



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:30 AM UTC

PDB ID : 8EPK / pdb_00008epk
Title : Complex of anticoagulant RNA aptamer and human coagulation factor IXa (S195A)
Authors : Kolyadko, V.N.; Krishnaswamy, S.
Deposited on : 2022-10-05
Resolution : 2.65 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)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

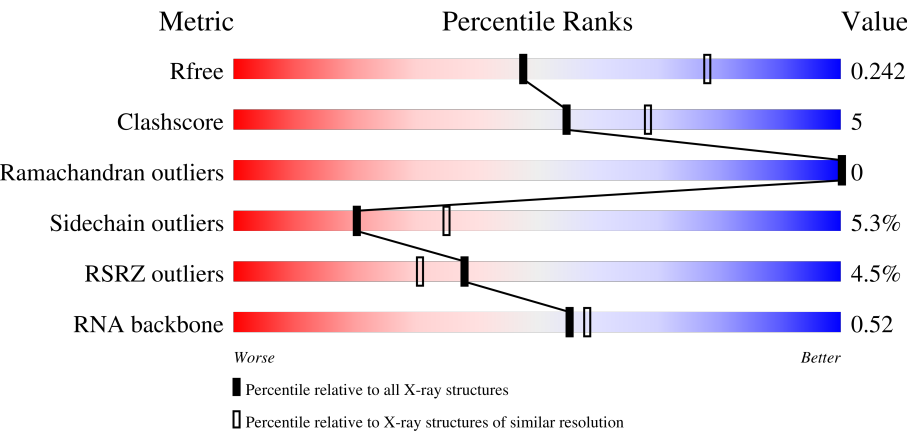
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



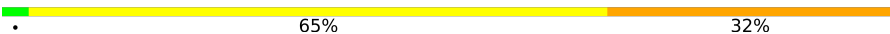
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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	65	2% 80% 5% 15%
1	C	65	6% 72% 12% 15%
2	B	235	4% 86% 13% .
2	D	235	5% 84% 16% .

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Mol	Chain	Length	Quality of chain
3	E	31	 58% 39%
3	F	31	 65% 32%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5870 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 Coagulation factor IXa light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	55	Total	C	N	O	S	0	0	0
			413	249	75	82	7			
1	C	55	Total	C	N	O	S	0	0	0
			413	249	75	82	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	ARG	-	insertion	UNP P00740
A	146	ARG	-	insertion	UNP P00740
A	147	LYS	-	insertion	UNP P00740
A	148	ARG	-	insertion	UNP P00740
C	145	ARG	-	insertion	UNP P00740
C	146	ARG	-	insertion	UNP P00740
C	147	LYS	-	insertion	UNP P00740
C	148	ARG	-	insertion	UNP P00740

- Molecule 2 is a protein called Coagulation factor IXa heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1843	1175	319	340	9			
2	D	235	Total	C	N	O	S	0	0	0
			1843	1175	319	340	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	engineered mutation	UNP P00740
D	195	ALA	SER	engineered mutation	UNP P00740

- Molecule 3 is a RNA chain called RNA (31-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	31	Total	C	F	N	O	P	0	0	0
			672	311	11	111	208	31			
3	F	31	Total	C	F	N	O	P	0	0	0
			672	311	11	111	208	31			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

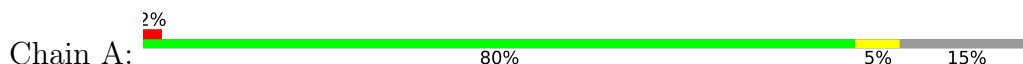
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	O	0	0
			3	3		
6	D	2	Total	O	0	0
			2	2		
6	E	2	Total	O	0	0
			2	2		
6	F	3	Total	O	0	0
			3	3		

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.

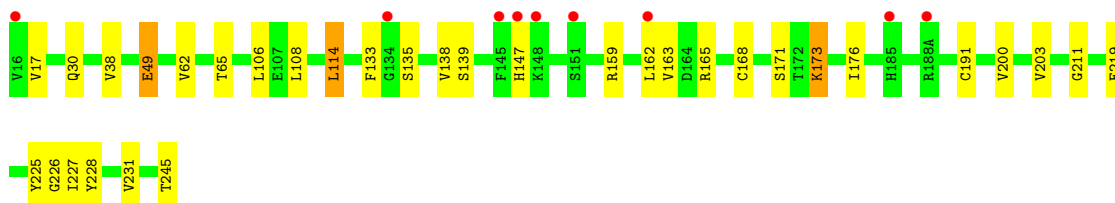
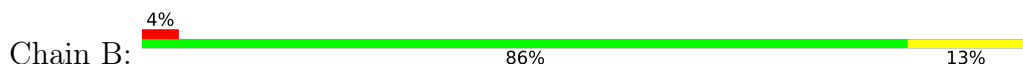
- Molecule 1: Coagulation factor IXa light chain



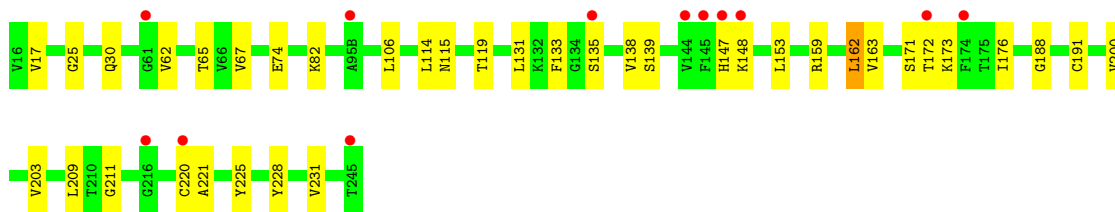
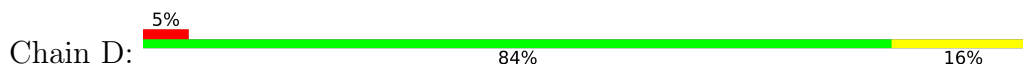
- Molecule 1: Coagulation factor IXa light chain



- Molecule 2: Coagulation factor IXa heavy chain



- Molecule 2: Coagulation factor IXa heavy chain



- Molecule 3: RNA (31-MER)

Chain E: . 58% 39%



• Molecule 3: RNA (31-MER)

Chain F: . 65% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.50Å 79.58Å 84.32Å 90.00° 101.78° 90.00°	Depositor
Resolution (Å)	60.24 – 2.65 60.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.6 (60.24-2.65) 96.9 (60.24-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.231 , 0.261 (Not available) , 0.242	Depositor DCC
R_{free} test set	1313 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5870	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, CA, ATD, CFZ, OMC, OMU, A2M, MG, UFT

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	0.56	0/418	0.90	1/563 (0.2%)
1	C	0.58	0/418	0.93	2/563 (0.4%)
2	B	0.53	0/1887	0.87	0/2557
2	D	0.52	0/1887	0.87	0/2557
3	E	0.78	0/26	0.68	0/41
3	F	0.84	0/26	0.72	0/41
All	All	0.54	0/4662	0.88	3/6322 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	CYS	N-CA-C	5.68	119.50	109.96
1	C	113	GLU	N-CA-C	5.54	120.45	111.37
1	C	84	LEU	N-CA-C	5.01	125.03	111.00

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	413	0	394	0	0
1	C	413	0	394	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1843	0	1807	15	0
2	D	1843	0	1807	19	0
3	E	672	0	361	12	0
3	F	672	0	361	9	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	3	0	0	0	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	3	0	0	0	0
All	All	5870	0	5124	53	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 5.

All (53) 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)
3:E:30:OMC:H3'	3:E:31:ATD:H4'	1.39	1.02
1:C:115:TYR:OH	1:C:134:ARG:HG2	1.94	0.67
3:E:6:CFZ:H6	3:E:6:CFZ:H5'	1.79	0.65
3:F:6:CFZ:H6	3:F:6:CFZ:H5'	1.79	0.65
2:B:173:LYS:HG2	2:D:148:LYS:HD3	1.80	0.64
3:F:30:OMC:H5'	3:F:30:OMC:H6	1.66	0.60
2:D:188:GLY:H	2:D:221:ALA:HB1	1.66	0.60
1:C:115:TYR:OH	1:C:134:ARG:CG	2.51	0.58
2:D:67:VAL:HG22	2:D:82:LYS:HG2	1.87	0.56
3:F:6:CFZ:H6	3:F:6:CFZ:C5'	2.37	0.55
2:B:147:HIS:CE1	2:B:219:GLU:HA	2.42	0.55
2:D:17:VAL:HG23	2:D:191:CYS:SG	2.47	0.55
3:E:6:CFZ:H6	3:E:6:CFZ:C5'	2.37	0.54
2:D:176:ILE:N	2:D:176:ILE:HD12	2.24	0.53
2:B:162:LEU:HD21	3:E:9:UFT:C2	2.38	0.53
3:F:28:OMC:HM22	3:F:29:A2M:O4'	2.09	0.52
2:B:17:VAL:HG23	2:B:191:CYS:SG	2.50	0.51
2:D:131:LEU:O	2:D:162:LEU:HD12	2.10	0.51
3:E:28:OMC:HM22	3:E:29:A2M:O4'	2.10	0.51
2:B:162:LEU:HD23	2:B:163:VAL:N	2.26	0.51
2:B:168:CYS:SG	2:B:176:ILE:HD11	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:LEU:HD21	3:E:9:UFT:N3	2.27	0.49
3:E:30:OMC:H6	3:E:30:OMC:H5'	1.78	0.48
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.96	0.47
2:D:138:VAL:HG11	2:D:228:TYR:CE2	2.50	0.47
2:D:148:LYS:HG3	3:E:27:OMC:HM21	1.97	0.46
3:F:31:ATD:O2	3:F:31:ATD:H2'	2.14	0.46
2:B:138:VAL:HG11	2:B:228:TYR:CE2	2.50	0.46
2:B:49:GLU:HG3	2:B:114:LEU:HD21	1.98	0.46
3:F:18:A2M:HM'2	3:F:20:OMG:H4'	1.99	0.45
3:F:30:OMC:H3'	3:F:31:ATD:H2'	1.97	0.45
2:B:226:GLY:C	2:B:227:ILE:HD12	2.42	0.45
2:D:162:LEU:HD23	2:D:163:VAL:N	2.32	0.45
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.98	0.44
3:E:16:UFT:O2	3:E:16:UFT:O4'	2.36	0.44
2:D:115:ASN:O	2:D:119:THR:HG22	2.18	0.44
2:B:30:GLN:NE2	2:B:139:SER:OG	2.51	0.43
2:D:133:PHE:CE2	2:D:203:VAL:HG12	2.53	0.43
2:D:172:THR:O	2:D:173:LYS:HB2	2.19	0.43
3:E:30:OMC:H5'	3:E:30:OMC:C6	2.53	0.43
2:B:133:PHE:CE2	2:B:203:VAL:HG12	2.53	0.42
3:E:18:A2M:HM'2	3:E:20:OMG:H4'	2.01	0.42
1:C:137:VAL:HG21	2:D:25:GLY:HA3	2.02	0.42
2:D:74:GLU:HG3	2:D:153:LEU:CD1	2.49	0.42
3:E:6:CFZ:H2'	3:E:7:UFT:O4'	2.20	0.42
2:D:30:GLN:NE2	2:D:139:SER:OG	2.53	0.42
2:D:163:VAL:HG21	2:D:225:TYR:CD1	2.55	0.42
3:F:16:UFT:O2	3:F:16:UFT:O4'	2.38	0.41
3:F:6:CFZ:H2'	3:F:7:UFT:O4'	2.21	0.41
2:D:135:SER:OG	2:D:159:ARG:NE	2.54	0.40
2:B:135:SER:OG	2:B:159:ARG:NE	2.55	0.40
2:B:163:VAL:HG21	2:B:225:TYR:CD1	2.56	0.40
2:D:209:LEU:HG	2:D:231:VAL:HG21	2.04	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	53/65 (82%)	48 (91%)	5 (9%)	0	100	100
1	C	53/65 (82%)	47 (89%)	6 (11%)	0	100	100
2	B	233/235 (99%)	219 (94%)	14 (6%)	0	100	100
2	D	233/235 (99%)	220 (94%)	13 (6%)	0	100	100
All	All	572/600 (95%)	534 (93%)	38 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	49/59 (83%)	47 (96%)	2 (4%)	27	46
1	C	49/59 (83%)	46 (94%)	3 (6%)	17	30
2	B	197/197 (100%)	185 (94%)	12 (6%)	17	30
2	D	197/197 (100%)	188 (95%)	9 (5%)	24	41
All	All	492/512 (96%)	466 (95%)	26 (5%)	20	35

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	VAL
1	A	135	VAL
2	B	38	VAL
2	B	49	GLU
2	B	62	VAL
2	B	65	THR
2	B	106	LEU
2	B	108	LEU

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Mol	Chain	Res	Type
2	B	114	LEU
2	B	165	ARG
2	B	171	SER
2	B	173	LYS
2	B	200	VAL
2	B	245	THR
1	C	90	ILE
1	C	104	ASP
1	C	135	VAL
2	D	62	VAL
2	D	65	THR
2	D	106	LEU
2	D	114	LEU
2	D	147	HIS
2	D	162	LEU
2	D	171	SER
2	D	200	VAL
2	D	220	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	30	GLN
2	D	30	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	10/31 (32%)	1 (10%)	0
3	F	10/31 (32%)	1 (10%)	0
All	All	20/62 (32%)	2 (10%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	E	24	OMC
3	F	24	OMC

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

60 non-standard protein/DNA/RNA residues 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
3	OMC	F	24	3	19,22,23	0.87	1 (5%)	25,31,34	1.26	3 (12%)
3	CFZ	F	12	3	18,21,22	0.90	0	25,30,33	1.26	3 (12%)
3	A2M	E	29	3	22,25,26	1.51	4 (18%)	30,36,39	2.16	8 (26%)
3	A2M	F	5	3	22,25,26	1.45	3 (13%)	30,36,39	2.26	8 (26%)
3	A2M	F	17	3	22,25,26	1.51	4 (18%)	30,36,39	2.20	10 (33%)
3	OMG	F	4	3	23,26,27	1.24	3 (13%)	32,38,41	2.01	6 (18%)
3	UFT	F	9	3	18,21,22	1.33	2 (11%)	25,30,33	1.91	6 (24%)
3	UFT	F	26	3	18,21,22	1.35	2 (11%)	25,30,33	2.07	5 (20%)
3	CFZ	E	21	3	18,21,22	0.93	1 (5%)	25,30,33	1.19	3 (12%)
3	OMC	F	27	3	19,22,23	0.83	0	25,31,34	1.22	3 (12%)
3	A2M	F	29	3	22,25,26	1.56	4 (18%)	30,36,39	2.12	9 (30%)
3	OMG	E	13	3	23,26,27	1.23	3 (13%)	32,38,41	2.06	7 (21%)
3	CFZ	E	14	3	18,21,22	0.94	0	25,30,33	1.11	2 (8%)
3	OMC	F	28	3	19,22,23	0.85	1 (5%)	25,31,34	1.18	3 (12%)
3	UFT	F	19	3	18,21,22	1.44	3 (16%)	25,30,33	1.70	4 (16%)
3	OMG	E	3	3	23,26,27	1.27	3 (13%)	32,38,41	2.01	6 (18%)
3	A2M	E	8	3	22,25,26	1.46	4 (18%)	30,36,39	2.22	11 (36%)
3	UFT	F	16	3	18,21,22	1.25	4 (22%)	25,30,33	2.08	7 (28%)
3	UFT	E	7	3	18,21,22	1.38	3 (16%)	25,30,33	1.87	6 (24%)
3	OMG	F	3	3	23,26,27	1.23	2 (8%)	32,38,41	2.09	7 (21%)
3	OMC	E	28	3	19,22,23	0.84	0	25,31,34	1.15	2 (8%)
3	A2M	F	8	3	22,25,26	1.48	4 (18%)	30,36,39	2.23	11 (36%)
3	OMC	E	24	3	19,22,23	0.86	1 (5%)	25,31,34	1.23	3 (12%)
3	CFZ	E	6	3	18,21,22	1.00	0	25,30,33	1.38	4 (16%)
3	OMU	F	2	3	19,22,23	1.20	3 (15%)	25,31,34	1.87	5 (20%)
3	OMU	F	22	3	19,22,23	1.28	3 (15%)	25,31,34	1.79	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	F	1	3	27,27,27	1.19	3 (11%)	39,41,41	1.98	6 (15%)
3	A2M	F	18	3	22,25,26	1.49	4 (18%)	30,36,39	2.25	9 (30%)
3	OMG	F	20	3	23,26,27	1.22	2 (8%)	32,38,41	2.22	7 (21%)
3	UFT	E	26	3	18,21,22	1.38	3 (16%)	25,30,33	2.06	5 (20%)
3	UFT	E	9	3	18,21,22	1.36	3 (16%)	25,30,33	1.92	7 (28%)
3	CFZ	E	12	3	18,21,22	0.93	0	25,30,33	1.20	3 (12%)
3	ATD	F	31	3	18,21,22	4.71	13 (72%)	26,30,33	2.57	10 (38%)
3	OMG	E	1	3	27,27,27	1.17	3 (11%)	39,41,41	1.95	5 (12%)
3	CFZ	F	6	3	18,21,22	0.96	0	25,30,33	1.36	3 (12%)
3	OMC	F	30	3	19,22,23	0.86	0	25,31,34	1.15	1 (4%)
3	A2M	E	10	3	22,25,26	1.52	4 (18%)	30,36,39	2.19	12 (40%)
3	CFZ	F	11	3	18,21,22	0.93	0	25,30,33	1.20	2 (8%)
3	A2M	E	5	3	22,25,26	1.49	4 (18%)	30,36,39	2.29	8 (26%)
3	A2M	E	17	3	22,25,26	1.56	5 (22%)	30,36,39	2.20	10 (33%)
3	OMC	E	27	3	19,22,23	0.81	0	25,31,34	1.25	3 (12%)
3	UFT	E	16	3	18,21,22	1.40	3 (16%)	25,30,33	2.01	6 (24%)
3	OMG	F	13	3	23,26,27	1.23	3 (13%)	32,38,41	2.04	7 (21%)
3	OMG	F	15	3	23,26,27	1.22	3 (13%)	32,38,41	2.10	8 (25%)
3	CFZ	F	21	3,5	18,21,22	0.95	1 (5%)	25,30,33	1.16	3 (12%)
3	A2M	F	10	3	22,25,26	1.51	5 (22%)	30,36,39	2.18	11 (36%)
3	UFT	E	19	3	18,21,22	1.49	4 (22%)	25,30,33	1.73	4 (16%)
3	CFZ	E	25	3	18,21,22	0.98	0	25,30,33	1.06	1 (4%)
3	OMG	E	15	3	23,26,27	1.20	3 (13%)	32,38,41	2.12	8 (25%)
3	OMU	E	2	3	19,22,23	1.19	3 (15%)	25,31,34	1.94	5 (20%)
3	OMG	E	20	3	23,26,27	1.25	3 (13%)	32,38,41	2.19	7 (21%)
3	CFZ	F	14	3	18,21,22	0.96	0	25,30,33	1.15	2 (8%)
3	OMU	E	22	3	19,22,23	1.23	3 (15%)	25,31,34	1.79	4 (16%)
3	CFZ	F	25	3	18,21,22	0.93	1 (5%)	25,30,33	1.10	1 (4%)
3	ATD	E	31	3	18,21,22	4.67	13 (72%)	26,30,33	2.42	9 (34%)
3	A2M	E	18	3	22,25,26	1.51	4 (18%)	30,36,39	2.26	9 (30%)
3	OMG	E	4	3	23,26,27	1.27	3 (13%)	32,38,41	2.00	6 (18%)
3	CFZ	E	11	3	18,21,22	0.94	1 (5%)	25,30,33	1.22	3 (12%)
3	UFT	F	7	3	18,21,22	1.30	1 (5%)	25,30,33	1.87	6 (24%)
3	OMC	E	30	3	19,22,23	0.93	0	25,31,34	1.14	1 (4%)

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	OMC	F	24	3	-	4/9/27/28	0/2/2/2
3	CFZ	F	12	3	-	3/7/25/26	0/2/2/2
3	A2M	E	29	3	-	0/9/27/28	0/3/3/3
3	A2M	F	5	3	-	2/9/27/28	0/3/3/3
3	A2M	F	17	3	-	3/9/27/28	0/3/3/3
3	OMG	F	4	3	-	0/9/27/28	0/3/3/3
3	UFT	F	9	3	-	0/7/25/26	0/2/2/2
3	UFT	F	26	3	-	0/7/25/26	0/2/2/2
3	CFZ	E	21	3	-	0/7/25/26	0/2/2/2
3	OMC	F	27	3	-	2/9/27/28	0/2/2/2
3	A2M	F	29	3	-	0/9/27/28	0/3/3/3
3	OMG	E	13	3	-	2/9/27/28	0/3/3/3
3	CFZ	E	14	3	-	2/7/25/26	0/2/2/2
3	OMC	F	28	3	-	0/9/27/28	0/2/2/2
3	UFT	F	19	3	-	0/7/25/26	0/2/2/2
3	OMG	E	3	3	-	0/9/27/28	0/3/3/3
3	A2M	E	8	3	-	3/9/27/28	0/3/3/3
3	UFT	F	16	3	-	3/7/25/26	0/2/2/2
3	UFT	E	7	3	-	0/7/25/26	0/2/2/2
3	OMG	F	3	3	-	0/9/27/28	0/3/3/3
3	OMC	E	28	3	-	0/9/27/28	0/2/2/2
3	A2M	F	8	3	-	3/9/27/28	0/3/3/3
3	OMC	E	24	3	-	4/9/27/28	0/2/2/2
3	CFZ	E	6	3	-	2/7/25/26	0/2/2/2
3	OMU	F	2	3	-	0/9/27/28	0/2/2/2
3	OMU	F	22	3	-	1/9/27/28	0/2/2/2
3	OMG	F	1	3	-	0/12/28/28	0/3/3/3
3	A2M	F	18	3	-	3/9/27/28	0/3/3/3
3	OMG	F	20	3	-	4/9/27/28	0/3/3/3
3	UFT	E	26	3	-	0/7/25/26	0/2/2/2
3	UFT	E	9	3	-	0/7/25/26	0/2/2/2
3	CFZ	E	12	3	-	2/7/25/26	0/2/2/2
3	ATD	F	31	3	-	5/8/22/23	0/2/2/2
3	OMG	E	1	3	-	2/12/28/28	0/3/3/3
3	CFZ	F	6	3	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	30	3	-	0/9/27/28	0/2/2/2
3	A2M	E	10	3	-	3/9/27/28	0/3/3/3
3	CFZ	F	11	3	-	2/7/25/26	0/2/2/2
3	A2M	E	5	3	-	2/9/27/28	0/3/3/3
3	A2M	E	17	3	-	3/9/27/28	0/3/3/3
3	OMC	E	27	3	-	2/9/27/28	0/2/2/2
3	UFT	E	16	3	-	4/7/25/26	0/2/2/2
3	OMG	F	13	3	-	3/9/27/28	0/3/3/3
3	OMG	F	15	3	-	2/9/27/28	0/3/3/3
3	CFZ	F	21	3,5	-	0/7/25/26	0/2/2/2
3	A2M	F	10	3	-	3/9/27/28	0/3/3/3
3	UFT	E	19	3	-	0/7/25/26	0/2/2/2
3	CFZ	E	25	3	-	0/7/25/26	0/2/2/2
3	OMG	E	15	3	-	2/9/27/28	0/3/3/3
3	OMU	E	2	3	-	0/9/27/28	0/2/2/2
3	OMG	E	20	3	-	3/9/27/28	0/3/3/3
3	CFZ	F	14	3	-	2/7/25/26	0/2/2/2
3	OMU	E	22	3	-	1/9/27/28	0/2/2/2
3	CFZ	F	25	3	-	0/7/25/26	0/2/2/2
3	ATD	E	31	3	-	6/8/22/23	0/2/2/2
3	A2M	E	18	3	-	3/9/27/28	0/3/3/3
3	OMG	E	4	3	-	0/9/27/28	0/3/3/3
3	CFZ	E	11	3	-	2/7/25/26	0/2/2/2
3	UFT	F	7	3	-	0/7/25/26	0/2/2/2
3	OMC	E	30	3	-	0/9/27/28	0/2/2/2

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	31	ATD	C6-C5	8.99	1.49	1.34
3	F	31	ATD	C6-C5	8.94	1.49	1.34
3	F	31	ATD	C2'-C1'	-7.44	1.32	1.52
3	E	31	ATD	C2'-C1'	-7.36	1.32	1.52
3	F	31	ATD	C2-N1	6.83	1.49	1.38
3	E	31	ATD	C3'-C4'	-6.42	1.29	1.52
3	E	31	ATD	C2-N1	6.28	1.48	1.38
3	F	31	ATD	C2-N3	6.27	1.48	1.38
3	F	31	ATD	C3'-C4'	-6.20	1.30	1.52
3	E	31	ATD	C2-N3	6.15	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	31	ATD	C2'-C3'	5.74	1.65	1.52
3	E	31	ATD	O4'-C4'	5.68	1.57	1.45
3	F	31	ATD	O4'-C4'	5.61	1.57	1.45
3	E	31	ATD	C2'-C3'	5.33	1.64	1.52
3	E	31	ATD	O4'-C1'	4.95	1.53	1.42
3	F	29	A2M	C5-C4	4.67	1.47	1.39
3	F	31	ATD	O4'-C1'	4.65	1.52	1.42
3	E	29	A2M	C5-C4	4.63	1.47	1.39
3	E	17	A2M	C5-C4	4.58	1.47	1.39
3	F	17	A2M	C5-C4	4.58	1.47	1.39
3	E	18	A2M	C5-C4	4.53	1.47	1.39
3	E	10	A2M	C5-C4	4.51	1.47	1.39
3	F	10	A2M	C5-C4	4.50	1.47	1.39
3	E	8	A2M	C5-C4	4.49	1.47	1.39
3	E	5	A2M	C5-C4	4.46	1.47	1.39
3	F	18	A2M	C5-C4	4.46	1.47	1.39
3	F	8	A2M	C5-C4	4.43	1.47	1.39
3	F	31	ATD	C6-N1	4.33	1.45	1.38
3	E	31	ATD	C6-N1	4.25	1.45	1.38
3	F	5	A2M	C5-C4	4.18	1.46	1.39
3	F	31	ATD	C4-N3	3.54	1.45	1.38
3	F	1	OMG	C5-C4	3.36	1.48	1.38
3	E	31	ATD	C4-N3	3.36	1.45	1.38
3	F	3	OMG	C5-C4	3.30	1.47	1.38
3	E	3	OMG	C5-C4	3.30	1.47	1.38
3	E	20	OMG	C5-C4	3.29	1.47	1.38
3	E	1	OMG	C5-C4	3.29	1.47	1.38
3	F	13	OMG	C5-C4	3.27	1.47	1.38
3	F	4	OMG	C5-C4	3.25	1.47	1.38
3	F	15	OMG	C5-C4	3.25	1.47	1.38
3	F	20	OMG	C5-C4	3.20	1.47	1.38
3	E	15	OMG	C5-C4	3.18	1.47	1.38
3	E	13	OMG	C5-C4	3.17	1.47	1.38
3	E	4	OMG	C5-C4	3.15	1.47	1.38
3	E	17	A2M	C5-C6	2.87	1.49	1.41
3	E	31	ATD	O4-C4	-2.86	1.18	1.23
3	F	22	OMU	C4-N3	-2.84	1.33	1.38
3	F	17	A2M	C5-C6	2.84	1.48	1.41
3	F	18	A2M	C5-C6	2.79	1.48	1.41
3	F	29	A2M	C5-C6	2.77	1.48	1.41
3	E	4	OMG	C6-N1	-2.77	1.33	1.38
3	F	5	A2M	C5-C6	2.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	18	A2M	C5-C6	2.77	1.48	1.41
3	E	7	UFT	C2-N1	2.77	1.42	1.38
3	E	19	UFT	C4-N3	-2.74	1.33	1.38
3	F	26	UFT	C2-N1	2.74	1.42	1.38
3	E	26	UFT	C2-N1	2.72	1.42	1.38
3	E	16	UFT	C4-N3	-2.71	1.34	1.38
3	E	5	A2M	C5-C6	2.68	1.48	1.41
3	F	31	ATD	O2-C2	-2.68	1.18	1.23
3	F	10	A2M	C5-C6	2.67	1.48	1.41
3	F	7	UFT	C2-N1	2.66	1.42	1.38
3	E	10	A2M	C5-C6	2.65	1.48	1.41
3	F	31	ATD	O4-C4	-2.63	1.18	1.23
3	E	31	ATD	C4-C5	2.62	1.49	1.44
3	E	3	OMG	C6-N1	-2.60	1.34	1.38
3	F	19	UFT	C4-N3	-2.60	1.34	1.38
3	E	5	A2M	C5-N7	-2.60	1.34	1.39
3	E	22	OMU	C4-N3	-2.59	1.34	1.38
3	E	16	UFT	C2-N1	2.58	1.42	1.38
3	E	31	ATD	O2-C2	-2.58	1.18	1.23
3	F	10	A2M	C5-N7	-2.57	1.34	1.39
3	E	20	OMG	C6-N1	-2.55	1.34	1.38
3	F	4	OMG	C6-N1	-2.55	1.34	1.38
3	E	17	A2M	C5-N7	-2.54	1.34	1.39
3	E	29	A2M	C5-N7	-2.52	1.34	1.39
3	E	10	A2M	C5-N7	-2.52	1.34	1.39
3	F	9	UFT	C2-N1	2.51	1.42	1.38
3	F	8	A2M	C5-N7	-2.50	1.34	1.39
3	F	8	A2M	C5-C6	2.50	1.47	1.41
3	E	9	UFT	C4-N3	-2.49	1.34	1.38
3	F	29	A2M	C5-N7	-2.49	1.34	1.39
3	F	5	A2M	C5-N7	-2.49	1.34	1.39
3	E	8	A2M	C5-C6	2.49	1.47	1.41
3	F	17	A2M	C8-N7	2.47	1.36	1.31
3	E	10	A2M	C8-N7	2.47	1.36	1.31
3	E	29	A2M	C5-C6	2.46	1.47	1.41
3	E	2	OMU	C2-N1	2.46	1.42	1.38
3	F	29	A2M	C8-N7	2.44	1.36	1.31
3	E	8	A2M	C5-N7	-2.42	1.34	1.39
3	F	31	ATD	C4-C5	2.41	1.48	1.44
3	E	18	A2M	C5-N7	-2.40	1.34	1.39
3	F	2	OMU	C4-N3	-2.39	1.34	1.38
3	F	9	UFT	C4-N3	-2.39	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMG	C5-N7	-2.37	1.34	1.39
3	F	18	A2M	C5-N7	-2.37	1.34	1.39
3	F	20	OMG	C6-N1	-2.37	1.34	1.38
3	F	1	OMG	C6-N1	-2.36	1.34	1.38
3	E	1	OMG	C6-N1	-2.34	1.34	1.38
3	E	19	UFT	C2-N3	-2.33	1.33	1.38
3	E	26	UFT	C4-N3	-2.33	1.34	1.38
3	F	15	OMG	C5-N7	-2.32	1.34	1.39
3	E	18	A2M	C8-N7	2.31	1.36	1.31
3	E	9	UFT	C2-N1	2.30	1.42	1.38
3	F	19	UFT	C2-N3	-2.30	1.34	1.38
3	E	19	UFT	C5-C4	-2.28	1.38	1.43
3	F	18	A2M	C8-N7	2.28	1.36	1.31
3	F	10	A2M	C8-N7	2.27	1.36	1.31
3	F	13	OMG	C6-N1	-2.26	1.34	1.38
3	E	13	OMG	C6-N1	-2.26	1.34	1.38
3	F	2	OMU	C2-N1	2.25	1.42	1.38
3	E	1	OMG	C5-N7	-2.25	1.34	1.39
3	F	24	OMC	C6-C5	2.24	1.40	1.35
3	F	28	OMC	C6-C5	2.23	1.40	1.35
3	E	8	A2M	C8-N7	2.23	1.36	1.31
3	F	15	OMG	C6-N1	-2.23	1.34	1.38
3	E	15	OMG	C5-N7	-2.22	1.34	1.39
3	F	1	OMG	C5-N7	-2.21	1.34	1.39
3	E	7	UFT	C4-N3	-2.21	1.34	1.38
3	F	26	UFT	C4-N3	-2.21	1.34	1.38
3	E	26	UFT	C5-C4	-2.20	1.38	1.43
3	F	4	OMG	C5-N7	-2.20	1.34	1.39
3	E	22	OMU	C2-N1	2.20	1.41	1.38
3	E	17	A2M	C8-N7	2.19	1.35	1.31
3	F	22	OMU	C2-N1	2.19	1.41	1.38
3	F	16	UFT	C2-N1	2.19	1.41	1.38
3	E	15	OMG	C6-N1	-2.19	1.34	1.38
3	F	16	UFT	C4-N3	-2.19	1.34	1.38
3	E	13	OMG	C5-N7	-2.18	1.34	1.39
3	F	3	OMG	C6-N1	-2.17	1.34	1.38
3	F	8	A2M	C8-N7	2.16	1.35	1.31
3	E	3	OMG	C5-N7	-2.15	1.34	1.39
3	E	24	OMC	C6-C5	2.15	1.40	1.35
3	E	5	A2M	C8-N7	2.14	1.35	1.31
3	F	22	OMU	C5-C4	-2.12	1.39	1.43
3	F	17	A2M	C5-N7	-2.12	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMU	C2-N3	-2.12	1.34	1.38
3	F	13	OMG	C5-N7	-2.09	1.34	1.39
3	E	7	UFT	C6-C5	2.09	1.39	1.35
3	E	29	A2M	C8-N7	2.08	1.35	1.31
3	F	21	CFZ	C6-C5	2.08	1.39	1.35
3	F	2	OMU	C6-C5	2.08	1.39	1.35
3	F	10	A2M	C4-N9	-2.06	1.33	1.37
3	F	16	UFT	C5-C4	-2.06	1.39	1.43
3	E	2	OMU	C5-C4	-2.06	1.39	1.43
3	F	25	CFZ	C6-C5	2.06	1.39	1.35
3	E	21	CFZ	C6-C5	2.05	1.39	1.35
3	E	16	UFT	C2-N3	-2.05	1.34	1.38
3	F	16	UFT	C2-N3	-2.04	1.34	1.38
3	E	20	OMG	C5-N7	-2.04	1.35	1.39
3	E	11	CFZ	C6-C5	2.02	1.39	1.35
3	E	17	A2M	C4-N9	-2.01	1.33	1.37
3	F	19	UFT	C5-C4	-2.01	1.39	1.43
3	E	19	UFT	C2-N1	2.01	1.41	1.38
3	E	9	UFT	C5-C4	-2.00	1.39	1.43
3	E	22	OMU	C2-N3	-2.00	1.34	1.38

All (339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	A2M	C5-C4-N3	-6.67	117.53	126.72
3	F	1	OMG	C5-C4-N3	-6.63	117.84	128.39
3	F	5	A2M	C5-C4-N3	-6.60	117.63	126.72
3	E	1	OMG	C5-C4-N3	-6.47	118.10	128.39
3	E	18	A2M	C5-C4-N3	-6.39	117.92	126.72
3	F	18	A2M	C5-C4-N3	-6.30	118.04	126.72
3	F	20	OMG	C5-C4-N3	-6.29	118.37	128.39
3	E	20	OMG	C5-C4-N3	-6.21	118.51	128.39
3	F	15	OMG	C5-C4-N3	-6.02	118.81	128.39
3	E	15	OMG	C5-C4-N3	-6.02	118.81	128.39
3	E	13	OMG	C5-C4-N3	-6.01	118.82	128.39
3	F	13	OMG	C5-C4-N3	-5.97	118.89	128.39
3	E	29	A2M	C5-C4-N3	-5.95	118.52	126.72
3	F	10	A2M	C5-C4-N3	-5.88	118.61	126.72
3	F	8	A2M	C5-C4-N3	-5.85	118.66	126.72
3	E	4	OMG	C5-C4-N3	-5.85	119.07	128.39
3	E	17	A2M	C5-C4-N3	-5.85	118.66	126.72
3	E	8	A2M	C5-C4-N3	-5.81	118.72	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	OMG	C5-C4-N3	-5.80	119.17	128.39
3	F	29	A2M	C5-C4-N3	-5.78	118.76	126.72
3	E	10	A2M	C5-C4-N3	-5.76	118.78	126.72
3	E	3	OMG	C5-C4-N3	-5.74	119.25	128.39
3	F	4	OMG	C5-C4-N3	-5.74	119.25	128.39
3	F	17	A2M	C5-C4-N3	-5.61	119.00	126.72
3	E	31	ATD	C4-N3-C2	-5.47	120.17	127.34
3	E	31	ATD	C5-C4-N3	5.46	120.07	115.32
3	E	5	A2M	N3-C4-N9	5.38	136.31	127.17
3	F	5	A2M	N3-C4-N9	5.38	136.31	127.17
3	F	1	OMG	C2-N3-C4	5.31	121.44	112.30
3	F	26	UFT	C4-N3-C2	-5.28	120.06	126.61
3	E	13	OMG	C2-N3-C4	5.25	121.34	112.30
3	F	20	OMG	C2-N3-C4	5.24	121.33	112.30
3	F	31	ATD	C5-C4-N3	5.18	119.83	115.32
3	E	26	UFT	C4-N3-C2	-5.17	120.19	126.61
3	E	1	OMG	C2-N3-C4	5.15	121.17	112.30
3	F	31	ATD	C4-N3-C2	-5.15	120.59	127.34
3	E	20	OMG	C2-N3-C4	5.13	121.14	112.30
3	F	13	OMG	C2-N3-C4	5.07	121.04	112.30
3	E	15	OMG	C2-N3-C4	5.05	121.00	112.30
3	F	31	ATD	O4-C4-C5	-5.01	119.19	124.92
3	F	18	A2M	N3-C4-N9	4.99	135.65	127.17
3	F	15	OMG	C2-N3-C4	4.97	120.86	112.30
3	E	18	A2M	N3-C4-N9	4.96	135.61	127.17
3	F	8	A2M	N3-C4-N9	4.89	135.49	127.17
3	E	16	UFT	C4-N3-C2	-4.89	120.54	126.61
3	F	3	OMG	C2-N3-C4	4.88	120.70	112.30
3	E	29	A2M	N3-C4-N9	4.87	135.45	127.17
3	E	8	A2M	N3-C4-N9	4.86	135.44	127.17
3	E	3	OMG	C2-N3-C4	4.75	120.47	112.30
3	F	16	UFT	C4-N3-C2	-4.74	120.72	126.61
3	F	9	UFT	C4-N3-C2	-4.71	120.77	126.61
3	E	1	OMG	N9-C4-N3	4.71	135.36	125.95
3	E	4	OMG	C2-N3-C4	4.68	120.36	112.30
3	F	29	A2M	N3-C4-N9	4.65	135.07	127.17
3	F	9	UFT	N3-C2-N1	4.64	120.93	114.89
3	E	9	UFT	N3-C2-N1	4.62	120.90	114.89
3	F	4	OMG	C2-N3-C4	4.61	120.24	112.30
3	E	31	ATD	O4-C4-C5	-4.61	119.64	124.92
3	E	2	OMU	C4-N3-C2	-4.59	120.92	126.61
3	F	1	OMG	N9-C4-N3	4.57	135.08	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	UFT	C4-N3-C2	-4.57	120.94	126.61
3	E	7	UFT	C4-N3-C2	-4.55	120.97	126.61
3	E	17	A2M	N3-C4-N9	4.54	134.89	127.17
3	F	2	OMU	C4-N3-C2	-4.53	120.99	126.61
3	E	22	OMU	C4-N3-C2	-4.45	121.09	126.61
3	E	22	OMU	N3-C2-N1	4.43	120.65	114.89
3	E	4	OMG	N9-C4-N3	4.42	134.80	125.95
3	F	22	OMU	C4-N3-C2	-4.40	121.15	126.61
3	F	17	A2M	N3-C4-N9	4.40	134.64	127.17
3	F	22	OMU	N3-C2-N1	4.39	120.61	114.89
3	F	2	OMU	N3-C2-N1	4.38	120.59	114.89
3	E	9	UFT	C4-N3-C2	-4.38	121.18	126.61
3	F	4	OMG	N9-C4-N3	4.36	134.66	125.95
3	E	10	A2M	N3-C4-N9	4.35	134.57	127.17
3	E	16	UFT	C5-C4-N3	4.34	120.87	114.80
3	F	16	UFT	C5-C4-N3	4.33	120.86	114.80
3	F	15	OMG	N9-C4-N3	4.32	134.59	125.95
3	F	26	UFT	N3-C2-N1	4.31	120.50	114.89
3	E	26	UFT	C5-C4-N3	4.30	120.82	114.80
3	E	15	OMG	N9-C4-N3	4.28	134.52	125.95
3	F	10	A2M	N3-C4-N9	4.28	134.44	127.17
3	F	18	A2M	C2-N3-C4	4.27	122.27	111.83
3	F	19	UFT	C4-N3-C2	-4.25	121.34	126.61
3	E	20	OMG	N9-C4-N3	4.25	134.44	125.95
3	E	18	A2M	C2-N3-C4	4.24	122.19	111.83
3	E	19	UFT	C4-N3-C2	-4.23	121.36	126.61
3	F	7	UFT	N3-C2-N1	4.22	120.39	114.89
3	F	20	OMG	N9-C4-N3	4.21	134.37	125.95
3	F	26	UFT	C5-C4-N3	4.20	120.68	114.80
3	E	7	UFT	N3-C2-N1	4.20	120.35	114.89
3	E	3	OMG	N9-C4-N3	4.19	134.34	125.95
3	E	26	UFT	N3-C2-N1	4.17	120.31	114.89
3	E	5	A2M	C2-N3-C4	4.16	122.00	111.83
3	F	8	A2M	N3-C2-N1	-4.15	122.30	128.58
3	F	5	A2M	C2-N3-C4	4.15	121.96	111.83
3	E	8	A2M	N3-C2-N1	-4.11	122.36	128.58
3	E	2	OMU	N3-C2-N1	4.11	120.24	114.89
3	E	16	UFT	N3-C2-N1	4.09	120.21	114.89
3	E	17	A2M	C4-C5-N7	-4.06	105.94	110.58
3	F	13	OMG	N9-C4-N3	4.04	134.04	125.95
3	E	13	OMG	N9-C4-N3	4.04	134.02	125.95
3	F	3	OMG	N9-C4-N3	4.03	134.00	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	19	UFT	C5-C4-N3	3.99	120.38	114.80
3	F	8	A2M	C2-N3-C4	3.99	121.56	111.83
3	E	8	A2M	C2-N3-C4	3.98	121.56	111.83
3	E	26	UFT	O4-C4-C5	-3.96	118.33	125.16
3	E	31	ATD	N3-C2-N1	3.95	120.03	114.89
3	E	29	A2M	C2-N3-C4	3.94	121.44	111.83
3	F	19	UFT	C5-C4-N3	3.92	120.29	114.80
3	E	2	OMU	C5-C4-N3	3.91	120.28	114.80
3	E	17	A2M	C2-N3-C4	3.90	121.36	111.83
3	F	17	A2M	C4-C5-N7	-3.90	106.13	110.58
3	F	18	A2M	N3-C2-N1	-3.88	122.71	128.58
3	E	10	A2M	C2-N3-C4	3.88	121.31	111.83
3	E	18	A2M	N3-C2-N1	-3.87	122.72	128.58
3	E	30	OMC	C2'-C1'-N1	-3.87	106.89	114.24
3	F	29	A2M	C2-N3-C4	3.87	121.27	111.83
3	F	17	A2M	C2-N3-C4	3.86	121.25	111.83
3	F	10	A2M	C2-N3-C4	3.85	121.24	111.83
3	E	29	A2M	N3-C2-N1	-3.84	122.77	128.58
3	F	31	ATD	C1'-N1-C2	3.84	125.16	117.66
3	F	10	A2M	C4-C5-N7	-3.79	106.25	110.58
3	F	31	ATD	N3-C2-N1	3.79	119.83	114.89
3	F	26	UFT	O4-C4-C5	-3.79	118.63	125.16
3	E	10	A2M	N3-C2-N1	-3.78	122.86	128.58
3	E	17	A2M	N3-C2-N1	-3.78	122.87	128.58
3	F	17	A2M	N3-C2-N1	-3.77	122.87	128.58
3	F	16	UFT	O4-C4-C5	-3.77	118.66	125.16
3	F	31	ATD	C4'-O4'-C1'	-3.77	100.56	109.51
3	F	3	OMG	C6-C5-N7	3.77	137.14	130.29
3	F	16	UFT	N3-C2-N1	3.76	119.79	114.89
3	E	28	OMC	C2'-C1'-N1	-3.75	107.13	114.24
3	F	10	A2M	N3-C2-N1	-3.74	122.92	128.58
3	F	19	UFT	N3-C2-N1	3.73	119.75	114.89
3	E	22	OMU	C5-C4-N3	3.70	119.98	114.80
3	E	13	OMG	C6-C5-N7	3.70	137.02	130.29
3	F	29	A2M	N3-C2-N1	-3.69	123.00	128.58
3	F	22	OMU	C5-C4-N3	3.68	119.95	114.80
3	F	20	OMG	C6-C5-N7	3.67	136.96	130.29
3	E	18	A2M	C4-C5-N7	-3.66	106.39	110.58
3	F	3	OMG	C2'-C1'-N9	-3.64	107.33	114.24
3	F	30	OMC	C2'-C1'-N1	-3.63	107.35	114.24
3	E	10	A2M	C4-C5-N7	-3.62	106.44	110.58
3	E	20	OMG	C6-C5-N7	3.62	136.87	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	13	OMG	C6-C5-N7	3.61	136.87	130.29
3	F	9	UFT	C5-C4-N3	3.61	119.86	114.80
3	E	19	UFT	N3-C2-N1	3.61	119.58	114.89
3	E	7	UFT	C5-C4-N3	3.57	119.81	114.80
3	F	7	UFT	C5-C4-N3	3.57	119.80	114.80
3	F	18	A2M	C4-C5-N7	-3.56	106.51	110.58
3	F	28	OMC	C2'-C1'-N1	-3.56	107.48	114.24
3	E	2	OMU	O4-C4-C5	-3.56	119.03	125.16
3	E	21	CFZ	C2'-C1'-N1	-3.54	108.83	114.27
3	E	3	OMG	C6-C5-N7	3.50	136.65	130.29
3	E	3	OMG	C2'-C1'-N9	-3.49	107.61	114.24
3	F	2	OMU	C5-C4-N3	3.49	119.69	114.80
3	E	5	A2M	N3-C2-N1	-3.48	123.31	128.58
3	E	7	UFT	O4-C4-C5	-3.46	119.20	125.16
3	E	20	OMG	C2'-C1'-N9	-3.45	107.69	114.24
3	E	5	A2M	C4-C5-N7	-3.43	106.66	110.58
3	F	5	A2M	N3-C2-N1	-3.43	123.39	128.58
3	F	7	UFT	O4-C4-C5	-3.42	119.26	125.16
3	F	20	OMG	C2'-C1'-N9	-3.40	107.78	114.24
3	E	9	UFT	C5-C4-N3	3.40	119.56	114.80
3	F	4	OMG	C6-C5-N7	3.38	136.44	130.29
3	E	27	OMC	C2'-C1'-N1	-3.38	107.83	114.24
3	F	17	A2M	C4-N9-C8	3.37	109.28	105.74
3	F	5	A2M	C4-C5-N7	-3.32	106.78	110.58
3	F	1	OMG	C6-C5-N7	3.29	136.29	130.29
3	F	27	OMC	C2'-C1'-N1	-3.29	108.00	114.24
3	E	15	OMG	C6-C5-N7	3.28	136.27	130.29
3	F	15	OMG	C6-C5-N7	3.28	136.27	130.29
3	E	4	OMG	C6-C5-N7	3.23	136.16	130.29
3	F	21	CFZ	C2'-C1'-N1	-3.22	109.33	114.27
3	E	6	CFZ	C2'-C1'-N1	-3.20	109.35	114.27
3	F	4	OMG	C2'-C1'-N9	-3.18	108.20	114.24
3	F	9	UFT	O4-C4-C5	-3.17	119.69	125.16
3	F	31	ATD	O4'-C1'-C2'	-3.17	100.33	106.25
3	E	4	OMG	C2'-C1'-N9	-3.16	108.24	114.24
3	F	6	CFZ	C2'-C1'-N1	-3.16	109.42	114.27
3	E	2	OMU	C2'-C1'-N1	-3.14	108.28	114.24
3	F	8	A2M	C4-C5-N7	-3.13	107.00	110.58
3	F	31	ATD	C1'-N1-C6	-3.13	115.49	120.74
3	E	31	ATD	C3'-C2'-C1'	3.13	108.85	102.89
3	F	29	A2M	C4-C5-N7	-3.11	107.02	110.58
3	E	29	A2M	C4-C5-N7	-3.09	107.05	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	9	UFT	O4-C4-C5	-3.09	119.83	125.16
3	F	17	A2M	C5-N7-C8	3.07	108.28	103.45
3	E	17	A2M	C5-N7-C8	3.05	108.24	103.45
3	E	1	OMG	C6-C5-N7	3.04	135.82	130.29
3	E	19	UFT	O4-C4-C5	-3.03	119.93	125.16
3	E	13	OMG	C4-C5-N7	-3.00	105.91	110.67
3	E	8	A2M	C4-C5-N7	-2.99	107.16	110.58
3	E	24	OMC	C2'-C1'-N1	-2.99	108.57	114.24
3	F	20	OMG	C4-C5-N7	-2.99	105.94	110.67
3	E	16	UFT	F2'-C2'-C3'	2.98	115.03	109.14
3	F	24	OMC	C2'-C1'-N1	-2.97	108.59	114.24
3	F	2	OMU	C2'-C1'-N1	-2.97	108.60	114.24
3	F	2	OMU	O4-C4-C5	-2.96	120.05	125.16
3	E	17	A2M	C4-N9-C8	2.96	108.84	105.74
3	E	15	OMG	O2'-C2'-C1'	2.93	114.54	108.99
3	F	13	OMG	C4-C5-N7	-2.93	106.03	110.67
3	F	1	OMG	C4-C5-N7	-2.92	106.04	110.67
3	F	3	OMG	C4-C5-N7	-2.92	106.04	110.67
3	E	20	OMG	C4-C5-N7	-2.92	106.05	110.67
3	F	15	OMG	O2'-C2'-C1'	2.91	114.52	108.99
3	E	29	A2M	C2'-C1'-N9	-2.90	108.97	113.75
3	F	8	A2M	C4-N9-C8	2.90	108.78	105.74
3	E	5	A2M	C5-N7-C8	2.90	108.01	103.45
3	E	8	A2M	C4-N9-C8	2.86	108.74	105.74
3	F	26	UFT	C2'-C1'-N1	-2.86	109.88	114.27
3	F	5	A2M	C5-N7-C8	2.83	107.89	103.45
3	E	31	ATD	C5-C6-N1	-2.82	120.25	123.31
3	F	17	A2M	N9-C8-N7	-2.80	109.96	113.94
3	F	18	A2M	C4-N9-C8	2.77	108.64	105.74
3	E	18	A2M	C5-N7-C8	2.75	107.77	103.45
3	E	10	A2M	C5-N7-C8	2.74	107.76	103.45
3	F	18	A2M	C5-N7-C8	2.73	107.75	103.45
3	E	26	UFT	C2'-C1'-N1	-2.72	110.09	114.27
3	E	16	UFT	O4-C4-C5	-2.71	120.48	125.16
3	F	10	A2M	C5-N7-C8	2.68	107.66	103.45
3	F	22	OMU	O4-C4-C5	-2.67	120.55	125.16
3	F	16	UFT	F2'-C2'-C3'	2.67	114.42	109.14
3	F	19	UFT	O4-C4-C5	-2.67	120.56	125.16
3	E	8	A2M	C5-N7-C8	2.66	107.63	103.45
3	F	14	CFZ	O2-C2-N3	-2.66	118.14	122.33
3	E	31	ATD	C5'-C4'-C3'	-2.65	109.39	115.22
3	F	29	A2M	C2'-C1'-N9	-2.65	109.40	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1	OMG	C4-C5-N7	-2.63	106.51	110.67
3	F	24	OMC	O2-C2-N3	-2.61	118.21	122.33
3	F	8	A2M	C5-N7-C8	2.61	107.56	103.45
3	F	12	CFZ	F2'-C2'-C3'	2.60	114.28	109.14
3	E	15	OMG	C4-C5-N7	-2.60	106.55	110.67
3	E	22	OMU	O4-C4-C5	-2.59	120.69	125.16
3	F	5	A2M	C4-N9-C8	2.59	108.45	105.74
3	E	6	CFZ	O4'-C1'-N1	2.59	114.22	108.36
3	F	29	A2M	C4-N9-C8	2.58	108.45	105.74
3	F	15	OMG	C4-C5-N7	-2.58	106.58	110.67
3	E	18	A2M	C4-N9-C8	2.56	108.43	105.74
3	E	16	UFT	C2'-C1'-N1	-2.55	110.35	114.27
3	E	3	OMG	C4-C5-N7	-2.55	106.62	110.67
3	E	5	A2M	C4-N9-C8	2.55	108.42	105.74
3	F	24	OMC	O4'-C1'-N1	2.53	114.09	108.36
3	F	25	CFZ	O2-C2-N3	-2.53	118.35	122.33
3	F	16	UFT	C2'-C1'-N1	-2.52	110.39	114.27
3	E	10	A2M	C4-N9-C8	2.51	108.37	105.74
3	E	24	OMC	O2-C2-N3	-2.49	118.41	122.33
3	E	14	CFZ	C2'-C1'-N1	-2.48	110.45	114.27
3	F	6	CFZ	O4'-C1'-N1	2.48	113.98	108.36
3	E	17	A2M	C6-C5-N7	2.48	136.86	132.09
3	E	24	OMC	O4'-C1'-N1	2.47	113.95	108.36
3	F	31	ATD	C5'-C4'-C3'	-2.47	109.79	115.22
3	F	10	A2M	C2'-C1'-N9	-2.47	109.69	113.75
3	F	29	A2M	C5-N7-C8	2.46	107.32	103.45
3	F	4	OMG	C4-C5-N7	-2.46	106.78	110.67
3	E	29	A2M	C4-N9-C8	2.45	108.31	105.74
3	E	27	OMC	O2'-C2'-C1'	2.44	113.63	108.99
3	F	17	A2M	C6-C5-N7	2.44	136.79	132.09
3	E	17	A2M	N9-C8-N7	-2.41	110.51	113.94
3	E	29	A2M	C5-N7-C8	2.41	107.24	103.45
3	E	31	ATD	C2'-C3'-C4'	2.40	107.59	102.93
3	E	25	CFZ	O2-C2-N3	-2.38	118.57	122.33
3	E	12	CFZ	C2'-C3'-C4'	2.38	105.56	102.43
3	E	4	OMG	C4-C5-N7	-2.37	106.91	110.67
3	F	14	CFZ	C2'-C1'-N1	-2.37	110.62	114.27
3	F	12	CFZ	O2-C2-N3	-2.37	118.59	122.33
3	F	21	CFZ	O4'-C1'-N1	2.35	113.69	108.36
3	E	15	OMG	C2'-C1'-N9	-2.35	109.78	114.24
3	E	11	CFZ	O2-C2-N3	-2.34	118.64	122.33
3	E	7	UFT	C2'-C1'-N1	-2.34	110.68	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	8	A2M	N9-C8-N7	-2.33	110.63	113.94
3	E	21	CFZ	O4'-C1'-N1	2.31	113.59	108.36
3	E	14	CFZ	O2-C2-N3	-2.30	118.70	122.33
3	F	9	UFT	C2'-C1'-N1	-2.29	110.75	114.27
3	F	13	OMG	C2'-C1'-N9	-2.29	109.89	114.24
3	F	11	CFZ	C2'-C1'-N1	-2.29	110.75	114.27
3	F	7	UFT	C2'-C1'-N1	-2.28	110.76	114.27
3	F	28	OMC	O2-C2-N3	-2.28	118.74	122.33
3	E	12	CFZ	O2-C2-N3	-2.27	118.75	122.33
3	E	10	A2M	C6-C5-N7	2.27	136.47	132.09
3	F	8	A2M	C2-N1-C6	2.27	122.46	118.73
3	E	10	A2M	C2'-C1'-N9	-2.27	110.02	113.75
3	E	9	UFT	C6-N1-C2	-2.26	118.24	121.00
3	E	12	CFZ	F2'-C2'-C3'	2.26	113.60	109.14
3	F	21	CFZ	O2-C2-N3	-2.25	118.78	122.33
3	F	18	A2M	C6-C5-N7	2.25	136.42	132.09
3	F	16	UFT	C1'-N1-C2	2.25	121.62	117.59
3	E	18	A2M	C6-C5-N7	2.24	136.42	132.09
3	F	10	A2M	C6-C5-N7	2.24	136.41	132.09
3	E	5	A2M	N9-C8-N7	-2.23	110.77	113.94
3	F	20	OMG	O4'-C4'-C5'	2.23	116.48	109.33
3	E	10	A2M	N9-C8-N7	-2.23	110.77	113.94
3	F	15	OMG	C2'-C1'-N9	-2.22	110.03	114.24
3	F	18	A2M	N9-C8-N7	-2.22	110.79	113.94
3	F	8	A2M	N9-C8-N7	-2.21	110.80	113.94
3	F	12	CFZ	C2'-C3'-C4'	2.21	105.35	102.43
3	E	13	OMG	C8-N7-C5	2.20	108.18	104.26
3	F	5	A2M	N9-C8-N7	-2.20	110.81	113.94
3	E	15	OMG	O6-C6-C5	-2.19	120.75	126.53
3	F	31	ATD	C5-C6-N1	-2.17	120.95	123.31
3	F	11	CFZ	C3'-C2'-C1'	2.17	105.61	103.10
3	F	6	CFZ	F2'-C2'-C3'	2.15	113.39	109.14
3	F	10	A2M	O2'-C2'-C1'	2.14	113.04	108.99
3	F	10	A2M	C4-N9-C8	2.13	107.98	105.74
3	E	10	A2M	C2-N1-C6	2.13	122.23	118.73
3	E	9	UFT	C2'-C1'-N1	-2.13	111.00	114.27
3	E	8	A2M	O4'-C1'-N9	2.13	112.18	108.09
3	F	28	OMC	O4'-C1'-N1	2.13	113.18	108.36
3	E	20	OMG	O4'-C1'-N9	2.12	113.16	108.36
3	E	18	A2M	N9-C8-N7	-2.11	110.94	113.94
3	E	27	OMC	O2-C2-N3	-2.11	119.00	122.33
3	F	10	A2M	C2-N1-C6	2.11	122.20	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	A2M	C6-C5-N7	2.11	136.16	132.09
3	F	8	A2M	O4'-C1'-N9	2.10	112.13	108.09
3	E	21	CFZ	O2-C2-N3	-2.10	119.02	122.33
3	F	15	OMG	O6-C6-C5	-2.10	120.99	126.53
3	E	8	A2M	C2-N1-C6	2.10	122.18	118.73
3	F	27	OMC	O2-C2-N3	-2.10	119.03	122.33
3	F	3	OMG	C8-N7-C5	2.10	107.99	104.26
3	E	11	CFZ	C2'-C1'-N1	-2.09	111.07	114.27
3	E	17	A2M	C2-N1-C6	2.08	122.15	118.73
3	F	22	OMU	C6-N1-C2	-2.08	118.47	121.00
3	E	9	UFT	C1'-N1-C2	2.07	121.31	117.59
3	F	9	UFT	C6-N1-C2	-2.07	118.48	121.00
3	F	7	UFT	O2-C2-N1	-2.06	120.12	122.80
3	F	27	OMC	O2'-C2'-C1'	2.05	112.88	108.99
3	F	29	A2M	N9-C8-N7	-2.04	111.03	113.94
3	E	7	UFT	O2-C2-N1	-2.04	120.14	122.80
3	E	31	ATD	O2-C2-N1	-2.03	120.15	122.80
3	E	13	OMG	C2'-C1'-N9	-2.03	110.38	114.24
3	E	8	A2M	C6-C5-N7	2.02	135.99	132.09
3	E	6	CFZ	F2'-C2'-C3'	2.02	113.14	109.14
3	E	10	A2M	O2'-C2'-C1'	2.02	112.83	108.99
3	F	1	OMG	C8-N7-C5	2.02	107.85	104.26
3	E	6	CFZ	C2'-C3'-C4'	2.02	105.09	102.43
3	F	13	OMG	C8-N7-C5	2.01	107.85	104.26
3	E	11	CFZ	C3'-C2'-C1'	2.01	105.44	103.10
3	F	17	A2M	C2-N1-C6	2.01	122.03	118.73
3	E	28	OMC	O4'-C1'-N1	2.00	112.89	108.36

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	OMG	C5'-O5'-P-OP2
3	E	1	OMG	C5'-O5'-P-OP3
3	E	6	CFZ	C3'-C4'-C5'-O5'
3	E	6	CFZ	O4'-C4'-C5'-O5'
3	F	6	CFZ	C3'-C4'-C5'-O5'
3	F	6	CFZ	O4'-C4'-C5'-O5'
3	E	10	A2M	C4'-C5'-O5'-P
3	E	10	A2M	C1'-C2'-O2'-CM'
3	F	10	A2M	C4'-C5'-O5'-P
3	F	10	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
3	E	11	CFZ	O4'-C1'-N1-C2
3	E	11	CFZ	O4'-C1'-N1-C6
3	F	11	CFZ	O4'-C1'-N1-C2
3	F	11	CFZ	O4'-C1'-N1-C6
3	E	12	CFZ	O4'-C1'-N1-C2
3	E	12	CFZ	O4'-C1'-N1-C6
3	F	12	CFZ	O4'-C1'-N1-C2
3	F	12	CFZ	O4'-C1'-N1-C6
3	E	14	CFZ	O4'-C4'-C5'-O5'
3	F	14	CFZ	O4'-C4'-C5'-O5'
3	E	15	OMG	C1'-C2'-O2'-CM2
3	F	15	OMG	C1'-C2'-O2'-CM2
3	E	16	UFT	O4'-C1'-N1-C6
3	E	16	UFT	O4'-C1'-N1-C2
3	F	16	UFT	O4'-C1'-N1-C6
3	F	16	UFT	O4'-C1'-N1-C2
3	E	20	OMG	O4'-C4'-C5'-O5'
3	F	20	OMG	O4'-C4'-C5'-O5'
3	F	20	OMG	C3'-C2'-O2'-CM2
3	E	24	OMC	O4'-C1'-N1-C2
3	E	24	OMC	O4'-C1'-N1-C6
3	F	24	OMC	O4'-C1'-N1-C2
3	F	24	OMC	O4'-C1'-N1-C6
3	E	27	OMC	C1'-C2'-O2'-CM2
3	F	27	OMC	C1'-C2'-O2'-CM2
3	E	31	ATD	C4'-C3'-O3'-P
3	E	31	ATD	C2'-C3'-O3'-P
3	E	31	ATD	O4'-C1'-N1-C2
3	F	31	ATD	C2'-C1'-N1-C2
3	F	31	ATD	C2'-C1'-N1-C6
3	F	31	ATD	O4'-C4'-C5'-O5'
3	F	31	ATD	C3'-C4'-C5'-O5'
3	E	31	ATD	O4'-C1'-N1-C6
3	E	31	ATD	O4'-C4'-C5'-O5'
3	E	17	A2M	O4'-C4'-C5'-O5'
3	F	17	A2M	O4'-C4'-C5'-O5'
3	E	24	OMC	C3'-C4'-C5'-O5'
3	E	24	OMC	O4'-C4'-C5'-O5'
3	F	24	OMC	C3'-C4'-C5'-O5'
3	F	24	OMC	O4'-C4'-C5'-O5'
3	E	31	ATD	C3'-C4'-C5'-O5'
3	E	10	A2M	C3'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
3	F	10	A2M	C3'-C2'-O2'-CM'
3	F	15	OMG	C3'-C2'-O2'-CM2
3	E	17	A2M	C3'-C2'-O2'-CM'
3	F	17	A2M	C3'-C2'-O2'-CM'
3	E	27	OMC	C3'-C2'-O2'-CM2
3	F	27	OMC	C3'-C2'-O2'-CM2
3	E	13	OMG	O4'-C4'-C5'-O5'
3	E	14	CFZ	C3'-C4'-C5'-O5'
3	F	14	CFZ	C3'-C4'-C5'-O5'
3	E	20	OMG	C3'-C4'-C5'-O5'
3	F	20	OMG	C3'-C4'-C5'-O5'
3	F	13	OMG	O4'-C4'-C5'-O5'
3	E	15	OMG	C3'-C2'-O2'-CM2
3	E	5	A2M	O4'-C4'-C5'-O5'
3	F	17	A2M	C3'-C4'-C5'-O5'
3	F	5	A2M	O4'-C4'-C5'-O5'
3	E	17	A2M	C3'-C4'-C5'-O5'
3	E	8	A2M	C2'-C1'-N9-C8
3	F	8	A2M	C2'-C1'-N9-C8
3	F	13	OMG	C3'-C4'-C5'-O5'
3	F	31	ATD	C2'-C3'-O3'-P
3	E	20	OMG	C4'-C5'-O5'-P
3	F	20	OMG	C4'-C5'-O5'-P
3	E	13	OMG	C3'-C4'-C5'-O5'
3	F	22	OMU	O4'-C4'-C5'-O5'
3	E	22	OMU	O4'-C4'-C5'-O5'
3	F	18	A2M	C2'-C1'-N9-C8
3	E	8	A2M	C2'-C1'-N9-C4
3	E	18	A2M	C2'-C1'-N9-C4
3	E	8	A2M	O4'-C1'-N9-C8
3	F	8	A2M	O4'-C1'-N9-C8
3	E	18	A2M	O4'-C1'-N9-C8
3	F	18	A2M	O4'-C1'-N9-C8
3	E	18	A2M	C2'-C1'-N9-C8
3	F	8	A2M	C2'-C1'-N9-C4
3	F	18	A2M	C2'-C1'-N9-C4
3	E	16	UFT	C2'-C1'-N1-C6
3	E	16	UFT	C2'-C1'-N1-C2
3	F	16	UFT	C2'-C1'-N1-C2
3	F	5	A2M	C3'-C4'-C5'-O5'
3	F	12	CFZ	C4'-C5'-O5'-P
3	E	5	A2M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	F	13	OMG	C4'-C5'-O5'-P

There are no ring outliers.

20 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	29	A2M	1	0
3	F	29	A2M	1	0
3	F	28	OMC	1	0
3	F	16	UFT	1	0
3	E	7	UFT	1	0
3	E	28	OMC	1	0
3	E	6	CFZ	3	0
3	F	18	A2M	1	0
3	F	20	OMG	1	0
3	E	9	UFT	2	0
3	F	31	ATD	2	0
3	F	6	CFZ	3	0
3	F	30	OMC	2	0
3	E	27	OMC	1	0
3	E	16	UFT	1	0
3	E	20	OMG	1	0
3	E	31	ATD	1	0
3	E	18	A2M	1	0
3	F	7	UFT	1	0
3	E	30	OMC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	55/65 (84%)	0.37	1 (1%) 67 63	69, 80, 102, 118	0
1	C	55/65 (84%)	0.66	4 (7%) 21 15	86, 104, 127, 140	0
2	B	235/235 (100%)	0.56	9 (3%) 44 36	59, 85, 126, 145	0
2	D	235/235 (100%)	0.48	12 (5%) 33 26	57, 90, 130, 149	0
3	E	1/31 (3%)	-0.59	0 100 100	91, 91, 91, 91	0
3	F	1/31 (3%)	0.09	0 100 100	84, 84, 84, 84	0
All	All	582/662 (87%)	0.52	26 (4%) 38 31	57, 90, 128, 149	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	147	HIS	3.5
2	D	145	PHE	3.4
1	C	85	ASP	3.2
2	D	216	GLY	3.1
2	B	188(A)	ARG	2.8
2	D	147	HIS	2.8
2	B	148	LYS	2.8
2	B	134	GLY	2.7
2	D	135	SER	2.6
2	B	145	PHE	2.6
1	A	84	LEU	2.5
2	B	185	HIS	2.5
1	C	84	LEU	2.5
1	C	90	ILE	2.4
2	B	151	SER	2.4
2	D	245	THR	2.3
2	D	174	PHE	2.3
2	D	95(B)	ALA	2.2
2	D	144	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	148	LYS	2.1
2	B	162	LEU	2.1
1	C	86	VAL	2.1
2	B	16	VAL	2.1
2	D	172	THR	2.0
2	D	220	CYS	2.0
2	D	61	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	CFZ	F	11	20/21	0.71	0.16	114,140,154,155	0
3	CFZ	F	12	20/21	0.71	0.16	111,121,137,143	0
3	CFZ	E	12	20/21	0.73	0.17	119,128,147,154	0
3	ATD	F	31	20/21	0.76	0.18	114,122,123,123	0
3	ATD	E	31	20/21	0.78	0.17	116,119,123,123	0
3	CFZ	E	11	20/21	0.78	0.15	117,145,160,162	0
3	OMC	F	30	21/22	0.79	0.13	119,128,135,140	0
3	UFT	F	16	20/21	0.82	0.15	101,108,125,130	0
3	A2M	F	29	23/24	0.84	0.12	110,114,122,125	0
3	OMG	F	1	25/25	0.84	0.11	117,123,128,132	0
3	CFZ	E	25	20/21	0.85	0.11	94,105,112,116	0
3	OMC	F	24	21/22	0.86	0.12	92,98,108,113	0
3	OMG	F	3	24/25	0.86	0.10	103,106,112,113	0
3	OMG	F	4	24/25	0.86	0.11	94,97,101,103	0
3	A2M	F	10	23/24	0.86	0.11	90,100,111,113	0
3	UFT	E	16	20/21	0.86	0.13	111,121,139,145	0
3	OMG	E	1	25/25	0.86	0.12	110,115,120,120	0
3	UFT	E	26	20/21	0.88	0.10	90,97,109,114	0
3	OMC	E	28	21/22	0.88	0.12	98,99,105,107	0
3	OMU	E	2	21/22	0.88	0.10	105,110,114,115	0
3	OMU	F	2	21/22	0.89	0.09	110,116,121,122	0
3	OMC	F	28	21/22	0.89	0.10	103,105,114,117	0
3	A2M	E	10	23/24	0.89	0.11	96,102,115,116	0
3	OMG	F	13	24/25	0.90	0.10	85,101,115,119	0
3	OMG	E	13	24/25	0.90	0.12	94,114,128,132	0
3	OMC	E	27	21/22	0.91	0.09	90,95,105,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	OMC	E	24	21/22	0.91	0.12	96,104,112,118	0
3	OMG	E	15	24/25	0.91	0.10	90,105,121,127	0
3	A2M	F	5	23/24	0.91	0.10	83,88,90,90	0
3	CFZ	F	25	20/21	0.91	0.08	91,104,111,113	0
3	UFT	F	9	20/21	0.91	0.13	84,97,103,106	0
3	UFT	F	26	20/21	0.91	0.09	94,102,112,117	0
3	OMG	E	4	24/25	0.92	0.08	90,93,100,103	0
3	CFZ	E	6	20/21	0.92	0.11	75,80,83,84	0
3	CFZ	F	6	20/21	0.92	0.10	75,79,82,83	0
3	OMC	E	30	21/22	0.92	0.09	109,114,119,122	0
3	OMG	E	3	24/25	0.92	0.08	99,103,108,111	0
3	CFZ	E	14	20/21	0.92	0.09	94,110,122,128	0
3	OMC	F	27	21/22	0.92	0.08	96,102,111,116	0
3	UFT	E	9	20/21	0.93	0.13	82,92,100,102	0
3	OMG	F	15	24/25	0.93	0.09	84,92,103,107	0
3	A2M	E	17	23/24	0.93	0.10	95,99,110,113	0
3	A2M	F	18	23/24	0.94	0.09	83,85,93,95	0
3	A2M	E	29	23/24	0.94	0.10	104,106,111,113	0
3	UFT	F	19	20/21	0.94	0.09	73,75,82,82	0
3	OMG	F	20	24/25	0.94	0.09	72,77,80,82	0
3	CFZ	F	14	20/21	0.94	0.08	85,95,106,111	0
3	A2M	E	5	23/24	0.94	0.08	83,86,91,92	0
3	A2M	F	17	23/24	0.94	0.09	91,95,99,101	0
3	UFT	E	19	20/21	0.95	0.09	72,75,81,81	0
3	A2M	E	8	23/24	0.95	0.08	75,84,94,97	0
3	A2M	F	8	23/24	0.95	0.08	73,80,86,88	0
3	CFZ	E	21	20/21	0.95	0.07	81,91,96,96	0
3	CFZ	F	21	20/21	0.95	0.07	74,80,84,84	0
3	A2M	E	18	23/24	0.95	0.08	83,89,94,97	0
3	UFT	E	7	20/21	0.95	0.08	73,76,79,81	0
3	OMU	E	22	21/22	0.96	0.07	83,90,96,99	0
3	OMU	F	22	21/22	0.96	0.07	77,81,85,88	0
3	OMG	E	20	24/25	0.96	0.08	74,83,89,93	0
3	UFT	F	7	20/21	0.97	0.07	71,74,77,78	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

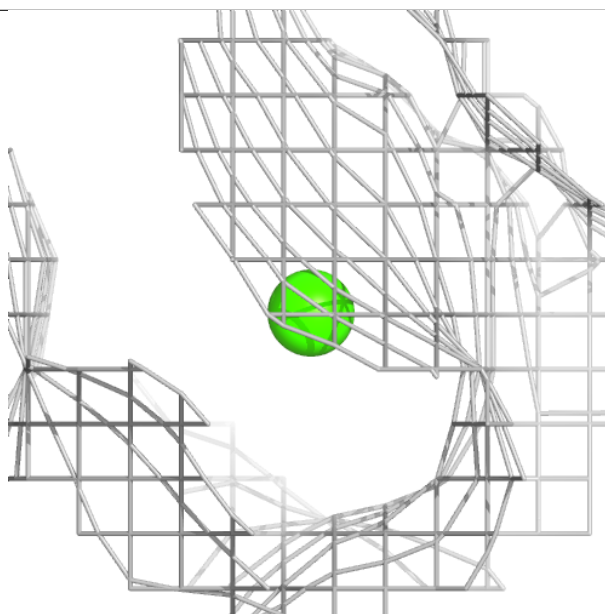
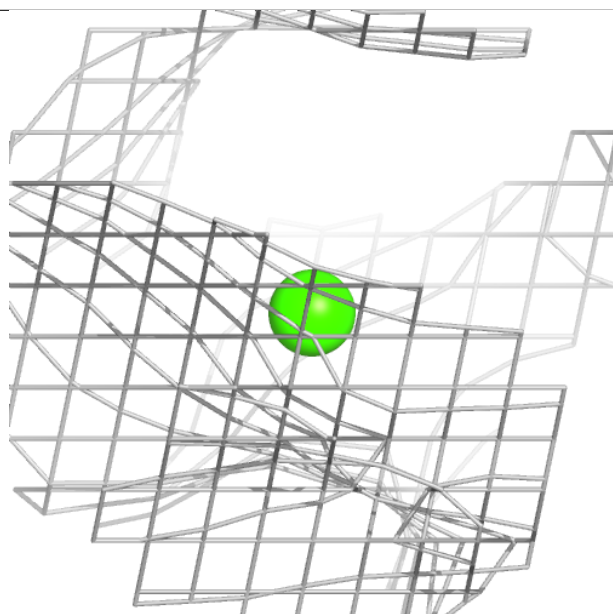
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	B	301	1/1	0.78	0.09	127,127,127,127	0
5	MG	E	101	1/1	0.86	0.14	78,78,78,78	0
4	CA	D	301	1/1	0.91	0.08	124,124,124,124	0
5	MG	F	101	1/1	0.92	0.12	97,97,97,97	0

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

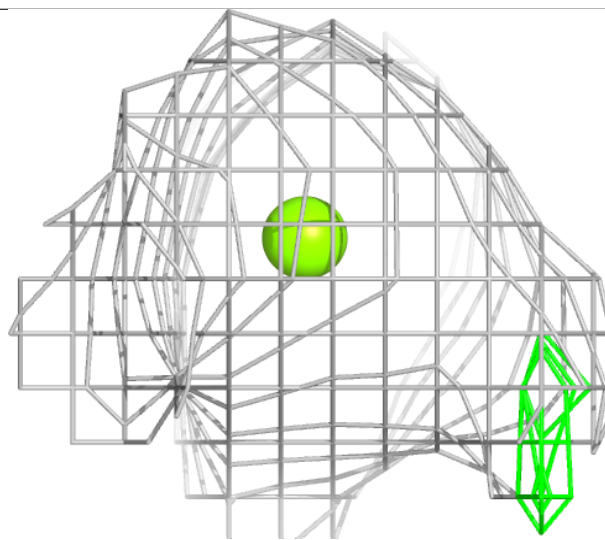
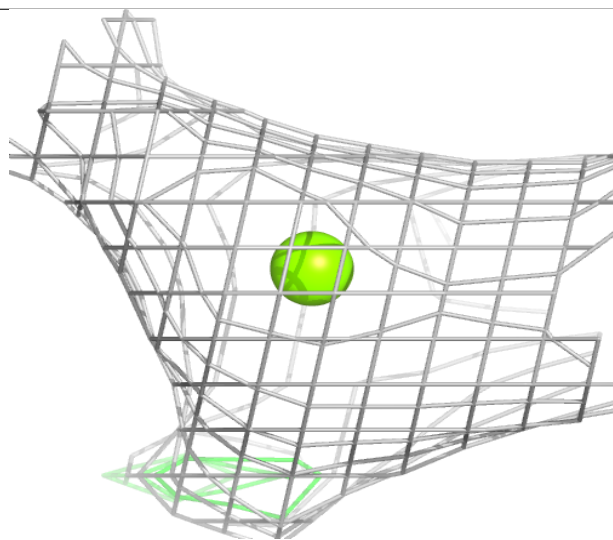
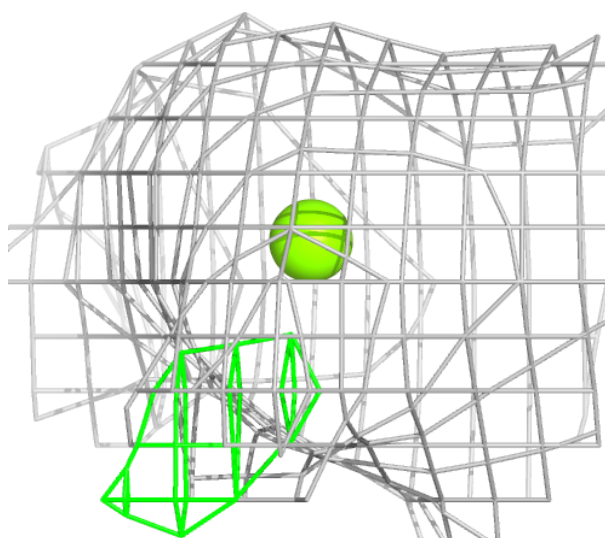
Electron density around CA B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



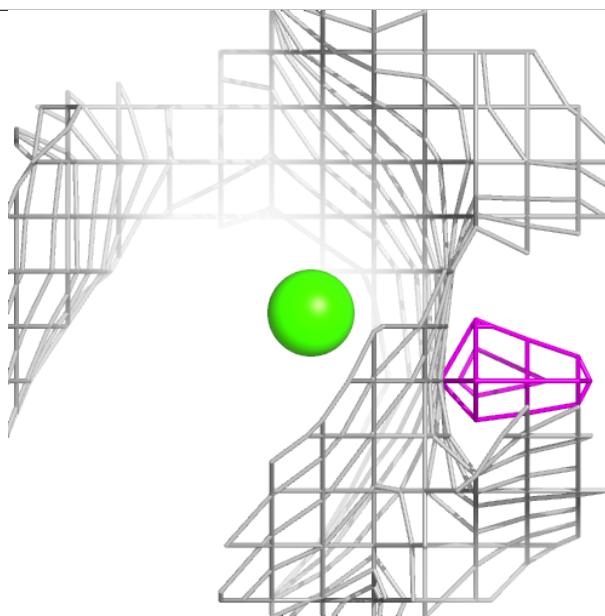
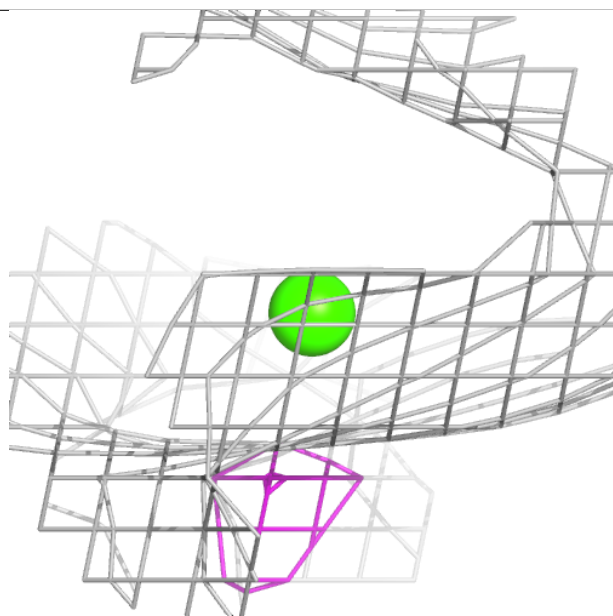
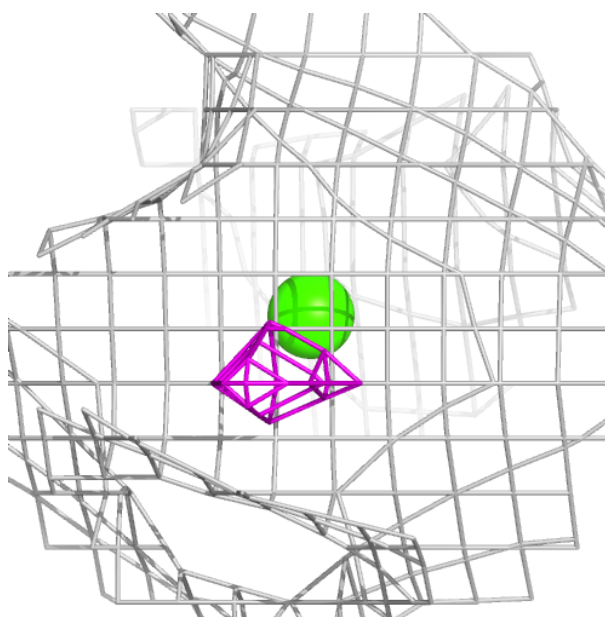
Electron density around MG E 101:

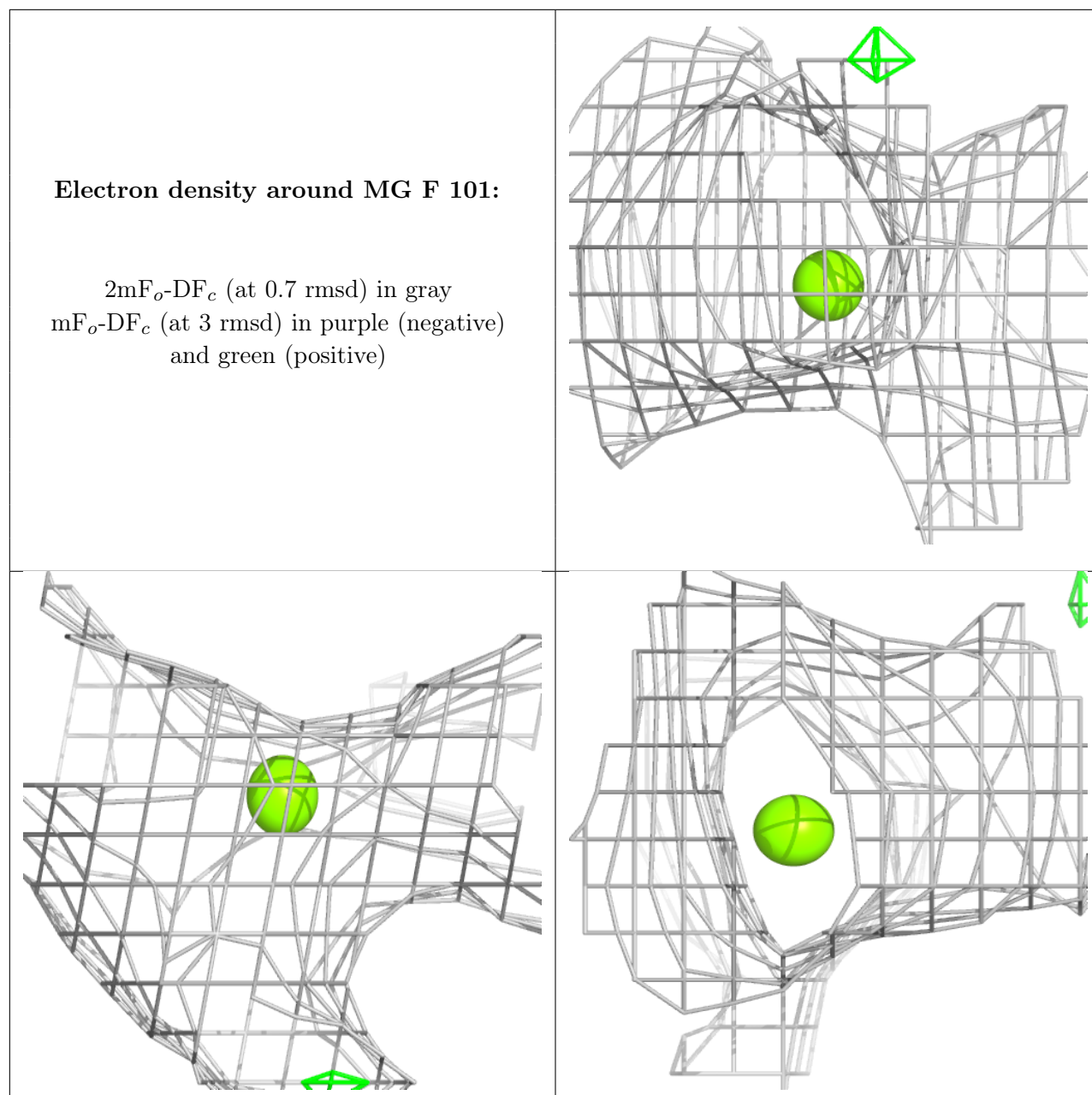
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA D 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.