



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2021 – 06:19 PM JST

PDB ID : 7BVR  
Title : DgpB-DgpC complex apo  
Authors : Mori, T.; He, H.; Abe, I.  
Deposited on : 2020-04-11  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

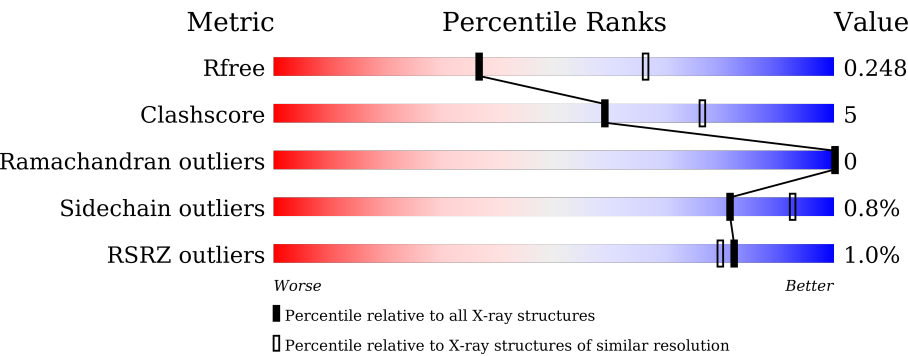
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	337	<div><div></div><div>80%16%.</div></div>
1	C	337	<div><div>2%</div><div>85%10%..</div></div>
1	E	337	<div><div>%</div><div>87%9%.</div></div>
1	G	337	<div><div>2%</div><div>83%12%.</div></div>
2	B	142	<div><div></div><div>89%8%..</div></div>
2	D	142	<div><div></div><div>88%9%.</div></div>

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Mol	Chain	Length	Quality of chain
2	F	142	<div><div>%</div><div><div></div></div><div>91%</div><div>7% ..</div></div>
2	H	142	<div><div></div><div>87%</div><div>11% .</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15165 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 AP\_endonuc\_2 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2550	1617	421	485	27			
1	C	323	Total	C	N	O	S	0	0	0
			2552	1619	419	487	27			
1	E	323	Total	C	N	O	S	0	0	0
			2557	1621	422	487	27			
1	G	323	Total	C	N	O	S	0	0	0
			2554	1619	421	487	27			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	LYS	-	expression tag	UNP A0A3Q9WXL1
A	326	LEU	-	expression tag	UNP A0A3Q9WXL1
A	327	ALA	-	expression tag	UNP A0A3Q9WXL1
A	328	ALA	-	expression tag	UNP A0A3Q9WXL1
A	329	ALA	-	expression tag	UNP A0A3Q9WXL1
A	330	LEU	-	expression tag	UNP A0A3Q9WXL1
A	331	GLU	-	expression tag	UNP A0A3Q9WXL1
A	332	HIS	-	expression tag	UNP A0A3Q9WXL1
A	333	HIS	-	expression tag	UNP A0A3Q9WXL1
A	334	HIS	-	expression tag	UNP A0A3Q9WXL1
A	335	HIS	-	expression tag	UNP A0A3Q9WXL1
A	336	HIS	-	expression tag	UNP A0A3Q9WXL1
A	337	HIS	-	expression tag	UNP A0A3Q9WXL1
C	325	LYS	-	expression tag	UNP A0A3Q9WXL1
C	326	LEU	-	expression tag	UNP A0A3Q9WXL1
C	327	ALA	-	expression tag	UNP A0A3Q9WXL1
C	328	ALA	-	expression tag	UNP A0A3Q9WXL1
C	329	ALA	-	expression tag	UNP A0A3Q9WXL1
C	330	LEU	-	expression tag	UNP A0A3Q9WXL1
C	331	GLU	-	expression tag	UNP A0A3Q9WXL1
C	332	HIS	-	expression tag	UNP A0A3Q9WXL1

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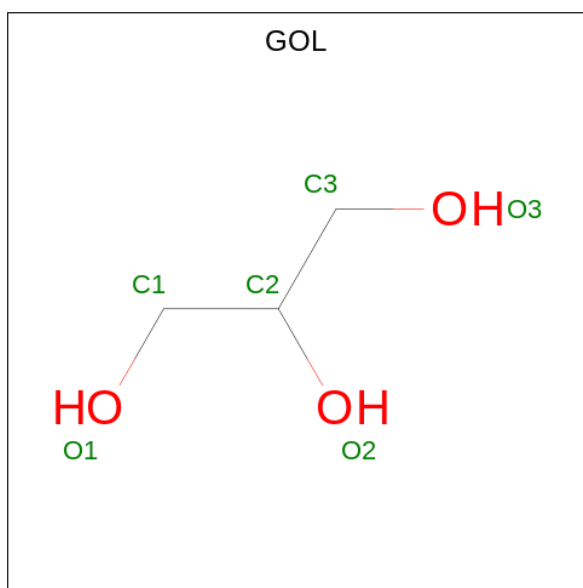
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Chain	Residue	Modelled	Actual	Comment	Reference
C	333	HIS	-	expression tag	UNP A0A3Q9WXL1
C	334	HIS	-	expression tag	UNP A0A3Q9WXL1
C	335	HIS	-	expression tag	UNP A0A3Q9WXL1
C	336	HIS	-	expression tag	UNP A0A3Q9WXL1
C	337	HIS	-	expression tag	UNP A0A3Q9WXL1
E	325	LYS	-	expression tag	UNP A0A3Q9WXL1
E	326	LEU	-	expression tag	UNP A0A3Q9WXL1
E	327	ALA	-	expression tag	UNP A0A3Q9WXL1
E	328	ALA	-	expression tag	UNP A0A3Q9WXL1
E	329	ALA	-	expression tag	UNP A0A3Q9WXL1
E	330	LEU	-	expression tag	UNP A0A3Q9WXL1
E	331	GLU	-	expression tag	UNP A0A3Q9WXL1
E	332	HIS	-	expression tag	UNP A0A3Q9WXL1
E	333	HIS	-	expression tag	UNP A0A3Q9WXL1
E	334	HIS	-	expression tag	UNP A0A3Q9WXL1
E	335	HIS	-	expression tag	UNP A0A3Q9WXL1
E	336	HIS	-	expression tag	UNP A0A3Q9WXL1
E	337	HIS	-	expression tag	UNP A0A3Q9WXL1
G	325	LYS	-	expression tag	UNP A0A3Q9WXL1
G	326	LEU	-	expression tag	UNP A0A3Q9WXL1
G	327	ALA	-	expression tag	UNP A0A3Q9WXL1
G	328	ALA	-	expression tag	UNP A0A3Q9WXL1
G	329	ALA	-	expression tag	UNP A0A3Q9WXL1
G	330	LEU	-	expression tag	UNP A0A3Q9WXL1
G	331	GLU	-	expression tag	UNP A0A3Q9WXL1
G	332	HIS	-	expression tag	UNP A0A3Q9WXL1
G	333	HIS	-	expression tag	UNP A0A3Q9WXL1
G	334	HIS	-	expression tag	UNP A0A3Q9WXL1
G	335	HIS	-	expression tag	UNP A0A3Q9WXL1
G	336	HIS	-	expression tag	UNP A0A3Q9WXL1
G	337	HIS	-	expression tag	UNP A0A3Q9WXL1

- Molecule 2 is a protein called DgpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total 1111	C 714	N 179	O 214	S 4	0	0	0
2	D	138	Total 1103	C 708	N 178	O 213	S 4	0	0	0
2	F	140	Total 1111	C 714	N 181	O 212	S 4	0	0	0
2	H	139	Total 1111	C 714	N 179	O 214	S 4	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

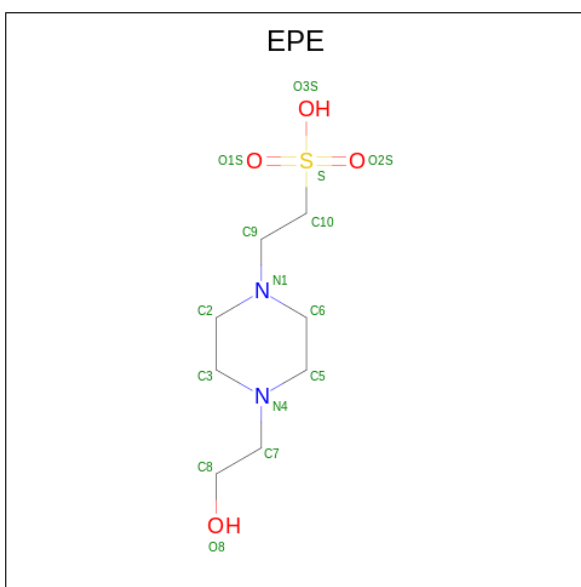


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	C	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		
4	G	1	Total	Mn	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	44	Total	O	0	0
			44	44		
6	B	57	Total	O	0	0
			57	57		
6	C	68	Total	O	0	0
			68	68		
6	D	35	Total	O	0	0
			35	35		
6	E	79	Total	O	0	0
			79	79		
6	F	49	Total	O	0	0
			49	49		
6	G	39	Total	O	0	0
			39	39		

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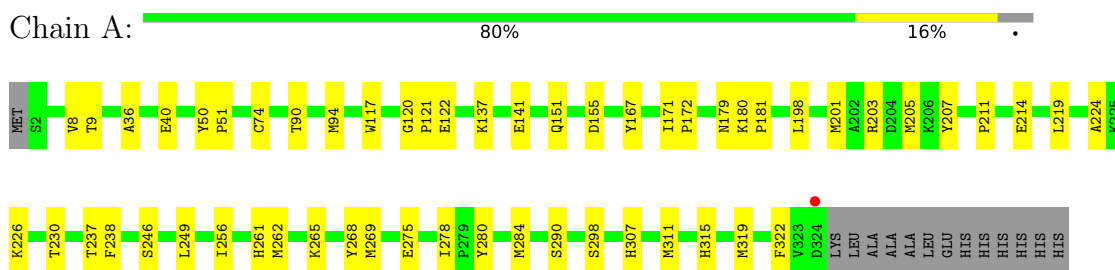
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	42	Total	O	0	0
			42	42		



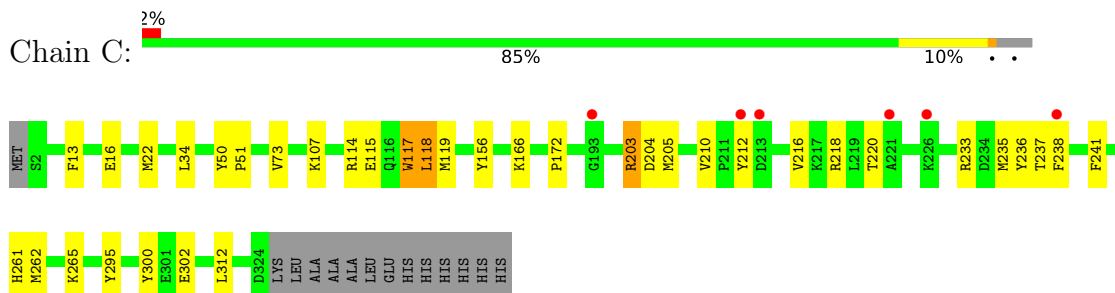
### 3 Residue-property plots [i](#)

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.

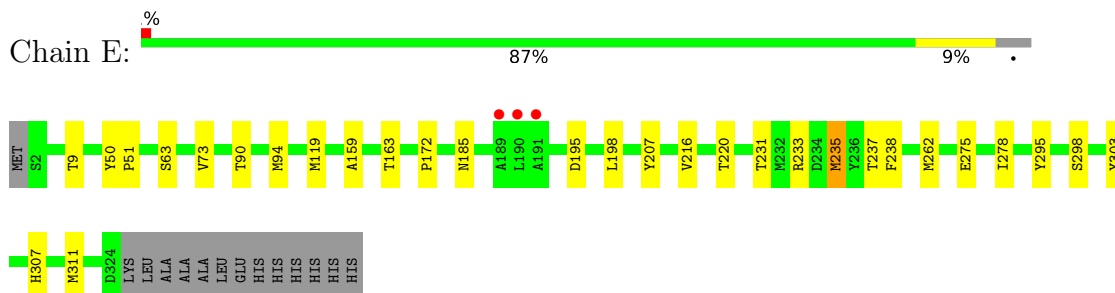
- Molecule 1: AP\_endonuc\_2 domain-containing protein



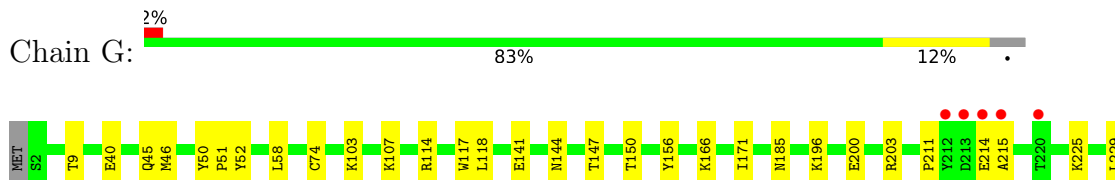
- Molecule 1: AP\_endonuc\_2 domain-containing protein

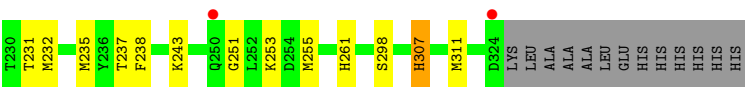


- Molecule 1: AP\_endonuc\_2 domain-containing protein

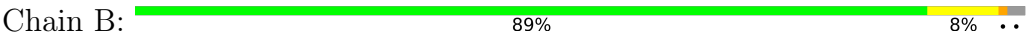


- Molecule 1: AP\_endonuc\_2 domain-containing protein

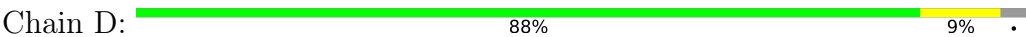




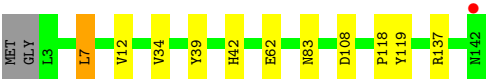
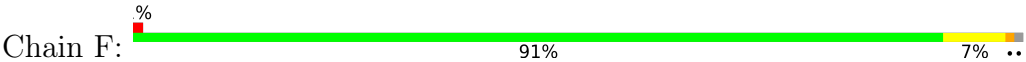
● Molecule 2: DgpB



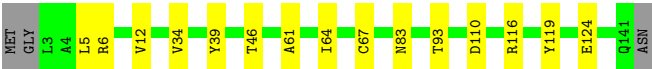
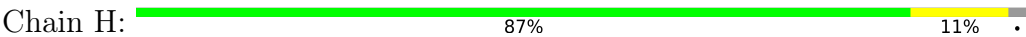
● Molecule 2: DgpB



● Molecule 2: DgpB



● Molecule 2: DgpB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.52Å 156.72Å 158.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.89 – 2.60 46.89 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.89-2.60) 100.0 (46.89-2.60)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.191 , 0.249 0.191 , 0.248	Depositor DCC
$R_{free}$ test set	2008 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15165	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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 20.49 % 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 8.5972e-03. 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: EPE, GOL, MN

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	0.26	0/2606	0.47	0/3517
1	C	0.26	0/2608	0.47	1/3519 (0.0%)
1	E	0.27	0/2613	0.47	0/3525
1	G	0.26	0/2610	0.46	0/3522
2	B	0.29	0/1137	0.51	0/1543
2	D	0.27	0/1129	0.50	0/1532
2	F	0.31	0/1137	0.53	0/1544
2	H	0.28	0/1137	0.51	0/1543
All	All	0.27	0/14977	0.48	1/20245 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	LEU	CA-CB-CG	5.05	126.91	115.30

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	2550	0	2471	35	0
1	C	2552	0	2475	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2557	0	2484	19	0
1	G	2554	0	2475	28	0
2	B	1111	0	1072	8	0
2	D	1103	0	1061	10	0
2	F	1111	0	1070	7	0
2	H	1111	0	1072	9	0
3	A	6	0	8	0	0
3	C	6	0	8	2	0
3	E	6	0	8	0	0
3	G	6	0	8	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	B	30	0	34	2	0
5	D	15	0	17	0	0
5	F	15	0	17	0	0
5	H	15	0	17	0	0
6	A	44	0	0	0	0
6	B	57	0	0	0	0
6	C	68	0	0	1	0
6	D	35	0	0	0	0
6	E	79	0	0	1	0
6	F	49	0	0	0	0
6	G	39	0	0	0	0
6	H	42	0	0	0	0
All	All	15165	0	14297	137	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 5.

All (137) 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:E:303:TYR:CE2	2:F:7:LEU:HD21	2.12	0.84
1:A:269:MET:H	1:A:311:MET:HE3	1.46	0.81
1:C:172:PRO:HG2	1:C:262:MET:HG2	1.65	0.77
2:B:49:GLU:HA	5:B:201:EPE:H101	1.68	0.76
2:D:83:ASN:HD21	2:H:83:ASN:HB3	1.47	0.76
1:A:269:MET:H	1:A:311:MET:CE	1.99	0.75
1:A:219:LEU:HG	1:A:224:ALA:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:PRO:HG2	1:A:262:MET:HG2	1.71	0.71
1:E:172:PRO:HG2	1:E:262:MET:HG2	1.73	0.70
1:G:114:ARG:HH22	3:G:401:GOL:H32	1.56	0.69
1:C:235:MET:HG2	1:C:241:PHE:HE1	1.57	0.68
1:A:268:TYR:HA	1:A:311:MET:CE	2.25	0.66
1:A:198:LEU:H	1:A:198:LEU:HD12	1.63	0.64
1:C:117:TRP:O	1:C:156:TYR:OH	2.17	0.63
2:H:39:TYR:HH	2:H:119:TYR:HH	1.49	0.61
2:D:39:TYR:HH	2:D:119:TYR:HH	1.49	0.60
1:A:284:MET:HG3	1:A:322:PHE:CD2	2.38	0.59
1:G:215:ALA:HB1	1:G:232:MET:HE2	1.84	0.59
1:C:203:ARG:NH1	1:C:204:ASP:OD1	2.36	0.58
1:G:215:ALA:HB1	1:G:232:MET:CE	2.33	0.57
2:B:53:LYS:HB3	2:B:110:ASP:HB2	1.86	0.57
2:D:53:LYS:HB3	2:D:110:ASP:HB2	1.85	0.57
1:G:211:PRO:O	1:G:215:ALA:N	2.37	0.56
1:G:171:ILE:HG12	1:G:261:HIS:HB3	1.88	0.56
1:G:45:GLN:HG2	1:G:46:MET:HG3	1.88	0.56
1:A:268:TYR:HA	1:A:311:MET:HE3	1.88	0.55
2:B:123:SER:OG	2:B:126:GLU:OE1	2.24	0.55
1:E:216:VAL:O	1:E:220:THR:OG1	2.16	0.54
1:E:275:GLU:HG2	1:E:278:ILE:HB	1.89	0.54
1:C:50:TYR:CG	1:C:51:PRO:HA	2.43	0.54
1:E:275:GLU:HG3	1:E:278:ILE:H	1.72	0.54
2:H:5:LEU:HD12	2:H:6:ARG:N	2.24	0.53
1:G:58:LEU:HD22	1:G:107:LYS:HG2	1.91	0.52
2:D:46:THR:HA	2:D:116:ARG:NH1	2.25	0.52
1:C:13:PHE:CD1	1:C:22:MET:HE1	2.45	0.52
1:E:159:ALA:O	1:E:163:THR:HG23	2.10	0.52
1:E:233:ARG:O	1:E:237:THR:HG23	2.10	0.52
1:A:226:LYS:O	1:A:230:THR:HG22	2.11	0.51
1:C:115:GLU:HG2	1:C:119:MET:CE	2.40	0.51
1:E:233:ARG:NH1	6:E:502:HOH:O	2.42	0.51
1:E:50:TYR:CG	1:E:51:PRO:HA	2.46	0.51
2:B:83:ASN:HD21	2:F:83:ASN:HB3	1.76	0.51
1:A:50:TYR:CG	1:A:51:PRO:HA	2.46	0.50
3:C:401:GOL:O3	3:C:401:GOL:O1	2.27	0.50
2:D:71:LYS:HD3	1:G:52:TYR:CE2	2.47	0.50
1:C:73:VAL:HG21	1:C:295:TYR:CZ	2.46	0.50
1:A:40:GLU:HB2	1:A:74:CYS:HB3	1.94	0.50
1:G:40:GLU:HB2	1:G:74:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:ALA:HA	2:H:64:ILE:HD12	1.92	0.50
1:A:90:THR:O	1:A:94:MET:HG3	2.12	0.50
2:B:28:ILE:HA	2:B:99:PRO:HA	1.94	0.49
1:E:237:THR:OG1	1:E:238:PHE:N	2.45	0.49
1:C:212:TYR:HB2	1:C:236:TYR:CD2	2.48	0.49
1:C:114:ARG:HH22	3:C:401:GOL:H32	1.78	0.49
1:A:201:MET:O	1:A:205:MET:HG3	2.12	0.48
1:A:122:GLU:H	1:A:122:GLU:CD	2.15	0.48
2:F:62:GLU:H	2:F:62:GLU:CD	2.17	0.48
1:E:195:ASP:HB3	1:E:198:LEU:HD12	1.95	0.48
1:G:50:TYR:CG	1:G:51:PRO:HA	2.48	0.48
1:A:179:ASN:OD1	1:A:180:LYS:HE3	2.13	0.48
2:D:72:GLU:OE1	1:G:103:LYS:NZ	2.31	0.48
1:C:115:GLU:HG2	1:C:119:MET:HE1	1.95	0.47
1:E:90:THR:O	1:E:94:MET:HG3	2.14	0.47
1:A:151:GLN:NE2	1:A:155:ASP:OD1	2.46	0.47
1:C:118:LEU:HD23	1:C:118:LEU:H	1.78	0.47
1:C:50:TYR:CD1	1:C:51:PRO:HA	2.50	0.47
1:A:307:HIS:O	1:A:311:MET:HG2	2.15	0.46
1:C:237:THR:OG1	1:C:238:PHE:N	2.48	0.46
1:A:203:ARG:HD3	1:A:207:TYR:CE2	2.51	0.46
1:G:243:LYS:HB3	1:G:243:LYS:HE2	1.54	0.46
2:H:12:VAL:O	2:H:34:VAL:HA	2.15	0.46
1:C:73:VAL:HG11	1:C:295:TYR:CD1	2.50	0.46
2:H:124:GLU:H	2:H:124:GLU:CD	2.19	0.46
2:F:108:ASP:OD1	2:F:137:ARG:HD2	2.16	0.46
2:B:50:ILE:HG22	5:B:201:EPE:H102	1.98	0.46
1:A:246:SER:HA	1:A:249:LEU:HD12	1.98	0.45
1:E:307:HIS:O	1:E:311:MET:HG2	2.16	0.45
2:F:39:TYR:OH	2:F:119:TYR:OH	2.33	0.45
1:G:118:LEU:HD11	2:H:119:TYR:HA	1.98	0.45
2:H:46:THR:HA	2:H:116:ARG:NH1	2.30	0.45
1:A:181:PRO:HG3	1:A:203:ARG:HG3	1.99	0.45
2:B:12:VAL:O	2:B:34:VAL:HA	2.17	0.45
2:D:67:CYS:HB2	2:D:93:THR:HB	1.97	0.45
1:E:50:TYR:CD1	1:E:51:PRO:HA	2.51	0.45
1:A:198:LEU:HB3	1:A:219:LEU:HD11	1.98	0.45
2:D:53:LYS:HE2	2:D:58:ASP:OD1	2.17	0.45
2:B:46:THR:HA	2:B:116:ARG:NH1	2.32	0.45
1:G:185:ASN:OD1	1:G:231:THR:HG23	2.17	0.45
1:C:265:LYS:NZ	6:C:503:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:TYR:O	1:C:216:VAL:HG13	2.16	0.44
1:G:307:HIS:O	1:G:311:MET:HG2	2.17	0.44
1:G:251:GLY:O	1:G:255:MET:HB2	2.18	0.44
1:C:107:LYS:HE3	1:E:63:SER:OG	2.18	0.44
1:C:205:MET:HG2	1:C:210:VAL:HG21	2.00	0.44
1:A:211:PRO:HG2	1:A:214:GLU:OE1	2.17	0.44
1:A:269:MET:HB3	1:A:269:MET:HE2	1.52	0.43
2:H:67:CYS:HB2	2:H:93:THR:HB	1.99	0.43
1:E:9:THR:HG22	1:E:298:SER:O	2.18	0.43
1:G:9:THR:HG22	1:G:298:SER:O	2.18	0.43
1:G:203:ARG:HE	1:G:203:ARG:HB3	1.62	0.43
1:C:16:GLU:HB2	1:C:22:MET:HE3	2.01	0.43
1:G:147:THR:OG1	1:G:150:THR:HG23	2.18	0.43
1:A:8:VAL:HG23	1:A:36:ALA:HB2	2.00	0.43
1:C:216:VAL:O	1:C:220:THR:OG1	2.20	0.43
1:A:265:LYS:O	1:A:280:TYR:OH	2.25	0.42
1:C:16:GLU:HB2	1:C:22:MET:CE	2.49	0.42
1:E:231:THR:O	1:E:235:MET:HG3	2.19	0.42
1:G:225:LYS:O	1:G:229:LEU:HG	2.19	0.42
1:G:166:LYS:HD2	1:G:166:LYS:HA	1.78	0.42
1:E:185:ASN:OD1	1:E:231:THR:HG23	2.20	0.42
1:A:269:MET:N	1:A:311:MET:CE	2.76	0.42
1:A:315:HIS:O	1:A:319:MET:HG2	2.20	0.42
2:D:71:LYS:HD3	1:G:52:TYR:CD2	2.55	0.42
1:A:9:THR:HG22	1:A:298:SER:O	2.20	0.42
1:C:233:ARG:O	1:C:237:THR:HG23	2.19	0.42
1:G:196:LYS:HE2	1:G:200:GLU:OE2	2.19	0.42
1:G:231:THR:O	1:G:235:MET:HG3	2.20	0.42
2:F:42:HIS:CE1	2:F:118:PRO:HD2	2.55	0.42
1:G:117:TRP:O	1:G:156:TYR:OH	2.38	0.41
1:G:253:LYS:HE3	1:G:253:LYS:HB3	1.91	0.41
1:C:300:TYR:CZ	1:C:302:GLU:HB2	2.55	0.41
1:A:141:GLU:HA	1:A:171:ILE:O	2.21	0.41
1:A:256:ILE:HG21	1:A:290:SER:HB2	2.02	0.41
1:E:73:VAL:HG21	1:E:295:TYR:CD1	2.55	0.41
2:F:12:VAL:O	2:F:34:VAL:HA	2.20	0.41
1:G:114:ARG:HD3	1:G:141:GLU:OE1	2.21	0.41
1:A:171:ILE:HG12	1:A:261:HIS:HB3	2.02	0.41
1:A:120:GLY:HA2	1:A:121:PRO:HD3	1.96	0.41
1:C:34:LEU:HD12	1:C:312:LEU:HD23	2.03	0.41
2:D:89:ILE:HD12	2:D:89:ILE:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:OE1	1:A:278:ILE:N	2.48	0.41
1:A:137:LYS:HG2	1:A:167:TYR:HA	2.04	0.40
1:C:218:ARG:HE	1:C:218:ARG:HB2	1.71	0.40
1:A:237:THR:OG1	1:A:238:PHE:N	2.53	0.40
1:C:172:PRO:HD2	1:C:261:HIS:O	2.21	0.40
1:G:237:THR:OG1	1:G:238:PHE:N	2.53	0.40
1:C:119:MET:HE3	1:C:119:MET:HB3	1.85	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	321/337 (95%)	313 (98%)	8 (2%)	0	100	100
1	C	321/337 (95%)	312 (97%)	9 (3%)	0	100	100
1	E	321/337 (95%)	311 (97%)	10 (3%)	0	100	100
1	G	321/337 (95%)	309 (96%)	12 (4%)	0	100	100
2	B	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
2	D	136/142 (96%)	131 (96%)	5 (4%)	0	100	100
2	F	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
2	H	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
All	All	1832/1916 (96%)	1777 (97%)	55 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	271/287 (94%)	270 (100%)	1 (0%)	91	97
1	C	272/287 (95%)	269 (99%)	3 (1%)	73	88
1	E	273/287 (95%)	270 (99%)	3 (1%)	73	88
1	G	272/287 (95%)	269 (99%)	3 (1%)	73	88
2	B	123/125 (98%)	122 (99%)	1 (1%)	81	92
2	D	122/125 (98%)	122 (100%)	0	100	100
2	F	122/125 (98%)	121 (99%)	1 (1%)	81	92
2	H	123/125 (98%)	122 (99%)	1 (1%)	81	92
All	All	1578/1648 (96%)	1565 (99%)	13 (1%)	81	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	TRP
2	B	126	GLU
1	C	117	TRP
1	C	166	LYS
1	C	203	ARG
1	E	119	MET
1	E	207	TYR
1	E	235	MET
2	F	7	LEU
1	G	144	ASN
1	G	214	GLU
1	G	307	HIS
2	H	110	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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$
5	EPE	H	201	-	15,15,15	0.80	1 (6%)	18,20,20	2.04	5 (27%)
3	GOL	G	401	-	5,5,5	0.81	0	5,5,5	1.04	0
5	EPE	D	201	-	15,15,15	0.82	1 (6%)	18,20,20	1.96	6 (33%)
3	GOL	A	401	-	5,5,5	0.92	0	5,5,5	0.95	0
3	GOL	E	401	-	5,5,5	0.77	0	5,5,5	0.99	0
5	EPE	F	201	-	15,15,15	0.84	1 (6%)	18,20,20	1.99	6 (33%)
5	EPE	B	201	-	15,15,15	0.81	1 (6%)	18,20,20	1.97	6 (33%)
5	EPE	B	202	-	15,15,15	0.87	1 (6%)	18,20,20	1.84	5 (27%)
3	GOL	C	401	-	5,5,5	0.88	0	5,5,5	0.97	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
5	EPE	H	201	-	-	3/9/19/19	0/1/1/1
3	GOL	G	401	-	-	4/4/4/4	-
5	EPE	D	201	-	-	2/9/19/19	0/1/1/1
3	GOL	A	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	E	401	-	-	2/4/4/4	-
5	EPE	F	201	-	-	4/9/19/19	0/1/1/1
5	EPE	B	201	-	-	7/9/19/19	0/1/1/1
5	EPE	B	202	-	-	3/9/19/19	0/1/1/1
3	GOL	C	401	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	202	EPE	C10-S	2.94	1.81	1.77
5	F	201	EPE	C10-S	2.75	1.81	1.77
5	D	201	EPE	C10-S	2.71	1.81	1.77
5	H	201	EPE	C10-S	2.71	1.81	1.77
5	B	201	EPE	C10-S	2.65	1.81	1.77

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	EPE	C5-N4-C3	5.46	121.11	108.83
5	B	201	EPE	C5-N4-C3	4.45	118.84	108.83
5	B	202	EPE	C5-N4-C3	4.35	118.62	108.83
5	D	201	EPE	C5-N4-C3	4.21	118.31	108.83
5	F	201	EPE	C5-N4-C3	4.07	117.98	108.83
5	B	201	EPE	C7-N4-C5	4.02	121.52	111.23
5	F	201	EPE	C7-N4-C3	3.78	120.89	111.23
5	F	201	EPE	C7-N4-C5	3.76	120.86	111.23
5	B	202	EPE	O1S-S-C10	3.55	111.19	106.92
5	H	201	EPE	C7-N4-C5	3.29	119.64	111.23
5	B	201	EPE	C7-N4-C3	3.28	119.62	111.23
5	B	202	EPE	C7-N4-C5	3.08	119.11	111.23
5	D	201	EPE	O1S-S-C10	3.06	110.60	106.92
5	F	201	EPE	O3S-S-C10	3.04	110.68	105.77
5	H	201	EPE	O1S-S-C10	2.99	110.51	106.92
5	B	202	EPE	C7-N4-C3	2.95	118.78	111.23
5	D	201	EPE	C7-N4-C3	2.92	118.71	111.23
5	H	201	EPE	C7-N4-C3	2.88	118.60	111.23
5	D	201	EPE	C6-N1-C2	2.83	115.21	108.83
5	D	201	EPE	C7-N4-C5	2.76	118.29	111.23
5	B	201	EPE	O1S-S-C10	2.70	110.17	106.92
5	D	201	EPE	O2S-S-C10	2.43	109.84	106.92
5	F	201	EPE	O2S-S-C10	2.37	109.77	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	201	EPE	O2S-S-C10	2.14	109.50	106.92
5	B	201	EPE	C6-N1-C2	2.10	113.56	108.83
5	F	201	EPE	C6-N1-C2	2.03	113.40	108.83
5	H	201	EPE	O2S-S-C10	2.03	109.36	106.92
5	B	202	EPE	O3S-S-C10	2.02	109.03	105.77

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	401	GOL	C1-C2-C3-O3
5	B	201	EPE	C8-C7-N4-C5
5	B	201	EPE	C9-C10-S-O1S
5	B	201	EPE	C9-C10-S-O3S
5	B	202	EPE	C9-C10-S-O2S
5	B	202	EPE	C9-C10-S-O3S
5	D	201	EPE	C10-C9-N1-C2
5	F	201	EPE	C8-C7-N4-C5
5	F	201	EPE	C9-C10-S-O2S
5	F	201	EPE	C9-C10-S-O3S
3	E	401	GOL	O1-C1-C2-C3
3	G	401	GOL	O1-C1-C2-C3
3	E	401	GOL	O1-C1-C2-O2
5	H	201	EPE	C8-C7-N4-C3
3	G	401	GOL	O2-C2-C3-O3
5	B	201	EPE	N4-C7-C8-O8
3	A	401	GOL	C1-C2-C3-O3
5	B	201	EPE	C10-C9-N1-C6
5	D	201	EPE	C10-C9-N1-C6
5	B	201	EPE	C9-C10-S-O2S
5	B	202	EPE	C9-C10-S-O1S
5	F	201	EPE	C9-C10-S-O1S
5	H	201	EPE	C9-C10-S-O2S
5	B	201	EPE	C10-C9-N1-C2
3	A	401	GOL	O1-C1-C2-C3
3	G	401	GOL	O1-C1-C2-O2
5	H	201	EPE	C9-C10-S-O1S

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	GOL	1	0
5	B	201	EPE	2	0
3	C	401	GOL	2	0

## 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	323/337 (95%)	-0.12	1 (0%) 94 93	25, 43, 60, 76	0
1	C	323/337 (95%)	-0.02	6 (1%) 66 62	24, 40, 76, 89	0
1	E	323/337 (95%)	-0.19	3 (0%) 84 82	22, 33, 55, 66	0
1	G	323/337 (95%)	0.11	7 (2%) 62 56	26, 44, 70, 86	0
2	B	139/142 (97%)	-0.29	0 100 100	25, 33, 43, 58	0
2	D	138/142 (97%)	-0.10	0 100 100	25, 38, 52, 58	0
2	F	140/142 (98%)	-0.18	1 (0%) 87 86	23, 35, 49, 60	0
2	H	139/142 (97%)	-0.30	0 100 100	26, 34, 50, 61	0
All	All	1848/1916 (96%)	-0.10	18 (0%) 82 80	22, 37, 62, 89	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	213	ASP	3.0
1	E	189	ALA	2.8
1	G	212	TYR	2.8
1	C	221	ALA	2.8
1	C	212	TYR	2.7
1	C	226	LYS	2.7
1	G	214	GLU	2.6
2	F	142	ASN	2.5
1	E	190	LEU	2.4
1	A	324	ASP	2.4
1	G	220	THR	2.3
1	C	213	ASP	2.3
1	G	215	ALA	2.2
1	G	324	ASP	2.2
1	C	193	GLY	2.1
1	C	238	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	191	ALA	2.1
1	G	250	GLN	2.1

## 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.

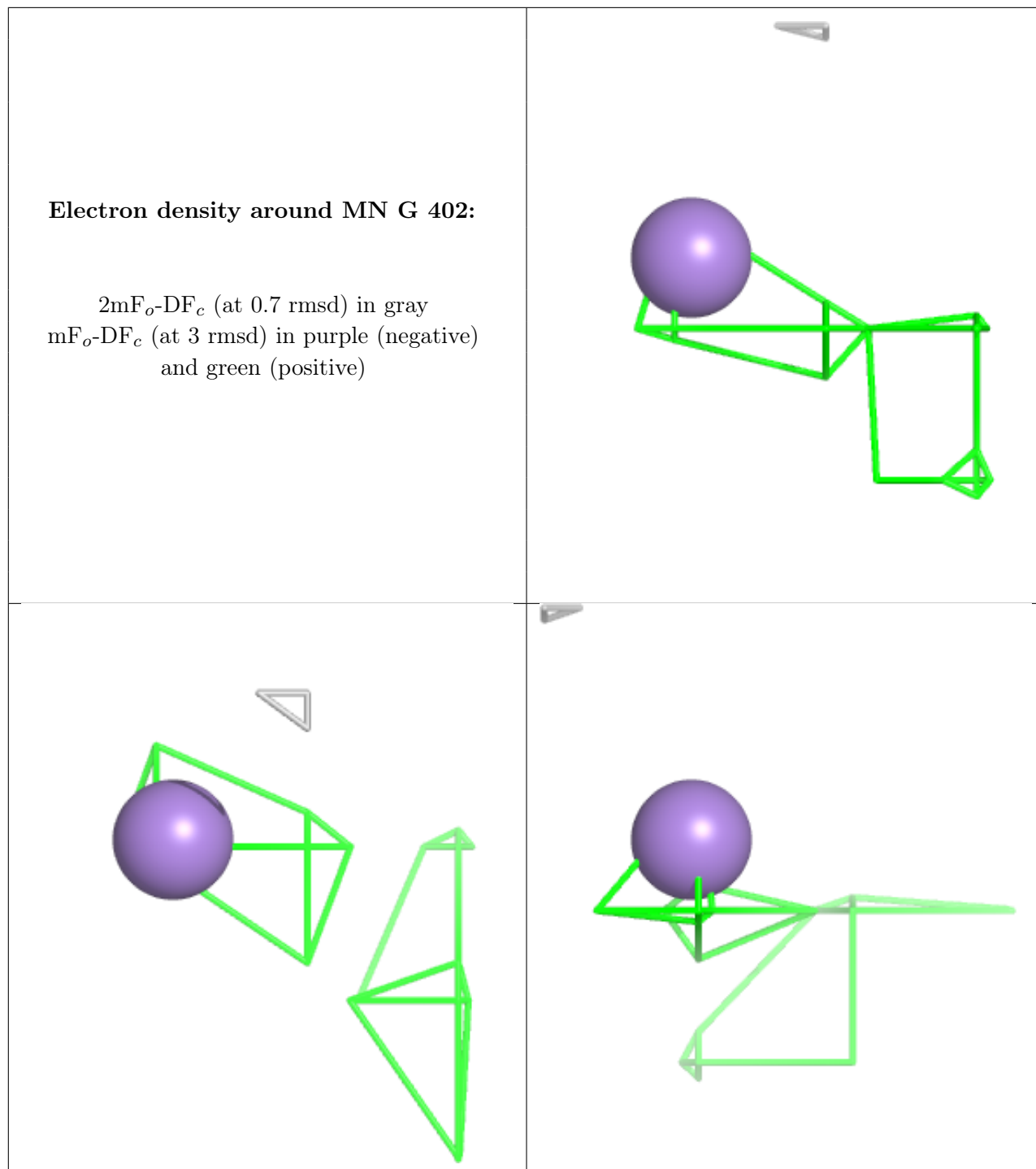
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	G	401	6/6	0.84	0.27	39,41,42,49	0
3	GOL	A	401	6/6	0.89	0.26	37,41,41,47	0
3	GOL	E	401	6/6	0.90	0.17	34,35,37,37	0
5	EPE	B	201	15/15	0.90	0.41	40,48,68,73	0
4	MN	G	402	1/1	0.93	0.19	32,32,32,32	1
3	GOL	C	401	6/6	0.94	0.15	38,39,43,46	0
5	EPE	B	202	15/15	0.94	0.26	37,59,77,77	0
5	EPE	D	201	15/15	0.94	0.34	42,57,73,74	0
5	EPE	F	201	15/15	0.95	0.30	38,50,70,71	0
5	EPE	H	201	15/15	0.95	0.30	35,60,82,87	0
4	MN	E	402	1/1	0.96	0.18	19,19,19,19	1
4	MN	C	402	1/1	0.97	0.17	29,29,29,29	1
4	MN	A	402	1/1	0.99	0.18	30,30,30,30	1

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



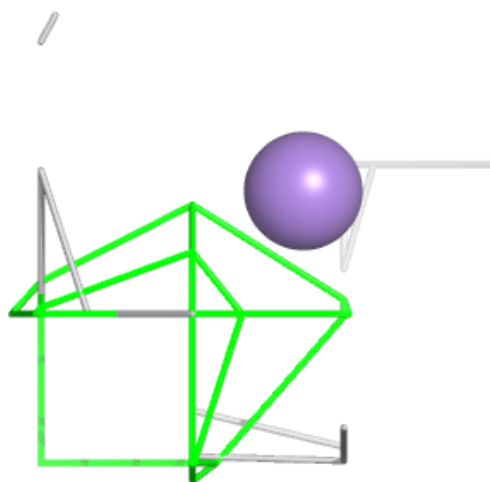
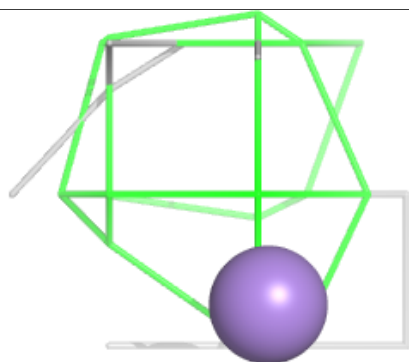
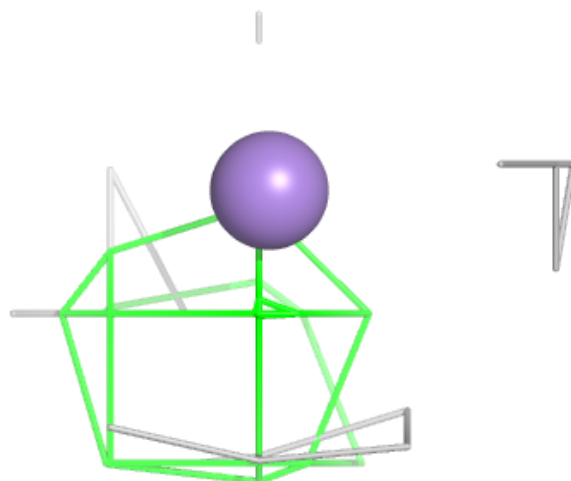
**Electron density around MN G 402:**

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



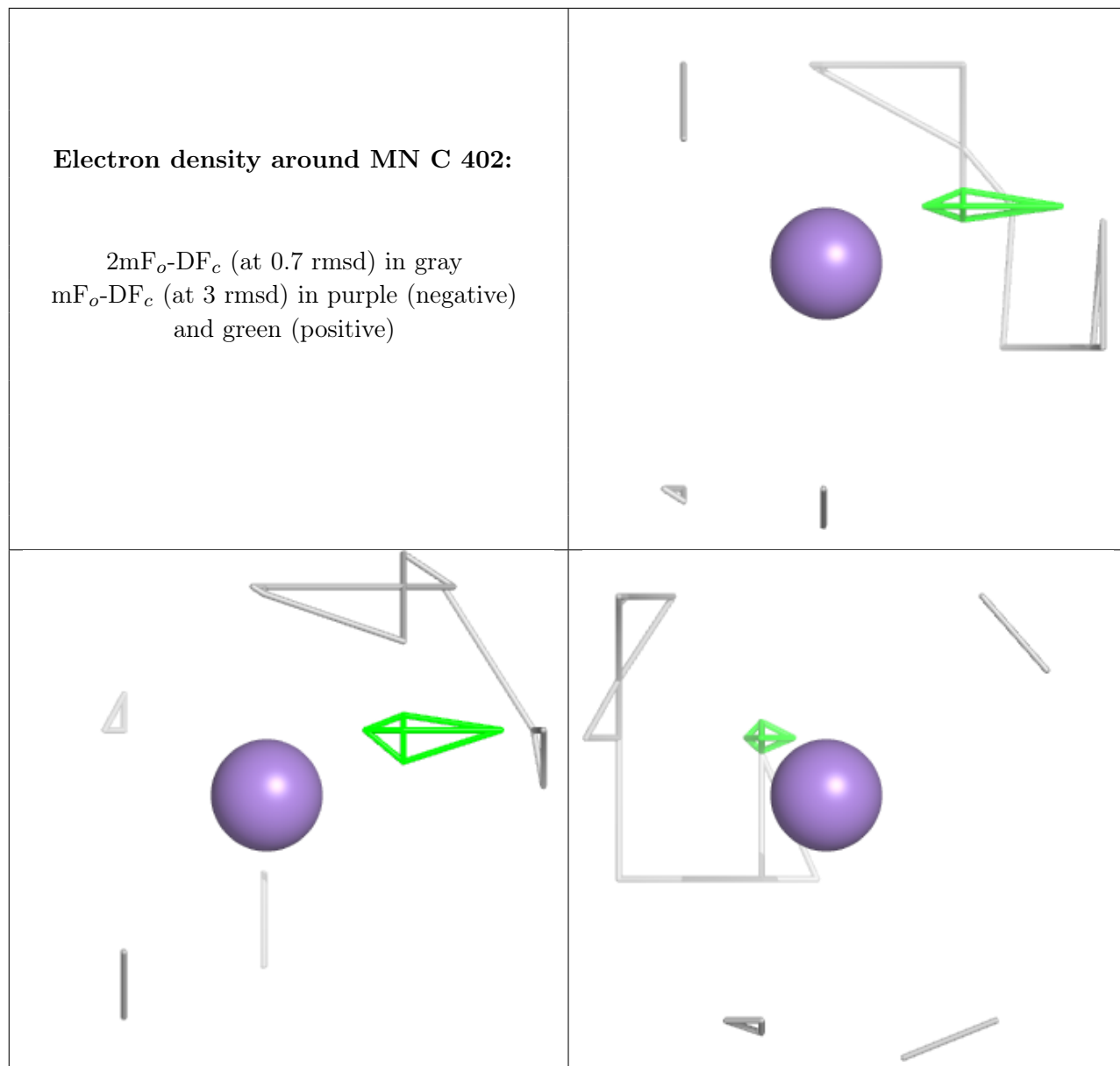
**Electron density around MN E 402:**

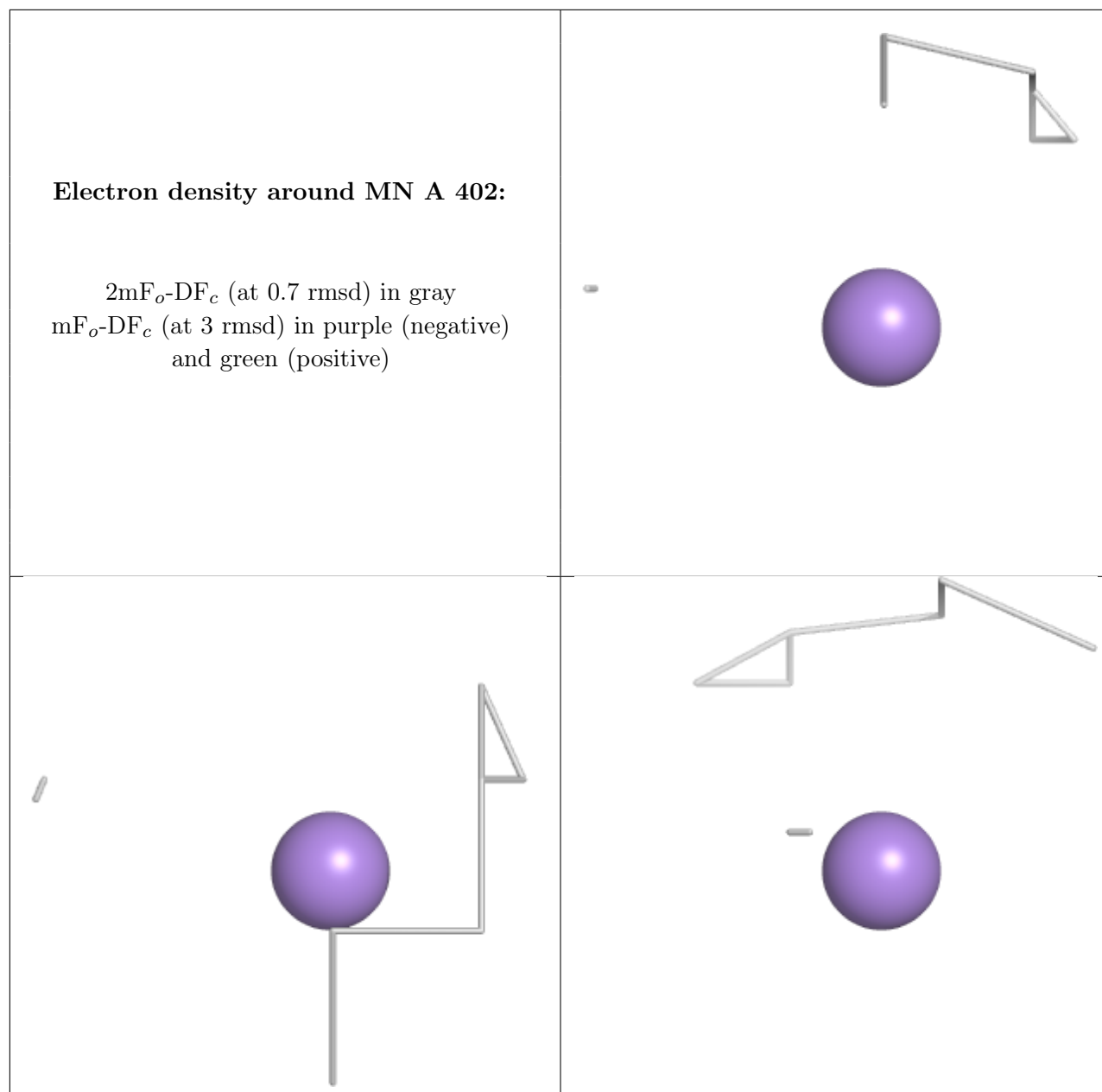
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MN C 402:**

$2mF_o-DF_c$  (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.