



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 07:10 am GMT

PDB ID : 5IIT
Title : Structure of SPX domain of the yeast inorganic polyphosphate polymerase Vtc4 crystallized by carrier-driven crystallization in fusion with the macro domain of human histone macroH2A1.1
Authors : Wild, R.; Hothorn, M.
Deposited on : 2016-03-01
Resolution : 2.13 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

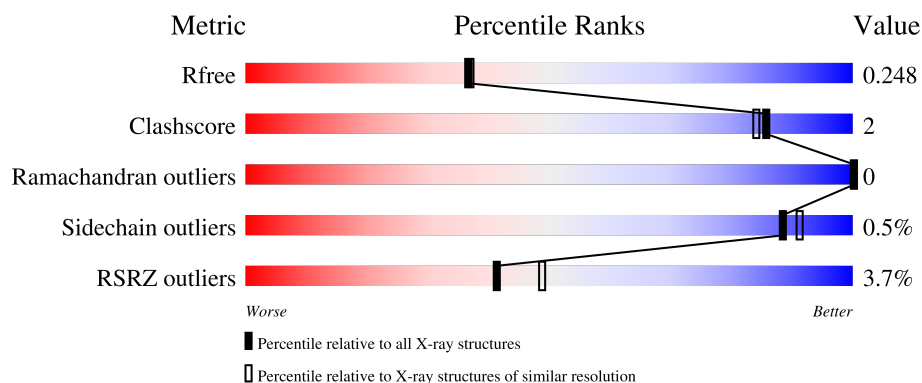
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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	374	 2% 89% 7% 5%
1	B	374	 % 92% • 5%
1	C	374	 5% 89% 6% 5%
1	D	374	 6% 93% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	403	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11622 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 Vacuolar transporter chaperone 4,Core histone macro-H2A.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	7	0
			2852	1828	469	549	6			
1	B	356	Total	C	N	O	S	0	3	0
			2837	1817	465	549	6			
1	C	357	Total	C	N	O	S	0	3	0
			2849	1825	469	549	6			
1	D	355	Total	C	N	O	S	0	0	0
			2810	1800	458	546	6			

There are 40 discrepancies between the modelled and reference sequences:

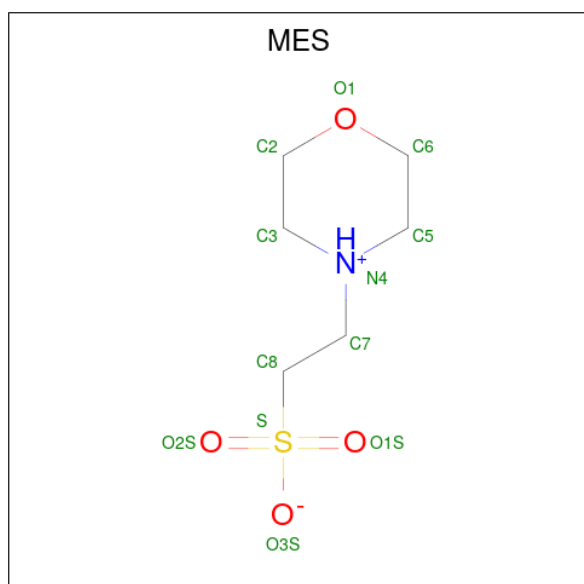
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ALA	-	linker	UNP P47075
A	180	GLY	-	linker	UNP P47075
A	181	SER	-	linker	UNP P47075
A	368	GLU	-	expression tag	UNP O75367
A	369	HIS	-	expression tag	UNP O75367
A	370	HIS	-	expression tag	UNP O75367
A	371	HIS	-	expression tag	UNP O75367
A	372	HIS	-	expression tag	UNP O75367
A	373	HIS	-	expression tag	UNP O75367
A	374	HIS	-	expression tag	UNP O75367
B	179	ALA	-	linker	UNP P47075
B	180	GLY	-	linker	UNP P47075
B	181	SER	-	linker	UNP P47075
B	368	GLU	-	expression tag	UNP O75367
B	369	HIS	-	expression tag	UNP O75367
B	370	HIS	-	expression tag	UNP O75367
B	371	HIS	-	expression tag	UNP O75367
B	372	HIS	-	expression tag	UNP O75367
B	373	HIS	-	expression tag	UNP O75367
B	374	HIS	-	expression tag	UNP O75367
C	179	ALA	-	linker	UNP P47075

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Chain	Residue	Modelled	Actual	Comment	Reference
C	180	GLY	-	linker	UNP P47075
C	181	SER	-	linker	UNP P47075
C	368	GLU	-	expression tag	UNP O75367
C	369	HIS	-	expression tag	UNP O75367
C	370	HIS	-	expression tag	UNP O75367
C	371	HIS	-	expression tag	UNP O75367
C	372	HIS	-	expression tag	UNP O75367
C	373	HIS	-	expression tag	UNP O75367
C	374	HIS	-	expression tag	UNP O75367
D	179	ALA	-	linker	UNP P47075
D	180	GLY	-	linker	UNP P47075
D	181	SER	-	linker	UNP P47075
D	368	GLU	-	expression tag	UNP O75367
D	369	HIS	-	expression tag	UNP O75367
D	370	HIS	-	expression tag	UNP O75367
D	371	HIS	-	expression tag	UNP O75367
D	372	HIS	-	expression tag	UNP O75367
D	373	HIS	-	expression tag	UNP O75367
D	374	HIS	-	expression tag	UNP O75367

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



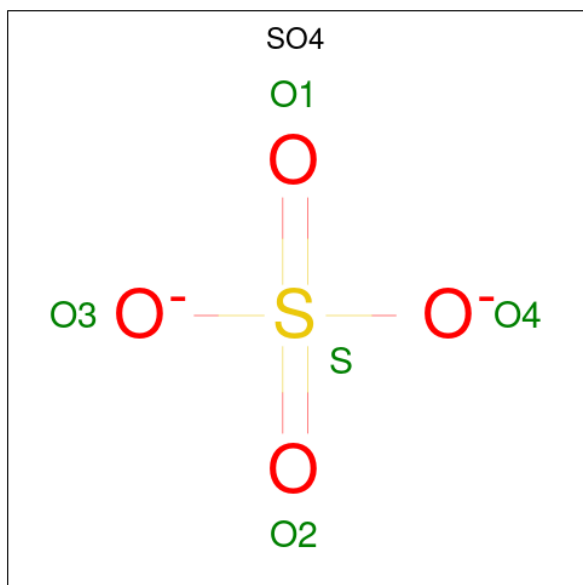
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

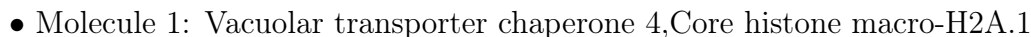
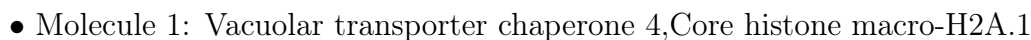
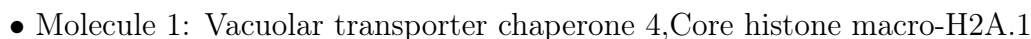
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	55	Total	O	0	0
			55	55		

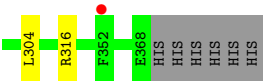
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	45	Total	O	0	0
			45	45		
6	D	40	Total	O	0	0
			40	40		

- Molecule 1: Vacuolar transporter chaperone 4,Core histone macro-H2A.1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.64Å 67.92Å 129.68Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	46.86 – 2.13 46.86 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.86-2.13) 99.1 (46.86-2.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.211 , 0.247 0.213 , 0.248	Depositor DCC
R_{free} test set	5075 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11622	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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: EDO, MG, MES, SO4

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	0.26	0/2920	0.40	0/3938
1	B	0.26	0/2900	0.41	0/3914
1	C	0.26	0/2912	0.41	0/3930
1	D	0.25	0/2863	0.39	0/3865
All	All	0.26	0/11595	0.40	0/15647

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2852	0	2876	15	0
1	B	2837	0	2845	10	0
1	C	2849	0	2862	18	0
1	D	2810	0	2812	7	0
2	A	12	0	12	4	0
2	B	12	0	12	4	0
2	C	12	0	12	2	0
2	D	12	0	12	1	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
4	C	8	0	12	3	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	44	0	0	0	0
6	B	55	0	0	0	0
6	C	45	0	0	0	0
6	D	40	0	0	1	0
All	All	11622	0	11473	51	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 2.

The worst 5 of 51 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:73:ARG:NH1	1:C:112:ASP:OD2	2.09	0.82
1:D:316:ARG:HD2	2:D:401:MES:H62	1.63	0.78
1:C:223:ILE:HD11	1:C:243:VAL:HG11	1.69	0.74
1:C:225:GLY:HA3	4:C:403:EDO:H11	1.76	0.66
1:B:216:PRO:HB2	2:B:402:MES:H71	1.80	0.63

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	360/374 (96%)	357 (99%)	3 (1%)	0	100	100
1	B	357/374 (96%)	352 (99%)	5 (1%)	0	100	100
1	C	358/374 (96%)	353 (99%)	5 (1%)	0	100	100
1	D	353/374 (94%)	351 (99%)	2 (1%)	0	100	100
All	All	1428/1496 (96%)	1413 (99%)	15 (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	319/331 (96%)	316 (99%)	3 (1%)	78	81
1	B	317/331 (96%)	316 (100%)	1 (0%)	92	94
1	C	318/331 (96%)	315 (99%)	3 (1%)	78	81
1	D	313/331 (95%)	313 (100%)	0	100	100
All	All	1267/1324 (96%)	1260 (99%)	7 (1%)	88	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	LEU
1	C	80[A]	GLN
1	C	326	GLN
1	C	80[B]	GLN
1	A	300	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.04	0
4	EDO	C	404	-	3,3,3	0.47	0	2,2,2	0.38	0
2	MES	A	401	-	12,12,12	2.21	1 (8%)	14,16,16	2.37	7 (50%)
2	MES	C	401	-	12,12,12	2.27	1 (8%)	14,16,16	2.20	7 (50%)
4	EDO	A	403	-	3,3,3	0.46	0	2,2,2	0.29	0
4	EDO	A	404	-	3,3,3	0.49	0	2,2,2	0.25	0
2	MES	B	402	-	12,12,12	2.29	1 (8%)	14,16,16	2.02	4 (28%)
3	SO4	B	403	-	4,4,4	0.15	0	6,6,6	0.04	0
3	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.06	0
2	MES	D	401	-	12,12,12	2.27	1 (8%)	14,16,16	1.95	3 (21%)
4	EDO	B	401	-	3,3,3	0.47	0	2,2,2	0.24	0
4	EDO	C	403	-	3,3,3	0.46	0	2,2,2	0.18	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	EDO	C	404	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	A	401	-	-	4/6/14/14	0/1/1/1
2	MES	C	401	-	-	5/6/14/14	0/1/1/1
4	EDO	A	403	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
2	MES	B	402	-	-	4/6/14/14	0/1/1/1
2	MES	D	401	-	-	2/6/14/14	0/1/1/1
4	EDO	B	401	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	MES	C8-S	-7.68	1.66	1.77
2	D	401	MES	C8-S	-7.59	1.66	1.77
2	C	401	MES	C8-S	-7.56	1.66	1.77
2	A	401	MES	C8-S	-7.38	1.67	1.77

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	402	MES	C5-N4-C3	5.78	121.85	108.83
2	A	401	MES	C5-N4-C3	5.11	120.32	108.83
2	C	401	MES	C5-N4-C3	4.74	119.51	108.83
2	D	401	MES	C5-N4-C3	4.70	119.41	108.83
2	A	401	MES	C7-N4-C3	3.20	119.43	111.23

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	MES	C8-C7-N4-C5
2	A	401	MES	C7-C8-S-O2S
2	A	401	MES	C7-C8-S-O3S
2	B	402	MES	C7-C8-S-O1S
2	B	402	MES	C7-C8-S-O2S

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	MES	4	0
2	C	401	MES	2	0
2	B	402	MES	4	0
2	D	401	MES	1	0
4	C	403	EDO	3	0

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	356/374 (95%)	0.16	8 (2%) 62 68	35, 49, 76, 128	0
1	B	356/374 (95%)	0.14	5 (1%) 75 80	31, 48, 68, 127	0
1	C	357/374 (95%)	0.35	19 (5%) 26 33	37, 56, 91, 145	0
1	D	355/374 (94%)	0.45	21 (5%) 22 28	39, 65, 105, 156	0
All	All	1424/1496 (95%)	0.27	53 (3%) 41 49	31, 53, 93, 156	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	PHE	8.8
1	C	146	PHE	6.1
1	A	12	ILE	5.1
1	D	37	ASN	4.3
1	C	145	VAL	4.1

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 monosaccharides 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(\AA^2)	Q<0.9
4	EDO	C	403	4/4	0.26	0.75	144,144,145,146	0
4	EDO	B	401	4/4	0.65	0.26	65,67,72,74	0
3	SO4	C	402	5/5	0.66	0.18	142,144,144,145	0
3	SO4	D	402	5/5	0.71	0.25	133,135,136,136	0
5	MG	C	405	1/1	0.75	0.09	73,73,73,73	0
4	EDO	A	404	4/4	0.79	0.17	54,55,56,61	0
2	MES	A	401	12/12	0.80	0.27	113,128,132,133	0
2	MES	B	402	12/12	0.82	0.28	120,134,135,136	0
2	MES	C	401	12/12	0.82	0.23	116,120,120,120	0
4	EDO	C	404	4/4	0.83	0.18	97,97,100,100	0
4	EDO	A	403	4/4	0.85	0.17	74,76,80,83	0
5	MG	B	404	1/1	0.88	0.05	61,61,61,61	0
3	SO4	A	402	5/5	0.89	0.16	134,135,135,135	0
3	SO4	B	403	5/5	0.92	0.15	128,129,129,129	0
2	MES	D	401	12/12	0.93	0.18	85,130,131,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.