



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 09:41 AM EDT

PDB ID : 2GD2
Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA racemase is catalyzed by an aspartate/histidine pair and involves a smooth, methionine-rich surface for binding the fatty acyl moiety
Authors : Bhaumik, P.; Wierenga, R.K.
Deposited on : 2006-03-15
Resolution : 1.70 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

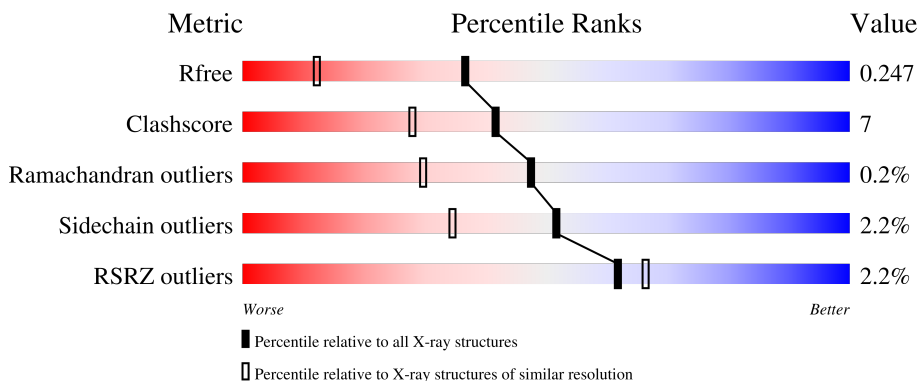
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	360	
1	B	360	
1	C	360	
1	D	360	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	2308	-	-	X	-
3	GOL	C	2307	-	-	X	-

2 Entry composition [i](#)

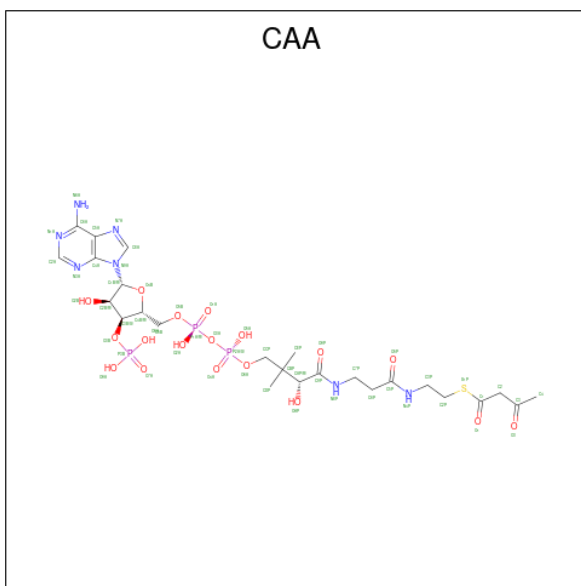
There are 4 unique types of molecules in this entry. The entry contains 12635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 probable alpha-methylacyl-CoA racemase MCR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	Total 2701	C 1693	N 488	O 504	S 16	0	6	0
1	B	354	Total 2718	C 1702	N 492	O 508	S 16	0	11	0
1	C	354	Total 2724	C 1705	N 494	O 509	S 16	0	11	0
1	D	354	Total 2722	C 1704	N 495	O 507	S 16	0	10	0

- Molecule 2 is ACETOACETYL-COENZYME A (three-letter code: CAA) (formula: C₂₅H₄₀N₇O₁₈P₃S).



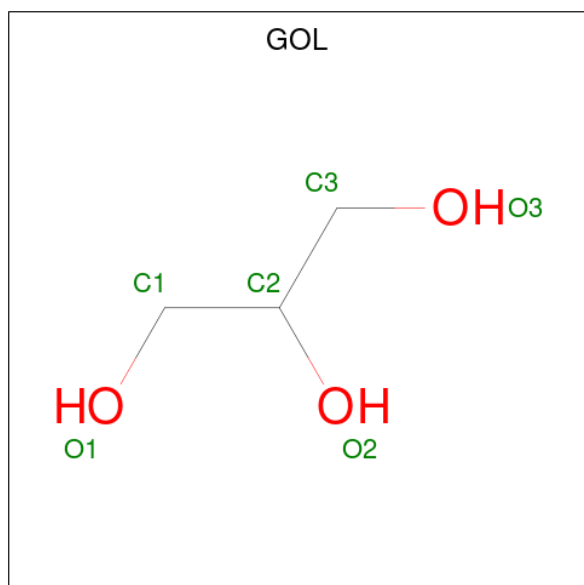
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total 54	C 25	N 7	O 18	P 3	S 1	0	0
2	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

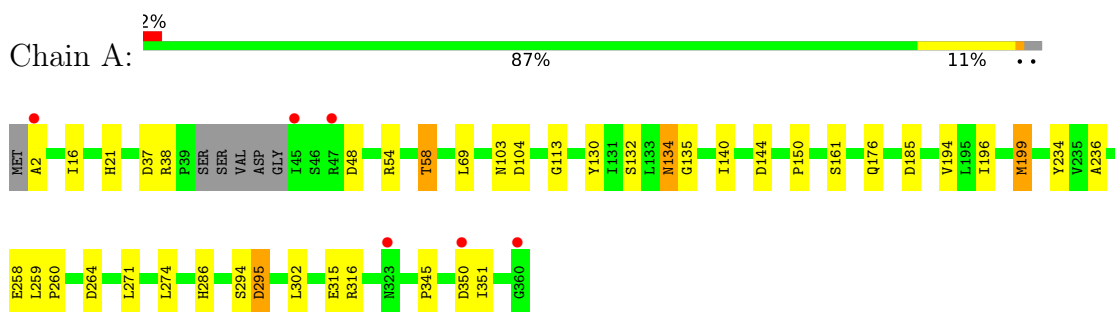
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	394	Total	O	0	0
			394	394		
4	B	388	Total	O	0	0
			388	388		
4	C	372	Total	O	0	0
			372	372		
4	D	400	Total	O	0	0
			400	400		

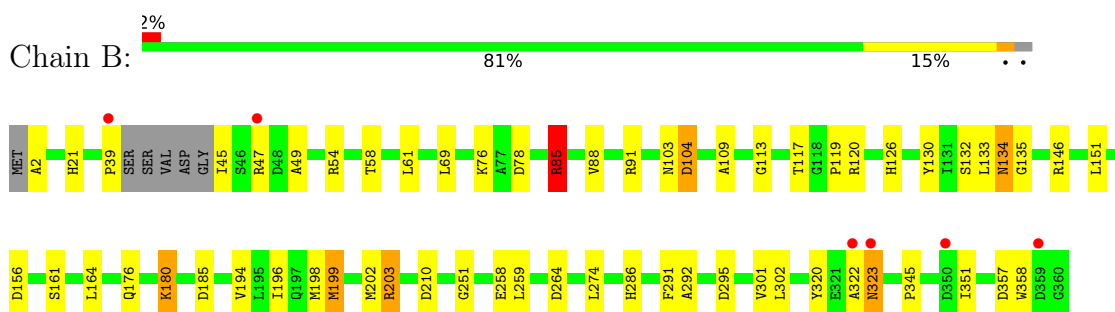
3 Residue-property plots [i](#)

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.

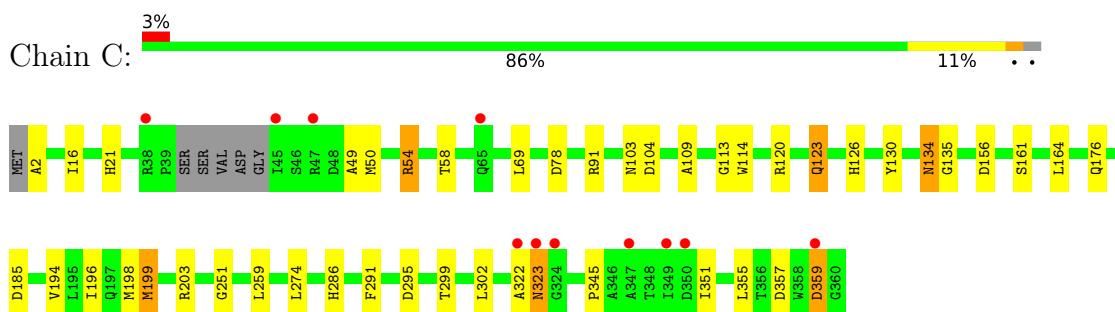
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



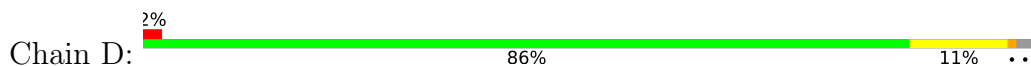
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR

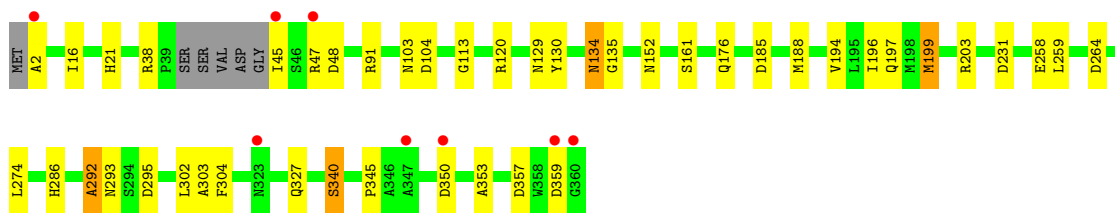


- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



- Molecule 1: probable alpha-methylacyl-CoA racemase MCR





4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.12Å 80.03Å 118.62Å 90.00° 91.58° 90.00°	Depositor
Resolution (Å)	19.80 – 1.70 19.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.80-1.70) 91.3 (19.80-1.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.250 0.209 , 0.247	Depositor DCC
R_{free} test set	8538 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.166 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12635	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2435e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CAA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.84	0/2792	0.93	8/3795 (0.2%)
1	B	0.84	0/2818	0.97	12/3830 (0.3%)
1	C	0.85	0/2822	0.92	7/3835 (0.2%)
1	D	0.88	0/2812	0.93	9/3822 (0.2%)
All	All	0.85	0/11244	0.94	36/15282 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	185	ASP	CB-CG-OD2	10.37	127.63	118.30
1	A	295	ASP	CB-CG-OD2	9.06	126.45	118.30
1	B	295	ASP	CB-CG-OD2	8.76	126.19	118.30
1	C	185	ASP	CB-CG-OD2	8.41	125.86	118.30
1	D	295	ASP	CB-CG-OD2	8.32	125.79	118.30
1	C	295	ASP	CB-CG-OD2	7.71	125.24	118.30
1	D	185	ASP	CB-CG-OD2	7.59	125.14	118.30
1	B	85	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	B	185	ASP	CB-CG-OD2	7.18	124.76	118.30
1	B	357	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C	104	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	104	ASP	CB-CG-OD2	6.86	124.48	118.30
1	A	264	ASP	CB-CG-OD2	6.39	124.06	118.30
1	B	91	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	104	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	78	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	264	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	357	ASP	CB-CG-OD2	5.90	123.61	118.30
1	C	359	ASP	CB-CG-OD2	5.53	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	ASP	CB-CG-OD2	5.53	123.27	118.30
1	D	231	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	144	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	350	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	292[A]	ALA	N-CA-C	5.34	125.41	111.00
1	D	292[B]	ALA	N-CA-C	5.34	125.41	111.00
1	B	292[A]	ALA	N-CA-C	5.29	125.29	111.00
1	B	292[B]	ALA	N-CA-C	5.29	125.29	111.00
1	D	357	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	54	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	37	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	54	ARG	CB-CA-C	-5.15	100.10	110.40
1	A	54	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	78	ASP	CB-CG-OD2	5.11	122.89	118.30
1	D	120	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	104	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2701	0	2641	31	0
1	B	2718	0	2651	52	0
1	C	2724	0	2662	43	0
1	D	2722	0	2660	35	0
2	A	54	0	36	3	0
2	B	48	0	31	8	0
2	C	48	0	31	5	0
2	D	54	0	36	3	0
3	B	6	0	8	11	0
3	C	6	0	8	4	0
4	A	394	0	0	14	0
4	B	388	0	0	6	0
4	C	372	0	0	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	400	0	0	10	1
All	All	12635	0	10764	151	1

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 7.

All (151) 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:2:ALA:HB1	4:D:2014:HOH:O	1.56	1.05
2:B:1752:CAA:S1P	3:B:2308:GOL:H31	2.12	0.89
1:C:322[B]:ALA:O	1:C:323[B]:ASN:O	1.94	0.86
1:C:176:GLN:HG3	4:D:1997:HOH:O	1.80	0.82
1:D:38:ARG:HH11	1:D:38:ARG:HG3	1.46	0.79
1:C:322[B]:ALA:O	1:C:323[B]:ASN:C	2.22	0.78
1:D:259:LEU:HD22	1:D:274:LEU:HD13	1.67	0.77
2:D:1754:CAA:H142	4:D:2152:HOH:O	1.87	0.73
1:B:322[A]:ALA:O	1:B:323[A]:ASN:C	2.26	0.72
2:B:1752:CAA:S1P	3:B:2308:GOL:C3	2.77	0.72
1:B:85:ARG:CD	2:B:1752:CAA:O1A	2.37	0.72
1:B:320:TYR:CE1	1:B:322[B]:ALA:HB2	2.25	0.71
1:D:259:LEU:CD2	1:D:274:LEU:HD13	2.21	0.71
1:B:286:HIS:HD2	4:B:2377:HOH:O	1.74	0.69
1:B:85:ARG:HD2	2:B:1752:CAA:O1A	1.93	0.69
1:B:126:HIS:HB3	3:B:2308:GOL:H32	1.75	0.68
2:A:1751:CAA:H4'3	2:A:1751:CAA:S1P	2.35	0.67
1:C:299:THR:HG22	4:C:2422:HOH:O	1.93	0.67
1:C:345:PRO:HB3	4:C:2392:HOH:O	1.95	0.66
1:B:126:HIS:ND1	3:B:2308:GOL:C3	2.59	0.65
1:A:345:PRO:HD3	4:A:2123:HOH:O	1.96	0.65
1:B:126:HIS:ND1	3:B:2308:GOL:H32	2.11	0.65
1:A:286:HIS:HE1	4:A:1818:HOH:O	1.79	0.65
1:C:91:ARG:NE	4:C:2420:HOH:O	1.94	0.65
4:A:2013:HOH:O	1:B:176:GLN:HG2	1.96	0.64
1:A:48:ASP:O	4:A:2104:HOH:O	2.14	0.64
1:B:85:ARG:HD3	2:B:1752:CAA:O1A	1.98	0.63
1:B:322[B]:ALA:O	1:B:323[B]:ASN:C	2.36	0.63
1:A:58:THR:HG21	4:A:2032:HOH:O	1.98	0.62
2:A:1751:CAA:S1P	2:A:1751:CAA:C4	2.88	0.61
1:A:140:ILE:HD12	1:A:150:PRO:HG3	1.81	0.61
1:C:91:ARG:HH12	2:C:1753:CAA:P3B	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:HD2	1:A:161:SER:OG	1.83	0.61
1:C:299:THR:HG21	1:D:129:ASN:HB3	1.82	0.60
1:B:258:GLU:HG3	4:B:2627:HOH:O	2.02	0.60
1:B:345:PRO:HD3	4:B:2617:HOH:O	2.02	0.60
1:B:259:LEU:HD22	1:B:274:LEU:HD13	1.84	0.59
1:B:126:HIS:CB	3:B:2308:GOL:H32	2.32	0.58
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.85	0.58
1:C:198:MET:HE1	1:D:152:ASN:HD21	1.69	0.57
1:D:345:PRO:HG2	4:D:2000:HOH:O	2.04	0.57
4:A:2003:HOH:O	1:B:119:PRO:HD3	2.04	0.56
1:C:126:HIS:ND1	3:C:2307:GOL:H2	2.20	0.56
1:A:294:SER:HA	4:A:2075:HOH:O	2.05	0.56
2:C:1753:CAA:S1P	3:C:2307:GOL:O3	2.51	0.56
1:B:156:ASP:OD2	3:B:2308:GOL:H2	2.07	0.55
1:A:176:GLN:NE2	1:B:176:GLN:HG2	2.21	0.55
1:D:38:ARG:HG3	1:D:38:ARG:NH1	2.20	0.55
1:B:126:HIS:ND1	3:B:2308:GOL:H31	2.21	0.55
4:A:1773:HOH:O	1:B:146:ARG:HB2	2.07	0.54
4:C:2633:HOH:O	1:D:16:ILE:HB	2.07	0.53
1:D:91:ARG:NH1	2:D:1754:CAA:O7A	2.41	0.53
2:C:1753:CAA:S1P	3:C:2307:GOL:O2	2.50	0.53
1:D:48:ASP:N	4:D:2000:HOH:O	2.41	0.53
1:B:69:LEU:HD13	1:B:351:ILE:HG21	1.90	0.53
1:A:16:ILE:HG23	4:A:1890:HOH:O	2.08	0.53
1:C:21:HIS:HD2	1:C:161:SER:OG	1.92	0.53
1:D:286:HIS:HE1	4:D:1799:HOH:O	1.92	0.53
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.44	0.52
1:D:134:ASN:C	1:D:134:ASN:HD22	2.12	0.52
1:B:39:PRO:HA	1:B:58:THR:OG1	2.09	0.52
1:D:21:HIS:HD2	1:D:161:SER:OG	1.92	0.52
1:A:302:LEU:O	1:B:135:GLY:HA2	2.10	0.52
1:A:316:ARG:HD2	1:B:117:THR:O	2.10	0.51
1:B:120:ARG:NE	1:B:133:LEU:HD11	2.25	0.51
1:D:47:ARG:NH1	4:D:2072:HOH:O	2.44	0.51
1:C:345:PRO:HD3	4:C:2541:HOH:O	2.11	0.51
1:A:134:ASN:C	1:A:134:ASN:HD22	2.12	0.51
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.46	0.50
1:B:21:HIS:HD2	1:B:161:SER:OG	1.94	0.50
1:C:49:ALA:HB2	4:C:2606:HOH:O	2.11	0.50
1:D:2:ALA:N	1:D:340:SER:HG	2.10	0.50
1:D:258:GLU:HG3	4:D:1934:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2572:HOH:O	1:D:327:GLN:HB3	2.12	0.50
1:A:258:GLU:HG3	4:A:1953:HOH:O	2.11	0.49
1:B:134:ASN:HD22	1:B:134:ASN:C	2.16	0.49
1:C:91:ARG:CZ	2:C:1753:CAA:O7A	2.58	0.49
1:A:260:PRO:HG2	1:A:271:LEU:HB2	1.94	0.49
1:C:194:VAL:O	1:D:21:HIS:HE1	1.96	0.49
1:B:47:ARG:NH2	4:B:2654:HOH:O	2.46	0.48
1:B:126:HIS:CG	3:B:2308:GOL:H32	2.48	0.48
1:C:135:GLY:HA2	1:D:302:LEU:O	2.14	0.48
1:A:21:HIS:CD2	1:A:161:SER:OG	2.67	0.48
1:C:302:LEU:O	1:D:135:GLY:HA2	2.14	0.48
1:C:109:ALA:HB1	1:C:164:LEU:HD11	1.96	0.48
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.49	0.48
2:D:1754:CAA:S1P	2:D:1754:CAA:C4	3.02	0.47
1:C:120:ARG:HH11	1:C:123[A]:GLN:HE22	1.62	0.47
1:A:16:ILE:HG22	2:A:1751:CAA:H4'3	1.96	0.47
1:A:194:VAL:O	1:B:21:HIS:HE1	1.96	0.47
1:B:286:HIS:HE1	4:B:2438:HOH:O	1.96	0.47
1:A:315:GLU:HG3	4:A:2003:HOH:O	2.14	0.47
1:C:134:ASN:HD22	1:C:134:ASN:C	2.17	0.47
1:C:156:ASP:OD2	3:C:2307:GOL:H32	2.15	0.47
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.50	0.47
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.50	0.47
1:D:176:GLN:NE2	4:D:1981:HOH:O	2.49	0.46
1:A:135:GLY:HA2	1:B:302:LEU:O	2.16	0.46
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.51	0.46
1:A:132[B]:SER:OG	1:B:301:VAL:HA	2.15	0.46
1:A:295:ASP:CG	1:B:85:ARG:HH22	2.18	0.46
1:C:198:MET:HE1	1:D:152:ASN:ND2	2.30	0.46
1:C:203[B]:ARG:HG2	4:C:2554:HOH:O	2.16	0.46
1:A:196:ILE:HG12	1:A:199:MET:HB2	1.97	0.45
1:C:198:MET:CE	1:D:152:ASN:HD21	2.28	0.45
1:B:88:VAL:HG13	2:B:1752:CAA:H3B	1.99	0.45
4:A:1857:HOH:O	1:B:49:ALA:HB1	2.15	0.45
1:C:114:TRP:HE1	1:C:123[A]:GLN:HG2	1.81	0.45
1:C:21:HIS:HE1	1:D:194:VAL:O	2.00	0.45
1:C:286:HIS:HE1	4:C:2461:HOH:O	1.99	0.45
1:C:50:MET:CA	1:D:197:GLN:HE22	2.30	0.44
1:A:234:TYR:HD1	4:A:1773:HOH:O	1.99	0.44
1:B:2:ALA:HA	4:B:2540:HOH:O	2.17	0.44
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:THR:CG2	4:C:2422:HOH:O	2.58	0.44
1:C:91:ARG:NH2	4:C:2420:HOH:O	2.50	0.44
1:C:355:LEU:HD23	1:C:355:LEU:HA	1.88	0.44
1:C:50:MET:N	1:D:197:GLN:HE22	2.15	0.44
1:B:109:ALA:HB1	1:B:164:LEU:HD11	2.00	0.44
1:C:259:LEU:HD22	1:C:274:LEU:HD13	2.00	0.44
1:A:38:ARG:HH11	1:A:38:ARG:HG3	1.83	0.43
1:B:203[A]:ARG:HD3	1:B:210:ASP:OD1	2.18	0.43
1:B:322[B]:ALA:O	1:B:323[B]:ASN:O	2.36	0.43
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.99	0.43
1:D:292[B]:ALA:O	1:D:293[B]:ASN:HB2	2.17	0.43
1:D:303:ALA:O	1:D:304:PHE:C	2.56	0.43
1:C:50:MET:HA	1:D:197:GLN:HE22	1.84	0.43
1:C:16:ILE:HB	4:D:2154:HOH:O	2.19	0.43
1:C:69:LEU:HD13	1:C:351:ILE:HG21	2.01	0.43
1:C:2:ALA:HB1	4:C:2551:HOH:O	2.18	0.43
1:A:21:HIS:HE1	1:B:194:VAL:O	2.02	0.43
1:A:69:LEU:HD13	1:A:351:ILE:HG21	2.01	0.42
1:C:16:ILE:HD13	4:C:2474:HOH:O	2.18	0.42
2:B:1752:CAA:H22	3:B:2308:GOL:O3	2.20	0.42
1:C:196:ILE:HG12	1:C:199:MET:HB2	2.01	0.42
1:A:2:ALA:HA	4:A:2131:HOH:O	2.19	0.42
1:D:350:ASP:O	1:D:353:ALA:HB3	2.19	0.42
1:B:198:MET:HG2	1:B:202:MET:HE2	2.02	0.42
1:C:251:GLY:HA3	1:C:291:PHE:CE2	2.54	0.42
1:B:76:LYS:HE2	1:B:358:TRP:O	2.20	0.41
1:B:104:ASP:OD2	1:B:180:LYS:HE2	2.20	0.41
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.55	0.41
1:B:196:ILE:HG12	1:B:199:MET:HB2	2.01	0.41
1:B:259:LEU:CD2	1:B:274:LEU:HD13	2.48	0.41
1:B:45:ILE:HG23	1:B:45:ILE:O	2.21	0.41
2:B:1752:CAA:S1P	3:B:2308:GOL:O3	2.79	0.41
1:D:113:GLY:CA	1:D:188:MET:HE3	2.51	0.41
1:A:236:ALA:HB2	1:B:132[B]:SER:OG	2.20	0.40
1:B:251:GLY:HA3	1:B:291:PHE:CE2	2.56	0.40
1:B:61:LEU:HD23	1:B:61:LEU:HA	1.86	0.40
1:C:91:ARG:NH2	2:C:1753:CAA:O7A	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2554:HOH:O	4:D:1998:HOH:O[4_656]	2.18	0.02

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	356/360 (99%)	345 (97%)	11 (3%)	0	100	100
1	B	361/360 (100%)	347 (96%)	11 (3%)	3 (1%)	19	6
1	C	361/360 (100%)	347 (96%)	12 (3%)	2 (1%)	25	11
1	D	360/360 (100%)	345 (96%)	15 (4%)	0	100	100
All	All	1438/1440 (100%)	1384 (96%)	49 (3%)	5 (0%)	47	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	323[A]	ASN
1	C	323[B]	ASN
1	B	323[A]	ASN
1	B	323[B]	ASN
1	B	151	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	272 (99%)	4 (1%)	67	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	277/275 (101%)	270 (98%)	7 (2%)	47	29
1	C	278/275 (101%)	270 (97%)	8 (3%)	42	23
1	D	276/275 (100%)	268 (97%)	8 (3%)	42	23
All	All	1107/1100 (101%)	1080 (98%)	27 (2%)	52	31

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	103	ASN
1	A	134	ASN
1	A	199	MET
1	B	85	ARG
1	B	103	ASN
1	B	134	ASN
1	B	180	LYS
1	B	199	MET
1	B	203[A]	ARG
1	B	203[B]	ARG
1	C	54	ARG
1	C	58	THR
1	C	103	ASN
1	C	123[A]	GLN
1	C	123[B]	GLN
1	C	134	ASN
1	C	199	MET
1	C	359	ASP
1	D	45	ILE
1	D	103	ASN
1	D	134	ASN
1	D	199	MET
1	D	203[A]	ARG
1	D	203[B]	ARG
1	D	340	SER
1	D	359	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS

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Mol	Chain	Res	Type
1	A	103	ASN
1	A	123	GLN
1	A	134	ASN
1	A	176	GLN
1	A	286	HIS
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	263	ASN
1	B	286	HIS
1	C	21	HIS
1	C	103	ASN
1	C	134	ASN
1	C	176	GLN
1	C	286	HIS
1	D	21	HIS
1	D	103	ASN
1	D	134	ASN
1	D	176	GLN
1	D	286	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	CAA	B	1752	-	41,50,56	1.12	4 (9%)	52,75,83	1.66	11 (21%)
3	GOL	C	2307	-	5,5,5	0.44	0	5,5,5	0.61	0
3	GOL	B	2308	-	5,5,5	0.56	0	5,5,5	0.70	0
2	CAA	D	1754	-	47,56,56	1.27	7 (14%)	60,83,83	2.55	13 (21%)
2	CAA	A	1751	1	47,56,56	1.21	5 (10%)	60,83,83	2.34	12 (20%)
2	CAA	C	1753	1	41,50,56	1.15	5 (12%)	52,75,83	1.69	13 (25%)

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	CAA	B	1752	-	-	3/44/64/71	0/3/3/3
3	GOL	C	2307	-	-	2/4/4/4	-
3	GOL	B	2308	-	-	2/4/4/4	-
2	CAA	D	1754	-	-	6/50/71/71	0/3/3/3
2	CAA	A	1751	1	-	7/50/71/71	0/3/3/3
2	CAA	C	1753	1	-	4/44/64/71	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1754	CAA	P3B-O7A	3.08	1.60	1.50
2	B	1752	CAA	P3B-O7A	2.97	1.60	1.50
2	A	1751	CAA	C1-S1P	-2.88	1.69	1.76
2	A	1751	CAA	P2A-O4A	2.67	1.60	1.50
2	A	1751	CAA	P3B-O7A	2.66	1.59	1.50
2	C	1753	CAA	P3B-O7A	2.62	1.59	1.50
2	D	1754	CAA	C1-S1P	-2.57	1.69	1.76
2	D	1754	CAA	C2A-N3A	2.46	1.36	1.32
2	C	1753	CAA	C8A-N7A	2.44	1.39	1.34
2	B	1752	CAA	O4B-C1B	2.33	1.44	1.41
2	C	1753	CAA	P1A-O1A	2.28	1.59	1.50
2	D	1754	CAA	OAP-CAP	2.24	1.46	1.42
2	D	1754	CAA	C2B-C1B	-2.24	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1752	CAA	C2A-N3A	2.20	1.35	1.32
2	C	1753	CAA	C2A-N3A	2.19	1.35	1.32
2	D	1754	CAA	C8A-N7A	2.19	1.38	1.34
2	C	1753	CAA	P2A-O4A	2.17	1.58	1.50
2	B	1752	CAA	C8A-N7A	2.11	1.38	1.34
2	D	1754	CAA	P1A-O1A	2.04	1.58	1.50
2	A	1751	CAA	C8A-N7A	2.03	1.38	1.34
2	A	1751	CAA	C2B-C1B	-2.01	1.50	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1754	CAA	C2-C1-S1P	13.34	130.31	113.69
2	A	1751	CAA	C2-C1-S1P	11.92	128.55	113.69
2	D	1754	CAA	O1-C1-C2	-6.74	111.67	123.35
2	A	1751	CAA	O1-C1-S1P	-6.23	114.52	122.61
2	D	1754	CAA	C1B-N9A-C4A	-5.34	117.27	126.64
2	A	1751	CAA	C1B-N9A-C4A	-5.08	117.71	126.64
2	B	1752	CAA	C1B-N9A-C4A	-4.68	118.42	126.64
2	C	1753	CAA	C1B-N9A-C4A	-4.60	118.55	126.64
2	C	1753	CAA	O6A-CCP-CBP	-4.28	103.67	110.55
2	C	1753	CAA	CDP-CBP-CAP	4.04	115.83	108.82
2	D	1754	CAA	O2B-C2B-C3B	3.80	121.95	111.17
2	B	1752	CAA	N3A-C2A-N1A	-3.75	122.82	128.68
2	A	1751	CAA	O1-C1-C2	-3.70	116.93	123.35
2	C	1753	CAA	N3A-C2A-N1A	-3.58	123.08	128.68
2	A	1751	CAA	O5P-C5P-C6P	-3.55	115.53	122.02
2	D	1754	CAA	O1-C1-S1P	-3.53	118.02	122.61
2	D	1754	CAA	O5P-C5P-C6P	-3.39	115.82	122.02
2	D	1754	CAA	O3B-C3B-C4B	-3.36	97.94	110.08
2	A	1751	CAA	N3A-C2A-N1A	-3.24	123.62	128.68
2	A	1751	CAA	O2B-C2B-C3B	3.16	120.14	111.17
2	D	1754	CAA	C6P-C5P-N4P	2.95	121.39	116.42
2	B	1752	CAA	O5P-C5P-C6P	-2.90	116.71	122.02
2	D	1754	CAA	N3A-C2A-N1A	-2.90	124.14	128.68
2	C	1753	CAA	CDP-CBP-CCP	-2.86	103.56	108.23
2	B	1752	CAA	O3B-C3B-C2B	-2.82	101.44	111.68
2	B	1752	CAA	O3B-C3B-C4B	-2.82	99.90	110.08
2	D	1754	CAA	N6A-C6A-N1A	2.81	124.41	118.57
2	B	1752	CAA	O6A-CCP-CBP	-2.79	106.06	110.55
2	A	1751	CAA	C6P-C5P-N4P	2.67	120.91	116.42
2	C	1753	CAA	O5P-C5P-C6P	-2.66	117.15	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1752	CAA	O2B-C2B-C1B	2.63	120.58	110.85
2	B	1752	CAA	C3B-C2B-C1B	2.61	105.68	99.89
2	D	1754	CAA	C3B-C2B-C1B	2.59	105.62	99.89
2	B	1752	CAA	CDP-CBP-CAP	2.57	113.28	108.82
2	C	1753	CAA	O3B-C3B-C2B	-2.49	102.67	111.68
2	D	1754	CAA	CEP-CBP-CCP	2.45	112.23	108.23
2	D	1754	CAA	O3B-C3B-C2B	-2.28	103.42	111.68
2	C	1753	CAA	O3B-C3B-C4B	-2.27	101.86	110.08
2	A	1751	CAA	N6A-C6A-N1A	2.26	123.27	118.57
2	A	1751	CAA	O4B-C1B-C2B	2.21	110.15	106.93
2	A	1751	CAA	CDP-CBP-CAP	2.19	112.62	108.82
2	C	1753	CAA	C3B-C2B-C1B	2.16	104.67	99.89
2	A	1751	CAA	O3B-C3B-C4B	-2.15	102.30	110.08
2	B	1752	CAA	C7P-N8P-C9P	2.15	126.42	122.59
2	C	1753	CAA	O2B-C2B-C3B	2.13	117.23	111.17
2	C	1753	CAA	C7P-N8P-C9P	2.11	126.35	122.59
2	C	1753	CAA	C2B-C3B-C4B	2.08	106.92	103.22
2	B	1752	CAA	C3P-N4P-C5P	2.02	126.58	122.84
2	C	1753	CAA	C2A-N1A-C6A	2.01	122.19	118.75

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1751	CAA	C3B-O3B-P3B-O8A
2	A	1751	CAA	C1-C2-C3-O3
2	A	1751	CAA	C1-C2-C3-C4
2	B	1752	CAA	C3B-O3B-P3B-O8A
2	C	1753	CAA	C3B-O3B-P3B-O8A
2	D	1754	CAA	C3B-O3B-P3B-O8A
2	D	1754	CAA	C5P-C6P-C7P-N8P
2	D	1754	CAA	C1-C2-C3-O3
2	D	1754	CAA	C1-C2-C3-C4
3	C	2307	GOL	O1-C1-C2-C3
3	C	2307	GOL	O1-C1-C2-O2
2	C	1753	CAA	C6P-C7P-N8P-C9P
2	A	1751	CAA	C6P-C7P-N8P-C9P
3	B	2308	GOL	O2-C2-C3-O3
2	D	1754	CAA	O1-C1-C2-C3
2	A	1751	CAA	P2A-O3A-P1A-O1A
2	A	1751	CAA	O1-C1-C2-C3
3	B	2308	GOL	C1-C2-C3-O3

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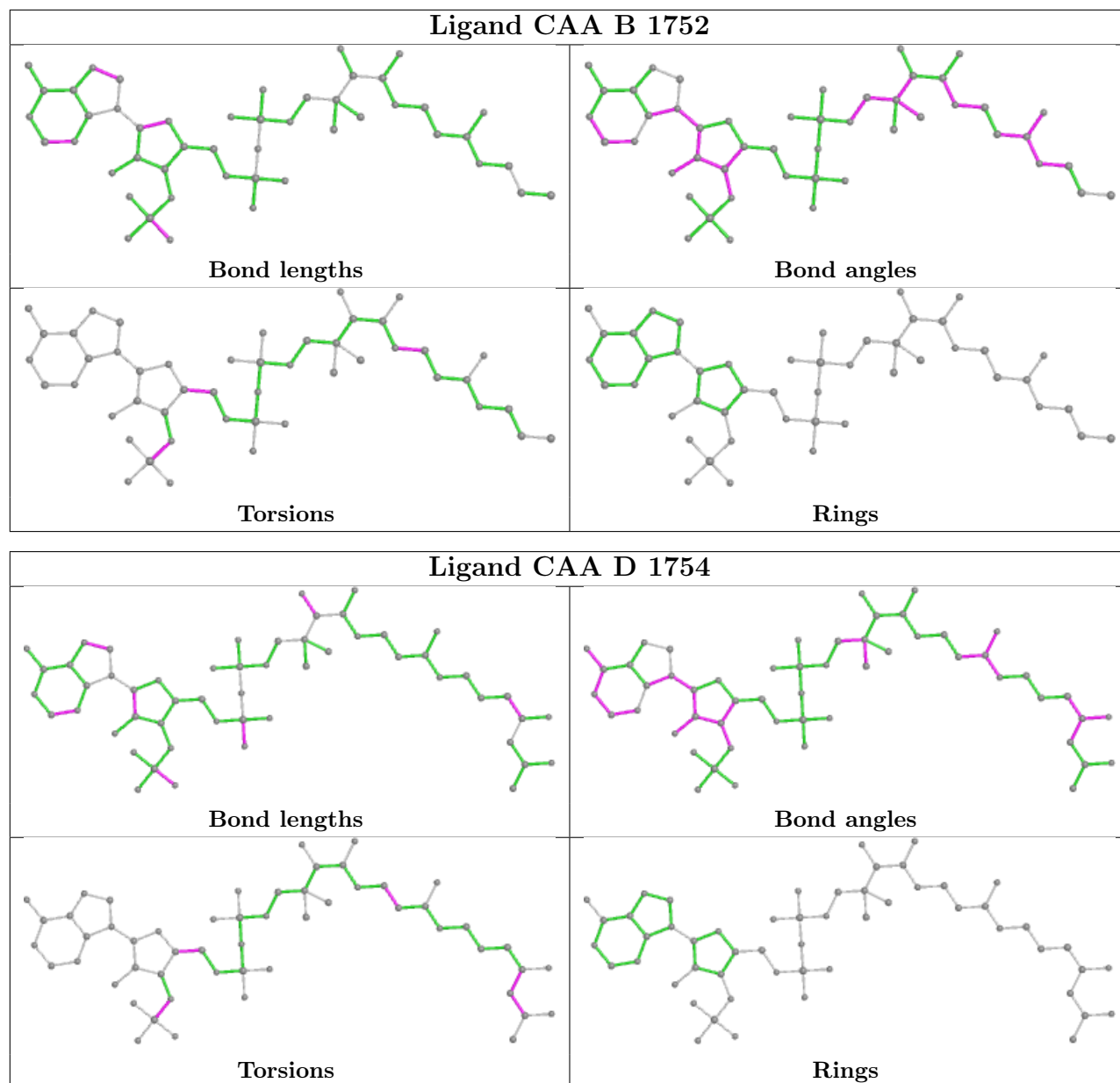
Mol	Chain	Res	Type	Atoms
2	A	1751	CAA	O4B-C4B-C5B-O5B
2	B	1752	CAA	O4B-C4B-C5B-O5B
2	C	1753	CAA	O4B-C4B-C5B-O5B
2	D	1754	CAA	O4B-C4B-C5B-O5B
2	C	1753	CAA	P2A-O3A-P1A-O1A
2	B	1752	CAA	C6P-C7P-N8P-C9P

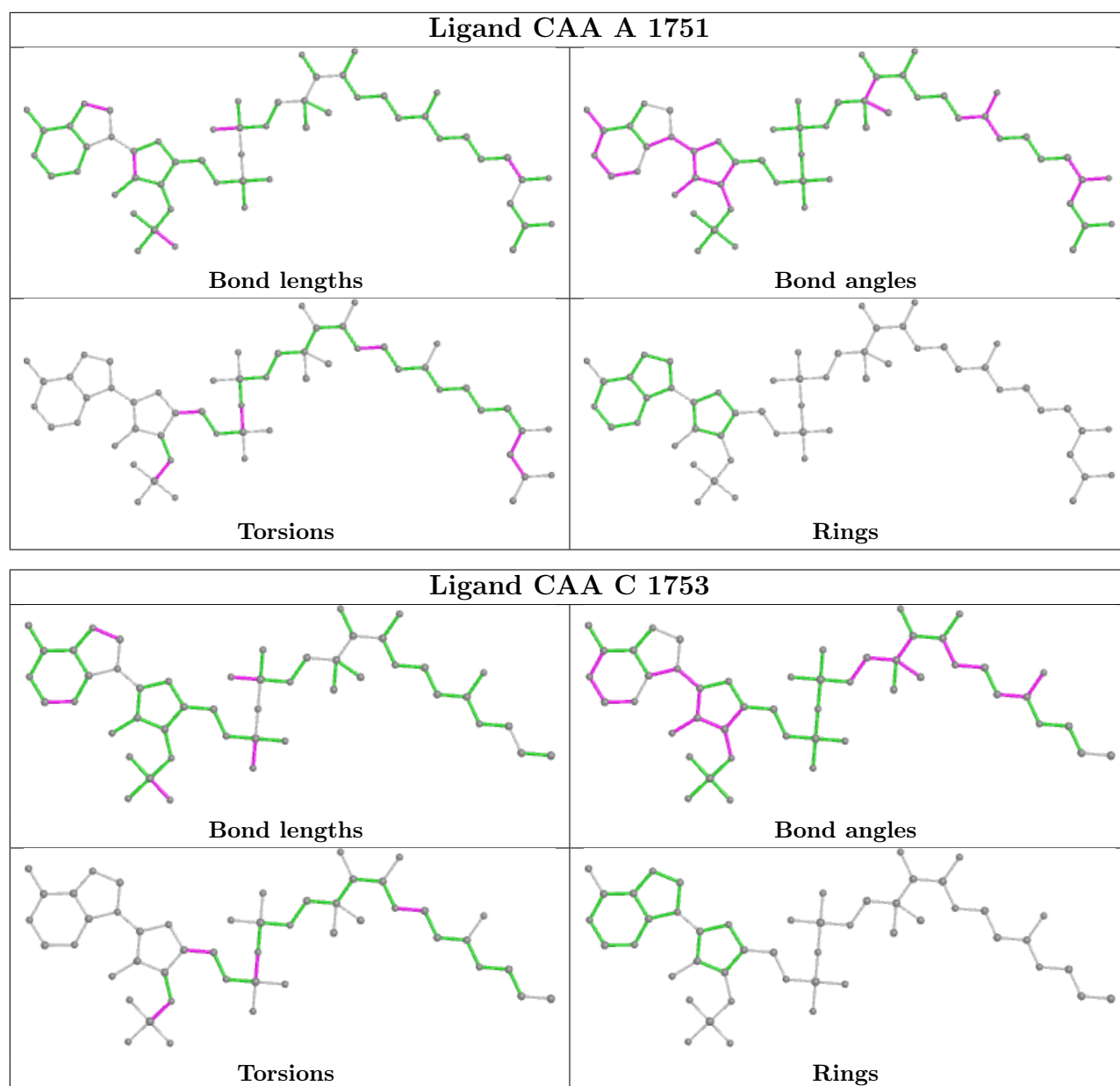
There are no ring outliers.

6 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1752	CAA	8	0
3	C	2307	GOL	4	0
3	B	2308	GOL	11	0
2	D	1754	CAA	3	0
2	A	1751	CAA	3	0
2	C	1753	CAA	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	354/360 (98%)	-0.16	6 (1%) 70 74	17, 25, 36, 46	0
1	B	354/360 (98%)	-0.11	6 (1%) 70 74	19, 26, 38, 47	0
1	C	354/360 (98%)	-0.14	11 (3%) 49 53	17, 23, 36, 49	0
1	D	354/360 (98%)	-0.20	8 (2%) 60 65	15, 24, 36, 44	0
All	All	1416/1440 (98%)	-0.15	31 (2%) 62 66	15, 24, 37, 49	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	ILE	4.7
1	C	45	ILE	4.0
1	A	323	ASN	3.5
1	B	322[A]	ALA	3.3
1	A	360	GLY	3.3
1	D	350	ASP	3.3
1	A	45	ILE	3.3
1	C	359	ASP	3.2
1	C	323[A]	ASN	3.1
1	B	350	ASP	3.1
1	B	323[A]	ASN	3.1
1	D	360	GLY	3.0
1	B	47	ARG	2.9
1	A	47	ARG	2.9
1	D	323[A]	ASN	2.9
1	C	47	ARG	2.9
1	C	347	ALA	2.8
1	A	350	ASP	2.7
1	B	359	ASP	2.6
1	C	38	ARG	2.6
1	D	45	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	347	ALA	2.3
1	D	2	ALA	2.3
1	C	350	ASP	2.3
1	D	359	ASP	2.3
1	D	47	ARG	2.2
1	C	65	GLN	2.2
1	C	324[A]	GLY	2.2
1	B	39	PRO	2.1
1	C	322[A]	ALA	2.1
1	A	2	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

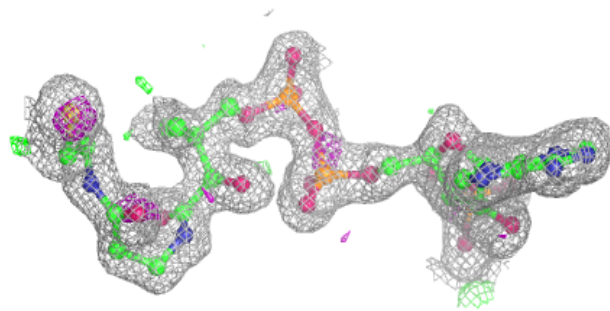
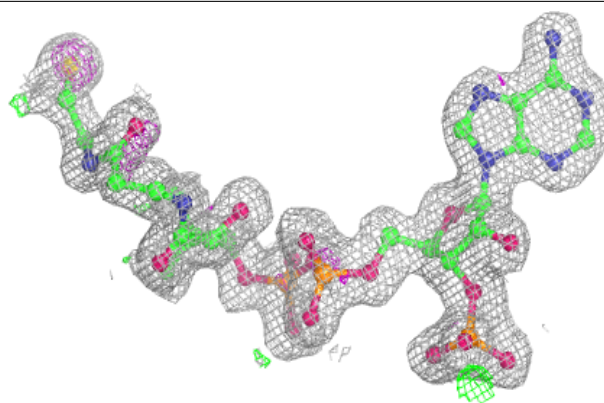
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	2308	6/6	0.79	0.15	40,43,45,46	0
3	GOL	C	2307	6/6	0.86	0.12	42,44,45,46	0
2	CAA	B	1752	48/54	0.96	0.08	20,28,36,37	0
2	CAA	D	1754	54/54	0.96	0.08	19,28,35,42	1
2	CAA	C	1753	48/54	0.97	0.07	16,26,34,37	0
2	CAA	A	1751	54/54	0.97	0.08	19,28,33,39	1

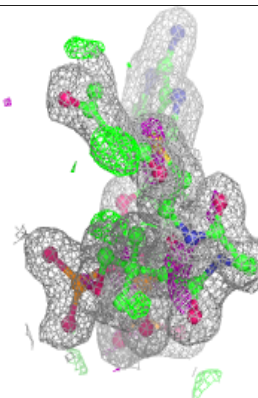
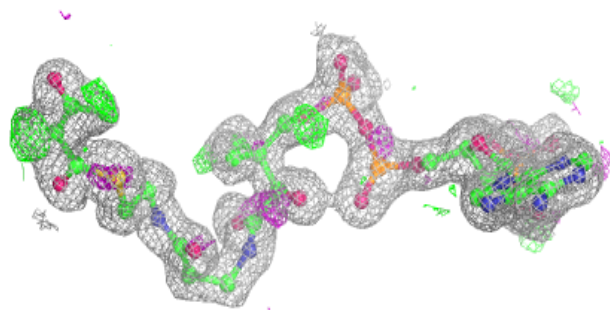
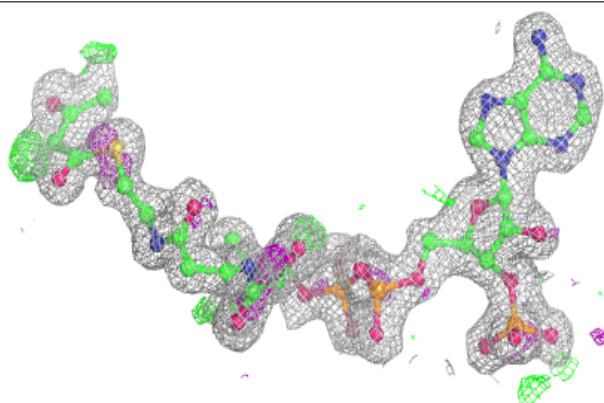
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAA B 1752:

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

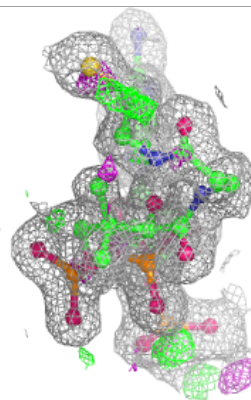
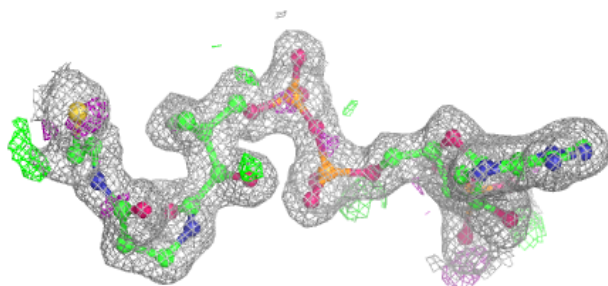
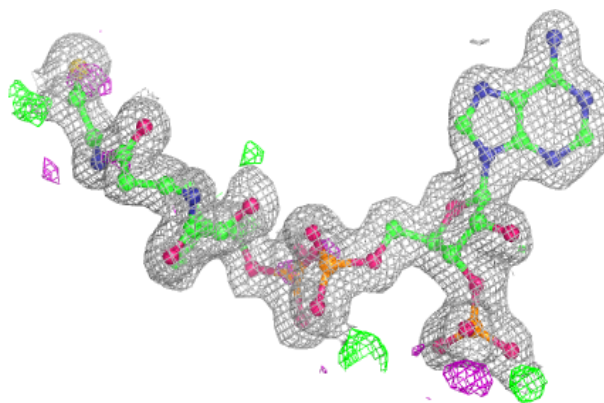
**Electron density around CAA D 1754:**

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

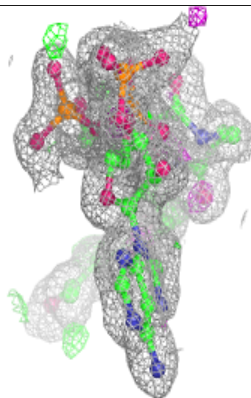
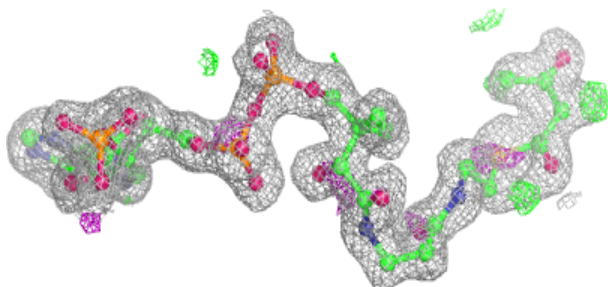
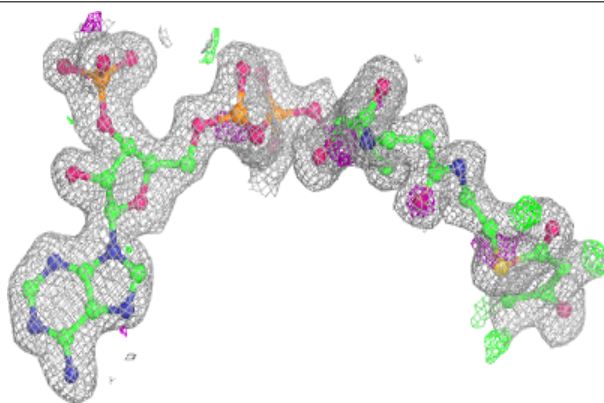


Electron density around CAA C 1753:

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

**Electron density around CAA A 1751:**

$2mF_o-DF_c$ (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.