



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 10:17 am BST

PDB ID : 9GZQ / pdb\_00009gzq  
Title : Structure of ForCE lacking the Helical Membrane Plug-in (HMP; DUF1641)  
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Deposited on : 2024-10-04  
Resolution : 3.63 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 : 1.8.4, 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

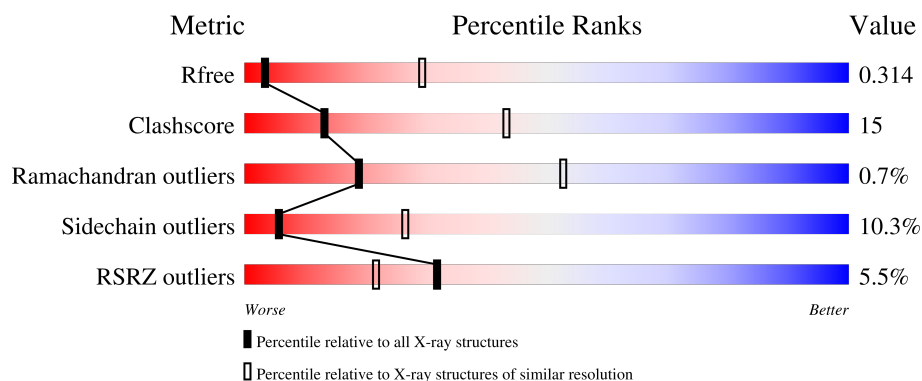
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.63 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	1619 (3.74-3.50)
Clashscore	180529	1721 (3.74-3.50)
Ramachandran outliers	177936	1694 (3.74-3.50)
Sidechain outliers	177891	1693 (3.74-3.50)
RSRZ outliers	164620	1618 (3.74-3.50)

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	1001	 6% 66% 27% . .
2	B	186	 42% 13% . 41%

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
4	SF4	A	1001	-	-	X	-
4	SF4	A	1002	-	-	X	-
4	SF4	A	1003	-	-	X	-
4	SF4	A	1004	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8632 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Probable oxidoreductase YjgC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	975	Total	C	N	O	S	0	0	0
			7636	4794	1307	1487	48			

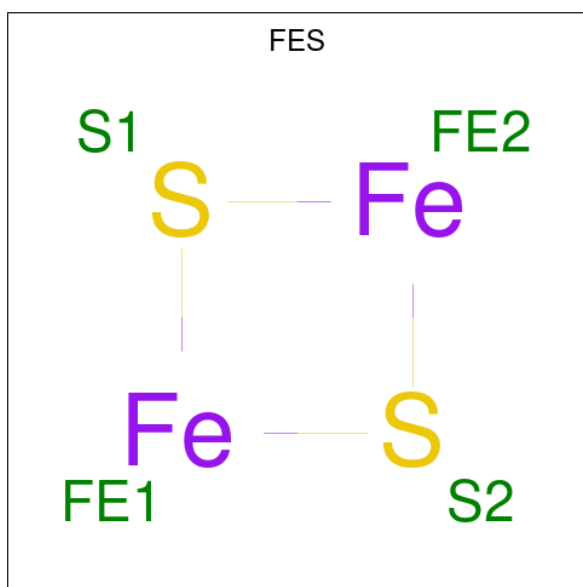
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP O34720
A	-14	HIS	-	expression tag	UNP O34720
A	-13	HIS	-	expression tag	UNP O34720
A	-12	HIS	-	expression tag	UNP O34720
A	-11	HIS	-	expression tag	UNP O34720
A	-10	HIS	-	expression tag	UNP O34720
A	-9	SER	-	expression tag	UNP O34720
A	-8	SER	-	expression tag	UNP O34720
A	-7	GLY	-	expression tag	UNP O34720
A	-6	GLU	-	expression tag	UNP O34720
A	-5	ASN	-	expression tag	UNP O34720
A	-4	LEU	-	expression tag	UNP O34720
A	-3	TYR	-	expression tag	UNP O34720
A	-2	PHE	-	expression tag	UNP O34720
A	-1	GLN	-	expression tag	UNP O34720
A	0	GLY	-	expression tag	UNP O34720

- Molecule 2 is a protein called ForE1.

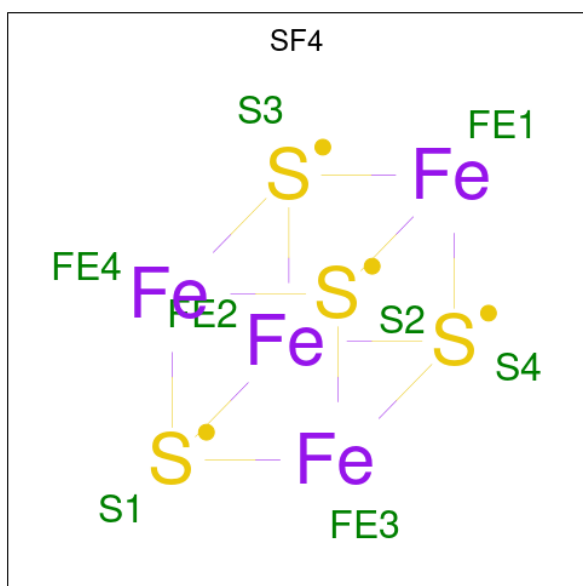
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total	C	N	O	S	0	0	0
			865	549	152	161	3			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



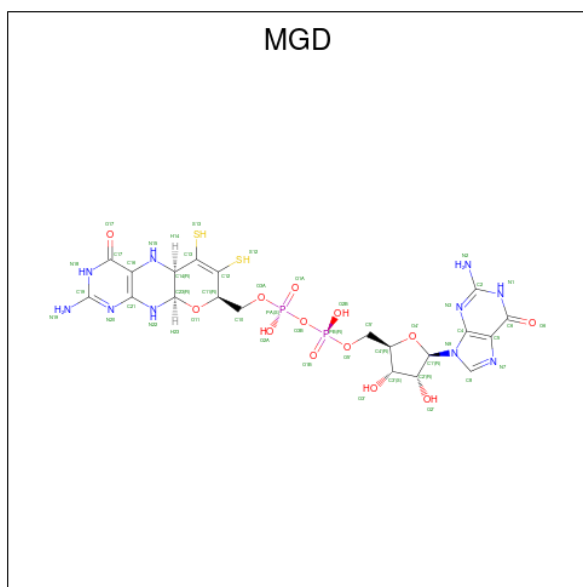
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula:  $C_{20}H_{26}N_{10}O_{13}P_2S_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

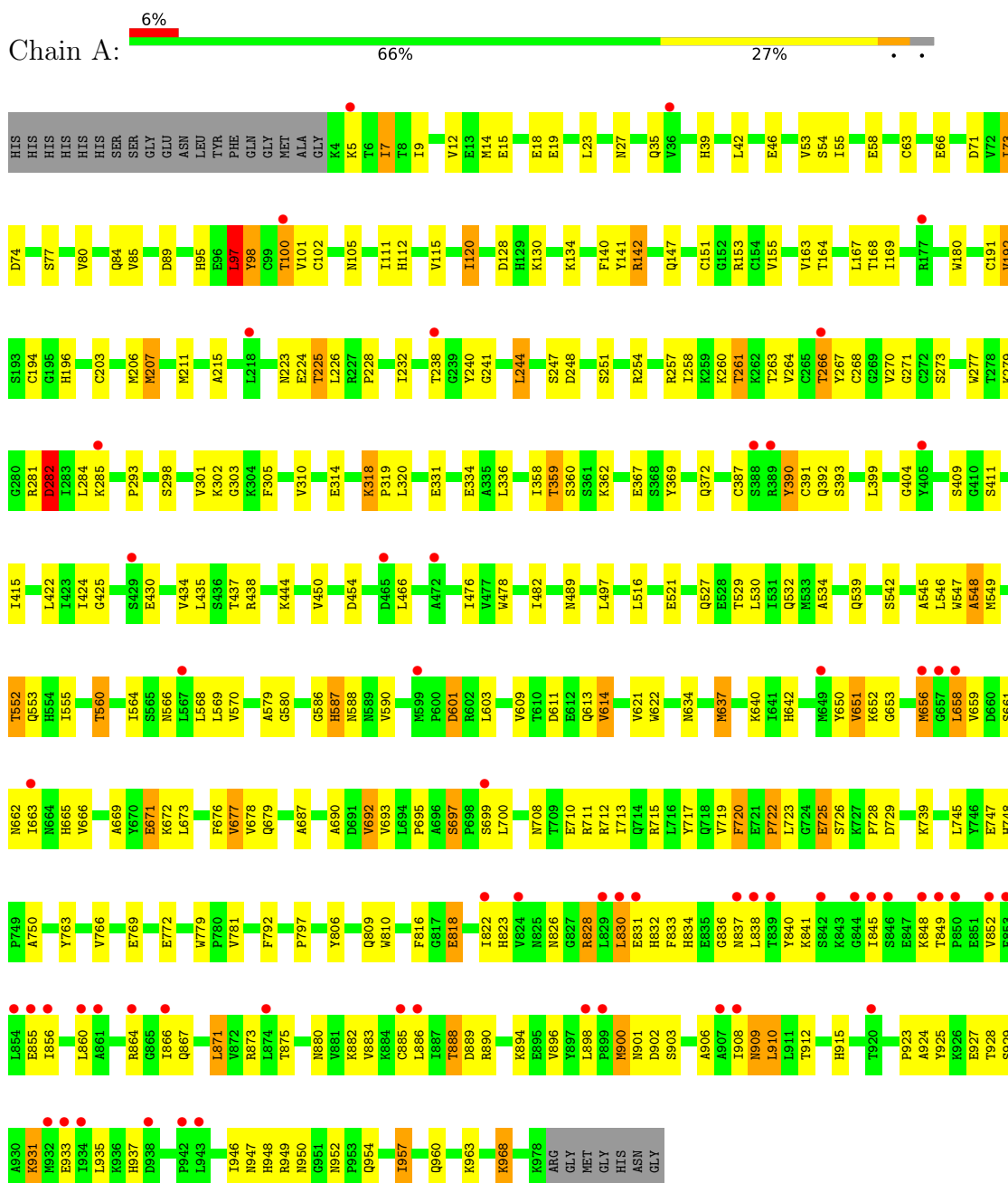
- Molecule 6 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		

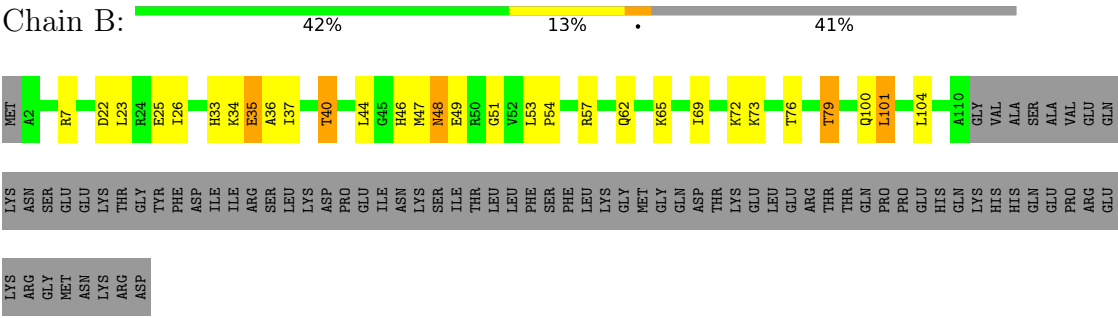
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Probable oxidoreductase YjgC



● Molecule 2: ForE1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	215.91Å 215.91Å 215.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.06 – 3.63 44.06 – 3.63	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.06-3.63) 99.5 (44.06-3.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 3.58Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.280 , 0.320 0.279 , 0.314	Depositor DCC
$R_{free}$ test set	1524 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	136.8	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 118.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.027 for l,-k,h 0.016 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8632	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: MGD, SF4, FES, 4MO

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	0.65	1/7797 (0.0%)	1.05	7/10558 (0.1%)
2	B	0.64	0/871	1.24	3/1168 (0.3%)
All	All	0.65	1/8668 (0.0%)	1.07	10/11726 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	548	ALA	CA-C	6.32	1.61	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	ASN	CA-CB-CG	6.64	119.24	112.60
1	A	601	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	282	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	84	GLN	CA-C-N	5.72	127.77	120.56
1	A	84	GLN	C-N-CA	5.72	127.77	120.56
1	A	164	THR	CB-CA-C	5.38	117.74	109.03
1	A	720	PHE	CA-CB-CG	5.28	119.08	113.80
2	B	48	ASN	CA-C-N	5.23	127.54	120.38
2	B	48	ASN	C-N-CA	5.23	127.54	120.38
2	B	35	GLU	CB-CG-CD	5.19	121.43	112.60

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	7636	0	7469	233	0
2	B	865	0	925	21	0
3	A	4	0	0	1	0
4	A	32	0	0	15	0
5	A	94	0	48	22	0
6	A	1	0	0	1	0
All	All	8632	0	8442	249	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 15.

All (249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:HB2	5:A:1006:MGD:H1'	1.36	1.04
1:A:555:ILE:HD11	1:A:915:HIS:CD2	2.01	0.96
1:A:360:SER:H	1:A:652:LYS:HZ2	0.95	0.95
2:B:62:GLN:HE21	2:B:65:LYS:HZ3	1.15	0.94
1:A:303:GLY:HA3	4:A:1004:SF4:S2	2.13	0.89
1:A:391:CYS:SG	6:A:1007:4MO:MO	1.82	0.88
1:A:360:SER:H	1:A:652:LYS:NZ	1.71	0.88
1:A:864:ARG:NH1	1:A:894:LYS:NZ	2.23	0.87
1:A:864:ARG:NH1	1:A:894:LYS:HZ3	1.75	0.85
1:A:362:LYS:NZ	1:A:833:PHE:HE2	1.74	0.84
1:A:834:HIS:HD2	1:A:900:MET:HE1	1.40	0.84
1:A:836:GLY:HA3	1:A:840:TYR:HD2	1.43	0.83
2:B:62:GLN:HE21	2:B:65:LYS:NZ	1.76	0.82
1:A:960:GLN:HG3	1:A:963:LYS:HZ1	1.46	0.80
1:A:832:HIS:CE1	1:A:845:ILE:HG22	2.15	0.80
1:A:362:LYS:HZ3	1:A:833:PHE:HE2	0.86	0.79
1:A:360:SER:N	1:A:652:LYS:HZ2	1.78	0.79
1:A:454:ASP:CB	5:A:1006:MGD:H1'	2.13	0.78
1:A:909:ASN:ND2	5:A:1005:MGD:N20	2.33	0.77
1:A:54:SER:HB3	1:A:74:ASP:HB3	1.67	0.77
1:A:642:HIS:CE1	1:A:669:ALA:HB2	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:HE3	5:A:1006:MGD:S12	2.27	0.74
1:A:566:ASN:HA	1:A:569:LEU:HB2	1.72	0.72
1:A:697:SER:HB2	1:A:728:PRO:HA	1.71	0.71
1:A:318:LYS:NZ	1:A:725:GLU:HG3	2.06	0.70
1:A:948:HIS:CE1	1:A:949:ARG:NH1	2.62	0.67
1:A:27:ASN:HD21	1:A:35:GLN:HE22	1.38	0.67
1:A:319:PRO:HA	1:A:695:PRO:HD3	1.76	0.67
1:A:318:LYS:HG3	1:A:319:PRO:HD2	1.77	0.66
1:A:391:CYS:HB2	5:A:1005:MGD:S13	2.36	0.66
1:A:748:HIS:NE2	1:A:750:ALA:HB3	2.10	0.66
1:A:155:VAL:HG21	1:A:169:ILE:HG13	1.79	0.65
1:A:241:GLY:HA3	2:B:73:LYS:HZ1	1.63	0.63
1:A:659:VAL:HB	5:A:1005:MGD:C23	2.28	0.63
1:A:411:SER:HA	1:A:710:GLU:HB2	1.80	0.63
1:A:642:HIS:HE1	1:A:669:ALA:HB2	1.63	0.63
1:A:834:HIS:CD2	1:A:900:MET:HE1	2.29	0.63
2:B:62:GLN:NE2	2:B:65:LYS:HZ3	1.92	0.63
2:B:65:LYS:O	2:B:69:ILE:HG12	1.97	0.63
1:A:425:GLY:HA2	1:A:454:ASP:HB3	1.80	0.62
1:A:826:ASN:HB3	1:A:908:ILE:HG12	1.82	0.62
1:A:832:HIS:NE2	1:A:849:THR:HB	2.14	0.62
1:A:663:ILE:HA	1:A:666:VAL:HG22	1.82	0.62
1:A:828:ARG:HH22	5:A:1005:MGD:H15	1.48	0.61
1:A:642:HIS:HA	1:A:672:LYS:NZ	2.15	0.61
1:A:267:TYR:HB3	1:A:302:LYS:HZ1	1.64	0.61
1:A:642:HIS:CA	1:A:672:LYS:HZ3	2.14	0.60
1:A:828:ARG:NE	5:A:1006:MGD:H102	2.17	0.60
1:A:134:LYS:NZ	1:A:142:ARG:HH21	1.99	0.60
1:A:46:GLU:HA	3:A:1000:FES:S2	2.42	0.60
2:B:35:GLU:HG2	2:B:36:ALA:N	2.18	0.59
1:A:656:MET:HA	1:A:659:VAL:HG22	1.85	0.59
1:A:611:ASP:HB2	1:A:614:VAL:HG22	1.83	0.59
1:A:444:LYS:HE2	1:A:957:ILE:HG13	1.84	0.59
1:A:834:HIS:HD2	1:A:900:MET:CE	2.14	0.59
1:A:434:VAL:HG23	4:A:1004:SF4:S1	2.43	0.58
1:A:960:GLN:HB2	1:A:963:LYS:HZ2	1.68	0.58
1:A:97:LEU:HA	4:A:1001:SF4:S3	2.44	0.57
1:A:838:LEU:HD21	5:A:1005:MGD:H8	1.85	0.57
1:A:360:SER:HB2	1:A:652:LYS:O	2.04	0.57
2:B:62:GLN:HG3	2:B:65:LYS:HZ2	1.68	0.56
1:A:318:LYS:HZ2	1:A:725:GLU:HG3	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TRP:O	1:A:482:ILE:HG12	2.05	0.56
1:A:112:HIS:ND1	1:A:244:LEU:HD21	2.20	0.56
1:A:555:ILE:HD11	1:A:915:HIS:HD2	1.65	0.56
1:A:837:ASN:HA	1:A:841:LYS:HZ3	1.71	0.56
1:A:542:SER:HB2	1:A:579:ALA:HB2	1.87	0.56
1:A:404:GLY:HA3	1:A:797:PRO:HG2	1.88	0.55
1:A:855:GLU:HG2	1:A:886:LEU:HD23	1.88	0.55
1:A:875:THR:HB	1:A:931:LYS:HD3	1.87	0.55
1:A:848:LYS:HD3	1:A:947:ASN:HA	1.89	0.55
1:A:266:THR:HG21	1:A:699:SER:HB2	1.89	0.55
1:A:359:THR:HB	1:A:652:LYS:HE3	1.89	0.55
1:A:257:ARG:HE	1:A:279:LYS:HD2	1.71	0.55
1:A:883:VAL:HG12	1:A:906:ALA:HB1	1.89	0.55
2:B:76:THR:HG1	2:B:79:THR:HG1	1.53	0.54
1:A:661:SER:HB3	1:A:923:PRO:HB3	1.90	0.54
2:B:48:ASN:HB2	2:B:53:LEU:HD12	1.89	0.54
1:A:909:ASN:HA	1:A:912:THR:HG22	1.90	0.54
1:A:642:HIS:HA	1:A:672:LYS:HD3	1.89	0.54
1:A:298:SER:HB2	1:A:438:ARG:HH22	1.73	0.53
1:A:437:THR:OG1	1:A:438:ARG:NH1	2.40	0.53
1:A:642:HIS:HA	1:A:672:LYS:HZ3	1.71	0.53
1:A:151:CYS:N	4:A:1002:SF4:S3	2.82	0.53
1:A:251:SER:HA	1:A:254:ARG:HD2	1.89	0.53
1:A:362:LYS:NZ	1:A:833:PHE:CE2	2.58	0.53
2:B:62:GLN:HG3	2:B:65:LYS:NZ	2.23	0.53
1:A:7:ILE:HD11	1:A:71:ASP:HB2	1.89	0.53
1:A:27:ASN:ND2	1:A:35:GLN:HE22	2.04	0.53
1:A:207:MET:HE3	1:A:211:MET:HB2	1.90	0.53
1:A:529:THR:HA	1:A:532:GLN:HG2	1.91	0.53
1:A:39:HIS:HB3	1:A:42:LEU:HB2	1.90	0.53
1:A:97:LEU:HD12	4:A:1001:SF4:S2	2.49	0.53
1:A:391:CYS:HB2	5:A:1005:MGD:S12	2.49	0.52
1:A:257:ARG:NE	1:A:279:LYS:HD2	2.25	0.52
1:A:320:LEU:HB2	1:A:693:VAL:HB	1.90	0.52
1:A:111:ILE:HD12	1:A:203:CYS:HB3	1.91	0.52
1:A:711:ARG:HB3	1:A:779:TRP:NE1	2.25	0.51
1:A:642:HIS:CE1	1:A:665:HIS:CE1	2.99	0.51
1:A:832:HIS:HE1	1:A:845:ILE:HG22	1.72	0.51
1:A:834:HIS:CE1	5:A:1006:MGD:H13	2.27	0.51
1:A:318:LYS:HZ3	1:A:725:GLU:HG3	1.75	0.51
1:A:115:VAL:HG13	1:A:120:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:ASN:HA	1:A:841:LYS:NZ	2.24	0.51
1:A:390:TYR:HB3	1:A:923:PRO:HD2	1.92	0.50
1:A:497:LEU:HD21	1:A:570:VAL:HA	1.92	0.50
1:A:960:GLN:HB2	1:A:963:LYS:NZ	2.26	0.50
1:A:77:SER:HB3	1:A:80:VAL:HG13	1.94	0.50
1:A:867:GLN:NE2	1:A:937:HIS:CE1	2.80	0.50
1:A:415:ILE:HD12	1:A:546:LEU:HD11	1.93	0.50
2:B:51:GLY:C	2:B:54:PRO:HD2	2.37	0.50
1:A:960:GLN:CG	1:A:963:LYS:HZ1	2.23	0.50
1:A:871:LEU:HB3	1:A:935:LEU:HB2	1.93	0.50
2:B:36:ALA:O	2:B:40:THR:OG1	2.30	0.50
1:A:241:GLY:HA3	2:B:73:LYS:NZ	2.27	0.50
1:A:391:CYS:HA	5:A:1005:MGD:S13	2.52	0.49
2:B:33:HIS:O	2:B:37:ILE:HG12	2.12	0.49
2:B:101:LEU:HG	2:B:104:LEU:HD23	1.95	0.49
1:A:241:GLY:CA	2:B:73:LYS:NZ	2.75	0.49
1:A:369:TYR:O	1:A:372:GLN:HG3	2.12	0.49
1:A:722:PRO:HB3	1:A:726:SER:O	2.13	0.49
1:A:387:CYS:HB2	5:A:1005:MGD:S12	2.53	0.49
1:A:763:TYR:HD2	1:A:766:VAL:HG21	1.76	0.49
1:A:241:GLY:CA	2:B:73:LYS:HZ1	2.26	0.48
1:A:391:CYS:SG	1:A:392:GLN:HG2	2.53	0.48
1:A:527:GLN:HA	1:A:530:LEU:HB3	1.94	0.48
1:A:832:HIS:CD2	1:A:849:THR:HB	2.48	0.48
1:A:310:VAL:HG21	1:A:700:LEU:HD12	1.95	0.48
1:A:603:LEU:HG	1:A:609:VAL:HG12	1.94	0.48
1:A:105:ASN:HB2	4:A:1001:SF4:S4	2.54	0.48
1:A:258:ILE:HD12	1:A:284:LEU:HD11	1.95	0.48
1:A:642:HIS:HA	1:A:672:LYS:CE	2.43	0.48
1:A:864:ARG:HH11	1:A:894:LYS:HZ3	1.59	0.48
1:A:873:ARG:HH21	1:A:882:LYS:HE3	1.78	0.48
1:A:134:LYS:HZ2	1:A:142:ARG:HH21	1.61	0.47
1:A:194:CYS:N	4:A:1003:SF4:S4	2.87	0.47
1:A:192:VAL:HA	1:A:948:HIS:HB2	1.97	0.47
1:A:303:GLY:CA	4:A:1004:SF4:S2	2.96	0.47
1:A:952:ASN:ND2	1:A:954:GLN:HE22	2.13	0.47
1:A:167:LEU:HD11	1:A:180:TRP:NE1	2.29	0.47
1:A:482:ILE:HD12	1:A:534:ALA:HB2	1.97	0.47
1:A:637:MET:HA	1:A:640:LYS:HG2	1.96	0.47
1:A:816:PHE:HB2	1:A:929:SER:HB2	1.96	0.47
1:A:924:ALA:HB1	1:A:927:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LYS:O	1:A:282:ASP:OD1	2.32	0.47
1:A:476:ILE:CG2	1:A:810:TRP:HD1	2.27	0.47
1:A:642:HIS:CE1	1:A:669:ALA:CB	2.96	0.47
1:A:676:PHE:HB3	1:A:690:ALA:HA	1.97	0.47
1:A:662:ASN:H	1:A:912:THR:HG23	1.80	0.47
1:A:270:VAL:HG11	1:A:434:VAL:HB	1.97	0.47
1:A:587:HIS:HB2	1:A:590:VAL:HB	1.97	0.47
1:A:586:GLY:HA3	5:A:1006:MGD:C12	2.45	0.46
1:A:948:HIS:NE2	1:A:949:ARG:NH1	2.64	0.46
1:A:267:TYR:HB2	4:A:1004:SF4:S3	2.56	0.46
1:A:85:VAL:O	1:A:89:ASP:OD1	2.33	0.46
1:A:399:LEU:HD21	1:A:547:TRP:HH2	1.81	0.46
2:B:47:MET:HE3	2:B:53:LEU:HD21	1.96	0.46
1:A:390:TYR:HB2	1:A:925:TYR:HE2	1.81	0.46
1:A:549:MET:HG3	1:A:828:ARG:NH2	2.31	0.46
1:A:823:HIS:HA	1:A:929:SER:HA	1.96	0.46
2:B:46:HIS:ND1	2:B:49:GLU:OE1	2.41	0.46
1:A:729:ASP:OD2	5:A:1005:MGD:N2	2.25	0.46
1:A:642:HIS:CA	1:A:672:LYS:NZ	2.76	0.45
1:A:832:HIS:CD2	1:A:849:THR:CG2	3.00	0.45
1:A:260:LYS:HG2	1:A:277:TRP:CD1	2.51	0.45
1:A:271:GLY:HA3	1:A:708:ASN:HD22	1.82	0.45
1:A:206:MET:HE2	4:A:1002:SF4:S1	2.56	0.45
1:A:362:LYS:HD3	1:A:588:ASN:HD21	1.82	0.45
1:A:553:GLN:HB3	1:A:925:TYR:H	1.82	0.45
1:A:134:LYS:CE	1:A:142:ARG:HE	2.30	0.45
1:A:548:ALA:HB1	5:A:1006:MGD:PA	2.57	0.45
1:A:864:ARG:NH1	1:A:894:LYS:HZ2	2.12	0.44
1:A:101:VAL:HG11	1:A:226:LEU:HD11	1.99	0.44
1:A:549:MET:HG2	5:A:1006:MGD:O2A	2.17	0.44
1:A:151:CYS:SG	1:A:153:ARG:HG3	2.57	0.44
1:A:621:VAL:HG13	1:A:622:TRP:CD1	2.52	0.44
1:A:98:TYR:N	4:A:1001:SF4:S3	2.80	0.44
1:A:240:TYR:O	1:A:244:LEU:HB2	2.17	0.44
1:A:715:ARG:NH2	1:A:717:TYR:CE1	2.86	0.44
1:A:836:GLY:HA3	1:A:840:TYR:CD2	2.35	0.44
1:A:167:LEU:HD11	4:A:1003:SF4:S1	2.57	0.44
1:A:659:VAL:HB	5:A:1005:MGD:H23	1.99	0.44
1:A:748:HIS:NE2	1:A:750:ALA:CB	2.78	0.44
1:A:856:ILE:HG13	1:A:860:LEU:HD23	1.98	0.44
1:A:898:LEU:HG	1:A:908:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:VAL:HG13	1:A:622:TRP:HD1	1.83	0.43
1:A:900:MET:H	1:A:900:MET:HG3	1.57	0.43
1:A:167:LEU:CD1	4:A:1003:SF4:S1	3.06	0.43
1:A:545:ALA:HB2	1:A:568:LEU:HD21	1.99	0.43
1:A:840:TYR:OH	1:A:901:ASN:ND2	2.50	0.43
1:A:358:ILE:HB	1:A:651:VAL:HB	2.00	0.43
1:A:261:THR:HG22	1:A:717:TYR:HB3	2.00	0.43
1:A:663:ILE:HD11	1:A:910:LEU:HD12	2.00	0.43
1:A:864:ARG:CZ	1:A:894:LYS:HZ3	2.30	0.43
1:A:302:LYS:HB2	1:A:302:LYS:HE3	1.88	0.43
1:A:549:MET:HG2	5:A:1006:MGD:H101	2.01	0.43
1:A:968:LYS:NZ	1:A:968:LYS:HA	2.34	0.43
1:A:560:THR:O	1:A:564:ILE:HG13	2.19	0.43
1:A:98:TYR:HD1	1:A:102:CYS:HB2	1.83	0.43
1:A:642:HIS:HB3	1:A:672:LYS:NZ	2.34	0.42
2:B:22:ASP:O	2:B:25:GLU:HB2	2.18	0.42
1:A:331:GLU:HB2	1:A:334:GLU:HG2	2.01	0.42
1:A:268:CYS:SG	1:A:270:VAL:HG23	2.60	0.42
1:A:391:CYS:SG	1:A:392:GLN:NE2	2.79	0.42
1:A:391:CYS:CB	5:A:1005:MGD:S13	3.05	0.42
1:A:422:LEU:HD21	1:A:424:ILE:HD11	2.00	0.42
1:A:678:VAL:HG11	1:A:687:ALA:HA	2.01	0.42
1:A:241:GLY:C	2:B:73:LYS:NZ	2.77	0.42
1:A:141:TYR:OH	1:A:191:CYS:SG	2.77	0.42
1:A:336:LEU:HB3	1:A:739:LYS:HG3	2.00	0.42
1:A:566:ASN:HD22	1:A:806:TYR:H	1.68	0.42
1:A:586:GLY:HA2	5:A:1006:MGD:H23	2.01	0.42
1:A:650:TYR:OH	1:A:679:GLN:NE2	2.52	0.42
1:A:671:GLU:H	1:A:671:GLU:HG2	1.70	0.42
1:A:873:ARG:NH2	1:A:880:ASN:HD21	2.16	0.42
1:A:912:THR:HA	1:A:928:THR:HG21	2.00	0.42
1:A:194:CYS:SG	1:A:196:HIS:ND1	2.89	0.42
1:A:871:LEU:HD22	1:A:935:LEU:HD12	2.01	0.42
1:A:888:THR:HG21	1:A:890:ARG:HE	1.85	0.42
1:A:769:GLU:HA	1:A:772:GLU:HG2	2.02	0.42
1:A:134:LYS:HE3	1:A:142:ARG:HE	1.85	0.41
1:A:267:TYR:CB	4:A:1004:SF4:S3	3.07	0.41
1:A:95:HIS:NE2	1:A:147:GLN:NE2	2.68	0.41
1:A:430:GLU:HG2	1:A:830:LEU:HB2	2.03	0.41
1:A:552:THR:HG22	1:A:553:GLN:HG3	2.02	0.41
1:A:586:GLY:CA	5:A:1006:MGD:H23	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:VAL:HB	1:A:902:ASP:HB2	2.02	0.41
1:A:281:ARG:HH21	1:A:723:LEU:HB2	1.85	0.41
1:A:409:SER:HB2	1:A:580:GLY:HA3	2.01	0.41
1:A:864:ARG:CZ	1:A:894:LYS:NZ	2.82	0.41
1:A:53:VAL:HG23	1:A:55:ILE:HG23	2.03	0.41
1:A:140:PHE:HB3	1:A:305:PHE:CD1	2.56	0.41
1:A:302:LYS:HE3	4:A:1004:SF4:S3	2.61	0.41
1:A:642:HIS:HA	1:A:672:LYS:CD	2.51	0.41
1:A:700:LEU:HD22	1:A:719:VAL:HG21	2.03	0.41
1:A:960:GLN:CB	1:A:963:LYS:NZ	2.84	0.41
1:A:100:THR:HG23	1:A:247:SER:HB3	2.03	0.41
1:A:266:THR:CG2	1:A:699:SER:HB2	2.51	0.41
1:A:9:ILE:HG13	1:A:12:VAL:HB	2.03	0.40
1:A:225:THR:C	1:A:228:PRO:HD2	2.47	0.40
1:A:549:MET:HG3	1:A:828:ARG:HH21	1.87	0.40
1:A:55:ILE:HG22	1:A:73:ILE:HG23	2.02	0.40
1:A:211:MET:HE2	1:A:215:ALA:HB2	2.02	0.40
1:A:822:ILE:HD11	1:A:896:VAL:HG13	2.04	0.40
1:A:23:LEU:HD22	1:A:63:CYS:HB3	2.04	0.40
1:A:677:VAL:HB	1:A:692:VAL:HG13	2.03	0.40
1:A:112:HIS:HE1	1:A:248:ASP:OD1	2.04	0.40
1:A:873:ARG:HB2	1:A:933:GLU:HB2	2.02	0.40
1:A:293:PRO:HB2	1:A:712:ARG:HD3	2.02	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	973/1001 (97%)	892 (92%)	73 (8%)	8 (1%)	16	50
2	B	107/186 (58%)	106 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1080/1187 (91%)	998 (92%)	74 (7%)	8 (1%)	19	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	818	GLU
1	A	5	LYS
1	A	97	LEU
1	A	18	GLU
1	A	658	LEU
1	A	722	PRO
1	A	653	GLY
1	A	946	ILE

### 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	840/859 (98%)	755 (90%)	85 (10%)	6	27
2	B	95/165 (58%)	84 (88%)	11 (12%)	4	23
All	All	935/1024 (91%)	839 (90%)	96 (10%)	6	26

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	14	MET
1	A	15	GLU
1	A	19	GLU
1	A	58	GLU
1	A	66	GLU
1	A	73	ILE
1	A	97	LEU
1	A	98	TYR
1	A	100	THR

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Mol	Chain	Res	Type
1	A	120	ILE
1	A	128	ASP
1	A	130	LYS
1	A	142	ARG
1	A	163	VAL
1	A	168	THR
1	A	192	VAL
1	A	207	MET
1	A	223	ASN
1	A	224	GLU
1	A	225	THR
1	A	232	ILE
1	A	238	THR
1	A	244	LEU
1	A	261	THR
1	A	263	THR
1	A	264	VAL
1	A	266	THR
1	A	273	SER
1	A	282	ASP
1	A	285	LYS
1	A	301	VAL
1	A	314	GLU
1	A	318	LYS
1	A	359	THR
1	A	367	GLU
1	A	390	TYR
1	A	393	SER
1	A	435	LEU
1	A	450	VAL
1	A	466	LEU
1	A	489	ASN
1	A	516	LEU
1	A	521	GLU
1	A	539	GLN
1	A	552	THR
1	A	560	THR
1	A	587	HIS
1	A	601	ASP
1	A	613	GLN
1	A	614	VAL
1	A	637	MET

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Mol	Chain	Res	Type
1	A	651	VAL
1	A	656	MET
1	A	658	LEU
1	A	671	GLU
1	A	673	LEU
1	A	677	VAL
1	A	692	VAL
1	A	697	SER
1	A	713	ILE
1	A	720	PHE
1	A	725	GLU
1	A	745	LEU
1	A	747	GLU
1	A	781	VAL
1	A	792	PHE
1	A	809	GLN
1	A	818	GLU
1	A	828	ARG
1	A	830	LEU
1	A	831	GLU
1	A	866	ILE
1	A	871	LEU
1	A	885	CYS
1	A	888	THR
1	A	889	ASP
1	A	900	MET
1	A	903	SER
1	A	909	ASN
1	A	910	LEU
1	A	931	LYS
1	A	950	ASN
1	A	957	ILE
1	A	968	LYS
2	B	7	ARG
2	B	23	LEU
2	B	26	ILE
2	B	34	LYS
2	B	40	THR
2	B	44	LEU
2	B	57	ARG
2	B	72	LYS
2	B	79	THR

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Mol	Chain	Res	Type
2	B	100	GLN
2	B	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	35	GLN
1	A	106	ASN
1	A	112	HIS
1	A	122	HIS
1	A	123	GLN
1	A	392	GLN
1	A	427	ASN
1	A	489	ASN
1	A	532	GLN
1	A	573	ASN
1	A	587	HIS
1	A	588	ASN
1	A	642	HIS
1	A	665	HIS
1	A	667	HIS
1	A	679	GLN
1	A	731	GLN
1	A	832	HIS
1	A	880	ASN
1	A	901	ASN
1	A	909	ASN
1	A	937	HIS
1	A	948	HIS
1	A	950	ASN
1	A	954	GLN
1	A	962	HIS
2	B	62	GLN
2	B	85	ASN
2	B	100	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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$
4	SF4	A	1004	1	0,12,12	-	-	-		
4	SF4	A	1003	1	0,12,12	-	-	-		
5	MGD	A	1006	-	41,52,52	0.67	0	40,81,81	0.96	2 (5%)
3	FES	A	1000	1	0,4,4	-	-	-		
5	MGD	A	1005	-	41,52,52	0.67	0	40,81,81	0.82	1 (2%)
4	SF4	A	1001	1	0,12,12	-	-	-		
4	SF4	A	1002	1	0,12,12	-	-	-		

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
4	SF4	A	1004	1	-	-	0/6/5/5
4	SF4	A	1003	1	-	-	0/6/5/5
5	MGD	A	1006	-	-	7/18/66/66	0/6/6/6
3	FES	A	1000	1	-	-	0/1/1/1
5	MGD	A	1005	-	-	4/18/66/66	0/6/6/6
4	SF4	A	1001	1	-	-	0/6/5/5
4	SF4	A	1002	1	-	-	0/6/5/5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1006	MGD	O11-C23-C14	3.51	111.30	108.96
5	A	1005	MGD	O11-C23-C14	-3.39	106.70	108.96
5	A	1006	MGD	O2A-PA-O1A	3.14	127.75	112.24

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1005	MGD	O3A-C10-C11-O11
5	A	1005	MGD	O3A-C10-C11-C12
5	A	1006	MGD	C5'-O5'-PB-O2B
5	A	1005	MGD	PB-O3B-PA-O1A
5	A	1006	MGD	PA-O3B-PB-O5'
5	A	1006	MGD	C5'-O5'-PB-O3B
5	A	1006	MGD	C5'-O5'-PB-O1B
5	A	1006	MGD	C11-C10-O3A-PA
5	A	1006	MGD	C10-O3A-PA-O3B
5	A	1005	MGD	PB-O3B-PA-O2A
5	A	1006	MGD	O4'-C4'-C5'-O5'

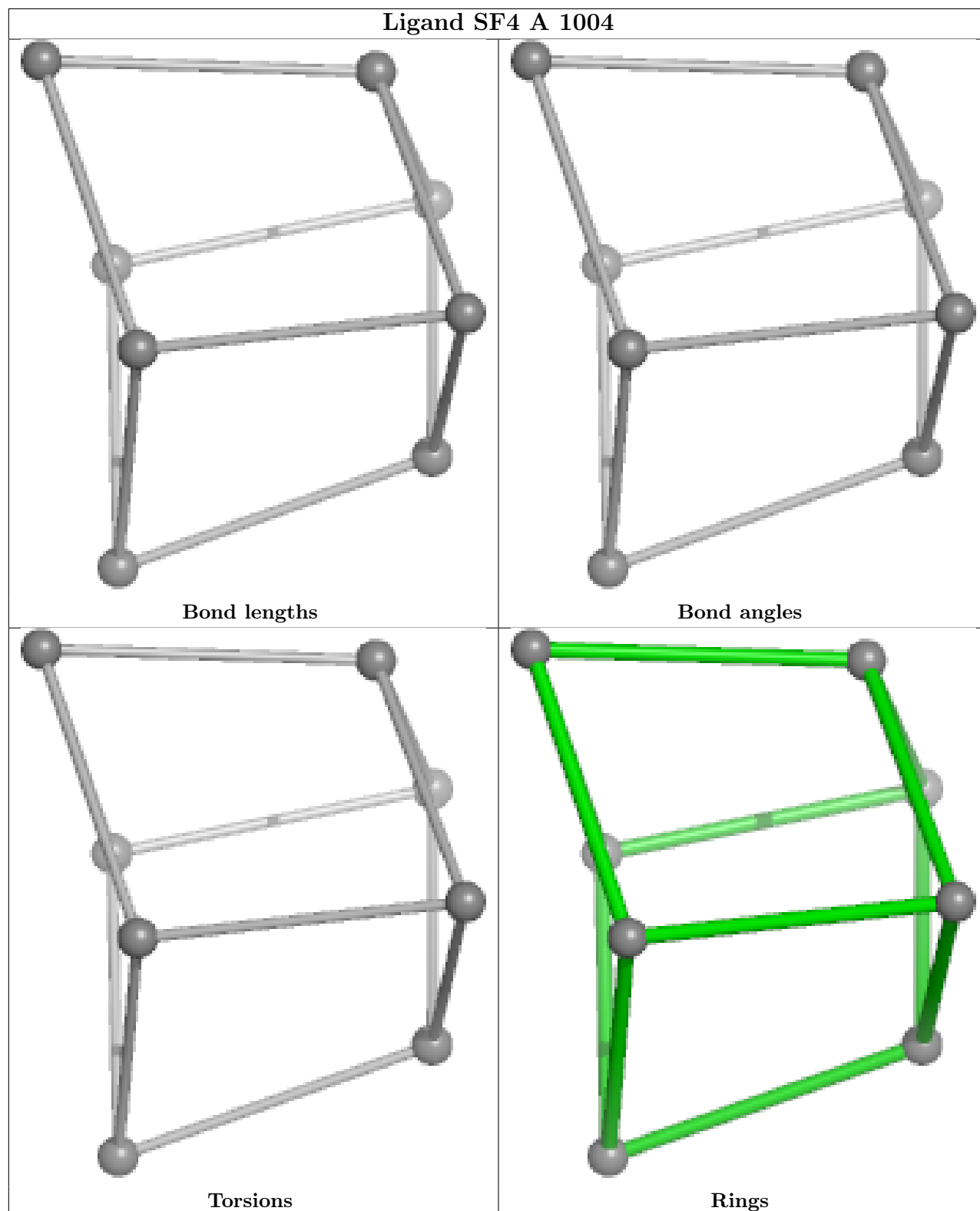
There are no ring outliers.

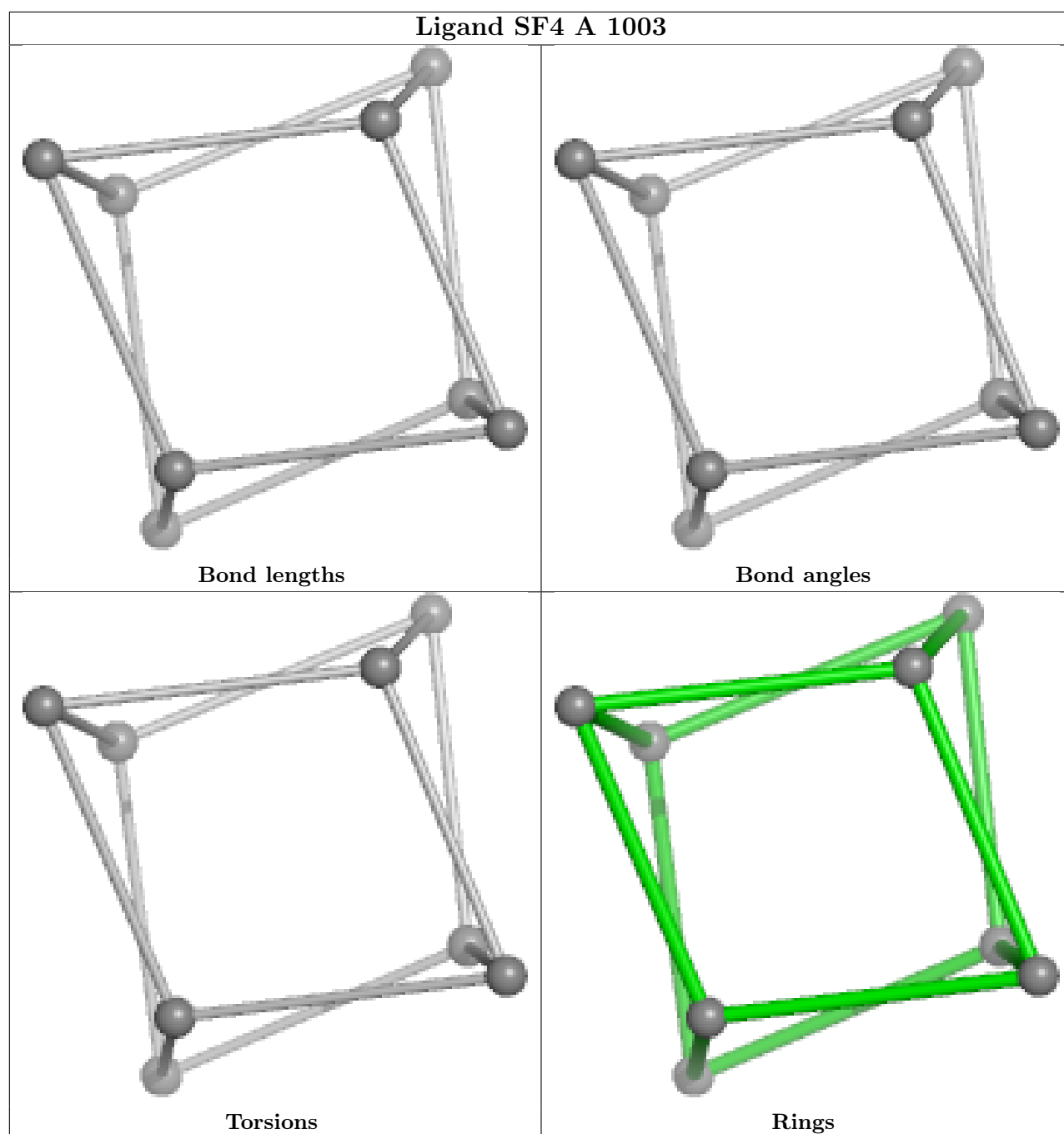
7 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	SF4	6	0
4	A	1003	SF4	3	0
5	A	1006	MGD	11	0
3	A	1000	FES	1	0
5	A	1005	MGD	11	0
4	A	1001	SF4	4	0
4	A	1002	SF4	2	0

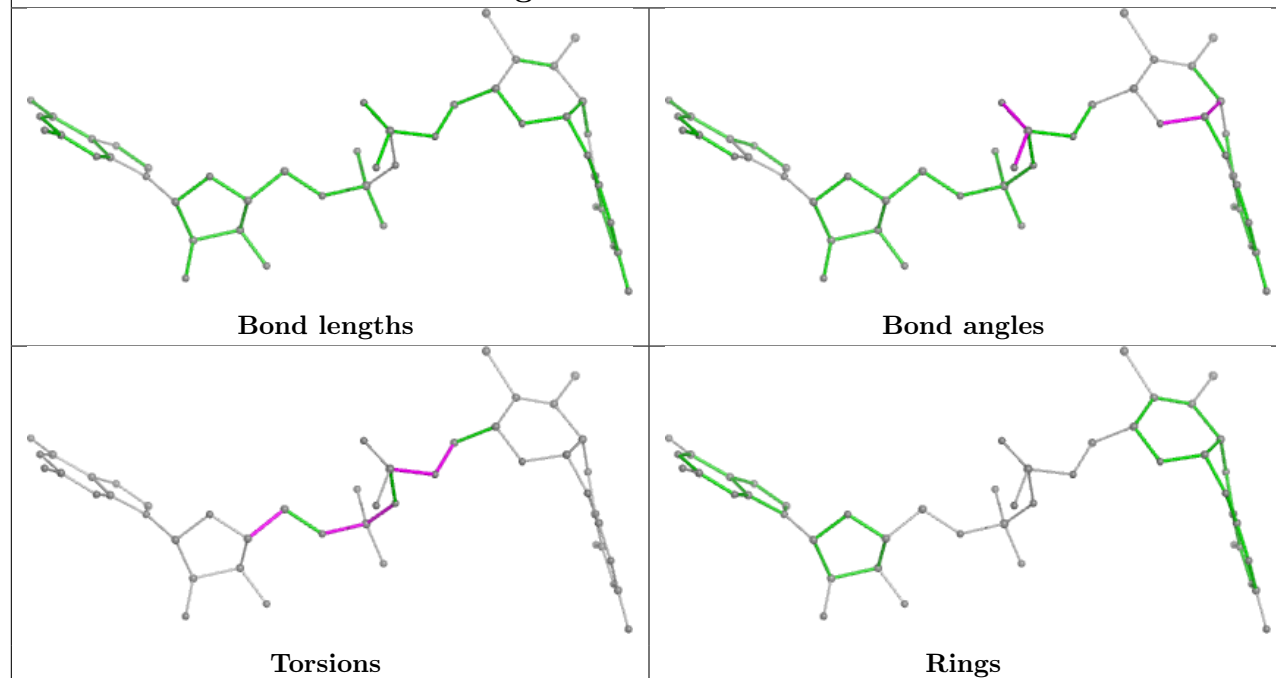
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

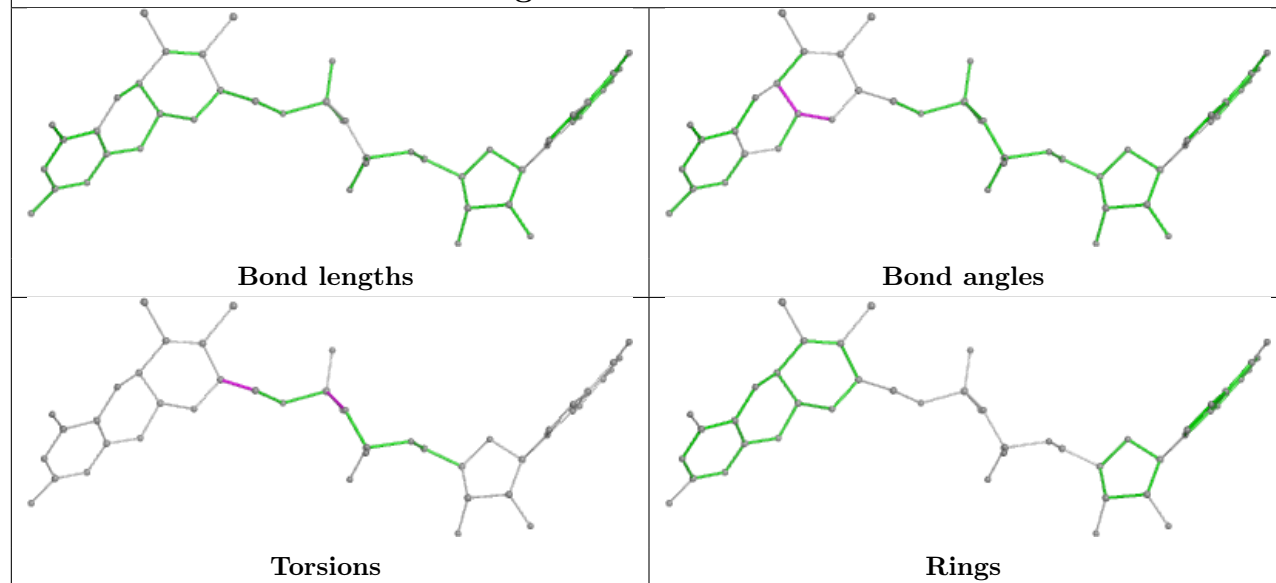


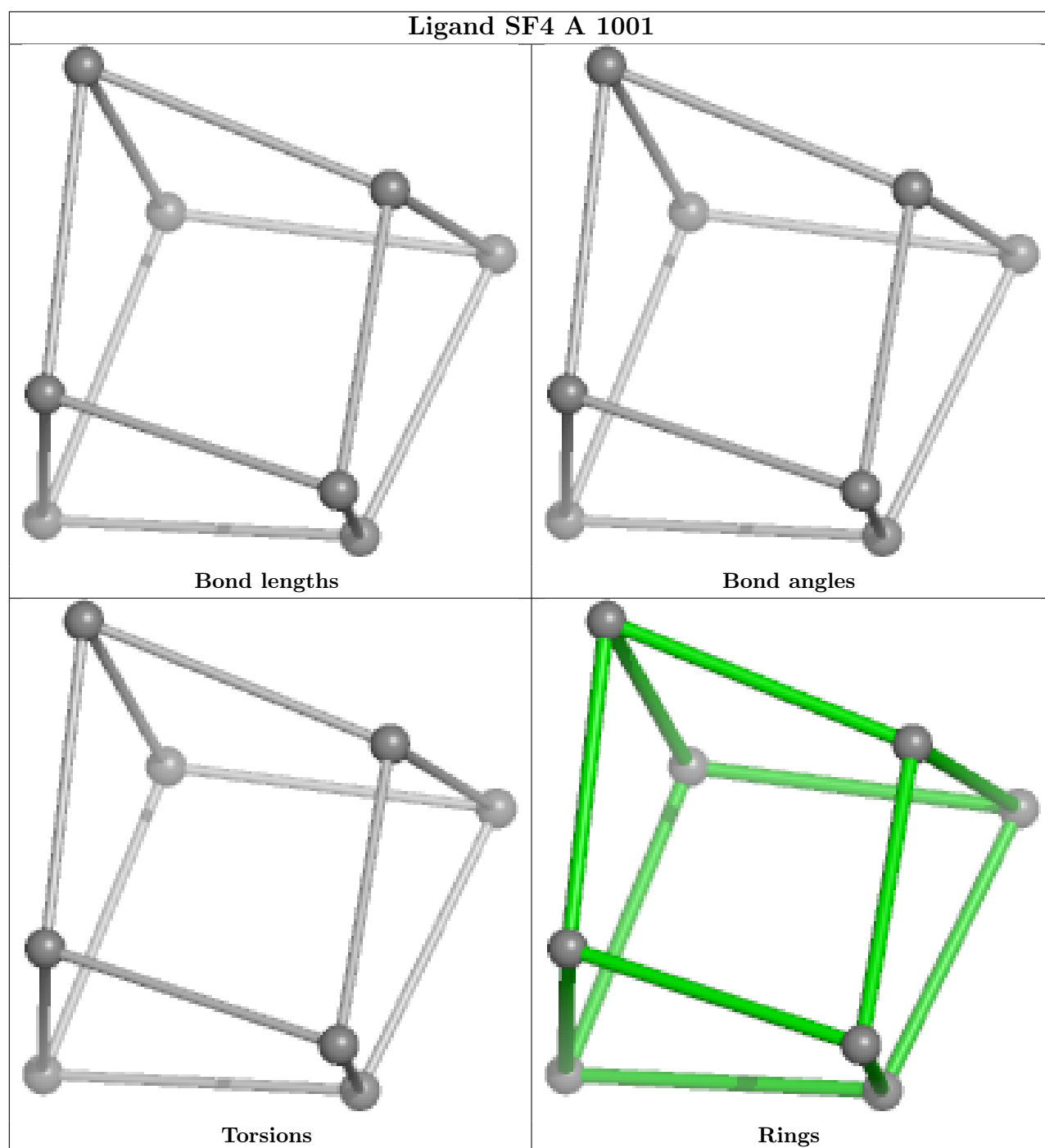


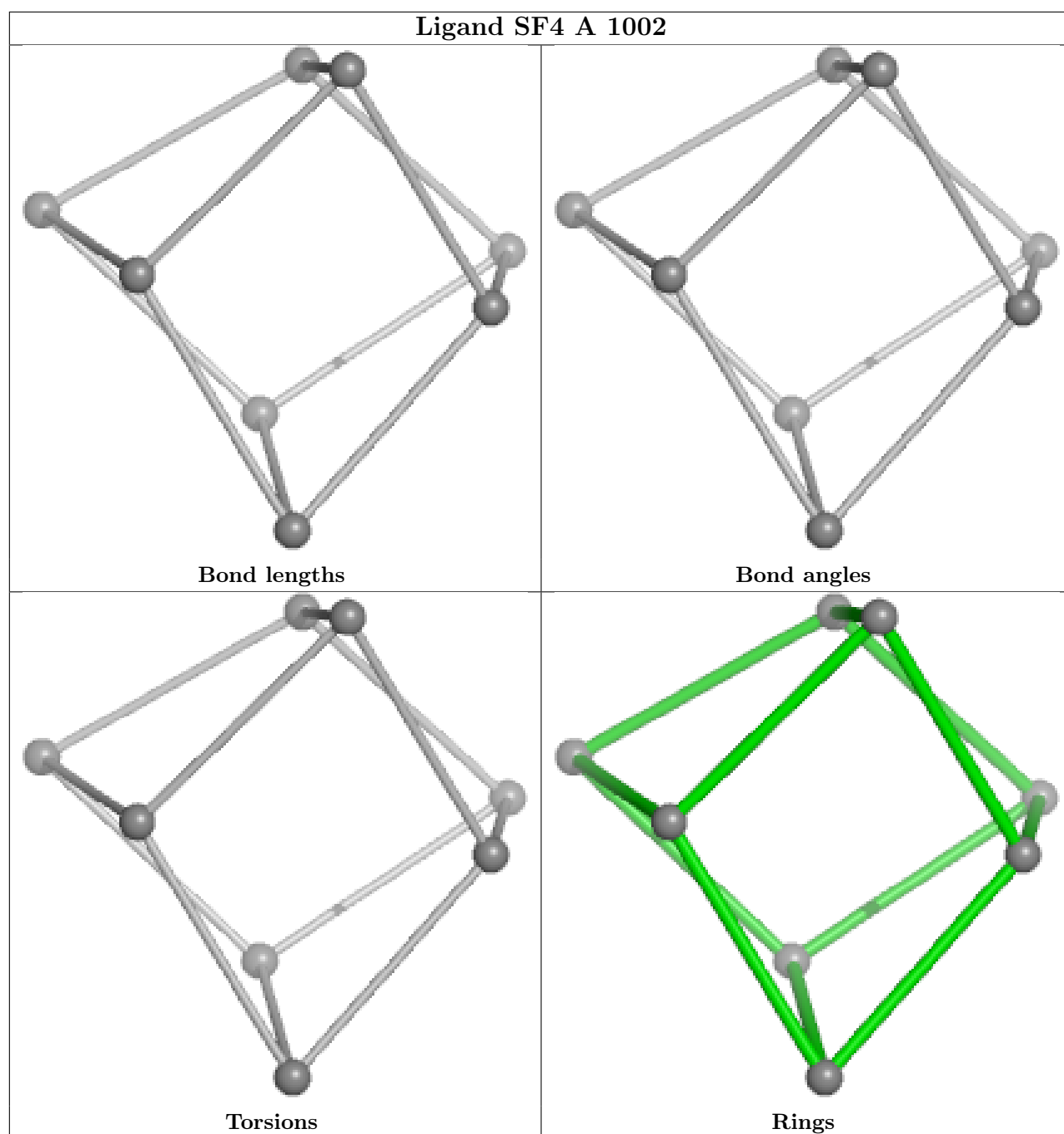
## Ligand MGD A 1006



## Ligand MGD A 1005







## 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	975/1001 (97%)	0.22	60 (6%) 28 20	99, 164, 198, 216	0
2	B	109/186 (58%)	-0.07	0 100 100	103, 145, 182, 198	0
All	All	1084/1187 (91%)	0.19	60 (5%) 32 22	99, 161, 198, 216	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	657	GLY	5.1
1	A	838	LEU	5.1
1	A	656	MET	4.7
1	A	829	LEU	4.6
1	A	658	LEU	4.4
1	A	874	LEU	3.8
1	A	842	SER	3.8
1	A	266	THR	3.7
1	A	844	GLY	3.6
1	A	932	MET	3.5
1	A	429	SER	3.5
1	A	885	CYS	3.1
1	A	846	SER	3.0
1	A	405	TYR	2.9
1	A	100	THR	2.8
1	A	699	SER	2.8
1	A	850	PRO	2.8
1	A	907	ALA	2.7
1	A	899	PRO	2.7
1	A	599	MET	2.7
1	A	839	THR	2.6
1	A	856	ILE	2.6
1	A	285	LYS	2.6
1	A	218	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	238	THR	2.5
1	A	831	GLU	2.5
1	A	845	ILE	2.5
1	A	908	ILE	2.5
1	A	938	ASP	2.4
1	A	864	ARG	2.4
1	A	822	ILE	2.3
1	A	920	THR	2.3
1	A	861	ALA	2.3
1	A	942	PRO	2.3
1	A	855	GLU	2.2
1	A	177	ARG	2.2
1	A	854	LEU	2.2
1	A	389	ARG	2.2
1	A	848	LYS	2.2
1	A	649	MET	2.2
1	A	36	VAL	2.2
1	A	849	THR	2.2
1	A	860	LEU	2.2
1	A	388	SER	2.2
1	A	5	LYS	2.1
1	A	934	ILE	2.1
1	A	824	VAL	2.1
1	A	465	ASP	2.1
1	A	866	ILE	2.1
1	A	472	ALA	2.1
1	A	663	ILE	2.1
1	A	830	LEU	2.1
1	A	567	LEU	2.0
1	A	852	VAL	2.0
1	A	853	PHE	2.0
1	A	886	LEU	2.0
1	A	933	GLU	2.0
1	A	837	ASN	2.0
1	A	898	LEU	2.0
1	A	943	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates

There are no oligosaccharides in this entry.

## 6.4 Ligands

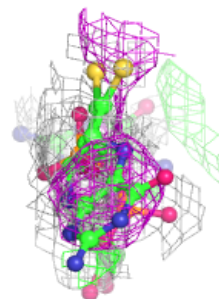
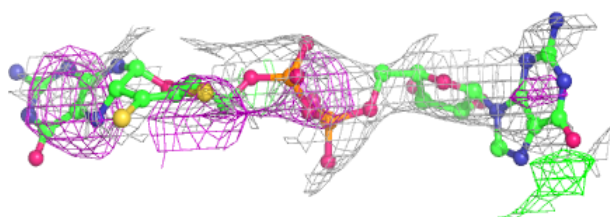
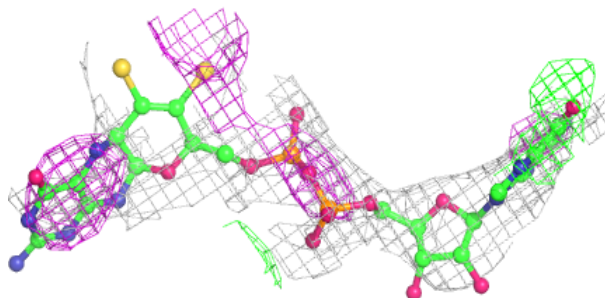
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	MGD	A	1005	47/47	0.86	0.13	143,154,160,164	0
5	MGD	A	1006	47/47	0.86	0.12	141,150,157,169	0
6	4MO	A	1007	1/1	0.96	0.15	172,172,172,172	0
3	FES	A	1000	4/4	0.98	0.04	140,144,145,154	0
4	SF4	A	1001	8/8	0.98	0.04	93,117,133,146	0
4	SF4	A	1003	8/8	0.98	0.07	109,125,131,151	0
4	SF4	A	1004	8/8	0.99	0.07	113,120,143,148	0
4	SF4	A	1002	8/8	0.99	0.06	104,118,132,148	0

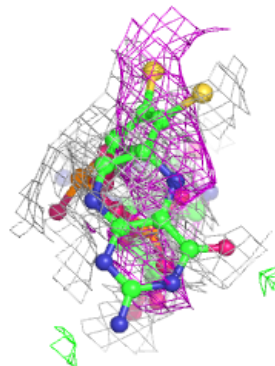
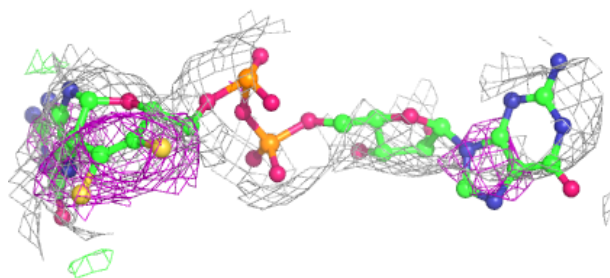
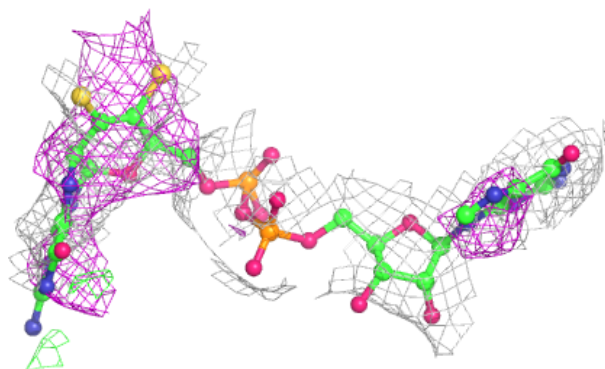
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around MGD A 1005:**

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

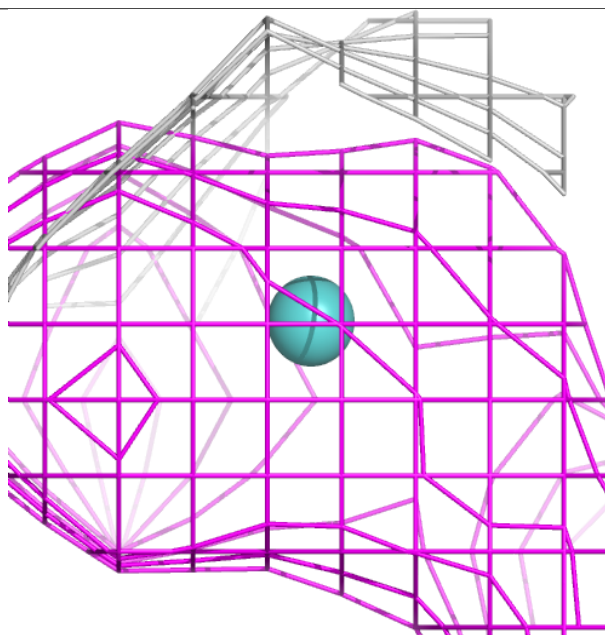
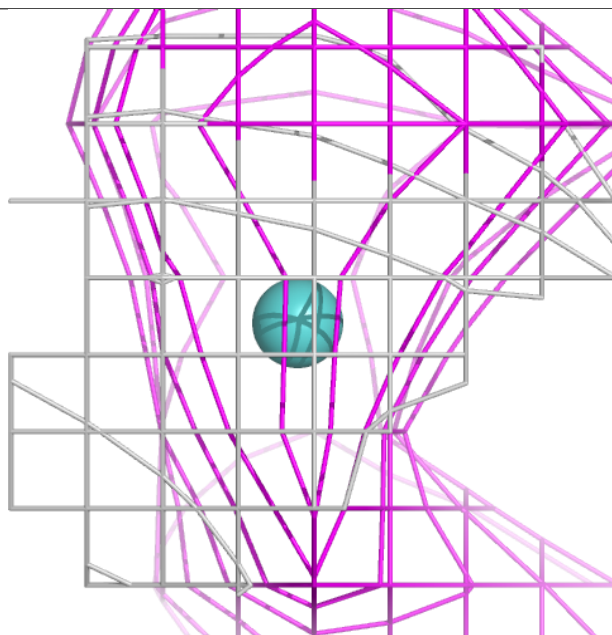
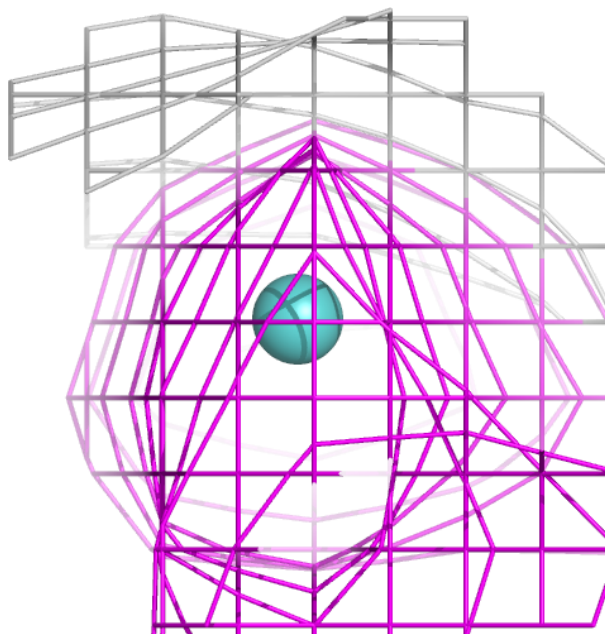
**Electron density around MGD A 1006:**

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



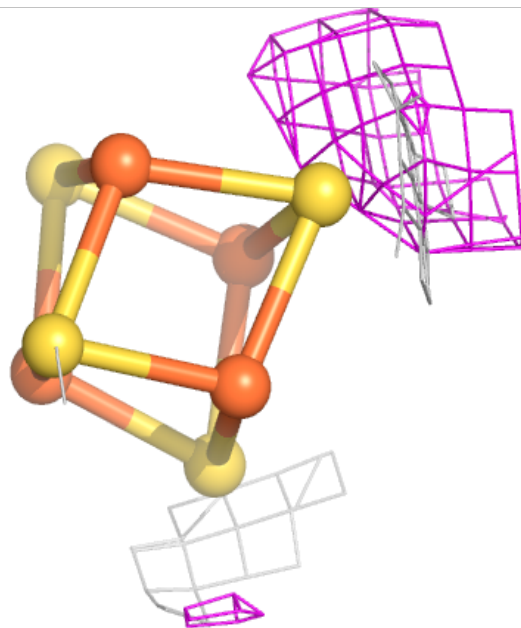
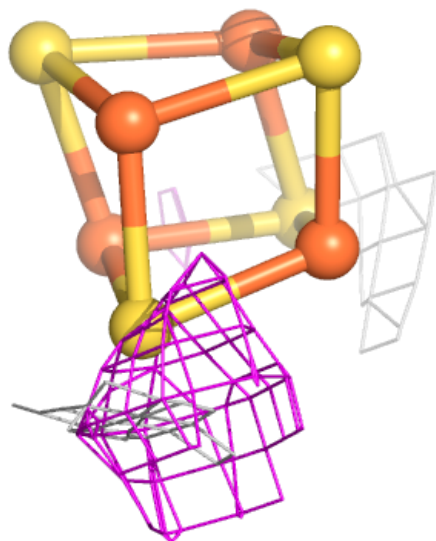
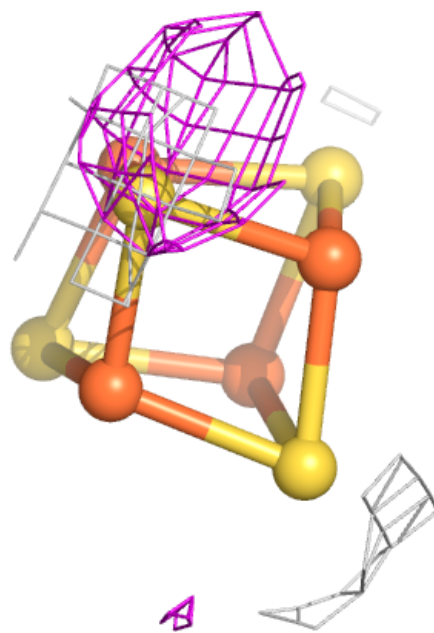
**Electron density around 4MO A 1007:**

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



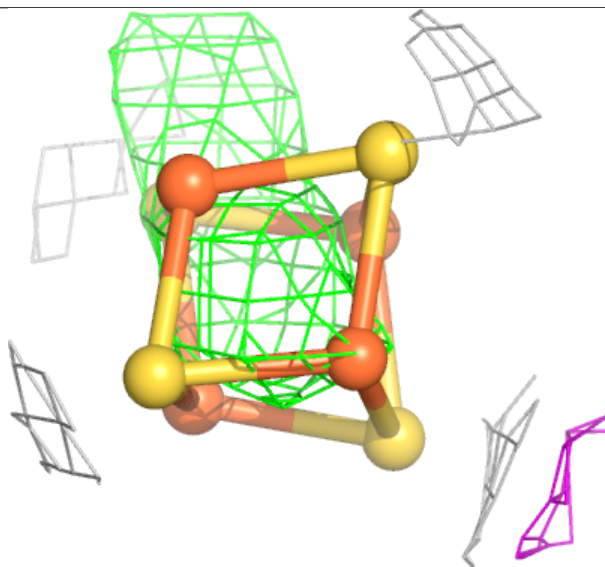
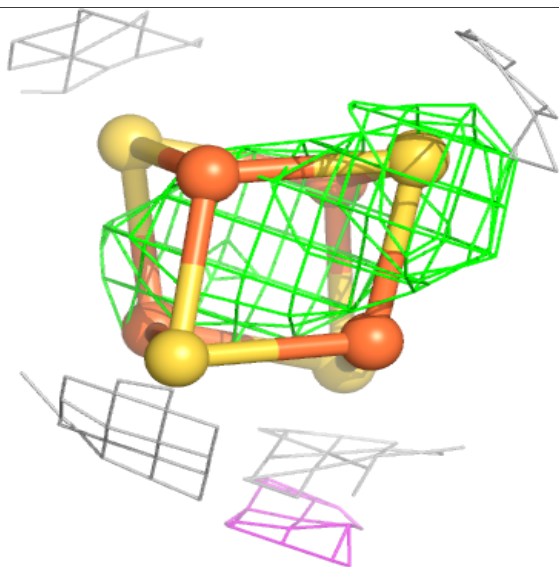
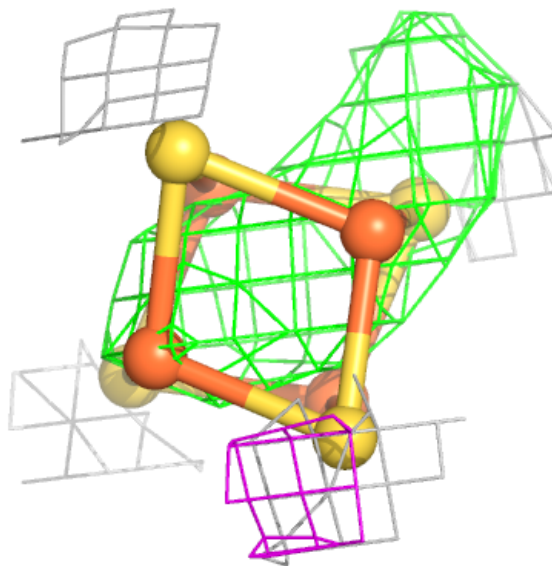
**Electron density around SF4 A 1001:**

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



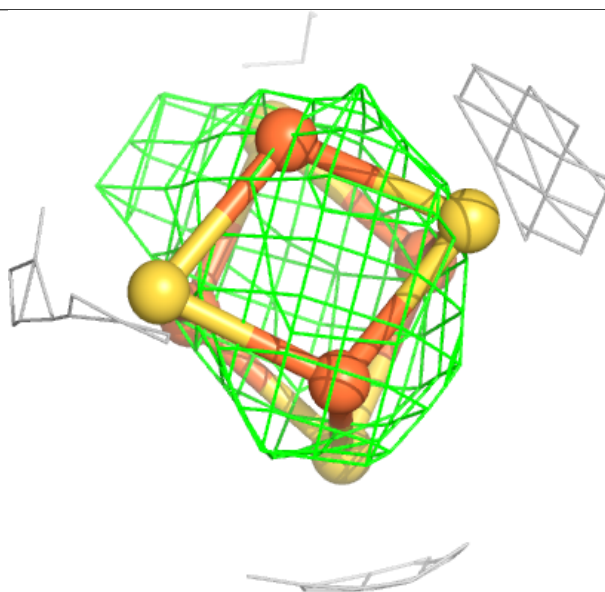
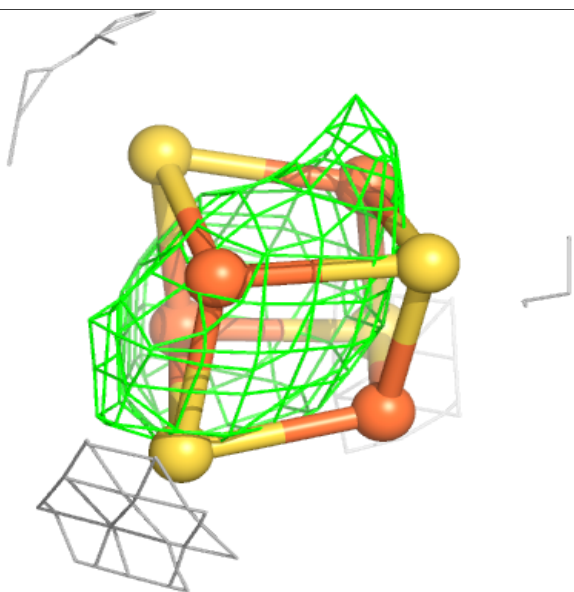
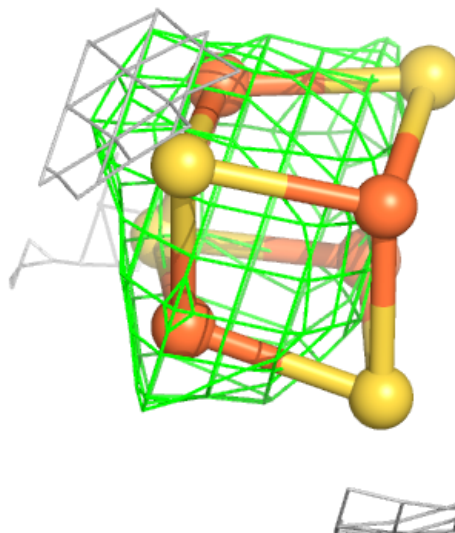
**Electron density around SF4 A 1003:**

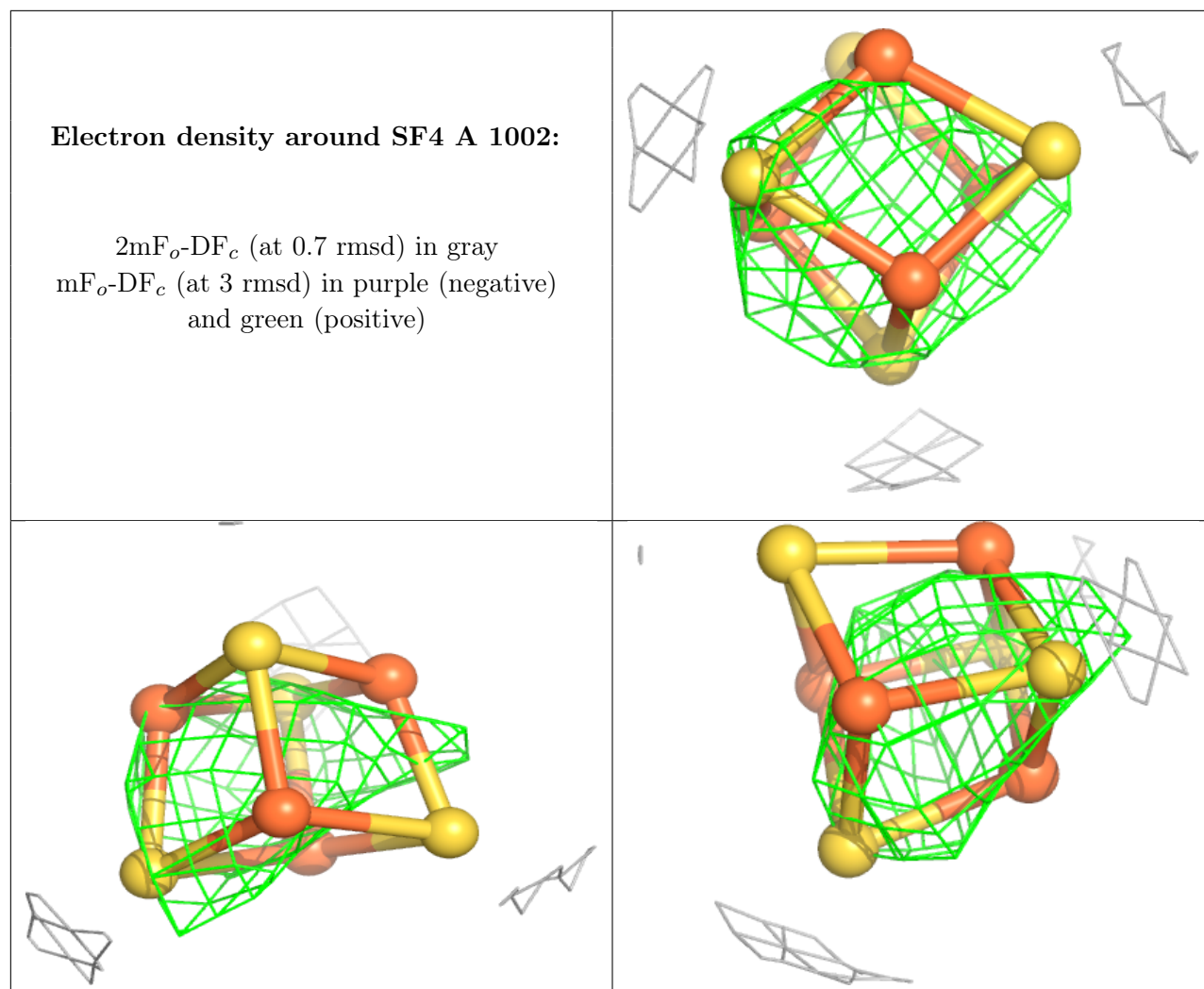
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around SF4 A 1004:**

$2mF_o-DF_c$  (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.