



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:29 PM GMT

PDB ID : 4LNB
Title : Aspergillus fumigatus protein farnesyltransferase ternary complex with farnesyl diphosphate and ethylenediamine scaffold inhibitor 5
Authors : Mabanglo, M.F.; Hast, M.A.; Beese, L.S.
Deposited on : 2013-07-11
Resolution : 1.75 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

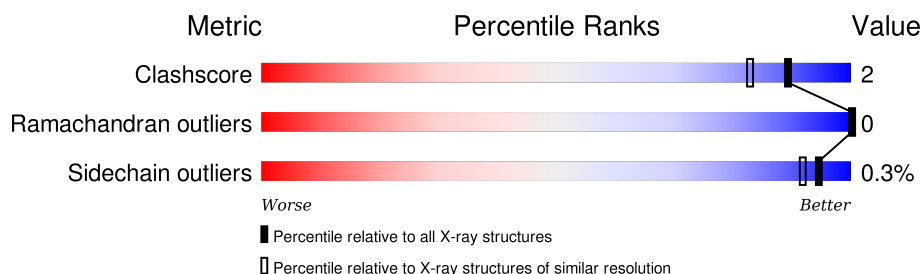
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)

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. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	367	
2	B	519	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6933 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 CaaX farnesyltransferase alpha subunit Ram2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	4	0
			2794	1777	490	518	9			

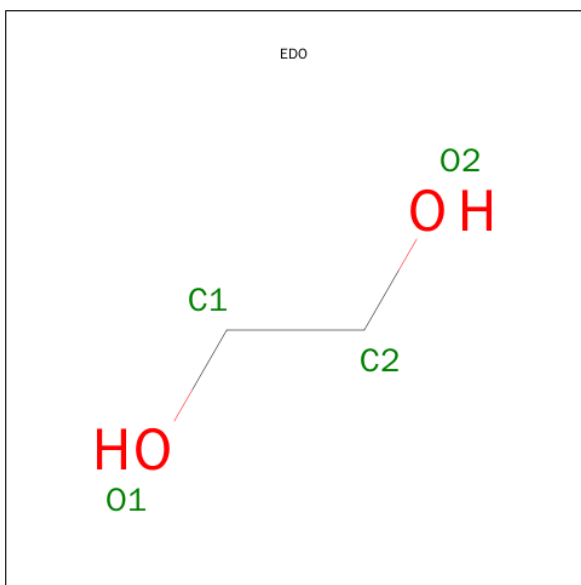
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	INITIATING METHIONINE	UNP Q4WP27
A	-12	GLY	-	EXPRESSION TAG	UNP Q4WP27
A	-11	SER	-	EXPRESSION TAG	UNP Q4WP27
A	-10	SER	-	EXPRESSION TAG	UNP Q4WP27
A	-9	HIS	-	EXPRESSION TAG	UNP Q4WP27
A	-8	HIS	-	EXPRESSION TAG	UNP Q4WP27
A	-7	HIS	-	EXPRESSION TAG	UNP Q4WP27
A	-6	HIS	-	EXPRESSION TAG	UNP Q4WP27
A	-5	HIS	-	EXPRESSION TAG	UNP Q4WP27
A	-4	HIS	-	EXPRESSION TAG	UNP Q4WP27
A	-3	SER	-	EXPRESSION TAG	UNP Q4WP27
A	-2	GLN	-	EXPRESSION TAG	UNP Q4WP27
A	-1	ASP	-	EXPRESSION TAG	UNP Q4WP27
A	0	PRO	-	EXPRESSION TAG	UNP Q4WP27
A	146	SER	ASN	ENGINEERED MUTATION	UNP Q4WP27

- Molecule 2 is a protein called CaaX farnesyltransferase beta subunit Ram1.

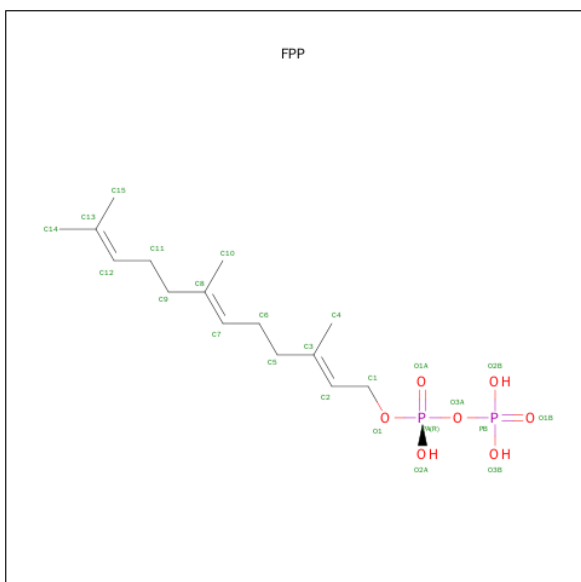
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	447	Total	C	N	O	S	0	11	0
			3518	2243	595	656	24			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is FARNESYL DIPHOSPHATE (three-letter code: FPP) (formula: $C_{15}H_{28}O_7P_2$).

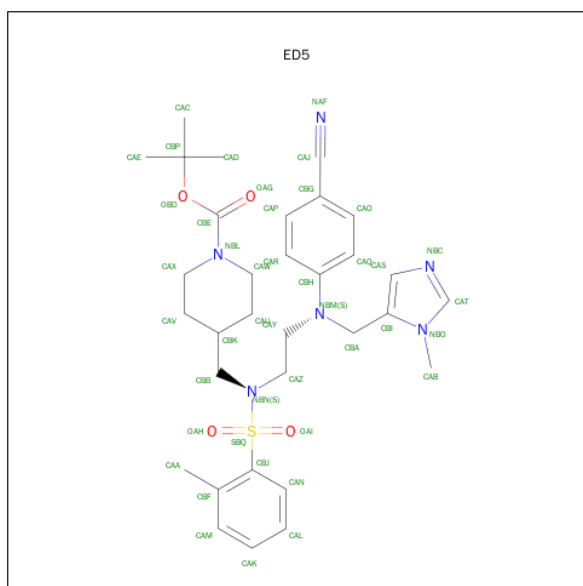


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			24	15	7	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is TERT-BUTYL 4-((2-((4-CYANOPHENYL)[(1-METHYL-1H-IMIDAZOL-5-YL)METHYL]AMINO)ETHYL)[(2-METHYLPHENYL)SULFONYL]AMINO}METHYL) PIPERIDINE-1-CARBOXYLATE (three-letter code: ED5) (formula: C₃₂H₄₂N₆O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			43	32	6	4	1		

- Molecule 7 is water.

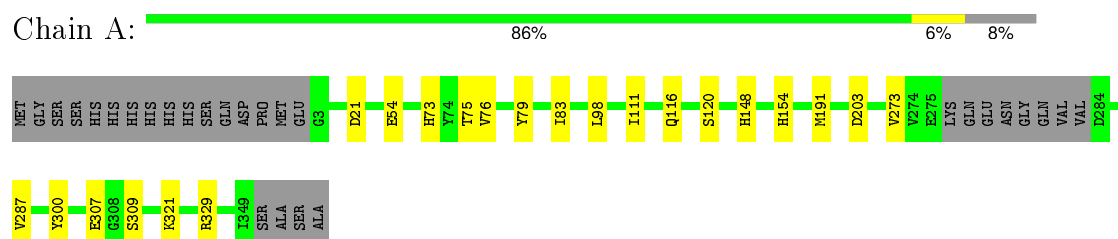
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	227	Total	O	0	0
			227	227		
7	B	306	Total	O	0	0
			306	306		

3 Residue-property plots

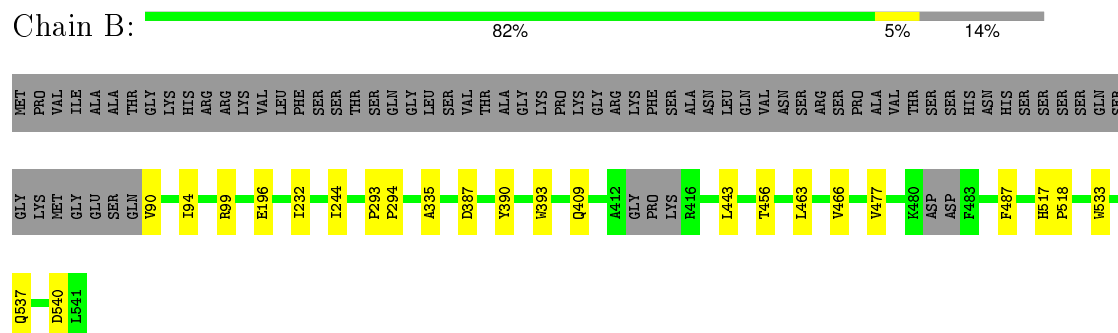
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS failed to run properly.

- Molecule 1: CaaX farnesyltransferase alpha subunit Ram2



- Molecule 2: CaaX farnesyltransferase beta subunit Ram1



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.32Å 91.25Å 83.05Å 90.00° 110.93° 90.00°	Depositor
Resolution (Å)	37.07 – 1.75	Depositor
% Data completeness (in resolution range)	94.0 (37.07-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.159 , 0.184	Depositor
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.342	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83348 reflections	Xtriage
Total number of atoms	6933	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ED5, EDO, FPP

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	0.23	0/2884	0.41	1/3914 (0.0%)
2	B	0.25	0/3642	0.44	0/4949
All	All	0.24	0/6526	0.43	1/8863 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	CB-CG-OD1	7.81	125.33	118.30

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	2794	0	2696	14	0
2	B	3518	0	3407	14	0
3	A	12	0	18	2	0
3	B	8	0	12	0	0
4	B	24	0	25	2	0
5	B	1	0	0	0	0
6	B	43	0	42	1	0
7	A	227	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	306	0	0	2	0
All	All	6933	0	6200	30	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 (30) 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:90:VAL:HG12	2:B:90:VAL:O	2.00	0.60
2:B:409:GLN:NE2	7:B:965:HOH:O	2.43	0.51
2:B:196:GLU:HG2	7:B:841:HOH:O	2.12	0.50
2:B:94:ILE:O	2:B:99:ARG:NH1	2.43	0.49
1:A:300:TYR:O	1:A:309:SER:OG	2.26	0.49
2:B:232:ILE:HD13	2:B:244:ILE:HD11	1.94	0.49
2:B:533:TRP:O	2:B:537:GLN:HG2	2.13	0.48
1:A:148:HIS:HE1	3:A:401:EDO:H22	1.80	0.47
1:A:154[A]:HIS:CD2	1:A:191:MET:HG3	2.50	0.47
1:A:154[A]:HIS:CD2	1:A:191:MET:HE2	2.50	0.46
1:A:154[A]:HIS:HE1	1:A:203:ASP:OD2	1.98	0.46
1:A:273:VAL:HG12	1:A:287:VAL:HG22	1.98	0.46
1:A:73:HIS:O	1:A:76:VAL:HG12	2.15	0.46
1:A:73:HIS:CE1	1:A:75:THR:HB	2.51	0.46
2:B:477:VAL:HG22	2:B:487:PHE:HB3	1.97	0.45
2:B:387:ASP:HB3	2:B:390:TYR:CD2	2.52	0.44
2:B:335:ALA:HB1	4:B:601:FPP:H92	1.98	0.44
2:B:443:LEU:HB2	2:B:456:THR:HA	1.99	0.44
1:A:148:HIS:CE1	3:A:401:EDO:H22	2.53	0.43
1:A:54:GLU:O	1:A:79:TYR:OH	2.26	0.43
2:B:463:LEU:O	2:B:466:VAL:HG22	2.18	0.43
1:A:321:LYS:HB2	1:A:329:ARG:HG3	2.01	0.42
1:A:98:LEU:HD11	1:A:111:ILE:HG23	2.01	0.42
2:B:517:HIS:HA	2:B:518:PRO:HD3	1.91	0.42
4:B:601:FPP:H61	4:B:601:FPP:H103	1.98	0.41
6:B:603:ED5:HAQ	6:B:603:ED5:HBAA	1.87	0.41
1:A:79:TYR:CE2	1:A:83:ILE:HD11	2.56	0.41
2:B:335:ALA:HA	2:B:393:TRP:HB3	2.03	0.40
2:B:293:PRO:HA	2:B:294:PRO:HD3	1.94	0.40
1:A:116:GLN:O	1:A:120[A]:SER:OG	2.24	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	339/367 (92%)	330 (97%)	9 (3%)	0	100	100
2	B	452/519 (87%)	448 (99%)	4 (1%)	0	100	100
All	All	791/886 (89%)	778 (98%)	13 (2%)	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	295/315 (94%)	294 (100%)	1 (0%)	94	92
2	B	379/428 (89%)	378 (100%)	1 (0%)	94	92
All	All	674/743 (91%)	672 (100%)	2 (0%)	94	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	GLU
2	B	540	ASP

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	EDO	A	401	-	3,3,3	0.56	0	2,2,2	0.69	0
3	EDO	A	402	-	3,3,3	0.54	0	2,2,2	0.68	0
3	EDO	A	403	-	3,3,3	0.57	0	2,2,2	0.62	0
4	FPP	B	601	-	21,23,23	3.62	7 (33%)	27,31,31	2.85	13 (48%)
6	ED5	B	603	5	44,46,46	2.26	9 (20%)	61,66,66	1.92	14 (22%)
3	EDO	B	604	-	3,3,3	0.54	0	2,2,2	0.66	0
3	EDO	B	605	-	3,3,3	0.55	0	2,2,2	0.66	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	EDO	A	401	-	-	0/1/1/1	0/0/0/0
3	EDO	A	402	-	-	0/1/1/1	0/0/0/0
3	EDO	A	403	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FPP	B	601	-	-	0/25/25/25	0/0/0/0
6	ED5	B	603	5	-	0/40/50/50	0/4/4/4
3	EDO	B	604	-	-	0/1/1/1	0/0/0/0
3	EDO	B	605	-	-	0/1/1/1	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	FPP	C11-C12	-3.84	1.39	1.50
4	B	601	FPP	C6-C7	-3.47	1.40	1.50
4	B	601	FPP	O1-C1	-2.97	1.39	1.43
4	B	601	FPP	C1-C2	-2.87	1.39	1.49
6	B	603	ED5	CBI-NBO	-2.27	1.33	1.38
6	B	603	ED5	OBD-CBP	-2.17	1.44	1.48
6	B	603	ED5	CBB-NBN	3.14	1.52	1.47
6	B	603	ED5	SBQ-NBN	3.34	1.68	1.63
6	B	603	ED5	CAZ-NBN	3.63	1.53	1.48
6	B	603	ED5	CBH-NBM	4.24	1.50	1.38
6	B	603	ED5	OBD-CBE	4.72	1.42	1.34
4	B	601	FPP	C12-C13	6.42	1.52	1.32
6	B	603	ED5	CBE-NBL	7.02	1.48	1.35
6	B	603	ED5	CAJ-NAF	7.73	1.32	1.14
4	B	601	FPP	C2-C3	9.56	1.51	1.33
4	B	601	FPP	C7-C8	9.69	1.52	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	FPP	C4-C3-C2	-6.62	110.50	123.50
6	B	603	ED5	OAH-SBQ-OAI	-6.27	108.65	119.47
4	B	601	FPP	C10-C8-C7	-5.72	112.27	123.50
4	B	601	FPP	C9-C8-C7	-5.27	111.06	121.05
4	B	601	FPP	C5-C3-C2	-5.12	111.34	121.05
6	B	603	ED5	OBD-CBE-OAG	-4.21	119.23	126.17
4	B	601	FPP	C10-C8-C9	-3.87	109.50	115.41
4	B	601	FPP	C6-C7-C8	-3.17	120.87	127.76
6	B	603	ED5	OAG-CBE-NBL	-3.05	118.51	124.32
6	B	603	ED5	CBB-NBN-SBQ	-2.80	111.36	117.46
4	B	601	FPP	C15-C13-C12	-2.70	113.93	122.61
4	B	601	FPP	C4-C3-C5	-2.62	111.40	115.41
4	B	601	FPP	C14-C13-C12	-2.61	114.21	122.61
6	B	603	ED5	CAA-CBF-CBJ	-2.40	121.60	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	603	ED5	NBC-CAT-NBO	-2.39	109.05	112.28
6	B	603	ED5	CAZ-NBN-CBB	-2.32	112.88	116.76
4	B	601	FPP	C11-C12-C13	-2.02	119.95	127.73
4	B	601	FPP	O3A-PA-O1	2.05	108.38	102.94
6	B	603	ED5	CBA-NBM-CAY	2.06	120.31	116.25
6	B	603	ED5	CBP-OBDB-CBE	2.23	123.56	121.00
6	B	603	ED5	CAM-CBF-CBJ	2.92	119.80	116.21
4	B	601	FPP	C9-C11-C12	2.94	119.40	111.69
6	B	603	ED5	OAH-SBQ-NBN	2.97	109.63	106.69
4	B	601	FPP	C5-C6-C7	3.09	119.77	111.69
6	B	603	ED5	CAY-CAZ-NBN	4.28	119.73	112.35
6	B	603	ED5	OAI-SBQ-NBN	4.82	111.45	106.69
6	B	603	ED5	OBDB-CBE-NBL	5.60	119.60	110.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	EDO	2	0
4	B	601	FPP	2	0
6	B	603	ED5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section will therefore be empty.