



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 04:03 am GMT

PDB ID : 3F98
Title : Crystal structure of human plasma platelet activating factor acetylhydrolase covalently inhibited by tabun
Authors : Samanta, U.; Bahnson, B.J.
Deposited on : 2008-11-13
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

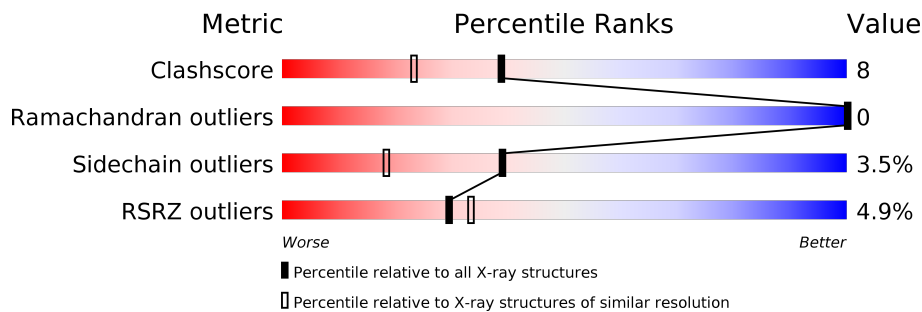
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	383	
1	B	383	
1	C	383	

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	FMT	A	513	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FMT	A	554	-	-	X	-
3	FMT	A	555	-	-	X	-
3	FMT	A	556	-	-	X	-
3	FMT	B	514	-	-	X	-
3	FMT	B	530	-	-	X	-
3	FMT	B	542	-	-	X	-
3	FMT	B	550	-	-	X	-
3	FMT	B	586	-	-	X	-
3	FMT	C	578	-	-	X	-
3	FMT	C	579	-	-	X	-
3	FMT	C	584	-	-	X	-
3	FMT	C	585	-	-	X	-

2 Entry composition [i](#)

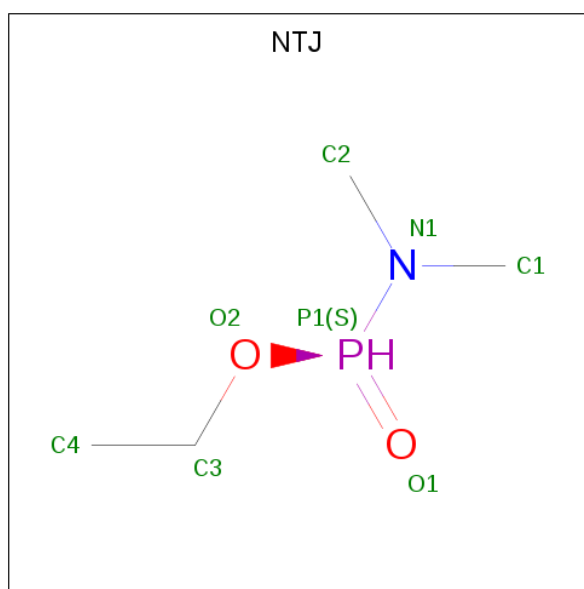
There are 4 unique types of molecules in this entry. The entry contains 10717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Platelet-activating factor acetylhydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	22	0
			3112	1996	530	572	14			
1	B	377	Total	C	N	O	S	0	24	0
			3125	2004	533	574	14			
1	C	377	Total	C	N	O	S	0	22	0
			3114	1996	532	572	14			

- Molecule 2 is R-ETHYL N,N-DIMETHYLPHOSPHONAMIDATE (three-letter code: NTJ) (formula: $C_4H_{12}NO_2P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
2	B	1	Total	C	N	O	P	0	0
			8	4	1	2	1		
2	C	1	Total	C	N	O	P	0	0
			8	4	1	2	1		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

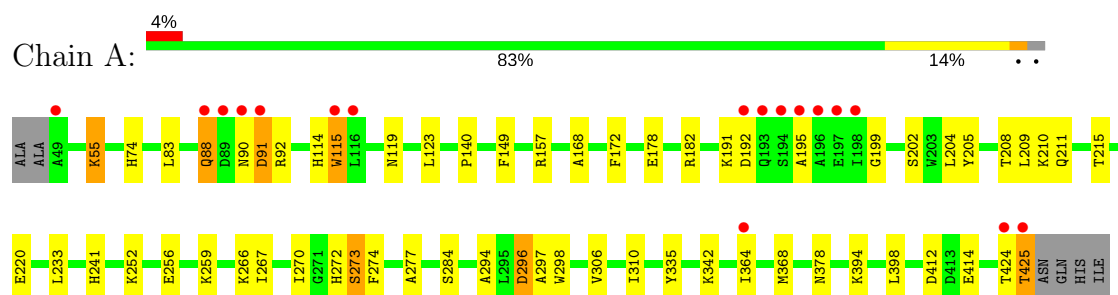
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	369	Total O 369 369	0	0
4	B	377	Total O 377 377	0	0
4	C	338	Total O 338 338	0	0

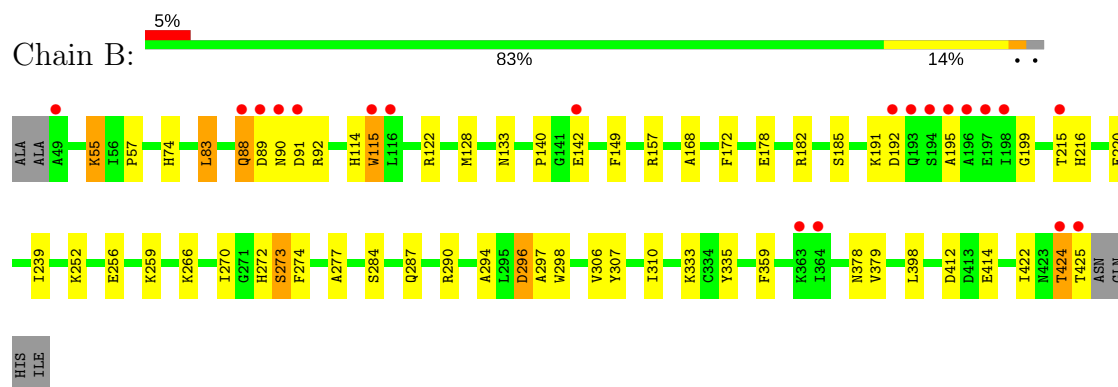
3 Residue-property plots [i](#)

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 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.

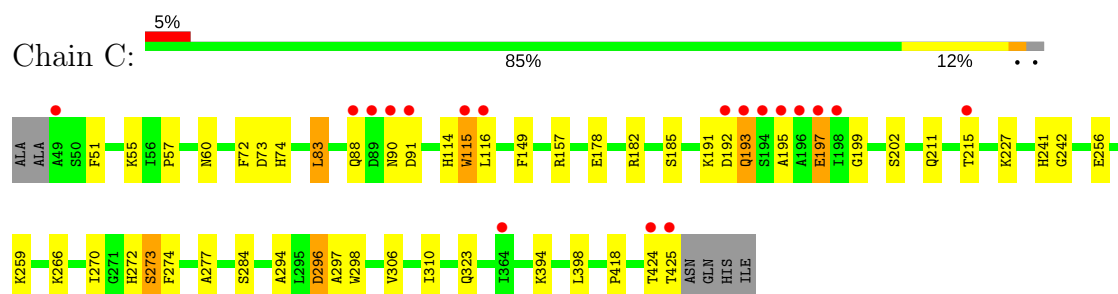
- Molecule 1: Platelet-activating factor acetylhydrolase



- Molecule 1: Platelet-activating factor acetylhydrolase



- Molecule 1: Platelet-activating factor acetylhydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	76.98Å 133.32Å 253.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 38.49 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-1.70) 98.8 (38.49-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.45 (at 1.70Å)	Xtriage
Refinement program	REFMAC OF CCP4I FOR REFINEMENT	Depositor
R, R_{free}	0.179 , 0.202 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.488 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.488 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10717	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.61	2/3276 (0.1%)	0.69	2/4426 (0.0%)
1	B	0.62	2/3289 (0.1%)	0.69	3/4442 (0.1%)
1	C	0.63	3/3279 (0.1%)	0.68	4/4430 (0.1%)
All	All	0.62	7/9844 (0.1%)	0.69	9/13298 (0.1%)

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	1
1	B	0	1
1	C	0	1
All	All	0	3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	HIS	C-N	12.49	1.62	1.34
1	B	272	HIS	C-N	12.49	1.62	1.34
1	C	272	HIS	C-N	12.16	1.62	1.34
1	B	273	SER	C-O	9.95	1.42	1.23
1	A	273	SER	C-O	9.93	1.42	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	SER	O-C-N	-10.51	105.89	122.70
1	B	273	SER	O-C-N	-9.16	108.04	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	SER	O-C-N	-9.15	108.06	122.70
1	C	273	SER	CA-C-N	8.52	135.93	117.20
1	B	273	SER	CA-C-N	8.37	135.62	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ASP	Peptide
1	B	91	ASP	Peptide
1	C	91	ASP	Peptide

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	3112	0	3066	47	0
1	B	3125	0	3083	57	0
1	C	3114	0	3062	44	0
2	A	8	0	11	3	0
2	B	8	0	11	1	0
2	C	8	0	11	1	0
3	A	93	0	31	15	0
3	B	81	0	27	22	0
3	C	84	0	28	19	0
4	A	369	0	0	9	0
4	B	377	0	0	9	0
4	C	338	0	0	11	0
All	All	10717	0	9330	154	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 8.

The worst 5 of 154 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:C:259[A]:LYS:HG3	3:C:578:FMT:H	1.21	1.13
1:B:256[A]:GLU:O	1:B:259[A]:LYS:HG3	1.63	0.99
3:A:554:FMT:H	4:A:1050:HOH:O	1.63	0.97
1:B:259[A]:LYS:HG2	3:B:550:FMT:H	1.47	0.95
1:C:259[A]:LYS:HG3	3:C:578:FMT:C	1.97	0.95

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	397/383 (104%)	386 (97%)	11 (3%)	0	100	100
1	B	399/383 (104%)	386 (97%)	13 (3%)	0	100	100
1	C	397/383 (104%)	386 (97%)	11 (3%)	0	100	100
All	All	1193/1149 (104%)	1158 (97%)	35 (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	347/329 (106%)	334 (96%)	13 (4%)	37	16
1	B	348/329 (106%)	333 (96%)	15 (4%)	32	12
1	C	347/329 (106%)	333 (96%)	14 (4%)	34	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1042/987 (106%)	1000 (96%)	42 (4%)	39 14

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	142[A]	GLU
1	B	215[B]	THR
1	C	274	PHE
1	B	142[B]	GLU
1	B	185[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	ASN
1	B	241	HIS
1	C	211	GLN
1	B	211	GLN
1	B	352	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

89 ligands are 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	NTJ	A	473	1	4,7,7	0.54	0	4,8,8	2.46	1 (25%)
3	FMT	A	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	506	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	509	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	510	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	511	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	513	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	518	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	521	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	522	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	524	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	527	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	528	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	531	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	533	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	534	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	536	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	538	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	539	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	540	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	541	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	544	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	546	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	547	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	551	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	552	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	553	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	554	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	555	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	556	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	558	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NTJ	B	473	1	4,7,7	0.51	0	4,8,8	2.38	1 (25%)
3	FMT	B	501	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	502	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	504	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	505	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	507	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	B	512	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	514	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	515	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	516	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	517	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	520	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	523	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	525	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	526	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	529	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	530	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	532	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	535	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	537	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	542	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	543	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	545	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	548	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	549	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	550	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	557	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	586	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NTJ	C	473	1	4,7,7	0.55	0	4,8,8	2.77	1 (25%)
3	FMT	C	519	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	559	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	560	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	561	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	562	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	563	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	564	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	565	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	566	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	567	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	568	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	569	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	570	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	571	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	572	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	573	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	574	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	575	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	576	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	577	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	C	578	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	579	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	580	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	581	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	582	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	583	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	584	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	585	-	0,2,2	0.00	-	0,1,1	0.00	-

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	NTJ	A	473	1	-	0/1/7/7	0/0/0/0
3	FMT	A	503	-	-	0/0/0/0	0/0/0/0
3	FMT	A	506	-	-	0/0/0/0	0/0/0/0
3	FMT	A	508	-	-	0/0/0/0	0/0/0/0
3	FMT	A	509	-	-	0/0/0/0	0/0/0/0
3	FMT	A	510	-	-	0/0/0/0	0/0/0/0
3	FMT	A	511	-	-	0/0/0/0	0/0/0/0
3	FMT	A	513	-	-	0/0/0/0	0/0/0/0
3	FMT	A	518	-	-	0/0/0/0	0/0/0/0
3	FMT	A	521	-	-	0/0/0/0	0/0/0/0
3	FMT	A	522	-	-	0/0/0/0	0/0/0/0
3	FMT	A	524	-	-	0/0/0/0	0/0/0/0
3	FMT	A	527	-	-	0/0/0/0	0/0/0/0
3	FMT	A	528	-	-	0/0/0/0	0/0/0/0
3	FMT	A	531	-	-	0/0/0/0	0/0/0/0
3	FMT	A	533	-	-	0/0/0/0	0/0/0/0
3	FMT	A	534	-	-	0/0/0/0	0/0/0/0
3	FMT	A	536	-	-	0/0/0/0	0/0/0/0
3	FMT	A	538	-	-	0/0/0/0	0/0/0/0
3	FMT	A	539	-	-	0/0/0/0	0/0/0/0
3	FMT	A	540	-	-	0/0/0/0	0/0/0/0
3	FMT	A	541	-	-	0/0/0/0	0/0/0/0
3	FMT	A	544	-	-	0/0/0/0	0/0/0/0
3	FMT	A	546	-	-	0/0/0/0	0/0/0/0
3	FMT	A	547	-	-	0/0/0/0	0/0/0/0
3	FMT	A	551	-	-	0/0/0/0	0/0/0/0
3	FMT	A	552	-	-	0/0/0/0	0/0/0/0
3	FMT	A	553	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMT	A	554	-	-	0/0/0/0	0/0/0/0
3	FMT	A	555	-	-	0/0/0/0	0/0/0/0
3	FMT	A	556	-	-	0/0/0/0	0/0/0/0
3	FMT	A	558	-	-	0/0/0/0	0/0/0/0
2	NTJ	B	473	1	-	0/1/7/7	0/0/0/0
3	FMT	B	501	-	-	0/0/0/0	0/0/0/0
3	FMT	B	502	-	-	0/0/0/0	0/0/0/0
3	FMT	B	504	-	-	0/0/0/0	0/0/0/0
3	FMT	B	505	-	-	0/0/0/0	0/0/0/0
3	FMT	B	507	-	-	0/0/0/0	0/0/0/0
3	FMT	B	512	-	-	0/0/0/0	0/0/0/0
3	FMT	B	514	-	-	0/0/0/0	0/0/0/0
3	FMT	B	515	-	-	0/0/0/0	0/0/0/0
3	FMT	B	516	-	-	0/0/0/0	0/0/0/0
3	FMT	B	517	-	-	0/0/0/0	0/0/0/0
3	FMT	B	520	-	-	0/0/0/0	0/0/0/0
3	FMT	B	523	-	-	0/0/0/0	0/0/0/0
3	FMT	B	525	-	-	0/0/0/0	0/0/0/0
3	FMT	B	526	-	-	0/0/0/0	0/0/0/0
3	FMT	B	529	-	-	0/0/0/0	0/0/0/0
3	FMT	B	530	-	-	0/0/0/0	0/0/0/0
3	FMT	B	532	-	-	0/0/0/0	0/0/0/0
3	FMT	B	535	-	-	0/0/0/0	0/0/0/0
3	FMT	B	537	-	-	0/0/0/0	0/0/0/0
3	FMT	B	542	-	-	0/0/0/0	0/0/0/0
3	FMT	B	543	-	-	0/0/0/0	0/0/0/0
3	FMT	B	545	-	-	0/0/0/0	0/0/0/0
3	FMT	B	548	-	-	0/0/0/0	0/0/0/0
3	FMT	B	549	-	-	0/0/0/0	0/0/0/0
3	FMT	B	550	-	-	0/0/0/0	0/0/0/0
3	FMT	B	557	-	-	0/0/0/0	0/0/0/0
3	FMT	B	586	-	-	0/0/0/0	0/0/0/0
2	NTJ	C	473	1	-	0/1/7/7	0/0/0/0
3	FMT	C	519	-	-	0/0/0/0	0/0/0/0
3	FMT	C	559	-	-	0/0/0/0	0/0/0/0
3	FMT	C	560	-	-	0/0/0/0	0/0/0/0
3	FMT	C	561	-	-	0/0/0/0	0/0/0/0
3	FMT	C	562	-	-	0/0/0/0	0/0/0/0
3	FMT	C	563	-	-	0/0/0/0	0/0/0/0
3	FMT	C	564	-	-	0/0/0/0	0/0/0/0
3	FMT	C	565	-	-	0/0/0/0	0/0/0/0
3	FMT	C	566	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMT	C	567	-	-	0/0/0/0	0/0/0/0
3	FMT	C	568	-	-	0/0/0/0	0/0/0/0
3	FMT	C	569	-	-	0/0/0/0	0/0/0/0
3	FMT	C	570	-	-	0/0/0/0	0/0/0/0
3	FMT	C	571	-	-	0/0/0/0	0/0/0/0
3	FMT	C	572	-	-	0/0/0/0	0/0/0/0
3	FMT	C	573	-	-	0/0/0/0	0/0/0/0
3	FMT	C	574	-	-	0/0/0/0	0/0/0/0
3	FMT	C	575	-	-	0/0/0/0	0/0/0/0
3	FMT	C	576	-	-	0/0/0/0	0/0/0/0
3	FMT	C	577	-	-	0/0/0/0	0/0/0/0
3	FMT	C	578	-	-	0/0/0/0	0/0/0/0
3	FMT	C	579	-	-	0/0/0/0	0/0/0/0
3	FMT	C	580	-	-	0/0/0/0	0/0/0/0
3	FMT	C	581	-	-	0/0/0/0	0/0/0/0
3	FMT	C	582	-	-	0/0/0/0	0/0/0/0
3	FMT	C	583	-	-	0/0/0/0	0/0/0/0
3	FMT	C	584	-	-	0/0/0/0	0/0/0/0
3	FMT	C	585	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	473	NTJ	C1-N1-C2	4.64	121.03	113.51
2	A	473	NTJ	C1-N1-C2	4.83	121.33	113.51
2	C	473	NTJ	C1-N1-C2	5.44	122.32	113.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

27 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	473	NTJ	3	0
3	A	506	FMT	1	0
3	A	513	FMT	2	0
3	A	518	FMT	1	0
3	A	533	FMT	1	0
3	A	551	FMT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	554	FMT	4	0
3	A	555	FMT	3	0
3	A	556	FMT	2	0
2	B	473	NTJ	1	0
3	B	514	FMT	2	0
3	B	515	FMT	1	0
3	B	517	FMT	1	0
3	B	529	FMT	1	0
3	B	530	FMT	2	0
3	B	535	FMT	1	0
3	B	542	FMT	2	0
3	B	550	FMT	8	0
3	B	557	FMT	1	0
3	B	586	FMT	3	0
2	C	473	NTJ	1	0
3	C	575	FMT	1	0
3	C	578	FMT	6	0
3	C	579	FMT	3	0
3	C	582	FMT	1	0
3	C	584	FMT	2	0
3	C	585	FMT	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	272:HIS	C	273:SER	N	1.62
1	B	272:HIS	C	273:SER	N	1.62
1	C	272:HIS	C	273:SER	N	1.62

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	377/383 (98%)	-0.02	17 (4%) 33 38	9, 15, 33, 45	0
1	B	377/383 (98%)	-0.01	20 (5%) 26 29	9, 15, 33, 44	0
1	C	377/383 (98%)	-0.00	18 (4%) 30 35	8, 15, 33, 45	0
All	All	1131/1149 (98%)	-0.01	55 (4%) 29 33	8, 15, 33, 45	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	89	ASP	11.2
1	A	89	ASP	10.6
1	B	89	ASP	9.4
1	A	115	TRP	8.1
1	B	90	ASN	8.0

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 carbohydrates 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(\AA^2)	Q<0.9
3	FMT	C	566	3/3	0.66	0.19	53,53,53,54	0
3	FMT	C	571	3/3	0.68	0.20	72,72,72,72	0
3	FMT	C	573	3/3	0.73	0.13	43,43,43,44	0
3	FMT	A	510	3/3	0.73	0.21	42,42,42,42	0
3	FMT	A	533	3/3	0.75	0.21	14,14,16,18	0
3	FMT	B	526	3/3	0.75	0.15	56,56,56,56	0
3	FMT	B	548	3/3	0.76	0.28	68,68,68,68	0
3	FMT	A	544	3/3	0.76	0.20	53,53,53,53	0
3	FMT	A	506	3/3	0.80	0.19	26,26,29,29	0
3	FMT	A	524	3/3	0.80	0.12	65,65,65,65	0
3	FMT	C	577	3/3	0.80	0.11	52,52,52,52	0
3	FMT	A	538	3/3	0.81	0.19	33,33,34,34	0
3	FMT	A	551	3/3	0.81	0.18	40,40,40,41	0
3	FMT	B	525	3/3	0.82	0.21	60,60,60,60	0
3	FMT	A	508	3/3	0.82	0.12	56,56,56,56	0
3	FMT	C	580	3/3	0.82	0.14	60,60,60,60	0
3	FMT	B	504	3/3	0.82	0.12	61,61,61,61	0
3	FMT	B	535	3/3	0.82	0.22	14,14,16,18	0
3	FMT	B	550	3/3	0.82	0.18	54,54,54,55	0
3	FMT	C	568	3/3	0.83	0.10	54,54,54,54	0
3	FMT	B	549	3/3	0.83	0.22	41,41,42,43	0
3	FMT	C	581	3/3	0.83	0.12	51,51,51,51	0
3	FMT	A	539	3/3	0.83	0.17	59,59,60,60	0
3	FMT	C	575	3/3	0.83	0.21	13,13,15,18	0
3	FMT	C	569	3/3	0.84	0.13	59,59,59,59	0
3	FMT	C	570	3/3	0.84	0.15	58,58,59,59	0
3	FMT	C	563	3/3	0.85	0.16	22,22,27,29	0
3	FMT	A	527	3/3	0.85	0.19	56,56,57,57	0
3	FMT	B	517	3/3	0.86	0.19	28,28,31,32	0
3	FMT	A	547	3/3	0.87	0.11	54,54,54,54	0
3	FMT	B	545	3/3	0.87	0.13	42,42,42,43	0
3	FMT	C	578	3/3	0.88	0.15	50,50,50,50	0
3	FMT	C	584	3/3	0.89	0.17	43,43,44,44	0
3	FMT	B	507	3/3	0.89	0.18	41,41,41,41	0
3	FMT	C	561	3/3	0.89	0.23	44,44,45,45	0
3	FMT	B	514	3/3	0.89	0.37	40,40,41,41	0
3	FMT	A	541	3/3	0.90	0.14	23,23,24,25	0
3	FMT	B	543	3/3	0.90	0.23	29,29,30,31	0
3	FMT	A	540	3/3	0.90	0.12	48,48,48,48	0
3	FMT	A	509	3/3	0.90	0.21	29,29,30,31	0
3	FMT	A	518	3/3	0.91	0.44	40,40,40,41	0
3	FMT	B	501	3/3	0.91	0.22	26,26,28,29	0
3	FMT	C	585	3/3	0.91	0.13	15,15,16,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMT	A	556	3/3	0.91	0.16	43,43,43,44	0
3	FMT	C	565	3/3	0.92	0.49	38,38,39,41	0
3	FMT	C	560	3/3	0.92	0.12	27,27,29,29	0
3	FMT	B	515	3/3	0.92	0.47	41,41,41,41	0
3	FMT	A	521	3/3	0.92	0.18	50,50,50,50	0
3	FMT	C	572	3/3	0.92	0.16	38,38,38,38	0
3	FMT	A	552	3/3	0.92	0.20	44,44,44,44	0
3	FMT	A	503	3/3	0.93	0.12	34,34,37,38	0
3	FMT	B	516	3/3	0.93	0.22	41,41,41,41	0
3	FMT	A	522	3/3	0.93	0.13	41,41,41,41	0
3	FMT	C	583	3/3	0.93	0.10	65,65,65,65	0
3	FMT	B	586	3/3	0.93	0.12	15,15,15,18	0
3	FMT	A	531	3/3	0.93	0.14	43,43,43,43	0
3	FMT	C	559	3/3	0.93	0.12	39,39,39,40	0
3	FMT	A	534	3/3	0.94	0.11	20,20,23,26	0
3	FMT	B	537	3/3	0.94	0.17	61,61,61,61	0
3	FMT	C	567	3/3	0.94	0.06	40,40,41,41	0
3	FMT	A	536	3/3	0.94	0.09	38,38,38,39	0
3	FMT	B	512	3/3	0.94	0.11	29,29,32,33	0
3	FMT	C	562	3/3	0.94	0.10	27,27,30,32	0
3	FMT	A	511	3/3	0.94	0.07	21,21,23,24	0
3	FMT	C	574	3/3	0.94	0.12	20,20,23,27	0
3	FMT	B	542	3/3	0.94	0.19	33,33,34,35	0
3	FMT	B	529	3/3	0.95	0.10	30,30,32,34	0
3	FMT	A	528	3/3	0.95	0.14	46,46,46,46	0
3	FMT	B	505	3/3	0.95	0.07	33,33,35,35	0
3	FMT	B	557	3/3	0.95	0.10	46,46,47,47	0
3	FMT	B	523	3/3	0.95	0.13	50,50,50,50	0
3	FMT	A	558	3/3	0.95	0.09	51,51,51,51	0
3	FMT	C	579	3/3	0.95	0.19	32,32,33,34	0
3	FMT	A	554	3/3	0.95	0.12	30,30,31,34	0
2	NTJ	C	473	8/8	0.96	0.11	13,15,19,22	0
3	FMT	B	502	3/3	0.96	0.11	19,19,22,25	0
3	FMT	A	553	3/3	0.96	0.12	36,36,37,37	0
3	FMT	C	564	3/3	0.96	0.17	40,40,41,41	0
3	FMT	C	582	3/3	0.96	0.28	43,43,43,44	0
2	NTJ	B	473	8/8	0.96	0.14	14,16,19,22	0
2	NTJ	A	473	8/8	0.96	0.13	13,16,19,22	0
3	FMT	C	519	3/3	0.97	0.15	14,14,16,16	0
3	FMT	C	576	3/3	0.97	0.13	38,38,38,38	0
3	FMT	B	530	3/3	0.97	0.10	25,25,28,31	0
3	FMT	A	555	3/3	0.97	0.15	25,25,28,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMT	B	532	3/3	0.97	0.15	14,14,15,16	0
3	FMT	B	520	3/3	0.97	0.07	32,32,34,35	0
3	FMT	A	546	3/3	0.98	0.06	21,21,24,24	0
3	FMT	A	513	3/3	0.98	0.13	39,39,39,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.