
1:B:110:ASN:ND2	1:B:204:TRP:CZ3	2.73	0.57
1:B:110:ASN:ND2	1:B:204:TRP:CE3	2.70	0.56
1:A:189:ARG:HH11	1:A:348:GLN:HE22	1.53	0.55
1:A:104:HIS:HB3	1:A:107:LEU:HD23	1.89	0.55
1:B:246:ASP:HB2	1:B:247:PRO:HD2	1.89	0.54
1:A:104:HIS:CG	1:A:105:PRO:HD2	2.42	0.54
1:A:348:GLN:HE21	1:A:349:SER:H	1.55	0.54
1:A:108:ARG:N	1:A:108:ARG:HD2	2.21	0.54
1:B:348:GLN:HE21	1:B:349:SER:H	1.58	0.52
1:A:246:ASP:HB2	1:A:247:PRO:HD2	1.92	0.52
1:B:184:GLN:NE2	1:B:188:ASN:HD22	2.07	0.52
1:A:184:GLN:HE21	1:A:188:ASN:HD22	1.58	0.52
1:A:104:HIS:CD2	1:A:105:PRO:HD2	2.45	0.52
1:B:189:ARG:HH11	1:B:348:GLN:NE2	2.07	0.51
1:B:386:LEU:HD11	1:B:417:VAL:HG21	1.92	0.51
1:A:147:GLU:OE1	1:A:149:SER:OG	2.21	0.51
1:B:401:LYS:NZ	5:B:8750:HOH:O	2.44	0.50
1:A:184:GLN:NE2	1:A:188:ASN:HD22	2.10	0.48
1:A:108:ARG:HD3	1:A:120:PRO:HB3	1.95	0.48
1:A:157:GLY:HA2	1:A:228:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:ARG:HH11	1:A:348:GLN:NE2	2.12	0.48
1:A:157:GLY:HA2	1:A:228:PHE:CZ	2.48	0.48
1:B:177[A]:HIS:CE1	1:B:218:ARG:HE	2.31	0.47
1:A:184:GLN:HE21	1:A:188:ASN:HB3	1.79	0.46
1:A:110:ASN:ND2	1:A:204:TRP:CE3	2.85	0.45
1:A:191:SER:HB3	5:A:7893:HOH:O	2.18	0.44
1:A:228:PHE:HB3	1:A:258:TYR:OH	2.19	0.43
1:B:240:PHE:HB2	1:B:300:VAL:HG21	2.01	0.42
1:A:197:ARG:HG2	1:A:198:PRO:HD2	2.02	0.41
1:A:346:PRO:HG2	1:A:455:THR:HG21	2.03	0.41
1:A:385:SER:O	1:A:427:ILE:HA	2.21	0.41
1:B:184:GLN:HE21	1:B:188:ASN:HB3	1.86	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	365/372 (98%)	360 (99%)	5 (1%)	0	100	100
1	B	359/372 (96%)	355 (99%)	4 (1%)	0	100	100
All	All	724/744 (97%)	715 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	301/302 (100%)	295 (98%)	6 (2%)	68	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	294/302 (97%)	286 (97%)	8 (3%)	57	33
All	All	595/604 (98%)	581 (98%)	14 (2%)	61	39

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LEU
1	A	124	LEU
1	A	138	ARG
1	A	410	TRP
1	A	417	VAL
1	A	441	ASP
1	B	124	LEU
1	B	138	ARG
1	B	219	LEU
1	B	401	LYS
1	B	410	TRP
1	B	441	ASP
1	B	449	LEU
1	B	466	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	HIS
1	A	184	GLN
1	A	319	GLN
1	A	343	GLN
1	A	348	GLN
1	A	353	GLN
1	A	465	GLN
1	B	184	GLN
1	B	319	GLN
1	B	343	GLN
1	B	348	GLN
1	B	465	GLN

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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
3	MTE	A	1501	4	26,26,26	1.80	4 (15%)	34,40,40	1.73	9 (26%)
2	SO4	A	7503	-	4,4,4	0.40	0	6,6,6	0.20	0
2	SO4	A	7504	-	4,4,4	0.28	0	6,6,6	0.17	0
3	MTE	B	4501	4	26,26,26	2.10	6 (23%)	34,40,40	1.75	10 (29%)
2	SO4	B	8503	-	4,4,4	0.55	0	6,6,6	0.44	0
2	SO4	B	8504	-	4,4,4	0.19	0	6,6,6	0.40	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
3	MTE	A	1501	4	-	0/6/34/34	0/0/3/3
2	SO4	A	7503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	7504	-	-	0/0/0/0	0/0/0/0
3	MTE	B	4501	4	-	0/6/34/34	0/0/3/3
2	SO4	B	8503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	8504	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4501	MTE	C6-C1'	-7.15	1.40	1.50
3	A	1501	MTE	C6-C1'	-5.78	1.42	1.50
3	A	1501	MTE	C6-N5	-4.68	1.38	1.45
3	B	4501	MTE	C6-N5	-4.23	1.39	1.45
3	B	4501	MTE	C4'-C3'	-3.80	1.46	1.52
3	A	1501	MTE	C7-N8	-2.53	1.39	1.44
3	B	4501	MTE	O3'-C7	2.32	1.47	1.44
3	B	4501	MTE	C7-C6	2.24	1.57	1.53
3	A	1501	MTE	C7-C6	2.10	1.57	1.53
3	B	4501	MTE	C7-N8	-2.08	1.40	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	4501	MTE	O3'-C7-C6	-4.04	104.01	109.50
3	B	4501	MTE	C6-C7-N8	3.91	115.34	110.01
3	A	1501	MTE	C6-C7-N8	3.83	115.23	110.01
3	B	4501	MTE	N3-C2-N1	-3.70	116.60	121.78
3	A	1501	MTE	O3'-C7-N8	-3.42	104.77	109.22
3	A	1501	MTE	C4-C9-N5	2.91	123.33	119.10
3	A	1501	MTE	C1'-C6-N5	2.56	116.54	111.70
3	B	4501	MTE	C4-C9-N5	2.44	122.64	119.10
3	A	1501	MTE	N3-C2-N1	-2.42	118.39	121.78
3	B	4501	MTE	O3'-C7-N8	-2.42	106.07	109.22
3	B	4501	MTE	C6-C1'-C2'	2.42	125.03	116.27
3	A	1501	MTE	O3'-C7-C6	-2.28	106.39	109.50
3	B	4501	MTE	C1'-C6-N5	2.26	115.96	111.70
3	B	4501	MTE	C4'-C3'-C2'	2.23	113.61	110.98
3	B	4501	MTE	N2-C2-N3	2.18	120.25	117.86
3	A	1501	MTE	C9-C10-N8	2.13	121.55	119.12
3	B	4501	MTE	C10-N8-C7	-2.11	120.28	124.01
3	A	1501	MTE	C4'-C3'-C2'	2.03	113.37	110.98
3	A	1501	MTE	C7-C6-N5	2.01	110.99	108.44

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	369/372 (99%)	0.19	24 (6%) 18 23	14, 21, 41, 57	0
1	B	359/372 (96%)	0.19	25 (6%) 16 20	14, 21, 38, 47	0
All	All	728/744 (97%)	0.19	49 (6%) 17 21	14, 21, 40, 57	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	PRO	6.5
1	A	97	PHE	6.1
1	A	96	PRO	5.3
1	B	248	GLY	5.2
1	B	111	SER	5.1
1	A	105	PRO	5.1
1	B	466	ASP	4.8
1	A	247	PRO	4.7
1	A	95	ASP	4.6
1	A	98	ALA	4.6
1	A	157	GLY	4.5
1	A	248	GLY	4.1
1	A	109	VAL	4.1
1	A	99	GLY	3.8
1	B	110	ASN	3.7
1	B	114	PRO	3.7
1	A	112	GLN	3.6
1	B	159	GLY	3.5
1	A	107	LEU	3.5
1	A	233	GLN	3.5
1	B	158	PRO	3.4
1	B	108	ARG	3.3
1	A	113	LYS	3.3
1	A	401	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	3.1
1	A	108	ARG	3.1
1	A	466	ASP	3.1
1	A	399	GLY	3.0
1	B	109	VAL	3.0
1	B	420	GLU	2.8
1	B	145	ALA	2.8
1	B	423	THR	2.8
1	B	249	GLY	2.7
1	A	162	THR	2.7
1	B	390	ARG	2.6
1	B	246	ASP	2.6
1	B	401	LYS	2.6
1	B	465	GLN	2.6
1	B	113	LYS	2.5
1	B	300	VAL	2.4
1	A	400	ASP	2.4
1	A	100	ASP	2.4
1	B	399	GLY	2.3
1	A	110	ASN	2.2
1	B	112	GLN	2.2
1	A	106	GLY	2.1
1	B	422	GLY	2.1
1	B	421	ALA	2.1
1	A	102	PRO	2.0

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(\AA^2)	Q<0.9
2	SO4	A	7504	5/5	0.12	3.10	59,59,60,60	0
2	SO4	B	8504	5/5	0.12	2.66	48,48,48,48	0
3	MTE	A	1501	24/24	0.10	-0.29	14,16,17,17	0
3	MTE	B	4501	24/24	0.10	-0.42	14,16,19,19	0
2	SO4	B	8503	5/5	0.04	-1.63	20,21,21,21	0
4	MO	B	5501	1/1	0.05	-2.31	16,16,16,16	0
2	SO4	A	7503	5/5	0.04	-2.33	22,22,23,24	0
4	MO	A	2501	1/1	0.04	-5.00	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.