



wwPDB X-ray Structure Validation Summary Report

Sep 4, 2014 – 11:35 PM EDT

PDB ID : 4C0C
Title : Crystal structure of Trypanosoma cruzi CYP51 bound to the inhibitor (R)-N-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-4-(4-(2,4-difluorophenyl)piperazin-1-yl)-2-fluorobenzamide.
Authors : Calvet, C.M.; Vieira, D.F.; Choi, J.Y.; Cameron, M.D.; Gut, J.; Kellar, D.; Siqueira-Neto, J.L.; McKerrow, J.H.; Roush, W.R.; Podust, L.M.
Deposited on : 2013-08-01
Resolution : 2.04 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>

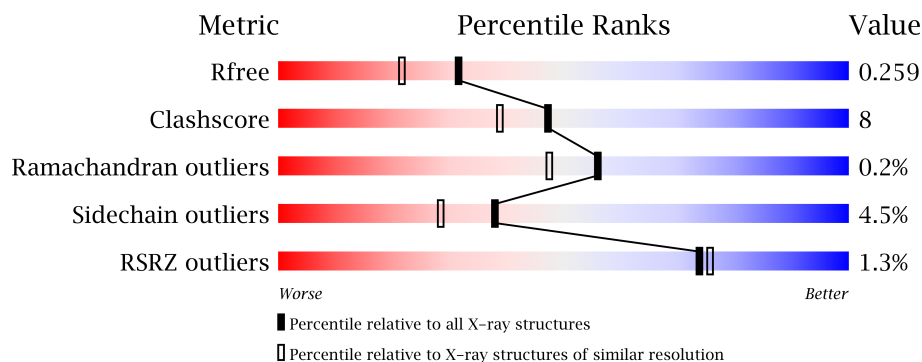
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.04 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	1380 (2.06-2.02)
Clashscore	79885	1577 (2.06-2.02)
Ramachandran outliers	78287	1565 (2.06-2.02)
Sidechain outliers	78261	1565 (2.06-2.02)
RSRZ outliers	66119	1381 (2.06-2.02)

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	467	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	1481	-	X
4	SO4	A	1483	-	X
4	SO4	A	1484	-	X
4	SO4	A	1485	-	X
4	SO4	A	1486	-	X
4	SO4	A	1487	-	X
4	SO4	A	1489	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	SO4	A	1490	-	X
4	SO4	A	1493	-	X
5	GOL	A	1491	-	X
5	GOL	A	1492	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3829 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.

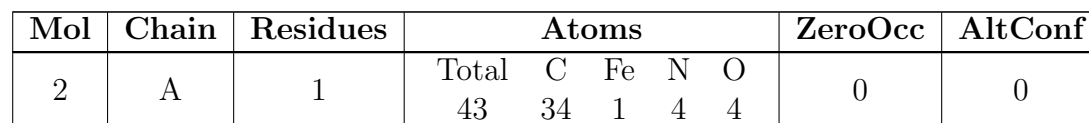
- Molecule 1 is a protein called STEROL 14-ALPHA DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3540	2270	613	629	28	0	1	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	EXPRESSION TAG	UNP Q5I4E1
A	22	ALA	-	EXPRESSION TAG	UNP Q5I4E1
A	23	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	24	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	25	THR	-	EXPRESSION TAG	UNP Q5I4E1
A	26	SER	-	EXPRESSION TAG	UNP Q5I4E1
A	27	SER	-	EXPRESSION TAG	UNP Q5I4E1
A	28	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	29	GLY	-	EXPRESSION TAG	UNP Q5I4E1
A	30	LYS	-	EXPRESSION TAG	UNP Q5I4E1
A	31	LEU	-	EXPRESSION TAG	UNP Q5I4E1
A	482	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	483	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	484	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	485	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	486	HIS	-	EXPRESSION TAG	UNP Q5I4E1
A	487	HIS	-	EXPRESSION TAG	UNP Q5I4E1

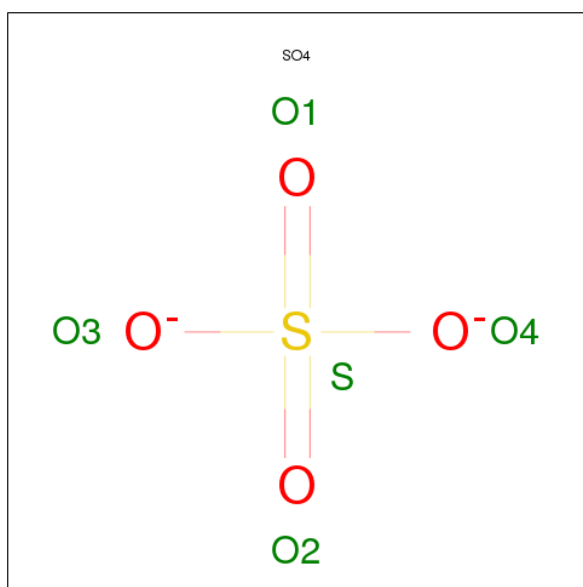
- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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- Chemical structure of compound WVH, showing a complex molecule with multiple rings and functional groups. The structure includes a central amide linkage connecting a substituted benzene ring (left) to a substituted benzene ring (right). The left benzene ring is substituted with a methyl group (C10) and a trifluoromethyl group (C11, C12, C13). The right benzene ring is substituted with a trifluoromethyl group (C14, C15, C16) and a trifluoromethyl group (C17, C18, C19). The central amide linkage is connected to a central carbon atom (C20) which is also bonded to a methyl group (C21) and a trifluoromethyl group (C22, C23, C24). The structure is labeled with atom names (C1-C24) and bond types (single, double, triple).

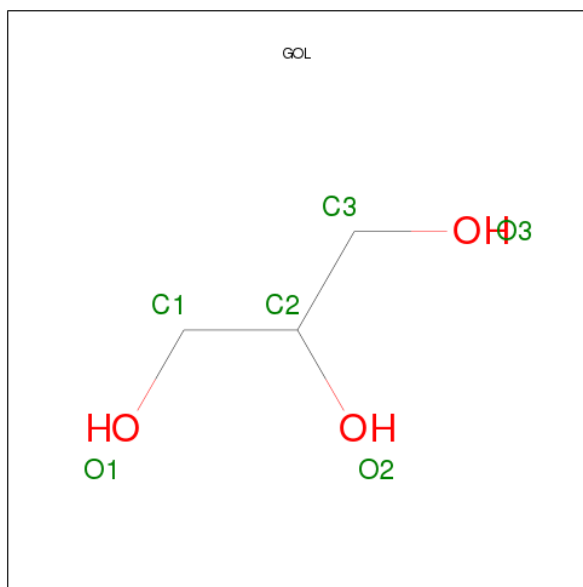
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			44	33	3	6	2		

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- WORLD WIDE
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PROTEIN DATA BANK



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

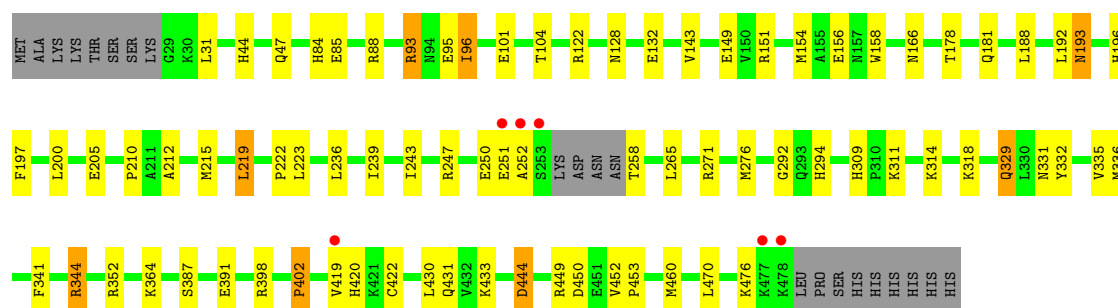
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		

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: STEROL 14-ALPHA DEMETHYLASE

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	128.53Å 128.53Å 116.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.68 – 2.04 80.55 – 2.04	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.68-2.04) 99.8 (80.55-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.199 , 0.254 0.206 , 0.259	Depositor DCC
R_{free} test set	1833 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 36661 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3829	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: GOL, WVH, SO4, HEM

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	0.90	0/3624	0.96	7/4904 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	344	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	449	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	444	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	314	LYS	N-CA-CB	-5.29	101.09	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts i

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	3540	0	3528	55	0
2	A	43	0	30	3	0
3	A	44	0	0	0	0
4	A	65	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	16	3	0
6	A	125	0	0	7	0
All	All	3829	0	3574	58	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 8.

The worst 5 of 58 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:387:SER:HB3	6:A:2097:HOH:O	1.07	1.19
1:A:247:ARG:O	1:A:251:GLU:HG2	1.61	1.01
1:A:387:SER:OG	6:A:2018:HOH:O	1.99	0.80
1:A:149:GLU:HG2	1:A:181:GLN:HG3	1.64	0.78
1:A:223:LEU:N	4:A:1490:SO4:O1	2.22	0.72

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	443/467 (95%)	428 (97%)	14 (3%)	1 (0%)	56 47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	ALA

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	377/408 (92%)	360 (96%)	17 (4%)	38	28

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	197	PHE
1	A	329	GLN
1	A	188	LEU
1	A	391	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	420	HIS
1	A	309	HIS
1	A	193	ASN
1	A	294	HIS

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 ⓘ

17 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	HEM	A	1450	1,3	42,50,50	3.38	17 (40%)	27,82,82	2.16	8 (29%)
3	WVH	A	1460	2	49,49,49	1.82	10 (20%)	69,69,69	2.30	22 (31%)
4	SO4	A	1479	-	4,4,4	0.56	0	6,6,6	0.44	0
4	SO4	A	1480	-	4,4,4	0.74	0	6,6,6	1.03	0
4	SO4	A	1481	-	4,4,4	0.19	0	6,6,6	0.72	0
4	SO4	A	1482	-	4,4,4	0.29	0	6,6,6	0.47	0
4	SO4	A	1483	-	4,4,4	0.55	0	6,6,6	0.53	0
4	SO4	A	1484	-	4,4,4	0.71	0	6,6,6	0.61	0
4	SO4	A	1485	-	4,4,4	0.63	0	6,6,6	0.30	0
4	SO4	A	1486	-	4,4,4	0.52	0	6,6,6	0.52	0
4	SO4	A	1487	-	4,4,4	0.53	0	6,6,6	0.18	0
4	SO4	A	1488	-	4,4,4	0.55	0	6,6,6	0.40	0
4	SO4	A	1489	-	4,4,4	0.59	0	6,6,6	0.16	0
4	SO4	A	1490	-	4,4,4	0.92	0	6,6,6	0.38	0
5	GOL	A	1491	-	5,5,5	0.19	0	5,5,5	0.74	0
5	GOL	A	1492	-	5,5,5	0.74	0	5,5,5	1.19	0
4	SO4	A	1493	-	4,4,4	0.36	0	6,6,6	0.20	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
2	HEM	A	1450	1,3	-	0/14/114/114	0/0/8/8
3	WVH	A	1460	2	-	0/28/38/38	0/6/6/6
4	SO4	A	1479	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1480	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1481	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1482	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1483	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1484	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1485	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1486	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1487	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	1488	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1489	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1490	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1491	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1492	-	-	0/4/4/4	0/0/0/0
4	SO4	A	1493	-	-	0/0/0/0	0/0/0/0

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1450	HEM	C3C-C2C	-11.83	1.36	1.45
2	A	1450	HEM	C3B-C2B	-11.60	1.34	1.45
2	A	1450	HEM	C3C-C4C	-6.30	1.40	1.45
3	A	1460	WVH	C8-C23	5.98	1.47	1.38
2	A	1450	HEM	CMD-C2D	5.18	1.54	1.45

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1460	WVH	C12-C13-N4	-6.09	98.93	110.67
2	A	1450	HEM	CMA-C3A-C4A	-5.21	120.46	128.46
3	A	1460	WVH	C8-C7-N2	4.98	125.34	116.92
2	A	1450	HEM	C4A-C3A-C2A	4.78	110.32	107.00
3	A	1460	WVH	F-C17-C16	4.56	126.75	118.52

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	446/467 (95%)	-0.08	6 (1%) 74 76	25, 41, 62, 104	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	478	LYS	6.6
1	A	251	GLU	4.7
1	A	477	LYS	4.2
1	A	252	ALA	3.8
1	A	253	SER	3.5

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
4	SO4	A	1486	5/5	0.33	7.16	91,100,106,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	A	1490	5/5	0.27	6.36	85,96,107,110	0
5	GOL	A	1491	6/6	0.35	6.01	51,54,59,59	0
4	SO4	A	1487	5/5	0.30	5.10	96,100,107,107	0
4	SO4	A	1483	5/5	0.16	4.30	75,86,90,96	0
4	SO4	A	1489	5/5	0.20	4.24	86,91,97,111	0
5	GOL	A	1492	6/6	0.18	3.20	43,43,48,55	0
4	SO4	A	1481	5/5	0.14	2.62	49,52,58,58	0
4	SO4	A	1493	5/5	0.16	2.30	79,79,86,86	0
4	SO4	A	1484	5/5	0.12	2.08	60,66,73,90	0
4	SO4	A	1485	5/5	0.18	2.05	93,94,98,98	0
4	SO4	A	1482	5/5	0.14	1.93	29,31,32,36	5
4	SO4	A	1488	5/5	0.14	1.52	73,74,81,82	5
4	SO4	A	1479	5/5	0.14	0.92	43,44,45,48	0
3	WVH	A	1460	44/44	0.13	0.81	25,37,47,65	0
2	HEM	A	1450	43/43	0.12	0.39	21,26,38,47	0
4	SO4	A	1480	5/5	0.11	-0.20	58,64,66,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.