



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 3, 2024 – 06:39 pm GMT

PDB ID : 5AEX  
Title : Crystal structure of *Saccharomyces cerevisiae* Mep2  
Authors : Rutherford, J.C.; Chembath, A.; van den Berg, B.  
Deposited on : 2015-01-12  
Resolution : 3.20 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](mailto: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>.

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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 : 1.8.4, 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

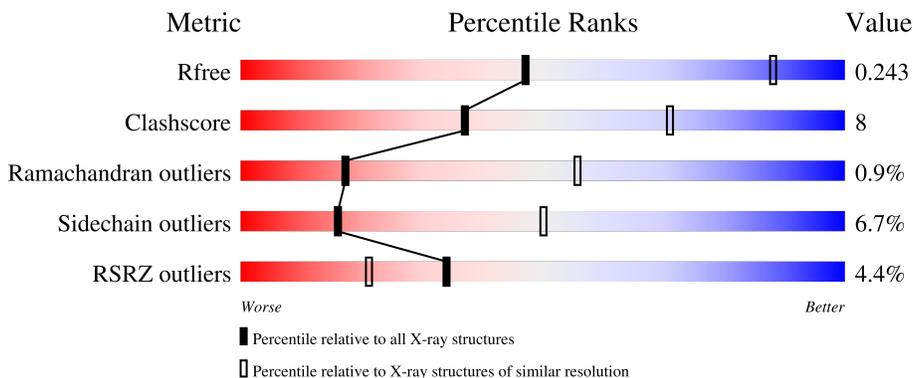
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 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	505	 % 73% 15% • 10%
1	B	505	 3% 66% 23% • 10%
1	C	505	 4% 70% 18% • 10%
1	D	505	 3% 70% 17% • 10%
1	E	505	 5% 66% 22% • 10%

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Mol	Chain	Length	Quality of chain
1	F	505	<p>2% 71% 18% 10%</p>
1	H	505	<p>8% 68% 17% 13%</p>
1	I	505	<p>5% 70% 17% 11%</p>
1	J	505	<p>5% 68% 16% 15%</p>

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
2	PO4	I	1455	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30576 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 AMMONIUM TRANSPORTER MEP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	456	3437	2242	561	608	26	41	0	0
1	B	456	3437	2242	561	608	26	65	0	0
1	C	456	3437	2242	561	608	26	69	0	0
1	D	455	3431	2239	560	606	26	60	0	0
1	E	456	3437	2242	561	608	26	95	0	0
1	F	456	3437	2242	561	608	26	57	0	0
1	H	440	3320	2175	541	578	26	117	0	0
1	I	447	3375	2206	549	594	26	204	0	0
1	J	427	3220	2115	519	561	25	258	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	500	HIS	-	expression tag	UNP P41948
A	501	HIS	-	expression tag	UNP P41948
A	502	HIS	-	expression tag	UNP P41948
A	503	HIS	-	expression tag	UNP P41948
A	504	HIS	-	expression tag	UNP P41948
A	505	HIS	-	expression tag	UNP P41948
B	500	HIS	-	expression tag	UNP P41948
B	501	HIS	-	expression tag	UNP P41948
B	502	HIS	-	expression tag	UNP P41948
B	503	HIS	-	expression tag	UNP P41948
B	504	HIS	-	expression tag	UNP P41948

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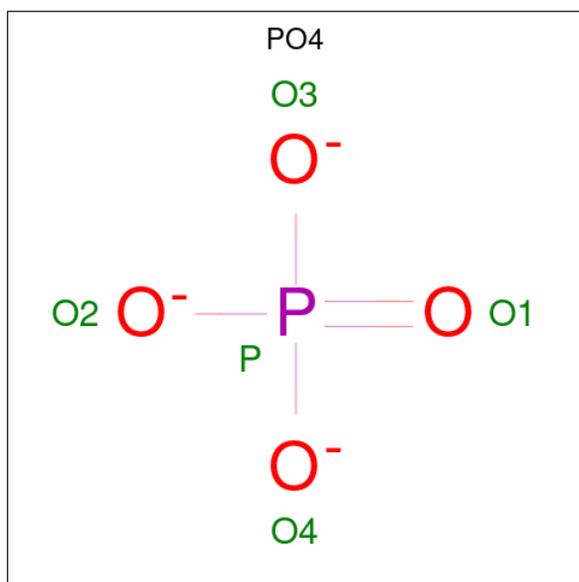
Chain	Residue	Modelled	Actual	Comment	Reference
B	505	HIS	-	expression tag	UNP P41948
C	500	HIS	-	expression tag	UNP P41948
C	501	HIS	-	expression tag	UNP P41948
C	502	HIS	-	expression tag	UNP P41948
C	503	HIS	-	expression tag	UNP P41948
C	504	HIS	-	expression tag	UNP P41948
C	505	HIS	-	expression tag	UNP P41948
D	500	HIS	-	expression tag	UNP P41948
D	501	HIS	-	expression tag	UNP P41948
D	502	HIS	-	expression tag	UNP P41948
D	503	HIS	-	expression tag	UNP P41948
D	504	HIS	-	expression tag	UNP P41948
D	505	HIS	-	expression tag	UNP P41948
E	500	HIS	-	expression tag	UNP P41948
E	501	HIS	-	expression tag	UNP P41948
E	502	HIS	-	expression tag	UNP P41948
E	503	HIS	-	expression tag	UNP P41948
E	504	HIS	-	expression tag	UNP P41948
E	505	HIS	-	expression tag	UNP P41948
F	500	HIS	-	expression tag	UNP P41948
F	501	HIS	-	expression tag	UNP P41948
F	502	HIS	-	expression tag	UNP P41948
F	503	HIS	-	expression tag	UNP P41948
F	504	HIS	-	expression tag	UNP P41948
F	505	HIS	-	expression tag	UNP P41948
H	500	HIS	-	expression tag	UNP P41948
H	501	HIS	-	expression tag	UNP P41948
H	502	HIS	-	expression tag	UNP P41948
H	503	HIS	-	expression tag	UNP P41948
H	504	HIS	-	expression tag	UNP P41948
H	505	HIS	-	expression tag	UNP P41948
I	500	HIS	-	expression tag	UNP P41948
I	501	HIS	-	expression tag	UNP P41948
I	502	HIS	-	expression tag	UNP P41948
I	503	HIS	-	expression tag	UNP P41948
I	504	HIS	-	expression tag	UNP P41948
I	505	HIS	-	expression tag	UNP P41948
J	500	HIS	-	expression tag	UNP P41948
J	501	HIS	-	expression tag	UNP P41948
J	502	HIS	-	expression tag	UNP P41948
J	503	HIS	-	expression tag	UNP P41948
J	504	HIS	-	expression tag	UNP P41948

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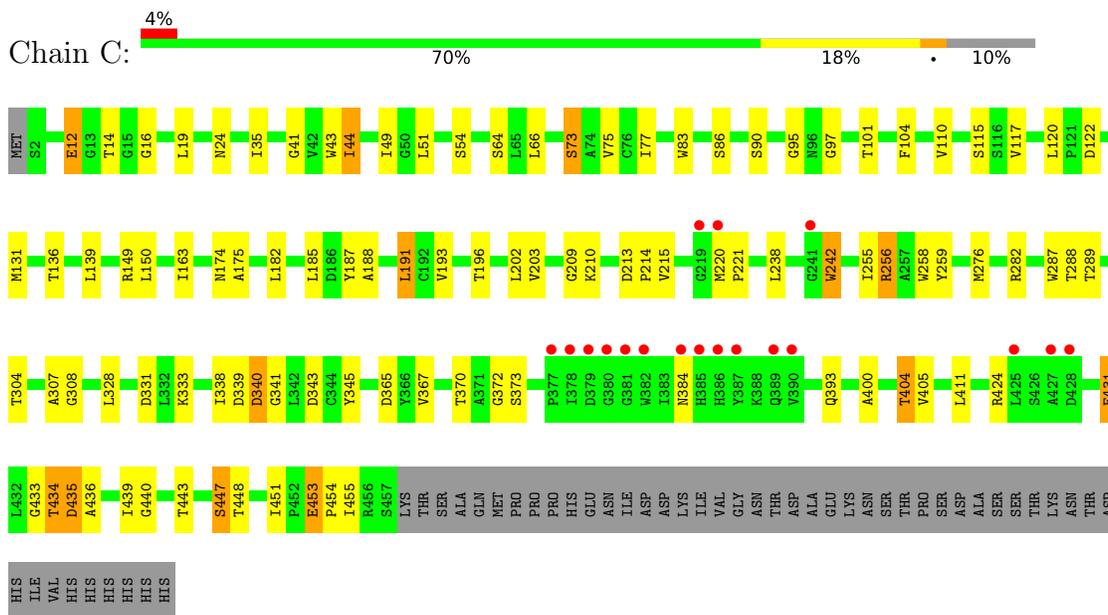
Chain	Residue	Modelled	Actual	Comment	Reference
J	505	HIS	-	expression tag	UNP P41948

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

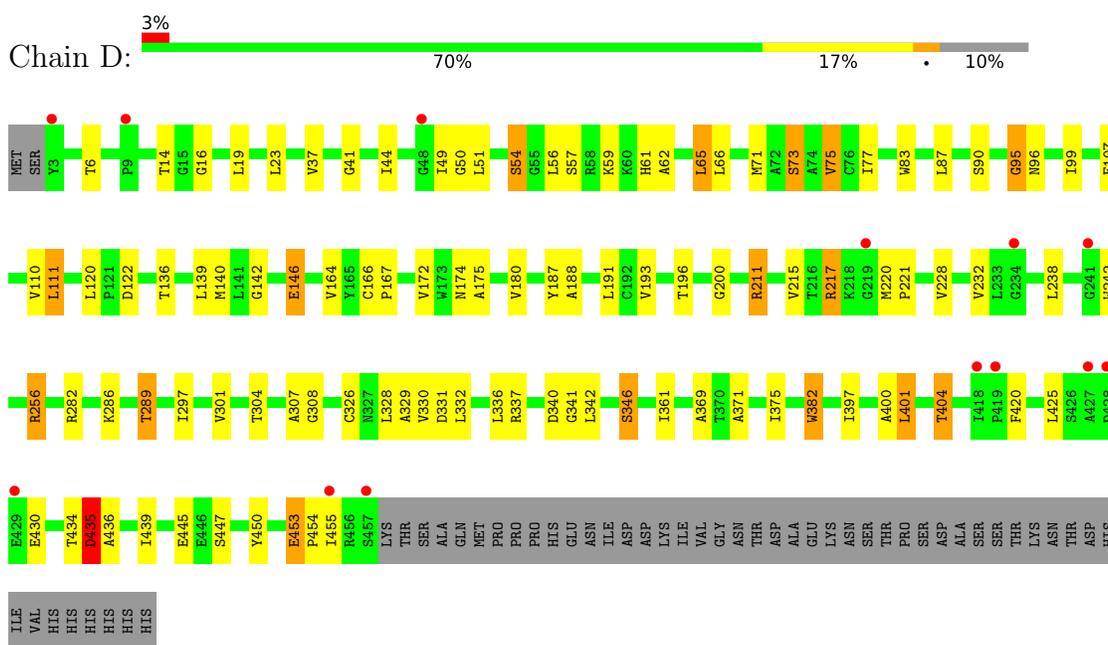


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0
2	H	1	5	4	1	0	0
2	I	1	5	4	1	0	0
2	J	1	5	4	1	0	0

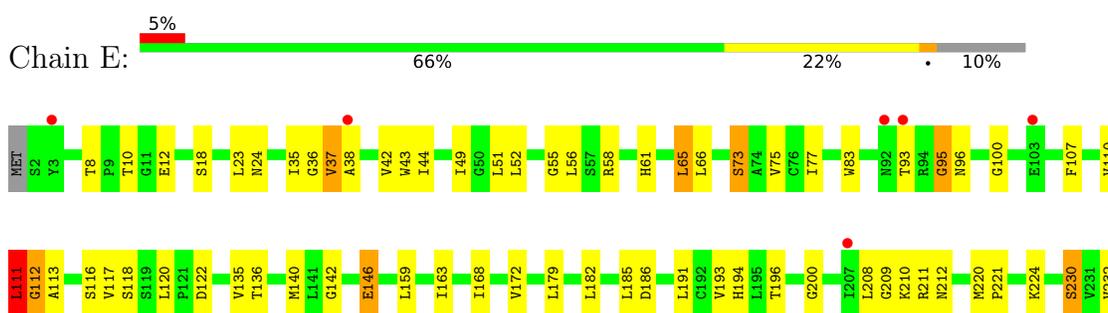




• Molecule 1: AMMONIUM TRANSPORTER MEP2



• Molecule 1: AMMONIUM TRANSPORTER MEP2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.69Å 232.35Å 279.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 3.20 49.28 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.28-3.20) 95.6 (49.28-3.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.189 , 0.241 0.193 , 0.243	Depositor DCC
$R_{free}$ test set	2453 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.6	Xtrriage
Anisotropy	0.267	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	30576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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: PO4

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	0.72	1/3534 (0.0%)	0.62	1/4818 (0.0%)
1	B	0.64	0/3534	0.61	2/4818 (0.0%)
1	C	0.54	0/3534	0.57	0/4818
1	D	0.65	0/3528	0.60	2/4810 (0.0%)
1	E	0.57	0/3534	0.59	1/4818 (0.0%)
1	F	0.69	0/3534	0.60	0/4818
1	H	0.53	0/3415	0.53	0/4654
1	I	0.41	0/3470	0.51	1/4729 (0.0%)
1	J	0.37	0/3313	0.48	0/4518
All	All	0.58	1/31396 (0.0%)	0.57	7/42801 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	VAL	CB-CG1	-5.34	1.41	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	111	LEU	CA-CB-CG	6.78	130.89	115.30
1	A	120	LEU	CA-CB-CG	5.57	128.11	115.30
1	B	340	ASP	N-CA-C	5.55	125.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	336	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	241	GLY	N-CA-C	-5.29	99.89	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	240	PHE	Peptide

## 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	3437	0	3401	37	0
1	B	3437	0	3401	69	0
1	C	3437	0	3401	53	1
1	D	3431	0	3396	52	0
1	E	3437	0	3401	63	0
1	F	3437	0	3401	47	0
1	H	3320	0	3295	48	0
1	I	3375	0	3337	53	1
1	J	3220	0	3188	51	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	2	0
2	J	5	0	0	0	0
All	All	30576	0	30221	454	1

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 8.

The worst 5 of 454 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:J:10:THR:HG22	1:J:12:GLU:H	1.37	0.88
1:F:256:ARG:NH1	1:F:308:GLY:O	2.10	0.84
1:A:10:THR:HG22	1:A:12:GLU:H	1.47	0.78
1:C:400:ALA:O	1:C:404:THR:OG1	2.01	0.78
1:H:49:ILE:HG13	1:H:238:LEU:HD21	1.65	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:GLU:OE2	1:I:387:TYR:OH[4_545]	2.19	0.01

## 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	454/505 (90%)	429 (94%)	21 (5%)	4 (1%)	17	56
1	B	454/505 (90%)	422 (93%)	29 (6%)	3 (1%)	22	61
1	C	454/505 (90%)	421 (93%)	29 (6%)	4 (1%)	17	56
1	D	453/505 (90%)	419 (92%)	29 (6%)	5 (1%)	14	51
1	E	454/505 (90%)	421 (93%)	28 (6%)	5 (1%)	14	51
1	F	454/505 (90%)	429 (94%)	24 (5%)	1 (0%)	47	79
1	H	434/505 (86%)	406 (94%)	20 (5%)	8 (2%)	8	41
1	I	441/505 (87%)	402 (91%)	34 (8%)	5 (1%)	14	51
1	J	421/505 (83%)	387 (92%)	32 (8%)	2 (0%)	29	67
All	All	4019/4545 (88%)	3736 (93%)	246 (6%)	37 (1%)	17	56

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	GLY
1	D	435	ASP
1	I	112	GLY
1	A	95	GLY
1	B	95	GLY

### 5.3.2 Protein sidechains [i](#)

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	353/398 (89%)	326 (92%)	27 (8%)	13	45
1	B	353/398 (89%)	328 (93%)	25 (7%)	14	47
1	C	353/398 (89%)	329 (93%)	24 (7%)	16	49
1	D	352/398 (88%)	322 (92%)	30 (8%)	10	38
1	E	353/398 (89%)	325 (92%)	28 (8%)	12	43
1	F	353/398 (89%)	329 (93%)	24 (7%)	16	49
1	H	341/398 (86%)	321 (94%)	20 (6%)	19	54
1	I	346/398 (87%)	325 (94%)	21 (6%)	18	54
1	J	330/398 (83%)	318 (96%)	12 (4%)	35	69
All	All	3134/3582 (88%)	2923 (93%)	211 (7%)	16	50

5 of 211 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	111	LEU
1	F	120	LEU
1	J	14	THR
1	E	146	GLU
1	E	428	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	368	ASN
1	E	384	ASN

### 5.3.3 RNA [i](#)

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](#)

9 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	PO4	J	1455	-	4,4,4	0.94	0	6,6,6	0.47	0
2	PO4	C	1458	-	4,4,4	1.07	0	6,6,6	0.43	0
2	PO4	D	1458	-	4,4,4	1.04	0	6,6,6	0.45	0
2	PO4	F	1458	-	4,4,4	1.15	0	6,6,6	0.57	0
2	PO4	H	1457	-	4,4,4	0.95	0	6,6,6	0.39	0
2	PO4	E	1458	-	4,4,4	1.13	0	6,6,6	0.39	0
2	PO4	A	1458	-	4,4,4	1.19	0	6,6,6	0.57	0
2	PO4	B	1458	-	4,4,4	1.02	0	6,6,6	0.51	0
2	PO4	I	1455	-	4,4,4	0.95	0	6,6,6	0.40	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1458	PO4	1	0
2	I	1455	PO4	2	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, 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	456/505 (90%)	-0.21	6 (1%) 77 65	45, 62, 92, 173	11 (2%)
1	B	456/505 (90%)	-0.02	17 (3%) 41 26	44, 71, 109, 192	18 (3%)
1	C	456/505 (90%)	-0.06	18 (3%) 39 25	49, 80, 122, 155	19 (4%)
1	D	455/505 (90%)	-0.12	13 (2%) 51 36	44, 69, 106, 158	16 (3%)
1	E	456/505 (90%)	0.02	24 (5%) 26 14	46, 76, 115, 211	25 (5%)
1	F	456/505 (90%)	-0.18	11 (2%) 59 44	42, 64, 99, 164	15 (3%)
1	H	440/505 (87%)	0.19	40 (9%) 9 5	57, 83, 138, 160	31 (7%)
1	I	447/505 (88%)	0.09	25 (5%) 24 13	64, 104, 151, 196	55 (12%)
1	J	426/505 (84%)	0.10	24 (5%) 24 13	68, 119, 158, 189	71 (16%)
All	All	4048/4545 (89%)	-0.02	178 (4%) 34 21	42, 77, 139, 211	261 (6%)

The worst 5 of 178 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	382	TRP	6.1
1	C	379	ASP	6.0
1	C	381	GLY	5.8
1	H	216	THR	5.5
1	C	219	GLY	5.4

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	I	1455	5/5	0.67	0.20	178,181,181,182	0
2	PO4	H	1457	5/5	0.81	0.23	200,202,202,204	0
2	PO4	J	1455	5/5	0.92	0.25	163,163,163,163	0
2	PO4	A	1458	5/5	0.94	0.19	98,101,104,105	0
2	PO4	F	1458	5/5	0.95	0.20	97,97,100,104	0
2	PO4	B	1458	5/5	0.95	0.21	99,100,101,102	0
2	PO4	D	1458	5/5	0.96	0.32	142,143,144,147	0
2	PO4	E	1458	5/5	0.96	0.24	113,113,114,114	0
2	PO4	C	1458	5/5	0.97	0.18	110,110,111,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.