



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:09 am BST

PDB ID : 1TCO  
Title : TERNARY COMPLEX OF A CALCINEURIN A FRAGMENT, CALCINEURIN B, FKBP12 AND THE IMMUNOSUPPRESSANT DRUG FK506 (TACROLIMUS)  
Authors : Griffith, J.P.; Kim, J.L.; Kim, E.E.; Sintchak, M.D.; Thomson, J.A.; Fitzgibbon, M.J.; Fleming, M.A.; Caron, P.R.; Hsiao, K.; Navia, M.A.  
Deposited on : 1996-08-21  
Resolution : 2.50 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

<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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

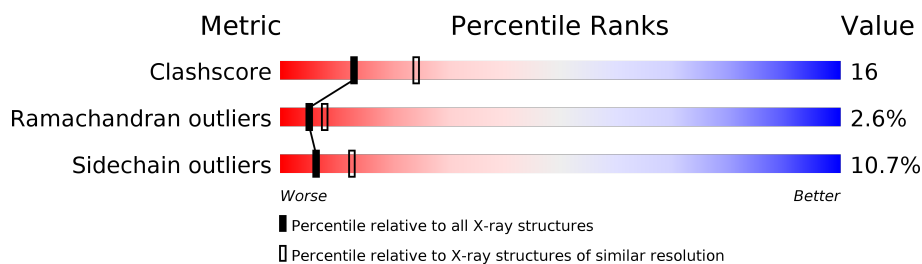
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	375	 64% 27% 6%
2	B	169	 57% 32% 10%
3	C	107	 65% 26% 8%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5827 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 SERINE/THREONINE PHOSPHATASE B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2863	1847	477	518	21	0	0	0

- Molecule 2 is a protein called SERINE/THREONINE PHOSPHATASE B2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	169	1345	847	223	267	8	0	0	0

- Molecule 3 is a protein called FK506-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	107	826	524	143	155	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	18	ALA	ARG	CONFLICT	UNP P62942

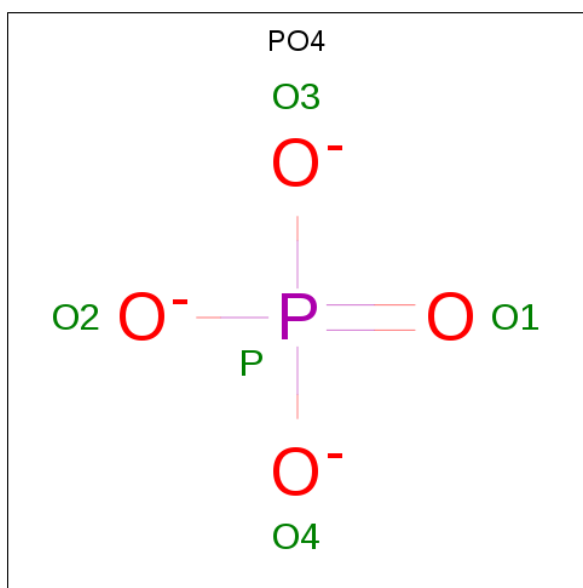
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
5	A	1	1	1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

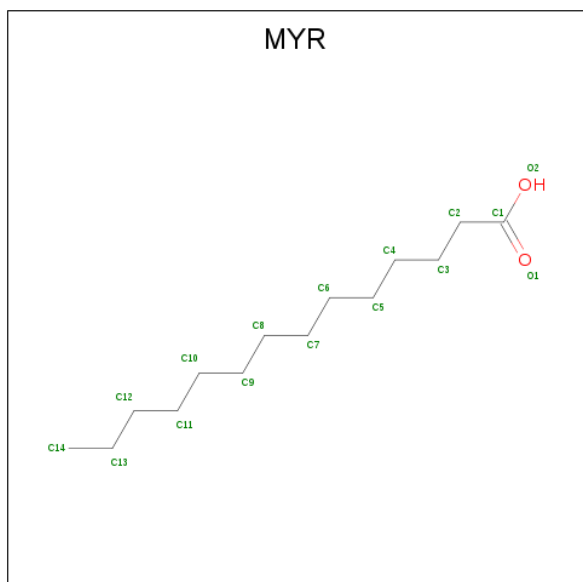


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

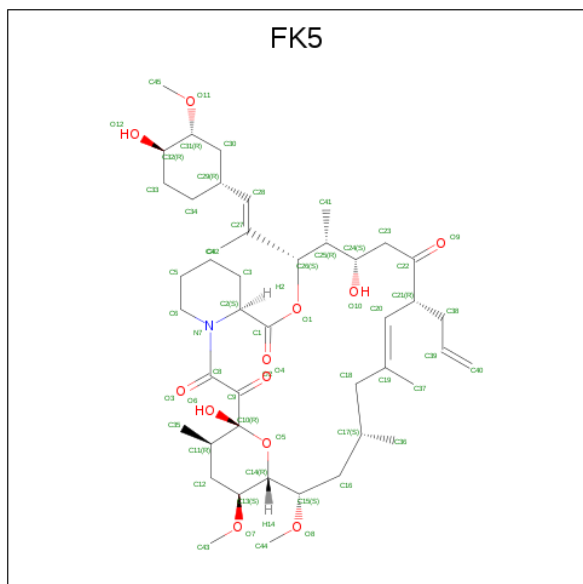
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	4	Total Ca 4 4	0	0

- Molecule 8 is MYRISTIC ACID (three-letter code: MYR) (formula:  $C_{14}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			15	14	1		

- Molecule 9 is 8-DEETHYL-8-[BUT-3-ENYL]-ASCOMYCIN (three-letter code: FK5) (formula:  $C_{44}H_{69}NO_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			57	44	1	12		

- Molecule 10 is water.

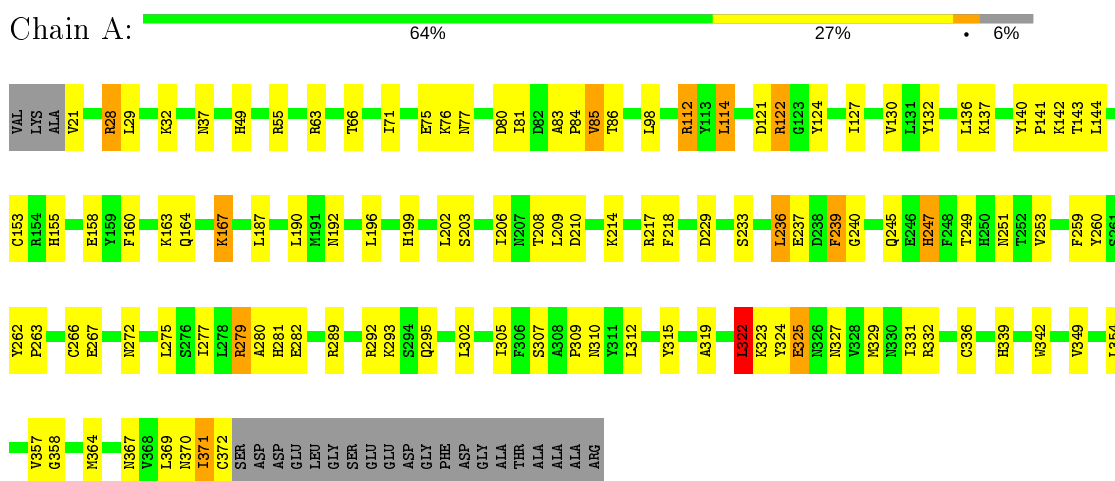
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	416	Total	O	0	0
			416	416		
10	B	185	Total	O	0	0
			185	185		
10	C	109	Total	O	0	0
			109	109		

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

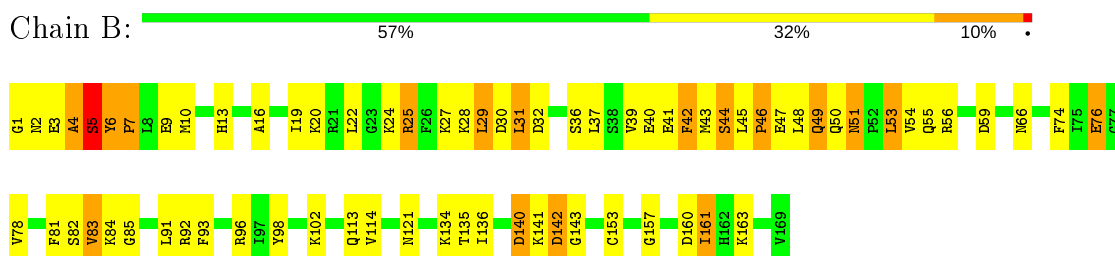
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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 was not executed.

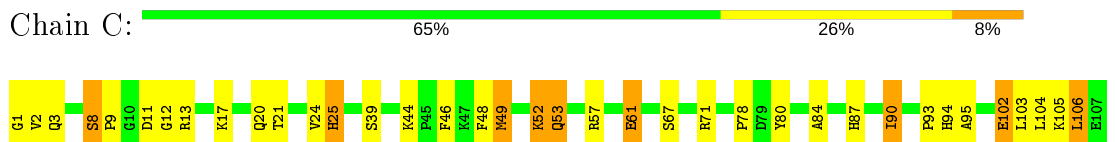
- Molecule 1: SERINE/THREONINE PHOSPHATASE B2



- Molecule 2: SERINE/THREONINE PHOSPHATASE B2



- Molecule 3: FK506-BINDING PROTEIN



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.05Å 94.43Å 116.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.195 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5827	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

## 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, PO4, MYR, FK5, FE, CA

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	0.43	0/2942	0.72	1/3993 (0.0%)
2	B	0.51	0/1364	0.84	3/1825 (0.2%)
3	C	0.41	0/845	0.74	0/1139
All	All	0.45	0/5151	0.76	4/6957 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	51	ASN	N-CA-C	-7.05	91.95	111.00
2	B	83	VAL	N-CA-C	-5.45	96.28	111.00
1	A	322	LEU	CA-CB-CG	5.26	127.40	115.30
2	B	143	GLY	N-CA-C	5.23	126.17	113.10

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	2863	0	2796	88	0
2	B	1345	0	1320	55	0
3	C	826	0	823	31	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
6	A	5	0	0	1	0
7	B	4	0	0	0	0
8	B	15	0	27	1	0
9	C	57	0	69	0	0
10	A	416	0	0	17	0
10	B	185	0	0	13	0
10	C	109	0	0	3	0
All	All	5827	0	5035	165	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 16.

All (165) 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:6:TYR:CD1	2:B:7:PRO:HD2	1.95	1.01
3:C:49:MET:SD	3:C:52:LYS:HG3	2.13	0.87
1:A:236:LEU:HD13	1:A:259:PHE:HB3	1.56	0.86
2:B:6:TYR:HD1	2:B:7:PRO:HD2	1.41	0.84
1:A:371:ILE:HD13	2:B:29:LEU:HD13	1.60	0.82
1:A:76:LYS:HE3	10:A:818:HOH:O	1.81	0.79
1:A:84:PRO:HB3	1:A:325:GLU:HG3	1.61	0.79
3:C:57:ARG:HB3	3:C:80:TYR:HD1	1.45	0.79
2:B:41:GLU:O	2:B:44:SER:HB2	1.85	0.77
3:C:8:SER:HB3	3:C:71:ARG:HB3	1.69	0.73
2:B:160:ASP:HB3	2:B:163:LYS:HE2	1.71	0.73
1:A:372:CYS:SG	2:B:28:LYS:HD3	2.30	0.72
1:A:84:PRO:O	1:A:112:ARG:HD3	1.91	0.71
1:A:323:LYS:HE2	1:A:332:ARG:HG3	1.72	0.70
2:B:16:ALA:O	2:B:20:LYS:HG3	1.92	0.69
3:C:1:GLY:HA2	3:C:80:TYR:CE2	2.28	0.69
3:C:57:ARG:HE	3:C:80:TYR:HE1	1.42	0.68
2:B:45:LEU:HB2	2:B:46:PRO:HD2	1.75	0.68
2:B:4:ALA:O	2:B:5:SER:HB2	1.94	0.67
1:A:239:PHE:O	1:A:262:TYR:HB2	1.96	0.66
1:A:32:LYS:N	1:A:32:LYS:HD2	2.10	0.66
1:A:160:PHE:HB3	10:A:630:HOH:O	1.96	0.65
2:B:98:TYR:HA	2:B:114:VAL:HG21	1.78	0.65
1:A:29:LEU:HG	1:A:49:HIS:CD2	2.32	0.64
1:A:122:ARG:HH11	1:A:122:ARG:HG3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:HB3	10:A:660:HOH:O	1.98	0.64
2:B:49:GLN:HG3	10:B:643:HOH:O	1.97	0.63
2:B:161:ILE:HB	10:B:577:HOH:O	1.99	0.62
1:A:364:MET:SD	2:B:54:VAL:HG22	2.39	0.62
3:C:24:VAL:HG12	3:C:103:LEU:HA	1.80	0.62
2:B:83:VAL:O	2:B:84:LYS:HB2	2.00	0.61
3:C:57:ARG:NE	3:C:80:TYR:HE1	1.98	0.61
1:A:164:GLN:O	1:A:167:LYS:HG2	2.00	0.61
3:C:57:ARG:HB3	3:C:80:TYR:CD1	2.33	0.60
1:A:349:VAL:HG22	2:B:135:THR:HG21	1.84	0.60
1:A:121:ASP:O	1:A:122:ARG:HB2	2.02	0.58
3:C:11:ASP:O	3:C:67:SER:HB2	2.02	0.58
3:C:105:LYS:HG2	3:C:106:LEU:H	1.67	0.58
2:B:136:ILE:O	2:B:140:ASP:HB2	2.04	0.58
3:C:90:ILE:HD12	3:C:90:ILE:H	1.68	0.58
1:A:203:SER:HB3	1:A:206:ILE:HD12	1.85	0.57
1:A:305:ILE:HD13	1:A:322:LEU:HD22	1.87	0.57
2:B:83:VAL:HG13	2:B:84:LYS:HD3	1.87	0.57
2:B:102:LYS:HG2	10:B:592:HOH:O	2.05	0.56
3:C:84:ALA:O	3:C:93:PRO:HB3	2.06	0.56
1:A:77:ASN:HB2	10:A:818:HOH:O	2.05	0.56
2:B:24:LYS:O	2:B:27:LYS:HB2	2.05	0.56
1:A:233:SER:HB3	1:A:260:TYR:CE2	2.41	0.56
1:A:210:ASP:O	1:A:214:LYS:HG3	2.06	0.56
3:C:20:GLN:HE22	3:C:106:LEU:HD23	1.71	0.56
3:C:17:LYS:O	3:C:20:GLN:HB2	2.06	0.55
3:C:52:LYS:C	3:C:53:GLN:HG3	2.26	0.55
3:C:105:LYS:HG2	3:C:106:LEU:N	2.22	0.55
1:A:371:ILE:O	1:A:372:CYS:SG	2.62	0.55
1:A:199:HIS:O	1:A:281:HIS:HB2	2.06	0.55
2:B:49:GLN:HG2	10:B:677:HOH:O	2.07	0.55
1:A:37:ASN:ND2	10:A:908:HOH:O	2.37	0.54
1:A:112:ARG:HG3	10:A:553:HOH:O	2.07	0.54
2:B:66:ASN:HB3	10:B:642:HOH:O	2.08	0.54
1:A:342:TRP:CE2	2:B:134:LYS:HE3	2.44	0.53
2:B:40:GLU:HB2	10:B:607:HOH:O	2.07	0.53
1:A:141:PRO:HG3	10:A:721:HOH:O	2.08	0.53
1:A:164:GLN:OE1	1:A:167:LYS:HD3	2.08	0.52
1:A:217:ARG:HG3	10:A:512:HOH:O	2.08	0.52
1:A:247:HIS:CD2	10:A:593:HOH:O	2.61	0.52
1:A:158:GLU:HG3	1:A:163:LYS:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:THR:HA	3:C:49:MET:HB3	1.91	0.52
2:B:19:ILE:HG22	8:B:508:MYR:H91	1.93	0.51
1:A:233:SER:HB3	1:A:260:TYR:HE2	1.75	0.51
2:B:13:HIS:NE2	2:B:85:GLY:HA2	2.25	0.51
1:A:310:ASN:HA	1:A:315:TYR:O	2.11	0.50
3:C:2:VAL:HG11	3:C:61:GLU:HB3	1.93	0.50
3:C:94:HIS:HD2	10:C:559:HOH:O	1.94	0.50
2:B:29:LEU:HD23	2:B:37:LEU:HD21	1.92	0.50
2:B:29:LEU:HB3	2:B:37:LEU:HD11	1.94	0.49
3:C:39:SER:HB2	3:C:44:LYS:O	2.13	0.49
2:B:74:PHE:O	2:B:78:VAL:HG23	2.12	0.49
1:A:28:ARG:HA	1:A:55:ARG:O	2.12	0.49
1:A:357:VAL:HA	2:B:53:LEU:HD21	1.94	0.49
1:A:339:HIS:HD2	10:A:603:HOH:O	1.96	0.49
1:A:280:ALA:O	1:A:281:HIS:HB3	2.12	0.49
1:A:208:THR:HA	1:A:272:ASN:OD1	2.13	0.48
2:B:49:GLN:NE2	10:B:685:HOH:O	2.46	0.48
1:A:75:GLU:O	1:A:217:ARG:NH2	2.46	0.48
1:A:127:ILE:HD12	1:A:130:VAL:CG2	2.44	0.48
2:B:92:ARG:HB3	2:B:96:ARG:NH2	2.29	0.48
1:A:322:LEU:HD12	1:A:329:MET:SD	2.54	0.48
1:A:84:PRO:HA	1:A:324:TYR:O	2.14	0.48
1:A:76:LYS:HE2	10:A:525:HOH:O	2.13	0.47
1:A:122:ARG:HG3	1:A:312:LEU:HD21	1.96	0.47
1:A:370:ASN:ND2	10:A:913:HOH:O	2.46	0.47
1:A:203:SER:HB2	1:A:229:ASP:HB2	1.96	0.47
1:A:322:LEU:HD13	1:A:331:ILE:HG13	1.96	0.47
3:C:90:ILE:N	3:C:90:ILE:HD12	2.28	0.47
1:A:81:ILE:CD1	1:A:114:LEU:HG	2.45	0.46
1:A:140:TYR:HB3	1:A:143:THR:OG1	2.15	0.46
1:A:192:ASN:HA	10:A:813:HOH:O	2.14	0.46
2:B:1:GLY:N	10:B:660:HOH:O	2.47	0.46
2:B:59:ASP:HB3	10:B:602:HOH:O	2.15	0.46
1:A:167:LYS:HB2	1:A:167:LYS:NZ	2.32	0.45
1:A:251:ASN:HA	1:A:259:PHE:CD2	2.51	0.45
2:B:42:PHE:O	2:B:48:LEU:HD22	2.16	0.45
3:C:25:HIS:CD2	3:C:104:LEU:HD11	2.51	0.45
1:A:132:TYR:O	1:A:136:LEU:HB2	2.16	0.45
1:A:71:ILE:HG21	1:A:137:LYS:HD2	1.98	0.45
2:B:55:GLN:HB3	10:B:608:HOH:O	2.17	0.45
10:A:626:HOH:O	2:B:47:GLU:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:57:ARG:NE	3:C:80:TYR:CE1	2.83	0.45
2:B:82:SER:C	2:B:83:VAL:O	2.54	0.45
1:A:83:ALA:HA	1:A:85:VAL:HG22	1.98	0.45
1:A:327:ASN:C	10:A:901:HOH:O	2.55	0.44
1:A:153:CYS:SG	1:A:155:HIS:CD2	3.11	0.44
2:B:31:LEU:HB2	2:B:41:GLU:HG2	1.99	0.44
2:B:30:ASP:O	2:B:32:ASP:N	2.51	0.44
1:A:239:PHE:CZ	1:A:262:TYR:HA	2.53	0.44
1:A:203:SER:HB2	1:A:229:ASP:CB	2.48	0.44
2:B:53:LEU:O	2:B:56:ARG:HB2	2.17	0.44
1:A:315:TYR:HE2	10:A:573:HOH:O	2.01	0.44
1:A:371:ILE:CD1	2:B:29:LEU:HD13	2.40	0.44
1:A:63:ARG:HA	1:A:66:THR:HG22	2.00	0.44
1:A:86:THR:HA	1:A:322:LEU:O	2.18	0.43
2:B:140:ASP:O	2:B:142:ASP:N	2.51	0.43
2:B:13:HIS:HE2	2:B:85:GLY:HA2	1.83	0.43
1:A:279:ARG:HH22	1:A:282:GLU:CG	2.31	0.43
3:C:71:ARG:HB2	3:C:102:GLU:HG2	1.99	0.43
1:A:142:LYS:HE3	1:A:142:LYS:HB2	1.83	0.43
2:B:81:PHE:HZ	2:B:93:PHE:CD1	2.36	0.43
1:A:358:GLY:HA3	10:B:577:HOH:O	2.18	0.43
1:A:122:ARG:HH21	6:A:507:PO4:P	2.40	0.43
1:A:262:TYR:N	1:A:263:PRO:HD2	2.34	0.43
1:A:309:PRO:HD3	1:A:319:ALA:HB2	2.00	0.43
1:A:124:TYR:CD1	1:A:124:TYR:N	2.86	0.43
1:A:83:ALA:HA	1:A:85:VAL:CG2	2.48	0.43
2:B:83:VAL:O	2:B:84:LYS:CB	2.65	0.43
1:A:310:ASN:ND2	1:A:315:TYR:O	2.52	0.43
3:C:87:HIS:CD2	10:C:517:HOH:O	2.71	0.43
1:A:251:ASN:HA	1:A:259:PHE:CE2	2.54	0.42
1:A:369:LEU:O	2:B:25:ARG:HD2	2.19	0.42
3:C:78:PRO:HG3	3:C:95:ALA:C	2.39	0.42
3:C:46:PHE:CE2	3:C:48:PHE:HB3	2.55	0.42
2:B:10:MET:HB2	2:B:76:GLU:OE1	2.19	0.42
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.88	0.42
2:B:51:ASN:HB3	2:B:54:VAL:HG23	2.01	0.42
2:B:81:PHE:HZ	2:B:93:PHE:CE1	2.37	0.42
2:B:91:LEU:HD21	10:B:662:HOH:O	2.19	0.41
3:C:1:GLY:HA2	3:C:80:TYR:CD2	2.54	0.41
1:A:293:LYS:HE2	1:A:293:LYS:HB3	1.80	0.41
1:A:293:LYS:HG2	10:A:726:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:C	2:B:85:GLY:H	2.21	0.41
2:B:31:LEU:HD12	10:B:682:HOH:O	2.19	0.41
3:C:94:HIS:CD2	10:C:564:HOH:O	2.73	0.41
2:B:3:GLU:HB3	2:B:4:ALA:H	1.69	0.41
1:A:279:ARG:HH22	1:A:282:GLU:HG3	1.84	0.41
1:A:124:TYR:HD1	1:A:124:TYR:N	2.18	0.41
1:A:277:ILE:O	1:A:302:LEU:HD12	2.21	0.41
1:A:367:ASN:ND2	2:B:47:GLU:HB3	2.35	0.41
3:C:11:ASP:O	3:C:11:ASP:OD1	2.38	0.41
1:A:253:VAL:HG23	1:A:259:PHE:HZ	1.87	0.41
1:A:307:SER:HA	1:A:319:ALA:HB1	2.02	0.41
2:B:160:ASP:CB	2:B:163:LYS:HE2	2.45	0.41
3:C:49:MET:SD	3:C:52:LYS:HE2	2.61	0.41
1:A:260:TYR:OH	1:A:279:ARG:HD3	2.20	0.40
1:A:305:ILE:HB	1:A:322:LEU:CD2	2.51	0.40
1:A:262:TYR:CE1	1:A:292:ARG:HG2	2.57	0.40
1:A:309:PRO:HD3	1:A:319:ALA:CB	2.51	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	350/375 (93%)	329 (94%)	17 (5%)	4 (1%)	14	26
2	B	167/169 (99%)	144 (86%)	14 (8%)	9 (5%)	2	2
3	C	105/107 (98%)	95 (90%)	7 (7%)	3 (3%)	4	6
All	All	622/651 (96%)	568 (91%)	38 (6%)	16 (3%)	5	8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	PHE
2	B	2	ASN
2	B	4	ALA
2	B	5	SER
2	B	31	LEU
2	B	46	PRO
2	B	141	LYS
1	A	240	GLY
2	B	140	ASP
3	C	9	PRO
3	C	52	LYS
2	B	7	PRO
2	B	157	GLY
1	A	218	PHE
3	C	12	GLY
1	A	371	ILE

### 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	315/330 (96%)	286 (91%)	29 (9%)	9	18
2	B	150/150 (100%)	130 (87%)	20 (13%)	4	7
3	C	88/88 (100%)	78 (89%)	10 (11%)	5	11
All	All	553/568 (97%)	494 (89%)	59 (11%)	6	13

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	28	ARG
1	A	80	ASP
1	A	85	VAL
1	A	98	LEU
1	A	112	ARG
1	A	114	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	122	ARG
1	A	144	LEU
1	A	167	LYS
1	A	187	LEU
1	A	190	LEU
1	A	196	LEU
1	A	202	LEU
1	A	209	LEU
1	A	236	LEU
1	A	237	GLU
1	A	245	GLN
1	A	247	HIS
1	A	249	THR
1	A	266	CYS
1	A	267	GLU
1	A	275	LEU
1	A	279	ARG
1	A	289	ARG
1	A	295	GLN
1	A	322	LEU
1	A	325	GLU
1	A	336	CYS
2	B	5	SER
2	B	6	TYR
2	B	9	GLU
2	B	22	LEU
2	B	25	ARG
2	B	29	LEU
2	B	36	SER
2	B	39	VAL
2	B	42	PHE
2	B	43	MET
2	B	44	SER
2	B	49	GLN
2	B	50	GLN
2	B	53	LEU
2	B	76	GLU
2	B	113	GLN
2	B	121	ASN
2	B	142	ASP
2	B	153	CYS
2	B	161	ILE

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Mol	Chain	Res	Type
3	C	3	GLN
3	C	8	SER
3	C	13	ARG
3	C	25	HIS
3	C	49	MET
3	C	53	GLN
3	C	61	GLU
3	C	90	ILE
3	C	102	GLU
3	C	106	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	155	HIS
1	A	245	GLN
1	A	250	HIS
1	A	273	ASN
1	A	330	ASN
1	A	367	ASN
2	B	49	GLN
3	C	53	GLN
3	C	94	HIS

### 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

Of 9 ligands modelled in this entry, 6 are 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
6	PO4	A	507	4	4,4,4	1.22	0	6,6,6	0.35	0
9	FK5	C	509	-	54,60,60	1.14	6 (11%)	64,86,86	1.81	12 (18%)
8	MYR	B	508	2	14,14,15	0.79	1 (7%)	13,13,15	0.74	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
9	FK5	C	509	-	-	3/68/114/114	0/3/4/4
8	MYR	B	508	2	-	7/11/12/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	509	FK5	O6-C10	3.59	1.45	1.39
9	C	509	FK5	C16-C15	2.54	1.57	1.52
8	B	508	MYR	O1-C1	2.52	1.34	1.19
9	C	509	FK5	C20-C19	2.46	1.37	1.33
9	C	509	FK5	C14-C15	2.25	1.56	1.52
9	C	509	FK5	C2-N7	-2.03	1.44	1.47
9	C	509	FK5	C14-C13	2.02	1.58	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	509	FK5	C21-C20-C19	4.91	132.67	127.64
9	C	509	FK5	C12-C11-C10	4.87	115.29	110.47
9	C	509	FK5	C15-C14-C13	4.45	120.39	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	509	FK5	O1-C26-C25	4.21	110.73	105.91
9	C	509	FK5	C23-C22-C21	-4.13	112.44	117.75
9	C	509	FK5	C1-C2-N7	3.73	119.00	112.05
9	C	509	FK5	O10-C24-C23	-2.96	102.42	109.56
9	C	509	FK5	O9-C22-C21	2.73	123.94	121.13
9	C	509	FK5	C3-C2-N7	-2.65	106.85	110.53
9	C	509	FK5	C30-C29-C34	2.20	111.18	108.66
9	C	509	FK5	O1-C1-C2	2.16	115.54	110.78
9	C	509	FK5	C6-N7-C2	2.02	120.05	115.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	508	MYR	C9-C10-C11-C12
8	B	508	MYR	C4-C5-C6-C7
8	B	508	MYR	C6-C7-C8-C9
8	B	508	MYR	C10-C11-C12-C13
8	B	508	MYR	C2-C3-C4-C5
8	B	508	MYR	C11-C10-C9-C8
9	C	509	FK5	C36-C17-C18-C19
9	C	509	FK5	C19-C20-C21-C22
8	B	508	MYR	C1-C2-C3-C4
9	C	509	FK5	O10-C24-C25-C41

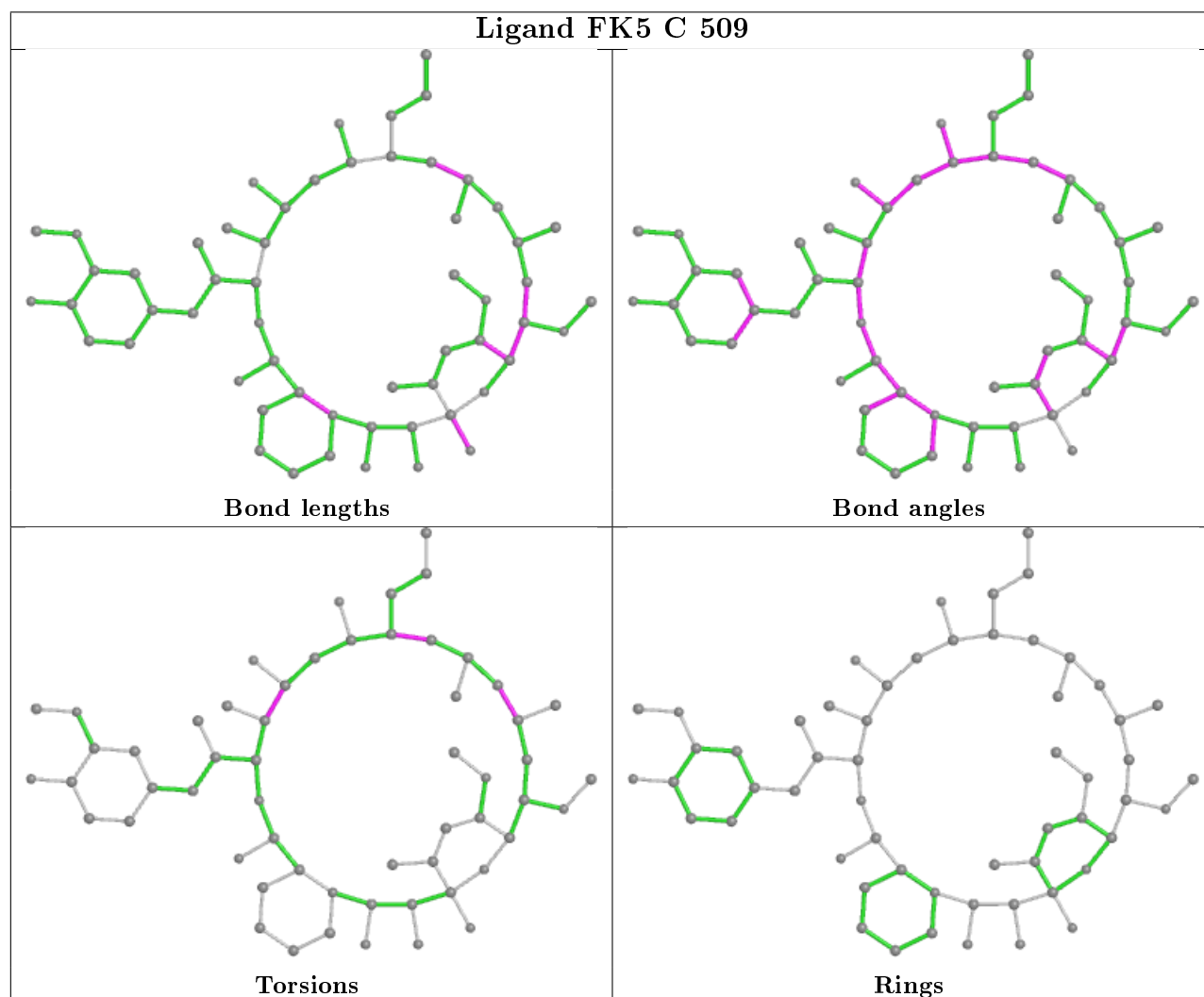
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	507	PO4	1	0
8	B	508	MYR	1	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 than 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.



## 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.