



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:29 PM UTC

PDB ID : 1CTR / pdb_00001ctr
Title : DRUG BINDING BY CALMODULIN: CRYSTAL STRUCTURE OF A CALMODULIN-TRIFLUOPERAZINE COMPLEX
Authors : Cook, W.J.; Walter, L.J.; Walter, M.R.
Deposited on : 1994-09-21
Resolution : 2.45 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

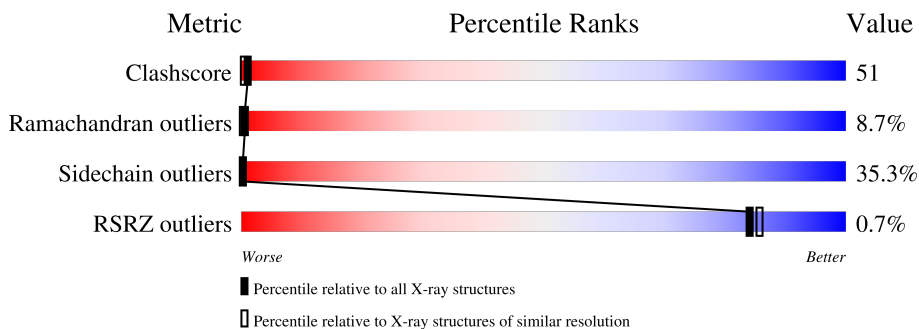
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 ≥ 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	148	

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	TFP	A	153	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1140 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.

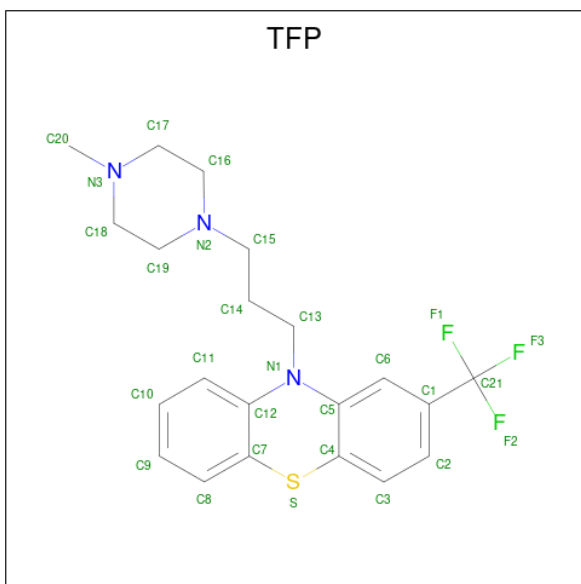
- Molecule 1 is a protein called CALMODULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	142	1108	679	179	242	8	0	0	1

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is 10-[3-(4-METHYL-PIPERAZIN-1-YL)-PROPYL]-2-TRIFLUOROMETHYL-10H-PHENOTHIAZINE (CCD ID: TFP) (formula: C₂₁H₂₄F₃N₃S).

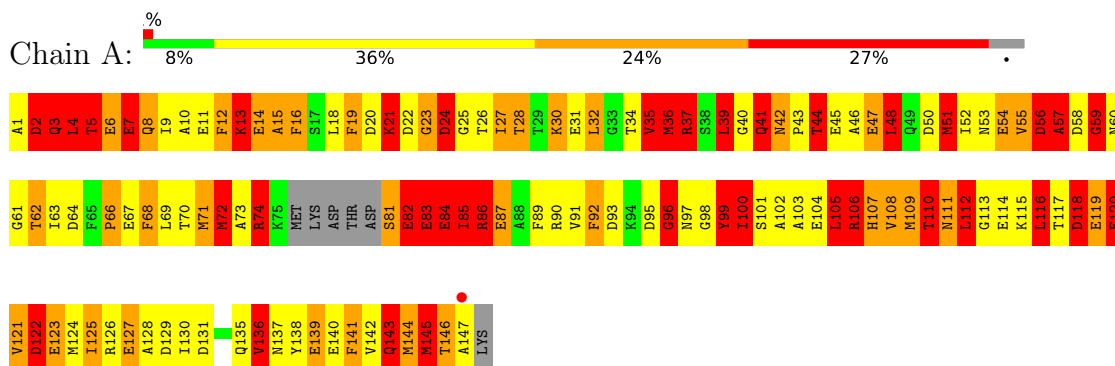


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	S		
3	A	1	28	21	3	3	1	0	0

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: CALMODULIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	41.00Å 41.00Å 178.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.45 6.00 – 2.46	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.45) 73.4 (6.00-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available) 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtrriage
Anisotropy	0.526	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 116.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1140	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: TFP, 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	1.08	3/1119 (0.3%)	1.88	29/1504 (1.9%)

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	A	0	92

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	107	HIS	CG-ND1	-5.22	1.32	1.38
1	A	74	ARG	C-N	-5.17	1.26	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ASN	CA-C-O	-7.80	112.41	119.59
1	A	122	ASP	CA-CB-CG	7.74	120.34	112.60
1	A	100	ILE	O-C-N	-7.60	114.86	122.99
1	A	24	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	14	GLU	N-CA-C	-6.09	104.27	111.03
1	A	106	ARG	N-CA-C	5.99	117.81	111.28
1	A	51	MET	O-C-N	-5.88	114.02	122.36
1	A	37	ARG	CD-NE-CZ	-5.87	116.19	124.40
1	A	136	VAL	O-C-N	-5.84	117.37	123.03
1	A	141	PHE	N-CA-C	-5.80	106.33	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	VAL	N-CA-CB	-5.79	104.68	112.10
1	A	7	GLU	N-CA-C	-5.66	104.59	112.45
1	A	5	THR	N-CA-C	5.62	117.33	110.41
1	A	44	THR	CA-CB-OG1	-5.61	101.18	109.60
1	A	41	GLN	O-C-N	-5.55	116.83	123.27
1	A	107	HIS	CA-CB-CG	-5.51	108.29	113.80
1	A	82	GLU	CA-C-O	-5.48	112.67	120.51
1	A	99	TYR	O-C-N	-5.42	117.41	123.48
1	A	55	VAL	O-C-N	-5.41	115.81	122.57
1	A	129	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	118	ASP	N-CA-C	-5.30	98.02	107.98
1	A	55	VAL	CA-C-N	-5.24	115.01	123.23
1	A	55	VAL	C-N-CA	-5.24	115.01	123.23
1	A	57	ALA	O-C-N	-5.12	116.01	122.20
1	A	16	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	118	ASP	CA-C-O	-5.11	115.85	121.58
1	A	21	LYS	CA-C-N	-5.11	114.63	122.60
1	A	21	LYS	C-N-CA	-5.11	114.63	122.60
1	A	131	ASP	N-CA-C	5.06	118.22	111.75

There are no chirality outliers.

All (92) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Mainchain
1	A	10	ALA	Mainchain
1	A	100	ILE	Mainchain
1	A	101	SER	Mainchain
1	A	102	ALA	Mainchain
1	A	103	ALA	Mainchain
1	A	105	LEU	Mainchain
1	A	106	ARG	Mainchain
1	A	107	HIS	Mainchain
1	A	108	VAL	Mainchain
1	A	109	MET	Mainchain
1	A	11	GLU	Mainchain
1	A	110	THR	Mainchain
1	A	111	ASN	Mainchain
1	A	112	LEU	Mainchain
1	A	113	GLY	Mainchain
1	A	116	LEU	Mainchain
1	A	117	THR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	118	ASP	Mainchain
1	A	120	GLU	Sidechain
1	A	127	GLU	Sidechain
1	A	13	LYS	Mainchain
1	A	135	GLN	Mainchain
1	A	136	VAL	Mainchain
1	A	137	ASN	Mainchain
1	A	138	TYR	Sidechain
1	A	139	GLU	Mainchain
1	A	140	GLU	Sidechain,Mainchain
1	A	143	GLN	Mainchain
1	A	144	MET	Mainchain
1	A	145	MET	Mainchain
1	A	146	THR	Mainchain
1	A	15	ALA	Mainchain
1	A	2	ASP	Mainchain
1	A	20	ASP	Mainchain
1	A	22	ASP	Mainchain
1	A	23	GLY	Mainchain
1	A	24	ASP	Sidechain,Mainchain
1	A	27	ILE	Mainchain
1	A	28	THR	Mainchain
1	A	3	GLN	Mainchain
1	A	30	LYS	Mainchain
1	A	32	LEU	Mainchain
1	A	34	THR	Mainchain
1	A	35	VAL	Mainchain
1	A	36	MET	Mainchain
1	A	37	ARG	Mainchain
1	A	39	LEU	Mainchain
1	A	4	LEU	Mainchain
1	A	40	GLY	Mainchain
1	A	41	GLN	Mainchain
1	A	42	ASN	Mainchain
1	A	44	THR	Mainchain
1	A	45	GLU	Mainchain
1	A	46	ALA	Mainchain
1	A	47	GLU	Mainchain
1	A	48	LEU	Mainchain
1	A	5	THR	Mainchain
1	A	50	ASP	Mainchain
1	A	51	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	A	54	GLU	Mainchain
1	A	55	VAL	Mainchain
1	A	56	ASP	Sidechain
1	A	57	ALA	Mainchain
1	A	59	GLY	Mainchain
1	A	60	ASN	Mainchain
1	A	61	GLY	Mainchain
1	A	62	THR	Mainchain
1	A	63	ILE	Mainchain
1	A	64	ASP	Sidechain
1	A	66	PRO	Mainchain
1	A	68	PHE	Mainchain
1	A	70	THR	Mainchain
1	A	73	ALA	Mainchain
1	A	81	SER	Mainchain
1	A	82	GLU	Mainchain
1	A	83	GLU	Mainchain
1	A	84	GLU	Mainchain
1	A	85	ILE	Mainchain
1	A	86	ARG	Sidechain
1	A	89	PHE	Mainchain
1	A	9	ILE	Mainchain
1	A	91	VAL	Mainchain
1	A	92	PHE	Mainchain
1	A	95	ASP	Mainchain
1	A	96	GLY	Mainchain
1	A	97	ASN	Mainchain
1	A	98	GLY	Mainchain
1	A	99	TYR	Sidechain,Mainchain

5.2 Too-close contacts

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	1108	0	1032	111	0
2	A	4	0	0	0	0
3	A	28	0	24	12	0
All	All	1140	0	1056	112	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 51.

All (112) 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:A:92:PHE:HB3	1:A:100:ILE:HD12	1.35	1.08
1:A:92:PHE:CB	1:A:100:ILE:HD12	1.92	0.98
1:A:144:MET:HA	3:A:153:TFP:H181	1.47	0.96
1:A:2:ASP:O	1:A:3:GLN:HB3	1.65	0.95
1:A:36:MET:HE1	1:A:51:MET:SD	2.14	0.87
1:A:37:ARG:HA	1:A:41:GLN:O	1.74	0.86
1:A:116:LEU:HD22	1:A:124:MET:HE1	1.63	0.81
1:A:125:ILE:CG2	1:A:136:VAL:HG23	2.12	0.79
1:A:82:GLU:O	1:A:84:GLU:N	2.16	0.79
1:A:110:THR:HG22	1:A:111:ASN:N	1.99	0.76
1:A:74:ARG:HD2	1:A:74:ARG:H	1.51	0.74
1:A:142:VAL:O	1:A:143:GLN:C	2.31	0.71
1:A:144:MET:HG3	3:A:153:TFP:H192	1.73	0.71
1:A:23:GLY:O	1:A:25:GLY:N	2.24	0.69
1:A:52:ILE:O	1:A:56:ASP:HB3	1.91	0.69
1:A:130:ILE:CD1	1:A:143:GLN:OE1	2.39	0.69
1:A:26:THR:HB	1:A:62:THR:HB	1.75	0.69
1:A:116:LEU:HD22	1:A:124:MET:CE	2.22	0.68
1:A:144:MET:HA	3:A:153:TFP:C18	2.24	0.67
1:A:116:LEU:CD2	1:A:124:MET:HE1	2.24	0.67
1:A:105:LEU:HD12	1:A:121:VAL:HG23	1.78	0.66
1:A:36:MET:CE	1:A:51:MET:SD	2.84	0.66
1:A:8:GLN:HB3	1:A:12:PHE:CE1	2.32	0.64
1:A:27:ILE:HG22	1:A:27:ILE:O	1.96	0.63
1:A:118:ASP:O	1:A:119:GLU:HB2	1.99	0.63
1:A:3:GLN:HG2	1:A:4:LEU:N	2.13	0.63
1:A:125:ILE:HG22	1:A:136:VAL:HG23	1.80	0.62
1:A:27:ILE:HA	1:A:31:GLU:OE1	2.01	0.61
1:A:83:GLU:O	1:A:85:ILE:N	2.34	0.60
1:A:109:MET:HB3	1:A:114:GLU:HB2	1.83	0.60
1:A:36:MET:SD	1:A:43:PRO:HG3	2.42	0.60
1:A:146:THR:OG1	1:A:147:ALA:N	2.35	0.60
1:A:32:LEU:HD22	1:A:52:ILE:HG13	1.85	0.59
1:A:83:GLU:O	1:A:86:ARG:N	2.34	0.59
1:A:19:PHE:N	1:A:19:PHE:CD1	2.69	0.59
1:A:71:MET:CE	1:A:72:MET:HG2	2.32	0.59
1:A:8:GLN:O	1:A:12:PHE:CD1	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ILE:CG2	1:A:136:VAL:CG2	2.81	0.59
1:A:24:ASP:OD2	1:A:26:THR:OG1	2.17	0.58
1:A:108:VAL:O	1:A:112:LEU:HB2	2.04	0.57
1:A:19:PHE:H	1:A:19:PHE:HD1	1.52	0.57
1:A:144:MET:O	1:A:144:MET:CG	2.53	0.56
1:A:121:VAL:O	1:A:125:ILE:HG12	2.05	0.56
1:A:120:GLU:O	1:A:124:MET:HG3	2.04	0.56
1:A:92:PHE:O	1:A:104:GLU:HG2	2.06	0.56
1:A:82:GLU:O	1:A:83:GLU:C	2.49	0.56
1:A:41:GLN:C	1:A:43:PRO:HD3	2.31	0.55
1:A:71:MET:HE2	1:A:72:MET:CG	2.36	0.55
1:A:128:ALA:HB3	3:A:153:TFP:H11	1.88	0.55
1:A:93:ASP:OD2	1:A:96:GLY:HA2	2.07	0.55
1:A:21:LYS:NZ	1:A:35:VAL:HG23	2.21	0.54
1:A:21:LYS:HZ3	1:A:35:VAL:HG23	1.73	0.54
1:A:19:PHE:O	1:A:31:GLU:HG2	2.08	0.54
1:A:14:GLU:O	1:A:15:ALA:C	2.49	0.53
1:A:136:VAL:HG21	3:A:153:TFP:H10	1.89	0.53
1:A:92:PHE:CB	1:A:100:ILE:CD1	2.78	0.53
1:A:68:PHE:CD1	1:A:68:PHE:C	2.86	0.52
1:A:87:GLU:HG2	1:A:90:ARG:NH2	2.24	0.52
1:A:128:ALA:HB2	3:A:153:TFP:H141	1.92	0.52
1:A:85:ILE:N	1:A:85:ILE:HD13	2.24	0.52
1:A:14:GLU:C	1:A:16:PHE:N	2.64	0.51
1:A:128:ALA:HB2	3:A:153:TFP:C14	2.40	0.51
1:A:26:THR:HB	1:A:62:THR:CB	2.40	0.51
1:A:109:MET:HB3	1:A:114:GLU:CB	2.41	0.51
1:A:83:GLU:O	1:A:84:GLU:C	2.54	0.50
1:A:83:GLU:HB3	1:A:84:GLU:OE1	2.11	0.50
1:A:139:GLU:O	1:A:142:VAL:N	2.44	0.50
1:A:82:GLU:HA	1:A:85:ILE:HG12	1.94	0.49
1:A:71:MET:HG2	1:A:72:MET:N	2.27	0.49
1:A:125:ILE:HG23	1:A:136:VAL:CG2	2.43	0.49
1:A:58:ASP:O	1:A:59:GLY:C	2.55	0.49
1:A:66:PRO:O	1:A:69:LEU:N	2.46	0.48
1:A:5:THR:OG1	1:A:6:GLU:N	2.47	0.48
1:A:99:TYR:HA	1:A:136:VAL:O	2.14	0.48
1:A:125:ILE:HG22	1:A:136:VAL:CG2	2.42	0.48
1:A:130:ILE:HD11	1:A:143:GLN:OE1	2.12	0.48
1:A:56:ASP:O	1:A:56:ASP:CG	2.55	0.48
1:A:44:THR:O	1:A:48:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MET:CE	1:A:72:MET:CG	2.92	0.47
1:A:14:GLU:O	1:A:16:PHE:N	2.48	0.47
1:A:123:GLU:O	1:A:127:GLU:HG3	2.16	0.46
1:A:105:LEU:HD11	1:A:124:MET:SD	2.55	0.46
1:A:39:LEU:O	1:A:41:GLN:NE2	2.39	0.46
1:A:144:MET:CA	3:A:153:TFP:H181	2.32	0.46
1:A:87:GLU:CD	1:A:90:ARG:NH2	2.74	0.46
1:A:5:THR:C	1:A:7:GLU:H	2.24	0.46
1:A:58:ASP:N	1:A:58:ASP:OD1	2.47	0.46
1:A:87:GLU:CD	1:A:90:ARG:HH21	2.23	0.46
1:A:81:SER:O	1:A:82:GLU:OE1	2.34	0.46
1:A:71:MET:HE2	1:A:72:MET:HG2	1.98	0.45
1:A:69:LEU:HD13	1:A:69:LEU:O	2.18	0.44
1:A:128:ALA:HB2	3:A:153:TFP:H132	1.99	0.44
1:A:71:MET:HE3	1:A:72:MET:HG2	1.99	0.43
1:A:92:PHE:CG	1:A:100:ILE:HD12	2.52	0.43
1:A:144:MET:CG	3:A:153:TFP:H192	2.46	0.43
1:A:92:PHE:CG	1:A:100:ILE:CD1	3.02	0.43
1:A:47:GLU:O	1:A:51:MET:HG3	2.19	0.43
1:A:13:LYS:HA	1:A:16:PHE:HB2	2.00	0.43
1:A:110:THR:C	1:A:112:LEU:N	2.75	0.43
1:A:139:GLU:O	1:A:141:PHE:N	2.51	0.42
1:A:19:PHE:N	1:A:19:PHE:HD1	2.10	0.42
1:A:21:LYS:NZ	1:A:35:VAL:CG2	2.82	0.42
1:A:139:GLU:HB3	1:A:143:GLN:HE22	1.83	0.42
3:A:153:TFP:H6	3:A:153:TFP:H131	1.64	0.42
1:A:144:MET:SD	3:A:153:TFP:H141	2.61	0.41
1:A:85:ILE:HD12	1:A:145:MET:HE2	2.03	0.41
1:A:125:ILE:HG12	1:A:125:ILE:H	1.58	0.41
1:A:122:ASP:O	1:A:123:GLU:C	2.63	0.41
1:A:28:THR:HG22	1:A:62:THR:HG22	2.03	0.41
1:A:120:GLU:HA	1:A:123:GLU:HB3	2.03	0.41
1:A:57:ALA:H	1:A:67:GLU:HG2	1.86	0.41
1:A:130:ILE:HD13	1:A:143:GLN:OE1	2.21	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	138/148 (93%)	109 (79%)	17 (12%)	12 (9%)	0 0

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	24	ASP
1	A	74	ARG
1	A	83	GLU
1	A	119	GLU
1	A	59	GLY
1	A	96	GLY
1	A	84	GLU
1	A	4	LEU
1	A	82	GLU
1	A	110	THR
1	A	72	MET

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	119/126 (94%)	77 (65%)	42 (35%)	0 0

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	GLN
1	A	5	THR
1	A	6	GLU
1	A	7	GLU
1	A	8	GLN
1	A	12	PHE
1	A	13	LYS
1	A	18	LEU
1	A	19	PHE
1	A	21	LYS
1	A	30	LYS
1	A	35	VAL
1	A	36	MET
1	A	39	LEU
1	A	48	LEU
1	A	53	ASN
1	A	54	GLU
1	A	56	ASP
1	A	71	MET
1	A	72	MET
1	A	74	ARG
1	A	82	GLU
1	A	83	GLU
1	A	85	ILE
1	A	86	ARG
1	A	87	GLU
1	A	100	ILE
1	A	105	LEU
1	A	106	ARG
1	A	110	THR
1	A	112	LEU
1	A	115	LYS
1	A	116	LEU
1	A	120	GLU
1	A	121	VAL
1	A	122	ASP
1	A	123	GLU
1	A	125	ILE
1	A	126	ARG
1	A	143	GLN
1	A	145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	TFP	A	153	-	31,31,31	1.54	3 (9%)	45,45,45	2.63	15 (33%)

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	TFP	A	153	-	-	2/12/34/34	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	153	TFP	C12-N1	5.87	1.50	1.40
3	A	153	TFP	C5-N1	2.16	1.44	1.40
3	A	153	TFP	C17-C16	-2.08	1.43	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	153	TFP	C18-N3-C17	6.39	119.72	109.54
3	A	153	TFP	C16-C17-N3	5.74	120.09	110.86
3	A	153	TFP	C19-C18-N3	5.49	119.68	110.86
3	A	153	TFP	C20-N3-C18	5.34	120.81	110.63
3	A	153	TFP	C17-C16-N2	5.14	121.02	110.65
3	A	153	TFP	C18-C19-N2	4.98	120.70	110.65
3	A	153	TFP	C20-N3-C17	4.64	119.47	110.63
3	A	153	TFP	C19-N2-C16	4.62	118.80	108.84
3	A	153	TFP	C15-N2-C19	4.27	122.63	111.24
3	A	153	TFP	C13-N1-C5	-3.82	113.70	119.03
3	A	153	TFP	C11-C12-C7	-3.21	114.23	118.59
3	A	153	TFP	C15-N2-C16	2.75	118.56	111.24
3	A	153	TFP	F3-C21-C1	2.56	118.38	112.90
3	A	153	TFP	C10-C11-C12	2.47	123.27	118.28
3	A	153	TFP	C8-C7-C12	2.19	122.36	120.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	153	TFP	C14-C15-N2-C19
3	A	153	TFP	C14-C13-N1-C12

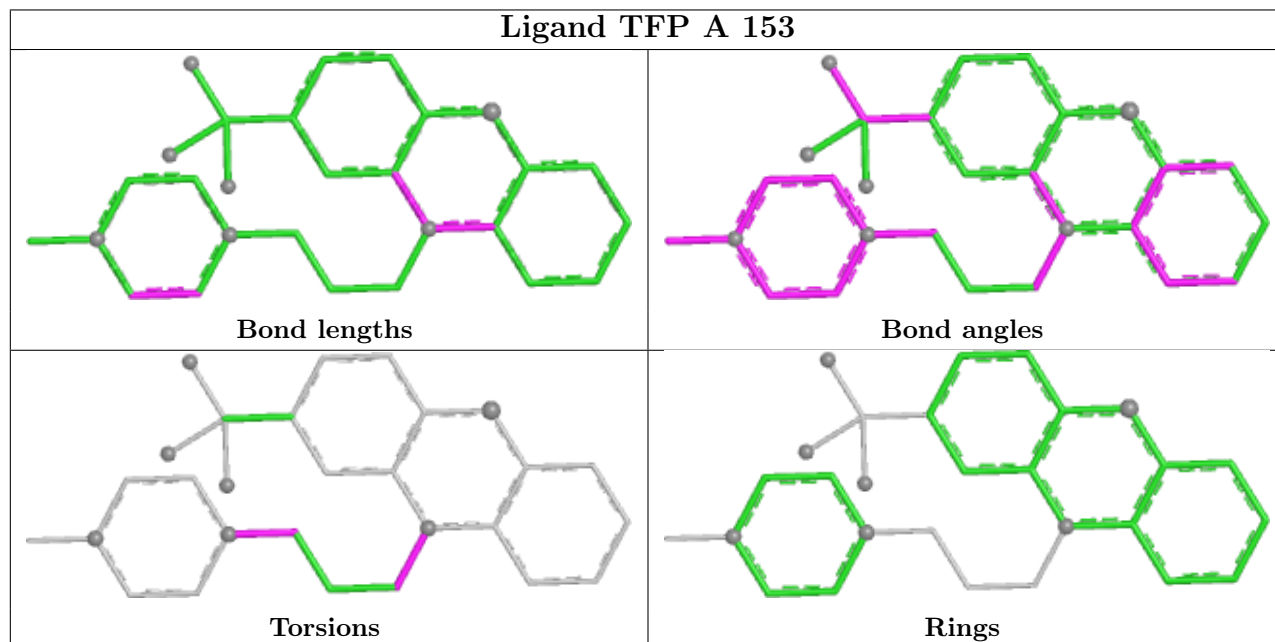
There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	153	TFP	12	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 [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	142/148 (95%)	-0.48	1 (0%) 84 86	8, 18, 27, 35	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	2.2

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 oligosaccharides in this entry.

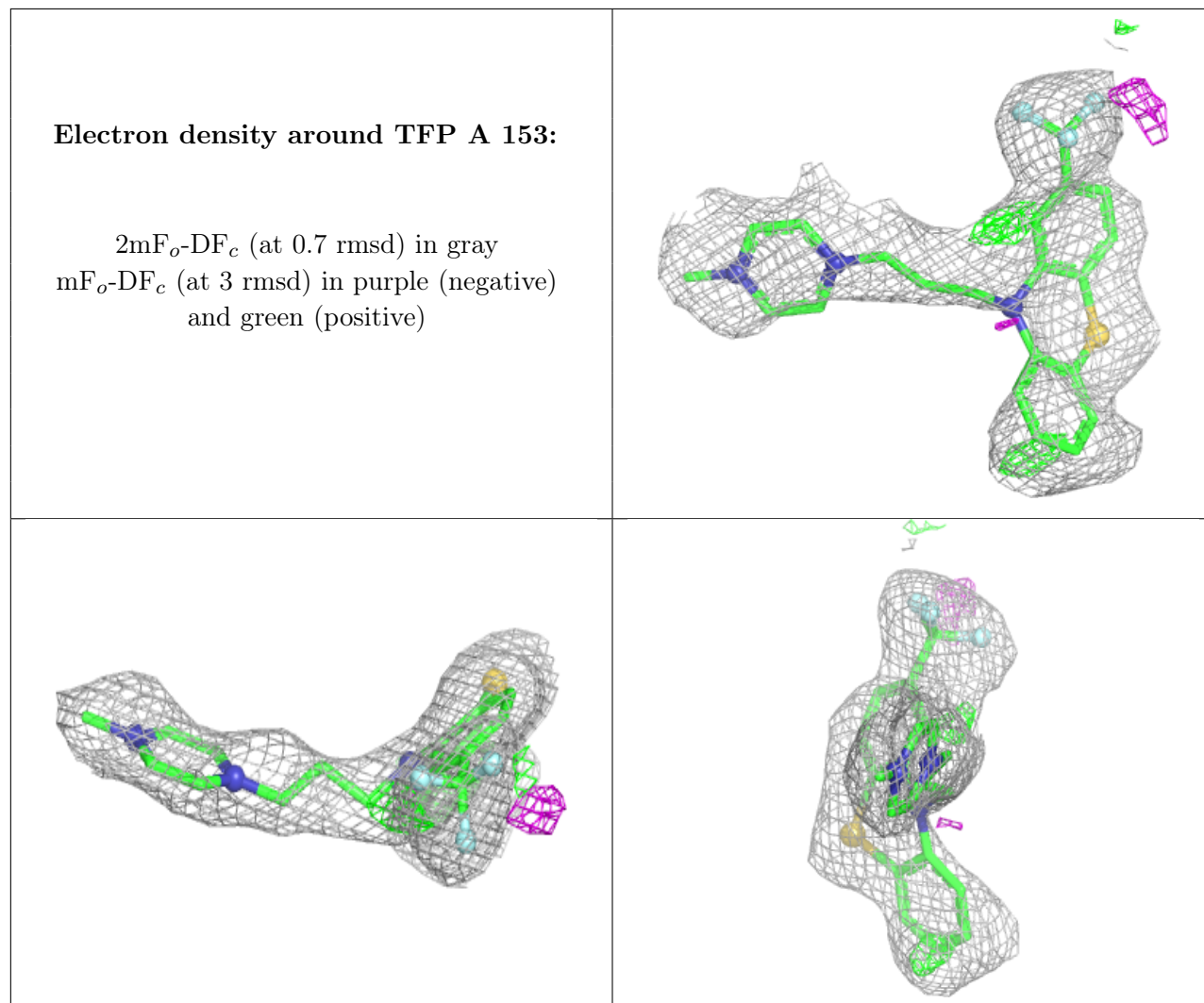
6.4 Ligands [i](#)

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
3	TFP	A	153	28/28	0.88	0.10	14,23,26,29	0
2	CA	A	149	1/1	0.95	0.02	15,15,15,15	0
2	CA	A	150	1/1	0.97	0.06	20,20,20,20	0
2	CA	A	152	1/1	0.98	0.07	12,12,12,12	0
2	CA	A	151	1/1	0.98	0.07	15,15,15,15	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.