



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:24 AM EDT

PDB ID : 2FS8 / pdb_00002fs8
Title : Human beta-tryptase II with inhibitor CRA-29382
Authors : Somoza, J.R.
Deposited on : 2006-01-21
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

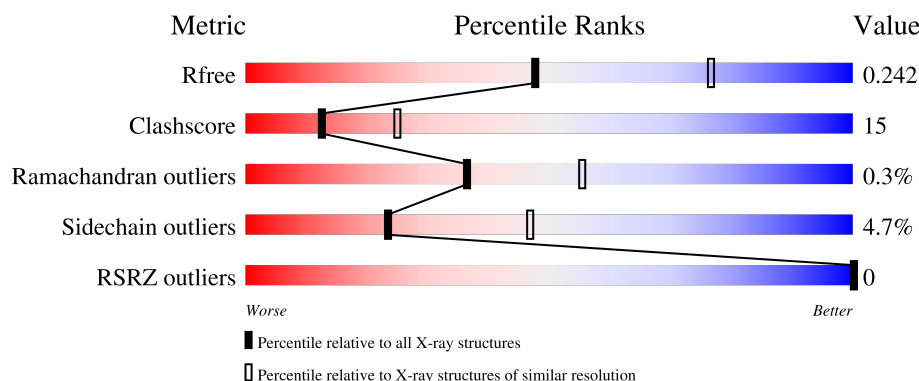
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	245	
1	B	245	
1	C	245	
1	D	245	

2 Entry composition [i](#)

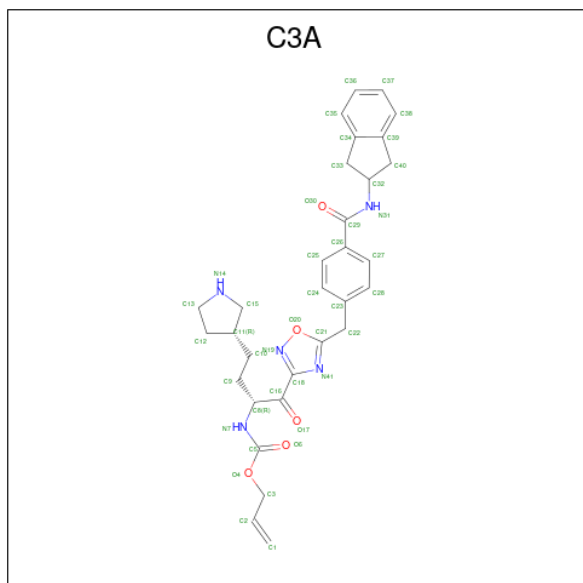
There are 3 unique types of molecules in this entry. The entry contains 8040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptase beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1920	1230	338	340	12			
1	B	243	Total	C	N	O	S	0	0	0
			1920	1230	338	340	12			
1	C	243	Total	C	N	O	S	0	0	0
			1920	1230	338	340	12			
1	D	243	Total	C	N	O	S	0	0	0
			1920	1230	338	340	12			

- Molecule 2 is ALLYL {(1S)-1-[(5-{4-[(2,3-DIHYDRO-1H-INDEN-2-YLAMINO)CARBONYL]BENZYL}-1,2,4-OXADIAZOL-3-YL)CARBONYL]-3-PYRROLIDIN-3-YLPROPYL}CARBAMATE (CCD ID: C3A) (formula: C₃₁H₃₅N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			41	31	5	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			41	31	5	5		
2	C	1	Total	C	N	O	0	0
			41	31	5	5		
2	D	1	Total	C	N	O	0	0
			41	31	5	5		

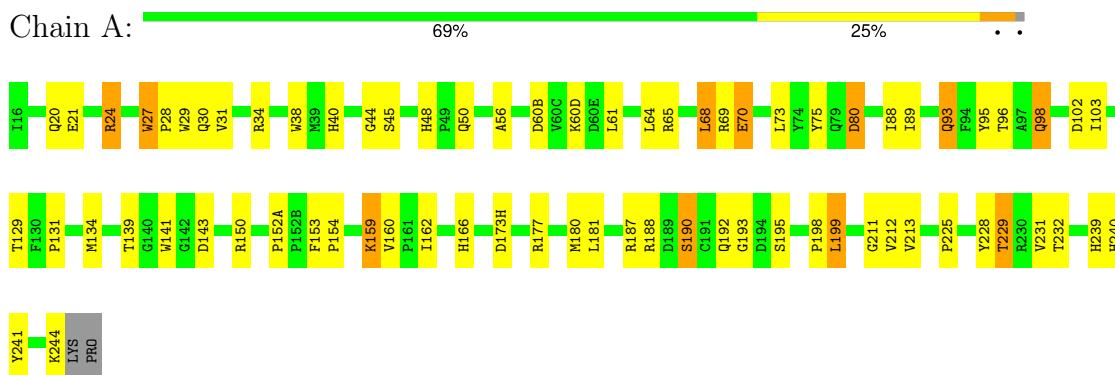
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	52	Total	O	0	0
			52	52		
3	B	43	Total	O	0	0
			43	43		
3	C	66	Total	O	0	0
			66	66		
3	D	35	Total	O	0	0
			35	35		

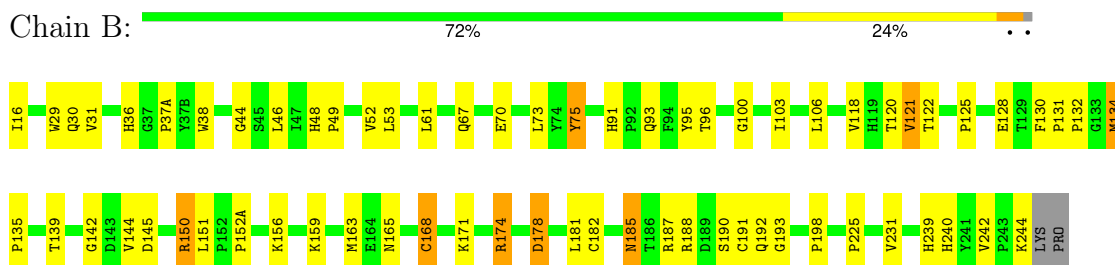
3 Residue-property plots

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 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.

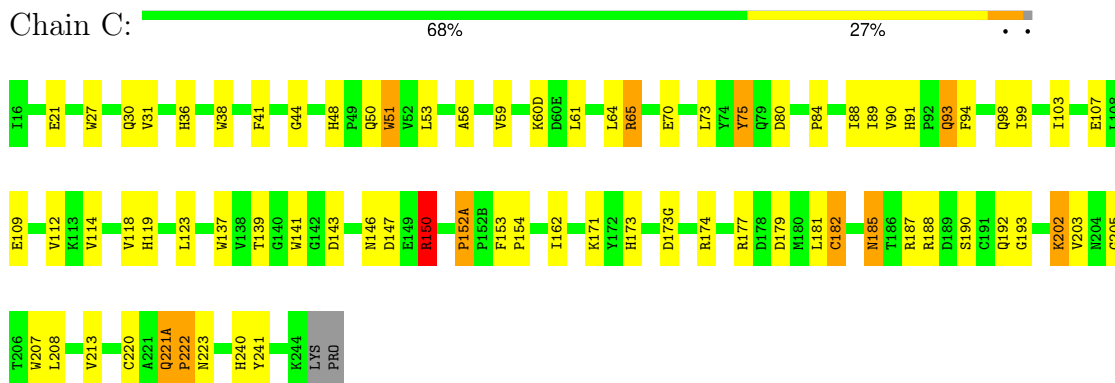
• Molecule 1: Tryptase beta-2



• Molecule 1: Tryptase beta-2



• Molecule 1: Tryptase beta-2



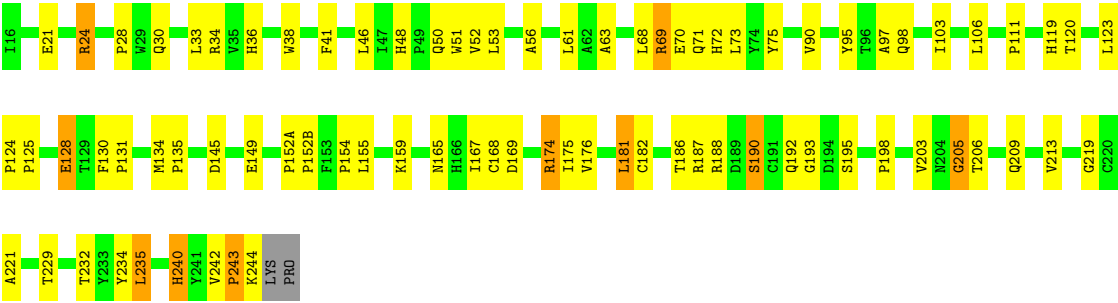
• Molecule 1: Tryptase beta-2

Chain D:

66%

29%

••



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	78.20Å 78.20Å 165.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.78 – 2.50 42.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (42.78-2.50) 92.7 (42.78-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.250 0.197 , 0.242	Depositor DCC
R_{free} test set	3931 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 8.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l 0.480 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8040	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: C3A

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	0.67	2/1985 (0.1%)	1.05	8/2720 (0.3%)
1	B	0.61	0/1985	1.06	13/2720 (0.5%)
1	C	0.59	0/1985	1.05	11/2720 (0.4%)
1	D	0.60	0/1985	1.01	7/2720 (0.3%)
All	All	0.62	2/7940 (0.0%)	1.04	39/10880 (0.4%)

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	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173(H)	ASP	CA-C	-7.21	1.42	1.52
1	A	173(H)	ASP	CG-OD2	5.08	1.34	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	HIS	N-CA-C	-7.08	104.61	113.18
1	D	175	ILE	N-CA-C	-6.70	105.80	111.56
1	D	152(A)	PRO	N-CA-C	-6.63	103.49	110.58
1	A	190	SER	N-CA-C	-6.46	100.90	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	130	PHE	CA-C-N	6.38	124.32	119.66
1	B	130	PHE	C-N-CA	6.38	124.32	119.66
1	B	75	TYR	N-CA-C	6.33	118.26	111.36
1	A	199	LEU	N-CA-C	-6.18	97.01	108.02
1	B	242	VAL	CA-C-N	6.13	126.15	119.90
1	B	242	VAL	C-N-CA	6.13	126.15	119.90
1	C	150	ARG	N-CA-C	6.12	118.68	110.35
1	A	80	ASP	N-CA-C	6.07	119.14	110.10
1	A	173(H)	ASP	N-CA-C	6.06	120.67	113.16
1	A	27	TRP	CA-C-N	5.95	125.57	119.56
1	A	27	TRP	C-N-CA	5.95	125.57	119.56
1	B	151	LEU	N-CA-C	-5.92	100.65	109.42
1	C	182	CYS	N-CA-C	5.92	118.55	108.90
1	A	240	HIS	N-CA-C	-5.91	105.57	112.89
1	A	160	VAL	N-CA-C	5.87	114.60	107.61
1	B	231	VAL	N-CA-C	5.83	116.02	110.42
1	C	94	PHE	N-CA-C	5.81	119.39	110.20
1	D	242	VAL	CA-C-N	5.79	127.07	119.84
1	D	242	VAL	C-N-CA	5.79	127.07	119.84
1	B	121	VAL	N-CA-C	-5.67	100.42	109.20
1	D	190	SER	N-CA-C	-5.57	101.79	110.42
1	B	178	ASP	N-CA-C	5.55	118.10	111.71
1	C	75	TYR	N-CA-C	5.51	117.36	111.36
1	B	100	GLY	N-CA-C	5.48	118.75	110.97
1	B	242	VAL	N-CA-C	5.45	112.52	107.56
1	B	152(A)	PRO	N-CA-C	-5.32	104.89	110.58
1	C	174	ARG	N-CA-C	5.31	117.87	109.96
1	C	51	TRP	N-CA-C	5.25	118.02	109.24
1	D	240	HIS	N-CA-C	-5.25	106.38	112.89
1	C	221(A)	GLN	CA-C-N	5.22	126.37	119.84
1	C	221(A)	GLN	C-N-CA	5.22	126.37	119.84
1	D	242	VAL	N-CA-C	5.16	113.55	107.77
1	C	152(A)	PRO	N-CA-C	-5.07	104.52	110.70
1	C	179	ASP	N-CA-C	-5.06	107.13	113.15
1	B	37(A)	PRO	N-CA-C	-5.04	106.84	113.65

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	TYR	Sidechain
1	B	95	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	95	TYR	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	1920	0	1854	50	0
1	B	1920	0	1854	57	0
1	C	1920	0	1854	59	0
1	D	1920	0	1854	68	0
2	A	41	0	31	5	0
2	B	41	0	34	4	0
2	C	41	0	33	9	0
2	D	41	0	33	10	0
3	A	52	0	0	3	0
3	B	43	0	0	2	0
3	C	66	0	0	5	0
3	D	35	0	0	4	0
All	All	8040	0	7547	235	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 15.

All (235) 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:D:24:ARG:HH11	1:D:24:ARG:HG2	1.16	1.09
1:D:125:PRO:HD2	1:D:128:GLU:OE1	1.60	1.00
1:B:185:ASN:ND2	1:B:188:ARG:H	1.61	0.97
1:A:24:ARG:HH11	1:A:24:ARG:HB3	1.30	0.94
1:C:146:ASN:HD21	1:C:220:CYS:H	1.17	0.91
1:A:102:ASP:O	1:A:229:THR:HG21	1.71	0.90
1:B:239:HIS:HB3	1:B:244:LYS:HE2	1.54	0.87
1:A:21:GLU:HG3	1:A:154:PRO:HB2	1.54	0.87
1:A:131:PRO:HD2	1:A:134:MET:HE2	1.56	0.86
1:B:91:HIS:HD2	1:B:93:GLN:H	1.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:HD21	1:B:188:ARG:H	1.23	0.82
2:C:997:C3A:O6	3:C:1047:HOH:O	1.99	0.81
1:A:24:ARG:HB3	1:A:24:ARG:NH1	1.97	0.80
1:D:24:ARG:HH11	1:D:24:ARG:CG	1.94	0.79
1:A:48:HIS:HD2	1:A:50:GLN:H	1.31	0.79
1:D:21:GLU:HG3	1:D:154:PRO:HB2	1.64	0.78
1:A:129:THR:HG23	1:A:131:PRO:HD3	1.64	0.78
1:D:24:ARG:HG2	1:D:24:ARG:NH1	1.86	0.78
1:C:192:GLN:HA	2:C:997:C3A:O17	1.85	0.77
1:A:159:LYS:O	1:A:188:ARG:HD3	1.86	0.76
1:B:163:MET:HB2	1:B:182:CYS:SG	2.26	0.76
1:D:243:PRO:C	1:D:244:LYS:HD2	2.11	0.76
1:D:24:ARG:CD	1:D:24:ARG:H	1.98	0.74
1:C:61:LEU:HD21	1:C:88:ILE:HG13	1.69	0.74
1:C:202:LYS:HE3	1:C:205:GLY:HA2	1.68	0.74
1:B:190:SER:O	2:B:998:C3A:H132	1.88	0.73
1:D:192:GLN:HA	2:D:996:C3A:O17	1.89	0.73
1:B:192:GLN:HA	2:B:998:C3A:O17	1.89	0.72
1:B:134:MET:SD	1:B:135:PRO:HD2	2.30	0.72
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.55	0.71
1:A:190:SER:O	2:A:999:C3A:H132	1.90	0.71
1:D:181:LEU:HD12	1:D:181:LEU:C	2.16	0.70
1:A:61:LEU:CD2	1:A:88:ILE:HG12	2.21	0.69
1:D:24:ARG:H	1:D:24:ARG:NE	1.90	0.69
1:C:137:TRP:HZ3	3:C:1052:HOH:O	1.74	0.69
1:C:48:HIS:HD2	1:C:50:GLN:H	1.42	0.68
1:B:185:ASN:HD21	1:B:188:ARG:N	1.91	0.68
1:A:61:LEU:HD21	1:A:88:ILE:HG12	1.76	0.66
1:C:59:VAL:O	1:C:60(D):LYS:HE2	1.94	0.66
1:C:114:VAL:HG13	1:C:119:HIS:HB3	1.78	0.65
1:C:84:PRO:HB2	1:C:109:GLU:OE2	1.96	0.65
1:D:190:SER:O	2:D:996:C3A:H132	1.96	0.65
1:C:185:ASN:HD22	1:C:185:ASN:C	2.05	0.65
1:D:24:ARG:HA	1:D:71:GLN:NE2	2.12	0.64
1:D:232:THR:HA	1:D:235:LEU:HD22	1.80	0.64
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.11	0.64
1:C:91:HIS:CE1	1:C:93:GLN:HB2	2.33	0.64
1:C:203:VAL:HG21	1:C:208:LEU:HD12	1.79	0.64
2:D:996:C3A:N7	2:D:996:C3A:N41	2.45	0.64
1:A:93:GLN:HA	1:A:93:GLN:HE21	1.63	0.63
1:D:36:HIS:HB2	1:D:38:TRP:CH2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:LYS:O	1:D:188:ARG:HD3	1.98	0.63
1:A:48:HIS:CD2	1:A:50:GLN:H	2.16	0.63
1:A:192:GLN:HA	2:A:999:C3A:O17	1.99	0.63
1:C:190:SER:O	2:C:997:C3A:H132	2.00	0.62
1:B:191:CYS:HA	2:B:998:C3A:H122	1.83	0.61
2:C:997:C3A:O4	2:C:997:C3A:N41	2.33	0.61
1:C:143:ASP:OD1	1:C:150:ARG:HD3	2.01	0.61
1:C:21:GLU:HG3	1:C:154:PRO:HB2	1.82	0.61
1:B:67:GLN:NE2	1:B:70:GLU:HG3	2.16	0.60
1:C:146:ASN:HD21	1:C:220:CYS:N	1.96	0.60
1:B:36:HIS:HB2	1:B:38:TRP:CH2	2.36	0.60
1:B:52:VAL:HB	1:B:106:LEU:HB2	1.82	0.60
1:D:181:LEU:HD12	1:D:182:CYS:N	2.17	0.59
1:B:185:ASN:C	1:B:185:ASN:HD22	2.11	0.59
1:C:150:ARG:HG2	1:C:150:ARG:HH11	1.68	0.58
1:B:29:TRP:CG	1:B:121:VAL:HB	2.39	0.58
1:B:163:MET:HE1	1:B:171:LYS:HZ1	1.68	0.58
1:B:163:MET:HE1	1:B:171:LYS:NZ	2.19	0.58
1:D:124:PRO:O	1:D:235:LEU:HD21	2.04	0.57
1:B:61:LEU:HD11	3:B:1020:HOH:O	2.04	0.57
1:D:52:VAL:HB	1:D:106:LEU:HB2	1.86	0.57
1:D:48:HIS:CD2	1:D:50:GLN:H	2.22	0.57
1:D:24:ARG:HA	1:D:71:GLN:HE21	1.69	0.56
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.69	0.56
1:C:48:HIS:CD2	1:C:50:GLN:H	2.23	0.56
1:C:31:VAL:HG22	1:C:44:GLY:C	2.31	0.56
1:D:48:HIS:HD2	1:D:50:GLN:H	1.53	0.55
1:C:64:LEU:HB2	2:C:997:C3A:H37	1.88	0.55
1:B:144:VAL:HG12	1:B:156:LYS:HE2	1.89	0.55
1:B:150:ARG:HD2	3:B:1031:HOH:O	2.06	0.55
1:D:193:GLY:N	2:D:996:C3A:O17	2.34	0.54
1:B:142:GLY:HA2	1:B:193:GLY:HA3	1.89	0.54
1:A:64:LEU:CD2	1:A:88:ILE:HD11	2.38	0.54
1:B:240:HIS:ND1	1:B:240:HIS:O	2.40	0.54
1:A:193:GLY:N	2:A:999:C3A:O17	2.38	0.53
1:C:150:ARG:HG2	1:C:150:ARG:NH1	2.22	0.53
1:D:72:HIS:HB3	1:D:152(B):PRO:O	2.09	0.53
1:B:174:ARG:HH22	1:B:178:ASP:CG	2.17	0.52
1:D:53:LEU:HD11	1:D:103:ILE:HD11	1.90	0.52
1:D:181:LEU:C	1:D:181:LEU:CD1	2.83	0.52
1:B:31:VAL:HG22	1:B:44:GLY:C	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:HB2	1:B:75:TYR:CE1	2.44	0.52
1:C:146:ASN:ND2	1:C:220:CYS:H	1.97	0.52
1:C:185:ASN:ND2	1:C:188:ARG:H	2.08	0.52
1:D:68:LEU:O	1:D:69:ARG:C	2.52	0.52
1:C:75:TYR:CE2	1:D:75:TYR:HB2	2.45	0.52
1:B:29:TRP:CD2	1:B:121:VAL:HB	2.44	0.51
1:B:67:GLN:HE21	1:B:70:GLU:HG3	1.75	0.51
1:A:211:GLY:HA2	1:A:231:VAL:HG23	1.92	0.51
1:C:202:LYS:HE3	1:C:205:GLY:CA	2.40	0.51
1:C:53:LEU:HD11	1:C:103:ILE:HD11	1.93	0.51
1:A:27:TRP:N	1:A:28:PRO:HD3	2.26	0.51
1:B:118:VAL:HG23	1:B:118:VAL:O	2.11	0.51
1:D:145:ASP:HB3	1:D:149:GLU:HG2	1.93	0.51
1:D:50:GLN:OE1	1:D:111:PRO:HG3	2.10	0.51
1:A:166:HIS:HD2	3:A:1050:HOH:O	1.94	0.50
1:B:188:ARG:HG2	1:B:188:ARG:HH11	1.77	0.50
1:C:56:ALA:HB2	1:C:103:ILE:O	2.11	0.50
1:B:144:VAL:O	1:B:145:ASP:HB2	2.11	0.50
1:C:41:PHE:CE2	2:C:997:C3A:H402	2.47	0.49
1:D:34:ARG:NH2	1:D:73:LEU:HD22	2.27	0.49
1:A:61:LEU:HD23	1:A:88:ILE:HG12	1.94	0.49
1:D:34:ARG:HH21	1:D:73:LEU:HD22	1.78	0.49
1:A:24:ARG:HH11	1:A:24:ARG:CB	2.13	0.49
1:B:168:CYS:SG	1:B:225:PRO:CG	3.01	0.49
1:D:28:PRO:HG3	1:D:119:HIS:CE1	2.47	0.49
1:A:96:THR:HG21	1:D:98:GLN:HG2	1.94	0.49
1:C:27:TRP:CD1	1:C:139:THR:HG21	2.48	0.49
1:D:186:THR:HA	1:D:221:ALA:O	2.12	0.49
1:C:70:GLU:OE1	1:C:80:ASP:OD1	2.31	0.48
1:D:69:ARG:HH22	1:D:71:GLN:NE2	2.10	0.48
1:A:31:VAL:HG22	1:A:44:GLY:C	2.39	0.48
1:C:185:ASN:ND2	1:C:187:ARG:H	2.11	0.48
1:A:212:VAL:HB	1:A:229:THR:HG23	1.96	0.48
1:D:63:ALA:HB3	2:D:996:C3A:H36	1.95	0.48
1:A:27:TRP:CD1	1:A:139:THR:HG21	2.48	0.48
1:B:125:PRO:HG2	1:B:128:GLU:HB2	1.95	0.48
1:D:134:MET:HG3	1:D:135:PRO:CD	2.44	0.48
1:C:147:ASP:C	1:C:150:ARG:HH12	2.21	0.47
1:B:46:LEU:O	1:B:120:THR:HA	2.14	0.47
1:B:131:PRO:O	1:B:134:MET:HB2	2.14	0.47
1:D:134:MET:HG3	1:D:135:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:C	1:D:205:GLY:H	2.22	0.47
1:B:185:ASN:ND2	1:B:187:ARG:H	2.12	0.47
1:A:70:GLU:OE1	1:A:80:ASP:OD1	2.33	0.47
1:A:177:ARG:HB2	1:A:180:MET:HE3	1.97	0.47
1:C:181:LEU:C	1:C:181:LEU:HD23	2.40	0.47
1:D:61:LEU:HD11	3:D:1026:HOH:O	2.14	0.47
1:D:234:TYR:HA	3:D:1030:HOH:O	2.15	0.47
1:B:91:HIS:CD2	1:B:93:GLN:H	2.17	0.46
1:C:193:GLY:N	2:C:997:C3A:O17	2.44	0.46
1:B:73:LEU:O	1:B:75:TYR:HD2	1.98	0.46
1:C:114:VAL:HG13	1:C:119:HIS:CB	2.42	0.46
1:D:240:HIS:O	1:D:240:HIS:ND1	2.45	0.46
1:B:73:LEU:O	1:B:75:TYR:CD2	2.69	0.46
1:D:149:GLU:HG3	1:D:149:GLU:O	2.16	0.46
1:D:195:SER:HA	1:D:213:VAL:CG1	2.45	0.46
1:A:34:ARG:HD3	1:A:40:HIS:HA	1.98	0.46
1:A:225:PRO:HA	3:A:1041:HOH:O	2.15	0.46
1:D:181:LEU:CD1	1:D:182:CYS:N	2.79	0.46
1:A:232:THR:HG23	3:A:1011:HOH:O	2.16	0.46
1:D:56:ALA:HB1	1:D:90:VAL:HG13	1.98	0.45
1:A:73:LEU:HG	1:A:141:TRP:CD1	2.51	0.45
1:B:30:GLN:NE2	1:B:139:THR:OG1	2.49	0.45
1:C:187:ARG:HE	1:C:187:ARG:HB2	1.43	0.45
1:D:33:LEU:HB3	1:D:41:PHE:CZ	2.50	0.45
1:D:219:GLY:O	2:D:996:C3A:H131	2.16	0.45
1:A:56:ALA:HB2	1:A:103:ILE:O	2.15	0.45
1:B:150:ARG:HD2	1:B:150:ARG:H	1.82	0.45
1:D:24:ARG:CD	1:D:24:ARG:N	2.73	0.45
1:C:38:TRP:CH2	1:C:65:ARG:HG3	2.52	0.45
1:C:173:HIS:CD2	1:C:173(G):ASP:HA	2.52	0.45
1:D:169:ASP:HA	1:D:176:VAL:HG23	1.99	0.45
1:A:98:GLN:H	1:A:98:GLN:HG2	1.28	0.45
1:B:181:LEU:HD23	1:B:182:CYS:N	2.31	0.45
1:D:124:PRO:HD3	1:D:209:GLN:O	2.17	0.45
1:D:195:SER:HA	1:D:213:VAL:HG12	1.98	0.45
1:B:185:ASN:ND2	1:B:188:ARG:N	2.45	0.45
1:B:188:ARG:HG2	1:B:188:ARG:NH1	2.32	0.44
1:C:202:LYS:CE	3:C:1038:HOH:O	2.65	0.44
1:D:34:ARG:HH21	1:D:73:LEU:CD2	2.31	0.44
1:A:60(B):ASP:O	1:A:60(D):LYS:HE3	2.18	0.44
1:C:36:HIS:HD2	1:C:38:TRP:CZ2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:HIS:CG	1:A:244:LYS:HE2	2.51	0.44
1:C:185:ASN:C	1:C:185:ASN:ND2	2.74	0.44
1:B:185:ASN:ND2	1:B:185:ASN:C	2.75	0.44
1:B:159:LYS:O	1:B:188:ARG:HD3	2.18	0.44
1:C:61:LEU:CD2	1:C:88:ILE:HG13	2.44	0.44
1:B:181:LEU:HD23	1:B:181:LEU:C	2.43	0.44
1:C:213:VAL:HG12	2:C:997:C3A:H101	1.98	0.43
1:B:240:HIS:HD1	1:B:240:HIS:C	2.26	0.43
1:D:130:PHE:HA	1:D:131:PRO:HD2	1.87	0.43
1:D:30:GLN:HG2	1:D:155:LEU:HD11	2.00	0.43
1:A:68:LEU:O	1:A:69:ARG:C	2.60	0.43
1:C:152(A):PRO:HG3	1:C:153:PHE:CZ	2.53	0.43
1:A:89:ILE:HD13	1:A:241:TYR:CD1	2.53	0.43
1:C:202:LYS:HG2	1:C:207:TRP:CE2	2.54	0.43
1:A:195:SER:HA	1:A:213:VAL:HG12	1.99	0.43
1:D:46:LEU:O	1:D:120:THR:HA	2.19	0.43
1:A:213:VAL:CG1	2:A:999:C3A:H101	2.49	0.43
1:A:228:TYR:CD1	1:A:228:TYR:N	2.87	0.43
1:B:168:CYS:SG	1:B:225:PRO:HG2	2.59	0.43
1:D:61:LEU:N	1:D:61:LEU:HD12	2.34	0.43
1:B:96:THR:HG21	1:C:98:GLN:HG2	2.00	0.42
2:B:998:C3A:H31	2:B:998:C3A:H27	1.51	0.42
1:D:103:ILE:HB	1:D:229:THR:HG21	2.01	0.42
1:C:51:TRP:CZ3	1:C:107:GLU:HB2	2.55	0.42
1:C:181:LEU:HD23	1:C:182:CYS:N	2.35	0.42
1:C:89:ILE:HD13	1:C:241:TYR:CD1	2.54	0.42
1:C:99:ILE:O	1:C:177:ARG:HD2	2.20	0.42
1:A:38:TRP:CZ3	1:A:65:ARG:HG3	2.54	0.42
1:B:131:PRO:HA	1:B:132:PRO:HD3	1.87	0.42
1:C:30:GLN:NE2	1:C:139:THR:OG1	2.52	0.42
1:C:171:LYS:HD2	1:C:223:ASN:HD22	1.84	0.42
1:A:143:ASP:OD2	1:A:150:ARG:NH1	2.53	0.42
1:C:60(D):LYS:NZ	3:C:1036:HOH:O	2.47	0.42
1:A:30:GLN:NE2	1:A:139:THR:OG1	2.52	0.42
1:C:56:ALA:HB1	1:C:90:VAL:HG13	2.02	0.42
1:C:190:SER:OG	2:C:997:C3A:H151	2.19	0.41
1:D:41:PHE:CE2	2:D:996:C3A:H402	2.55	0.41
1:D:69:ARG:HH22	1:D:71:GLN:HE21	1.67	0.41
1:C:171:LYS:HD2	1:C:223:ASN:ND2	2.35	0.41
1:C:202:LYS:HE2	3:C:1038:HOH:O	2.20	0.41
1:D:48:HIS:CD2	1:D:51:TRP:HD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ARG:HG3	1:D:187:ARG:HH21	1.85	0.41
1:D:244:LYS:HD2	1:D:244:LYS:N	2.34	0.41
1:B:53:LEU:HD11	1:B:103:ILE:HD11	2.02	0.41
1:A:29:TRP:O	1:A:45:SER:HA	2.20	0.41
1:A:181:LEU:C	1:A:181:LEU:HD23	2.45	0.41
1:D:119:HIS:HB2	3:D:1004:HOH:O	2.19	0.41
1:B:240:HIS:ND1	1:B:240:HIS:C	2.79	0.41
1:B:187:ARG:CZ	1:B:187:ARG:HB2	2.50	0.41
2:D:996:C3A:H121	3:D:1009:HOH:O	2.21	0.41
1:A:190:SER:OG	2:A:999:C3A:H151	2.20	0.41
1:B:16:ILE:O	1:B:144:VAL:HA	2.20	0.41
1:B:48:HIS:CG	1:B:49:PRO:HD2	2.55	0.41
1:D:174:ARG:HB3	1:D:174:ARG:HH21	1.85	0.41
1:D:123:LEU:HD23	1:D:123:LEU:HA	1.89	0.41
1:A:152(A):PRO:HA	1:A:153:PHE:N	2.36	0.40
1:C:73:LEU:HG	1:C:141:TRP:CD1	2.56	0.40
1:C:221(A):GLN:HA	1:C:222:PRO:HD3	1.98	0.40
1:A:187:ARG:HE	1:A:187:ARG:HB2	1.68	0.40
1:D:97:ALA:HB3	2:D:996:C3A:C1	2.50	0.40
1:D:97:ALA:HB3	2:D:996:C3A:H12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/245 (98%)	230 (95%)	11 (5%)	0	100	100
1	B	241/245 (98%)	224 (93%)	17 (7%)	0	100	100
1	C	241/245 (98%)	228 (95%)	13 (5%)	0	100	100
1	D	241/245 (98%)	221 (92%)	17 (7%)	3 (1%)	10	20
All	All	964/980 (98%)	903 (94%)	58 (6%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	243	PRO
1	D	69	ARG
1	D	205	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	208/210 (99%)	198 (95%)	10 (5%)	23	46
1	B	208/210 (99%)	200 (96%)	8 (4%)	29	56
1	C	208/210 (99%)	198 (95%)	10 (5%)	23	46
1	D	208/210 (99%)	197 (95%)	11 (5%)	20	42
All	All	832/840 (99%)	793 (95%)	39 (5%)	23	47

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ARG
1	A	68	LEU
1	A	70	GLU
1	A	93	GLN
1	A	98	GLN
1	A	159	LYS
1	A	162	ILE
1	A	199	LEU
1	A	229	THR
1	B	122	THR
1	B	134	MET
1	B	150	ARG
1	B	165	ASN
1	B	168	CYS
1	B	174	ARG
1	B	185	ASN

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Mol	Chain	Res	Type
1	B	198	PRO
1	C	65	ARG
1	C	93	GLN
1	C	112	VAL
1	C	118	VAL
1	C	123	LEU
1	C	150	ARG
1	C	162	ILE
1	C	185	ASN
1	C	202	LYS
1	C	222	PRO
1	D	24	ARG
1	D	70	GLU
1	D	128	GLU
1	D	165	ASN
1	D	167	ILE
1	D	168	CYS
1	D	174	ARG
1	D	181	LEU
1	D	198	PRO
1	D	206	THR
1	D	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	30	GLN
1	A	48	HIS
1	A	72	HIS
1	A	79	GLN
1	A	93	GLN
1	A	119	HIS
1	A	165	ASN
1	A	166	HIS
1	A	223	ASN
1	A	240	HIS
1	B	30	GLN
1	B	36	HIS
1	B	50	GLN
1	B	91	HIS
1	B	165	ASN

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Mol	Chain	Res	Type
1	B	185	ASN
1	B	204	ASN
1	B	221(A)	GLN
1	C	30	GLN
1	C	36	HIS
1	C	48	HIS
1	C	72	HIS
1	C	79	GLN
1	C	119	HIS
1	C	146	ASN
1	C	165	ASN
1	C	166	HIS
1	C	185	ASN
1	C	223	ASN
1	D	30	GLN
1	D	36	HIS
1	D	48	HIS
1	D	71	GLN
1	D	79	GLN
1	D	93	GLN
1	D	119	HIS
1	D	223	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	C3A	B	998	1	43,45,45	3.89	21 (48%)	50,61,61	4.39	20 (40%)
2	C3A	D	996	1	43,45,45	3.70	28 (65%)	50,61,61	5.44	20 (40%)
2	C3A	C	997	1	43,45,45	3.80	27 (62%)	50,61,61	4.61	22 (44%)
2	C3A	A	999	1	43,45,45	4.05	29 (67%)	50,61,61	4.77	20 (40%)

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	C3A	B	998	1	-	13/33/48/48	0/5/5/5
2	C3A	D	996	1	-	14/33/48/48	0/5/5/5
2	C3A	C	997	1	-	14/33/48/48	0/5/5/5
2	C3A	A	999	1	-	13/33/48/48	0/5/5/5

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	C3A	O17-C16	12.70	1.44	1.22
2	A	999	C3A	C22-C21	-12.05	1.36	1.50
2	C	997	C3A	C22-C21	-11.77	1.36	1.50
2	D	996	C3A	O17-C16	11.28	1.41	1.22
2	B	998	C3A	C22-C21	-10.44	1.38	1.50
2	C	997	C3A	O17-C16	9.55	1.38	1.22
2	A	999	C3A	O6-C5	8.09	1.36	1.21
2	A	999	C3A	O17-C16	7.97	1.36	1.22
2	D	996	C3A	C22-C21	-7.75	1.41	1.50
2	B	998	C3A	C24-C23	6.91	1.52	1.38
2	D	996	C3A	C24-C23	6.81	1.52	1.38
2	C	997	C3A	C24-C23	6.55	1.51	1.38
2	A	999	C3A	C24-C23	6.41	1.51	1.38
2	A	999	C3A	O4-C3	6.20	1.62	1.46
2	D	996	C3A	C25-C26	6.11	1.48	1.39
2	D	996	C3A	O4-C3	6.02	1.62	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	C3A	O20-N19	-5.86	1.31	1.42
2	B	998	C3A	C25-C26	5.83	1.48	1.39
2	C	997	C3A	O20-N19	-5.51	1.32	1.42
2	A	999	C3A	O20-C21	5.36	1.39	1.34
2	A	999	C3A	C40-C32	5.35	1.62	1.53
2	C	997	C3A	C40-C32	5.35	1.62	1.53
2	B	998	C3A	C40-C32	5.21	1.61	1.53
2	D	996	C3A	C25-C24	5.21	1.47	1.38
2	C	997	C3A	C25-C26	5.09	1.47	1.39
2	A	999	C3A	O20-N19	-4.97	1.33	1.42
2	A	999	C3A	C25-C26	4.92	1.46	1.39
2	C	997	C3A	C25-C24	4.85	1.46	1.38
2	D	996	C3A	C40-C32	4.84	1.61	1.53
2	B	998	C3A	C25-C24	4.74	1.46	1.38
2	A	999	C3A	C25-C24	4.64	1.46	1.38
2	C	997	C3A	O6-C5	4.60	1.30	1.21
2	D	996	C3A	O20-N19	-4.59	1.34	1.42
2	B	998	C3A	C37-C36	4.48	1.48	1.38
2	B	998	C3A	C37-C38	4.42	1.46	1.38
2	C	997	C3A	C37-C36	4.32	1.47	1.38
2	B	998	C3A	C35-C34	4.20	1.46	1.39
2	B	998	C3A	C27-C26	4.20	1.45	1.39
2	A	999	C3A	O4-C5	4.16	1.43	1.35
2	D	996	C3A	C37-C36	4.16	1.47	1.38
2	C	997	C3A	O4-C3	4.15	1.57	1.46
2	A	999	C3A	C21-N41	4.14	1.33	1.29
2	A	999	C3A	C37-C36	4.02	1.47	1.38
2	A	999	C3A	O30-C29	-3.98	1.14	1.23
2	C	997	C3A	O30-C29	-3.88	1.14	1.23
2	A	999	C3A	C16-C18	-3.88	1.42	1.50
2	D	996	C3A	C37-C38	3.87	1.45	1.38
2	C	997	C3A	C35-C34	3.87	1.45	1.39
2	C	997	C3A	C37-C38	3.86	1.45	1.38
2	D	996	C3A	C33-C34	-3.84	1.44	1.50
2	D	996	C3A	O6-C5	3.82	1.28	1.21
2	C	997	C3A	C16-C18	-3.75	1.42	1.50
2	B	998	C3A	C16-C18	-3.72	1.42	1.50
2	B	998	C3A	O20-C21	3.70	1.37	1.34
2	C	997	C3A	C27-C26	3.70	1.45	1.39
2	A	999	C3A	C3-C2	3.69	1.67	1.48
2	B	998	C3A	C33-C34	-3.65	1.44	1.50
2	A	999	C3A	C27-C26	3.64	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	999	C3A	C37-C38	3.62	1.45	1.38
2	D	996	C3A	C27-C26	3.60	1.44	1.39
2	D	996	C3A	C36-C35	3.58	1.45	1.38
2	B	998	C3A	C39-C34	3.56	1.45	1.39
2	D	996	C3A	C35-C34	3.55	1.45	1.39
2	D	996	C3A	C3-C2	3.47	1.66	1.48
2	B	998	C3A	C36-C35	3.46	1.44	1.38
2	A	999	C3A	C35-C34	3.45	1.45	1.39
2	A	999	C3A	C36-C35	3.39	1.44	1.38
2	C	997	C3A	O20-C21	3.38	1.37	1.34
2	C	997	C3A	C36-C35	3.37	1.44	1.38
2	C	997	C3A	C39-C34	3.30	1.45	1.39
2	D	996	C3A	O4-C5	3.29	1.41	1.35
2	D	996	C3A	C39-C34	3.28	1.45	1.39
2	A	999	C3A	C38-C39	3.26	1.44	1.39
2	B	998	C3A	O6-C5	3.23	1.27	1.21
2	A	999	C3A	C33-C34	-3.19	1.45	1.50
2	A	999	C3A	C33-C32	-3.16	1.48	1.53
2	A	999	C3A	C39-C34	3.16	1.45	1.39
2	C	997	C3A	C38-C39	3.09	1.44	1.39
2	B	998	C3A	C38-C39	3.05	1.44	1.39
2	C	997	C3A	C33-C34	-3.05	1.45	1.50
2	D	996	C3A	C38-C39	3.04	1.44	1.39
2	D	996	C3A	O30-C29	-2.84	1.16	1.23
2	A	999	C3A	C32-N31	-2.84	1.41	1.46
2	B	998	C3A	C32-N31	-2.84	1.41	1.46
2	D	996	C3A	C32-N31	-2.72	1.41	1.46
2	C	997	C3A	C3-C2	2.67	1.62	1.48
2	C	997	C3A	C33-C32	-2.63	1.49	1.53
2	A	999	C3A	C26-C29	-2.60	1.44	1.50
2	B	998	C3A	O30-C29	-2.58	1.17	1.23
2	B	998	C3A	C33-C32	-2.48	1.49	1.53
2	C	997	C3A	C32-N31	-2.47	1.41	1.46
2	C	997	C3A	C22-C23	-2.47	1.47	1.51
2	D	996	C3A	C33-C32	-2.46	1.49	1.53
2	A	999	C3A	C28-C23	2.43	1.43	1.38
2	D	996	C3A	C28-C23	2.36	1.43	1.38
2	C	997	C3A	O4-C5	2.31	1.39	1.35
2	A	999	C3A	C10-C9	2.30	1.59	1.53
2	D	996	C3A	O20-C21	2.28	1.36	1.34
2	A	999	C3A	C1-C2	2.23	1.43	1.29
2	C	997	C3A	C26-C29	-2.23	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	997	C3A	C21-N41	2.23	1.31	1.29
2	D	996	C3A	C18-N41	2.10	1.41	1.37
2	D	996	C3A	C18-N19	2.05	1.36	1.31
2	D	996	C3A	C16-C18	-2.04	1.46	1.50
2	D	996	C3A	C1-C2	2.01	1.42	1.29

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	996	C3A	O4-C5-N7	17.30	147.44	110.45
2	B	998	C3A	O17-C16-C18	-16.18	99.15	120.14
2	D	996	C3A	O6-C5-N7	-16.02	98.61	124.86
2	D	996	C3A	C21-N41-C18	15.85	108.95	102.01
2	C	997	C3A	O17-C16-C18	-14.82	100.91	120.14
2	A	999	C3A	O17-C16-C18	-14.68	101.09	120.14
2	D	996	C3A	O17-C16-C18	-13.58	102.53	120.14
2	A	999	C3A	O4-C5-N7	13.54	139.40	110.45
2	B	998	C3A	C21-N41-C18	12.29	107.39	102.01
2	C	997	C3A	O4-C5-N7	11.88	135.86	110.45
2	C	997	C3A	C21-N41-C18	11.41	107.00	102.01
2	A	999	C3A	O6-C5-N7	-11.39	106.20	124.86
2	A	999	C3A	C8-N7-C5	10.74	147.65	120.93
2	B	998	C3A	C3-O4-C5	10.33	131.70	116.11
2	C	997	C3A	O6-C5-N7	-10.11	108.30	124.86
2	C	997	C3A	C8-N7-C5	9.68	145.02	120.93
2	A	999	C3A	C21-N41-C18	9.12	106.00	102.01
2	D	996	C3A	C8-N7-C5	8.70	142.59	120.93
2	A	999	C3A	C32-N31-C29	8.70	139.02	122.56
2	D	996	C3A	O4-C5-O6	-8.30	108.35	124.26
2	B	998	C3A	C9-C8-N7	-8.19	94.69	110.91
2	D	996	C3A	N41-C18-N19	-7.98	104.60	115.62
2	A	999	C3A	O20-N19-C18	7.60	110.63	102.84
2	C	997	C3A	C32-N31-C29	7.28	136.33	122.56
2	A	999	C3A	C33-C32-N31	7.16	126.16	112.32
2	C	997	C3A	O20-N19-C18	7.16	110.17	102.84
2	C	997	C3A	C33-C32-N31	6.89	125.64	112.32
2	D	996	C3A	C32-N31-C29	6.84	135.51	122.56
2	B	998	C3A	C32-N31-C29	6.77	135.36	122.56
2	D	996	C3A	O20-N19-C18	6.76	109.76	102.84
2	B	998	C3A	O6-C5-N7	-6.70	113.89	124.86
2	D	996	C3A	C33-C32-N31	6.46	124.79	112.32
2	D	996	C3A	O20-C21-N41	-6.26	108.55	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	C3A	O4-C3-C2	6.16	130.06	109.44
2	A	999	C3A	O4-C5-O6	-6.06	112.65	124.26
2	B	998	C3A	O4-C5-N7	5.84	122.93	110.45
2	B	998	C3A	N41-C18-N19	-5.83	107.58	115.62
2	C	997	C3A	N41-C18-N19	-5.74	107.70	115.62
2	C	997	C3A	O20-C21-N41	-5.72	108.99	113.62
2	B	998	C3A	O20-N19-C18	5.71	108.69	102.84
2	A	999	C3A	O20-C21-N41	-5.61	109.08	113.62
2	B	998	C3A	C33-C32-N31	5.55	123.04	112.32
2	B	998	C3A	O20-C21-N41	-5.33	109.31	113.62
2	C	997	C3A	O4-C5-O6	-5.24	114.22	124.26
2	C	997	C3A	O4-C3-C2	5.18	126.76	109.44
2	D	996	C3A	O4-C3-C2	4.96	126.04	109.44
2	A	999	C3A	N41-C18-N19	-4.86	108.92	115.62
2	B	998	C3A	O4-C3-C2	4.77	125.42	109.44
2	C	997	C3A	C9-C8-N7	-4.72	101.56	110.91
2	B	998	C3A	C8-N7-C5	4.01	130.90	120.93
2	D	996	C3A	C21-O20-N19	3.73	108.14	106.10
2	A	999	C3A	C26-C29-N31	-3.41	110.72	117.04
2	B	998	C3A	C34-C33-C32	3.20	106.04	102.89
2	A	999	C3A	C24-C25-C26	-3.10	117.48	120.80
2	B	998	C3A	C39-C40-C32	-3.03	99.91	102.89
2	C	997	C3A	C24-C25-C26	-2.96	117.63	120.80
2	B	998	C3A	C24-C25-C26	-2.90	117.70	120.80
2	C	997	C3A	C34-C33-C32	2.88	105.73	102.89
2	D	996	C3A	C39-C40-C32	-2.76	100.17	102.89
2	A	999	C3A	C34-C33-C32	2.71	105.56	102.89
2	D	996	C3A	C34-C33-C32	2.65	105.50	102.89
2	B	998	C3A	C26-C29-N31	-2.64	112.15	117.04
2	A	999	C3A	C39-C40-C32	-2.62	100.31	102.89
2	C	997	C3A	C9-C10-C11	2.62	119.07	115.03
2	C	997	C3A	C28-C27-C26	2.58	123.56	120.80
2	C	997	C3A	C3-O4-C5	2.58	120.01	116.11
2	B	998	C3A	C40-C32-N31	2.57	117.29	112.32
2	A	999	C3A	C28-C27-C26	2.57	123.54	120.80
2	D	996	C3A	C24-C25-C26	-2.57	118.06	120.80
2	D	996	C3A	C26-C29-N31	-2.51	112.38	117.04
2	C	997	C3A	C36-C35-C34	-2.47	117.25	120.88
2	B	998	C3A	C36-C35-C34	-2.43	117.33	120.88
2	A	999	C3A	C33-C34-C39	2.42	112.13	110.50
2	A	999	C3A	C9-C8-N7	-2.40	106.15	110.91
2	B	998	C3A	C28-C27-C26	2.35	123.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	996	C3A	C36-C35-C34	-2.35	117.44	120.88
2	A	999	C3A	C36-C35-C34	-2.32	117.49	120.88
2	C	997	C3A	C33-C34-C39	2.15	111.94	110.50
2	C	997	C3A	C26-C29-N31	-2.15	113.06	117.04
2	D	996	C3A	C33-C34-C39	2.09	111.90	110.50
2	C	997	C3A	C39-C40-C32	-2.08	100.83	102.89
2	D	996	C3A	C28-C27-C26	2.06	123.00	120.80

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	C3A	C2-C3-O4-C5
2	A	999	C3A	C18-C16-C8-C9
2	A	999	C3A	C18-C16-C8-N7
2	A	999	C3A	C9-C10-C11-C12
2	A	999	C3A	C8-C16-C18-N19
2	A	999	C3A	O17-C16-C18-N19
2	A	999	C3A	C33-C32-N31-C29
2	B	998	C3A	C18-C16-C8-C9
2	B	998	C3A	O17-C16-C8-N7
2	B	998	C3A	C18-C16-C8-N7
2	B	998	C3A	C11-C10-C9-C8
2	B	998	C3A	C8-C16-C18-N19
2	B	998	C3A	C8-C16-C18-N41
2	B	998	C3A	O17-C16-C18-N19
2	B	998	C3A	C33-C32-N31-C29
2	C	997	C3A	C2-C3-O4-C5
2	C	997	C3A	C16-C8-N7-C5
2	C	997	C3A	C18-C16-C8-N7
2	C	997	C3A	C9-C10-C11-C12
2	C	997	C3A	C8-C16-C18-N19
2	C	997	C3A	C8-C16-C18-N41
2	C	997	C3A	O17-C16-C18-N19
2	C	997	C3A	C33-C32-N31-C29
2	D	996	C3A	O6-C5-N7-C8
2	D	996	C3A	C2-C3-O4-C5
2	D	996	C3A	C9-C8-N7-C5
2	D	996	C3A	C18-C16-C8-N7
2	D	996	C3A	C8-C16-C18-N19
2	D	996	C3A	O17-C16-C18-N19
2	D	996	C3A	C33-C32-N31-C29

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Mol	Chain	Res	Type	Atoms
2	A	999	C3A	C16-C8-N7-C5
2	D	996	C3A	N7-C8-C9-C10
2	B	998	C3A	C16-C8-C9-C10
2	D	996	C3A	C16-C8-C9-C10
2	B	998	C3A	N7-C8-C9-C10
2	A	999	C3A	O6-C5-N7-C8
2	D	996	C3A	O6-C5-O4-C3
2	A	999	C3A	C1-C2-C3-O4
2	B	998	C3A	C1-C2-C3-O4
2	A	999	C3A	C9-C10-C11-C15
2	C	997	C3A	C9-C10-C11-C15
2	D	996	C3A	C9-C10-C11-C15
2	D	996	C3A	C1-C2-C3-O4
2	C	997	C3A	O6-C5-N7-C8
2	D	996	C3A	C9-C10-C11-C12
2	C	997	C3A	C18-C16-C8-C9
2	C	997	C3A	O17-C16-C8-N7
2	A	999	C3A	C11-C10-C9-C8
2	C	997	C3A	C11-C10-C9-C8
2	B	998	C3A	O4-C5-N7-C8
2	C	997	C3A	O4-C5-N7-C8
2	A	999	C3A	O4-C5-N7-C8
2	D	996	C3A	O4-C5-N7-C8
2	B	998	C3A	O6-C5-N7-C8

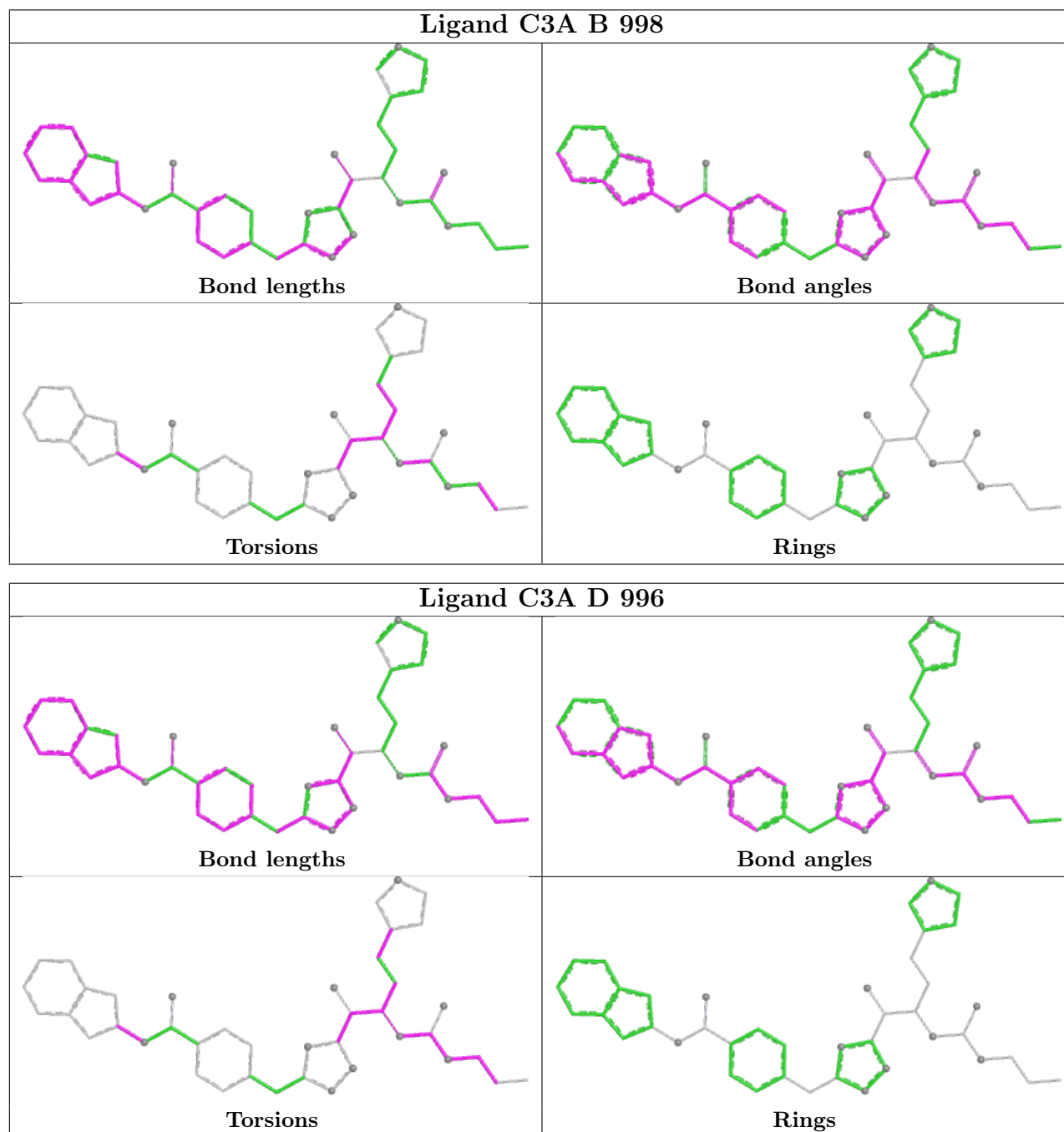
There are no ring outliers.

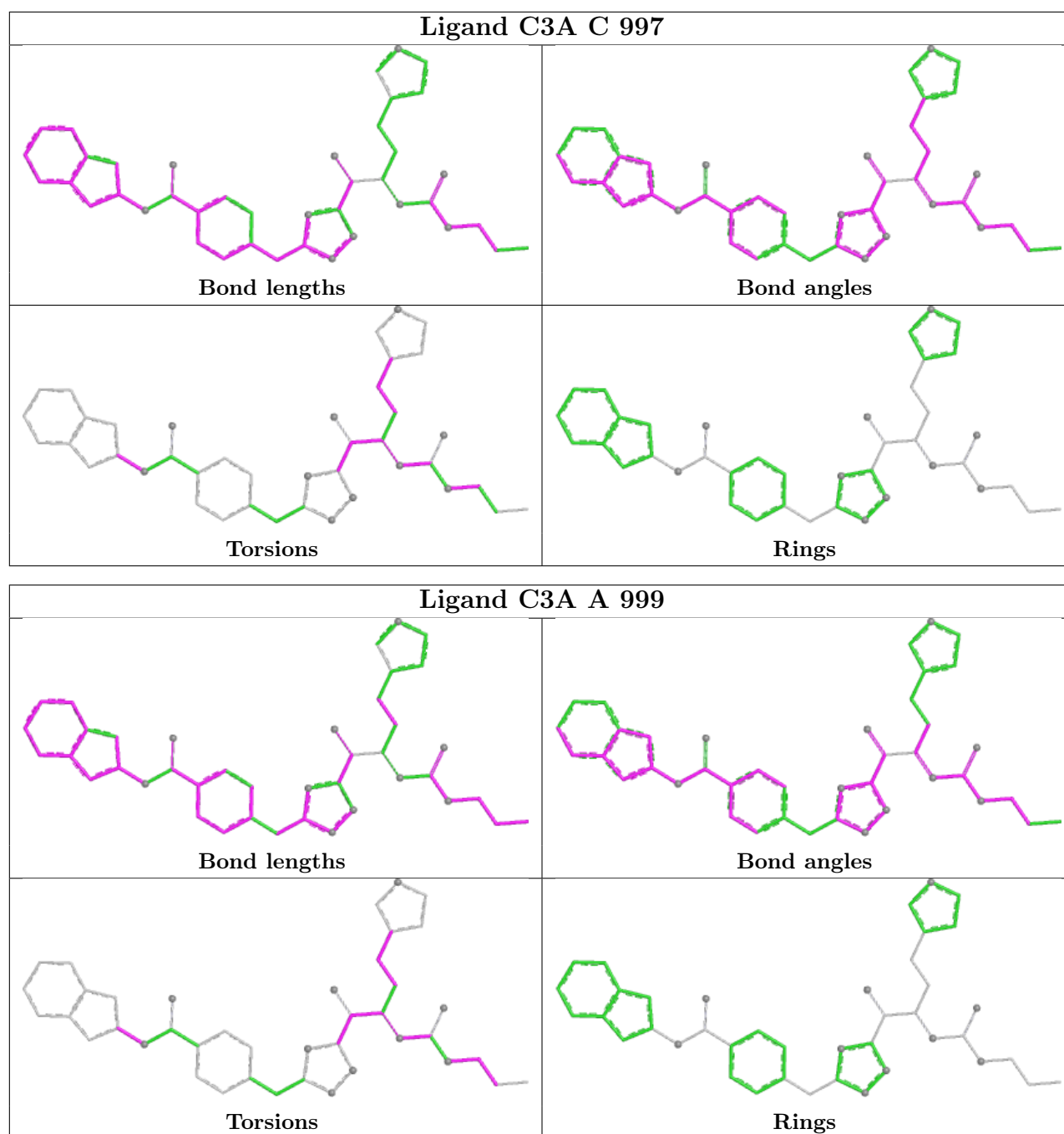
4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	998	C3A	4	0
2	D	996	C3A	10	0
2	C	997	C3A	9	0
2	A	999	C3A	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	243/245 (99%)	-1.66	0 100 100	12, 23, 45, 62	0
1	B	243/245 (99%)	-1.59	0 100 100	14, 28, 53, 71	0
1	C	243/245 (99%)	-1.67	0 100 100	13, 24, 46, 67	0
1	D	243/245 (99%)	-1.57	0 100 100	15, 29, 54, 69	0
All	All	972/980 (99%)	-1.62	0 100 100	12, 26, 50, 71	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

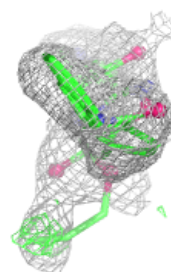
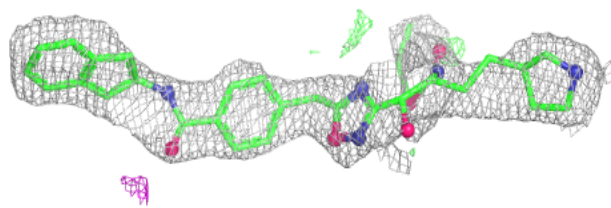
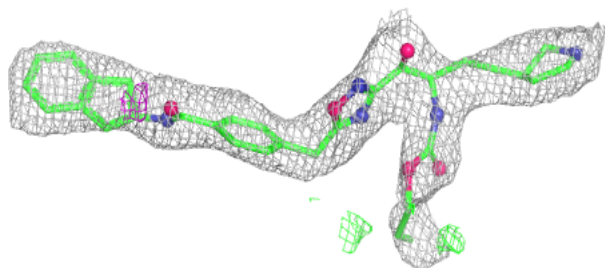
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	C3A	A	999	41/41	0.99	0.04	30,45,50,53	0
2	C3A	B	998	41/41	0.99	0.03	34,42,48,50	0
2	C3A	C	997	41/41	0.99	0.04	31,42,53,54	0
2	C3A	D	996	41/41	0.99	0.04	36,40,56,59	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.

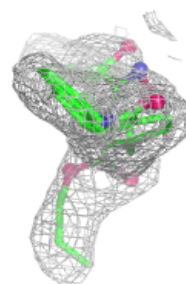
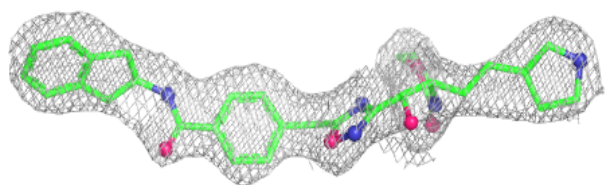
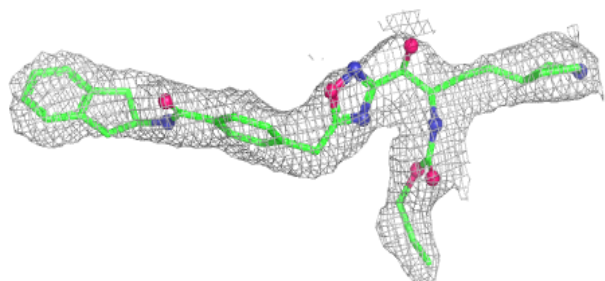
Electron density around C3A A 999:

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

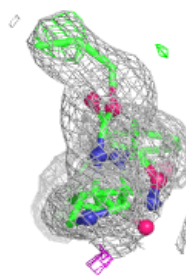
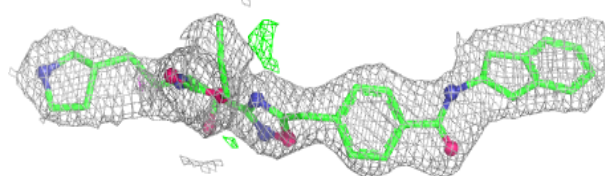
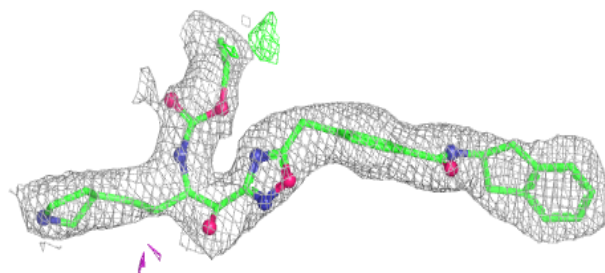


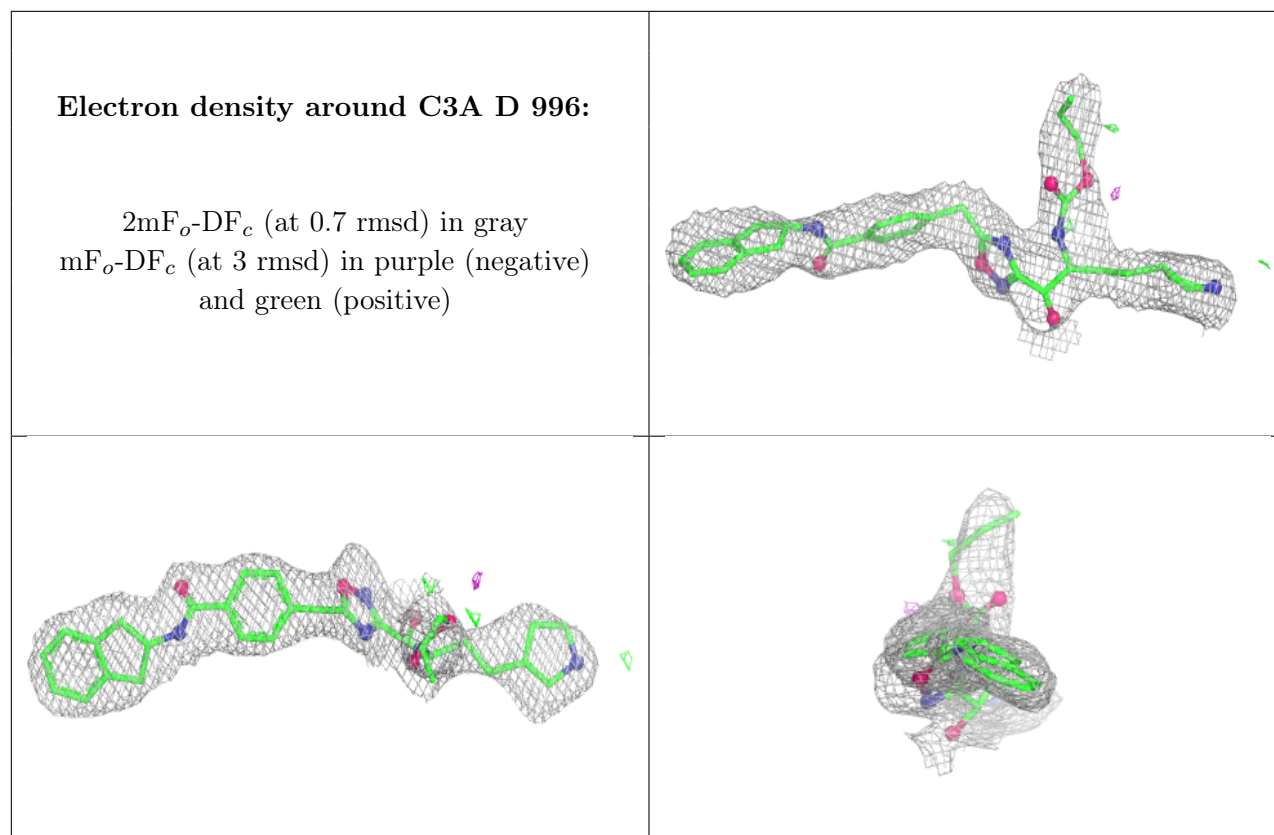
Electron density around C3A B 998:

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

**Electron density around C3A C 997:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.