



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 07:04 am GMT

PDB ID : 3Q7F  
Title : Cryptococcus neoformans protein farnesyltransferase in complex with FPP and ethylenediamine inhibitor 1  
Authors : Hast, M.A.; Beese, L.S.  
Deposited on : 2011-01-04  
Resolution : 2.20 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

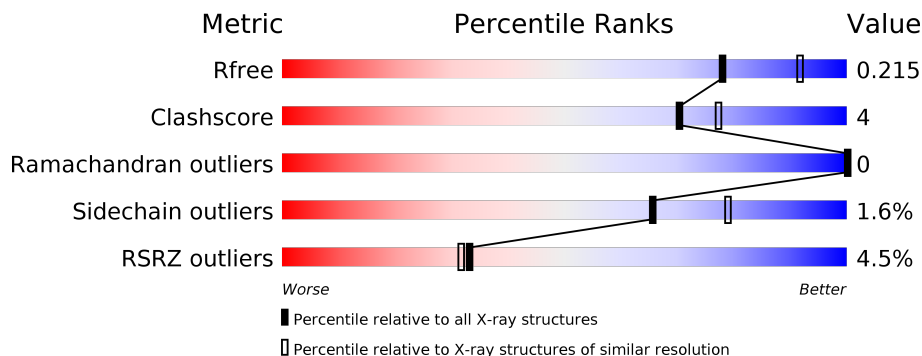
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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 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	349	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>5%</div> <div>10%</div> </div> </div>
2	B	520	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>7%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SUC	A	3010	X	-	-	-
3	SUC	B	1002	X	-	-	-
3	SUC	B	3010	X	-	-	-
5	3CX	B	522	X	-	-	-
5	3CX	B	523	X	-	-	-
5	3CX	B	524	X	-	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7003 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.

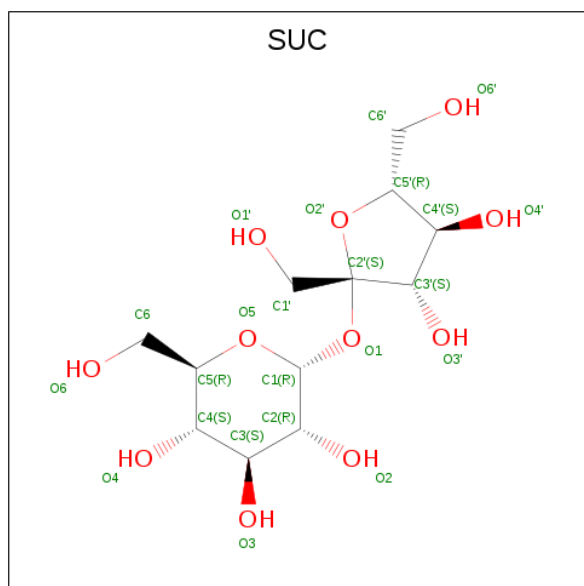
- Molecule 1 is a protein called Farnesyltransferase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2606	1680	444	471	11			

- Molecule 2 is a protein called Farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	1	0
			3730	2366	649	700	15			

- Molecule 3 is SUCROSE (three-letter code: SUC) (formula:  $C_{12}H_{22}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	12	11		
3	B	1	Total	C	O	0	0
			23	12	11		

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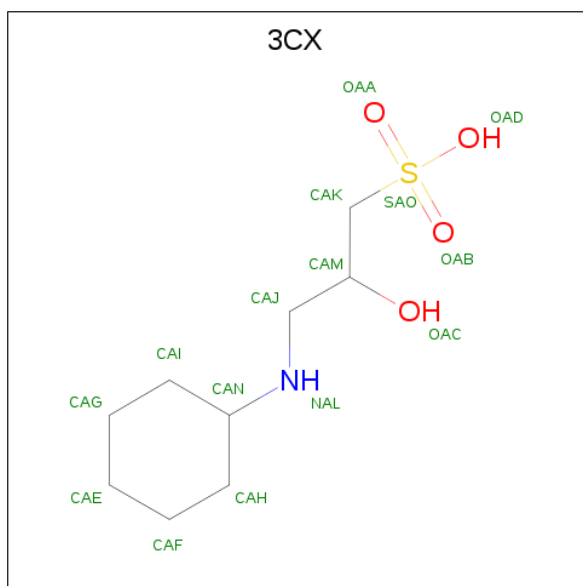
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

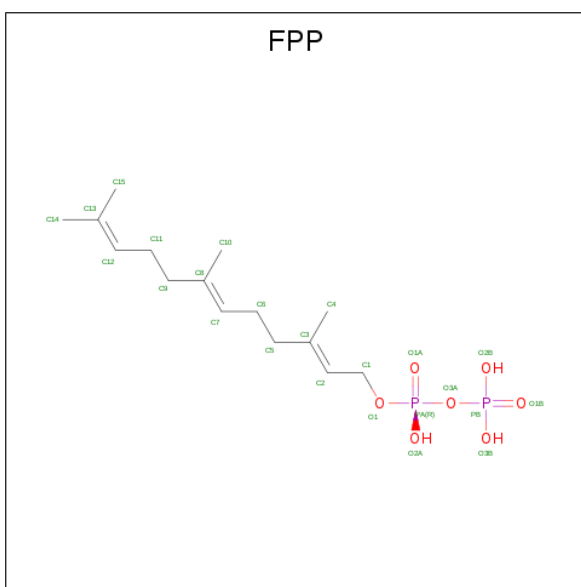
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2S)-3-(cyclohexylamino)-2-hydroxypropane-1-sulfonic acid (three-letter code: 3CX) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>4</sub>S).



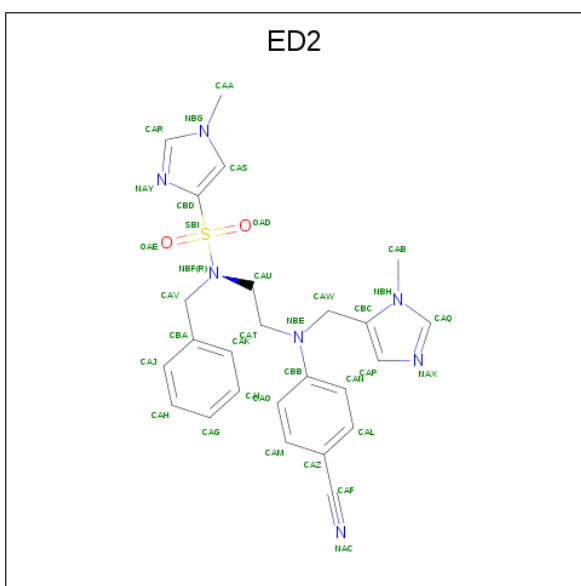
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		

- Molecule 6 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>7</sub>P<sub>2</sub>).



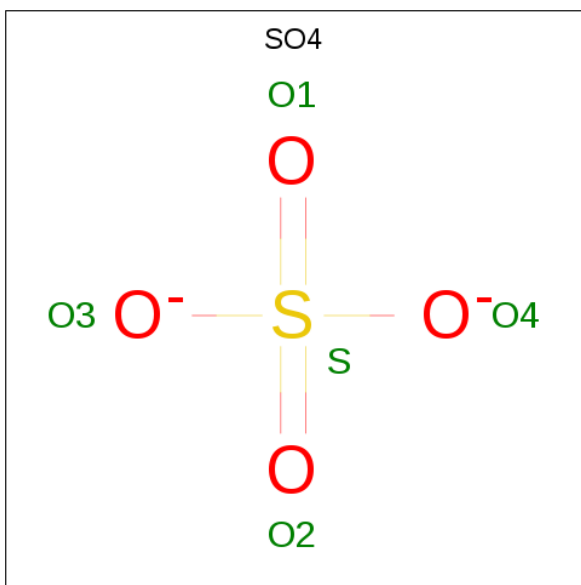
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 7 is N-benzyl-N-(2-{(4-cyanophenyl)[(1-methyl-1H-imidazol-5-yl)methyl]amino}ethyl)-1-methyl-1H-imidazole-4-sulfonamide (three-letter code: ED2) (formula:  $C_{25}H_{27}N_7O_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			35	25	7	2	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

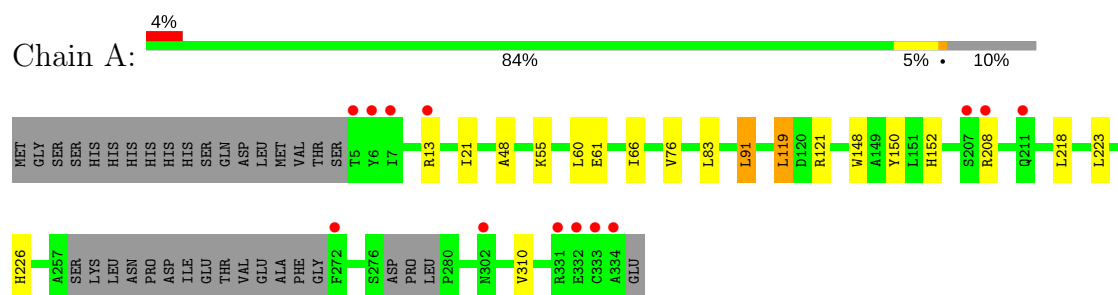
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	171	Total	O	0	0
			171	171		
9	B	317	Total	O	0	0
			317	317		

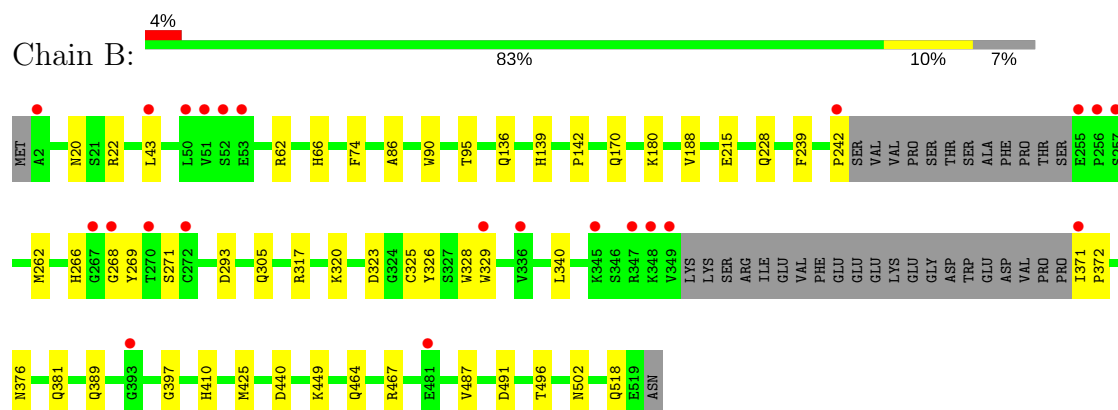
### 3 Residue-property plots [i](#)

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: Farnesyltransferase alpha subunit



#### • Molecule 2: Farnesyltransferase beta subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.58Å 143.58Å 130.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.94 – 2.20 44.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.94-2.20) 99.1 (44.94-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.191 , 0.213 0.194 , 0.215	Depositor DCC
$R_{free}$ test set	3447 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7003	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: ZN, SUC, ED2, SO4, FPP, 3CX

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	0.35	0/2687	0.47	0/3657
2	B	0.37	0/3827	0.50	1/5198 (0.0%)
All	All	0.36	0/6514	0.48	1/8855 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	242	PRO	CA-N-CD	-8.53	99.56	111.50

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	2606	0	2526	10	0
2	B	3730	0	3657	37	0
3	A	23	0	22	0	0
3	B	46	0	44	1	0
4	B	1	0	0	0	0
5	B	45	0	48	1	0
6	B	24	0	25	3	0
7	B	35	0	27	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	5	0	0	0	0
9	A	171	0	0	1	0
9	B	317	0	0	1	0
All	All	7003	0	6349	50	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 4.

The worst 5 of 50 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)
2:B:228:GLN:HE22	2:B:293:ASP:H	1.19	0.89
2:B:62:ARG:H	2:B:389:GLN:HE22	1.20	0.86
2:B:464:GLN:HE22	2:B:467:ARG:HH11	1.25	0.82
2:B:66:HIS:HD1	2:B:397:GLY:H	1.28	0.82
2:B:440:ASP:H	2:B:518:GLN:HE22	1.29	0.79

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	307/349 (88%)	298 (97%)	9 (3%)	0	100	100
2	B	480/520 (92%)	472 (98%)	8 (2%)	0	100	100
All	All	787/869 (91%)	770 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	283/316 (90%)	275 (97%)	8 (3%)	47	59
2	B	404/436 (93%)	401 (99%)	3 (1%)	85	93
All	All	687/752 (91%)	676 (98%)	11 (2%)	65	79

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	ARG
1	A	218	LEU
2	B	22	ARG
1	A	119	LEU
1	A	310	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	219	ASN
2	B	266	HIS
2	B	414	ASN
2	B	170	GLN
2	B	464	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	SUC	A	3010	-	24,24,24	1.06	1 (4%)	36,36,36	0.95	2 (5%)
3	SUC	B	1002	-	24,24,24	1.05	1 (4%)	36,36,36	1.01	2 (5%)
7	ED2	B	1003	4	34,38,38	1.95	7 (20%)	41,53,53	1.62	6 (14%)
3	SUC	B	3010	-	24,24,24	1.07	1 (4%)	36,36,36	0.99	1 (2%)
5	3CX	B	522	-	15,15,15	1.92	1 (6%)	17,20,20	1.77	5 (29%)
5	3CX	B	523	-	15,15,15	1.97	1 (6%)	17,20,20	2.00	4 (23%)
5	3CX	B	524	-	15,15,15	2.01	1 (6%)	17,20,20	2.01	4 (23%)
6	FPP	B	525	-	22,23,23	1.30	2 (9%)	25,31,31	1.28	5 (20%)
8	SO4	B	526	-	4,4,4	0.14	0	6,6,6	0.11	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	SUC	A	3010	-	4/4/9/9	0/12/51/51	0/2/2/2
3	SUC	B	1002	-	4/4/9/9	0/12/51/51	0/2/2/2
7	ED2	B	1003	4	-	0/25/31/31	0/4/4/4
3	SUC	B	3010	-	4/4/9/9	0/12/51/51	0/2/2/2
5	3CX	B	522	-	1/1/3/4	0/10/18/18	0/1/1/1
5	3CX	B	523	-	1/1/3/4	0/10/18/18	0/1/1/1
5	3CX	B	524	-	1/1/3/4	0/10/18/18	0/1/1/1
6	FPP	B	525	-	-	0/25/25/25	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	B	526	-	-	0/0/0/0	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	524	3CX	OAC-CAM	-7.13	1.22	1.43
5	B	523	3CX	OAC-CAM	-7.11	1.22	1.43
5	B	522	3CX	OAC-CAM	-6.81	1.23	1.43
6	B	525	FPP	O1-C1	-3.74	1.38	1.43
7	B	1003	ED2	CBD-SBI	-2.78	1.76	1.78

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1003	ED2	OAD-SBI-OAE	-6.35	109.06	119.50
7	B	1003	ED2	NAX-CAQ-NBH	-2.56	108.35	112.18
3	B	1002	SUC	C1-O5-C5	-2.41	108.96	113.71
6	B	525	FPP	PA-O3A-PB	-2.26	125.04	132.63
6	B	525	FPP	C4-C3-C2	-2.18	117.97	123.70

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	522	3CX	CAM
5	B	524	3CX	CAM
5	B	523	3CX	CAM
3	B	3010	SUC	C2
3	B	3010	SUC	C4'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1003	ED2	5	0
3	B	3010	SUC	1	0
5	B	522	3CX	1	0
6	B	525	FPP	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, 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	313/349 (89%)	-0.10	13 (4%) 36 34	26, 41, 62, 71	0
2	B	485/520 (93%)	0.10	23 (4%) 31 30	21, 33, 49, 71	0
All	All	798/869 (91%)	0.02	36 (4%) 33 32	21, 36, 59, 71	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	349	VAL	8.0
2	B	255	GLU	5.8
1	A	5	THR	5.4
2	B	257	SER	5.3
1	A	333	CYS	5.0

### 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 [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( $\text{\AA}^2$ )	Q<0.9
3	SUC	A	3010	23/23	0.66	0.30	79,80,81,81	0
3	SUC	B	3010	23/23	0.80	0.24	72,72,73,73	0
5	3CX	B	524	15/15	0.80	0.20	64,67,73,73	0
3	SUC	B	1002	23/23	0.85	0.16	44,47,47,48	0
7	ED2	B	1003	35/35	0.86	0.21	45,52,62,62	0
8	SO4	B	526	5/5	0.92	0.25	79,79,79,79	0
6	FPP	B	525	24/24	0.95	0.22	33,37,41,42	0
5	3CX	B	523	15/15	0.96	0.14	46,47,48,50	0
5	3CX	B	522	15/15	0.98	0.11	27,28,30,31	0
4	ZN	B	521	1/1	1.00	0.14	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.