



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 12:12 PM JST

PDB ID : 5H92  
Title : Crystal structure of the complex between maize Sulfite Reductase and ferredoxin in the form-3 crystal  
Authors : Kurisu, G.; Nakayama, M.; Hase, T.  
Deposited on : 2015-12-25  
Resolution : 2.08 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

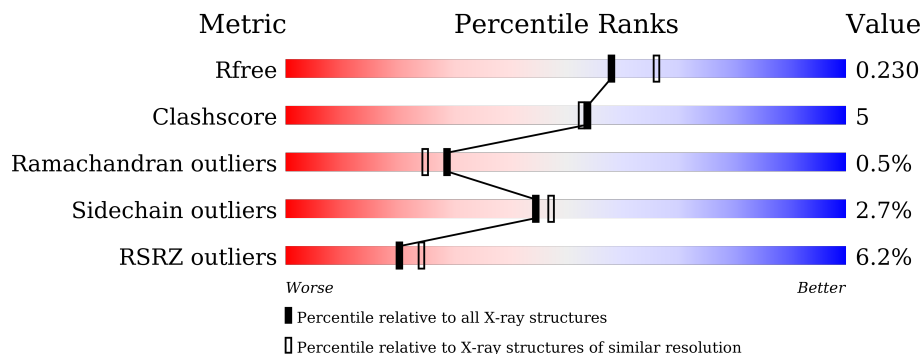
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	583	 87% 10% .
1	B	583	 86% 12% ..
2	C	98	 73% 19% 5% .

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	SRM	A	702	X	-	-	-
4	SRM	B	702	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10157 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.

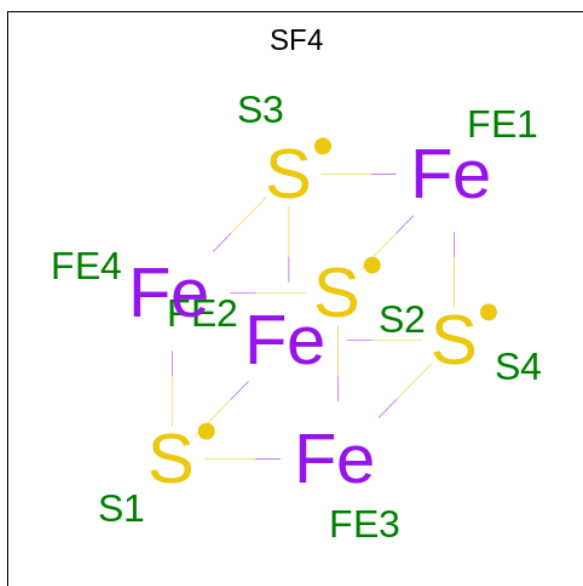
- Molecule 1 is a protein called Sulfite reductase [ferredoxin], chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	567	Total 4441	C 2822	N 768	O 834	S 17	0	0	0
1	B	572	Total 4457	C 2835	N 766	O 840	S 16	0	0	0

- Molecule 2 is a protein called Ferredoxin-1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	96	Total 720	C 444	N 111	O 161	S 4	0	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



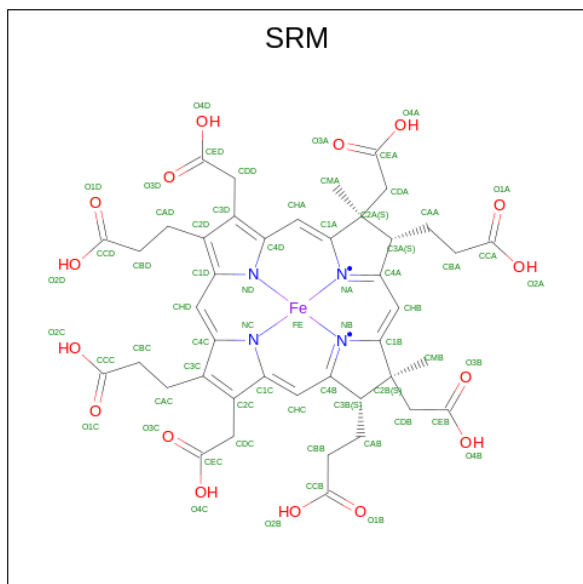
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	A	1	Total 8	Fe 4	S 4	0	0

*Continued on next page...*

Continued from previous page...

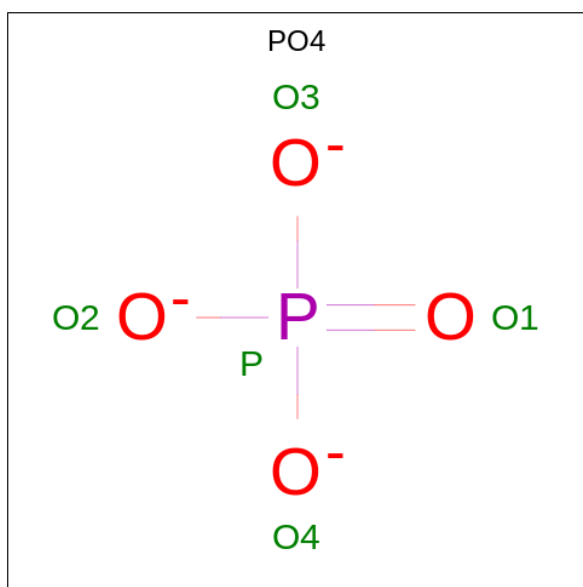
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
3	B	1	8	4	4	0	0

- Molecule 4 is SIROHEME (three-letter code: SRM) (formula:  $C_{42}H_{44}FeN_4O_{16}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
4	A	1	63	42	1	4	16	0	0
4	B	1	63	42	1	4	16	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

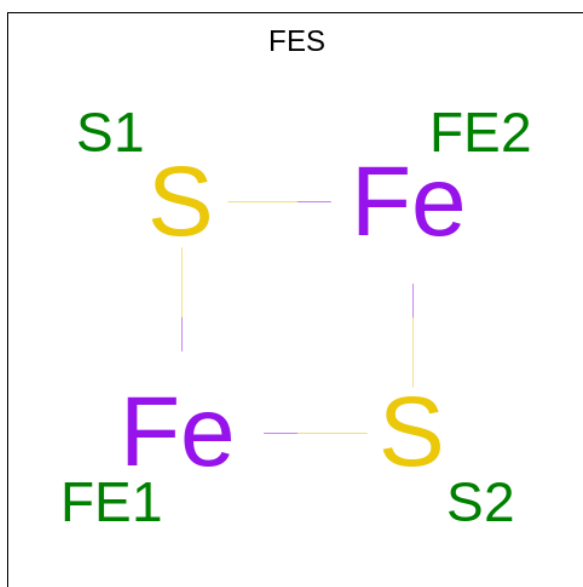


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Fe	S	0	0
			4	2	2		

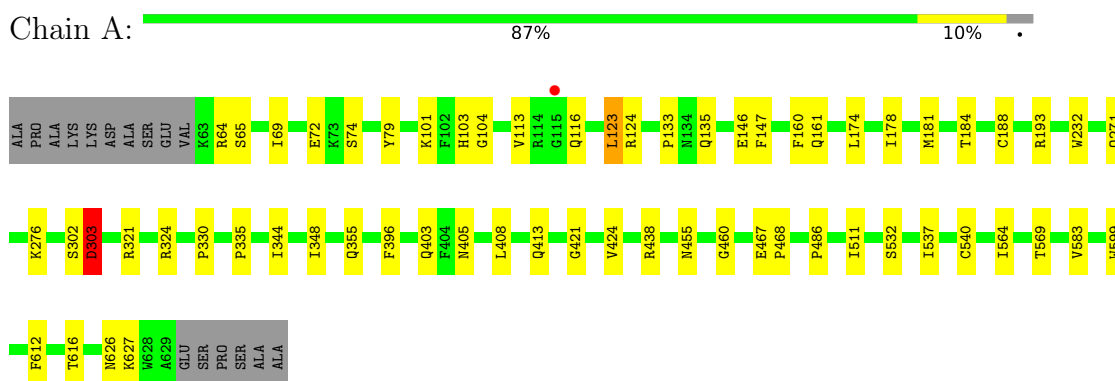
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	220	Total	O	0	0
			220	220		
8	B	156	Total	O	0	0
			156	156		
8	C	5	Total	O	0	0
			5	5		

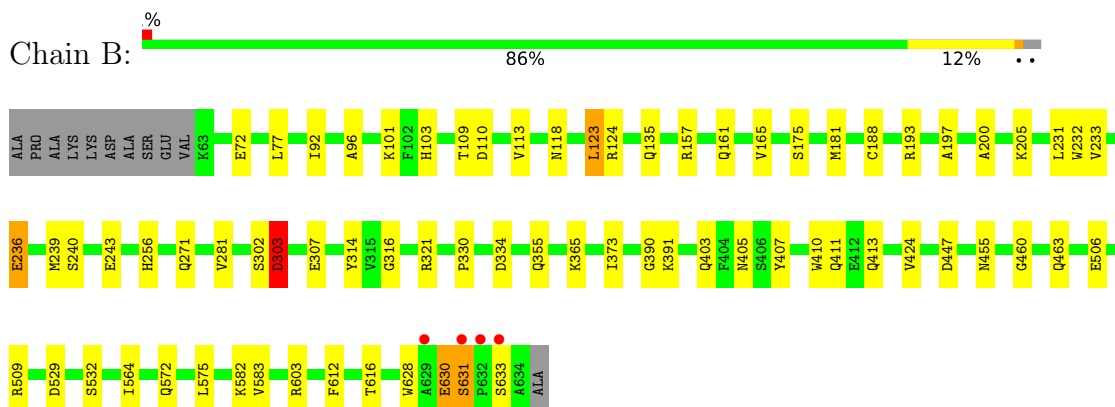
### 3 Residue-property plots [i](#)

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.

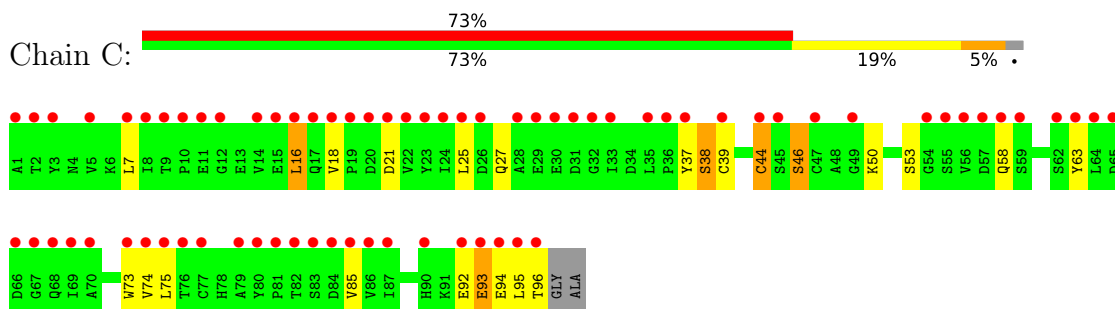
- Molecule 1: Sulfite reductase [ferredoxin], chloroplastic



- Molecule 1: Sulfite reductase [ferredoxin], chloroplastic



- Molecule 2: Ferredoxin-1, chloroplastic





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.41Å 103.41Å 122.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.27 – 2.08 43.26 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.27-2.08) 99.8 (43.26-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.50 (at 2.08Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.179 , 0.232 0.181 , 0.230	Depositor DCC
$R_{free}$ test set	3972 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtrriage
Anisotropy	0.477	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.30 % 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 1.1328e-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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SRM, MG, PO4, FES, SF4

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	0.81	1/4537 (0.0%)	0.78	5/6153 (0.1%)
1	B	0.69	0/4554	0.74	5/6180 (0.1%)
2	C	0.61	0/732	0.63	0/1001
All	All	0.74	1/9823 (0.0%)	0.75	10/13334 (0.1%)

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	A	0	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	599	TRP	CB-CG	5.04	1.59	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	193	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	B	631	SER	N-CA-C	7.87	132.26	111.00
1	A	123	LEU	CA-CB-CG	7.86	133.39	115.30
1	B	603	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	193	ARG	NE-CZ-NH1	-5.89	117.36	120.30
1	A	627	LYS	N-CA-C	-5.83	95.26	111.00
1	A	303	ASP	N-CA-C	5.69	126.35	111.00

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	160	PHE	CB-CA-C	-5.05	100.30	110.40
1	B	157	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	302	SER	Peptide
1	A	626	ASN	Peptide
1	B	302	SER	Peptide
1	B	630	GLU	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4441	0	4405	40	0
1	B	4457	0	4396	49	0
2	C	720	0	658	14	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
4	A	63	0	34	2	0
4	B	63	0	34	2	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	C	4	0	0	0	0
8	A	220	0	0	0	0
8	B	156	0	0	2	0
8	C	5	0	0	0	0
All	All	10157	0	9527	102	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 (102) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLN:HB3	1:B:181:MET:HE2	1.37	1.04
1:B:124:ARG:HE	1:B:161:GLN:HE21	1.10	0.95
1:A:124:ARG:HE	1:A:161:GLN:HE21	1.12	0.91
1:A:324:ARG:HD2	2:C:37:TYR:CZ	2.10	0.87
1:A:135:GLN:HB3	1:A:181:MET:HE2	1.56	0.87
1:B:403:GLN:HE21	1:B:405:ASN:HD21	1.20	0.86
1:B:135:GLN:HB3	1:B:181:MET:CE	2.06	0.84
1:B:303:ASP:HB2	1:B:307:GLU:O	1.78	0.84
1:B:109:THR:HG22	1:B:118:ASN:O	1.78	0.82
1:B:233:VAL:O	1:B:236:GLU:HG3	1.82	0.80
1:B:124:ARG:HE	1:B:161:GLN:NE2	1.79	0.79
1:A:135:GLN:HB3	1:A:181:MET:CE	2.13	0.78
2:C:92:GLU:O	2:C:96:THR:HB	1.83	0.78
1:A:413:GLN:NE2	1:A:460:GLY:H	1.82	0.77
1:A:612:PHE:O	1:A:616:THR:HG23	1.84	0.76
1:B:233:VAL:O	1:B:236:GLU:CG	2.35	0.75
1:B:612:PHE:O	1:B:616:THR:HG23	1.87	0.74
1:B:403:GLN:HE21	1:B:405:ASN:ND2	1.90	0.69
1:A:413:GLN:HE22	1:A:460:GLY:H	1.41	0.66
1:B:413:GLN:NE2	1:B:460:GLY:H	1.96	0.64
1:B:424:VAL:H	1:B:455:ASN:ND2	1.97	0.63
1:B:101:LYS:O	1:B:188:CYS:HB2	2.00	0.62
1:B:72:GLU:HB2	1:B:271:GLN:HE22	1.65	0.61
1:A:467:GLU:HB3	1:A:468:PRO:HD3	1.83	0.61
1:A:133:PRO:HB2	1:A:181:MET:HE3	1.83	0.60
2:C:93:GLU:O	2:C:96:THR:C	2.40	0.60
1:B:103:HIS:CD2	1:B:232:TRP:HE1	2.20	0.59
1:B:135:GLN:CB	1:B:181:MET:HE2	2.21	0.59
2:C:58:GLN:HE22	2:C:74:VAL:HA	1.67	0.58
1:A:101:LYS:O	1:A:188:CYS:HB2	2.04	0.57
1:A:403:GLN:HE21	1:A:405:ASN:HD21	1.53	0.56
1:A:424:VAL:H	1:A:455:ASN:ND2	2.03	0.56
1:A:72:GLU:HB2	1:A:271:GLN:HE22	1.71	0.55
1:B:424:VAL:H	1:B:455:ASN:HD22	1.54	0.55
1:A:103:HIS:CD2	1:A:232:TRP:HE1	2.26	0.55
1:A:511:ILE:HD12	1:A:537:ILE:HG13	1.87	0.55
1:B:124:ARG:HH21	1:B:161:GLN:HE22	1.55	0.54
1:B:355:GLN:HE21	1:B:355:GLN:HA	1.71	0.54
1:B:413:GLN:HE22	1:B:460:GLY:H	1.56	0.54
1:A:124:ARG:NE	1:A:161:GLN:HE21	1.94	0.54
1:B:233:VAL:O	1:B:236:GLU:HG2	2.06	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ARG:NE	1:B:161:GLN:HE21	1.92	0.53
1:B:175:SER:HB2	1:B:233:VAL:HG12	1.89	0.53
1:B:135:GLN:CB	1:B:181:MET:CE	2.82	0.53
1:A:276:LYS:NZ	5:A:703:PO4:O4	2.42	0.53
2:C:18:VAL:HG22	2:C:27:GLN:HG2	1.91	0.52
1:B:303:ASP:HB3	1:B:307:GLU:H	1.75	0.52
2:C:63:TYR:HB3	2:C:75:LEU:HD11	1.91	0.52
2:C:7:LEU:CD1	2:C:16:LEU:HD21	2.40	0.51
1:A:124:ARG:HH21	1:A:161:GLN:HE22	1.59	0.50
1:A:124:ARG:HH21	1:A:161:GLN:NE2	2.10	0.49
2:C:38:SER:HB3	2:C:46:SER:OG	2.12	0.49
2:C:44:CYS:SG	2:C:46:SER:HB2	2.53	0.49
1:A:65:SER:O	1:A:69:ILE:HD12	2.12	0.49
1:A:424:VAL:H	1:A:455:ASN:HD22	1.59	0.49
4:A:702:SRM:HBB1	4:A:702:SRM:CHC	2.42	0.49
1:B:92:ILE:HD12	1:B:96:ALA:HB1	1.95	0.48
1:A:104:GLY:HA3	1:A:184:THR:O	2.14	0.48
1:A:324:ARG:HD2	2:C:37:TYR:CE2	2.49	0.48
1:A:69:ILE:HD12	1:A:69:ILE:H	1.79	0.47
1:A:146:GLU:HG3	1:A:147:PHE:CD2	2.49	0.47
1:B:197:ALA:HA	1:B:281:VAL:O	2.14	0.47
1:A:324:ARG:HD2	2:C:37:TYR:OH	2.14	0.47
1:B:200:ALA:HB2	1:B:407:TYR:CD1	2.50	0.47
1:A:486:PRO:HB2	1:A:532:SER:HB2	1.97	0.47
1:B:316:GLY:HA3	1:B:373:ILE:HD12	1.97	0.46
1:A:74:SER:HA	1:A:79:TYR:O	2.15	0.45
1:A:344:ILE:O	1:A:348:ILE:HG12	2.15	0.45
1:A:413:GLN:HE22	1:A:460:GLY:N	2.12	0.45
1:B:181:MET:HE3	8:B:922:HOH:O	2.15	0.45
1:B:205:LYS:HE3	1:B:307:GLU:OE1	2.16	0.45
2:C:73:TRP:CE3	2:C:95:LEU:HD13	2.52	0.44
1:B:564:ILE:HD12	1:B:583:VAL:HG21	1.99	0.44
1:A:355:GLN:HE21	1:A:355:GLN:HA	1.82	0.44
1:B:403:GLN:NE2	1:B:405:ASN:HD21	2.00	0.44
1:B:77:LEU:O	1:B:103:HIS:HE1	2.00	0.44
1:A:174:LEU:O	1:A:178:ILE:HG13	2.17	0.44
1:A:324:ARG:CD	2:C:37:TYR:CZ	2.93	0.44
4:A:702:SRM:HBB1	4:A:702:SRM:HHC	1.99	0.44
1:B:123:LEU:HD21	1:B:165:VAL:HG21	2.00	0.44
1:B:321:ARG:HD2	1:B:330:PRO:HD3	1.99	0.43
1:A:72:GLU:CB	1:A:271:GLN:HE22	2.31	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:GLU:OE1	1:B:509:ARG:HB2	2.17	0.43
1:B:572:GLN:HA	8:B:815:HOH:O	2.18	0.43
1:B:314:TYR:HA	1:B:334:ASP:O	2.19	0.43
1:A:564:ILE:HD12	1:A:583:VAL:HG21	2.00	0.42
1:B:103:HIS:NE2	1:B:231:LEU:HD22	2.35	0.42
1:A:135:GLN:CB	1:A:181:MET:CE	2.91	0.42
1:B:113:VAL:O	1:B:113:VAL:HG23	2.19	0.42
2:C:53:SER:O	2:C:85:VAL:HA	2.20	0.42
1:A:335:PRO:HB3	1:A:396:PHE:CD1	2.54	0.42
1:A:408:LEU:HA	1:A:421:GLY:HA3	2.01	0.41
1:A:321:ARG:HD2	1:A:330:PRO:HD3	2.02	0.41
1:B:256:HIS:CE1	1:B:390:GLY:HA3	2.55	0.41
1:B:628:TRP:CH2	1:B:633:SER:HB3	2.55	0.41
1:B:110:ASP:O	1:B:113:VAL:HG22	2.19	0.41
4:B:702:SRM:CHC	4:B:702:SRM:HBB1	2.50	0.41
1:B:330:PRO:HB2	1:B:575:LEU:HD11	2.03	0.41
1:B:410:TRP:C	1:B:411:GLN:HG2	2.41	0.41
1:A:124:ARG:HE	1:A:161:GLN:NE2	1.96	0.41
1:B:161:GLN:NE2	4:B:702:SRM:HMB3	2.36	0.40
1:B:355:GLN:HA	1:B:355:GLN:NE2	2.35	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	565/583 (97%)	555 (98%)	8 (1%)	2 (0%)	34 31
1	B	570/583 (98%)	552 (97%)	14 (2%)	4 (1%)	22 17
2	C	94/98 (96%)	89 (95%)	5 (5%)	0	100 100
All	All	1229/1264 (97%)	1196 (97%)	27 (2%)	6 (0%)	29 25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	ASP
1	B	239	MET
1	B	303	ASP
1	A	116	GLN
1	B	240	SER
1	B	631	SER

### 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	474/493 (96%)	467 (98%)	7 (2%)	65 69
1	B	471/493 (96%)	460 (98%)	11 (2%)	50 53
2	C	81/83 (98%)	71 (88%)	10 (12%)	4 2
All	All	1026/1069 (96%)	998 (97%)	28 (3%)	44 47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	113	VAL
1	A	123	LEU
1	A	303	ASP
1	A	438	ARG
1	A	540	CYS
1	A	569	THR
1	B	123	LEU
1	B	236	GLU
1	B	243	GLU
1	B	303	ASP
1	B	365	LYS
1	B	391	LYS
1	B	463	GLN
1	B	529	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	532	SER
1	B	582	LYS
1	B	630	GLU
2	C	16	LEU
2	C	21	ASP
2	C	25	LEU
2	C	38	SER
2	C	39	CYS
2	C	44	CYS
2	C	46	SER
2	C	50	LYS
2	C	93	GLU
2	C	94	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	161	GLN
1	A	271	GLN
1	A	355	GLN
1	A	403	GLN
1	A	413	GLN
1	A	445	ASN
1	A	455	ASN
1	A	488	ASN
1	B	103	HIS
1	B	161	GLN
1	B	169	ASN
1	B	224	GLN
1	B	271	GLN
1	B	355	GLN
1	B	405	ASN
1	B	411	GLN
1	B	413	GLN
1	B	445	ASN
1	B	455	ASN
1	B	488	ASN
2	C	58	GLN



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are 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	SRM	B	702	5,1	68,70,70	2.33	19 (27%)	81,112,112	2.88	30 (37%)
7	FES	C	101	2	0,4,4	-	-	-	-	-
5	PO4	B	703	4	4,4,4	0.85	0	6,6,6	0.48	0
3	SF4	B	701	1	0,12,12	-	-	-	-	-
3	SF4	A	701	1	0,12,12	-	-	-	-	-
4	SRM	A	702	5,1	68,70,70	2.23	20 (29%)	81,112,112	2.90	32 (39%)
5	PO4	A	703	4	4,4,4	1.03	0	6,6,6	1.15	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
4	SRM	B	702	5,1	2/2/19/23	12/38/126/126	-
7	FES	C	101	2	-	-	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	B	701	1	-	-	0/6/5/5
3	SF4	A	701	1	-	-	0/6/5/5
4	SRM	A	702	5,1	2/2/19/23	11/38/126/126	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	SRM	CHD-C4C	9.25	1.48	1.35
4	A	702	SRM	CHD-C4C	8.94	1.47	1.35
4	B	702	SRM	CHA-C1A	7.52	1.48	1.35
4	A	702	SRM	CHA-C1A	6.16	1.46	1.35
4	A	702	SRM	CHC-C1C	5.69	1.49	1.38
4	B	702	SRM	C3C-C2C	5.29	1.48	1.36
4	A	702	SRM	C3C-C2C	4.75	1.46	1.36
4	B	702	SRM	CHC-C1C	4.62	1.47	1.38
4	B	702	SRM	C4D-CHA	3.44	1.50	1.41
4	B	702	SRM	C4A-NA	3.42	1.37	1.35
4	A	702	SRM	C1D-CHD	3.37	1.50	1.41
4	B	702	SRM	C3A-C4A	-3.10	1.44	1.51
4	B	702	SRM	C1C-C2C	-3.06	1.39	1.45
4	A	702	SRM	CHB-C4A	3.01	1.47	1.39
4	B	702	SRM	CHB-C4A	2.99	1.47	1.39
4	A	702	SRM	C4C-NC	-2.94	1.34	1.39
4	A	702	SRM	C3A-C4A	-2.93	1.44	1.51
4	B	702	SRM	C4C-NC	-2.88	1.34	1.39
4	A	702	SRM	FE-NC	2.87	2.06	1.95
4	A	702	SRM	C4D-CHA	2.82	1.48	1.41
4	B	702	SRM	CHB-C1B	2.81	1.45	1.37
4	B	702	SRM	C1D-CHD	2.81	1.48	1.41
4	B	702	SRM	FE-NC	2.76	2.06	1.95
4	B	702	SRM	C4B-NB	-2.63	1.33	1.35
4	A	702	SRM	CDC-CEC	-2.61	1.47	1.51
4	B	702	SRM	C4C-C3C	-2.60	1.40	1.45
4	A	702	SRM	C1C-C2C	-2.44	1.40	1.45
4	B	702	SRM	C2B-C3B	-2.42	1.48	1.55
4	B	702	SRM	CHC-C4B	2.41	1.46	1.39
4	A	702	SRM	C4C-C3C	-2.39	1.41	1.45
4	A	702	SRM	O4B-CEB	-2.34	1.22	1.30
4	A	702	SRM	CHB-C1B	2.23	1.43	1.37
4	A	702	SRM	C1C-NC	-2.23	1.35	1.39
4	B	702	SRM	FE-NA	2.15	2.09	1.97
4	A	702	SRM	C2B-C3B	-2.11	1.49	1.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	SRM	O4C-CEC	-2.09	1.23	1.30
4	A	702	SRM	O4D-CED	-2.06	1.23	1.30
4	A	702	SRM	C2B-C1B	-2.05	1.49	1.54
4	B	702	SRM	O2D-CCD	-2.05	1.23	1.30

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	SRM	CAB-C3B-C4B	-12.42	89.29	111.19
4	B	702	SRM	CAA-C3A-C4A	10.49	129.69	111.19
4	A	702	SRM	CAA-C3A-C4A	9.95	128.73	111.19
4	B	702	SRM	CAB-C3B-C4B	-9.59	94.28	111.19
4	A	702	SRM	C2A-C3A-C4A	6.45	109.15	100.90
4	B	702	SRM	CAB-C3B-C2B	-6.26	96.88	114.14
4	A	702	SRM	CMB-C2B-C3B	5.76	122.72	112.08
4	B	702	SRM	CMB-C2B-C3B	5.57	122.38	112.08
4	B	702	SRM	CAC-CBC-CCC	-5.53	101.70	113.60
4	B	702	SRM	C2A-C3A-C4A	5.38	107.78	100.90
4	A	702	SRM	CAC-CBC-CCC	-5.34	102.11	113.60
4	B	702	SRM	CHC-C1C-NC	-5.23	118.78	124.44
4	A	702	SRM	CAB-C3B-C2B	-5.09	100.12	114.14
4	B	702	SRM	CMA-C2A-C3A	-5.02	102.80	112.08
4	B	702	SRM	CDA-C2A-C3A	4.72	121.04	108.39
4	B	702	SRM	C2C-C1C-NC	4.70	114.90	110.32
4	A	702	SRM	CDA-C2A-C3A	4.40	120.18	108.39
4	A	702	SRM	CMA-C2A-C3A	-4.37	104.01	112.08
4	B	702	SRM	C3B-C4B-NB	4.34	119.39	110.85
4	B	702	SRM	C1C-C2C-C3C	-4.27	101.92	106.86
4	A	702	SRM	CDB-C2B-C3B	-4.08	97.47	108.39
4	A	702	SRM	CBD-CAD-C2D	-3.83	106.08	112.62
4	B	702	SRM	C4A-CHB-C1B	-3.76	120.33	125.88
4	A	702	SRM	CHD-C4C-NC	-3.72	120.41	124.43
4	B	702	SRM	CDB-C2B-C3B	-3.67	98.55	108.39
4	A	702	SRM	C3C-C4C-NC	3.67	113.89	110.32
4	A	702	SRM	C3B-C4B-NB	3.46	117.64	110.85
4	B	702	SRM	C2B-C1B-CHB	-3.44	120.40	123.54
4	B	702	SRM	CHD-C4C-NC	-3.21	120.96	124.43
4	A	702	SRM	CDA-C2A-C1A	3.19	117.14	107.12
4	A	702	SRM	C2B-C1B-CHB	-3.19	120.63	123.54
4	B	702	SRM	CAB-CBB-CCB	3.16	120.89	112.51
4	A	702	SRM	O2B-CCB-CBB	3.01	123.69	114.03
4	B	702	SRM	O3C-CEC-CDC	-2.99	113.35	122.08

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	SRM	C2A-C1A-NA	2.94	115.94	111.21
4	B	702	SRM	C3C-C4C-NC	2.91	113.15	110.32
4	A	702	SRM	C4C-C3C-C2C	-2.88	103.53	106.86
4	B	702	SRM	C2B-C3B-C4B	-2.84	97.27	100.90
4	A	702	SRM	C2C-C1C-NC	2.82	113.06	110.32
4	B	702	SRM	O3D-CED-CDD	-2.81	115.01	123.04
4	A	702	SRM	CHC-C1C-NC	-2.80	121.41	124.44
4	A	702	SRM	O2B-CCB-O1B	-2.76	116.42	123.30
4	A	702	SRM	C4A-CHB-C1B	-2.69	121.92	125.88
4	A	702	SRM	C3A-C2A-C1A	-2.67	96.34	100.92
4	A	702	SRM	C1C-C2C-C3C	-2.56	103.90	106.86
4	A	702	SRM	C2B-C3B-C4B	-2.49	97.71	100.90
4	B	702	SRM	CAA-C3A-C2A	2.36	120.63	114.14
4	A	702	SRM	CMA-C2A-CDA	2.35	114.68	110.80
4	B	702	SRM	C2A-C1A-NA	2.34	114.98	111.21
4	A	702	SRM	CAC-C3C-C4C	2.34	129.30	124.89
4	B	702	SRM	C4B-NB-C1B	-2.31	102.62	105.23
4	B	702	SRM	CDA-C2A-C1A	2.29	114.33	107.12
4	A	702	SRM	C3B-C2B-C1B	2.28	104.83	100.92
4	A	702	SRM	O4B-CEB-O3B	-2.22	117.77	123.30
4	A	702	SRM	C4D-CHA-C1A	-2.20	125.75	130.12
4	B	702	SRM	O2B-CCB-CBB	2.20	121.08	114.03
4	B	702	SRM	O2B-CCB-O1B	-2.17	117.90	123.30
4	A	702	SRM	O3C-CEC-CDC	-2.16	115.76	122.08
4	A	702	SRM	CAA-C3A-C2A	2.14	120.04	114.14
4	B	702	SRM	C4D-CHA-C1A	-2.13	125.90	130.12
4	B	702	SRM	CAC-C3C-C4C	2.10	128.85	124.89
4	B	702	SRM	CBD-CAD-C2D	-2.04	109.14	112.62

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	702	SRM	C3A
4	A	702	SRM	NC
4	B	702	SRM	C3A
4	B	702	SRM	NC

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	SRM	C1A-C2A-CDA-CEA
4	A	702	SRM	CMA-C2A-CDA-CEA

Continued on next page...

*Continued from previous page...*

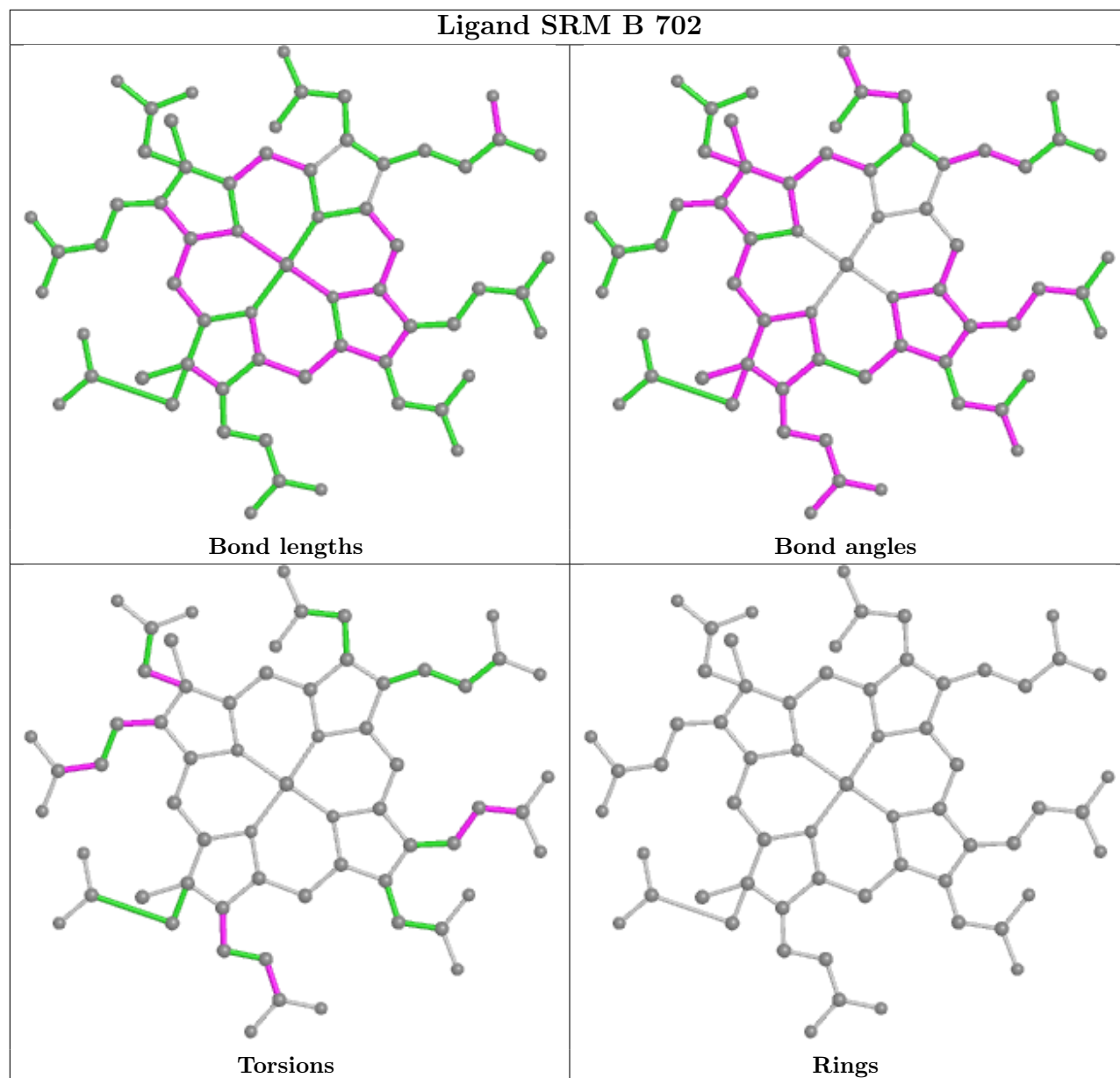
Mol	Chain	Res	Type	Atoms
4	A	702	SRM	C2A-C3A-CAA-CBA
4	B	702	SRM	C1A-C2A-CDA-CEA
4	B	702	SRM	CMA-C2A-CDA-CEA
4	B	702	SRM	C3A-C2A-CDA-CEA
4	B	702	SRM	C2A-C3A-CAA-CBA
4	A	702	SRM	C3C-CAC-CBC-CCC
4	B	702	SRM	C3C-CAC-CBC-CCC
4	B	702	SRM	C4B-C3B-CAB-CBB
4	A	702	SRM	C4B-C3B-CAB-CBB
4	A	702	SRM	CAA-CBA-CCA-O1A
4	A	702	SRM	CAB-CBB-CCB-O1B
4	B	702	SRM	CAC-CBC-CCC-O2C
4	B	702	SRM	CAC-CBC-CCC-O1C
4	A	702	SRM	CAA-CBA-CCA-O2A
4	B	702	SRM	CAB-CBB-CCB-O2B
4	A	702	SRM	CAB-CBB-CCB-O2B
4	B	702	SRM	CAA-CBA-CCA-O2A
4	A	702	SRM	CAC-CBC-CCC-O1C
4	B	702	SRM	CAA-CBA-CCA-O1A
4	A	702	SRM	CAC-CBC-CCC-O2C
4	B	702	SRM	CAB-CBB-CCB-O1B

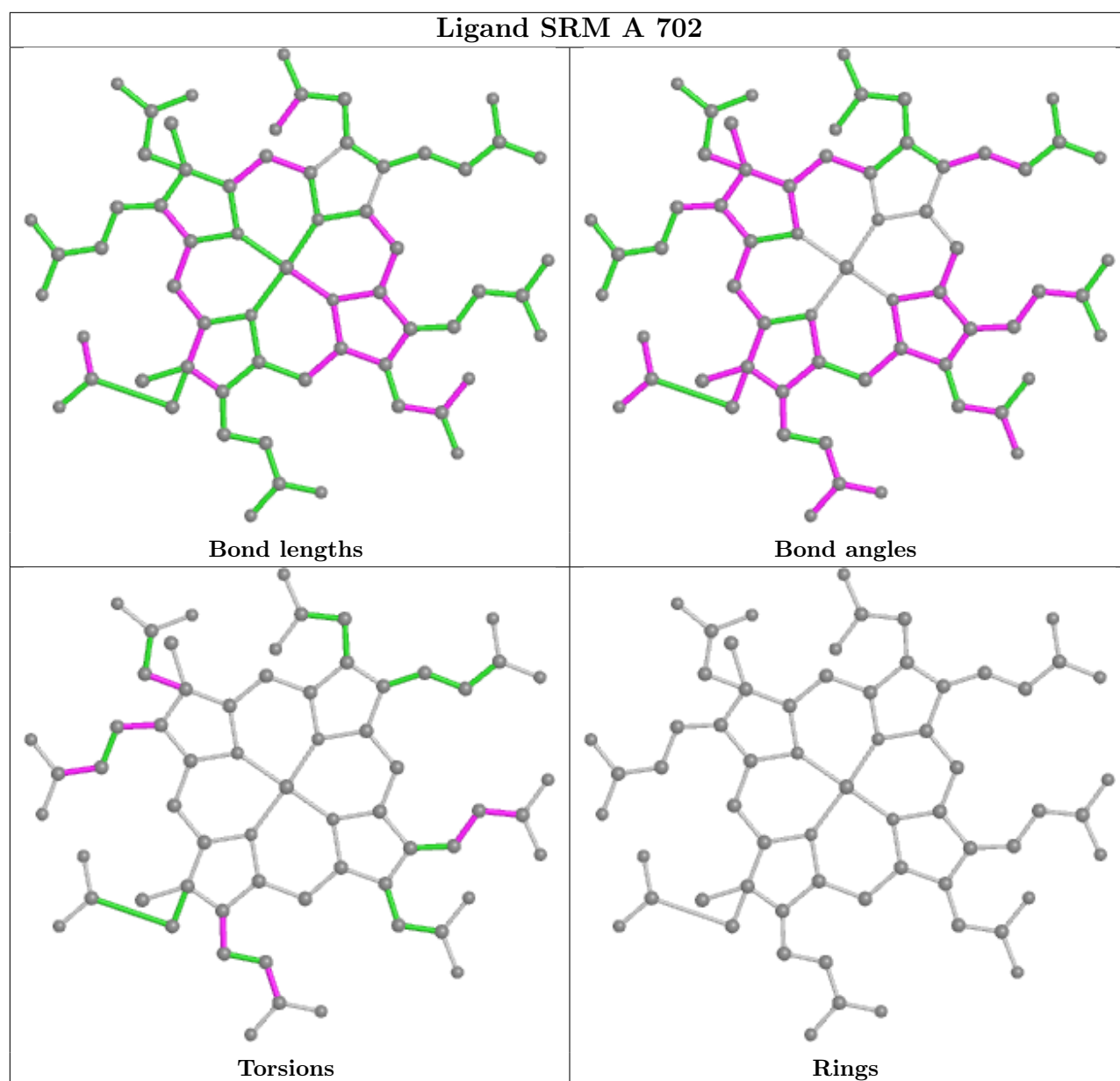
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	702	SRM	2	0
4	A	702	SRM	2	0
5	A	703	PO4	1	0

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





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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	567/583 (97%)	-0.30	1 (0%) 95 95	22, 31, 44, 72	0
1	B	572/583 (98%)	-0.17	4 (0%) 87 89	25, 37, 55, 68	0
2	C	96/98 (97%)	3.02	72 (75%) 0 0	49, 69, 102, 117	0
All	All	1235/1264 (97%)	0.02	77 (6%) 20 24	22, 35, 67, 117	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	35	LEU	6.1
2	C	28	ALA	5.9
2	C	24	ILE	5.4
2	C	33	ILE	5.4
2	C	83	SER	5.3
2	C	31	ASP	5.3
2	C	64	LEU	5.2
2	C	95	LEU	5.1
2	C	65	ASP	5.0
2	C	76	THR	4.9
2	C	8	ILE	4.7
2	C	25	LEU	4.6
2	C	70	ALA	4.6
2	C	3	TYR	4.6
2	C	7	LEU	4.5
2	C	9	THR	4.5
2	C	19	PRO	4.4
2	C	10	PRO	4.4
2	C	82	THR	4.3
2	C	32	GLY	4.3
2	C	86	VAL	4.2
2	C	11	GLU	4.1
2	C	63	TYR	4.1

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	C	56	VAL	4.1
2	C	37	TYR	4.0
2	C	66	ASP	3.8
2	C	73	TRP	3.8
2	C	30	GLU	3.7
2	C	62	SER	3.7
2	C	96	THR	3.7
2	C	44	CYS	3.6
2	C	5	VAL	3.6
2	C	87	ILE	3.5
2	C	47	CYS	3.5
2	C	58	GLN	3.5
2	C	23	TYR	3.5
2	C	57	ASP	3.4
2	C	93	GLU	3.4
2	C	79	ALA	3.3
2	C	1	ALA	3.3
2	C	67	GLY	3.3
2	C	18	VAL	3.2
2	C	15	GLU	3.0
2	C	94	GLU	3.0
2	C	17	GLN	2.9
2	C	22	VAL	2.9
2	C	69	ILE	2.9
2	C	59	SER	2.9
2	C	16	LEU	2.8
2	C	21	ASP	2.8
2	C	75	LEU	2.8
2	C	45	SER	2.8
2	C	84	ASP	2.7
2	C	74	VAL	2.7
2	C	85	VAL	2.7
2	C	77	CYS	2.7
2	C	80	TYR	2.7
2	C	2	THR	2.7
1	A	115	GLY	2.6
2	C	12	GLY	2.5
2	C	55	SER	2.5
2	C	39	CYS	2.5
2	C	92	GLU	2.5
2	C	49	GLY	2.4
1	B	629	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	26	ASP	2.4
2	C	81	PRO	2.4
2	C	36	PRO	2.3
1	B	632	PRO	2.2
2	C	54	GLY	2.2
2	C	90	HIS	2.1
2	C	68	GLN	2.1
1	B	631	SER	2.1
2	C	14	VAL	2.1
1	B	633	SER	2.1
2	C	29	GLU	2.0
2	C	20	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

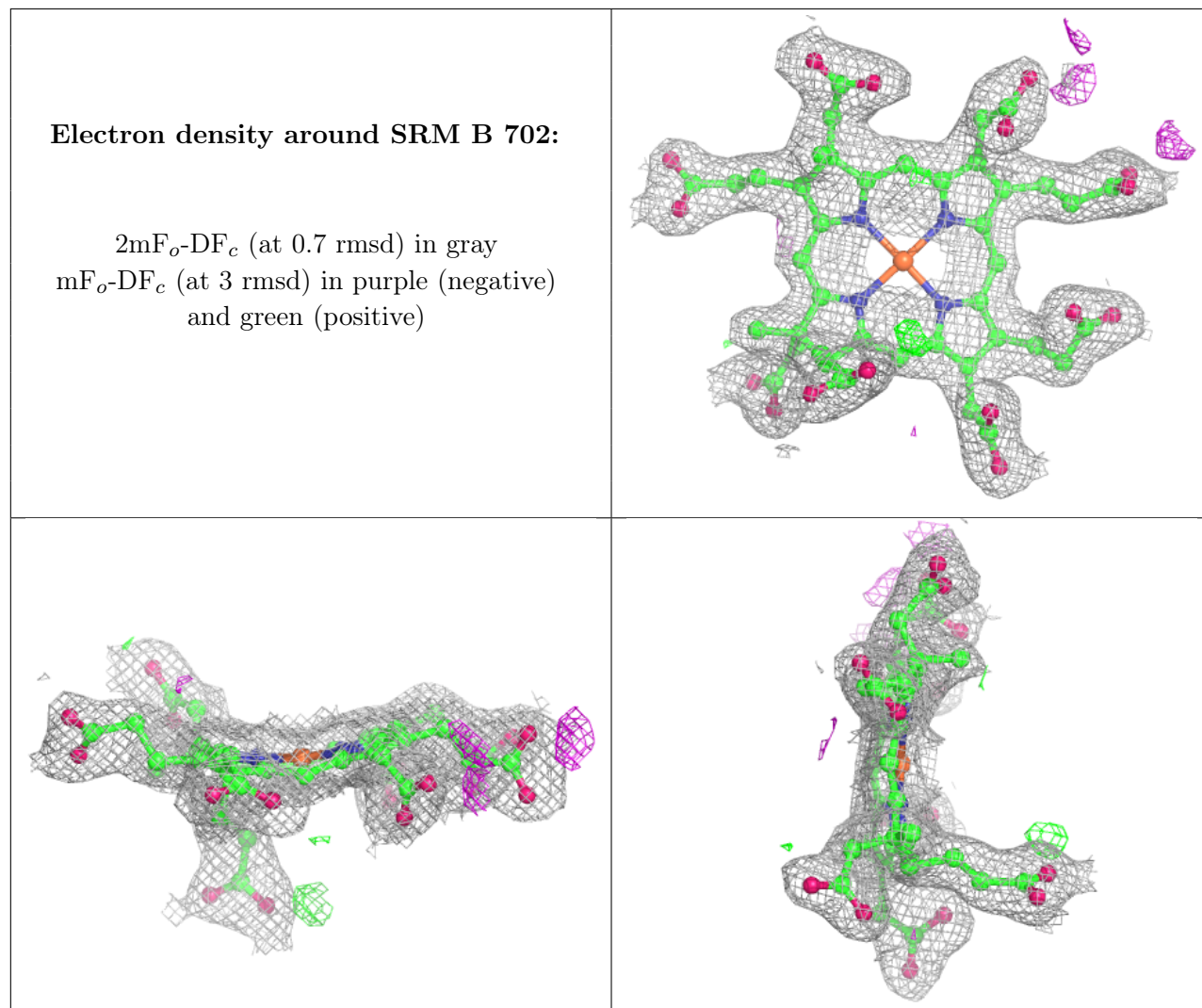
## 6.4 Ligands [i](#)

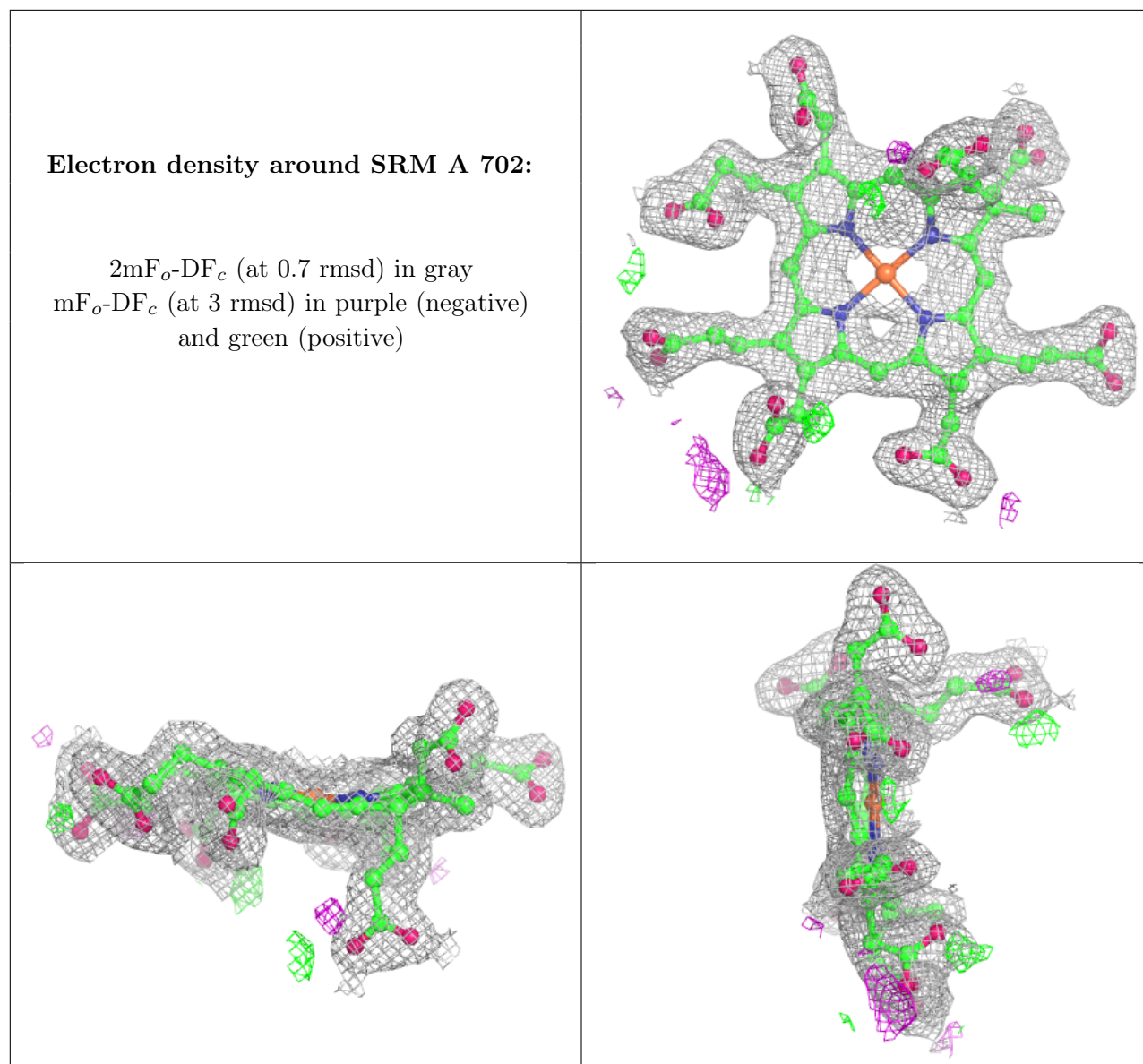
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	FES	C	101	4/4	0.93	0.17	57,59,61,66	0
5	PO4	A	703	5/5	0.97	0.13	38,44,45,48	0
4	SRM	B	702	63/63	0.97	0.13	28,33,40,49	0
5	PO4	B	703	5/5	0.98	0.10	42,43,49,51	0
6	MG	A	704	1/1	0.98	0.22	20,20,20,20	0
4	SRM	A	702	63/63	0.98	0.15	20,27,35,41	0
6	MG	B	704	1/1	0.99	0.22	22,22,22,22	0
3	SF4	B	701	8/8	0.99	0.12	31,34,34,35	0
3	SF4	A	701	8/8	1.00	0.13	24,25,26,27	0

The following is a graphical depiction of the model fit to experimental electron density of all

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.