



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:53 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

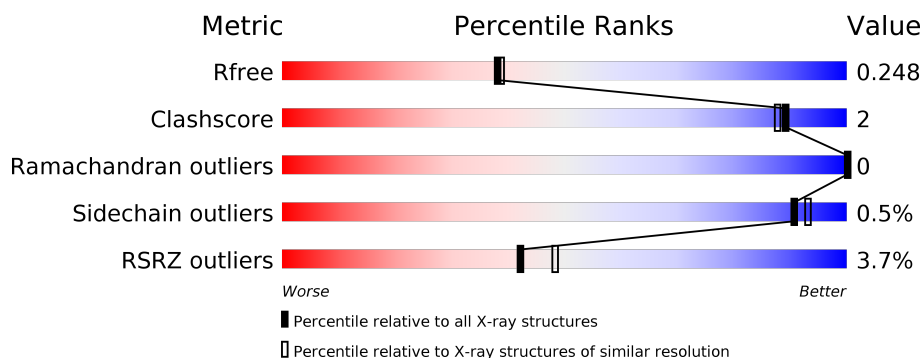
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	374	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>• 5%</div> </div> </div>
1	C	374	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	D	374	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>• 5%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MES	A	401	-	-	-	X
2	MES	B	402	-	-	-	X
2	MES	C	401	-	-	-	X
3	SO4	D	402	-	-	-	X
4	EDO	B	401	-	-	-	X
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:

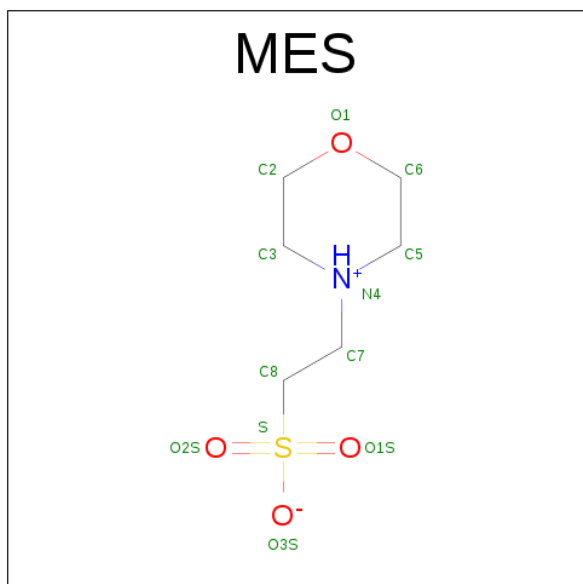
Chain	Residue	Modelled	Actual	Comment	Reference
A	179	ALA	-	linker	UNP P47075
A	180	GLY	-	linker	UNP P47075
A	181	SER	-	linker	UNP P47075
A	368	GLU	-	expression tag	UNP O75367
A	369	HIS	-	expression tag	UNP O75367
A	370	HIS	-	expression tag	UNP O75367
A	371	HIS	-	expression tag	UNP O75367
A	372	HIS	-	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: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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: O<sub>4</sub>S).



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: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

- Molecule 6 is water.

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

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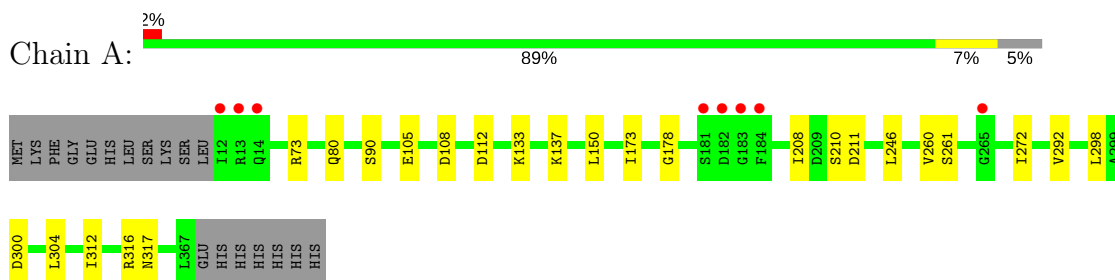
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	45	Total	O	0	0
			45	45		
6	D	40	Total	O	0	0
			40	40		



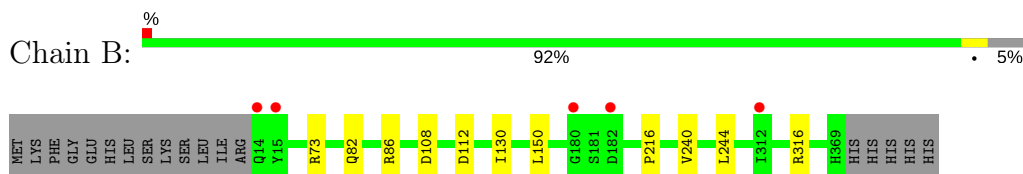
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

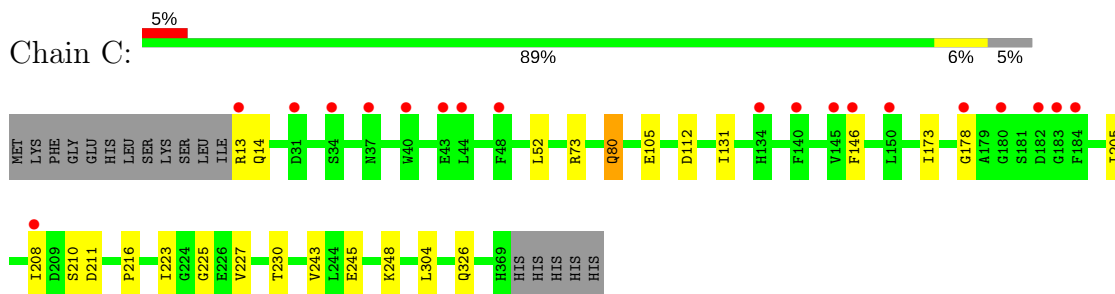
- Molecule 1: Vacuolar transporter chaperone 4,Core histone macro-H2A.1



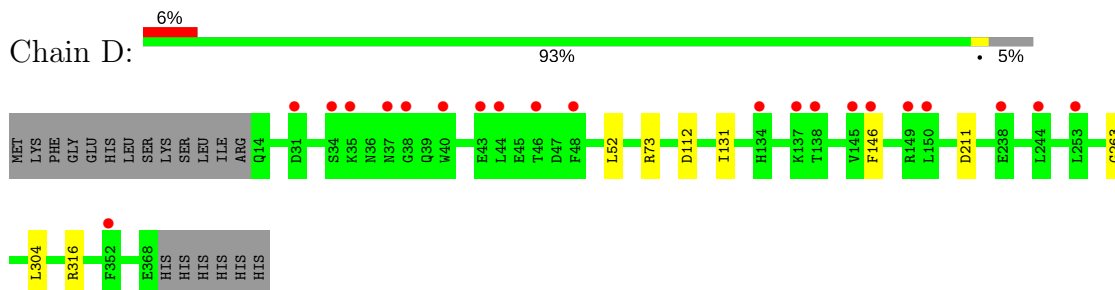
- Molecule 1: Vacuolar transporter chaperone 4,Core histone macro-H2A.1



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



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.14Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.211 , 0.247 0.212 , 0.248	Depositor DCC
$R_{free}$ test set	5072 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtrriage
Anisotropy	0.651	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, SO4, MES, EDO

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.

All (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
1:B:316:ARG:HD3	2:B:402:MES:H62	1.82	0.62
1:C:216:PRO:O	4:C:403:EDO:O1	2.17	0.62
1:A:316:ARG:HD2	2:A:401:MES:H62	1.83	0.61
1:C:216:PRO:HB2	2:C:401:MES:H71	1.84	0.60
1:C:227:VAL:HB	4:C:403:EDO:H21	1.84	0.59
1:A:73:ARG:NH1	1:A:112:ASP:OD2	2.36	0.58
1:C:131:ILE:HD11	1:C:146:PHE:HD2	1.68	0.58
1:C:245:GLU:HA	1:C:248:LYS:HD2	1.87	0.56
1:A:260[B]:VAL:HG23	1:A:298:LEU:HD13	1.88	0.56
1:A:316:ARG:HD2	2:A:401:MES:H31	1.90	0.54
1:C:173:ILE:HG23	1:C:178:GLY:HA2	1.90	0.54
1:D:131:ILE:HD11	1:D:146:PHE:HD2	1.74	0.53
1:C:131:ILE:HD11	1:C:146:PHE:CD2	2.44	0.52
1:C:80[B]:GLN:NE2	1:C:105:GLU:OE2	2.42	0.52
1:B:216:PRO:O	2:B:402:MES:H32	2.11	0.51
1:C:205:ILE:HG21	1:C:227:VAL:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD22	1:A:261:SER:HB3	1.94	0.50
1:C:52:LEU:HB3	1:C:146:PHE:CE1	2.47	0.50
1:A:260[B]:VAL:HG22	1:A:272:ILE:HG12	1.94	0.49
1:D:131:ILE:HD11	1:D:146:PHE:CD2	2.48	0.49
1:D:263:GLY:O	6:D:501:HOH:O	2.19	0.48
1:A:133:LYS:O	1:A:137[B]:LYS:HG2	2.14	0.47
1:C:13:ARG:HG3	1:C:14:GLN:N	2.30	0.47
1:B:73:ARG:NH1	1:B:112:ASP:OD2	2.48	0.46
1:C:211:ASP:HB3	1:C:304:LEU:HD22	1.97	0.46
1:D:52:LEU:HB3	1:D:146:PHE:CE1	2.51	0.46
1:A:80[B]:GLN:NE2	1:A:105:GLU:OE2	2.49	0.46
1:B:73:ARG:NH2	1:B:108:ASP:HB3	2.31	0.45
2:C:401:MES:H82	2:C:401:MES:H31	1.73	0.44
1:A:317:ASN:OD1	2:A:401:MES:H51	2.18	0.43
1:C:227:VAL:O	1:C:230:THR:HG22	2.19	0.43
1:B:73:ARG:HH22	1:B:108:ASP:HB3	1.83	0.43
1:B:316:ARG:HG2	2:B:402:MES:H81	2.00	0.43
1:B:240:VAL:O	1:B:244:LEU:HD13	2.19	0.42
1:A:292:VAL:HG22	1:A:312:ILE:HD11	2.01	0.42
1:B:82:GLN:O	1:B:86:ARG:HG2	2.19	0.42
1:A:73:ARG:NH2	1:A:108:ASP:HB3	2.33	0.42
1:C:208:ILE:HG22	1:C:210:SER:H	1.85	0.42
1:D:73:ARG:NH2	1:D:112:ASP:OD2	2.47	0.42
1:A:208:ILE:HG22	1:A:210[B]:SER:H	1.85	0.42
1:A:316:ARG:HG2	2:A:401:MES:H81	2.01	0.42
1:D:211:ASP:HB3	1:D:304:LEU:HD22	2.02	0.41
1:A:211:ASP:HB3	1:A:304:LEU:HD22	2.03	0.41
1:A:173:ILE:HG23	1:A:178:GLY:HA2	2.03	0.40
1:C:13:ARG:NH1	1:C:14:GLN:H	2.19	0.40
1:B:130:ILE:HD12	1:B:130:ILE:HA	1.97	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	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%)	82	85
1	B	317/331 (96%)	316 (100%)	1 (0%)	94	96
1	C	318/331 (96%)	315 (99%)	3 (1%)	82	85
1	D	313/331 (95%)	313 (100%)	0	100	100
All	All	1267/1324 (96%)	1260 (99%)	7 (1%)	91	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	A	150	LEU
1	A	300	ASP
1	B	150	LEU
1	C	80[A]	GLN
1	C	80[B]	GLN
1	C	326	GLN

Some 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 ⓘ

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 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	$\# Z  > 2$
2	MES	A	401	-	12,12,12	2.10	1 (8%)	14,16,16	2.61	8 (57%)
3	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.31	0
4	EDO	A	404	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	B	401	-	3,3,3	0.47	0	2,2,2	0.26	0
2	MES	B	402	-	12,12,12	2.18	1 (8%)	14,16,16	2.21	5 (35%)
3	SO4	B	403	-	4,4,4	0.15	0	6,6,6	0.04	0
2	MES	C	401	-	12,12,12	2.16	1 (8%)	14,16,16	2.43	7 (50%)
3	SO4	C	402	-	4,4,4	0.13	0	6,6,6	0.08	0
4	EDO	C	403	-	3,3,3	0.45	0	2,2,2	0.20	0
4	EDO	C	404	-	3,3,3	0.46	0	2,2,2	0.40	0
2	MES	D	401	-	12,12,12	2.15	1 (8%)	14,16,16	2.23	5 (35%)
3	SO4	D	402	-	4,4,4	0.15	0	6,6,6	0.06	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	MES	A	401	-	-	0/6/14/14	0/1/1/1
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
4	EDO	B	401	-	-	0/1/1/1	0/0/0/0
2	MES	B	402	-	-	0/6/14/14	0/1/1/1
3	SO4	B	403	-	-	0/0/0/0	0/0/0/0
2	MES	C	401	-	-	0/6/14/14	0/1/1/1
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
4	EDO	C	403	-	-	0/1/1/1	0/0/0/0
4	EDO	C	404	-	-	0/1/1/1	0/0/0/0
2	MES	D	401	-	-	0/6/14/14	0/1/1/1
3	SO4	D	402	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	MES	C8-S	-7.28	1.66	1.77
2	D	401	MES	C8-S	-7.20	1.66	1.77
2	C	401	MES	C8-S	-7.16	1.66	1.77
2	A	401	MES	C8-S	-6.99	1.67	1.77

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	MES	C2-C3-N4	-2.49	106.62	110.11
2	C	401	MES	C6-C5-N4	-2.41	106.72	110.11
2	A	401	MES	C6-C5-N4	-2.34	106.82	110.11
2	D	401	MES	C7-N4-C5	2.02	116.42	111.26
2	B	402	MES	C7-N4-C3	2.20	116.89	111.26
2	D	401	MES	O3S-S-C8	2.27	108.84	106.06
2	D	401	MES	O2S-S-C8	2.49	108.93	106.79
2	C	401	MES	O3S-S-C8	2.56	109.20	106.06
2	A	401	MES	O2S-S-C8	2.63	109.05	106.79
2	B	402	MES	O2S-S-C8	2.64	109.06	106.79
2	C	401	MES	C7-N4-C5	2.68	118.13	111.26
2	A	401	MES	C7-N4-C5	2.77	118.35	111.26
2	B	402	MES	O3S-S-C8	2.81	109.51	106.06
2	C	401	MES	C7-N4-C3	2.88	118.63	111.26
2	A	401	MES	O3S-S-C8	3.07	109.84	106.06
2	C	401	MES	O2S-S-C8	3.11	109.46	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	MES	C7-N4-C3	3.19	119.43	111.26
2	B	402	MES	O1S-S-C8	3.21	109.55	106.79
2	C	401	MES	O1S-S-C8	3.57	109.86	106.79
2	A	401	MES	O1S-S-C8	4.04	110.26	106.79
2	D	401	MES	O1S-S-C8	4.57	110.72	106.79
2	D	401	MES	C5-N4-C3	4.65	119.41	108.87
2	C	401	MES	C5-N4-C3	4.70	119.51	108.87
2	A	401	MES	C5-N4-C3	5.06	120.32	108.87
2	B	402	MES	C5-N4-C3	5.73	121.85	108.87

There are no chirality outliers.

There are no torsion outliers.

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	B	402	MES	4	0
2	C	401	MES	2	0
4	C	403	EDO	3	0
2	D	401	MES	1	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	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%) 27 33	37, 56, 91, 145	0
1	D	355/374 (94%)	0.45	21 (5%) 23 28	39, 65, 105, 156	0
All	All	1424/1496 (95%)	0.27	53 (3%) 42 48	31, 53, 93, 156	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	PHE	8.7
1	C	146	PHE	6.1
1	A	12	ILE	5.1
1	D	37	ASN	4.3
1	D	352	PHE	4.0
1	C	145	VAL	4.0
1	C	208	ILE	3.9
1	A	183	GLY	3.9
1	B	182	ASP	3.8
1	D	44	LEU	3.6
1	C	182	ASP	3.5
1	D	134	HIS	3.5
1	A	181	SER	3.3
1	D	43	GLU	3.2
1	D	48	PHE	3.2
1	D	40	TRP	3.1
1	C	140	PHE	3.0
1	C	40	TRP	2.9
1	D	138	THR	2.9
1	B	14	GLN	2.9
1	D	150	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	38	GLY	2.8
1	D	238	GLU	2.8
1	C	37	ASN	2.7
1	A	182	ASP	2.7
1	C	150	LEU	2.7
1	D	46	THR	2.6
1	D	145	VAL	2.5
1	C	43	GLU	2.5
1	D	35	LYS	2.5
1	C	13	ARG	2.5
1	C	44	LEU	2.5
1	C	178	GLY	2.4
1	A	14	GLN	2.4
1	A	184	PHE	2.4
1	C	184	PHE	2.4
1	D	31	ASP	2.4
1	D	253	LEU	2.4
1	C	134	HIS	2.4
1	B	180	GLY	2.3
1	C	183	GLY	2.3
1	D	149	ARG	2.3
1	B	15	TYR	2.2
1	D	137	LYS	2.2
1	A	13	ARG	2.1
1	A	265	GLY	2.1
1	C	34	SER	2.1
1	C	180	GLY	2.1
1	D	34	SER	2.1
1	B	312	ILE	2.0
1	C	48	PHE	2.0
1	C	31	ASP	2.0
1	D	244	LEU	2.0

## 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 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	C	403	4/4	0.26	0.75	11.41	144,144,145,146	0
3	SO4	D	402	5/5	0.71	0.25	5.87	133,135,136,136	0
2	MES	A	401	12/12	0.79	0.27	3.85	113,128,132,133	0
4	EDO	B	401	4/4	0.65	0.26	3.81	65,67,72,74	0
2	MES	B	402	12/12	0.82	0.28	3.48	120,134,135,136	0
2	MES	C	401	12/12	0.82	0.23	2.77	116,120,120,120	0
4	EDO	A	403	4/4	0.86	0.16	1.31	74,76,80,83	0
3	SO4	B	403	5/5	0.92	0.15	0.96	128,129,129,129	0
4	EDO	A	404	4/4	0.79	0.17	0.90	54,55,56,61	0
2	MES	D	401	12/12	0.93	0.17	0.73	85,130,131,132	0
3	SO4	C	402	5/5	0.67	0.18	0.32	142,144,144,145	0
4	EDO	C	404	4/4	0.83	0.18	-0.07	97,97,100,100	0
5	MG	C	405	1/1	0.76	0.09	-1.87	73,73,73,73	0
5	MG	B	404	1/1	0.88	0.05	-2.39	61,61,61,61	0
3	SO4	A	402	5/5	0.89	0.16	-	134,135,135,135	0

## 6.5 Other polymers

There are no such residues in this entry.