



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:26 AM UTC

PDB ID : 2GCI / pdb_00002gci
Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA race-
mase is catalyzed by an asparte/histidine pair and involves a smooth,
methionine-rich surface for binding the fatty acyl moiety
Authors : Bhaumik, P.; Wierenga, R.K.
Deposited on : 2006-03-14
Resolution : 1.60 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

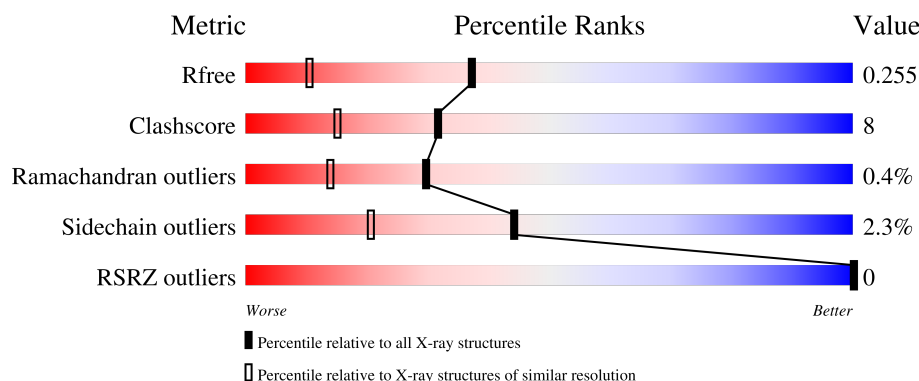
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	 86% 12% ..
1	B	360	 84% 13% ..
1	C	360	 85% 13% ..
1	D	360	 84% 12% ..

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	C	1302	-	-	X	-

2 Entry composition [i](#)

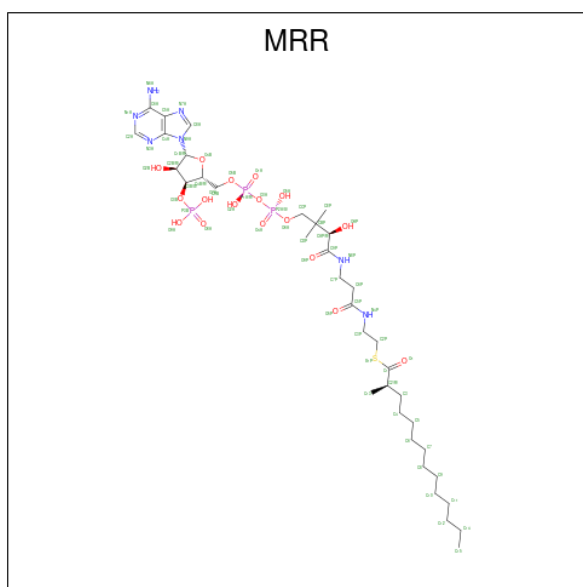
There are 4 unique types of molecules in this entry. The entry contains 12207 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			
1	B	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			
1	C	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			
1	D	354	Total	C	N	O	S	0	0	0
			2679	1683	481	500	15			

- Molecule 2 is (R)-2-METHYLMYRISTOYL-COENZYME A (CCD ID: MRR) (formula: $C_{36}H_{64}N_7O_{17}P_3S$).



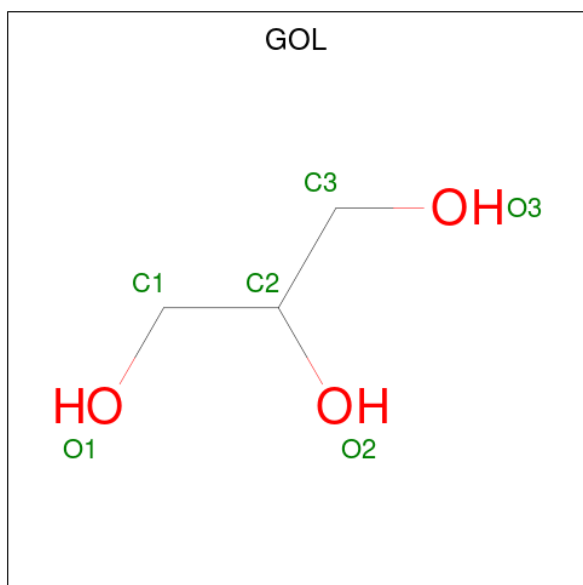
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P S	0	0
			55	27	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	1
			74	46	7	17	3 1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			54	26	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			64	36	7	17	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		

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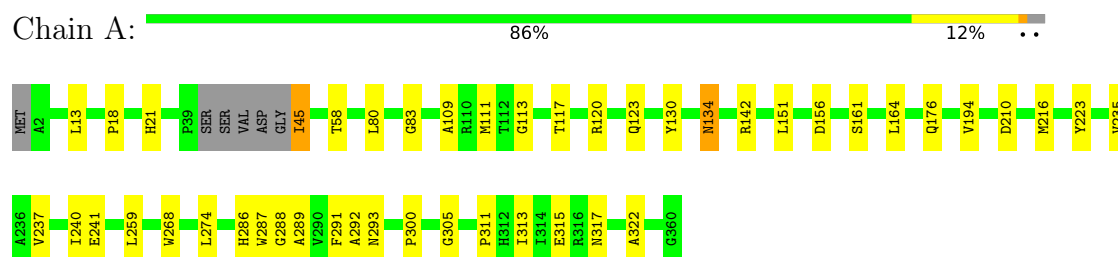
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	243	Total 243	O 243	0	0
4	C	349	Total 349	O 349	0	0
4	D	370	Total 370	O 370	0	0

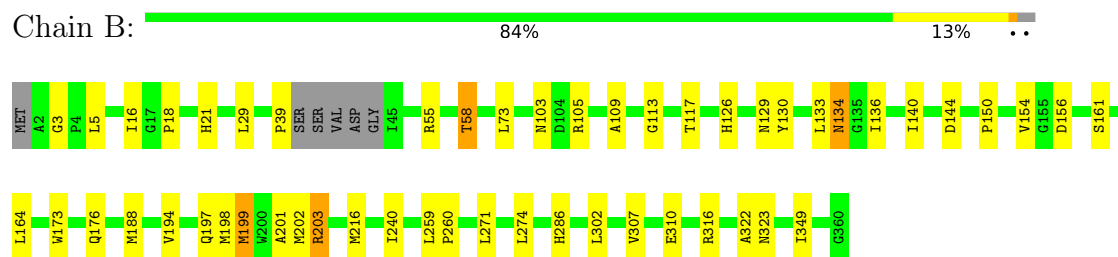
3 Residue-property plots

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.

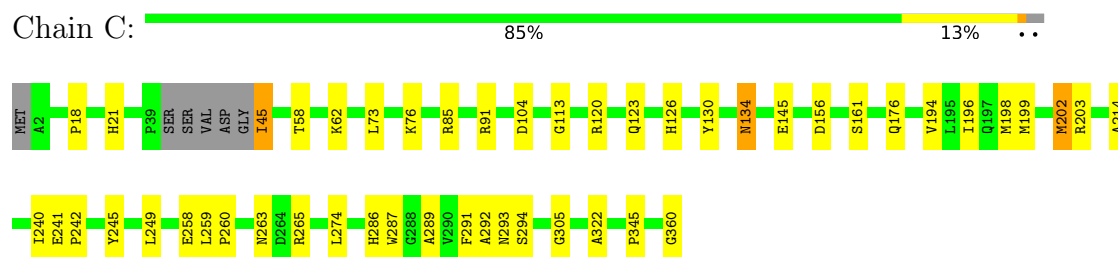
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



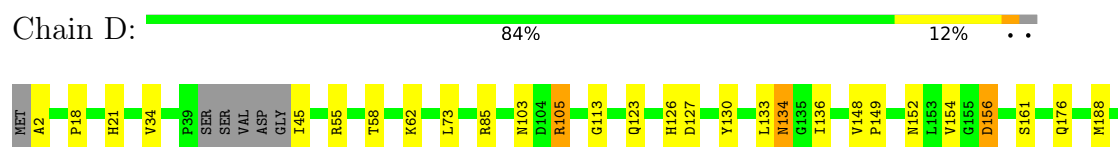
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



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



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.70Å 79.81Å 118.06Å 90.00° 89.93° 90.00°	Depositor
Resolution (Å)	19.83 – 1.60 19.83 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.83-1.60) 96.7 (19.83-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.58 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , 0.244 0.244 , 0.255	Depositor DCC
R_{free} test set	10825 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.458 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12207	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.75 % 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 7.8953e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MRR, 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	0.79	0/2740	0.97	3/3727 (0.1%)
1	B	0.80	0/2740	0.98	2/3727 (0.1%)
1	C	1.05	1/2740 (0.0%)	1.05	3/3727 (0.1%)
1	D	1.03	2/2740 (0.1%)	1.03	1/3727 (0.0%)
All	All	0.93	3/10960 (0.0%)	1.01	9/14908 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	202	MET	SD-CE	-6.77	1.62	1.79
1	D	105	ARG	CZ-NH1	5.61	1.40	1.32
1	D	156	ASP	C-O	5.37	1.30	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	287	TRP	N-CA-C	-7.05	103.67	111.36
1	C	289	ALA	N-CA-C	6.81	120.07	111.69
1	D	203	ARG	NE-CZ-NH1	6.68	128.18	121.50
1	C	260	PRO	CB-CA-C	-6.03	105.72	111.39
1	B	3	GLY	CA-C-N	5.55	125.07	119.19
1	B	3	GLY	C-N-CA	5.55	125.07	119.19
1	A	287	TRP	N-CA-C	-5.54	105.32	111.36
1	A	322	ALA	N-CA-C	-5.51	101.81	110.36
1	A	289	ALA	N-CA-C	5.49	118.44	111.69

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	2679	0	2623	40	0
1	B	2679	0	2623	40	0
1	C	2679	0	2623	49	1
1	D	2679	0	2623	56	0
2	A	55	0	39	0	0
2	B	74	0	46	7	0
2	C	54	0	39	3	0
2	D	64	0	60	14	0
3	A	6	0	8	2	0
3	B	12	0	16	1	1
3	C	12	0	16	7	0
3	D	6	0	8	1	1
4	A	246	0	0	21	1
4	B	243	0	0	6	0
4	C	349	0	0	11	1
4	D	370	0	0	16	1
All	All	12207	0	10724	176	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (176) 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:A:237:VAL:HG12	4:A:1988:HOH:O	1.31	1.29
1:A:300:PRO:HA	4:A:1986:HOH:O	1.13	1.25
1:C:242:PRO:HD3	2:D:1754:MRR:H151	1.32	1.10
1:C:202:MET:HE2	4:C:2002:HOH:O	1.54	1.08
1:D:283:ASP:HB2	4:D:2112:HOH:O	1.54	1.07
1:D:285:ASP:OD1	4:D:2051:HOH:O	1.76	1.00
1:D:156:ASP:OD2	2:D:1754:MRR:H2	1.63	0.98
3:C:1302:GOL:O2	2:D:1754:MRR:H153	1.70	0.91
1:D:198:MET:HG2	1:D:202:MET:HE2	1.51	0.91
1:C:242:PRO:CD	2:D:1754:MRR:H151	2.02	0.90
4:A:1946:HOH:O	2:B:1752[B]:MRR:H142	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLN:NE2	4:B:1988:HOH:O	2.09	0.83
3:C:1301:GOL:H11	1:D:202:MET:HG2	1.62	0.80
1:C:199:MET:SD	4:C:2002:HOH:O	2.39	0.80
2:C:1753:MRR:N3A	2:C:1753:MRR:C5A	2.45	0.78
1:C:176:GLN:HE21	1:D:176:GLN:HE21	1.34	0.76
1:A:288:GLY:HA2	4:A:1984:HOH:O	1.84	0.76
1:B:129:ASN:OD1	4:B:1983:HOH:O	2.03	0.75
1:C:241:GLU:HG3	2:D:1754:MRR:H142	1.68	0.75
3:C:1301:GOL:H11	1:D:202:MET:CG	2.18	0.74
1:C:305:GLY:HA2	1:D:203:ARG:HH22	1.54	0.73
1:A:305:GLY:HA2	1:B:203:ARG:HH22	1.54	0.73
1:A:240:ILE:O	3:A:1306:GOL:H31	1.90	0.72
1:A:291:PHE:O	1:A:293:ASN:N	2.22	0.72
1:C:291:PHE:O	1:C:293:ASN:N	2.22	0.72
1:A:142:ARG:NH2	4:A:1985:HOH:O	2.12	0.71
1:C:203:ARG:NH2	4:C:1860:HOH:O	2.20	0.70
2:B:1752[A]:MRR:H72	2:B:1752[A]:MRR:H141	1.74	0.69
1:A:311:PRO:O	1:A:315:GLU:HG2	1.92	0.69
1:B:198:MET:HG2	1:B:202:MET:HE2	1.72	0.69
1:A:216:MET:HE1	2:B:1752[B]:MRR:H152	1.74	0.69
1:D:259:LEU:HD22	1:D:274:LEU:HD13	1.74	0.68
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.74	0.68
1:C:21:HIS:HD2	1:C:161:SER:OG	1.77	0.68
1:B:16:ILE:HG21	2:B:1752[A]:MRR:H82	1.75	0.67
1:B:140:ILE:HD13	1:B:150:PRO:HG3	1.77	0.67
1:C:45:ILE:HG23	4:C:1973:HOH:O	1.95	0.66
1:C:76:LYS:HE3	1:C:360:GLY:HA2	1.78	0.66
1:A:120:ARG:HH11	1:A:123:GLN:HE22	1.42	0.65
1:A:223:TYR:O	4:A:1988:HOH:O	2.14	0.65
4:A:1993:HOH:O	1:B:302:LEU:HD12	1.95	0.65
1:D:85:ARG:HD2	4:D:1909:HOH:O	1.96	0.65
1:D:126:HIS:HB3	2:D:1754:MRR:H133	1.79	0.65
1:D:358:TRP:O	1:D:359:ASP:HB2	1.95	0.65
1:D:127:ASP:H	2:D:1754:MRR:H132	1.62	0.64
1:B:113:GLY:HA2	1:B:188:MET:HB2	1.79	0.64
1:C:120:ARG:HH11	1:C:123:GLN:HE22	1.46	0.64
1:C:258:GLU:HG3	4:C:1960:HOH:O	1.97	0.63
1:A:21:HIS:HD2	1:A:161:SER:OG	1.81	0.62
1:D:188:MET:SD	4:D:2019:HOH:O	2.56	0.60
1:D:288:GLY:HA2	4:D:2027:HOH:O	2.02	0.59
1:C:126:HIS:HB3	2:C:1753:MRR:H133	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:ILE:HD11	4:C:1859:HOH:O	2.03	0.59
1:A:235:VAL:HG12	4:A:1986:HOH:O	2.03	0.59
1:A:240:ILE:O	3:A:1306:GOL:C3	2.51	0.58
1:B:173:TRP:HA	1:B:176:GLN:HE21	1.68	0.58
1:D:258:GLU:HG3	4:D:2029:HOH:O	2.03	0.58
1:D:62:LYS:HE2	4:D:2017:HOH:O	2.03	0.58
1:D:21:HIS:HD2	1:D:161:SER:OG	1.88	0.57
1:D:320:TYR:OH	4:D:2116:HOH:O	2.09	0.57
1:A:120:ARG:NH1	1:A:123:GLN:HE22	2.02	0.57
1:B:136:ILE:HG21	1:B:154:VAL:HG11	1.87	0.56
1:B:201:ALA:HB2	4:B:1988:HOH:O	2.06	0.56
1:C:214:ALA:O	1:C:265:ARG:NH2	2.39	0.55
1:B:21:HIS:HD2	1:B:161:SER:OG	1.89	0.55
1:D:286:HIS:HE1	4:D:1815:HOH:O	1.89	0.55
1:D:320:TYR:CE1	1:D:322:ALA:HB2	2.42	0.55
1:D:286:HIS:HD2	4:D:1950:HOH:O	1.90	0.54
1:A:286:HIS:HE1	4:A:1888:HOH:O	1.91	0.54
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.43	0.54
1:A:286:HIS:HD2	4:C:1816:HOH:O	1.90	0.53
1:C:198:MET:HG2	4:C:2002:HOH:O	2.08	0.53
1:B:286:HIS:HE1	4:B:1771:HOH:O	1.92	0.53
1:B:260:PRO:HG2	1:B:271:LEU:HB2	1.90	0.53
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.90	0.53
1:B:134:ASN:HD22	1:B:134:ASN:C	2.17	0.53
1:C:241:GLU:HA	2:D:1754:MRR:H142	1.90	0.52
1:A:109:ALA:HB1	1:A:164:LEU:HD11	1.91	0.52
1:B:199:MET:HE3	1:B:202:MET:HE1	1.91	0.52
1:D:345:PRO:HD3	4:D:2119:HOH:O	2.08	0.52
1:A:313:ILE:HG22	4:A:1830:HOH:O	2.08	0.52
1:B:109:ALA:HB1	1:B:164:LEU:HD11	1.92	0.52
1:D:127:ASP:HA	4:D:2019:HOH:O	2.09	0.52
1:A:21:HIS:HE1	1:B:194:VAL:O	1.94	0.51
1:D:156:ASP:OD2	2:D:1754:MRR:C2	2.50	0.51
1:A:176:GLN:NE2	4:A:1930:HOH:O	2.43	0.50
1:D:134:ASN:C	1:D:134:ASN:HD22	2.19	0.50
1:D:263:ASN:OD1	3:D:1303:GOL:H32	2.11	0.50
1:C:305:GLY:HA2	1:D:203:ARG:NH2	2.25	0.50
3:C:1302:GOL:O2	2:D:1754:MRR:C15	2.50	0.50
1:A:241:GLU:OE2	2:B:1752[A]:MRR:H92	2.11	0.50
1:C:45:ILE:HD11	1:C:345:PRO:O	2.12	0.50
1:D:55:ARG:HD2	1:D:349:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PRO:CD	2:D:1754:MRR:C15	2.84	0.49
1:D:2:ALA:HA	4:D:2052:HOH:O	2.11	0.49
1:C:241:GLU:HA	2:D:1754:MRR:C14	2.42	0.49
1:C:286:HIS:HE1	4:C:1982:HOH:O	1.94	0.49
1:D:198:MET:HE1	1:D:217:LEU:CD1	2.43	0.49
1:A:235:VAL:HA	4:A:1986:HOH:O	2.12	0.49
1:D:18:PRO:HB3	1:D:156:ASP:O	2.12	0.49
1:B:5:LEU:HD12	1:B:29:LEU:HB2	1.95	0.49
1:C:263:ASN:HD21	3:C:1302:GOL:C3	2.26	0.49
1:B:126:HIS:HB2	4:B:1983:HOH:O	2.13	0.48
1:A:194:VAL:O	1:B:21:HIS:HE1	1.95	0.48
1:C:240:ILE:O	3:C:1302:GOL:H31	2.13	0.48
1:C:176:GLN:HG2	1:D:176:GLN:NE2	2.28	0.48
4:A:1774:HOH:O	1:C:286:HIS:HD2	1.95	0.48
1:C:134:ASN:HD22	1:C:134:ASN:C	2.21	0.48
1:A:120:ARG:HH11	1:A:123:GLN:NE2	2.10	0.48
1:A:216:MET:CE	2:B:1752[B]:MRR:H152	2.41	0.48
1:A:13:LEU:HG	1:A:80:LEU:HD11	1.97	0.47
1:C:156:ASP:OD2	2:C:1753:MRR:H2	2.14	0.47
1:D:127:ASP:H	2:D:1754:MRR:C13	2.27	0.47
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.50	0.46
1:C:291:PHE:C	1:C:293:ASN:N	2.73	0.46
1:D:322:ALA:O	1:D:323:ASN:C	2.57	0.46
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.50	0.46
1:B:259:LEU:HD22	1:B:274:LEU:HD13	1.97	0.46
1:C:194:VAL:O	1:D:21:HIS:HE1	1.99	0.46
1:B:240:ILE:O	3:B:1304:GOL:H2	2.16	0.46
1:C:62:LYS:NZ	4:C:2071:HOH:O	2.46	0.45
1:C:198:MET:HE1	1:D:152:ASN:ND2	2.32	0.45
1:B:18:PRO:HB3	1:B:156:ASP:O	2.17	0.45
1:C:21:HIS:HE1	1:D:194:VAL:O	1.99	0.45
1:D:85:ARG:HG2	4:D:2011:HOH:O	2.17	0.45
1:D:103:ASN:ND2	1:D:105:ARG:H	2.14	0.45
1:B:322:ALA:O	1:B:323:ASN:C	2.60	0.44
1:B:103:ASN:ND2	1:B:105:ARG:H	2.16	0.44
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.52	0.44
1:B:286:HIS:HD2	4:B:1869:HOH:O	2.00	0.44
1:D:130:TYR:HD2	4:D:2019:HOH:O	2.00	0.44
1:A:18:PRO:HB3	1:A:156:ASP:O	2.17	0.44
1:D:136:ILE:HG21	1:D:154:VAL:HG11	2.00	0.44
1:A:134:ASN:C	1:A:134:ASN:HD22	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TRP:HD1	4:A:1769:HOH:O	2.01	0.44
1:B:103:ASN:HD22	1:B:105:ARG:H	1.66	0.44
1:D:148:VAL:HG22	1:D:149:PRO:HD2	2.00	0.43
1:C:91:ARG:NH2	4:C:2089:HOH:O	2.14	0.43
1:D:34:VAL:HG11	1:D:73:LEU:HD21	2.00	0.43
1:C:241:GLU:HG3	2:D:1754:MRR:H102	2.00	0.43
4:A:1993:HOH:O	1:B:302:LEU:CD1	2.61	0.43
1:C:198:MET:HE1	1:D:152:ASN:HD21	1.83	0.43
1:D:198:MET:HE3	1:D:202:MET:CE	2.49	0.43
1:A:291:PHE:C	1:A:293:ASN:N	2.77	0.42
1:A:291:PHE:C	4:A:1797:HOH:O	2.61	0.42
1:C:18:PRO:HB3	1:C:156:ASP:O	2.19	0.42
1:C:245:TYR:CE2	1:C:249:LEU:HD11	2.53	0.42
1:D:103:ASN:C	1:D:103:ASN:HD22	2.27	0.42
1:A:45:ILE:N	4:A:1994:HOH:O	2.52	0.42
1:D:198:MET:HE3	1:D:202:MET:HE1	2.01	0.42
4:A:1993:HOH:O	1:B:307:VAL:HA	2.20	0.42
3:C:1301:GOL:H11	1:D:202:MET:HG3	2.00	0.42
1:A:210:ASP:OD2	4:A:1982:HOH:O	2.22	0.42
1:D:199:MET:HE3	1:D:202:MET:HE1	2.02	0.42
1:A:305:GLY:HA2	1:B:203:ARG:NH2	2.30	0.42
1:D:103:ASN:HD22	1:D:105:ARG:H	1.67	0.42
1:C:196:ILE:HG12	1:C:199:MET:HB2	2.01	0.41
1:A:317:ASN:HA	4:A:1858:HOH:O	2.19	0.41
1:C:294:SER:O	1:D:123:GLN:HG3	2.21	0.41
4:A:1993:HOH:O	1:B:310:GLU:HB2	2.21	0.41
1:B:39:PRO:HA	1:B:58:THR:HG21	2.03	0.41
1:C:104:ASP:OD1	1:C:104:ASP:C	2.62	0.41
1:D:148:VAL:CG2	1:D:149:PRO:HD2	2.51	0.41
1:C:76:LYS:HE3	1:C:360:GLY:CA	2.47	0.41
1:C:120:ARG:NH1	1:C:123:GLN:HE22	2.16	0.41
1:B:216:MET:HE3	1:B:216:MET:HB2	1.92	0.41
1:D:203:ARG:NH2	4:D:1969:HOH:O	2.53	0.41
1:A:117:THR:O	1:B:316:ARG:HD2	2.21	0.41
1:B:55:ARG:HD2	1:B:349:ILE:HD11	2.02	0.41
1:C:305:GLY:CA	1:D:203:ARG:HH22	2.29	0.40
1:C:291:PHE:C	1:C:293:ASN:H	2.28	0.40
1:A:83:GLY:HA2	1:A:111:MET:O	2.20	0.40

All (3) 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)
3:D:1303:GOL:C3	4:C:1853:HOH:O[4_543]	1.94	0.26
1:C:265:ARG:NH2	4:D:1881:HOH:O[4_553]	2.11	0.09
3:B:1304:GOL:C3	4:A:1810:HOH:O[4_554]	2.15	0.05

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	350/360 (97%)	338 (97%)	10 (3%)	2 (1%)	21	7
1	B	350/360 (97%)	337 (96%)	13 (4%)	0	100	100
1	C	350/360 (97%)	336 (96%)	12 (3%)	2 (1%)	21	7
1	D	350/360 (97%)	337 (96%)	12 (3%)	1 (0%)	36	20
All	All	1400/1440 (97%)	1348 (96%)	47 (3%)	5 (0%)	30	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ALA
1	C	292	ALA
1	D	323	ASN
1	C	322	ALA
1	A	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	270/275 (98%)	267 (99%)	3 (1%)	65	46
1	B	270/275 (98%)	262 (97%)	8 (3%)	36	13
1	C	270/275 (98%)	264 (98%)	6 (2%)	45	22
1	D	270/275 (98%)	262 (97%)	8 (3%)	36	13
All	All	1080/1100 (98%)	1055 (98%)	25 (2%)	44	20

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	58	THR
1	A	134	ASN
1	B	58	THR
1	B	73	LEU
1	B	117	THR
1	B	133	LEU
1	B	134	ASN
1	B	144	ASP
1	B	199	MET
1	B	203	ARG
1	C	45	ILE
1	C	58	THR
1	C	73	LEU
1	C	85	ARG
1	C	134	ASN
1	C	145	GLU
1	D	45	ILE
1	D	58	THR
1	D	133	LEU
1	D	134	ASN
1	D	199	MET
1	D	203	ARG
1	D	294	SER
1	D	359	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	103	ASN

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Mol	Chain	Res	Type
1	A	123	GLN
1	A	134	ASN
1	A	286	HIS
1	A	293	ASN
1	A	327	GLN
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	176	GLN
1	B	286	HIS
1	C	21	HIS
1	C	103	ASN
1	C	123	GLN
1	C	134	ASN
1	C	263	ASN
1	C	286	HIS
1	C	327	GLN
1	D	21	HIS
1	D	103	ASN
1	D	134	ASN
1	D	176	GLN
1	D	286	HIS
1	D	309	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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
3	GOL	C	1301	-	5,5,5	0.34	0	5,5,5	0.51	0
3	GOL	C	1302	-	5,5,5	0.42	0	5,5,5	0.44	0
2	MRR	A	1751	-	54,57,66	1.12	5 (9%)	75,84,93	1.63	12 (16%)
3	GOL	B	1304	-	5,5,5	0.40	0	5,5,5	0.31	0
2	MRR	D	1754	-	63,66,66	1.17	6 (9%)	85,93,93	1.55	12 (14%)
3	GOL	D	1303	-	5,5,5	0.51	0	5,5,5	0.48	0
2	MRR	B	1752[A]	-	63,66,66	1.03	5 (7%)	85,93,93	1.58	14 (16%)
3	GOL	B	1305	-	5,5,5	0.29	0	5,5,5	0.50	0
2	MRR	C	1753	-	47,54,66	1.67	5 (10%)	61,76,93	1.74	9 (14%)
3	GOL	A	1306	-	5,5,5	0.36	0	5,5,5	0.59	0
2	MRR	B	1752[B]	-	63,66,66	1.02	5 (7%)	85,93,93	1.59	14 (16%)

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	GOL	C	1301	-	-	3/4/4/4	-
3	GOL	C	1302	-	-	2/4/4/4	-
2	MRR	A	1751	-	-	5/57/74/83	0/3/3/3
3	GOL	B	1304	-	-	2/4/4/4	-
2	MRR	D	1754	-	-	12/66/83/83	0/3/3/3
3	GOL	D	1303	-	-	2/4/4/4	-
2	MRR	B	1752[A]	-	-	15/66/83/83	0/3/3/3
3	GOL	B	1305	-	-	1/4/4/4	-
2	MRR	C	1753	-	-	3/54/72/83	0/1/1/3
3	GOL	A	1306	-	-	2/4/4/4	-
2	MRR	B	1752[B]	-	-	12/66/83/83	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1753	MRR	C5A-N7A	-6.39	1.36	1.46
2	C	1753	MRR	P1A-O3A	4.86	1.64	1.59
2	C	1753	MRR	C1B-N9A	3.94	1.48	1.43
2	D	1754	MRR	P2A-O3A	3.92	1.63	1.59
2	C	1753	MRR	C6A-N1A	3.78	1.36	1.31
2	D	1754	MRR	P1A-O3A	3.73	1.63	1.59
2	A	1751	MRR	P1A-O3A	3.72	1.63	1.59
2	C	1753	MRR	P2A-O3A	3.61	1.63	1.59
2	A	1751	MRR	C5A-C6A	3.24	1.50	1.41
2	B	1752[A]	MRR	C5A-C6A	3.20	1.49	1.41
2	B	1752[B]	MRR	C5A-C6A	3.20	1.49	1.41
2	A	1751	MRR	P2A-O3A	3.10	1.62	1.59
2	B	1752[A]	MRR	P2A-O3A	3.10	1.62	1.59
2	B	1752[B]	MRR	P2A-O3A	3.10	1.62	1.59
2	D	1754	MRR	C5A-C6A	3.08	1.49	1.41
2	B	1752[A]	MRR	P1A-O3A	2.95	1.62	1.59
2	B	1752[B]	MRR	P1A-O3A	2.95	1.62	1.59
2	D	1754	MRR	C1-S1P	-2.37	1.67	1.75
2	D	1754	MRR	C8A-N7A	2.36	1.36	1.31
2	D	1754	MRR	O1-C1	2.27	1.24	1.20
2	A	1751	MRR	C8A-N7A	2.22	1.36	1.31
2	B	1752[A]	MRR	C8A-N7A	2.22	1.35	1.31
2	B	1752[B]	MRR	C8A-N7A	2.22	1.35	1.31
2	B	1752[A]	MRR	C1-S1P	-2.11	1.68	1.75
2	B	1752[B]	MRR	C1-S1P	-2.11	1.68	1.75
2	A	1751	MRR	C1-S1P	-2.04	1.68	1.75

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1753	MRR	N9A-C8A-N7A	-8.02	110.22	122.27
2	A	1751	MRR	C5A-C4A-N3A	-5.52	119.12	126.72
2	D	1754	MRR	C5A-C4A-N3A	-5.43	119.24	126.72
2	B	1752[A]	MRR	C5A-C4A-N3A	-5.39	119.30	126.72
2	B	1752[B]	MRR	C5A-C4A-N3A	-5.39	119.30	126.72
2	C	1753	MRR	O1-C1-S1P	-4.73	117.44	123.80
2	D	1754	MRR	O1-C1-S1P	-4.62	117.59	123.80
2	A	1751	MRR	N1A-C2A-N3A	-4.30	122.07	128.58
2	C	1753	MRR	C5A-N7A-C8A	-4.25	108.87	117.20
2	A	1751	MRR	C2A-N3A-C4A	4.22	122.15	111.83
2	B	1752[A]	MRR	O1-C1-S1P	-4.21	118.13	123.80
2	B	1752[B]	MRR	O1-C1-S1P	-4.21	118.13	123.80
2	A	1751	MRR	O1-C1-S1P	-4.17	118.19	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1752[A]	MRR	N1A-C2A-N3A	-4.09	122.38	128.58
2	B	1752[B]	MRR	N1A-C2A-N3A	-4.09	122.38	128.58
2	C	1753	MRR	C7P-N8P-C9P	4.09	129.89	122.55
2	A	1751	MRR	C7P-N8P-C9P	4.06	129.84	122.55
2	B	1752[A]	MRR	C2A-N3A-C4A	4.04	121.70	111.83
2	B	1752[B]	MRR	C2A-N3A-C4A	4.04	121.70	111.83
2	D	1754	MRR	N1A-C2A-N3A	-4.04	122.47	128.58
2	D	1754	MRR	C2A-N3A-C4A	3.99	121.58	111.83
2	B	1752[A]	MRR	C7P-N8P-C9P	3.71	129.22	122.55
2	B	1752[B]	MRR	C7P-N8P-C9P	3.71	129.22	122.55
2	D	1754	MRR	C7P-N8P-C9P	3.60	129.01	122.55
2	B	1752[A]	MRR	N9A-C8A-N7A	-3.56	108.89	113.94
2	B	1752[B]	MRR	N9A-C8A-N7A	-3.56	108.89	113.94
2	A	1751	MRR	N3A-C4A-N9A	3.46	133.05	127.17
2	D	1754	MRR	N3A-C4A-N9A	3.45	133.03	127.17
2	B	1752[A]	MRR	N3A-C4A-N9A	3.44	133.01	127.17
2	B	1752[B]	MRR	N3A-C4A-N9A	3.44	133.01	127.17
2	B	1752[A]	MRR	C3P-N4P-C5P	3.31	128.99	122.82
2	B	1752[B]	MRR	C3P-N4P-C5P	3.31	128.99	122.82
2	A	1751	MRR	N9A-C8A-N7A	-3.30	109.25	113.94
2	A	1751	MRR	C3P-N4P-C5P	3.19	128.75	122.82
2	B	1752[A]	MRR	C4A-C5A-N7A	-2.92	107.24	110.58
2	B	1752[B]	MRR	C4A-C5A-N7A	-2.92	107.24	110.58
2	D	1754	MRR	N9A-C8A-N7A	-2.91	109.80	113.94
2	C	1753	MRR	C2B-C1B-N9A	2.89	115.88	112.11
2	C	1753	MRR	C5A-C6A-N6A	2.81	121.22	117.40
2	A	1751	MRR	C4A-C5A-N7A	-2.80	107.38	110.58
2	B	1752[A]	MRR	C2P-S1P-C1	2.78	109.70	101.73
2	B	1752[B]	MRR	C2P-S1P-C1	2.78	109.70	101.73
2	B	1752[A]	MRR	C5A-N7A-C8A	2.71	107.71	103.45
2	B	1752[B]	MRR	C5A-N7A-C8A	2.71	107.71	103.45
2	B	1752[A]	MRR	C4A-N9A-C8A	2.60	108.47	105.74
2	B	1752[B]	MRR	C4A-N9A-C8A	2.60	108.47	105.74
2	A	1751	MRR	C5A-N7A-C8A	2.55	107.46	103.45
2	D	1754	MRR	C3P-N4P-C5P	2.50	127.48	122.82
2	A	1751	MRR	C2P-S1P-C1	2.40	108.60	101.73
2	D	1754	MRR	C4A-C5A-N7A	-2.37	107.88	110.58
2	D	1754	MRR	O5P-C5P-C6P	-2.35	117.77	122.02
2	C	1753	MRR	C3P-N4P-C5P	2.33	127.17	122.82
2	B	1752[A]	MRR	C6P-C7P-N8P	-2.29	107.12	112.00
2	B	1752[B]	MRR	C6P-C7P-N8P	-2.29	107.12	112.00
2	B	1752[A]	MRR	C2P-C3P-N4P	-2.28	107.65	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1752[B]	MRR	C2P-C3P-N4P	-2.28	107.65	112.41
2	C	1753	MRR	CDP-CBP-CAP	2.22	112.56	108.77
2	A	1751	MRR	C4A-N9A-C8A	2.22	108.07	105.74
2	D	1754	MRR	C5A-N7A-C8A	2.13	106.79	103.45
2	C	1753	MRR	O2A-P1A-O1A	2.03	121.89	112.44
2	D	1754	MRR	O2A-P1A-O1A	2.03	121.88	112.44

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1751	MRR	S1P-C1-C2-C13
2	A	1751	MRR	C1-C2-C3-C4
2	A	1751	MRR	C13-C2-C3-C4
2	B	1752[A]	MRR	S1P-C1-C2-C13
2	B	1752[A]	MRR	C1-C2-C3-C4
2	B	1752[A]	MRR	C13-C2-C3-C4
2	B	1752[B]	MRR	S1P-C1-C2-C13
2	B	1752[B]	MRR	C1-C2-C3-C4
2	B	1752[B]	MRR	C13-C2-C3-C4
2	D	1754	MRR	C2P-C3P-N4P-C5P
2	D	1754	MRR	C3-C4-C5-C6
2	B	1752[A]	MRR	C3-C4-C5-C6
3	C	1302	GOL	O1-C1-C2-O2
2	A	1751	MRR	C2-C3-C4-C5
3	A	1306	GOL	C1-C2-C3-O3
3	B	1304	GOL	O1-C1-C2-C3
3	C	1301	GOL	O1-C1-C2-C3
3	C	1302	GOL	O1-C1-C2-C3
3	D	1303	GOL	O1-C1-C2-C3
2	D	1754	MRR	C11-C10-C9-C8
2	D	1754	MRR	C7-C8-C9-C10
3	D	1303	GOL	O1-C1-C2-O2
2	B	1752[A]	MRR	C10-C11-C12-C14
2	B	1752[B]	MRR	C2-C3-C4-C5
2	B	1752[A]	MRR	C5-C6-C7-C8
2	B	1752[B]	MRR	C11-C10-C9-C8
2	B	1752[A]	MRR	C6-C7-C8-C9
2	D	1754	MRR	C4-C5-C6-C7
2	D	1754	MRR	C5-C6-C7-C8
2	B	1752[A]	MRR	C4-C5-C6-C7
2	B	1752[A]	MRR	C2-C3-C4-C5

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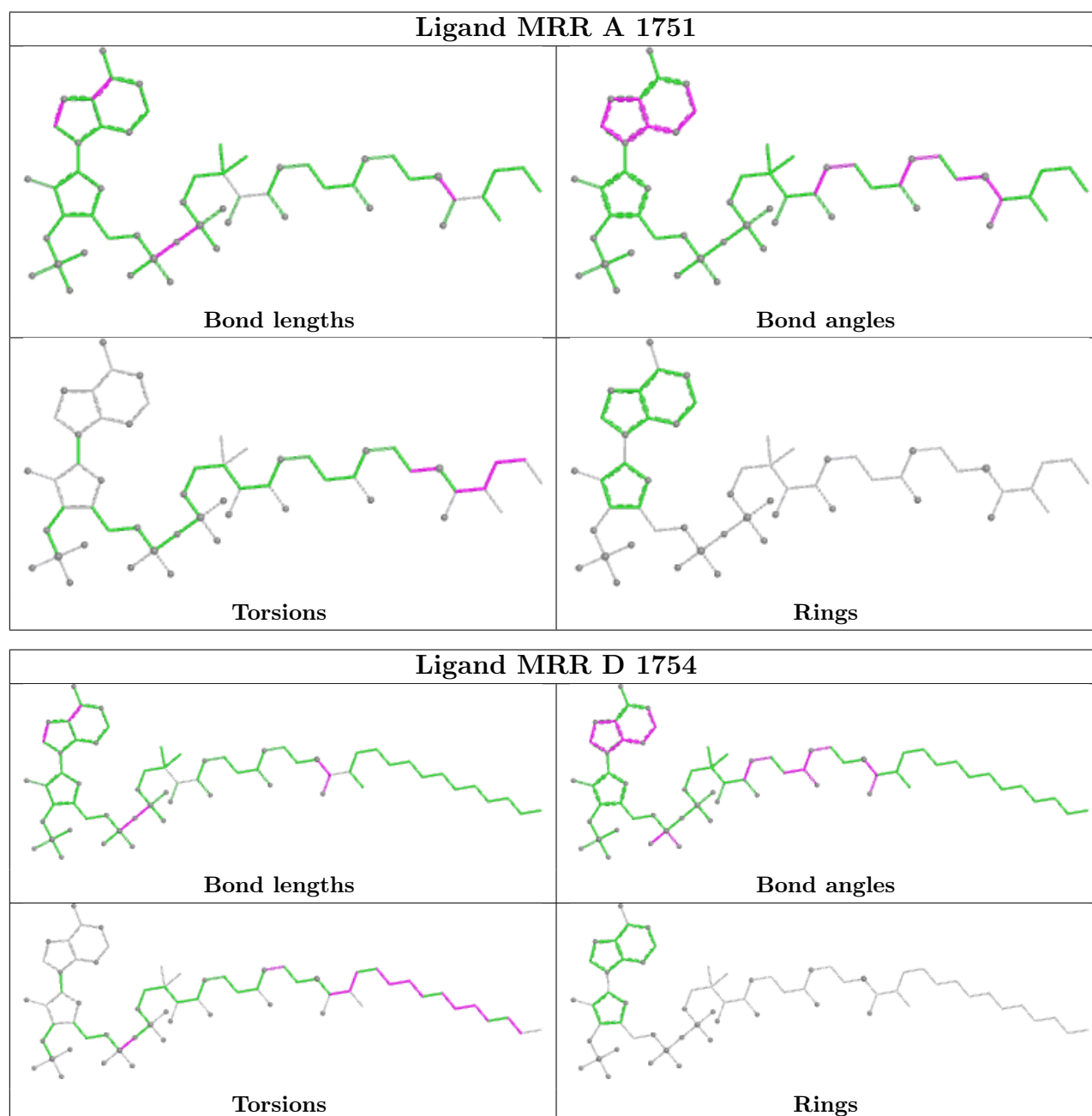
Mol	Chain	Res	Type	Atoms
2	B	1752[B]	MRR	C6-C7-C8-C9
2	C	1753	MRR	C2-C3-C4-C5
2	B	1752[A]	MRR	C7-C8-C9-C10
2	D	1754	MRR	C9-C10-C11-C12
2	B	1752[B]	MRR	C5-C6-C7-C8
3	A	1306	GOL	O2-C2-C3-O3
3	B	1304	GOL	O1-C1-C2-O2
3	C	1301	GOL	O1-C1-C2-O2
2	B	1752[B]	MRR	C3-C4-C5-C6
2	C	1753	MRR	C13-C2-C3-C4
2	D	1754	MRR	C13-C2-C3-C4
2	B	1752[B]	MRR	C9-C10-C11-C12
2	C	1753	MRR	C1-C2-C3-C4
2	D	1754	MRR	C1-C2-C3-C4
2	B	1752[A]	MRR	C11-C10-C9-C8
2	D	1754	MRR	C11-C12-C14-C15
2	B	1752[A]	MRR	O4B-C4B-C5B-O5B
2	B	1752[B]	MRR	O4B-C4B-C5B-O5B
3	B	1305	GOL	O1-C1-C2-O2
2	B	1752[A]	MRR	C11-C12-C14-C15
2	B	1752[A]	MRR	P1A-O3A-P2A-O5A
2	B	1752[B]	MRR	P1A-O3A-P2A-O5A
2	D	1754	MRR	P2A-O3A-P1A-O1A
2	B	1752[A]	MRR	C3B-O3B-P3B-O7A
2	B	1752[B]	MRR	C3B-O3B-P3B-O7A
2	D	1754	MRR	O1-C1-C2-C3
3	C	1301	GOL	C1-C2-C3-O3
2	A	1751	MRR	C3P-C2P-S1P-C1

There are no ring outliers.

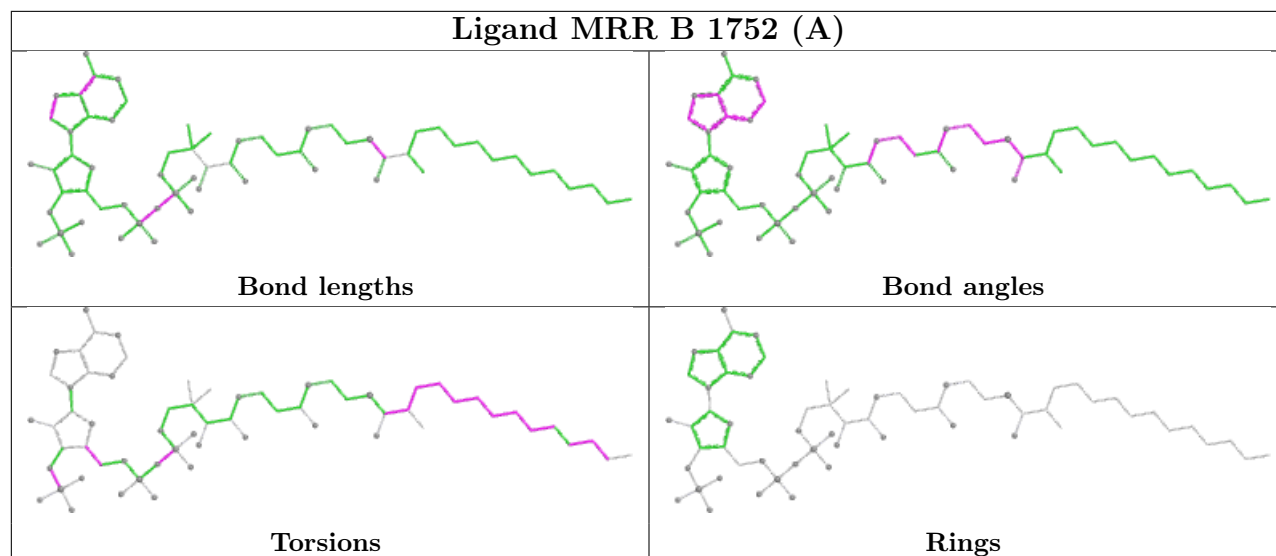
9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1301	GOL	3	0
3	C	1302	GOL	4	0
3	B	1304	GOL	1	1
2	D	1754	MRR	14	0
3	D	1303	GOL	1	1
2	B	1752[A]	MRR	4	0
2	C	1753	MRR	3	0
3	A	1306	GOL	2	0
2	B	1752[B]	MRR	3	0

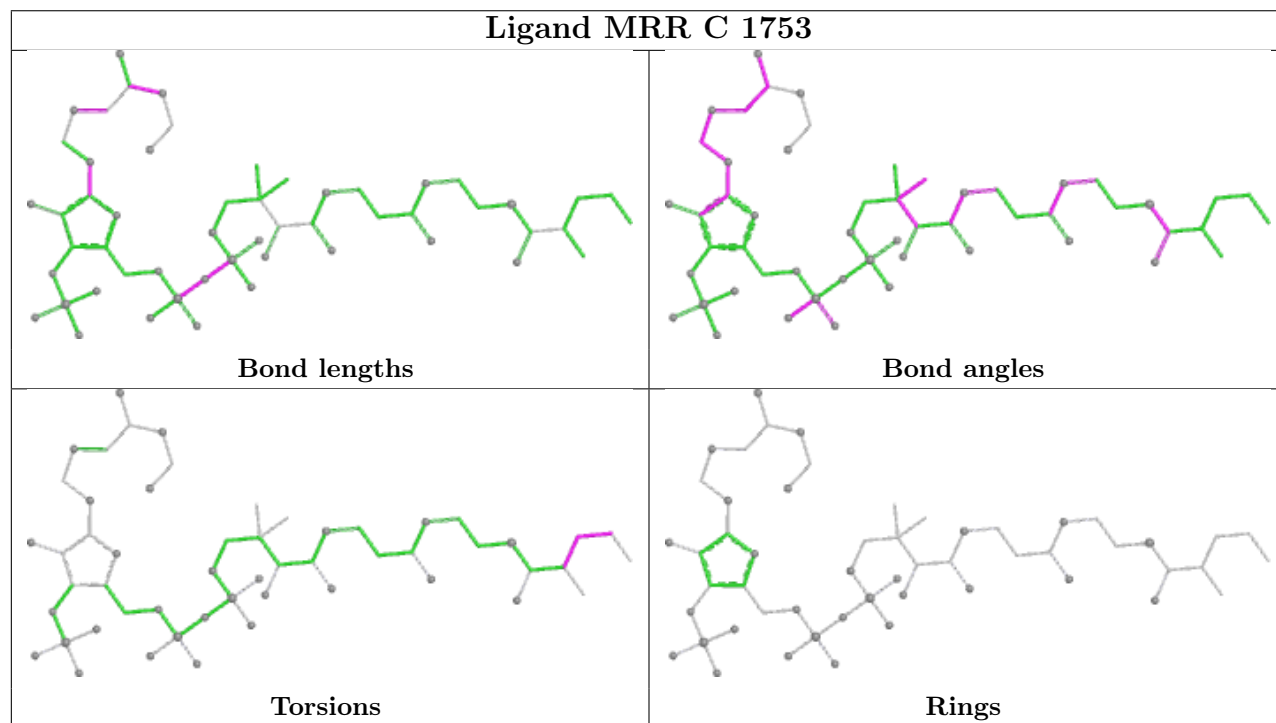
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

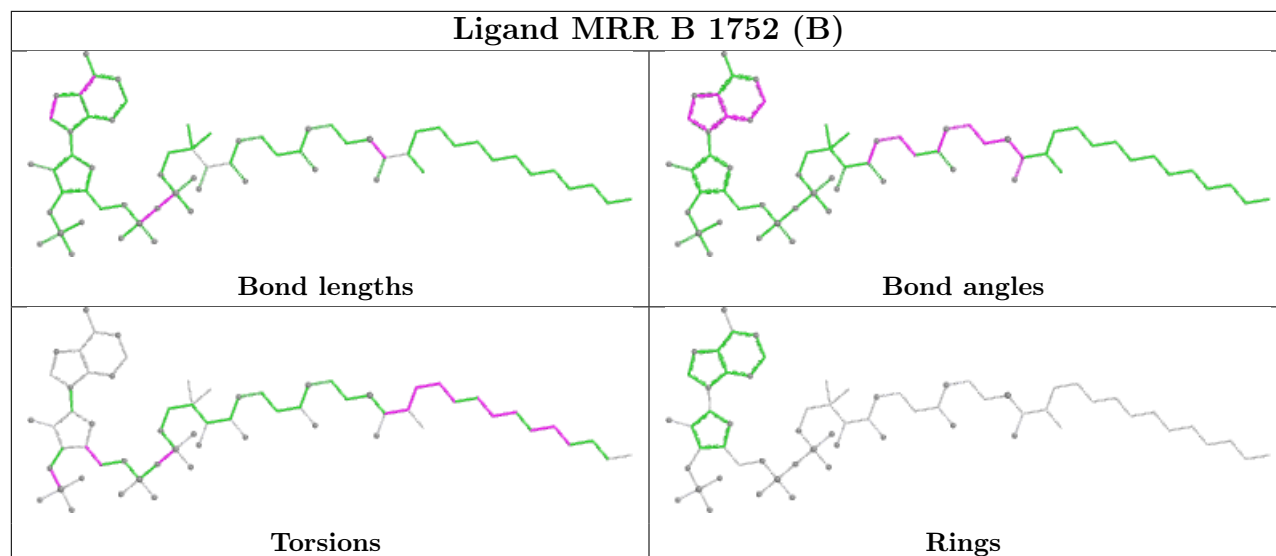


Ligand MRR B 1752 (A)



Ligand MRR C 1753





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%)	-0.62	0 100 100	20, 29, 42, 46	0
1	B	354/360 (98%)	-0.61	0 100 100	19, 28, 40, 48	0
1	C	354/360 (98%)	-0.76	0 100 100	16, 22, 34, 44	0
1	D	354/360 (98%)	-0.80	0 100 100	16, 22, 33, 42	0
All	All	1416/1440 (98%)	-0.70	0 100 100	16, 26, 37, 48	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	MRR	A	1751	55/64	0.96	0.07	54,62,65,66	0
2	MRR	B	1752[A]	64/64	0.96	0.08	34,57,69,69	10
2	MRR	B	1752[B]	64/64	0.96	0.08	18,57,69,69	10
3	GOL	B	1304	6/6	0.96	0.09	56,57,58,58	0

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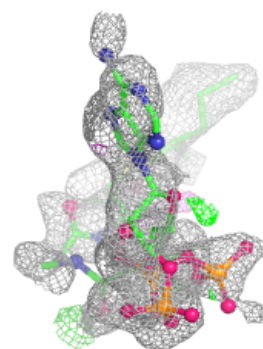
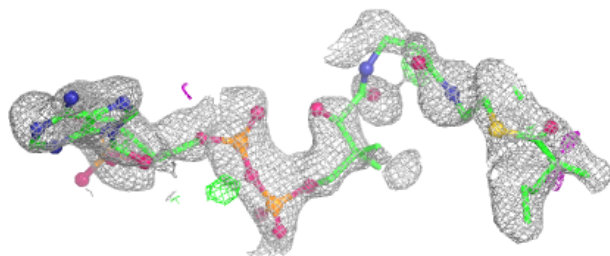
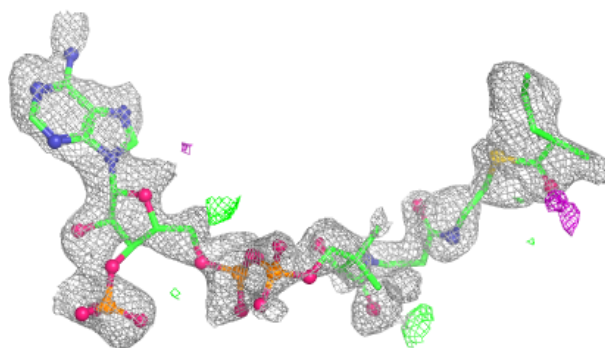
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MRR	D	1754	64/64	0.97	0.07	31,41,49,52	0
3	GOL	A	1306	6/6	0.97	0.07	39,40,41,42	0
2	MRR	C	1753	54/64	0.97	0.07	34,45,51,52	0
3	GOL	C	1301	6/6	0.97	0.10	85,85,86,86	0
3	GOL	C	1302	6/6	0.97	0.06	30,33,36,37	0
3	GOL	B	1305	6/6	0.98	0.07	54,59,61,64	0
3	GOL	D	1303	6/6	0.98	0.06	38,40,43,44	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.

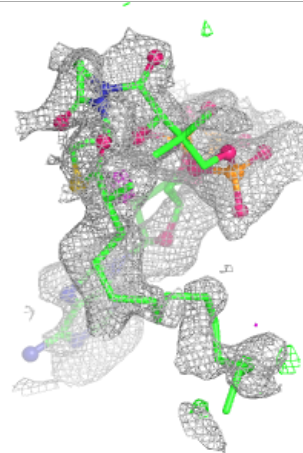
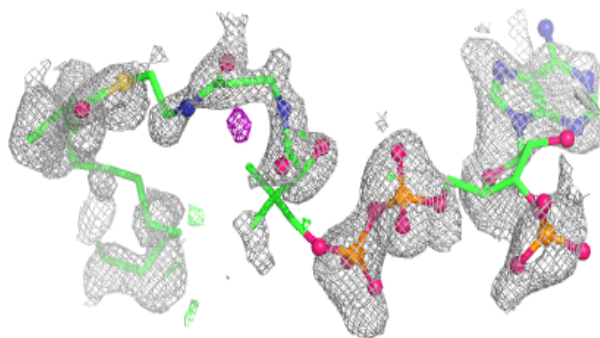
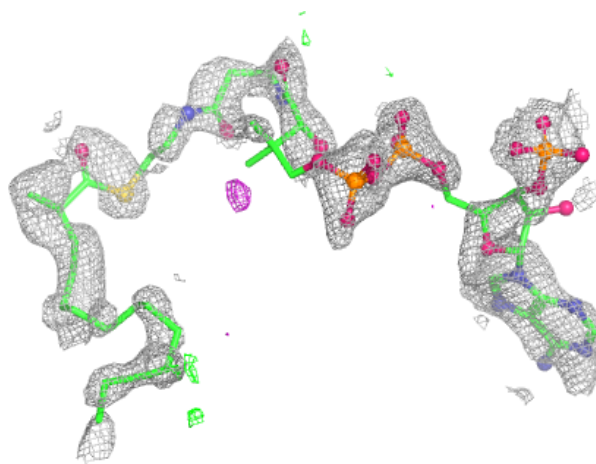
Electron density around MRR A 1751:

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



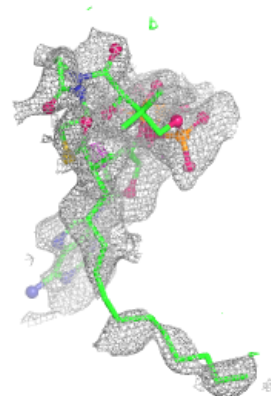
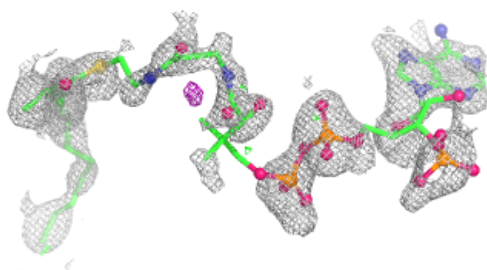
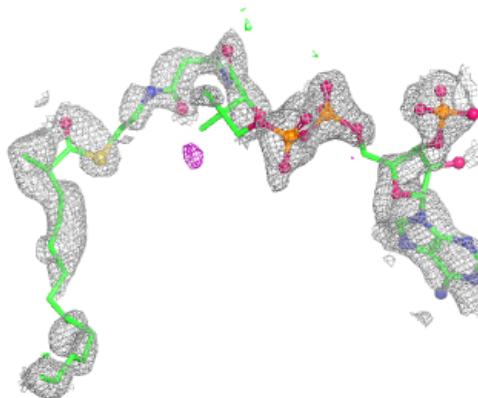
Electron density around MRR B 1752 (A):

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

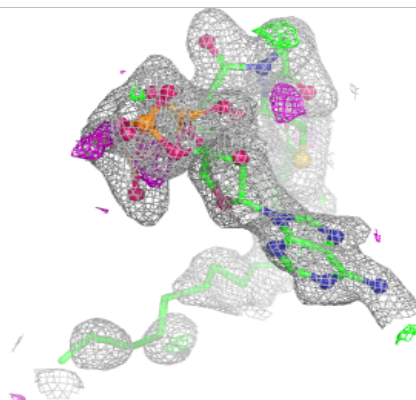
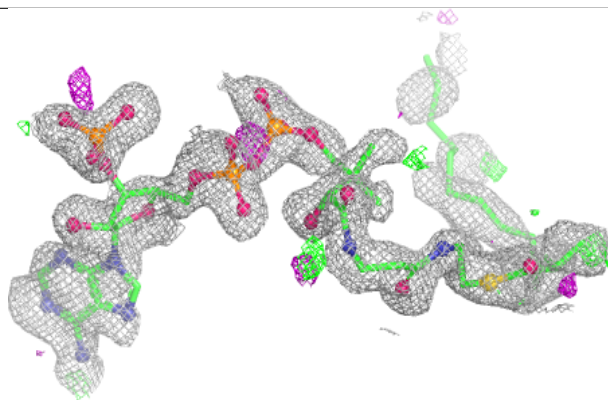
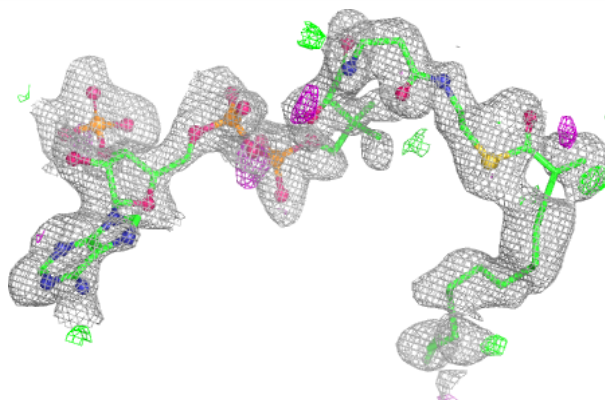


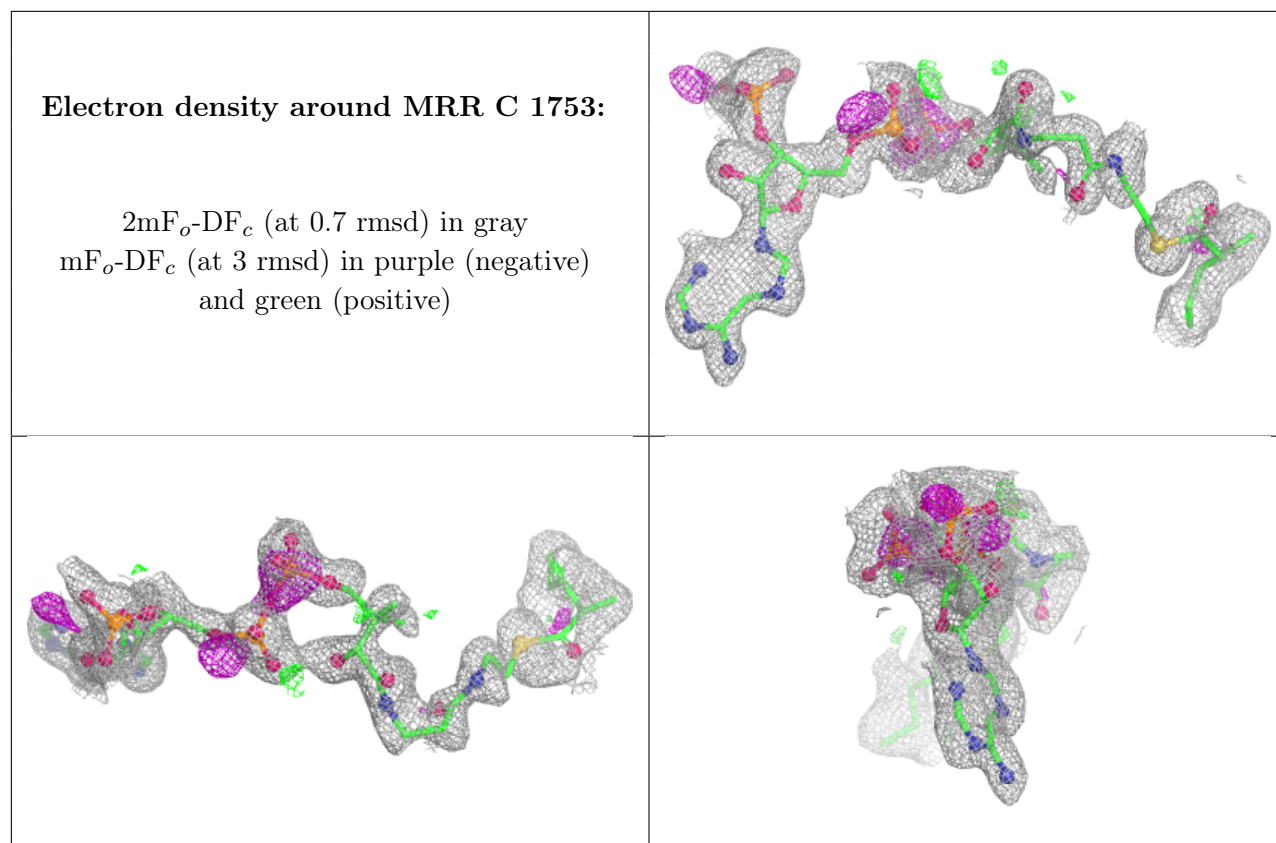
Electron density around MRR B 1752 (B):

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

**Electron density around MRR 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.