



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 05:45 AM EDT

PDB ID : 2GD0  
Title : The 1,1-proton transfer reaction mechanism by alpha-methylacyl-CoA race-  
mase 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](mailto: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>.

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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)
Xtriage (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

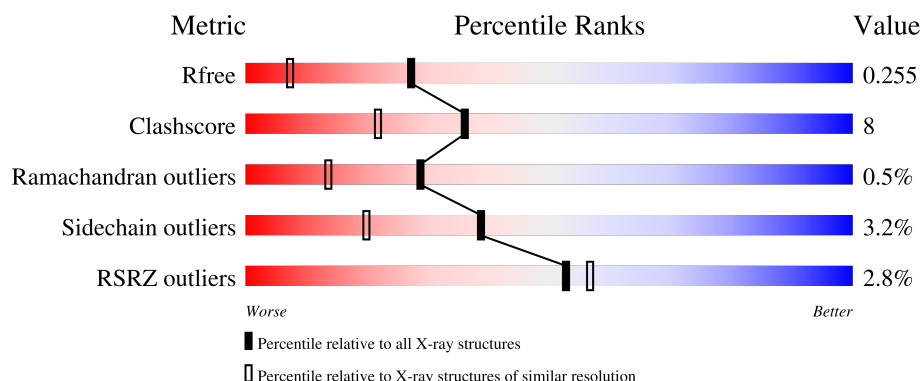
# 1 Overall quality at a glance

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	360	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	360	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	360	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>

## 2 Entry composition [i](#)

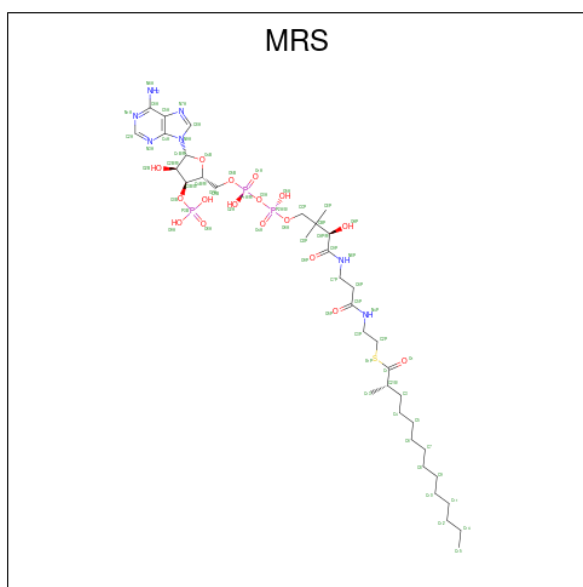
There are 4 unique types of molecules in this entry. The entry contains 12376 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (S)-2-METHYLMYRISTOYL-COENZYME A (three-letter code: MRS) (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
			64	36	7	17	3 1		
2	B	1	Total	C	N	O	P S	0	0
			64	36	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
			64	36	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 (three-letter code: 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	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	349	Total	O	0	0
			349	349		
4	B	341	Total	O	0	0
			341	341		
4	C	357	Total	O	0	0
			357	357		

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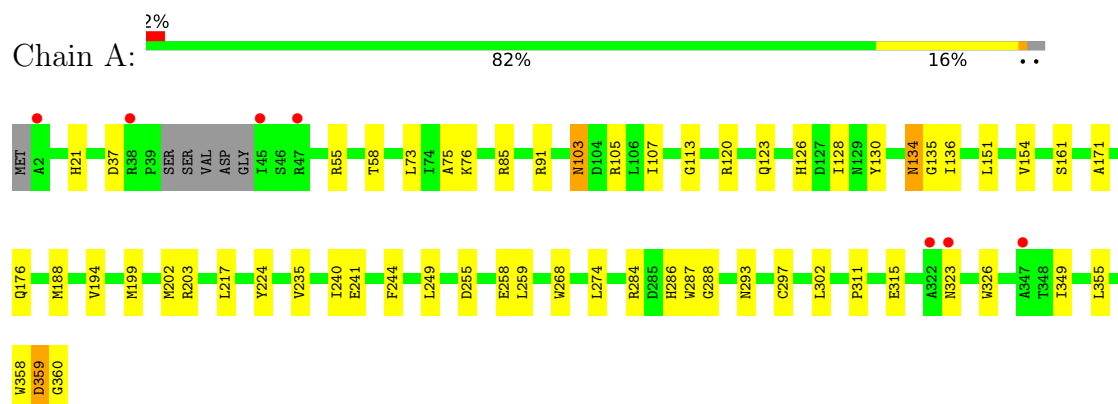
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	333	Total 333	O 333	0	0

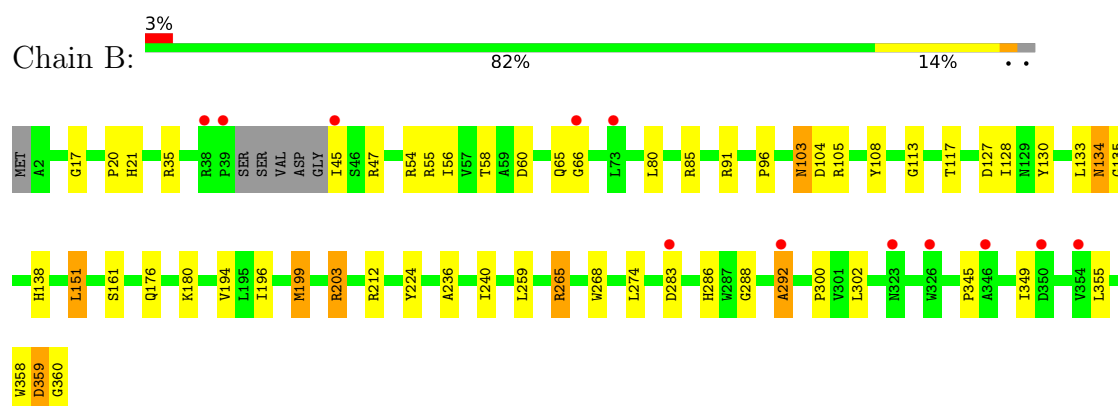
### 3 Residue-property plots [i](#)

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.

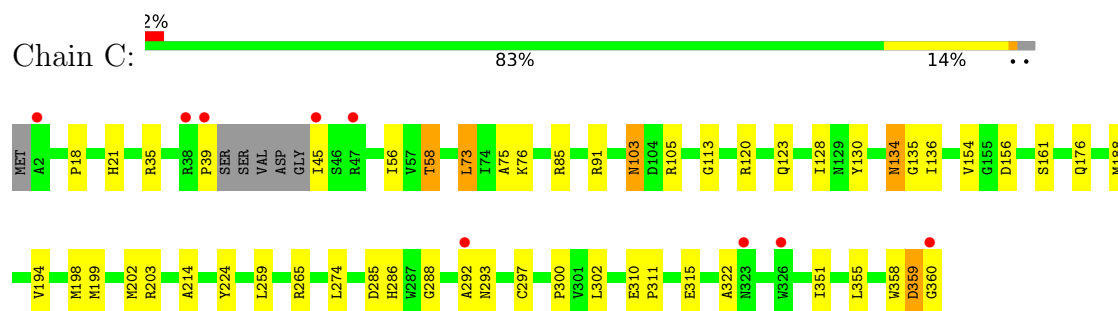
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



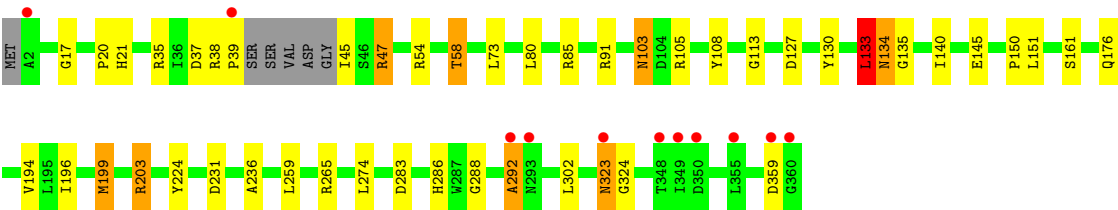
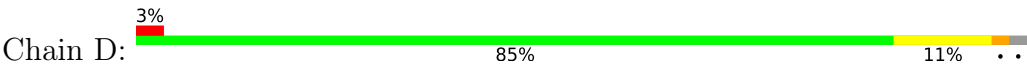
- Molecule 1: probable alpha-methylacyl-CoA racemase MCR



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.74Å 79.75Å 117.92Å 90.00° 123.14° 90.00°	Depositor
Resolution (Å)	19.80 – 1.70 19.79 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.4 (19.80-1.70) 97.4 (19.79-1.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.07 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.236 , 0.276 0.219 , 0.255	Depositor DCC
$R_{free}$ test set	8946 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.477 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12376	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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 76.91 % 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 9.4635e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MRS, 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	0.89	4/2740 (0.1%)	0.84	1/3727 (0.0%)
1	B	0.87	4/2740 (0.1%)	0.84	3/3727 (0.1%)
1	C	0.88	3/2740 (0.1%)	0.83	0/3727
1	D	0.85	2/2740 (0.1%)	0.85	5/3727 (0.1%)
All	All	0.87	13/10960 (0.1%)	0.84	9/14908 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	TYR	CE1-CZ	7.33	1.48	1.38
1	C	297	CYS	CB-SG	-7.07	1.70	1.82
1	C	224	TYR	CE1-CZ	6.99	1.47	1.38
1	A	297	CYS	CB-SG	-6.90	1.70	1.82
1	A	224	TYR	CG-CD2	6.36	1.47	1.39
1	D	224	TYR	CG-CD2	5.93	1.46	1.39
1	C	224	TYR	CG-CD2	5.81	1.46	1.39
1	B	128	ILE	CB-CG2	5.42	1.69	1.52
1	B	224	TYR	CE1-CZ	5.23	1.45	1.38
1	D	224	TYR	CE1-CZ	5.22	1.45	1.38
1	B	224	TYR	CG-CD2	5.14	1.45	1.39
1	A	268	TRP	CG-CD1	5.11	1.44	1.36
1	B	268	TRP	CG-CD1	5.04	1.43	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	B	127	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	265	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	203	ARG	NE-CZ-NH1	5.83	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	203	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	203	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	265	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	D	133	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	D	127	ASP	OD1-CG-OD2	5.07	132.93	123.30

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	2679	0	2623	54	0
1	B	2679	0	2623	47	0
1	C	2679	0	2623	51	0
1	D	2679	0	2623	40	0
2	A	64	0	60	5	0
2	B	64	0	60	2	0
2	C	64	0	60	2	0
2	D	64	0	60	1	0
3	A	6	0	8	2	0
3	B	6	0	8	1	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	A	349	0	0	14	0
4	B	341	0	0	20	0
4	C	357	0	0	10	0
4	D	333	0	0	16	0
All	All	12376	0	10764	174	0

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

All (174) 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:B:292:ALA:HB1	4:B:2640:HOH:O	1.14	1.27
1:D:35:ARG:HB2	4:D:2633:HOH:O	1.47	1.15
1:B:35:ARG:HB2	4:B:2641:HOH:O	1.43	1.14
1:D:283:ASP:HB2	4:D:2628:HOH:O	1.55	1.06
1:B:345:PRO:HG2	4:B:2636:HOH:O	1.68	0.94
1:D:288:GLY:O	4:D:2624:HOH:O	1.92	0.88
1:B:288:GLY:O	4:B:2412:HOH:O	1.92	0.86
1:B:283:ASP:HB2	4:B:2638:HOH:O	1.75	0.85
1:C:286:HIS:CD2	4:C:2652:HOH:O	2.29	0.84
1:D:288:GLY:HA2	4:D:2461:HOH:O	1.75	0.83
1:B:288:GLY:HA2	4:B:2427:HOH:O	1.81	0.79
1:C:176:GLN:HE21	1:D:176:GLN:HE21	1.32	0.76
1:A:315:GLU:HG3	4:A:2448:HOH:O	1.84	0.75
1:C:300:PRO:HB3	4:C:2501:HOH:O	1.87	0.75
1:B:259:LEU:HD22	1:B:274:LEU:HD13	1.69	0.74
1:A:176:GLN:HE21	1:B:176:GLN:HE21	1.34	0.73
1:C:120:ARG:HH11	1:C:123:GLN:HE22	1.34	0.72
1:A:259:LEU:HD22	1:A:274:LEU:HD13	1.72	0.72
1:C:355:LEU:HD22	1:C:360:GLY:HA3	1.71	0.70
1:D:259:LEU:HD22	1:D:274:LEU:HD13	1.74	0.69
1:B:85:ARG:HH12	1:B:91:ARG:HH22	1.39	0.69
1:A:91:ARG:NH1	2:A:1751:MRS:O7A	2.22	0.69
1:A:287:TRP:HB2	4:A:2650:HOH:O	1.93	0.69
1:A:85:ARG:NH1	4:A:2456:HOH:O	2.19	0.68
1:C:358:TRP:O	1:C:359:ASP:HB2	1.94	0.68
1:A:286:HIS:HE1	4:A:2398:HOH:O	1.77	0.67
1:A:284:ARG:HA	4:A:2650:HOH:O	1.95	0.67
1:C:286:HIS:HE1	4:C:2355:HOH:O	1.78	0.67
1:D:47:ARG:HG2	4:D:2572:HOH:O	1.96	0.65
1:D:286:HIS:HE1	4:D:2427:HOH:O	1.79	0.65
1:A:85:ARG:HD3	4:A:2351:HOH:O	1.97	0.64
1:C:259:LEU:HD22	1:C:274:LEU:HD13	1.80	0.64
1:A:235:VAL:CG1	4:A:2650:HOH:O	2.44	0.63
1:D:38:ARG:HD3	4:D:2549:HOH:O	1.97	0.63
1:A:120:ARG:HH11	1:A:123:GLN:HE22	1.46	0.62
1:C:85:ARG:HD3	4:C:2348:HOH:O	2.00	0.62
1:B:286:HIS:HE1	4:B:2414:HOH:O	1.82	0.62
1:A:311:PRO:O	1:A:315:GLU:HG2	2.00	0.61
1:A:358:TRP:O	1:A:359:ASP:HB2	2.02	0.58
1:B:292:ALA:HA	4:B:2412:HOH:O	2.04	0.57
1:D:91:ARG:NH1	2:D:1754:MRS:O7A	2.26	0.57
1:A:76:LYS:HE3	1:A:359:ASP:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:HD2	1:B:349:ILE:HD11	1.86	0.57
1:D:85:ARG:NH1	4:D:2618:HOH:O	2.37	0.56
1:A:286:HIS:HD2	4:C:2438:HOH:O	1.89	0.55
1:C:91:ARG:NH1	2:C:1753:MRS:O7A	2.38	0.55
1:A:55:ARG:HD2	1:A:349:ILE:HD11	1.88	0.55
1:D:134:ASN:C	1:D:134:ASN:HD22	2.09	0.55
1:C:21:HIS:HD2	1:C:161:SER:OG	1.90	0.54
2:A:1751:MRS:H72	4:B:2431:HOH:O	2.06	0.54
1:A:113:GLY:HA3	1:A:130:TYR:CZ	2.42	0.54
1:D:140:ILE:HD13	1:D:150:PRO:HG3	1.90	0.54
1:A:288:GLY:HA2	4:A:2606:HOH:O	2.07	0.54
1:C:176:GLN:NE2	1:D:176:GLN:HE21	2.04	0.54
1:C:285:ASP:OD1	4:C:2650:HOH:O	2.19	0.54
1:A:103:ASN:C	1:A:103:ASN:HD22	2.11	0.53
1:C:302:LEU:O	1:D:135:GLY:HA2	2.07	0.53
1:C:176:GLN:HG2	4:D:2634:HOH:O	2.08	0.53
1:B:358:TRP:O	1:B:359:ASP:HB2	2.08	0.53
1:D:103:ASN:ND2	1:D:105:ARG:H	2.07	0.53
1:A:302:LEU:O	1:B:135:GLY:HA2	2.09	0.53
1:D:292:ALA:HA	4:D:2624:HOH:O	2.09	0.53
1:C:322:ALA:HB1	4:C:2643:HOH:O	2.09	0.52
1:B:134:ASN:HD22	1:B:134:ASN:C	2.11	0.52
1:C:113:GLY:HA3	1:C:130:TYR:CZ	2.44	0.51
1:C:176:GLN:HE21	1:D:176:GLN:NE2	2.05	0.51
1:D:323:ASN:HB2	4:D:2497:HOH:O	2.10	0.51
1:A:21:HIS:HD2	1:A:161:SER:OG	1.92	0.51
1:C:103:ASN:HD22	1:C:103:ASN:C	2.12	0.51
1:A:235:VAL:HG13	4:A:2650:HOH:O	2.08	0.51
1:D:37:ASP:O	1:D:58:THR:HA	2.11	0.51
1:B:300:PRO:HB3	4:B:2427:HOH:O	2.10	0.50
1:A:103:ASN:ND2	1:A:105:ARG:H	2.09	0.50
1:B:103:ASN:ND2	1:B:105:ARG:H	2.10	0.50
1:C:120:ARG:NH1	1:C:123:GLN:HE22	2.04	0.50
1:C:45:ILE:O	1:C:45:ILE:HG23	2.11	0.50
1:C:76:LYS:HE3	1:C:359:ASP:O	2.12	0.50
1:B:288:GLY:CA	4:B:2427:HOH:O	2.52	0.49
1:C:214:ALA:O	1:C:265:ARG:NH2	2.45	0.49
1:C:203:ARG:NH2	4:C:2540:HOH:O	2.45	0.49
1:C:286:HIS:CE1	4:C:2355:HOH:O	2.61	0.48
4:A:2498:HOH:O	1:C:286:HIS:HD2	1.95	0.48
1:D:85:ARG:HD3	4:D:2360:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLN:NE2	1:B:176:GLN:HE21	2.08	0.48
1:A:103:ASN:HD22	1:A:105:ARG:H	1.59	0.48
1:C:103:ASN:ND2	1:C:105:ARG:H	2.11	0.48
1:A:113:GLY:HA3	1:A:130:TYR:CE1	2.49	0.48
1:C:135:GLY:HA2	1:D:302:LEU:O	2.12	0.47
1:B:17:GLY:O	1:B:20:PRO:HD2	2.14	0.47
1:C:39:PRO:O	4:C:2651:HOH:O	2.20	0.47
1:A:176:GLN:HE21	1:B:176:GLN:NE2	2.08	0.47
1:D:54:ARG:NE	4:D:2633:HOH:O	2.48	0.47
1:D:286:HIS:HD2	4:D:2396:HOH:O	1.97	0.47
1:C:35:ARG:HB3	1:C:56:ILE:HD13	1.97	0.47
1:A:130:TYR:CE2	1:A:188:MET:HE3	2.50	0.47
1:A:194:VAL:O	1:B:21:HIS:HE1	1.97	0.47
1:B:355:LEU:HD22	1:B:360:GLY:HA3	1.97	0.47
1:A:176:GLN:HG2	4:B:2597:HOH:O	2.15	0.47
1:D:21:HIS:HD2	1:D:161:SER:OG	1.97	0.47
1:A:135:GLY:HA2	1:B:302:LEU:O	2.14	0.47
1:A:85:ARG:NE	2:A:1751:MRS:O1A	2.48	0.46
1:C:176:GLN:HG2	1:D:176:GLN:NE2	2.30	0.46
1:D:85:ARG:HG3	4:D:2590:HOH:O	2.16	0.46
1:A:126:HIS:HA	2:A:1751:MRS:H22	1.98	0.46
1:B:80:LEU:HD23	1:B:108:TYR:CE1	2.51	0.46
1:D:196:ILE:HG12	1:D:199:MET:HB2	1.97	0.46
1:C:134:ASN:HD22	1:C:134:ASN:C	2.19	0.46
1:A:355:LEU:HD22	1:A:360:GLY:HA3	1.98	0.46
1:C:39:PRO:HA	1:C:58:THR:CG2	2.46	0.46
1:B:265:ARG:NH1	4:B:2379:HOH:O	2.43	0.45
1:D:324:GLY:C	4:D:2614:HOH:O	2.53	0.45
1:C:103:ASN:HD22	1:C:105:ARG:H	1.64	0.45
1:D:80:LEU:HD23	1:D:108:TYR:CE1	2.51	0.45
1:B:117:THR:HB	4:B:2559:HOH:O	2.15	0.45
1:B:196:ILE:HG12	1:B:199:MET:HB2	1.97	0.45
1:D:231:ASP:OD1	1:D:231:ASP:N	2.50	0.45
1:A:134:ASN:C	1:A:134:ASN:HD22	2.18	0.45
1:A:240:ILE:CG2	3:A:2306:GOL:H31	2.47	0.45
1:D:113:GLY:HA3	1:D:130:TYR:CZ	2.52	0.45
2:C:1753:MRS:H41	2:C:1753:MRS:H71	1.78	0.45
1:C:176:GLN:CG	1:D:176:GLN:HE21	2.31	0.44
1:C:39:PRO:HA	1:C:58:THR:HG21	1.99	0.44
1:C:194:VAL:O	1:D:21:HIS:HE1	2.00	0.44
1:A:21:HIS:HE1	1:B:194:VAL:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:NH1	1:A:123:GLN:HE22	2.14	0.44
1:C:21:HIS:HE1	1:D:194:VAL:O	2.01	0.44
1:C:113:GLY:HA3	1:C:130:TYR:CE1	2.52	0.44
1:A:287:TRP:HD1	4:A:2650:HOH:O	2.00	0.44
1:B:85:ARG:CZ	4:B:2568:HOH:O	2.66	0.44
1:A:176:GLN:HG2	1:B:176:GLN:NE2	2.33	0.44
1:B:113:GLY:HA3	1:B:130:TYR:CE1	2.53	0.44
1:A:255:ASP:HB3	1:A:258:GLU:HG3	1.99	0.44
1:B:265:ARG:NH2	4:B:2626:HOH:O	1.92	0.44
1:B:47:ARG:HB2	4:B:2599:HOH:O	2.18	0.43
1:B:96:PRO:HG2	4:B:2552:HOH:O	2.18	0.43
1:A:188:MET:HE1	2:A:1751:MRS:H21	2.00	0.43
4:A:2476:HOH:O	2:B:1752:MRS:H72	2.18	0.43
1:B:60:ASP:O	1:B:66:GLY:HA3	2.19	0.43
1:D:113:GLY:HA3	1:D:130:TYR:CE1	2.54	0.43
1:B:54:ARG:NE	4:B:2641:HOH:O	2.52	0.42
1:D:17:GLY:O	1:D:20:PRO:HD2	2.19	0.42
1:B:113:GLY:HA3	1:B:130:TYR:CZ	2.53	0.42
1:D:39:PRO:HG3	1:D:58:THR:HG23	2.01	0.42
1:C:130:TYR:CE2	1:C:188:MET:HE3	2.55	0.42
1:A:103:ASN:C	1:A:103:ASN:ND2	2.73	0.42
1:B:240:ILE:O	3:B:2304:GOL:H32	2.20	0.42
1:A:235:VAL:HG11	4:A:2650:HOH:O	2.13	0.42
1:B:286:HIS:HD2	4:B:2375:HOH:O	2.02	0.42
1:C:310:GLU:HG2	1:D:133:LEU:HD13	2.01	0.42
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.88	0.41
1:C:103:ASN:C	1:C:103:ASN:ND2	2.72	0.41
1:A:241:GLU:HB2	1:A:244:PHE:CD2	2.56	0.41
1:C:311:PRO:O	1:C:315:GLU:HG3	2.19	0.41
1:A:75:ALA:HA	1:A:103:ASN:HB2	2.02	0.41
1:A:136:ILE:HG21	1:A:154:VAL:HG11	2.01	0.41
1:C:136:ILE:HG21	1:C:154:VAL:HG11	2.03	0.41
1:B:104:ASP:OD2	1:B:180:LYS:HE3	2.20	0.41
1:B:85:ARG:NH1	1:B:91:ARG:HH22	2.11	0.41
1:A:326:TRP:HD1	4:A:2630:HOH:O	2.03	0.41
1:B:21:HIS:HD2	1:B:161:SER:OG	2.04	0.41
1:A:202:MET:HG2	2:B:1752:MRS:H122	2.01	0.41
1:C:73:LEU:CD2	1:C:351:ILE:HD11	2.51	0.41
1:A:217:LEU:O	1:B:151:LEU:HA	2.21	0.41
1:A:240:ILE:HG22	3:A:2306:GOL:H31	2.02	0.41
1:C:18:PRO:HB3	1:C:156:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ALA:HA	1:C:103:ASN:HB2	2.03	0.40
1:B:138:HIS:O	1:B:212:ARG:HD3	2.21	0.40
1:C:198:MET:HG2	1:C:202:MET:HE2	2.03	0.40
1:B:35:ARG:HB3	1:B:56:ILE:HD13	2.03	0.40
1:A:107:ILE:HD12	1:A:171:ALA:HB1	2.04	0.40
1:A:128:ILE:HG12	1:B:236:ALA:HB1	2.02	0.40
1:C:128:ILE:HG12	1:D:236:ALA:HB1	2.03	0.40
1:C:288:GLY:O	1:C:292:ALA:HB2	2.20	0.40
1:C:85:ARG:HH12	1:C:91:ARG:NH2	2.19	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/360 (97%)	335 (96%)	13 (4%)	2 (1%)	25	11
1	B	350/360 (97%)	334 (95%)	14 (4%)	2 (1%)	25	11
1	C	350/360 (97%)	335 (96%)	14 (4%)	1 (0%)	41	24
1	D	350/360 (97%)	336 (96%)	12 (3%)	2 (1%)	25	11
All	All	1400/1440 (97%)	1340 (96%)	53 (4%)	7 (0%)	29	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	292	ALA
1	C	359	ASP
1	D	292	ALA
1	A	359	ASP
1	A	151	LEU
1	B	151	LEU

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Mol	Chain	Res	Type
1	D	151	LEU

### 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	270/275 (98%)	262 (97%)	8 (3%)	41	22
1	B	270/275 (98%)	261 (97%)	9 (3%)	38	19
1	C	270/275 (98%)	264 (98%)	6 (2%)	52	34
1	D	270/275 (98%)	258 (96%)	12 (4%)	28	11
All	All	1080/1100 (98%)	1045 (97%)	35 (3%)	39	20

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASP
1	A	58	THR
1	A	73	LEU
1	A	103	ASN
1	A	134	ASN
1	A	199	MET
1	A	293	ASN
1	A	323	ASN
1	B	45	ILE
1	B	58	THR
1	B	65	GLN
1	B	103	ASN
1	B	133	LEU
1	B	134	ASN
1	B	199	MET
1	B	203	ARG
1	B	359	ASP
1	C	58	THR
1	C	73	LEU
1	C	103	ASN

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Mol	Chain	Res	Type
1	C	134	ASN
1	C	199	MET
1	C	293	ASN
1	D	45	ILE
1	D	47	ARG
1	D	58	THR
1	D	73	LEU
1	D	103	ASN
1	D	133	LEU
1	D	134	ASN
1	D	145	GLU
1	D	199	MET
1	D	203	ARG
1	D	323	ASN
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
1	A	123	GLN
1	A	134	ASN
1	A	176	GLN
1	A	286	HIS
1	A	293	ASN
1	A	323	ASN
1	B	21	HIS
1	B	103	ASN
1	B	134	ASN
1	B	176	GLN
1	B	263	ASN
1	B	286	HIS
1	C	21	HIS
1	C	103	ASN
1	C	123	GLN
1	C	134	ASN
1	C	286	HIS
1	D	21	HIS
1	D	103	ASN
1	D	134	ASN
1	D	176	GLN

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Mol	Chain	Res	Type
1	D	263	ASN
1	D	286	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

8 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	MRS	C	1753	-	57,66,66	0.78	1 (1%)	68,93,93	1.34	6 (8%)
2	MRS	D	1754	-	57,66,66	0.75	0	68,93,93	1.27	7 (10%)
3	GOL	D	2303	-	5,5,5	0.34	0	5,5,5	1.02	0
2	MRS	B	1752	-	57,66,66	0.80	1 (1%)	68,93,93	1.27	6 (8%)
2	MRS	A	1751	-	57,66,66	0.77	1 (1%)	68,93,93	1.36	9 (13%)
3	GOL	A	2306	-	5,5,5	0.32	0	5,5,5	0.77	0
3	GOL	B	2304	-	5,5,5	0.30	0	5,5,5	0.66	0
3	GOL	C	2302	-	5,5,5	0.39	0	5,5,5	0.52	0

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	MRS	C	1753	-	-	12/62/83/83	0/3/3/3
2	MRS	D	1754	-	-	12/62/83/83	0/3/3/3
3	GOL	D	2303	-	-	0/4/4/4	-
2	MRS	B	1752	-	-	12/62/83/83	0/3/3/3
2	MRS	A	1751	-	-	16/62/83/83	0/3/3/3
3	GOL	A	2306	-	-	3/4/4/4	-
3	GOL	B	2304	-	-	4/4/4/4	-
3	GOL	C	2302	-	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1753	MRS	O4B-C1B	2.38	1.44	1.41
2	A	1751	MRS	O4B-C1B	2.23	1.44	1.41
2	B	1752	MRS	O4B-C1B	2.19	1.44	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1751	MRS	C7P-N8P-C9P	4.98	131.47	122.59
2	C	1753	MRS	C2P-S1P-C1	4.45	115.13	101.75
2	D	1754	MRS	C7P-N8P-C9P	4.40	130.44	122.59
2	C	1753	MRS	C7P-N8P-C9P	4.33	130.31	122.59
2	A	1751	MRS	N3A-C2A-N1A	-4.07	122.32	128.68
2	D	1754	MRS	N3A-C2A-N1A	-3.96	122.48	128.68
2	C	1753	MRS	N3A-C2A-N1A	-3.90	122.58	128.68
2	B	1752	MRS	N3A-C2A-N1A	-3.81	122.73	128.68
2	B	1752	MRS	C7P-N8P-C9P	3.77	129.31	122.59
2	A	1751	MRS	C2P-S1P-C1	3.69	112.86	101.75
2	B	1752	MRS	C3P-N4P-C5P	3.00	128.41	122.84
2	B	1752	MRS	CDP-CBP-CAP	2.98	113.99	108.82
2	D	1754	MRS	C3P-N4P-C5P	2.96	128.33	122.84
2	B	1752	MRS	O1-C1-S1P	-2.78	120.06	123.80
2	A	1751	MRS	C2P-C3P-N4P	-2.70	106.74	112.42
2	A	1751	MRS	C3P-N4P-C5P	2.49	127.47	122.84
2	D	1754	MRS	CDP-CBP-CAP	2.42	113.01	108.82
2	C	1753	MRS	O1-C1-C2	-2.36	115.61	122.53
2	D	1754	MRS	O1-C1-S1P	-2.25	120.77	123.80
2	B	1752	MRS	C2P-C3P-N4P	-2.22	107.76	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1751	MRS	C4-C3-C2	-2.19	110.32	114.82
2	C	1753	MRS	C3P-N4P-C5P	2.19	126.90	122.84
2	A	1751	MRS	O1-C1-C2	-2.08	116.45	122.53
2	D	1754	MRS	C6P-C7P-N8P	-2.07	107.71	111.90
2	D	1754	MRS	C2P-S1P-C1	2.05	107.92	101.75
2	A	1751	MRS	O1-C1-S1P	-2.04	121.05	123.80
2	A	1751	MRS	C4A-C5A-N7A	-2.03	107.28	109.40
2	C	1753	MRS	C2P-C3P-N4P	-2.03	108.15	112.42

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1751	MRS	O1-C1-S1P-C2P
2	A	1751	MRS	C2-C1-S1P-C2P
2	A	1751	MRS	S1P-C1-C2-C13
2	B	1752	MRS	S1P-C1-C2-C13
2	C	1753	MRS	C2-C1-S1P-C2P
2	D	1754	MRS	S1P-C1-C2-C13
2	D	1754	MRS	C1-C2-C3-C4
2	D	1754	MRS	C13-C2-C3-C4
3	B	2304	GOL	O1-C1-C2-O2
3	B	2304	GOL	O1-C1-C2-C3
3	B	2304	GOL	C1-C2-C3-O3
2	C	1753	MRS	C4-C5-C6-C7
2	A	1751	MRS	C13-C2-C3-C4
2	B	1752	MRS	C13-C2-C3-C4
2	A	1751	MRS	C6-C7-C8-C9
2	B	1752	MRS	C6-C7-C8-C9
2	C	1753	MRS	C6-C7-C8-C9
2	D	1754	MRS	C4-C5-C6-C7
2	C	1753	MRS	C10-C11-C12-C14
3	A	2306	GOL	O1-C1-C2-C3
3	A	2306	GOL	C1-C2-C3-O3
3	C	2302	GOL	O1-C1-C2-C3
2	A	1751	MRS	C10-C11-C12-C14
2	D	1754	MRS	C10-C11-C12-C14
2	B	1752	MRS	C4-C5-C6-C7
2	A	1751	MRS	C4-C5-C6-C7
3	B	2304	GOL	O2-C2-C3-O3
2	B	1752	MRS	C11-C10-C9-C8
2	A	1751	MRS	C2-C3-C4-C5

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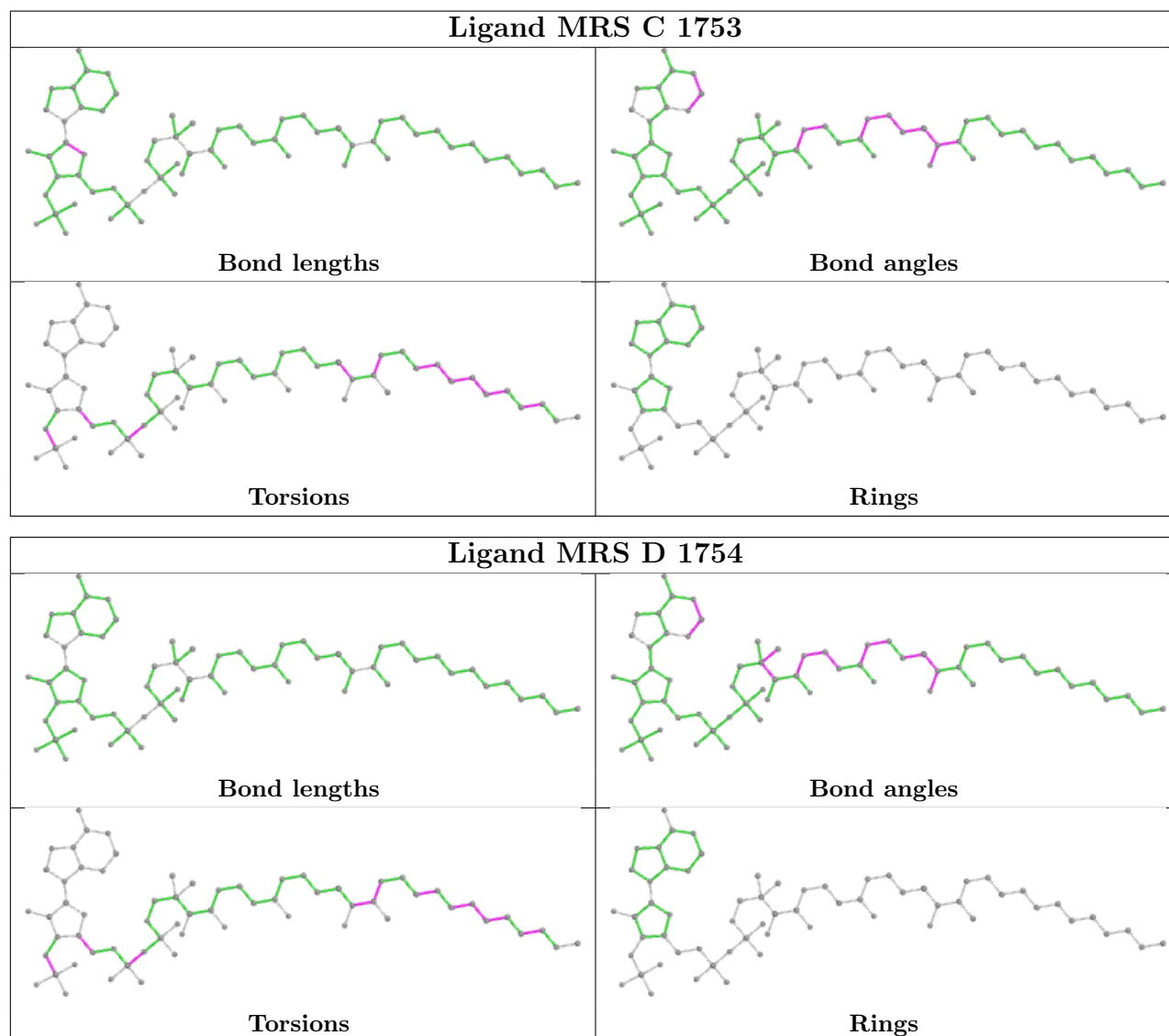
Mol	Chain	Res	Type	Atoms
2	C	1753	MRS	C7-C8-C9-C10
2	A	1751	MRS	C1-C2-C3-C4
2	B	1752	MRS	C1-C2-C3-C4
2	D	1754	MRS	C6-C7-C8-C9
2	C	1753	MRS	O1-C1-S1P-C2P
2	D	1754	MRS	C11-C10-C9-C8
2	D	1754	MRS	C7-C8-C9-C10
2	A	1751	MRS	C5-C6-C7-C8
2	C	1753	MRS	C5-C6-C7-C8
2	A	1751	MRS	S1P-C2P-C3P-N4P
2	B	1752	MRS	C10-C11-C12-C14
2	C	1753	MRS	C11-C10-C9-C8
2	D	1754	MRS	P2A-O3A-P1A-O1A
2	B	1752	MRS	C5-C6-C7-C8
2	A	1751	MRS	C11-C10-C9-C8
2	C	1753	MRS	C1-C2-C3-C4
2	B	1752	MRS	O4B-C4B-C5B-O5B
2	A	1751	MRS	C3P-C2P-S1P-C1
2	D	1754	MRS	P2A-O3A-P1A-O2A
3	A	2306	GOL	O1-C1-C2-O2
2	B	1752	MRS	C7-C8-C9-C10
2	D	1754	MRS	O4B-C4B-C5B-O5B
2	A	1751	MRS	C3B-O3B-P3B-O9A
2	C	1753	MRS	C3B-O3B-P3B-O9A
2	D	1754	MRS	C3B-O3B-P3B-O9A
2	A	1751	MRS	O4B-C4B-C5B-O5B
2	C	1753	MRS	O4B-C4B-C5B-O5B
2	A	1751	MRS	P2A-O3A-P1A-O1A
2	B	1752	MRS	P2A-O3A-P1A-O1A
2	C	1753	MRS	P2A-O3A-P1A-O1A
2	B	1752	MRS	C2-C3-C4-C5

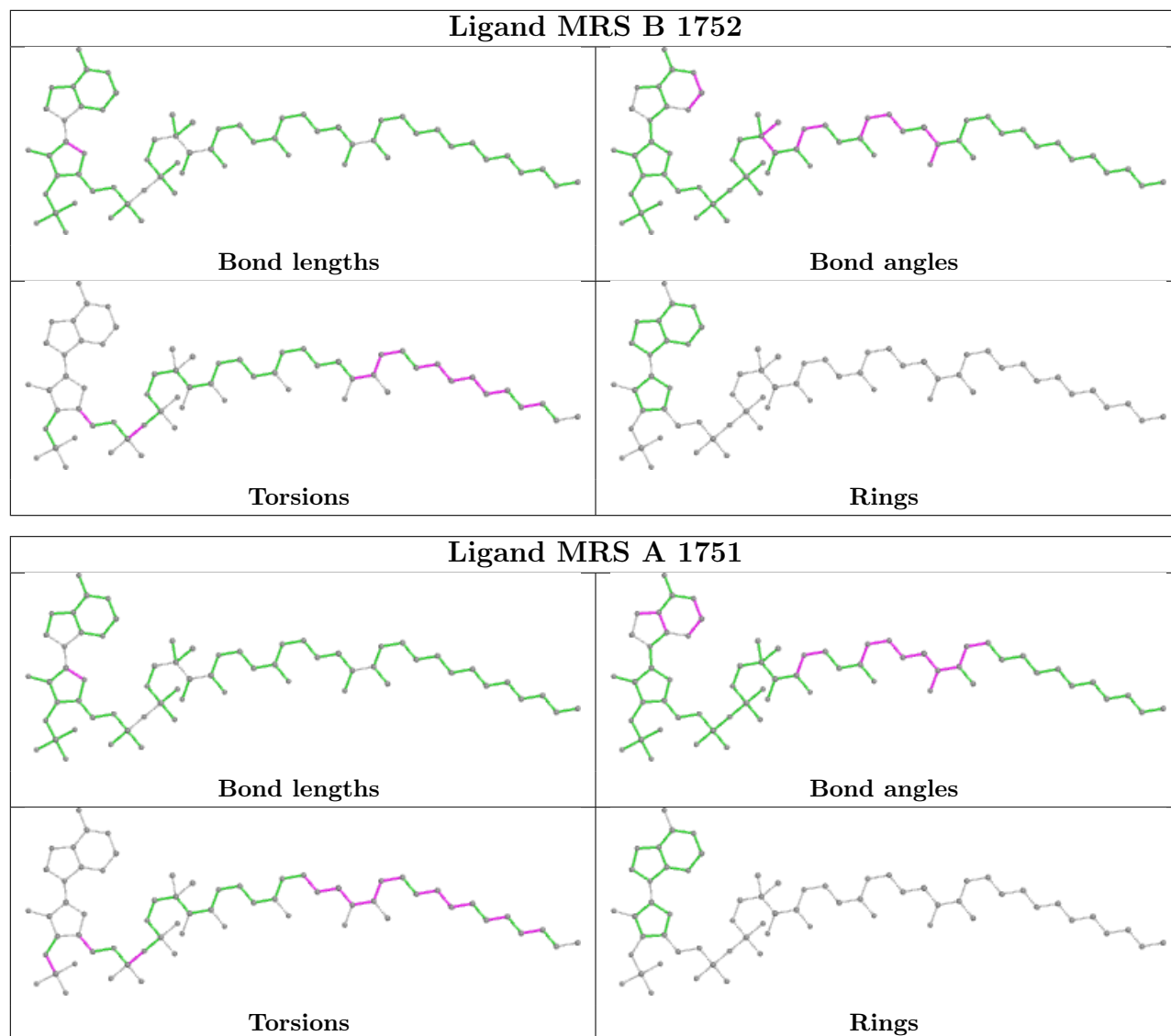
There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1753	MRS	2	0
2	D	1754	MRS	1	0
2	B	1752	MRS	2	0
2	A	1751	MRS	5	0
3	A	2306	GOL	2	0
3	B	2304	GOL	1	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	354/360 (98%)	0.10	7 (1%) 65 69	9, 24, 46, 57	0
1	B	354/360 (98%)	0.15	12 (3%) 45 50	9, 25, 49, 59	0
1	C	354/360 (98%)	0.04	9 (2%) 57 61	9, 24, 46, 56	0
1	D	354/360 (98%)	0.11	11 (3%) 49 53	9, 25, 49, 59	0
All	All	1416/1440 (98%)	0.10	39 (2%) 53 57	9, 25, 48, 59	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ILE	6.0
1	B	323	ASN	5.1
1	B	39	PRO	4.5
1	C	360	GLY	4.2
1	C	45	ILE	4.1
1	C	39	PRO	3.8
1	C	323	ASN	3.8
1	D	292	ALA	3.7
1	B	350	ASP	3.6
1	A	347	ALA	3.5
1	C	326	TRP	3.4
1	D	360	GLY	3.4
1	B	292	ALA	3.3
1	D	293	ASN	3.0
1	D	350	ASP	3.0
1	A	322	ALA	3.0
1	C	2	ALA	2.9
1	D	355	LEU	2.8
1	D	349	ILE	2.8
1	C	38	ARG	2.8
1	C	292	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	323	ASN	2.7
1	D	323	ASN	2.7
1	B	354	VAL	2.7
1	D	39	PRO	2.6
1	B	45	ILE	2.5
1	C	47	ARG	2.4
1	A	38	ARG	2.3
1	B	38	ARG	2.3
1	A	2	ALA	2.3
1	D	359	ASP	2.3
1	B	346	ALA	2.2
1	B	326	TRP	2.2
1	A	47	ARG	2.1
1	D	2	ALA	2.1
1	D	348	THR	2.0
1	B	73	LEU	2.0
1	B	66	GLY	2.0
1	B	283	ASP	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MRS	D	1754	64/64	0.80	0.17	38,52,59,61	0
3	GOL	A	2306	6/6	0.80	0.16	38,42,42,45	0
3	GOL	C	2302	6/6	0.83	0.18	39,42,42,43	0
2	MRS	C	1753	64/64	0.84	0.17	39,50,65,65	0
2	MRS	B	1752	64/64	0.84	0.16	36,50,63,63	0

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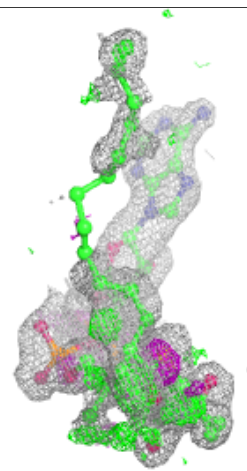
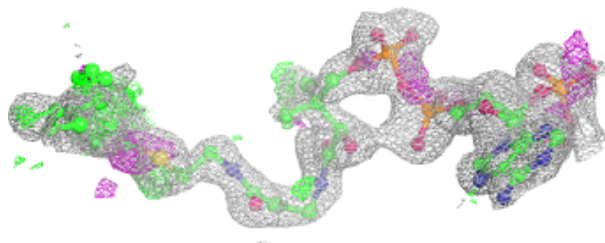
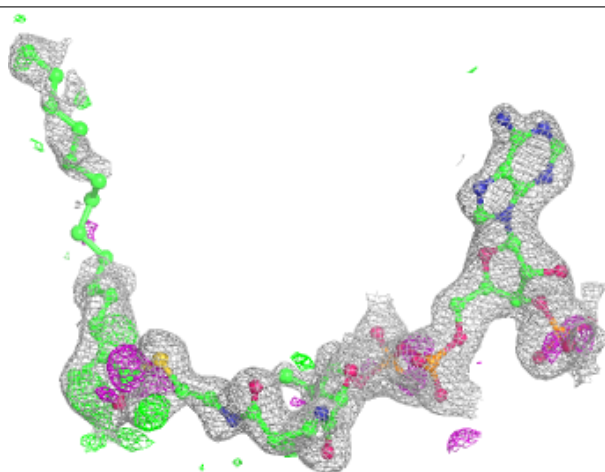
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	B	2304	6/6	0.85	0.13	39,40,42,43	0
2	MRS	A	1751	64/64	0.86	0.14	36,50,58,59	0
3	GOL	D	2303	6/6	0.91	0.10	30,34,35,35	0

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.

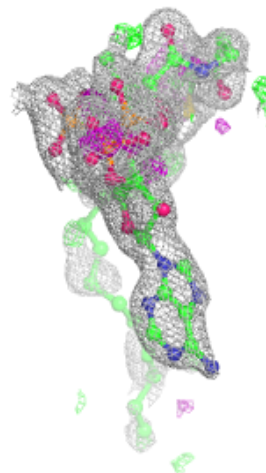
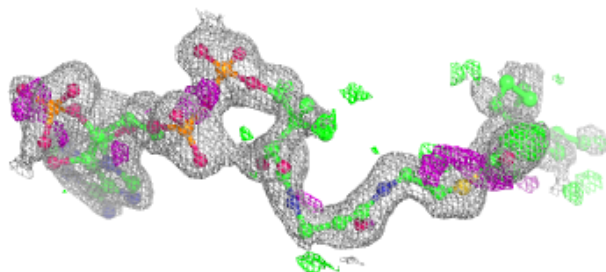
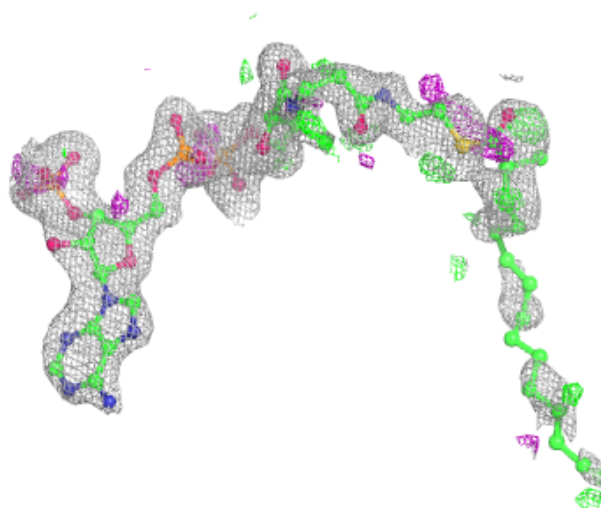
**Electron density around MRS D 1754:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



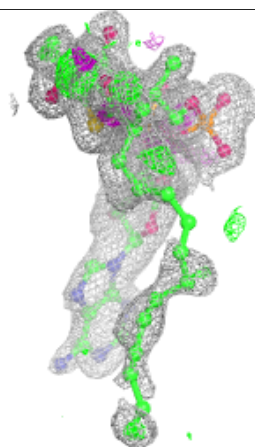
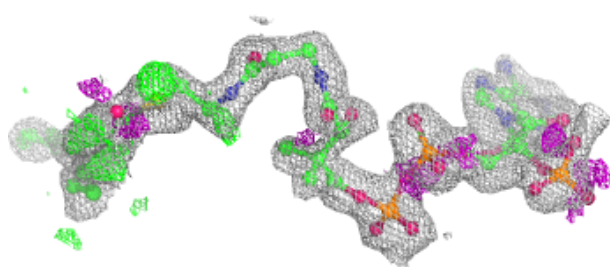
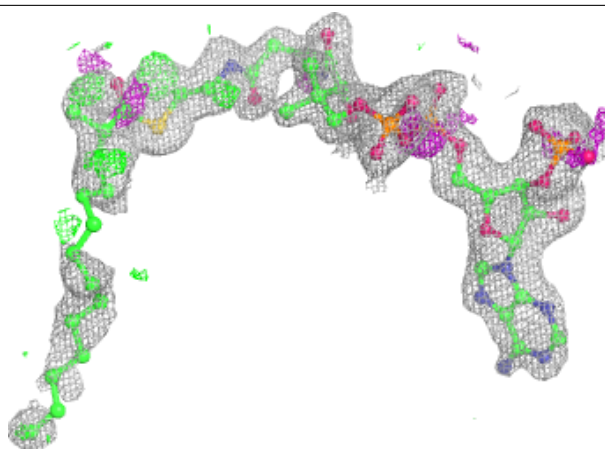
**Electron density around MRS C 1753:**

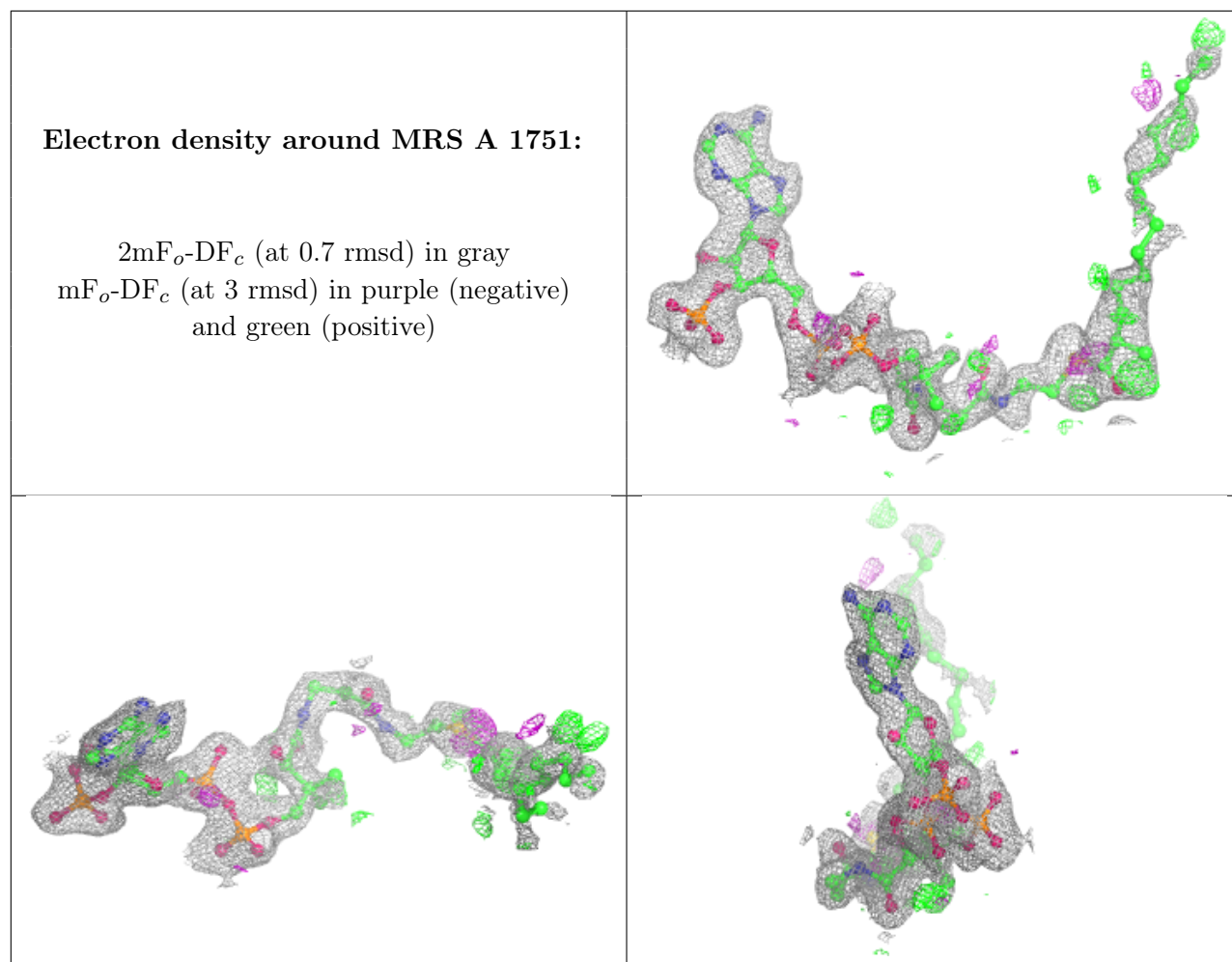
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MRS 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.