



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:10 AM UTC

PDB ID : 2FEU / pdb\_00002feu  
Title : P45OCAM from *Pseudomonas putida* reconstituted with manganic protoporphyrin IX  
Authors : von Koenig, K.; Makris, T.M.; Sligar, S.G.; Schlichting, I.  
Deposited on : 2005-12-16  
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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

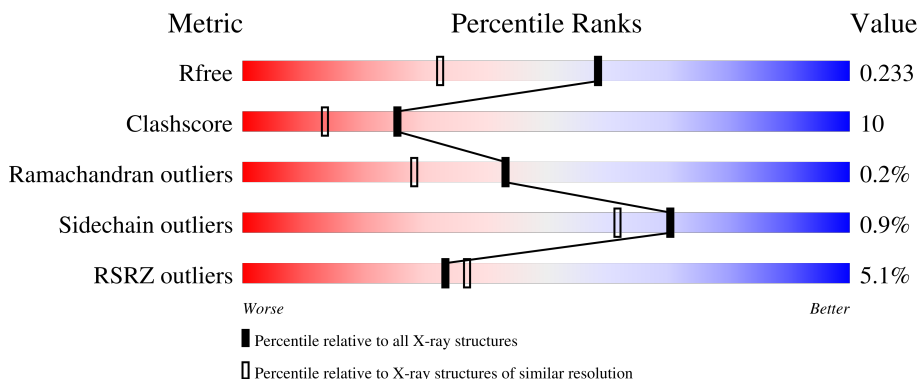
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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	411	
1	B	411	

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
5	TRS	A	1430	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7252 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 Cytochrome P450-cam.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3199	2029	558	594	18	0	0	0
1	B	405	3207	2033	560	596	18	0	0	0

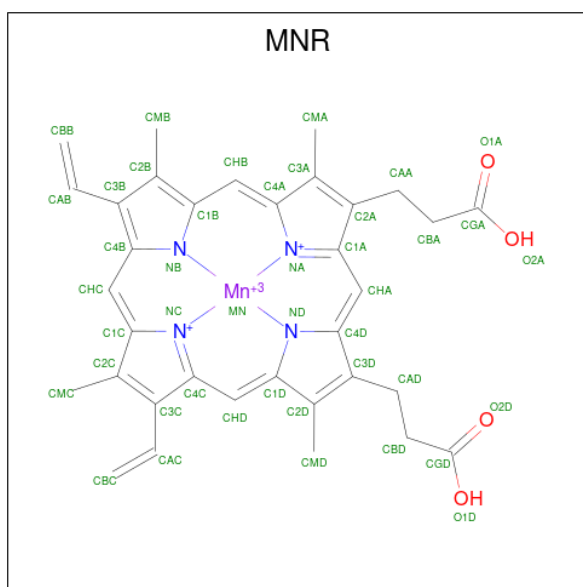
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	415	HIS	-	expression tag	UNP P00183
A	416	HIS	-	expression tag	UNP P00183
A	417	HIS	-	expression tag	UNP P00183
A	418	HIS	-	expression tag	UNP P00183
A	419	HIS	-	expression tag	UNP P00183
A	420	HIS	-	expression tag	UNP P00183
B	415	HIS	-	expression tag	UNP P00183
B	416	HIS	-	expression tag	UNP P00183
B	417	HIS	-	expression tag	UNP P00183
B	418	HIS	-	expression tag	UNP P00183
B	419	HIS	-	expression tag	UNP P00183
B	420	HIS	-	expression tag	UNP P00183

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

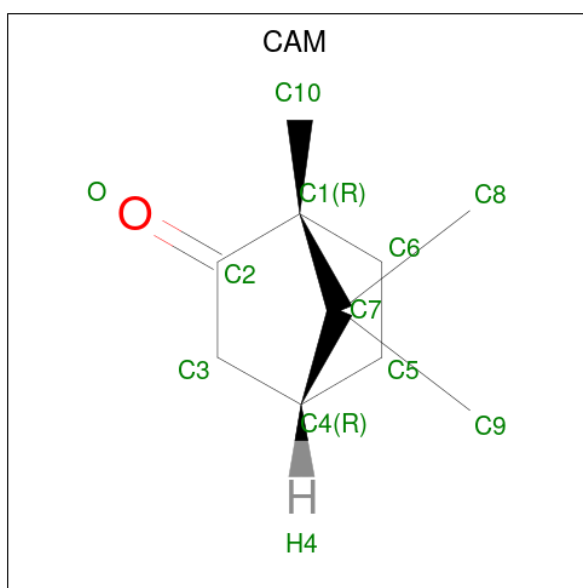
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	2	Total K 2 2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING MN (CCD ID: MNR) (formula: C<sub>34</sub>H<sub>32</sub>MnN<sub>4</sub>O<sub>4</sub>).



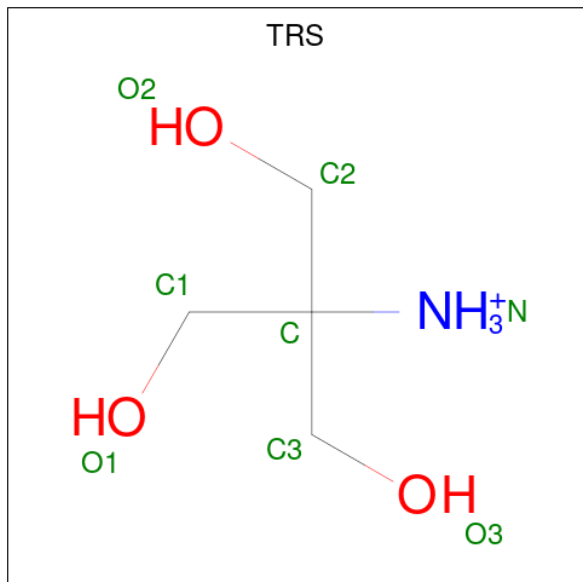
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Mn	N			O
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0

- Molecule 4 is CAMPHOR (CCD ID: CAM) (formula:  $C_{10}H_{16}O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	11	10	1	0	0
4	B	1	11	10	1	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	8	4	1	3	0	0

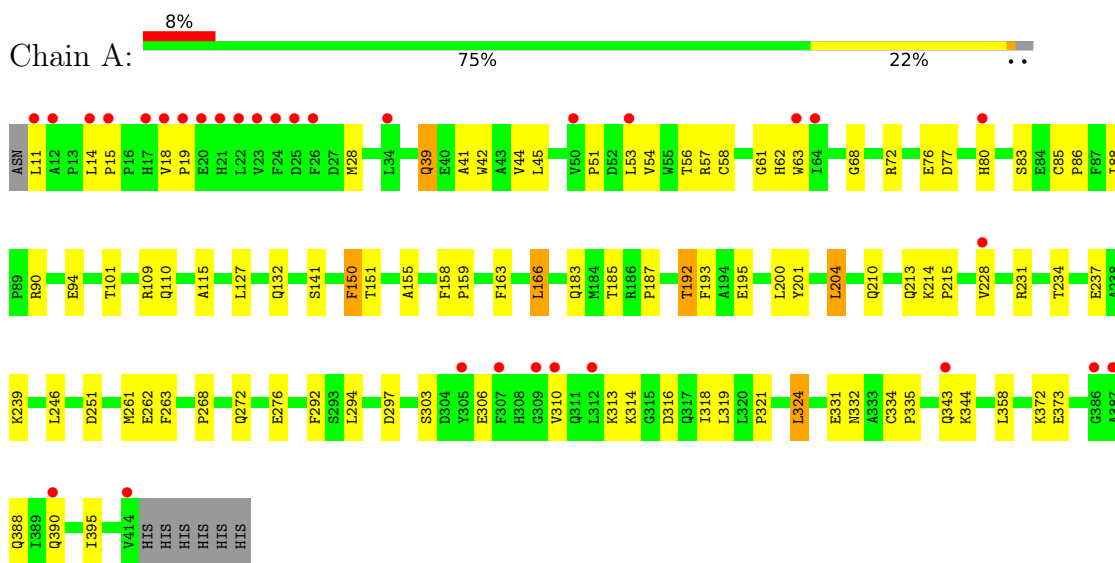
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		
6	B	427	Total	O	0	0
			427	427		

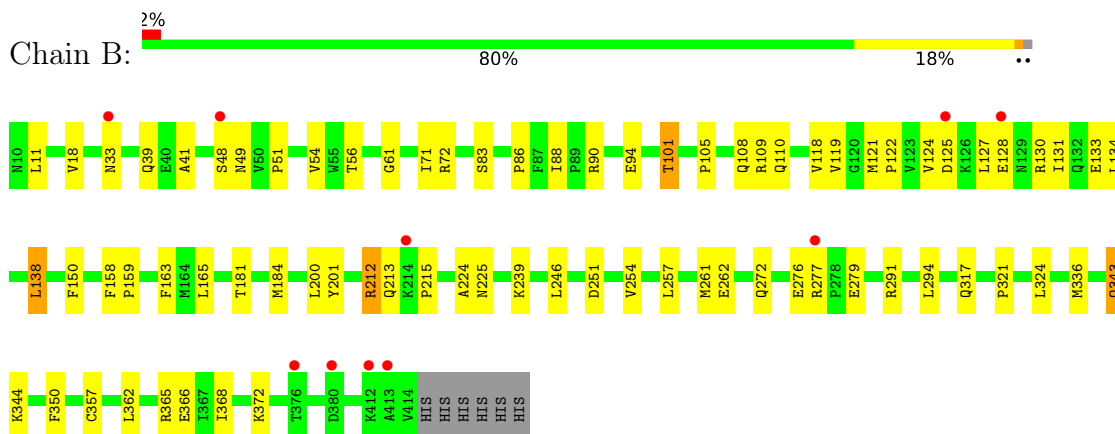
### 3 Residue-property plots [i](#)

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: Cytochrome P450-cam



- Molecule 1: Cytochrome P450-cam



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.13Å 62.23Å 94.71Å 90.00° 90.64° 90.00°	Depositor
Resolution (Å)	19.80 – 1.70 19.80 – 1.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (19.80-1.70) 97.2 (19.80-1.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 1.70Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.238 0.210 , 0.233	Depositor DCC
$R_{free}$ test set	4183 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAM, TRS, MNR, K

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	0.36	0/3278	0.89	11/4454 (0.2%)
1	B	0.38	0/3286	0.91	11/4465 (0.2%)
All	All	0.37	0/6564	0.90	22/8919 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	LEU	N-CA-C	7.33	120.32	111.82
1	B	109	ARG	N-CA-C	6.99	119.49	111.11
1	B	105	PRO	N-CA-C	-6.97	102.19	110.70
1	A	85	CYS	CA-C-N	6.69	126.40	119.64
1	A	85	CYS	C-N-CA	6.69	126.40	119.64
1	A	101	THR	N-CA-C	6.35	119.01	111.33
1	A	324	LEU	N-CA-C	6.28	119.11	111.82
1	A	150	PHE	N-CA-C	6.17	118.51	111.11
1	A	204	LEU	N-CA-C	5.93	117.82	111.36
1	A	192	THR	N-CA-C	-5.89	102.92	110.53
1	B	251	ASP	N-CA-C	5.59	117.60	110.61
1	A	251	ASP	N-CA-C	5.58	117.58	110.61
1	A	334	CYS	CA-C-N	5.39	125.47	119.32
1	A	334	CYS	C-N-CA	5.39	125.47	119.32
1	B	212	ARG	N-CA-C	-5.39	106.54	113.23
1	B	343	GLN	N-CA-C	5.39	116.83	111.07
1	B	48	SER	N-CA-C	5.37	122.23	110.80
1	B	101	THR	N-CA-C	5.37	117.13	111.28
1	B	108	GLN	N-CA-C	5.35	117.11	111.28
1	A	262	GLU	N-CA-C	-5.16	105.57	111.14
1	B	262	GLU	N-CA-C	-5.15	105.74	111.36
1	B	18	VAL	N-CA-C	5.04	112.85	107.76

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3199	0	3150	74	0
1	B	3207	0	3156	48	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	11	0	16	0	0
4	B	11	0	16	0	0
5	A	8	0	12	1	0
6	A	300	0	0	13	0
6	B	427	0	0	6	0
All	All	7252	0	6410	124	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 10.

All (124) 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:130:ARG:HD2	1:B:165:LEU:HD21	1.53	0.90
1:B:121:MET:HE3	1:B:124:VAL:HB	1.64	0.79
1:A:332:ASN:HB2	6:A:1476:HOH:O	1.85	0.76
1:B:72:ARG:HG3	6:B:1668:HOH:O	1.84	0.76
1:A:163:PHE:HE2	1:A:246:LEU:HD23	1.53	0.74
1:A:158:PHE:HB3	1:A:159:PRO:HD3	1.71	0.73
1:A:335:PRO:HB3	6:A:1476:HOH:O	1.89	0.72
1:A:51:PRO:HG2	1:A:54:VAL:HG12	1.72	0.71
1:A:313:LYS:HB3	1:A:316:ASP:OD2	1.91	0.69
1:A:200:LEU:HD11	1:A:246:LEU:HD13	1.73	0.69
1:A:56:THR:HG23	6:A:1496:HOH:O	1.94	0.68
1:A:56:THR:O	1:A:61:GLY:HA2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD11	1:A:166:LEU:HD12	1.77	0.65
1:B:150:PHE:CZ	1:B:261:MET:HG3	2.33	0.64
1:B:184:MET:HE1	1:B:200:LEU:HD22	1.80	0.64
1:A:15:PRO:HB2	1:A:18:VAL:HG23	1.80	0.63
1:A:268:PRO:HB3	5:A:1430:TRS:H21	1.80	0.63
1:A:90:ARG:O	1:A:94:GLU:HG3	1.99	0.62
1:A:110:GLN:NE2	1:A:228:VAL:HG12	2.14	0.62
1:A:192:THR:OG1	1:A:195:GLU:HG3	1.98	0.62
1:A:321:PRO:HB2	1:A:324:LEU:HD13	1.81	0.61
1:B:372:LYS:NZ	1:B:372:LYS:HB3	2.16	0.61
1:A:11:LEU:HD22	1:A:11:LEU:N	2.16	0.61
1:A:53:LEU:HD11	1:A:63:TRP:HB3	1.82	0.61
1:B:133:GLU:HG2	6:B:1787:HOH:O	1.98	0.61
1:A:294:LEU:HD23	1:A:294:LEU:H	1.65	0.61
1:A:303:SER:HA	1:A:314:LYS:HB2	1.83	0.60
1:B:134:LEU:CD2	1:B:138:LEU:HD22	2.32	0.60
1:B:200:LEU:HD11	1:B:246:LEU:HD13	1.83	0.59
1:A:306:GLU:HG3	6:A:1470:HOH:O	2.01	0.58
1:A:372:LYS:HD2	6:A:1669:HOH:O	2.02	0.58
1:B:181:THR:HA	1:B:184:MET:HE3	1.84	0.58
1:A:321:PRO:CB	1:A:324:LEU:HD13	2.32	0.58
1:B:118:VAL:HG23	1:B:119:VAL:HG13	1.87	0.57
1:B:257:LEU:HA	6:B:1488:HOH:O	2.03	0.57
1:A:45:LEU:HG	6:A:1518:HOH:O	2.06	0.56
1:A:185:THR:HG22	6:A:1529:HOH:O	2.04	0.56
1:A:313:LYS:HE3	6:A:1656:HOH:O	2.06	0.56
1:B:277:ARG:HB3	1:B:279:GLU:OE2	2.07	0.55
1:B:128:GLU:HB2	1:B:365:ARG:HH12	1.71	0.55
1:A:72:ARG:O	1:A:76:GLU:HG3	2.05	0.55
1:B:201:TYR:HB3	1:B:239:LYS:HD2	1.89	0.54
1:A:68:GLY:HA3	1:A:331:GLU:OE2	2.08	0.54
1:B:368:ILE:O	1:B:372:LYS:HG3	2.07	0.54
1:A:310:VAL:N	6:A:1470:HOH:O	2.39	0.54
1:A:344:LYS:N	1:A:344:LYS:HD3	2.23	0.54
1:A:234:THR:OG1	1:A:237:GLU:HG3	2.06	0.54
1:A:42:TRP:HA	6:A:1518:HOH:O	2.08	0.54
1:A:163:PHE:CE2	1:A:246:LEU:HD23	2.40	0.53
1:A:294:LEU:HD23	1:A:294:LEU:N	2.23	0.53
1:B:90:ARG:O	1:B:94:GLU:HG3	2.09	0.53
1:A:83:SER:O	1:A:86:PRO:HD3	2.10	0.52
1:A:150:PHE:CZ	1:A:261:MET:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PRO:HG2	1:B:254:VAL:HG22	1.90	0.51
1:A:28:MET:HE1	1:A:395:ILE:HD13	1.93	0.51
1:A:39:GLN:NE2	1:A:39:GLN:H	2.08	0.51
1:B:134:LEU:HD23	1:B:134:LEU:O	2.10	0.51
1:B:272:GLN:O	1:B:276:GLU:HG3	2.10	0.51
1:B:213:GLN:C	1:B:215:PRO:HD3	2.36	0.50
1:A:77:ASP:OD2	1:A:80:HIS:HB2	2.11	0.50
1:A:62:HIS:CD2	1:A:88:ILE:HD13	2.47	0.50
1:B:294:LEU:H	1:B:294:LEU:HD23	1.76	0.50
1:A:343:GLN:CB	1:A:344:LYS:HD3	2.41	0.49
1:A:110:GLN:HB2	1:A:228:VAL:HG12	1.94	0.49
3:B:731:MNR:HBB1	3:B:731:MNR:HMB1	1.94	0.49
1:A:210:GLN:HE22	1:A:214:LYS:CE	2.26	0.48
1:B:372:LYS:HB3	1:B:372:LYS:HZ3	1.76	0.48
1:B:130:ARG:HD2	1:B:165:LEU:CD2	2.35	0.48
1:A:110:GLN:HE21	1:A:228:VAL:HG12	1.79	0.48
1:B:291:ARG:CZ	1:B:336:MET:HE3	2.44	0.48
1:B:83:SER:HB3	1:B:101:THR:O	2.13	0.48
1:A:51:PRO:HG2	1:A:54:VAL:CG1	2.40	0.48
1:A:201:TYR:HB3	1:A:239:LYS:HD2	1.98	0.46
1:B:121:MET:HB3	1:B:122:PRO:HD3	1.98	0.45
1:B:71:ILE:HB	6:B:1668:HOH:O	2.17	0.45
1:A:158:PHE:CB	1:A:159:PRO:HD3	2.45	0.45
1:B:127:LEU:O	1:B:131:ILE:HG13	2.17	0.45
1:B:158:PHE:HB3	1:B:159:PRO:CD	2.47	0.45
1:A:151:THR:HA	1:A:155:ALA:HB3	1.99	0.45
1:A:272:GLN:O	1:A:276:GLU:HG3	2.17	0.45
1:A:213:GLN:C	1:A:215:PRO:HD3	2.41	0.45
1:A:204:LEU:HD21	1:A:246:LEU:HD11	1.98	0.45
1:A:210:GLN:NE2	1:A:214:LYS:HE2	2.32	0.45
1:B:213:GLN:O	1:B:215:PRO:HD3	2.17	0.44
1:A:57:ARG:HG2	6:A:1528:HOH:O	2.17	0.44
1:A:15:PRO:HB2	1:A:18:VAL:CG2	2.47	0.44
1:A:14:LEU:HD12	1:A:15:PRO:HD2	1.99	0.43
1:B:343:GLN:O	1:B:344:LYS:HD3	2.17	0.43
1:A:388:GLN:O	1:A:390:GLN:OE1	2.36	0.43
1:A:58:CYS:N	6:A:1437:HOH:O	2.51	0.43
1:A:313:LYS:HG2	1:A:314:LYS:N	2.34	0.43
1:B:294:LEU:HD23	1:B:294:LEU:N	2.33	0.43
1:A:41:ALA:O	1:A:44:VAL:HG22	2.19	0.43
1:A:109:ARG:HH11	1:A:109:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:HA	1:B:225:ASN:HD21	1.83	0.43
1:B:362:LEU:O	1:B:366:GLU:HG3	2.19	0.43
1:A:88:ILE:HD12	1:A:319:LEU:HD13	2.01	0.42
1:B:163:PHE:CE2	1:B:246:LEU:HD23	2.53	0.42
1:A:343:GLN:HB3	1:A:344:LYS:HD3	2.00	0.42
1:B:121:MET:HE2	1:B:125:ASP:OD1	2.19	0.42
1:B:350:PHE:HB3	1:B:357:CYS:HB3	2.01	0.42
1:A:115:ALA:HB3	1:A:358:LEU:HD13	2.00	0.42
1:A:318:ILE:O	1:A:318:ILE:HG23	2.19	0.42
1:B:279:GLU:H	1:B:279:GLU:CD	2.27	0.42
1:A:297:ASP:OD2	3:A:730:MNR:O2A	2.37	0.42
1:B:49:ASN:ND2	6:B:1584:HOH:O	2.51	0.42
1:B:212:ARG:HG3	1:B:224:ALA:HB1	2.01	0.42
1:B:272:GLN:HG3	1:B:276:GLU:HG3	2.01	0.42
1:A:183:GLN:O	1:A:187:PRO:HB3	2.21	0.41
1:A:210:GLN:HE22	1:A:214:LYS:HE3	1.85	0.41
3:A:730:MNR:HMB1	3:A:730:MNR:HBB1	2.01	0.41
1:B:33:ASN:HB3	1:B:41:ALA:HA	2.02	0.41
1:A:231:ARG:HD2	1:A:231:ARG:C	2.46	0.41
1:B:56:THR:O	1:B:61:GLY:HA2	2.20	0.41
1:B:88:ILE:HD11	1:B:317:GLN:HB3	2.01	0.41
1:A:263:PHE:HB2	1:A:292:PHE:CZ	2.56	0.41
1:A:42:TRP:HB3	1:A:324:LEU:HD11	2.03	0.41
1:A:141:SER:HB3	6:A:1633:HOH:O	2.21	0.41
1:B:110:GLN:NE2	6:B:1657:HOH:O	2.51	0.40
1:B:291:ARG:NH2	1:B:336:MET:HE3	2.37	0.40
1:A:132:GLN:HE22	1:A:373:GLU:CD	2.29	0.40
1:A:294:LEU:N	1:A:294:LEU:CD2	2.84	0.40
1:A:193:PHE:CD1	1:A:193:PHE:C	2.99	0.40
1:B:51:PRO:HG2	1:B:54:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/411 (98%)	386 (96%)	15 (4%)	1 (0%)	43	28
1	B	403/411 (98%)	392 (97%)	10 (2%)	1 (0%)	43	28
All	All	805/822 (98%)	778 (97%)	25 (3%)	2 (0%)	43	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
1	B	321	PRO

### 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	349/356 (98%)	347 (99%)	2 (1%)	78	72
1	B	350/356 (98%)	346 (99%)	4 (1%)	65	54
All	All	699/712 (98%)	693 (99%)	6 (1%)	70	62

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	166	LEU
1	B	11	LEU
1	B	39	GLN
1	B	86	PRO
1	B	138	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	39	GLN
1	A	46	GLN
1	A	110	GLN
1	A	117	GLN
1	A	132	GLN
1	A	145	GLN
1	A	210	GLN
1	A	225	ASN
1	A	229	ASN
1	A	272	GLN
1	A	311	GLN
1	A	337	HIS
1	B	30	ASN
1	B	33	ASN
1	B	39	GLN
1	B	46	GLN
1	B	49	ASN
1	B	69	GLN
1	B	110	GLN
1	B	132	GLN
1	B	210	GLN
1	B	225	ASN
1	B	227	GLN
1	B	272	GLN
1	B	317	GLN
1	B	388	GLN
1	B	400	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	MNR	B	731	1	37,50,50	2.04	6 (16%)	34,82,82	1.70	8 (23%)
4	CAM	B	1421	-	12,12,12	1.42	2 (16%)	20,21,21	1.17	2 (10%)
3	MNR	A	730	1	37,50,50	2.24	4 (10%)	34,82,82	1.80	8 (23%)
5	TRS	A	1430	-	7,7,7	0.80	0	9,9,9	5.91	5 (55%)
4	CAM	A	1420	-	12,12,12	1.49	4 (33%)	20,21,21	1.21	2 (10%)

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	MNR	B	731	1	-	2/12/94/94	-
4	CAM	B	1421	-	-	-	0/3/2/2
3	MNR	A	730	1	-	1/12/94/94	-
5	TRS	A	1430	-	-	6/9/9/9	-
4	CAM	A	1420	-	-	-	0/3/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	730	MNR	CAC-C3C	-6.78	1.39	1.47
3	A	730	MNR	C1D-C2D	6.71	1.47	1.39
3	B	731	MNR	C1D-C2D	5.76	1.46	1.39
3	A	730	MNR	C1B-C2B	5.71	1.46	1.39
3	B	731	MNR	CAC-C3C	-5.59	1.40	1.47
3	A	730	MNR	C3B-C4B	5.58	1.46	1.41
3	B	731	MNR	C3B-C4B	5.21	1.46	1.41
3	B	731	MNR	C1B-C2B	4.64	1.44	1.39
4	A	1420	CAM	C1-C2	2.96	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	731	MNR	CMA-C3A	2.82	1.55	1.50
4	B	1421	CAM	C1-C2	2.38	1.56	1.52
4	A	1420	CAM	C3-C4	2.13	1.58	1.53
4	B	1421	CAM	C3-C4	2.12	1.58	1.53
3	B	731	MNR	CMC-C2C	2.09	1.53	1.50
4	A	1420	CAM	C5-C4	2.04	1.59	1.53
4	A	1420	CAM	C6-C1	2.03	1.62	1.55

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1430	TRS	C1-C-N	-10.31	81.87	108.17
5	A	1430	TRS	C2-C-N	-9.81	83.15	108.17
5	A	1430	TRS	C3-C-N	-8.94	85.38	108.17
5	A	1430	TRS	C2-C-C1	4.33	122.19	110.66
3	A	730	MNR	CHA-C1A-NA	4.28	125.14	120.60
3	A	730	MNR	CHB-C4A-NA	4.00	124.85	120.60
3	B	731	MNR	CHC-C1C-NC	3.89	124.73	120.60
3	A	730	MNR	CHC-C1C-NC	3.85	124.69	120.60
3	B	731	MNR	CHB-C4A-NA	3.40	124.21	120.60
5	A	1430	TRS	C3-C-C1	3.25	119.31	110.66
4	A	1420	CAM	C7-C1-C2	3.24	105.85	100.33
4	B	1421	CAM	C7-C1-C2	3.21	105.81	100.33
3	A	730	MNR	CHD-C4C-NC	3.19	123.99	120.60
3	B	731	MNR	C1A-CHA-C4D	3.01	126.84	116.07
3	A	730	MNR	C1C-CHC-C4B	2.87	126.36	116.07
3	B	731	MNR	C1C-CHC-C4B	2.87	126.35	116.07
3	B	731	MNR	C4A-CHB-C1B	2.86	126.31	116.07
3	B	731	MNR	C4C-CHD-C1D	2.85	126.26	116.07
3	A	730	MNR	C1A-CHA-C4D	2.78	126.02	116.07
3	B	731	MNR	CHD-C4C-NC	2.72	123.49	120.60
3	A	730	MNR	C4C-CHD-C1D	2.63	125.47	116.07
3	A	730	MNR	C4A-CHB-C1B	2.51	125.05	116.07
3	B	731	MNR	CHA-C1A-NA	2.43	123.17	120.60
4	A	1420	CAM	O-C2-C1	2.27	128.05	125.33
4	B	1421	CAM	O-C2-C1	2.05	127.79	125.33

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1430	TRS	C3-C-C1-O1

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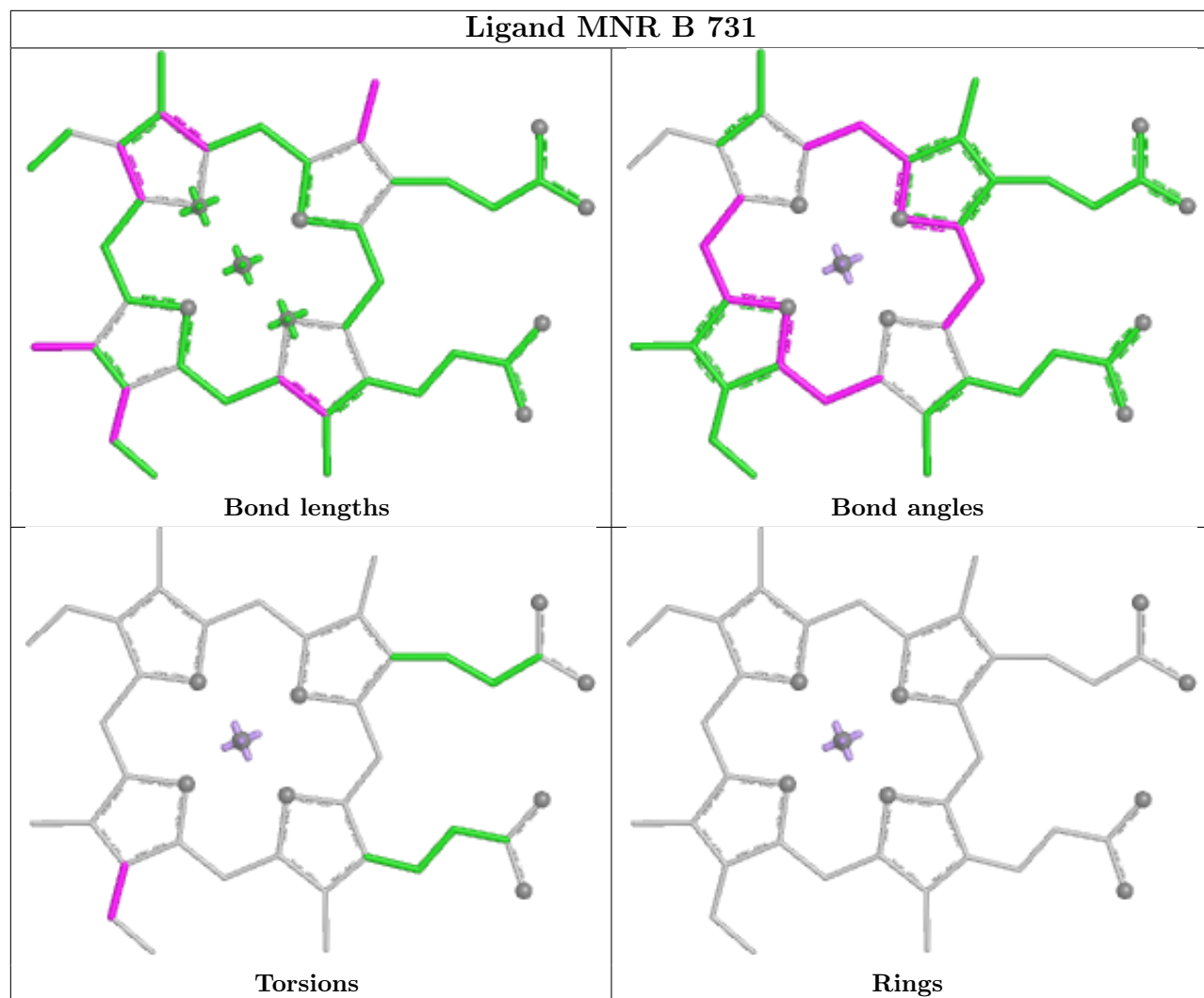
Mol	Chain	Res	Type	Atoms
5	A	1430	TRS	N-C-C1-O1
5	A	1430	TRS	C3-C-C2-O2
5	A	1430	TRS	N-C-C2-O2
5	A	1430	TRS	C1-C-C3-O3
5	A	1430	TRS	N-C-C3-O3
3	B	731	MNR	C2C-C3C-CAC-CBC
3	A	730	MNR	C2C-C3C-CAC-CBC
3	B	731	MNR	C4C-C3C-CAC-CBC

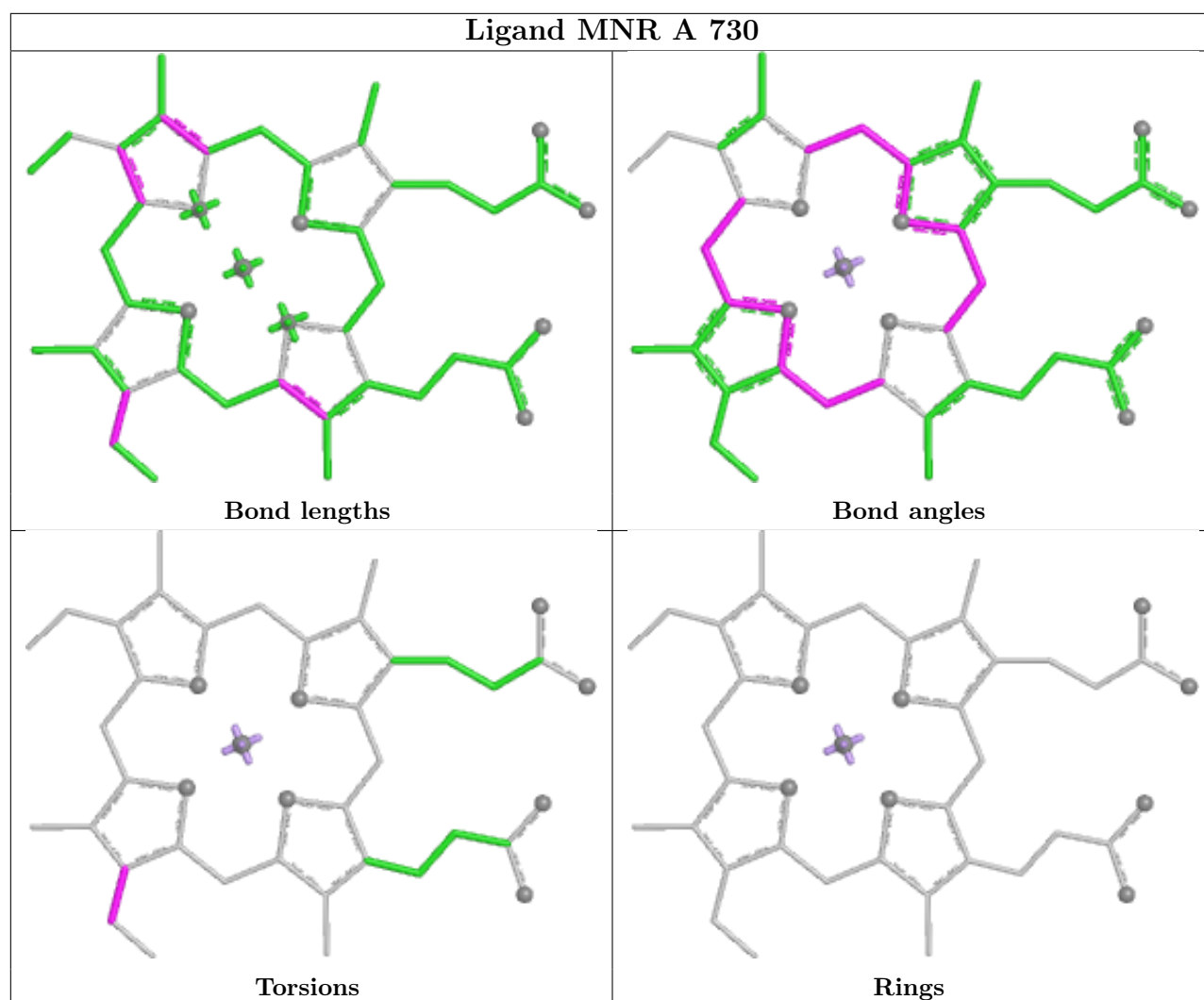
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	731	MNR	1	0
3	A	730	MNR	2	0
5	A	1430	TRS	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	404/411 (98%)	0.66	31 (7%) 19 21	13, 24, 32, 35	0
1	B	405/411 (98%)	0.17	10 (2%) 58 62	9, 19, 30, 33	1 (0%)
All	All	809/822 (98%)	0.42	41 (5%) 33 37	9, 22, 31, 35	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	GLY	4.0
1	A	11	LEU	4.0
1	A	15	PRO	3.4
1	A	19	PRO	3.4
1	A	414	VAL	3.4
1	A	24	PHE	3.2
1	A	228	VAL	3.2
1	A	18	VAL	3.0
1	A	17	HIS	2.9
1	A	63	TRP	2.8
1	B	413	ALA	2.8
1	A	25	ASP	2.8
1	A	26	PHE	2.7
1	A	14	LEU	2.7
1	A	390	GLN	2.7
1	B	277	ARG	2.6
1	A	307	PHE	2.6
1	A	53	LEU	2.6
1	A	12	ALA	2.6
1	A	386	GLY	2.5
1	A	22	LEU	2.5
1	A	50	VAL	2.5
1	A	21	HIS	2.4
1	B	33	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	312	LEU	2.4
1	A	20	GLU	2.4
1	A	23	VAL	2.3
1	B	128	GLU	2.3
1	B	376	THR	2.3
1	A	305	TYR	2.3
1	A	64	ILE	2.2
1	A	310	VAL	2.2
1	A	387	ALA	2.2
1	A	343	GLN	2.1
1	A	34	LEU	2.1
1	A	80	HIS	2.1
1	B	125	ASP	2.1
1	B	380	ASP	2.0
1	B	214	LYS	2.0
1	B	48	SER	2.0
1	B	412	LYS	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 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, 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.

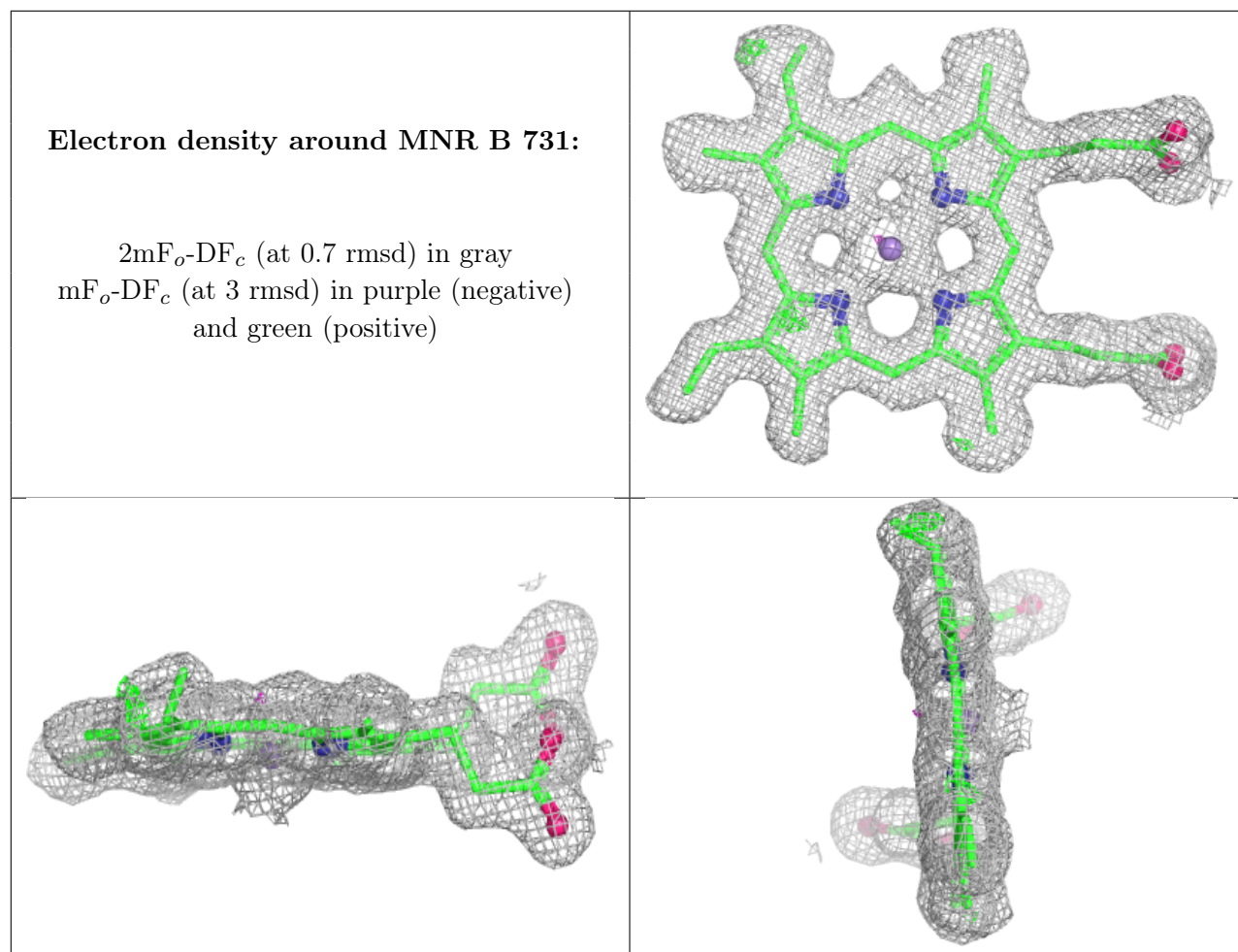
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TRS	A	1430	8/8	0.68	0.21	14,21,25,28	0
4	CAM	B	1421	11/11	0.93	0.07	12,14,16,17	0
4	CAM	A	1420	11/11	0.94	0.06	20,21,21,22	0
2	K	A	729	1/1	0.97	0.04	24,24,24,24	0
3	MNR	B	731	43/43	0.98	0.06	8,14,18,25	0
3	MNR	A	730	43/43	0.98	0.06	15,19,21,24	0

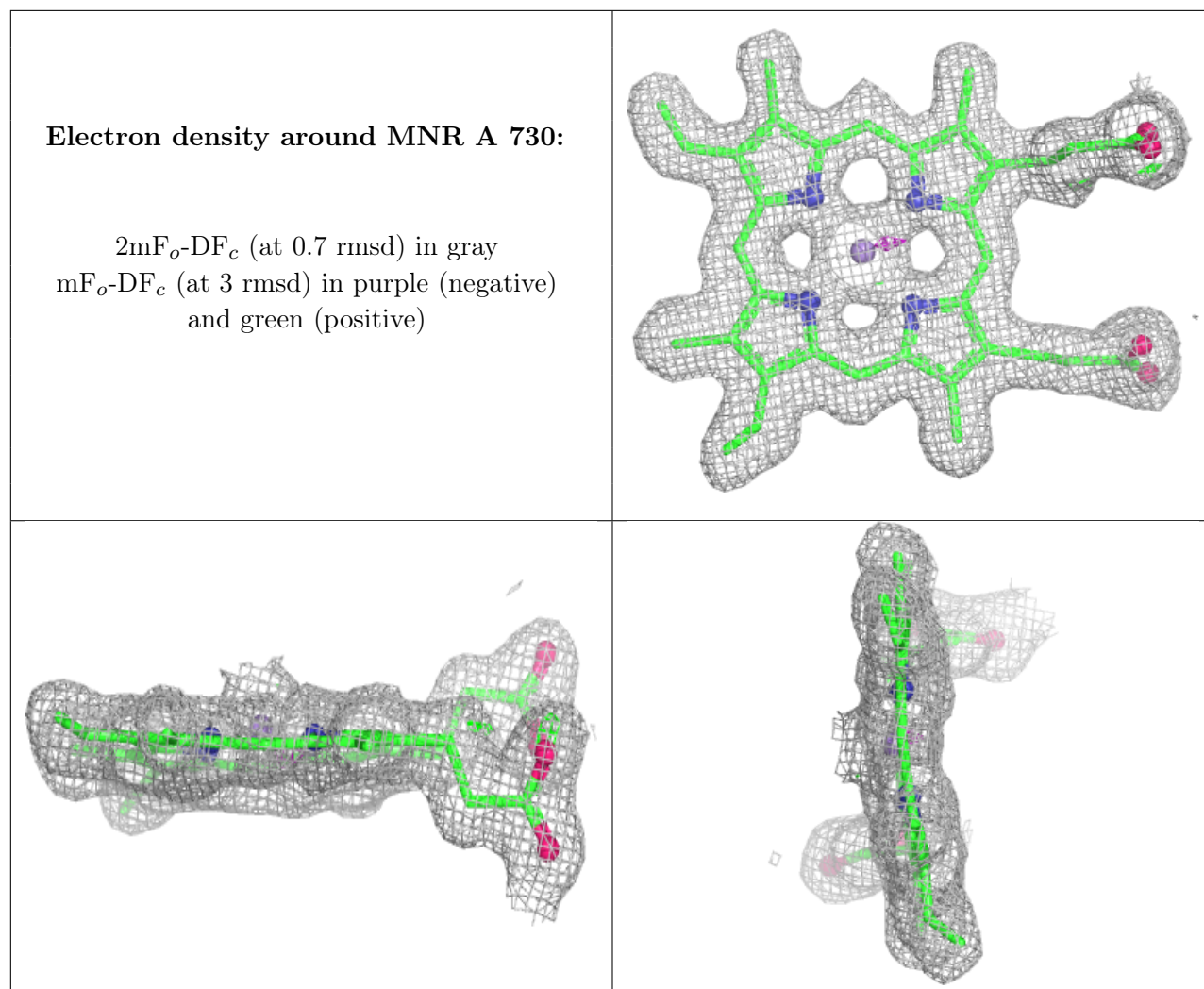
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	B	730	1/1	1.00	0.04	16,16,16,16	0
2	K	B	728	1/1	1.00	0.02	14,14,14,14	0

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.





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.