Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2020 – 03:49 PM BST

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PDB ID	:	3Q78
Title	:	Cryptococcus neoformans protein farnesyltransferase in complex with FSPP and DDPTASACNIQ peptide
Authors	:	Hast, M.A.; Beese, L.S.
Deposited on	:	2011-01-04
Resolution	:	2.20 Å(reported)

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1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
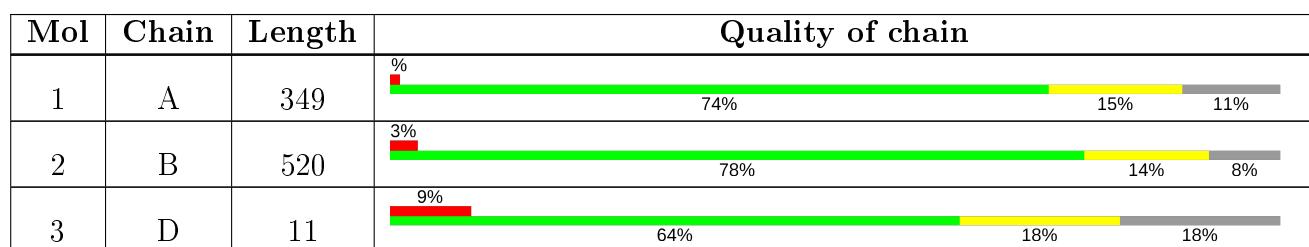
The reported resolution of this entry is 2.20 Å.

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 >=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 <=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	
2	B	520	
3	D	11	

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
5	3CX	B	522	X	-	-	-
5	3CX	B	523	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6742 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	312	Total	C	N	O	S	0	0	0
			2603	1680	443	469	11			

- Molecule 2 is a protein called Farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	478	Total	C	N	O	S	0	0	0
			3678	2334	642	688	14			
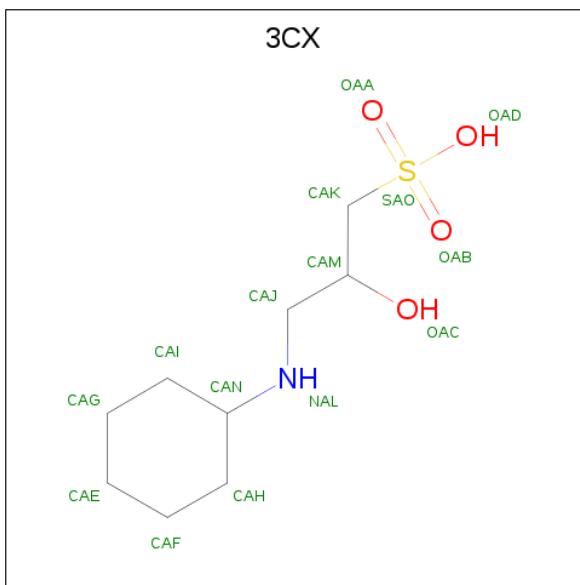
- Molecule 3 is a protein called peptide substrate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	9	Total	C	N	O	S	0	0	0
			62	36	11	14	1			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).
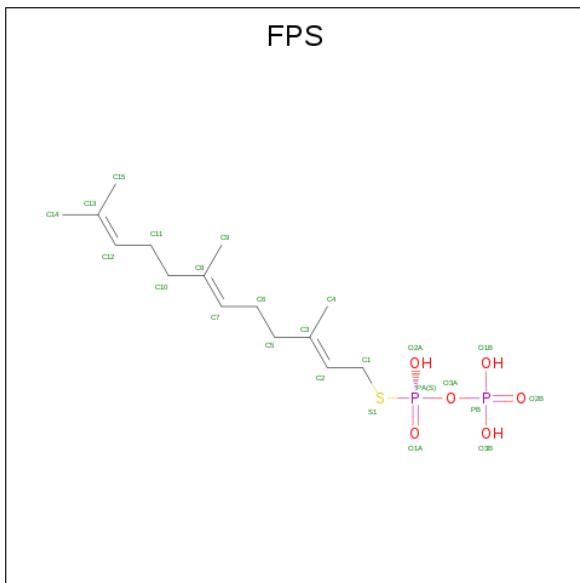
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is (2S)-3-(cyclohexylamino)-2-hydroxypropane-1-sulfonic acid (three-letter code: 3CX) (formula: $C_9H_{19}NO_4S$).

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		

- Molecule 6 is S-[(2E,6E)-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENYL] TRIHYDRO-GEN THIODIPHOSPHATE (three-letter code: FPS) (formula: $C_{15}H_{28}O_6P_2S$).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	113	Total 113	O 113	0	0
7	B	227	Total 227	O 227	0	0
7	D	4	Total 4	O 4	0	0
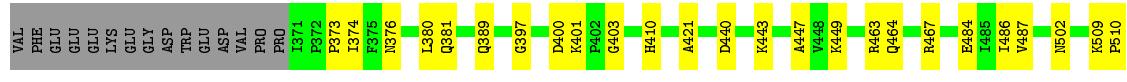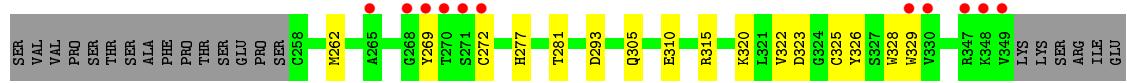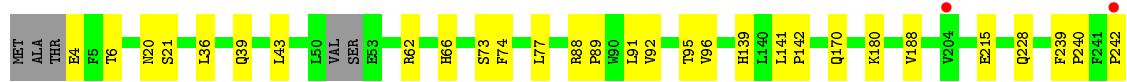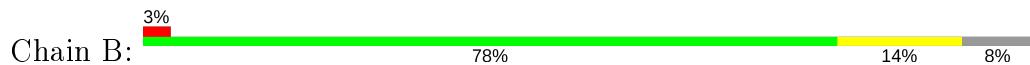
3 Residue-property plots (i)

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

- Molecule 3: peptide substrate

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.02Å 143.02Å 130.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.23 – 2.20 45.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.23-2.20) 100.0 (45.23-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.01 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.6.1_336	Depositor
R, R_{free}	0.183 , 0.214 0.178 , 0.208	Depositor DCC
R_{free} test set	3452 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.9	EDS
L-test for twinning[2]	$<\left|L\right|> = 0.45$, $<L^2> = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6742	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<\left|L\right|>$, $<L^2>$ 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, 3CX, FPS

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	0.21	0/2683	0.36	0/3651
2	B	0.22	0/3770	0.41	1/5118 (0.0%)
3	D	0.19	0/62	0.35	0/82
All	All	0.22	0/6515	0.39	1/8851 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	242	PRO	CA-N-CD	-8.59	99.47	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	2603	0	2525	38	0
2	B	3678	0	3603	61	0
3	D	62	0	58	2	0
4	B	1	0	0	0	0
5	B	30	0	33	0	0
6	B	24	0	25	8	0
7	A	113	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	227	0	0	2	0
7	D	4	0	0	0	0
All	All	6742	0	6244	94	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 7.

All (94) 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:62:ARG:H	2:B:389:GLN:HE22	1.15	0.92
2:B:440:ASP:H	2:B:518:GLN:HE22	1.20	0.88
2:B:228:GLN:HE22	2:B:293:ASP:H	1.20	0.88
2:B:66:HIS:HD1	2:B:397:GLY:H	1.28	0.77
2:B:464:GLN:HE22	2:B:467:ARG:HE	1.32	0.77
2:B:139:HIS:HD2	2:B:141:LEU:H	1.32	0.76
2:B:170:GLN:HE22	2:B:449:LYS:H	1.32	0.76
2:B:305:GLN:HE22	2:B:376:ASN:H	1.38	0.71
6:B:524:FPS:H12	3:D:10:ILE:HB	1.75	0.66
1:A:226:HIS:H	2:B:20:ASN:HD21	1.41	0.64
2:B:464:GLN:NE2	2:B:467:ARG:HE	1.96	0.63
2:B:381:GLN:HE22	2:B:487:VAL:H	1.48	0.61
2:B:323:ASP:HB3	2:B:326:TYR:CD2	2.35	0.61
2:B:74:PHE:CD2	2:B:95:THR:HG21	2.38	0.59
2:B:170:GLN:NE2	2:B:449:LYS:H	2.00	0.59
2:B:62:ARG:H	2:B:389:GLN:NE2	1.93	0.58
2:B:329:TRP:CH2	6:B:524:FPS:H142	2.38	0.58
1:A:145:TYR:HB3	6:B:524:FPS:H42	1.84	0.58
2:B:320:LYS:HE3	6:B:524:FPS:O3B	2.04	0.57
2:B:170:GLN:HE22	2:B:449:LYS:N	2.02	0.56
2:B:447:ALA:HB2	2:B:463:ARG:CZ	2.36	0.56
1:A:9:MET:HA	1:A:12:ARG:HG3	1.89	0.55
1:A:152:HIS:HE1	7:A:1787:HOH:O	1.90	0.55
2:B:328:TRP:CZ2	2:B:502:ASN:HB2	2.42	0.55
1:A:31:VAL:HG21	2:B:91:LEU:HB3	1.89	0.55
2:B:73:SER:HB3	2:B:77:LEU:HD21	1.89	0.54
2:B:272:CYS:SG	6:B:524:FPS:H143	2.48	0.53
2:B:180:LYS:HE2	2:B:215:GLU:O	2.08	0.53
2:B:239:PHE:HB2	2:B:262:MET:SD	2.49	0.53
2:B:440:ASP:H	2:B:518:GLN:NE2	1.99	0.52
2:B:381:GLN:NE2	2:B:487:VAL:H	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:N	1:A:248:ILE:HD12	2.26	0.51
1:A:226:HIS:H	2:B:20:ASN:ND2	2.08	0.51
1:A:148:TRP:O	1:A:152:HIS:HD2	1.94	0.50
1:A:131:ILE:HD13	1:A:155:TYR:CZ	2.47	0.50
1:A:23:GLN:HB2	1:A:47:ARG:NH2	2.27	0.50
1:A:252:ILE:HD12	1:A:252:ILE:N	2.28	0.49
1:A:31:VAL:HG21	2:B:91:LEU:CB	2.43	0.49
1:A:91:LEU:HD11	1:A:121:ARG:HD3	1.94	0.49
1:A:119:LEU:HD13	1:A:150:TYR:OH	2.13	0.48
2:B:39:GLN:O	2:B:43:LEU:HD13	2.13	0.48
1:A:143:LYS:HD3	2:B:320:LYS:HD3	1.94	0.48
2:B:269:TYR:CZ	6:B:524:FPS:H52	2.49	0.48
1:A:195:TYR:HA	1:A:199:SER:OG	2.13	0.47
1:A:222:HIS:HD2	1:A:255:TYR:OH	1.96	0.47
1:A:9:MET:HG2	1:A:12:ARG:NH2	2.29	0.47
2:B:509:LYS:HB3	2:B:510:PRO:HD3	1.95	0.47
2:B:320:LYS:CE	6:B:524:FPS:O3B	2.63	0.47
2:B:66:HIS:HD1	2:B:397:GLY:N	2.03	0.47
2:B:88:ARG:HD3	7:B:1773:HOH:O	2.14	0.47
2:B:380:LEU:HD23	2:B:421:ALA:HB2	1.96	0.46
2:B:403:GLY:O	3:D:4:THR:HG22	2.15	0.46
2:B:62:ARG:N	2:B:389:GLN:HE22	1.98	0.46
1:A:31:VAL:N	1:A:32:PRO:HD3	2.31	0.46
1:A:156:SER:O	1:A:160:THR:HG23	2.16	0.46
1:A:60:LEU:HA	1:A:83:LEU:HD13	1.98	0.45
1:A:211:GLN:O	1:A:215:ILE:HG13	2.17	0.45
2:B:6:THR:CG2	2:B:373:PRO:HG2	2.47	0.45
1:A:137:SER:O	1:A:140:PRO:HD2	2.16	0.45
1:A:246:VAL:HB	1:A:247:PRO:HD3	1.99	0.45
1:A:124:PRO:HD2	1:A:158:PHE:CE2	2.52	0.45
2:B:325:CYS:HB3	2:B:410:HIS:CD2	2.52	0.44
2:B:6:THR:HG23	2:B:373:PRO:HG2	1.98	0.44
2:B:88:ARG:N	2:B:89:PRO:CD	2.80	0.44
2:B:323:ASP:HA	2:B:400:ASP:OD1	2.18	0.44
2:B:92:VAL:O	2:B:96:VAL:HG22	2.18	0.44
1:A:25:ASP:HB3	1:A:29:PRO:HG3	2.00	0.43
1:A:124:PRO:HD2	1:A:158:PHE:CZ	2.54	0.43
2:B:89:PRO:HG2	2:B:142:PRO:HB3	2.00	0.43
1:A:23:GLN:OE1	1:A:47:ARG:NH2	2.51	0.43
2:B:36:LEU:HA	2:B:36:LEU:HD12	1.87	0.43
2:B:443:LYS:HB3	2:B:443:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HG21	1:A:76:VAL:HG21	2.00	0.42
2:B:484:GLU:HG2	2:B:486:ILE:HD11	2.01	0.42
1:A:231:TRP:HH2	1:A:252:ILE:HG23	1.84	0.42
2:B:269:TYR:CE2	6:B:524:FPS:H52	2.55	0.42
1:A:119:LEU:CD2	1:A:130:GLU:HG2	2.49	0.42
2:B:374:ILE:HD12	2:B:374:ILE:HA	1.86	0.42
1:A:281:GLU:HB3	2:B:21:SER:OG	2.20	0.42
2:B:139:HIS:NE2	2:B:188:VAL:HB	2.34	0.42
2:B:239:PHE:HA	2:B:240:PRO:HD3	1.90	0.42
2:B:139:HIS:HB3	2:B:142:PRO:HD2	2.01	0.42
2:B:310:GLU:OE1	2:B:315:ARG:NH2	2.52	0.42
1:A:291:LEU:HB2	1:A:314:LEU:HD21	2.02	0.42
2:B:4:GLU:HB2	7:B:2008:HOH:O	2.19	0.42
2:B:464:GLN:HA	2:B:464:GLN:NE2	2.35	0.41
2:B:322:VAL:O	2:B:401:LYS:HD3	2.21	0.41
1:A:243:LEU:HA	1:A:244:PRO:HD3	1.91	0.41
2:B:277:HIS:O	2:B:281:THR:HG23	2.21	0.41
1:A:213:GLU:O	1:A:217:ILE:HG13	2.21	0.41
1:A:139:LEU:N	1:A:140:PRO:CD	2.84	0.40
1:A:31:VAL:HG13	1:A:31:VAL:O	2.21	0.40
1:A:99:ASN:O	1:A:103:VAL:HG23	2.20	0.40
2:B:139:HIS:CD2	2:B:142:PRO:HD2	2.57	0.40

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	304/349 (87%)	293 (96%)	11 (4%)	0	100	100
2	B	470/520 (90%)	462 (98%)	8 (2%)	0	100	100
3	D	7/11 (64%)	6 (86%)	1 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	781/880 (89%)	761 (97%)	20 (3%)	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%)	280 (99%)	3 (1%)	73 85
2	B	397/436 (91%)	397 (100%)	0	100 100
3	D	7/9 (78%)	7 (100%)	0	100 100
All	All	687/761 (90%)	684 (100%)	3 (0%)	91 96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	223	LEU
1	A	310	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	187	ASN
1	A	222	HIS
1	A	226	HIS
2	B	20	ASN
2	B	136	GLN
2	B	139	HIS
2	B	170	GLN
2	B	219	ASN
2	B	228	GLN

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Mol	Chain	Res	Type
2	B	304	GLN
2	B	305	GLN
2	B	319	ASN
2	B	381	GLN
2	B	389	GLN
2	B	414	ASN
2	B	464	GLN
2	B	495	ASN
2	B	518	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	#$|Z| > 2$
5	3CX	B	523	-	15,15,15	2.15	1 (6%)	16,20,20	5.13	8 (50%)
6	FPS	B	524	-	19,23,23	1.92	6 (31%)	23,31,31	1.18	3 (13%)
5	3CX	B	522	-	15,15,15	2.11	1 (6%)	16,20,20	5.42	11 (68%)

Full wwPDB X-ray Structure Validation Report

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
5	3CX	B	523	-	1/1/3/4	9/10/18/18	0/1/1/1
6	FPS	B	524	-	-	6/19/25/25	-
5	3CX	B	522	-	1/1/3/4	3/10/18/18	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	523	3CX	OAC-CAM	-7.36	1.21	1.43
5	B	522	3CX	OAC-CAM	-7.22	1.21	1.43
6	B	524	FPS	C6-C7	-3.36	1.39	1.50
6	B	524	FPS	C11-C12	-3.34	1.39	1.50
6	B	524	FPS	PA-O2A	-3.07	1.48	1.56
6	B	524	FPS	C7-C8	2.71	1.39	1.33
6	B	524	FPS	C2-C3	2.68	1.39	1.33
6	B	524	FPS	C12-C13	2.46	1.39	1.32

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	522	3CX	OAB-SAO-CAK	-12.65	91.90	106.94
5	B	523	3CX	OAB-SAO-CAK	-11.53	93.23	106.94
5	B	522	3CX	OAD-SAO-CAK	10.63	122.68	105.74
5	B	523	3CX	OAD-SAO-CAK	10.02	121.70	105.74
5	B	523	3CX	OAA-SAO-CAK	8.83	117.44	106.94
5	B	522	3CX	OAA-SAO-CAK	8.37	116.89	106.94
5	B	523	3CX	OAD-SAO-OAB	-8.05	91.61	111.27
5	B	522	3CX	OAD-SAO-OAB	-7.96	91.82	111.27
5	B	522	3CX	OAB-SAO-OAA	-3.97	100.20	113.95
5	B	523	3CX	OAB-SAO-OAA	-3.80	100.80	113.95
5	B	522	3CX	OAC-CAM-CAJ	3.32	120.66	109.32
5	B	522	3CX	CAM-CAJ-NAL	3.27	120.84	112.17
5	B	523	3CX	OAC-CAM-CAJ	3.15	120.07	109.32
5	B	522	3CX	OAD-SAO-OAA	2.98	118.56	111.27
5	B	523	3CX	OAD-SAO-OAA	2.94	118.47	111.27
6	B	524	FPS	C9-C8-C10	2.83	120.04	115.27
6	B	524	FPS	C4-C3-C5	2.80	119.98	115.27
5	B	522	3CX	CAI-CAN-CAH	2.64	115.40	110.82
5	B	523	3CX	CAM-CAJ-NAL	2.49	118.77	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	524	FPS	C15-C13-C14	2.46	120.03	114.60
5	B	522	3CX	CAG-CAI-CAN	2.20	115.25	111.11
5	B	522	3CX	CAF-CAH-CAN	2.14	115.14	111.11

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	523	3CX	CAM
5	B	522	3CX	CAM

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	523	3CX	CAM-CAJ-NAL-CAN
5	B	523	3CX	NAL-CAJ-CAM-OAC
5	B	523	3CX	CAM-CAK-SAO-OAA
5	B	523	3CX	CAM-CAK-SAO-OAB
6	B	524	FPS	C8-C10-C11-C12
5	B	522	3CX	NAL-CAJ-CAM-OAC
5	B	522	3CX	CAM-CAK-SAO-OAD
5	B	523	3CX	CAI-CAN-NAL-CAJ
5	B	523	3CX	SAO-CAK-CAM-OAC
5	B	523	3CX	CAM-CAK-SAO-OAD
6	B	524	FPS	C4-C3-C5-C6
6	B	524	FPS	PB-O3A-PA-O2A
6	B	524	FPS	C2-C3-C5-C6
5	B	523	3CX	CAH-CAN-NAL-CAJ
5	B	523	3CX	SAO-CAK-CAM-CAJ
5	B	522	3CX	SAO-CAK-CAM-CAJ
6	B	524	FPS	PB-O3A-PA-O1A
6	B	524	FPS	C11-C10-C8-C9
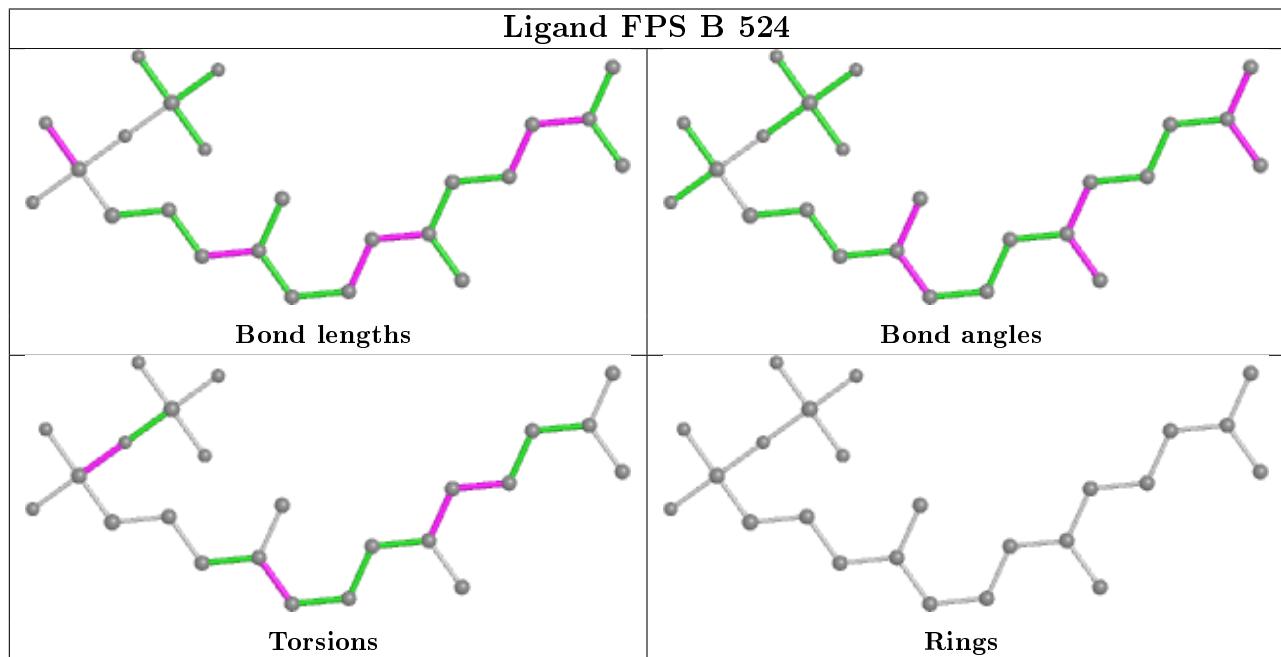
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	524	FPS	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FPS B 524

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	312/349 (89%)	-0.31	4 (1%) 77	75	30, 48, 85, 104	0
2	B	478/520 (91%)	-0.23	13 (2%) 54	52	27, 39, 68, 120	0
3	D	9/11 (81%)	0.97	1 (11%) 5	4	43, 71, 87, 116	0
All	All	799/880 (90%)	-0.25	18 (2%) 60	58	27, 43, 78, 120	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	349	VAL	4.9
2	B	348	LYS	3.4
1	A	334	ALA	3.3
1	A	208	ARG	3.2
3	D	3	PRO	3.0
2	B	242	PRO	2.8
2	B	347	ARG	2.7
2	B	268	GLY	2.6
1	A	5	THR	2.4
2	B	271	SER	2.4
2	B	204	VAL	2.3
1	A	7	ILE	2.3
2	B	272	CYS	2.3
2	B	269	TYR	2.2
2	B	330	VAL	2.2
2	B	329	TRP	2.2
2	B	270	THR	2.1
2	B	265	ALA	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.

WORLDWIDE PDB
PROTEIN DATA BANK

6.3 Carbohydrates (i)
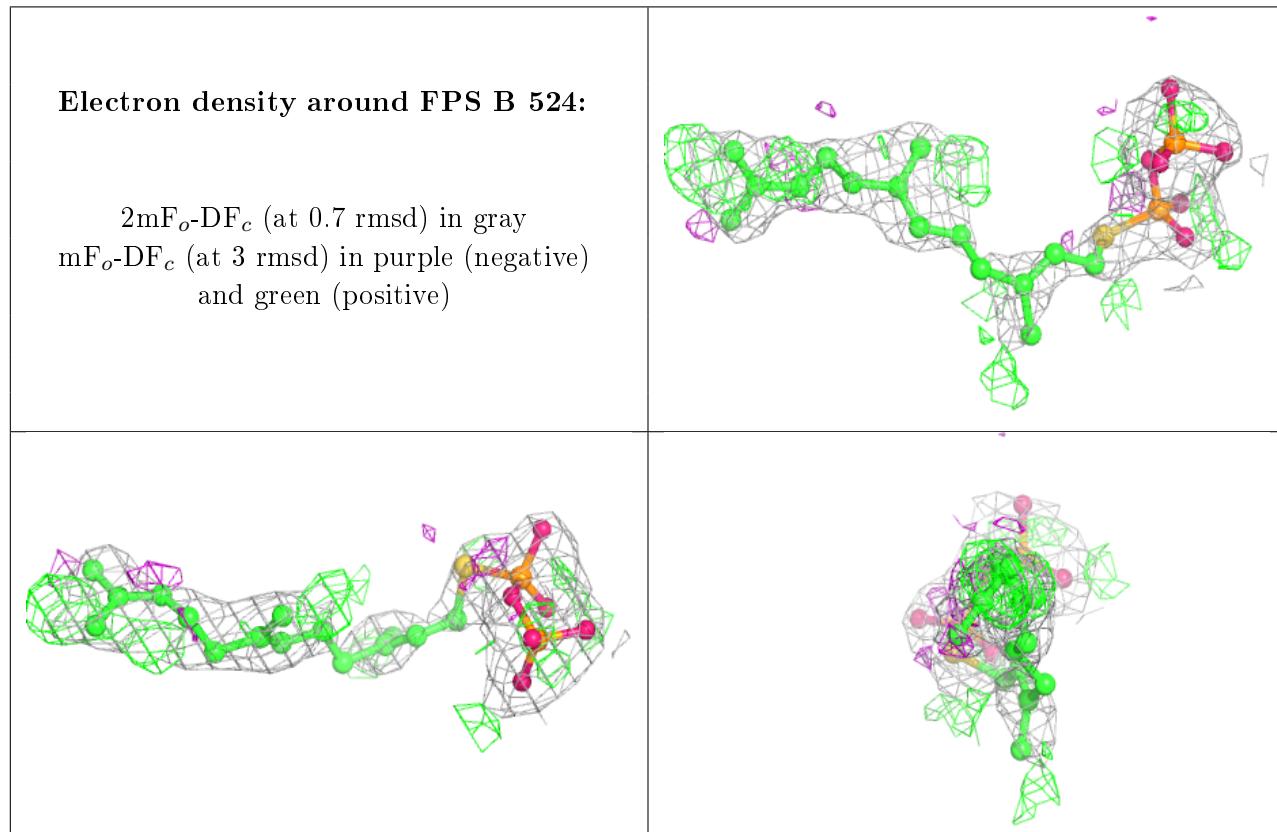
There are no monosaccharides in this entry.

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(Å^2)	Q<0.9
6	FPS	B	524	24/24	0.91	0.40	25,51,72,88	9
5	3CX	B	523	15/15	0.97	0.13	46,72,83,88	0
5	3CX	B	522	15/15	0.97	0.11	37,46,53,53	0
4	ZN	B	521	1/1	0.99	0.09	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FPS B 524:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.