



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 1, 2025 – 10:10 PM JST

PDB ID : 9JFC / pdb\_00009jfc  
Title : Crystal structure of Pseudomonas aeruginosa SuhB complexed with Gallic acid  
in monoclinic space group  
Authors : Yadav, V.K.; Shukla, M.; Maji, S.; Bhattacharyya, S.  
Deposited on : 2024-09-04  
Resolution : 2.20 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 Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

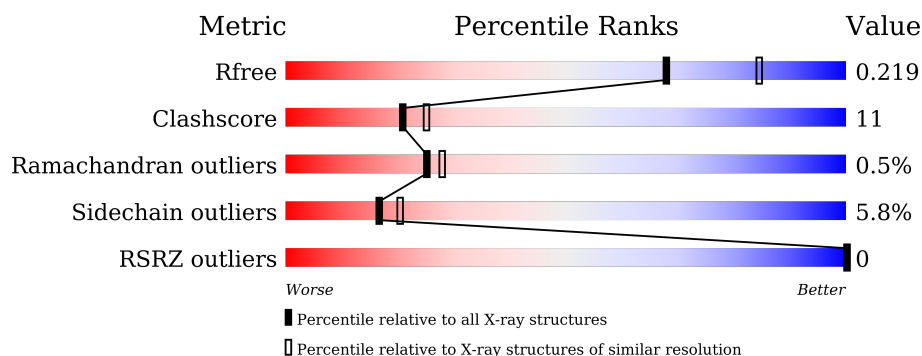
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	273	 73% 23% ..
1	E	273	 74% 21% ..
1	I	273	 73% 23% ..
1	M	273	 83% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	E	302	-	-	X	-
3	GDE	A	304	-	-	X	-
3	GDE	M	301	-	-	X	-
4	DTT	I	403	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8715 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 Nus factor SuhB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2067	1305	370	385	7			
1	E	270	Total	C	N	O	S	0	0	0
			2067	1305	370	385	7			
1	I	272	Total	C	N	O	S	0	0	0
			2077	1310	372	388	7			
1	M	272	Total	C	N	O	S	0	0	0
			2077	1310	372	388	7			

There are 12 discrepancies between the modelled and reference sequences:

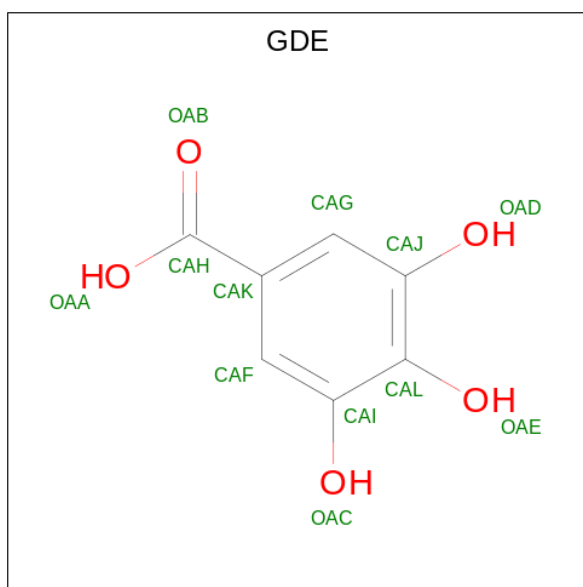
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q9HXI4
A	0	SER	-	cloning artifact	UNP Q9HXI4
A	71	LEU	PHE	cloning artifact	UNP Q9HXI4
E	-1	GLY	-	cloning artifact	UNP Q9HXI4
E	0	SER	-	cloning artifact	UNP Q9HXI4
E	71	LEU	PHE	cloning artifact	UNP Q9HXI4
I	-1	GLY	-	cloning artifact	UNP Q9HXI4
I	0	SER	-	cloning artifact	UNP Q9HXI4
I	71	LEU	PHE	cloning artifact	UNP Q9HXI4
M	-1	GLY	-	cloning artifact	UNP Q9HXI4
M	0	SER	-	cloning artifact	UNP Q9HXI4
M	71	LEU	PHE	cloning artifact	UNP Q9HXI4

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



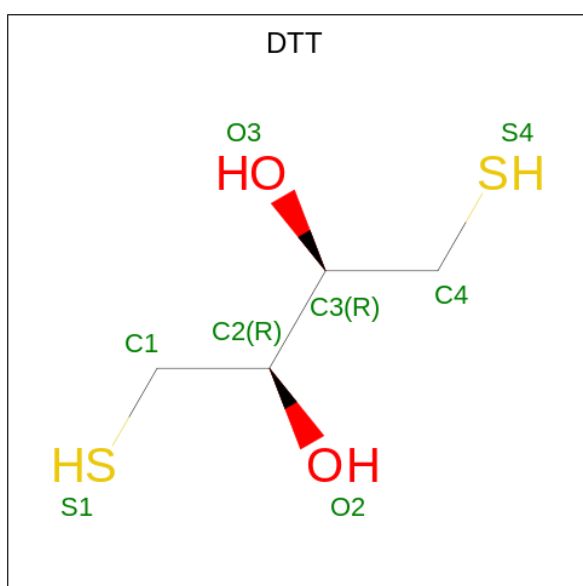
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 3,4,5-trihydroxybenzoic acid (CCD ID: GDE) (formula:  $C_7H_6O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		
3	A	1	Total	C	O	0	0
			12	7	5		
3	I	1	Total	C	O	0	0
			12	7	5		
3	M	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	O	S	0	0
			8	4	2	2		
4	I	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is water.

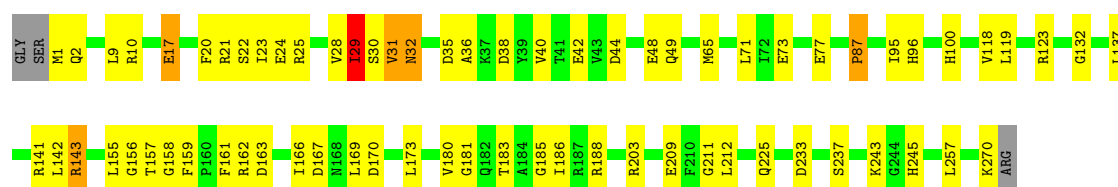
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	E	83	Total	O	0	0
			83	83		
5	I	92	Total	O	0	0
			92	92		
5	M	77	Total	O	0	0
			77	77		

### 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.

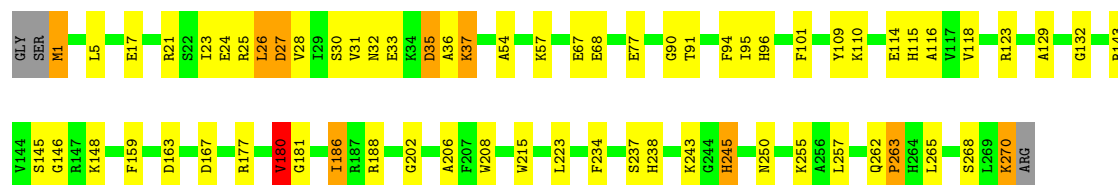
#### • Molecule 1: Nus factor SuhB

Chain A: 



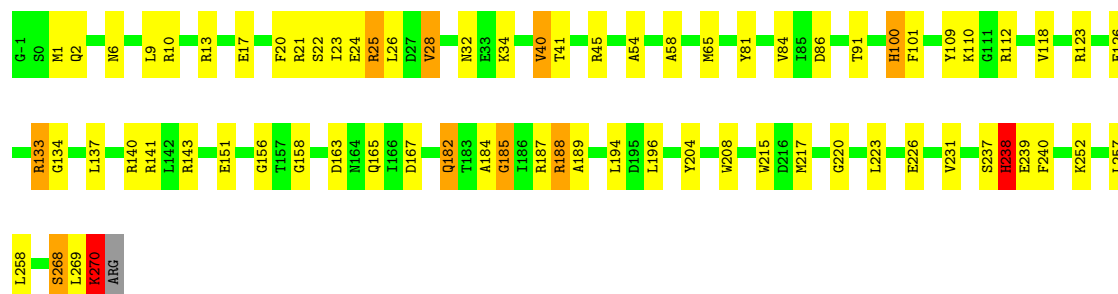
#### • Molecule 1: Nus factor SuhB

Chain E: 




#### • Molecule 1: Nus factor SuhB

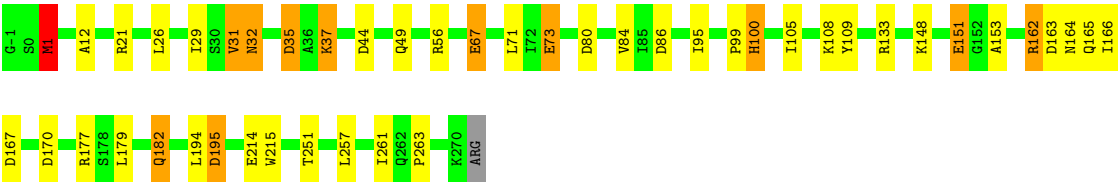
Chain I: 



#### • Molecule 1: Nus factor SuhB

Chain M: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.17Å 90.60Å 89.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.98 – 2.20 44.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.98-2.20) 99.5 (44.98-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.30 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.21.2-5419	Depositor
R, $R_{free}$	0.182 , 0.234 0.171 , 0.219	Depositor DCC
$R_{free}$ test set	2505 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 22.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.015 for -h,l,k 0.469 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTT, GOL, GDE

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	1.26	7/2107 (0.3%)	1.45	5/2849 (0.2%)
1	E	1.29	8/2107 (0.4%)	1.49	2/2849 (0.1%)
1	I	1.33	10/2117 (0.5%)	1.47	9/2862 (0.3%)
1	M	1.28	4/2117 (0.2%)	1.43	4/2862 (0.1%)
All	All	1.29	29/8448 (0.3%)	1.46	20/11422 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	I	0	1
All	All	0	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	238	HIS	CE1-NE2	8.65	1.41	1.32
1	I	101	PHE	C-O	8.31	1.33	1.23
1	E	101	PHE	C-O	7.01	1.31	1.23
1	A	100	HIS	CE1-NE2	6.94	1.39	1.32
1	M	100	HIS	CE1-NE2	6.90	1.39	1.32
1	A	119	LEU	C-O	-6.63	1.16	1.24
1	E	245	HIS	C-O	6.47	1.31	1.24
1	I	156	GLY	C-O	6.47	1.32	1.23
1	I	100	HIS	CE1-NE2	6.02	1.38	1.32
1	I	185	GLY	C-O	-5.97	1.17	1.24
1	M	195	ASP	CG-OD2	-5.77	1.14	1.25
1	E	263	PRO	C-O	-5.68	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	118	VAL	C-O	5.57	1.30	1.24
1	I	239	GLU	C-O	-5.47	1.16	1.24
1	E	206	ALA	C-O	5.40	1.30	1.23
1	E	35	ASP	C-O	5.38	1.30	1.24
1	E	167	ASP	C-O	5.38	1.30	1.24
1	A	118	VAL	C-O	5.37	1.30	1.24
1	E	202	GLY	C-O	5.32	1.31	1.24
1	A	158	GLY	C-O	5.27	1.29	1.24
1	I	40	VAL	C-O	5.26	1.30	1.24
1	M	153	ALA	C-O	5.23	1.30	1.23
1	A	209	GLU	CD-OE1	-5.20	1.15	1.25
1	E	118	VAL	C-O	5.18	1.29	1.24
1	I	188	ARG	CD-NE	-5.18	1.39	1.46
1	A	87	PRO	C-O	-5.14	1.18	1.24
1	A	212	LEU	C-O	5.14	1.30	1.23
1	I	208	TRP	C-O	5.12	1.30	1.23
1	M	263	PRO	C-O	-5.00	1.17	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	182	GLN	CB-CG-CD	7.09	124.66	112.60
1	I	270	LYS	CA-C-O	6.31	131.52	120.80
1	E	27	ASP	N-CA-C	-6.22	104.61	111.82
1	A	270	LYS	CA-C-O	5.77	130.61	120.80
1	A	157	THR	CA-CB-OG1	5.74	118.20	109.60
1	I	165	GLN	CA-C-O	-5.66	114.96	121.47
1	E	24	GLU	CA-C-O	-5.48	115.07	120.82
1	M	73	GLU	N-CA-CB	5.30	118.51	110.45
1	I	187	ARG	CA-C-O	-5.22	115.07	120.70
1	I	182	GLN	N-CA-CB	-5.21	102.93	110.70
1	A	38	ASP	CA-CB-CG	-5.20	107.40	112.60
1	I	258	LEU	CA-C-N	5.18	127.18	120.44
1	I	258	LEU	C-N-CA	5.18	127.18	120.44
1	A	42	GLU	N-CA-CB	5.18	117.52	110.01
1	A	156	GLY	CA-C-O	-5.12	115.92	120.94
1	I	40	VAL	O-C-N	5.07	126.88	121.91
1	M	67	GLU	CA-C-N	5.04	127.29	120.44
1	M	67	GLU	C-N-CA	5.04	127.29	120.44
1	I	133	ARG	N-CA-CB	5.01	119.26	110.98
1	M	182	GLN	CB-CG-CD	5.01	121.12	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	180	VAL	Peptide
1	I	269	LEU	Peptide

## 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	2067	0	2054	46	1
1	E	2067	0	2054	46	3
1	I	2077	0	2062	62	2
1	M	2077	0	2062	37	2
2	A	12	0	16	2	0
2	E	6	0	8	6	0
2	I	6	0	8	3	0
2	M	6	0	8	0	0
3	A	24	0	8	4	0
3	I	12	0	4	2	0
3	M	12	0	4	6	0
4	E	8	0	10	0	0
4	I	8	0	10	7	0
5	A	81	0	0	10	0
5	E	83	0	0	9	0
5	I	92	0	0	22	0
5	M	77	0	0	12	0
All	All	8715	0	8308	182	4

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 11.

All (182) 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:I:54:ALA:O	5:I:501:HOH:O	1.66	1.13
1:A:65:MET:HE3	1:A:71:LEU:HB2	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:LYS:NZ	5:E:402:HOH:O	1.92	1.01
1:A:29:ILE:HG21	1:A:95:ILE:O	1.66	0.94
1:I:163:ASP:OD1	5:I:503:HOH:O	1.89	0.88
1:E:68:GLU:OE2	5:E:401:HOH:O	1.91	0.88
1:A:170:ASP:OD1	1:E:177:ARG:NH1	2.06	0.88
1:M:67:GLU:OE2	5:M:401:HOH:O	1.91	0.86
1:M:109:TYR:HA	5:M:402:HOH:O	1.77	0.85
1:M:80:ASP:O	5:M:402:HOH:O	1.93	0.83
1:I:1:MET:SD	5:I:581:HOH:O	2.36	0.83
1:I:140:ARG:O	5:I:504:HOH:O	1.97	0.82
1:I:151:GLU:HA	1:I:182:GLN:CG	2.10	0.81
1:I:137:LEU:HB3	5:I:504:HOH:O	1.82	0.79
1:I:151:GLU:HA	1:I:182:GLN:HG2	1.68	0.75
1:E:116:ALA:HB3	5:E:411:HOH:O	1.85	0.75
1:M:108:LYS:NZ	1:M:214:GLU:OE2	2.19	0.74
3:I:401:GDE:OAA	5:I:505:HOH:O	2.04	0.74
1:I:252:LYS:NZ	5:I:502:HOH:O	1.82	0.74
1:A:17:GLU:OE1	1:A:21:ARG:NH2	2.21	0.73
1:I:270:LYS:NZ	5:I:509:HOH:O	2.18	0.73
1:A:20:PHE:O	1:A:23:ILE:HG22	1.88	0.73
1:A:31:VAL:HG23	1:A:32:ASN:H	1.51	0.73
3:A:304:GDE:CAH	1:E:188:ARG:HD3	2.19	0.73
1:I:184:ALA:O	5:I:506:HOH:O	2.07	0.72
1:I:189:ALA:HB1	4:I:403:DTT:H42	1.71	0.72
1:E:54:ALA:O	5:E:403:HOH:O	2.09	0.71
1:E:91:THR:HG23	2:E:302:GOL:H11	1.73	0.69
1:E:1:MET:HB3	1:E:5:LEU:HD23	1.74	0.68
1:M:151:GLU:HA	1:M:182:GLN:HG2	1.75	0.68
1:M:162:ARG:NH2	3:M:301:GDE:OAD	2.26	0.68
1:I:141:ARG:NE	5:I:511:HOH:O	2.21	0.67
1:A:21:ARG:NH2	5:A:404:HOH:O	2.28	0.66
1:M:151:GLU:HA	1:M:182:GLN:CG	2.25	0.66
1:A:132:GLY:O	5:A:402:HOH:O	2.11	0.66
1:M:165:GLN:O	5:M:404:HOH:O	2.13	0.66
1:I:23:ILE:HD12	1:I:26:LEU:HD13	1.78	0.66
1:M:162:ARG:NH1	3:M:301:GDE:OAD	2.30	0.65
1:I:41:THR:OG1	5:I:508:HOH:O	2.15	0.65
1:A:143:ARG:O	5:A:403:HOH:O	2.15	0.65
1:I:20:PHE:O	1:I:23:ILE:HG22	1.96	0.64
1:M:71:LEU:HD23	5:M:473:HOH:O	1.97	0.63
1:E:208:TRP:HB3	1:E:257:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:ASP:OD2	2:I:402:GOL:O2	2.10	0.63
1:I:151:GLU:HA	1:I:182:GLN:HG3	1.81	0.63
1:I:189:ALA:CB	4:I:403:DTT:H42	2.29	0.62
1:M:29:ILE:HG22	1:M:31:VAL:HG22	1.82	0.62
1:M:148:LYS:NZ	5:M:403:HOH:O	2.13	0.62
1:E:234:PHE:H	1:E:245:HIS:HD2	1.48	0.61
1:I:84:VAL:HG12	1:I:215:TRP:HA	1.84	0.60
1:A:29:ILE:CG2	1:A:95:ILE:O	2.46	0.60
1:E:91:THR:HG23	2:E:302:GOL:C1	2.31	0.60
1:M:86:ASP:OD2	5:M:405:HOH:O	2.16	0.60
1:E:26:LEU:HD23	1:E:30:SER:OG	2.02	0.59
1:I:217:MET:HE1	1:I:240:PHE:C	2.28	0.58
1:A:233:ASP:OD2	1:A:237:SER:OG	2.15	0.58
1:A:225:GLN:HB3	5:A:474:HOH:O	2.03	0.58
1:A:141:ARG:HD2	1:I:167:ASP:OD2	2.04	0.57
1:A:40:VAL:HG23	1:A:95:ILE:HD13	1.86	0.57
1:E:270:LYS:O	5:E:404:HOH:O	2.17	0.57
1:I:220:GLY:HA2	5:I:517:HOH:O	2.04	0.57
1:E:90:GLY:H	2:E:302:GOL:H12	1.68	0.57
1:A:243:LYS:HE2	1:A:245:HIS:HE2	1.70	0.57
1:E:33:GLU:O	1:E:37:LYS:HG2	2.03	0.57
1:I:231:VAL:O	1:I:238:HIS:CE1	2.57	0.57
1:A:143:ARG:HD3	1:I:268:SER:O	2.05	0.57
1:I:100:HIS:CE1	4:I:403:DTT:H11	2.40	0.57
1:E:36:ALA:HB1	1:E:95:ILE:HD11	1.86	0.56
1:A:36:ALA:HB1	1:A:95:ILE:HD11	1.88	0.56
1:I:223:LEU:HB2	5:I:517:HOH:O	2.05	0.55
1:A:161:PHE:CZ	1:A:211:GLY:HA3	2.41	0.55
1:I:185:GLY:HA2	3:M:301:GDE:CAJ	2.37	0.55
1:M:164:ASN:ND2	5:M:411:HOH:O	2.40	0.55
1:I:182:GLN:HG2	1:I:182:GLN:O	2.05	0.55
1:A:21:ARG:O	1:A:24:GLU:HG2	2.07	0.54
1:A:203:ARG:HA	1:E:96:HIS:O	2.07	0.54
1:I:141:ARG:HD3	5:I:550:HOH:O	2.07	0.54
1:E:91:THR:CG2	2:E:302:GOL:H11	2.38	0.54
1:E:109:TYR:CE2	1:E:110:LYS:HG3	2.43	0.54
1:E:265:LEU:O	1:E:270:LYS:NZ	2.38	0.54
1:A:143:ARG:CD	1:I:268:SER:O	2.57	0.53
1:I:54:ALA:HA	5:I:552:HOH:O	2.08	0.53
1:I:140:ARG:NH2	5:I:521:HOH:O	2.41	0.53
1:I:17:GLU:HG3	1:I:21:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:403:DTT:H2	1:M:100:HIS:HB2	1.91	0.52
1:E:26:LEU:O	1:E:30:SER:N	2.41	0.52
1:I:9:LEU:HD21	1:I:13:ARG:NH1	2.25	0.52
1:I:13:ARG:NE	1:I:126:GLU:OE2	2.42	0.52
1:I:91:THR:HG23	2:I:402:GOL:H31	1.93	0.51
1:M:162:ARG:HH22	3:M:301:GDE:CAJ	2.24	0.51
1:E:146:GLY:O	1:E:148:LYS:HD2	2.10	0.51
1:A:166:ILE:HD13	1:E:177:ARG:NH2	2.26	0.51
1:I:270:LYS:CD	1:I:270:LYS:C	2.84	0.51
1:E:129:ALA:HB3	5:E:411:HOH:O	2.10	0.50
1:I:58:ALA:N	5:I:501:HOH:O	2.04	0.50
1:I:21:ARG:O	1:I:24:GLU:HG2	2.11	0.50
1:A:48:GLU:HB2	1:A:87:PRO:HG3	1.94	0.50
1:A:155:LEU:HD12	5:A:406:HOH:O	2.12	0.50
2:A:301:GOL:H12	1:E:159:PHE:CD2	2.47	0.50
3:I:401:GDE:OAD	5:I:507:HOH:O	2.12	0.49
1:M:56:ARG:NH1	5:M:409:HOH:O	2.30	0.49
1:M:195:ASP:OD1	5:M:406:HOH:O	2.20	0.49
1:A:180:VAL:HG13	2:A:301:GOL:H31	1.94	0.49
1:M:31:VAL:HG12	1:M:35:ASP:HB3	1.95	0.49
1:E:223:LEU:N	5:E:411:HOH:O	2.46	0.49
1:A:21:ARG:NH1	5:A:417:HOH:O	2.46	0.48
1:A:49:GLN:NE2	5:A:401:HOH:O	2.06	0.48
1:M:84:VAL:HG12	1:M:215:TRP:HA	1.95	0.48
1:I:189:ALA:HB3	5:I:519:HOH:O	2.14	0.48
1:M:80:ASP:C	5:M:402:HOH:O	2.49	0.48
1:E:23:ILE:HD13	1:E:94:PHE:CE1	2.49	0.48
1:E:91:THR:N	2:E:302:GOL:O3	2.43	0.47
1:I:81:TYR:CE2	1:I:109:TYR:HD2	2.32	0.47
1:E:32:ASN:HB3	1:E:35:ASP:HB3	1.97	0.47
1:E:109:TYR:CD2	1:E:110:LYS:HG3	2.49	0.47
1:I:238:HIS:ND1	5:I:515:HOH:O	2.36	0.47
1:I:204:TYR:OH	4:I:403:DTT:S1	2.71	0.47
1:M:26:LEU:HD23	1:M:26:LEU:HA	1.76	0.47
1:A:22:SER:HA	1:A:25:ARG:NH1	2.29	0.47
4:I:403:DTT:H2	1:M:100:HIS:CB	2.45	0.47
1:I:257:LEU:O	1:I:257:LEU:HD23	2.15	0.46
1:M:32:ASN:ND2	1:M:35:ASP:HB2	2.30	0.46
1:M:86:ASP:HB2	1:M:215:TRP:CD1	2.50	0.46
1:I:1:MET:HE1	1:I:9:LEU:HD22	1.97	0.46
1:A:167:ASP:O	1:A:170:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:VAL:O	1:I:238:HIS:HE1	1.96	0.46
1:E:31:VAL:HG13	5:E:463:HOH:O	2.16	0.46
1:M:166:ILE:O	1:M:170:ASP:N	2.40	0.46
1:M:162:ARG:CZ	3:M:301:GDE:OAD	2.63	0.46
1:A:137:LEU:HB3	1:A:142:LEU:HD21	1.98	0.46
1:I:13:ARG:NH2	1:I:126:GLU:OE1	2.49	0.45
1:I:185:GLY:HA2	3:M:301:GDE:OAD	2.17	0.45
1:A:1:MET:HE1	1:A:9:LEU:HD22	1.99	0.45
1:I:2:GLN:OE1	1:I:133:ARG:NH1	2.49	0.45
3:A:304:GDE:CAF	1:E:159:PHE:H	2.29	0.45
1:M:109:TYR:CD1	5:M:402:HOH:O	2.56	0.45
1:A:173:LEU:CD1	1:E:177:ARG:HG2	2.47	0.45
1:E:180:VAL:HA	1:E:186:ILE:HD11	1.99	0.45
1:A:166:ILE:CG1	1:A:169:LEU:HD23	2.47	0.44
1:I:32:ASN:OD1	1:I:34:LYS:HG2	2.18	0.44
1:I:196:LEU:C	5:I:517:HOH:O	2.60	0.44
1:A:123:ARG:NH2	1:E:123:ARG:NH2	2.66	0.43
1:I:158:GLY:HA2	1:I:188:ARG:HG3	2.00	0.43
1:I:215:TRP:NE1	2:I:402:GOL:O1	2.45	0.43
1:I:257:LEU:HD23	1:I:257:LEU:C	2.43	0.43
1:I:109:TYR:CE1	1:I:110:LYS:HG3	2.54	0.43
1:E:17:GLU:OE2	1:E:21:ARG:HG3	2.18	0.43
1:A:185:GLY:HA2	3:A:304:GDE:HAG	2.00	0.43
1:I:123:ARG:NE	1:M:99:PRO:HG2	2.34	0.43
1:M:1:MET:HE3	1:M:1:MET:HB3	1.84	0.43
1:E:243:LYS:HE2	5:E:426:HOH:O	2.18	0.42
1:I:137:LEU:N	5:I:504:HOH:O	2.50	0.42
1:M:95:ILE:HD12	1:M:95:ILE:HA	1.89	0.42
3:A:304:GDE:OAB	1:E:188:ARG:HD3	2.19	0.42
1:M:182:GLN:CD	1:M:182:GLN:H	2.26	0.42
4:I:403:DTT:H2	1:M:100:HIS:CG	2.53	0.42
1:A:162:ARG:HD2	1:E:181:GLY:O	2.19	0.42
1:A:186:ILE:HD11	5:A:406:HOH:O	2.17	0.42
1:I:25:ARG:O	1:I:28:VAL:HG23	2.19	0.42
1:A:243:LYS:HE2	1:A:245:HIS:NE2	2.34	0.42
1:E:114:GLU:HG3	1:E:115:HIS:CD2	2.54	0.42
1:A:29:ILE:HD13	1:A:96:HIS:HA	2.01	0.42
1:A:95:ILE:HD12	1:A:95:ILE:HA	1.82	0.41
1:A:183:THR:HG21	5:A:406:HOH:O	2.20	0.41
1:A:257:LEU:C	1:A:257:LEU:HD23	2.46	0.41
1:I:151:GLU:HG2	1:I:182:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:GLN:HB2	1:E:263:PRO:HD3	2.02	0.41
1:I:134:GLY:C	1:I:226:GLU:HB3	2.46	0.41
1:M:37:LYS:HE3	1:M:37:LYS:HB3	1.90	0.41
1:E:90:GLY:N	2:E:302:GOL:H12	2.34	0.41
1:M:12:ALA:HB2	1:M:105:ILE:HD12	2.03	0.41
1:A:44:ASP:OD1	1:A:87:PRO:HG2	2.20	0.41
1:I:65:MET:HE2	1:I:215:TRP:CZ3	2.56	0.41
1:E:143:ARG:HD2	1:E:143:ARG:HA	1.88	0.40
1:E:145:SER:OG	1:E:250:ASN:ND2	2.54	0.40
1:I:194:LEU:HD23	1:I:194:LEU:HA	1.89	0.40
1:M:194:LEU:HD23	1:M:194:LEU:HA	1.98	0.40
1:A:77:GLU:N	5:A:427:HOH:O	2.55	0.40
1:A:159:PHE:N	1:A:188:ARG:HH22	2.18	0.40
1:E:67:GLU:HG3	1:E:215:TRP:CZ2	2.55	0.40
1:M:179:LEU:HD11	1:M:257:LEU:CD1	2.52	0.40
1:A:188:ARG:HD2	1:E:188:ARG:NH1	2.36	0.40

All (4) 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)
1:E:132:GLY:O	1:I:182:GLN:NE2[2_656]	1.55	0.65
1:I:45:ARG:NH1	1:M:49:GLN:OE1[2_555]	2.06	0.14
1:A:35:ASP:O	1:E:25:ARG:NH1[2_656]	2.09	0.11
1:E:163:ASP:OD2	1:M:133:ARG:NH1[1_556]	2.11	0.09

## 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	268/273 (98%)	263 (98%)	2 (1%)	3 (1%)	<b>12</b> <b>10</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	268/273 (98%)	265 (99%)	3 (1%)	0	100	100
1	I	270/273 (99%)	262 (97%)	7 (3%)	1 (0%)	30	34
1	M	270/273 (99%)	264 (98%)	5 (2%)	1 (0%)	30	34
All	All	1076/1092 (98%)	1054 (98%)	17 (2%)	5 (0%)	25	28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	1	MET
1	A	29	ILE
1	A	31	VAL
1	A	181	GLY
1	I	28	VAL

### 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	209/211 (99%)	199 (95%)	10 (5%)	21	28
1	E	209/211 (99%)	196 (94%)	13 (6%)	15	18
1	I	210/211 (100%)	199 (95%)	11 (5%)	19	24
1	M	210/211 (100%)	195 (93%)	15 (7%)	12	13
All	All	838/844 (99%)	789 (94%)	49 (6%)	17	20

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	10	ARG
1	A	17	GLU
1	A	28	VAL
1	A	29	ILE
1	A	30	SER

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Mol	Chain	Res	Type
1	A	32	ASN
1	A	73	GLU
1	A	143	ARG
1	A	163	ASP
1	E	1	MET
1	E	26	LEU
1	E	27	ASP
1	E	28	VAL
1	E	37	LYS
1	E	77	GLU
1	E	180	VAL
1	E	186	ILE
1	E	237	SER
1	E	238	HIS
1	E	255	LYS
1	E	268	SER
1	E	270	LYS
1	I	6	ASN
1	I	10	ARG
1	I	22	SER
1	I	25	ARG
1	I	40	VAL
1	I	112	ARG
1	I	143	ARG
1	I	237	SER
1	I	238	HIS
1	I	268	SER
1	I	270	LYS
1	M	1	MET
1	M	21	ARG
1	M	31	VAL
1	M	32	ASN
1	M	35	ASP
1	M	37	LYS
1	M	44	ASP
1	M	73	GLU
1	M	151	GLU
1	M	162	ARG
1	M	163	ASP
1	M	167	ASP
1	M	177	ARG
1	M	251	THR

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Mol	Chain	Res	Type
1	M	261	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	32	ASN
1	A	164	ASN
1	E	245	HIS
1	M	164	ASN
1	M	171	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	GDE	M	301	-	12,12,12	1.21	1 (8%)	17,17,17	1.55	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GDE	A	302	-	12,12,12	1.22	3 (25%)	17,17,17	0.82	1 (5%)
3	GDE	A	304	-	12,12,12	1.80	3 (25%)	17,17,17	1.44	2 (11%)
3	GDE	I	401	-	12,12,12	0.76	0	17,17,17	1.25	2 (11%)
2	GOL	A	301	-	5,5,5	0.18	0	5,5,5	0.75	0
2	GOL	E	302	-	5,5,5	0.41	0	5,5,5	0.67	0
2	GOL	I	402	-	5,5,5	0.47	0	5,5,5	0.63	0
4	DTT	I	403	-	7,7,7	0.31	0	4,8,8	1.06	0
2	GOL	M	302	-	5,5,5	0.13	0	5,5,5	0.59	0
2	GOL	A	303	-	5,5,5	0.30	0	5,5,5	0.83	0
4	DTT	E	301	-	7,7,7	0.88	0	4,8,8	1.43	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
3	GDE	M	301	-	-	0/4/4/4	0/1/1/1
3	GDE	A	302	-	-	0/4/4/4	0/1/1/1
3	GDE	A	304	-	-	4/4/4/4	0/1/1/1
3	GDE	I	401	-	-	0/4/4/4	0/1/1/1
2	GOL	A	301	-	-	0/4/4/4	-
2	GOL	E	302	-	-	2/4/4/4	-
2	GOL	I	402	-	-	4/4/4/4	-
4	DTT	I	403	-	-	6/8/8/8	-
2	GOL	M	302	-	-	0/4/4/4	-
2	GOL	A	303	-	-	1/4/4/4	-
4	DTT	E	301	-	-	6/8/8/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	304	GDE	OAA-CAH	-3.94	1.18	1.30
3	A	304	GDE	CAI-CAL	-2.71	1.36	1.40
3	A	304	GDE	CAG-CAJ	-2.57	1.35	1.38
3	M	301	GDE	CAI-CAL	-2.20	1.37	1.40
3	A	302	GDE	CAG-CAJ	2.14	1.42	1.38
3	A	302	GDE	CAK-CAH	2.09	1.53	1.49
3	A	302	GDE	OAB-CAH	2.07	1.28	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	301	GDE	CAJ-CAL-CAI	-2.89	117.67	119.51
3	M	301	GDE	CAF-CAI-CAL	2.72	122.34	120.47
3	I	401	GDE	OAD-CAJ-CAL	2.59	124.59	117.90
3	M	301	GDE	OAC-CAI-CAL	-2.55	111.32	117.90
3	M	301	GDE	OAC-CAI-CAF	2.52	126.22	119.46
3	A	304	GDE	OAD-CAJ-CAL	2.42	124.16	117.90
3	A	304	GDE	CAG-CAJ-CAL	-2.23	118.93	120.47
3	I	401	GDE	OAE-CAL-CAJ	2.13	125.17	119.50
3	A	302	GDE	OAC-CAI-CAL	2.04	123.17	117.90

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	402	GOL	O1-C1-C2-C3
4	E	301	DTT	C1-C2-C3-C4
4	E	301	DTT	O2-C2-C3-O3
4	E	301	DTT	O2-C2-C3-C4
4	E	301	DTT	C2-C3-C4-S4
4	E	301	DTT	O3-C3-C4-S4
4	I	403	DTT	S1-C1-C2-O2
4	I	403	DTT	S1-C1-C2-C3
4	I	403	DTT	C1-C2-C3-O3
4	I	403	DTT	C1-C2-C3-C4
4	I	403	DTT	O2-C2-C3-C4
3	A	304	GDE	OAB-CAH-CAK-CAG
3	A	304	GDE	OAB-CAH-CAK-CAF
3	A	304	GDE	OAA-CAH-CAK-CAG
3	A	304	GDE	OAA-CAH-CAK-CAF
2	E	302	GOL	C1-C2-C3-O3
2	I	402	GOL	C1-C2-C3-O3
2	I	402	GOL	O1-C1-C2-O2
4	I	403	DTT	O2-C2-C3-O3
2	E	302	GOL	O2-C2-C3-O3
4	E	301	DTT	C1-C2-C3-O3
2	I	402	GOL	O2-C2-C3-O3
2	A	303	GOL	O1-C1-C2-O2

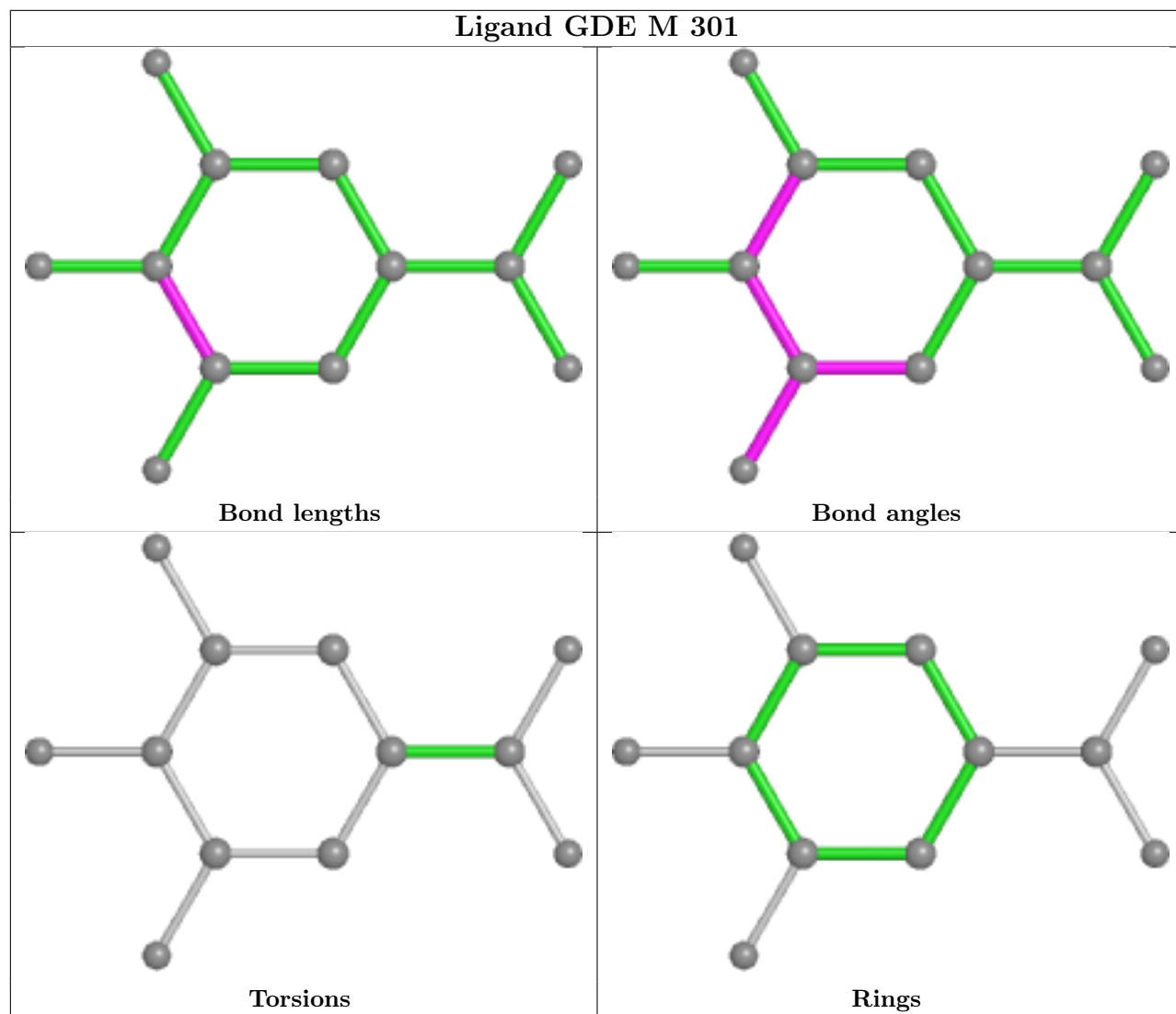
There are no ring outliers.

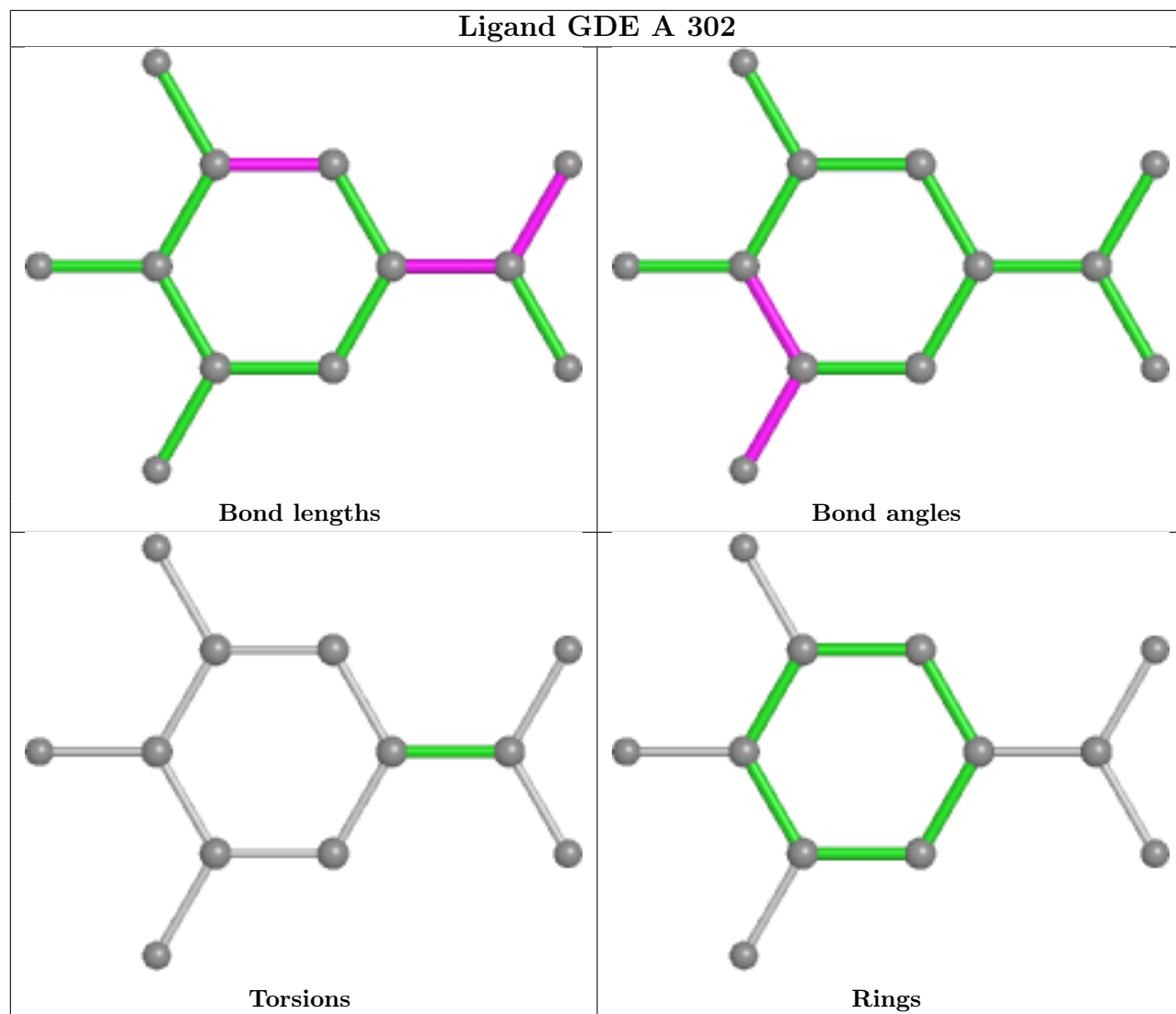
7 monomers are involved in 30 short contacts:

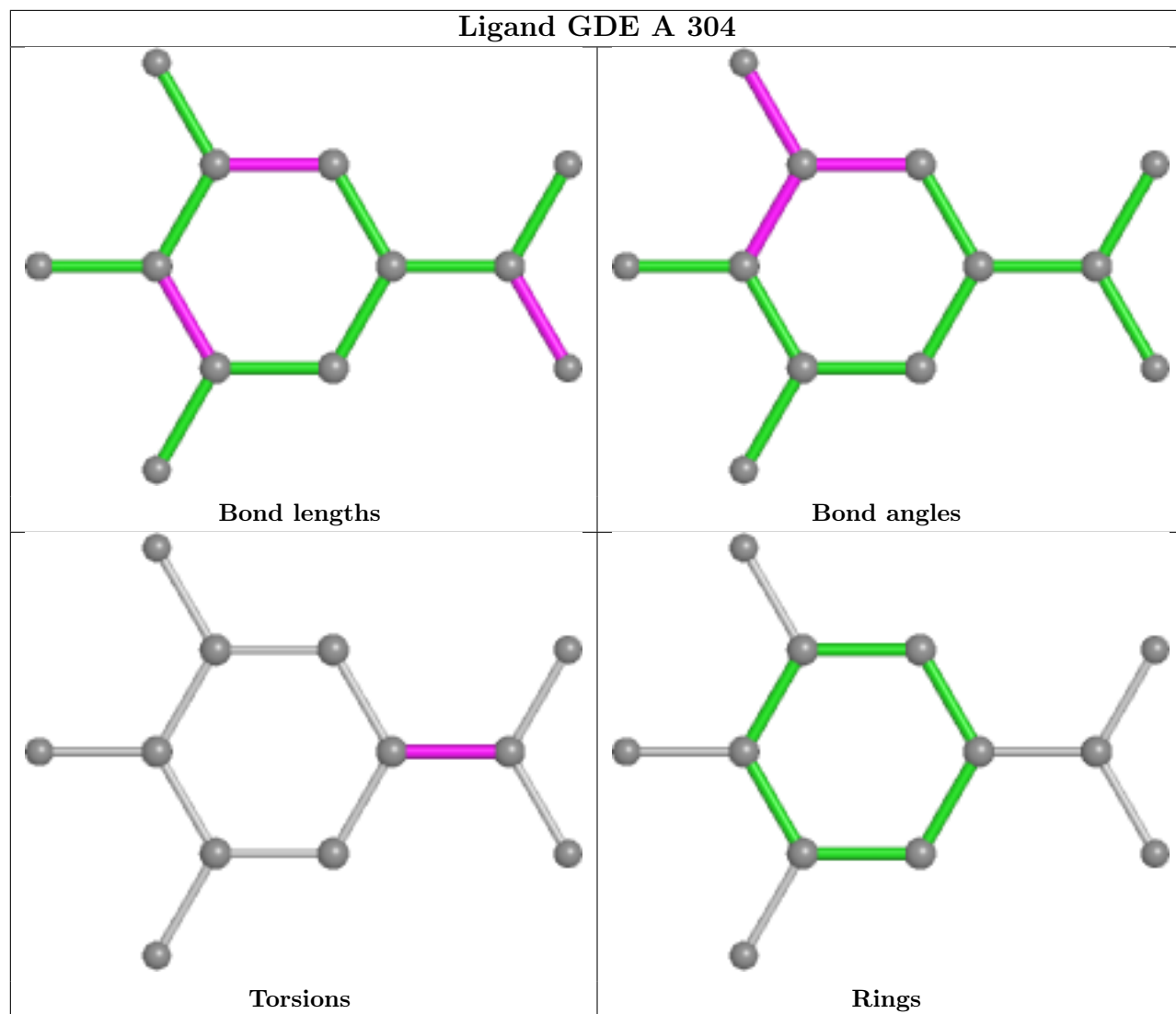
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	301	GDE	6	0
3	A	304	GDE	4	0
3	I	401	GDE	2	0
2	A	301	GOL	2	0
2	E	302	GOL	6	0
2	I	402	GOL	3	0
4	I	403	DTT	7	0

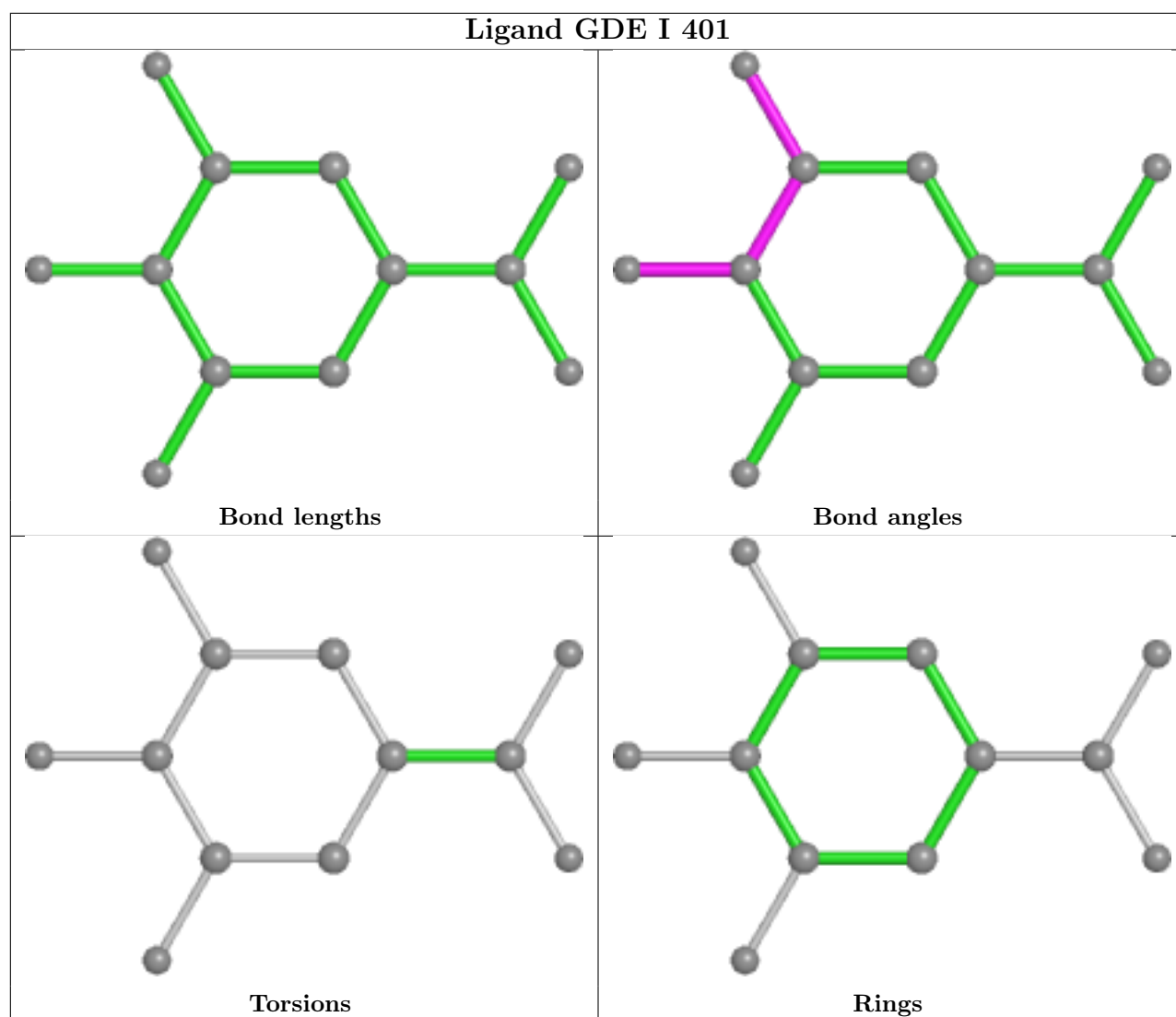
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	270/273 (98%)	-1.61	0 100 100	15, 25, 46, 73	0
1	E	270/273 (98%)	-1.68	0 100 100	14, 22, 34, 46	0
1	I	272/273 (99%)	-1.64	0 100 100	11, 24, 45, 69	0
1	M	272/273 (99%)	-1.62	0 100 100	15, 25, 53, 72	0
All	All	1084/1092 (99%)	-1.64	0 100 100	11, 24, 45, 73	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, 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.

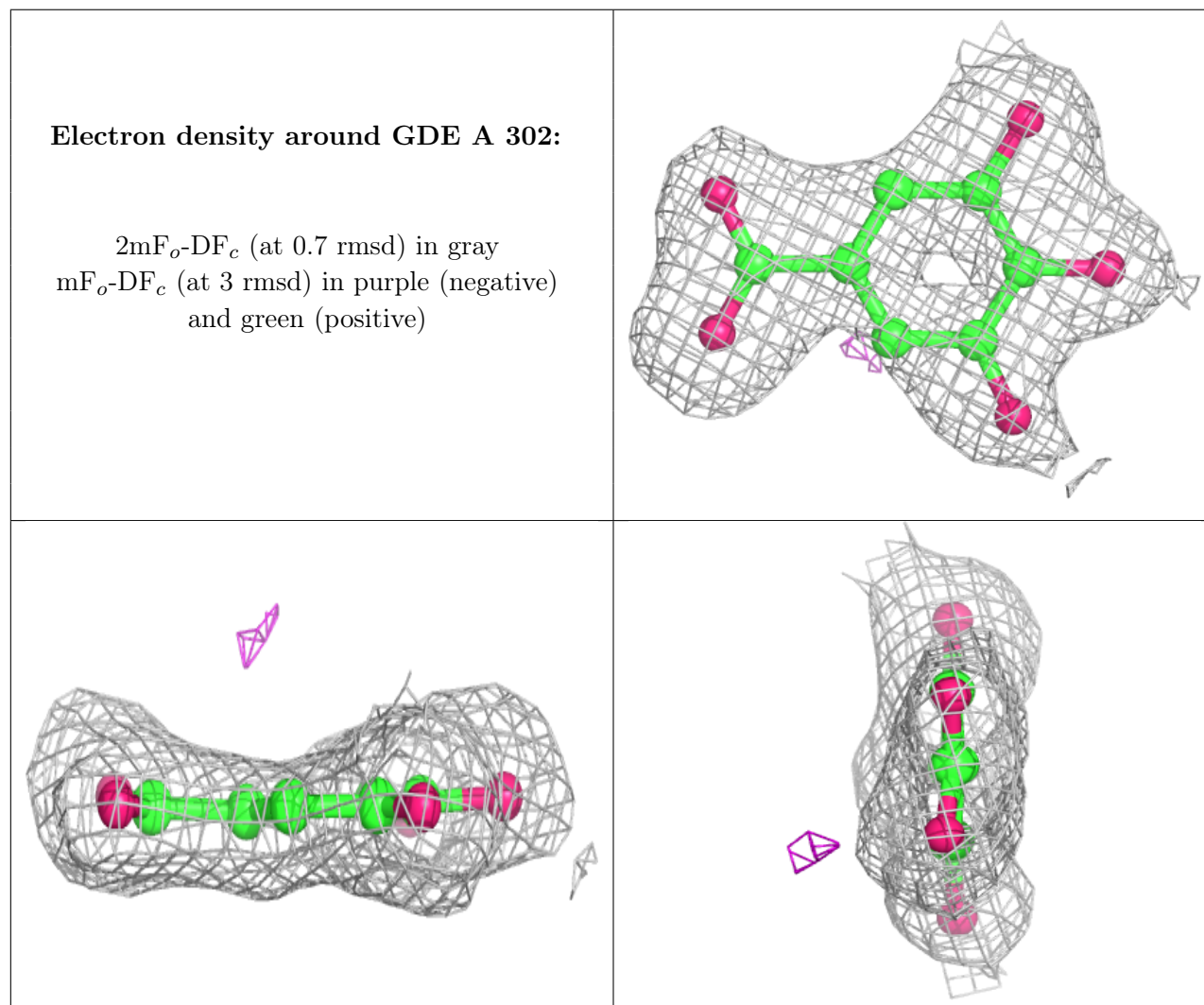
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GOL	A	301	6/6	0.99	0.03	22,27,28,29	0
2	GOL	A	303	6/6	0.99	0.03	22,23,24,25	0
2	GOL	I	402	6/6	0.99	0.03	22,24,27,28	0
2	GOL	M	302	6/6	0.99	0.06	29,32,34,38	0

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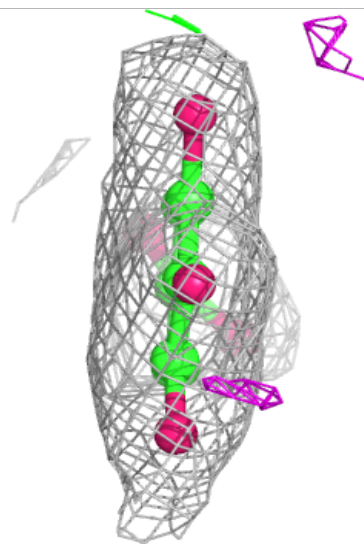
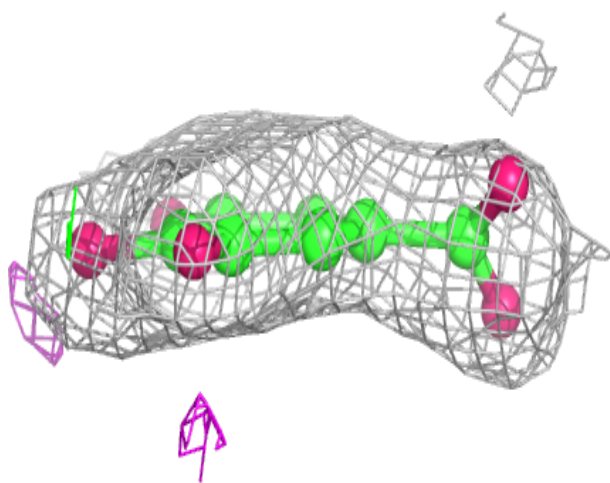
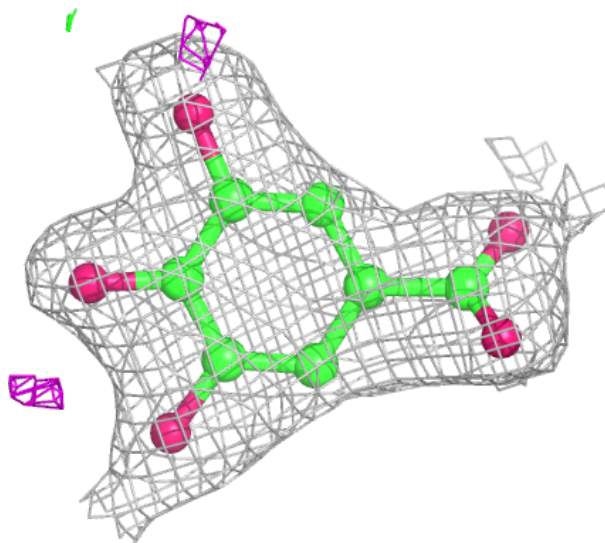
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GDE	A	302	12/12	0.99	0.03	19,27,30,35	0
3	GDE	A	304	12/12	0.99	0.03	18,20,31,38	0
3	GDE	I	401	12/12	0.99	0.03	31,35,39,40	0
4	DTT	E	301	8/8	0.99	0.04	27,31,34,35	0
3	GDE	M	301	12/12	1.00	0.02	27,36,41,45	0
2	GOL	E	302	6/6	1.00	0.03	35,36,39,40	0
4	DTT	I	403	8/8	1.00	0.03	40,46,48,52	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.



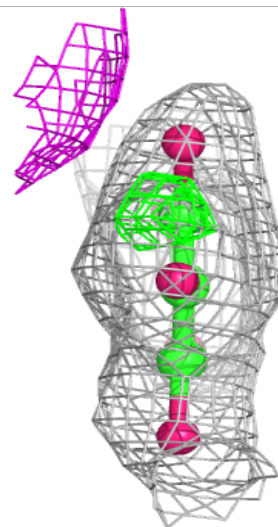
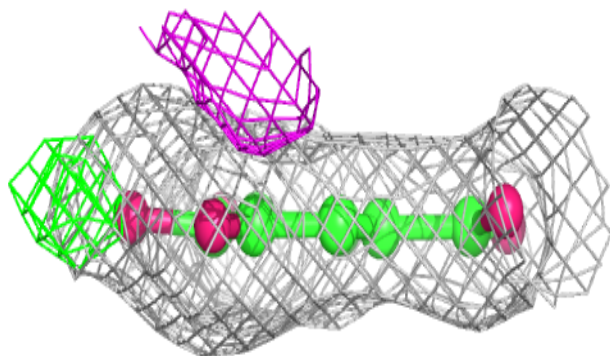
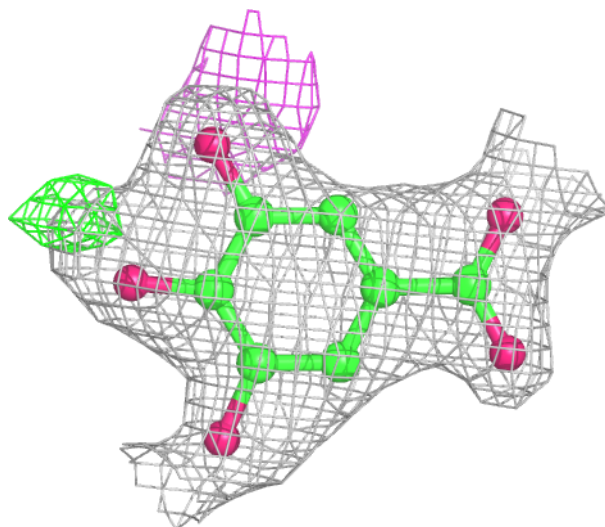
**Electron density around GDE A 304:**

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

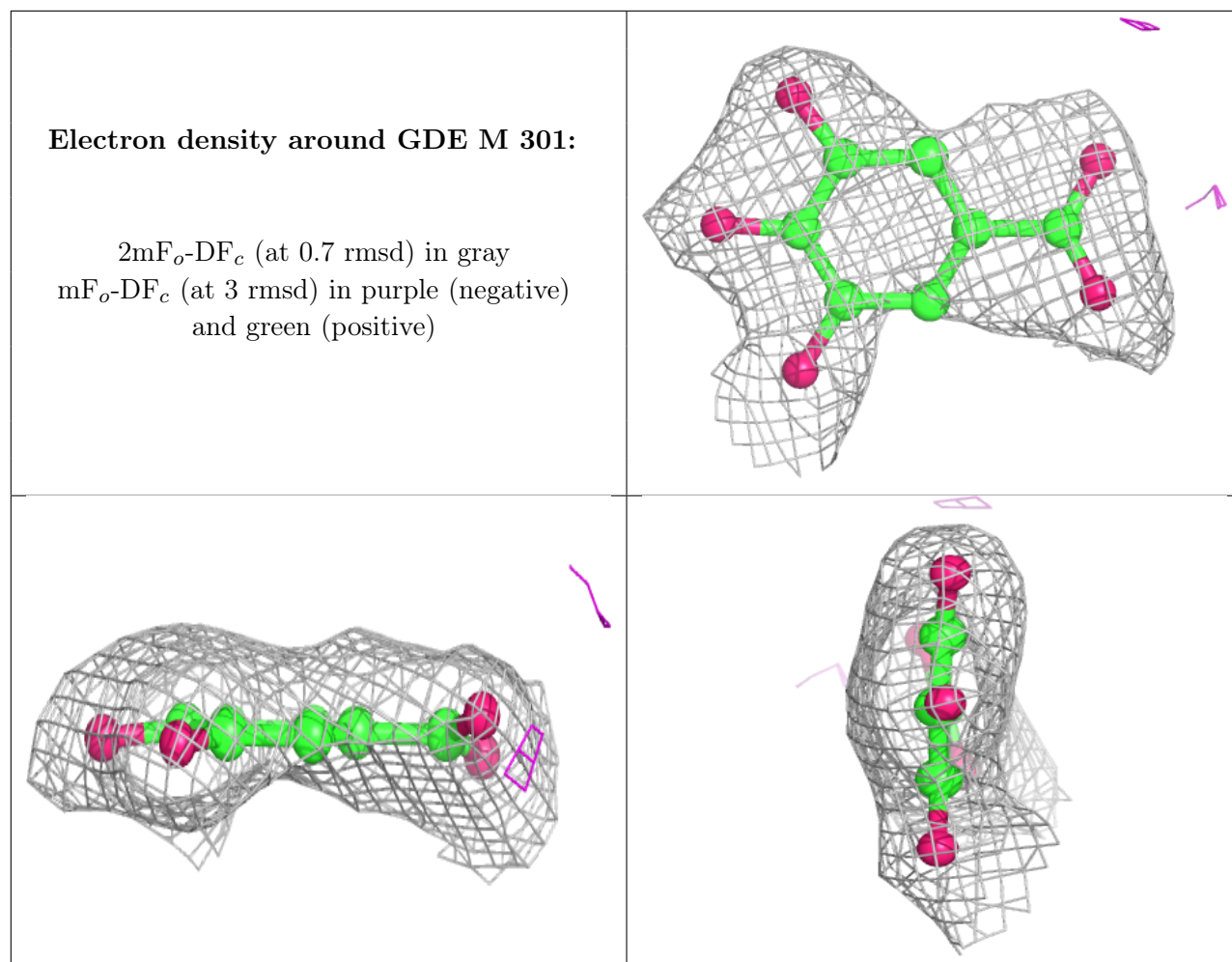


**Electron density around GDE I 401:**

$2mF_o-DF_c$  (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.