



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 11:33 PM EDT

PDB ID : 1FT4  
Title : PHOTOCHEMICALLY-ENHANCED BINDING OF SMALL MOLECULES  
TO THE TUMOR NECROSIS FACTOR RECEPTOR-1  
Authors : Muckelbauer, J.K.; Chang, C.-H.  
Deposited on : 2000-09-11  
Resolution : 2.90 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)
Xtriage (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)	:	2.36.2

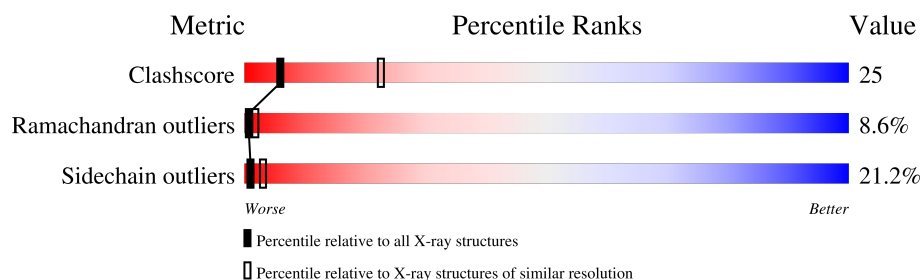
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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  $\geq 3$ , 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	162	
1	B	162	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2232 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.

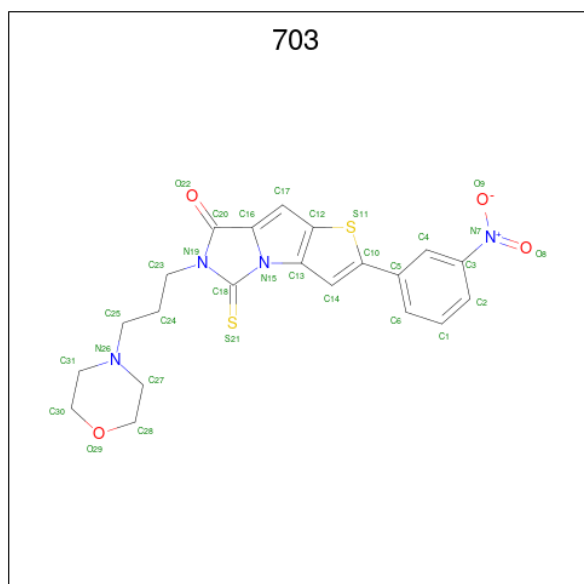
- Molecule 1 is a protein called SOLUBLE TUMOR NECROSIS FACTOR RECEPTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1095	658	201	214	22			
1	B	142	Total	C	N	O	S	0	0	0
			1106	664	204	216	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	cloning artifact	UNP P19438
B	11	MET	-	cloning artifact	UNP P19438

- Molecule 2 is 5-(3-MORPHOLIN-4-YL-PROPYL)-2-(3-NITRO-PHENYL)-4-THIOXO-4,5-DIHYDRO-1-THIA-3B,5-DIAZA-CYCLOPENTA[A]PENTALEN-6-ONE (three-letter code: 703) (formula: C<sub>21</sub>H<sub>20</sub>N<sub>4</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	21	4	4	2		

### 3 Residue-property plots

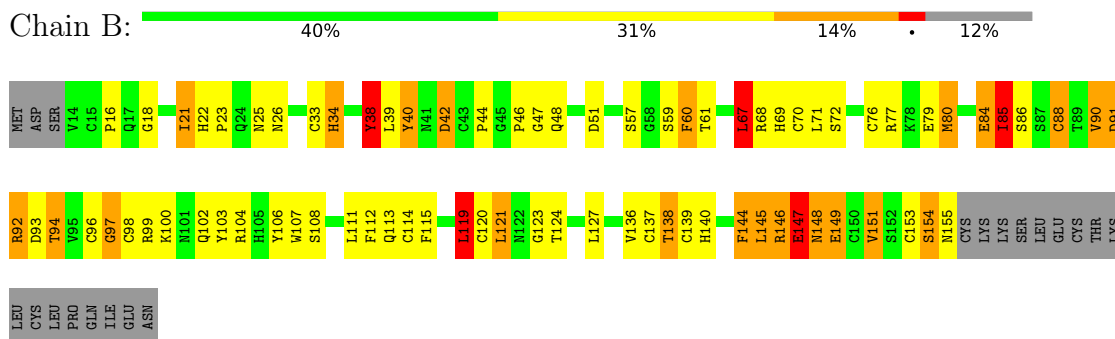
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: SOLUBLE TUMOR NECROSIS FACTOR RECEPTOR 1



#### • Molecule 1: SOLUBLE TUMOR NECROSIS FACTOR RECEPTOR 1



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.80Å 67.80Å 190.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.274 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
703

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	0.84	1/1117 (0.1%)	1.51	11/1504 (0.7%)
1	B	0.78	0/1128	1.52	10/1520 (0.7%)
All	All	0.81	1/2245 (0.0%)	1.52	21/3024 (0.7%)

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	6
1	B	0	7
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	THR	C-N	6.57	1.49	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	PHE	CB-CG-CD2	-6.76	116.07	120.80
1	A	115	PHE	C-N-CA	-6.74	104.84	121.70
1	B	40	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	20	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	B	97	GLY	C-N-CA	-6.13	106.37	121.70
1	A	112	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	A	38	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	103	TYR	CB-CG-CD2	-5.95	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	LEU	CA-C-N	-5.92	104.17	117.20
1	B	67	LEU	C-N-CA	-5.89	106.97	121.70
1	A	50	THR	C-N-CA	-5.89	106.98	121.70
1	B	38	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	B	51	ASP	C-N-CA	-5.58	107.75	121.70
1	B	21	ILE	CA-CB-CG1	-5.45	100.66	111.00
1	A	143	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	A	46	PRO	N-CA-C	5.33	125.95	112.10
1	B	46	PRO	C-N-CA	-5.33	111.12	122.30
1	A	70	CYS	C-N-CA	-5.28	108.50	121.70
1	B	68	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	119	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	38	TYR	CD1-CG-CD2	5.00	123.40	117.90

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	TYR	Sidechain
1	A	11	MET	Peptide
1	A	119	LEU	Peptide
1	A	142	GLY	Peptide
1	A	20	TYR	Sidechain
1	A	62	ALA	Peptide
1	B	107	TRP	Peptide
1	B	154	SER	Peptide
1	B	38	TYR	Sidechain
1	B	40	TYR	Sidechain
1	B	60	PHE	Peptide
1	B	85	ILE	Peptide
1	B	99	ARG	Sidechain

## 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	1095	0	992	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1106	0	1005	52	0
2	A	31	0	19	4	0
All	All	2232	0	2016	106	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 25.

All (106) 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:B:84:GLU:HA	1:B:96:CYS:HA	1.48	0.92
1:A:25:ASN:HD22	1:A:28:ILE:HG13	1.38	0.89
1:A:120:CYS:SG	1:A:125:VAL:HA	2.26	0.76
1:B:138:THR:HA	1:B:145:LEU:HD11	1.67	0.75
1:A:98:CYS:SG	1:A:104:ARG:HG2	2.27	0.75
1:A:35:LYS:HB3	1:A:63:SER:HA	1.71	0.73
1:A:122:ASN:O	1:A:139:CYS:HA	1.93	0.68
1:A:15:CYS:SG	1:A:21:ILE:HG22	2.35	0.67
1:B:103:TYR:CE1	1:B:115:PHE:HB2	2.30	0.67
1:A:107:TRP:O	1:A:111:LEU:HB2	1.96	0.65
1:B:77:ARG:HD2	1:B:111:LEU:HD13	1.79	0.65
1:A:103:TYR:CE1	1:A:115:PHE:HB3	2.32	0.64
1:A:32:LYS:HD3	1:A:64:GLU:HB3	1.80	0.64
1:A:38:TYR:H	1:A:38:TYR:HD1	1.47	0.63
1:B:76:CYS:SG	1:B:84:GLU:HB3	2.41	0.61
1:B:92:ARG:HG3	1:B:93:ASP:O	2.01	0.61
1:B:59:SER:OG	1:B:70:CYS:HB2	2.01	0.60
1:B:80:MET:HG3	1:B:113:GLN:HB3	1.84	0.59
1:A:11:MET:N	1:A:13:SER:HG	2.01	0.59
1:A:78:LYS:HD3	1:A:78:LYS:H	1.66	0.59
1:B:44:PRO:HD2	1:B:48:GLN:HB3	1.86	0.58
1:B:80:MET:SD	1:B:80:MET:N	2.76	0.58
1:B:146:ARG:HA	1:B:146:ARG:HE	1.68	0.58
1:A:35:LYS:HB3	1:A:63:SER:CA	2.34	0.57
1:B:106:TYR:HA	1:B:112:PHE:CB	2.35	0.56
1:A:61:THR:HG23	1:A:70:CYS:HA	1.86	0.56
1:A:62:ALA:HB2	2:A:962:703:C2	2.35	0.56
1:B:22:HIS:NE2	1:B:42:ASP:HB2	2.20	0.56
1:B:22:HIS:HD2	1:B:23:PRO:HD2	1.71	0.55
1:A:71:LEU:HD11	2:A:962:703:H14	1.88	0.54
1:A:65:ASN:HB2	1:A:67:LEU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HB3	1:B:149:GLU:HA	1.90	0.54
1:B:85:ILE:HD11	1:B:97:GLY:HA3	1.91	0.52
1:B:103:TYR:O	1:B:114:CYS:HA	2.10	0.51
1:A:104:ARG:HD2	1:A:112:PHE:HE2	1.75	0.51
1:B:111:LEU:HD12	1:B:112:PHE:H	1.75	0.51
1:B:127:LEU:HB2	1:B:136:VAL:HB	1.93	0.51
1:A:88:CYS:HB2	1:A:94:THR:HG23	1.93	0.51
1:A:28:ILE:HG12	1:A:46:PRO:HD3	1.92	0.50
1:A:71:LEU:N	1:A:71:LEU:HD22	2.25	0.50
1:B:79:GLU:C	1:B:80:MET:SD	2.90	0.50
1:A:71:LEU:HD22	1:A:71:LEU:H	1.77	0.50
1:A:60:PHE:HA	1:A:90:VAL:HA	1.93	0.50
1:B:22:HIS:CD2	1:B:23:PRO:HD2	2.47	0.49
1:A:129:CYS:SG	1:A:134:ASN:HA	2.52	0.49
1:B:102:GLN:HB3	1:B:115:PHE:O	2.12	0.49
1:A:11:MET:SD	1:A:11:MET:O	2.71	0.49
1:A:138:THR:HG21	1:B:145:LEU:HG	1.95	0.48
1:B:123:GLY:HA2	1:B:140:HIS:H	1.79	0.48
1:A:76:CYS:SG	1:A:84:GLU:HA	2.52	0.48
1:A:122:ASN:HB3	1:A:139:CYS:SG	2.53	0.48
1:A:48:GLN:HA	1:B:47:GLY:O	2.14	0.48
1:A:102:GLN:HB3	1:A:115:PHE:O	2.13	0.48
1:B:44:PRO:O	1:B:48:GLN:HG3	2.14	0.48
1:B:61:THR:O	1:B:91:ASP:HA	2.14	0.48
1:A:71:LEU:HD21	2:A:962:703:C6	2.44	0.48
1:A:105:HIS:HE2	1:A:107:TRP:HZ3	1.63	0.47
1:B:121:LEU:HB2	1:B:148:ASN:OD1	2.14	0.47
1:A:81:GLY:O	1:A:114:CYS:SG	2.73	0.47
1:B:60:PHE:HA	1:B:90:VAL:HA	1.96	0.47
1:A:34:HIS:HD2	1:B:18:GLY:HA3	1.81	0.46
1:A:82:GLN:HA	1:A:97:GLY:O	2.16	0.45
1:A:107:TRP:HA	1:A:107:TRP:CE3	2.51	0.45
1:B:120:CYS:HA	1:B:148:ASN:ND2	2.31	0.45
1:A:104:ARG:HD2	1:A:112:PHE:CE2	2.52	0.45
1:B:106:TYR:HA	1:B:112:PHE:HB3	1.98	0.45
1:A:38:TYR:HB2	1:A:67:LEU:O	2.17	0.44
1:B:144:PHE:CD1	1:B:151:VAL:HG13	2.52	0.44
1:A:34:HIS:CE1	1:B:34:HIS:CE1	3.05	0.44
1:A:143:PHE:HB3	1:A:150:CYS:C	2.37	0.44
1:A:118:SER:HB3	1:A:121:LEU:HD12	1.99	0.43
1:B:38:TYR:HD2	1:B:39:LEU:O	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:CYS:SG	1:B:104:ARG:HG3	2.58	0.43
1:B:144:PHE:HD1	1:B:151:VAL:O	2.00	0.43
1:B:76:CYS:SG	1:B:84:GLU:CB	3.06	0.43
1:B:106:TYR:HA	1:B:112:PHE:HB2	2.00	0.43
1:B:137:CYS:SG	1:B:148:ASN:HA	2.59	0.43
1:A:56:GLU:O	1:A:59:SER:HB2	2.17	0.43
1:B:121:LEU:CB	1:B:149:GLU:HA	2.49	0.42
1:A:32:LYS:HB2	1:B:34:HIS:NE2	2.34	0.42
1:A:19:LYS:HA	1:A:30:CYS:O	2.19	0.42
1:A:105:HIS:O	1:A:112:PHE:HA	2.19	0.42
1:B:76:CYS:SG	1:B:84:GLU:HG3	2.59	0.42
1:A:120:CYS:SG	1:A:125:VAL:CA	3.03	0.42
1:A:122:ASN:ND2	1:A:150:CYS:SG	2.92	0.42
1:A:98:CYS:HB3	1:A:102:GLN:HB2	2.01	0.42
1:A:106:TYR:HB3	1:A:109:GLU:H	1.84	0.42
1:A:100:LYS:HA	1:A:101:ASN:HA	1.58	0.41
1:B:146:ARG:C	1:B:147:GLU:HG3	2.40	0.41
1:A:20:TYR:CE1	1:A:30:CYS:HB2	2.54	0.41
1:B:80:MET:HG2	1:B:111:LEU:HD11	2.03	0.41
1:B:139:CYS:SG	1:B:145:LEU:HD13	2.60	0.41
1:B:22:HIS:HB3	1:B:25:ASN:O	2.20	0.41
1:B:44:PRO:HD2	1:B:48:GLN:CB	2.49	0.41
1:A:18:GLY:O	1:A:31:THR:HA	2.20	0.41
1:A:33:CYS:HB2	1:A:65:ASN:O	2.20	0.41
2:A:962:703:O22	2:A:962:703:H242	2.20	0.41
1:B:21:ILE:HD13	1:B:21:ILE:HA	1.60	0.41
1:B:67:LEU:HA	1:B:67:LEU:HD22	1.77	0.41
1:B:119:LEU:H	1:B:119:LEU:HD13	1.85	0.41
1:B:88:CYS:HB2	1:B:94:THR:H	1.86	0.41
1:A:89:THR:O	1:A:91:ASP:N	2.54	0.40
1:A:100:LYS:C	1:A:100:LYS:HD3	2.41	0.40
1:A:16:PRO:HD2	1:A:19:LYS:HD3	2.04	0.40
1:A:22:HIS:ND1	1:A:23:PRO:HD2	2.36	0.40
1:A:123:GLY:HA3	1:A:138:THR:O	2.22	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	138/162 (85%)	97 (70%)	23 (17%)	18 (13%)	0	0
1	B	140/162 (86%)	117 (84%)	17 (12%)	6 (4%)	2	10
All	All	278/324 (86%)	214 (77%)	40 (14%)	24 (9%)	1	2

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ALA
1	A	73	CYS
1	A	90	VAL
1	A	141	ALA
1	B	90	VAL
1	B	100	LYS
1	A	14	VAL
1	A	64	GLU
1	A	106	TYR
1	B	26	ASN
1	B	33	CYS
1	A	131	GLU
1	B	147	GLU
1	A	39	LEU
1	A	63	SER
1	A	79	GLU
1	A	110	ASN
1	A	145	LEU
1	A	147	GLU
1	A	46	PRO
1	A	108	SER
1	A	149	GLU
1	B	16	PRO
1	A	47	GLY

### 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	129/151 (85%)	104 (81%)	25 (19%)	1	4
1	B	131/151 (87%)	101 (77%)	30 (23%)	1	2
All	All	260/302 (86%)	205 (79%)	55 (21%)	1	3

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET
1	A	21	ILE
1	A	31	THR
1	A	38	TYR
1	A	43	CYS
1	A	53	ARG
1	A	54	GLU
1	A	57	SER
1	A	61	THR
1	A	71	LEU
1	A	78	LYS
1	A	79	GLU
1	A	83	VAL
1	A	94	THR
1	A	107	TRP
1	A	108	SER
1	A	112	PHE
1	A	115	PHE
1	A	120	CYS
1	A	121	LEU
1	A	130	GLN
1	A	133	GLN
1	A	135	THR
1	A	140	HIS
1	A	143	PHE
1	B	34	HIS
1	B	42	ASP

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Mol	Chain	Res	Type
1	B	57	SER
1	B	67	LEU
1	B	69	HIS
1	B	71	LEU
1	B	72	SER
1	B	80	MET
1	B	84	GLU
1	B	85	ILE
1	B	86	SER
1	B	88	CYS
1	B	91	ASP
1	B	92	ARG
1	B	94	THR
1	B	108	SER
1	B	119	LEU
1	B	121	LEU
1	B	124	THR
1	B	138	THR
1	B	144	PHE
1	B	145	LEU
1	B	146	ARG
1	B	147	GLU
1	B	148	ASN
1	B	149	GLU
1	B	151	VAL
1	B	153	CYS
1	B	154	SER
1	B	155	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	48	GLN
1	A	66	HIS
1	B	69	HIS
1	B	102	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
2	703	A	962	1	31,35,35	2.05	8 (25%)	31,51,51	3.30	14 (45%)

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
2	703	A	962	1	-	6/8/22/22	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	962	703	O22-C20	5.50	1.33	1.22
2	A	962	703	C1-C6	4.20	1.46	1.36
2	A	962	703	C16-N15	-3.61	1.30	1.36
2	A	962	703	C16-C20	-3.45	1.43	1.50
2	A	962	703	C18-S21	2.87	1.75	1.67
2	A	962	703	C18-N19	2.47	1.41	1.37
2	A	962	703	O8-N7	2.43	1.26	1.22
2	A	962	703	C12-S11	-2.23	1.72	1.74

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	962	703	C2-C3-N7	7.98	125.38	119.38
2	A	962	703	C17-C12-C13	7.34	112.63	106.24
2	A	962	703	C16-C20-N19	-6.95	105.06	112.65
2	A	962	703	C4-C3-N7	-5.58	113.83	118.75
2	A	962	703	C23-N19-C20	5.19	129.10	123.88
2	A	962	703	O22-C20-C16	4.94	128.64	120.32
2	A	962	703	C13-C12-S11	-4.28	106.18	111.85
2	A	962	703	S21-C18-N15	-4.22	120.98	126.75
2	A	962	703	C23-N19-C18	3.51	127.81	124.03
2	A	962	703	C6-C1-C2	-2.76	116.58	120.99
2	A	962	703	S21-C18-N19	-2.42	124.48	126.50
2	A	962	703	C20-C16-N15	-2.22	113.34	116.16
2	A	962	703	C3-C4-C5	2.22	123.82	120.26
2	A	962	703	C25-N26-C31	2.17	116.77	111.23

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	962	703	C24-C23-N19-C18
2	A	962	703	C24-C23-N19-C20
2	A	962	703	N19-C23-C24-C25
2	A	962	703	C24-C25-N26-C31
2	A	962	703	C24-C25-N26-C27
2	A	962	703	C4-C3-N7-O8

There are no ring outliers.

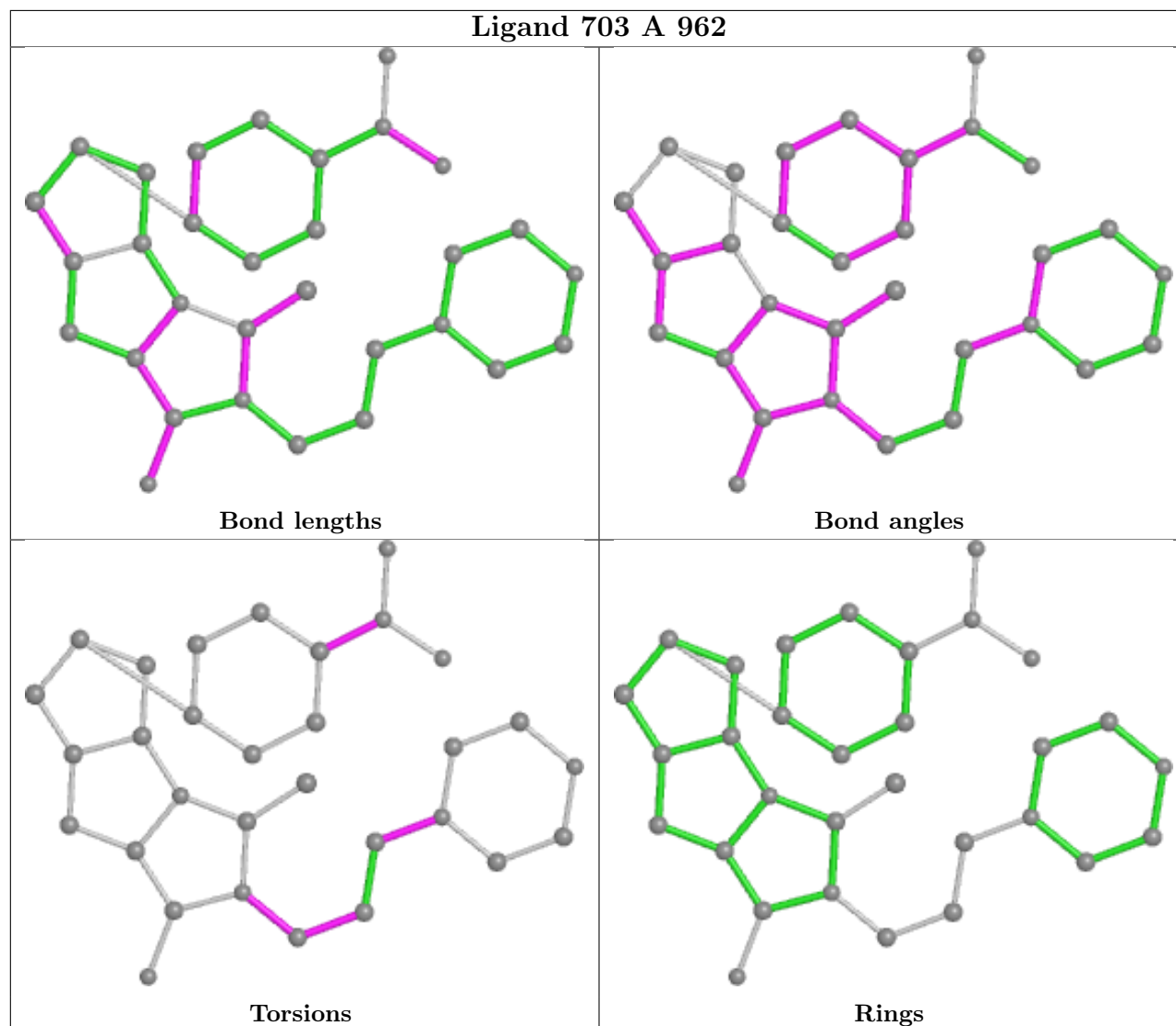
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	962	703	4	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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.