Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 04:44 PM JST

PDB ID	:	7E0L
Title	:	Class III hybrid cluster protein (HCP) from Methanothermobacter marburgensis
Authors	:	Fujishiro, T.
Deposited on	:	2021-01-28
Resolution	:	2.82 Å(reported)

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

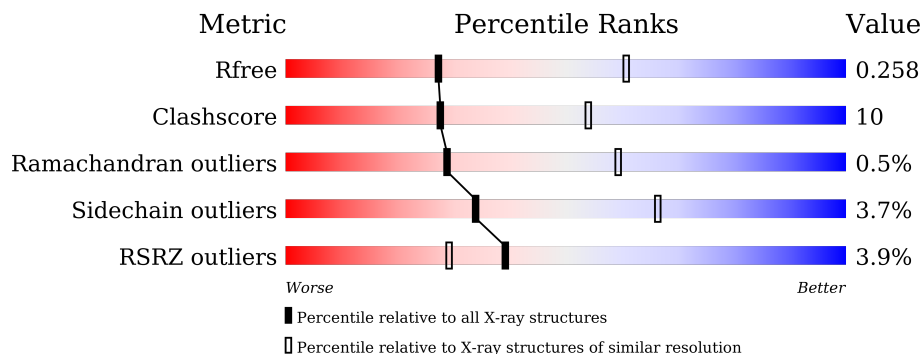|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.82 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		10
Ramachandran outliers		0.5%
Sidechain outliers		3.7%
RSRZ outliers		3.9%

Worse　　　　　　　　　　　　　　　　　　　　Better

▮ Percentile relative to all X-ray structures

❒ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 >=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 <=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	506	2% / 71% / 25% / • •
1	B	506	5% / 73% / 23% / • •
1	K	506	2% / 74% / 21% / • •
1	M	506	6% / 73% / 21% / • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FS2	K	601	-	-	X	-
2	FS2	M	601	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15353 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 Hydroxylamine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total 3837	C 2445	N 635	O 731	S 26	0	0	0
1	B	491	Total 3835	C 2443	N 634	O 733	S 25	0	0	0
1	K	487	Total 3796	C 2421	N 622	O 727	S 26	0	0	0
1	M	484	Total 3773	C 2408	N 616	O 724	S 25	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	VAL	-	expression tag	UNP D9PYV4
A	493	ASP	-	expression tag	UNP D9PYV4
A	494	LYS	-	expression tag	UNP D9PYV4
A	495	LEU	-	expression tag	UNP D9PYV4
A	496	ALA	-	expression tag	UNP D9PYV4
A	497	ALA	-	expression tag	UNP D9PYV4
A	498	ALA	-	expression tag	UNP D9PYV4
A	499	LEU	-	expression tag	UNP D9PYV4
A	500	GLU	-	expression tag	UNP D9PYV4
A	501	HIS	-	expression tag	UNP D9PYV4
A	502	HIS	-	expression tag	UNP D9PYV4
A	503	HIS	-	expression tag	UNP D9PYV4
A	504	HIS	-	expression tag	UNP D9PYV4
A	505	HIS	-	expression tag	UNP D9PYV4
A	506	HIS	-	expression tag	UNP D9PYV4
B	492	VAL	-	expression tag	UNP D9PYV4
B	493	ASP	-	expression tag	UNP D9PYV4
B	494	LYS	-	expression tag	UNP D9PYV4
B	495	LEU	-	expression tag	UNP D9PYV4
B	496	ALA	-	expression tag	UNP D9PYV4
B	497	ALA	-	expression tag	UNP D9PYV4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	498	ALA	-	expression tag	UNP D9PYV4
B	499	LEU	-	expression tag	UNP D9PYV4
B	500	GLU	-	expression tag	UNP D9PYV4
B	501	HIS	-	expression tag	UNP D9PYV4
B	502	HIS	-	expression tag	UNP D9PYV4
B	503	HIS	-	expression tag	UNP D9PYV4
B	504	HIS	-	expression tag	UNP D9PYV4
B	505	HIS	-	expression tag	UNP D9PYV4
B	506	HIS	-	expression tag	UNP D9PYV4
K	492	VAL	-	expression tag	UNP D9PYV4
K	493	ASP	-	expression tag	UNP D9PYV4
K	494	LYS	-	expression tag	UNP D9PYV4
K	495	LEU	-	expression tag	UNP D9PYV4
K	496	ALA	-	expression tag	UNP D9PYV4
K	497	ALA	-	expression tag	UNP D9PYV4
K	498	ALA	-	expression tag	UNP D9PYV4
K	499	LEU	-	expression tag	UNP D9PYV4
K	500	GLU	-	expression tag	UNP D9PYV4
K	501	HIS	-	expression tag	UNP D9PYV4
K	502	HIS	-	expression tag	UNP D9PYV4
K	503	HIS	-	expression tag	UNP D9PYV4
K	504	HIS	-	expression tag	UNP D9PYV4
K	505	HIS	-	expression tag	UNP D9PYV4
K	506	HIS	-	expression tag	UNP D9PYV4
M	492	VAL	-	expression tag	UNP D9PYV4
M	493	ASP	-	expression tag	UNP D9PYV4
M	494	LYS	-	expression tag	UNP D9PYV4
M	495	LEU	-	expression tag	UNP D9PYV4
M	496	ALA	-	expression tag	UNP D9PYV4
M	497	ALA	-	expression tag	UNP D9PYV4
M	498	ALA	-	expression tag	UNP D9PYV4
M	499	LEU	-	expression tag	UNP D9PYV4
M	500	GLU	-	expression tag	UNP D9PYV4
M	501	HIS	-	expression tag	UNP D9PYV4
M	502	HIS	-	expression tag	UNP D9PYV4
M	503	HIS	-	expression tag	UNP D9PYV4
M	504	HIS	-	expression tag	UNP D9PYV4
M	505	HIS	-	expression tag	UNP D9PYV4
M	506	HIS	-	expression tag	UNP D9PYV4

- Molecule 2 is FE-S-O HYBRID CLUSTER (three-letter code: FS2) (formula: $Fe_4O_3S_2$) (labeled as "Ligand of Interest" by depositor).
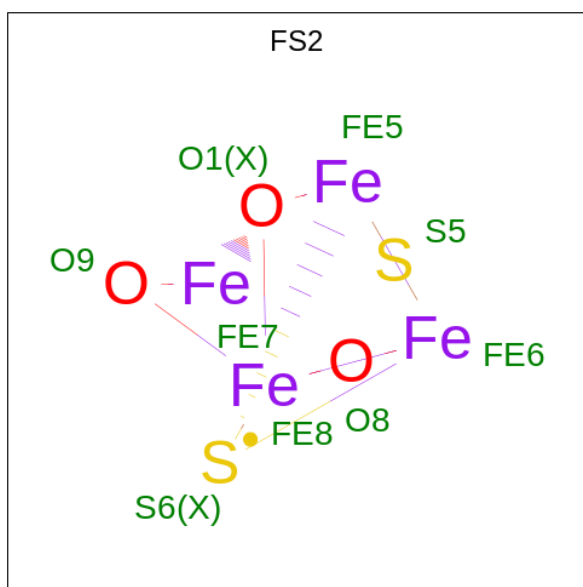
FS2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total Fe O S				0	0
			9 4 3 2					
2	B	1	Total Fe O S				0	0
			9 4 3 2					
2	K	1	Total Fe O S				0	0
			9 4 3 2					
2	M	1	Total Fe O S				0	0
			9 4 3 2					

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

SF4
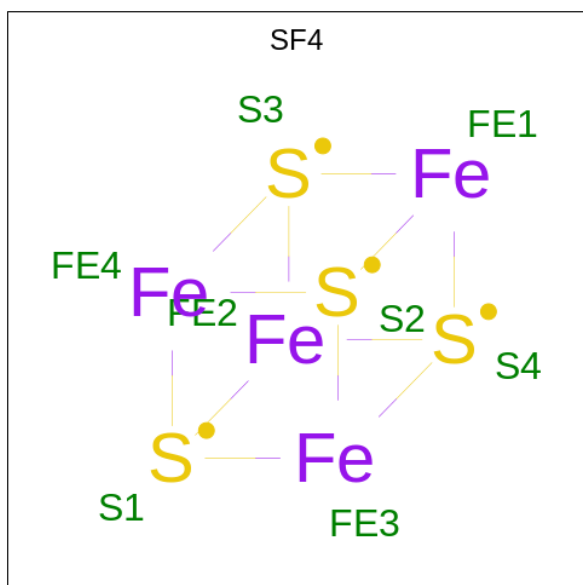
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	Fe 4	S 4	0	0
3	B	1	Total 8	Fe 4	S 4	0	0
3	K	1	Total 8	Fe 4	S 4	0	0
3	M	1	Total 8	Fe 4	S 4	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Fe 1	0	0
4	B	1	Total 1	Fe 1	0	0
4	K	1	Total 1	Fe 1	0	0
4	M	1	Total 1	Fe 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	O 2	0	0
5	B	15	Total 15	O 15	0	0
5	K	8	Total 8	O 8	0	0
5	M	15	Total 15	O 15	0	0

3 Residue-property plots ⓘ

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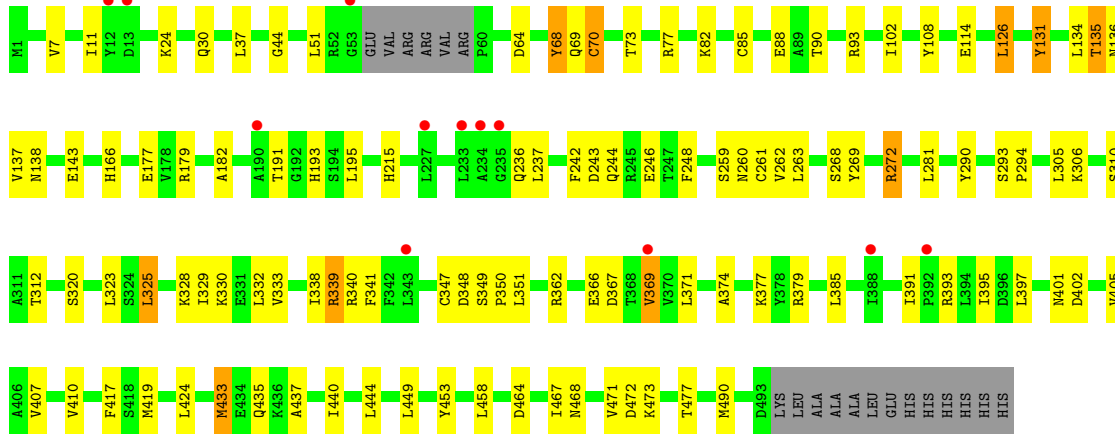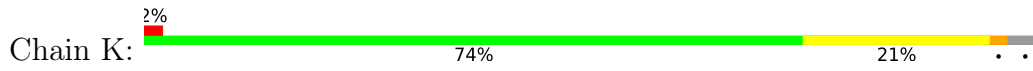
• Molecule 1: Hydroxylamine reductase
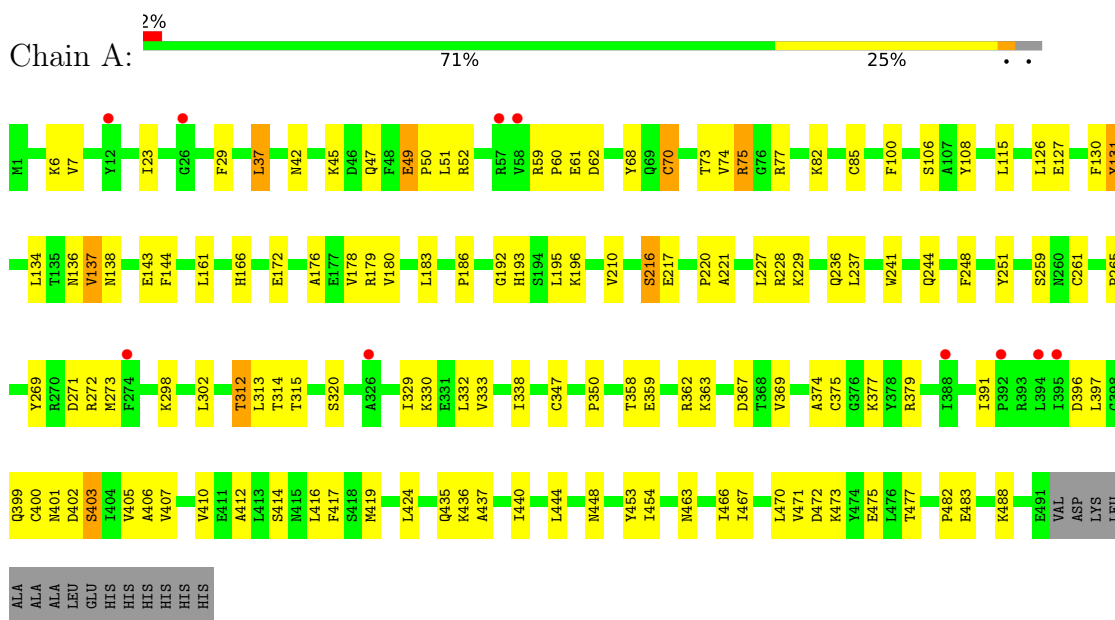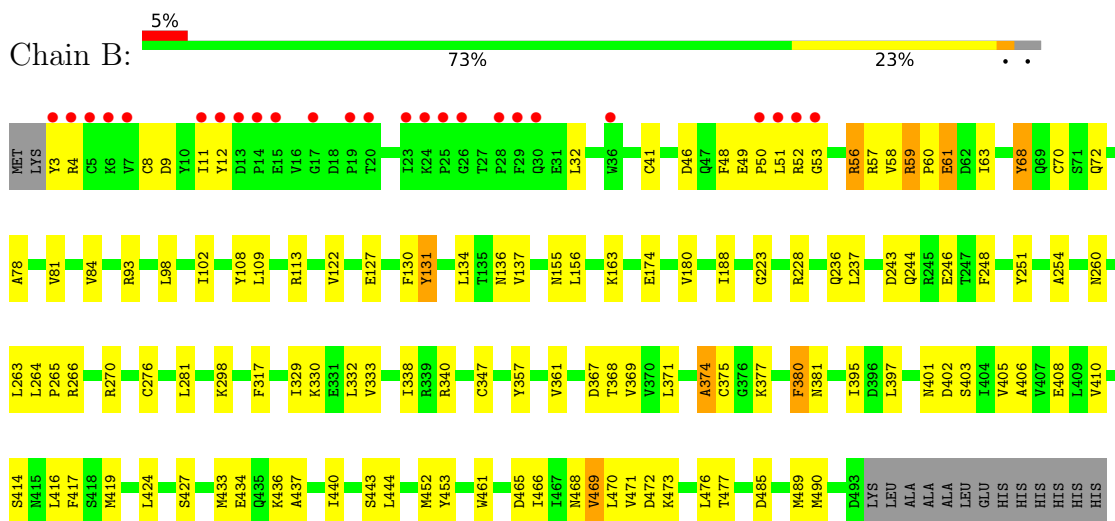
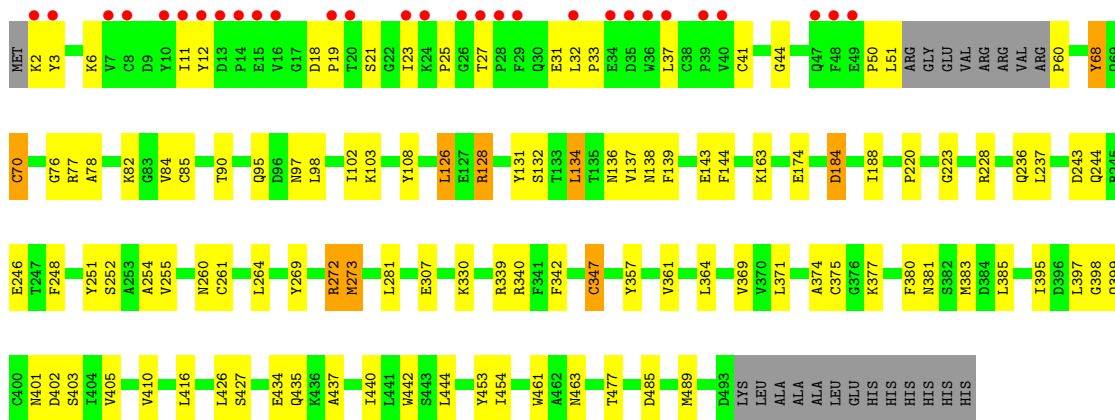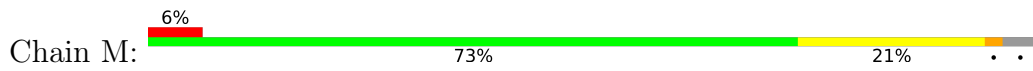Chain A:

• Molecule 1: Hydroxylamine reductase

Chain B:

• Molecule 1: Hydroxylamine reductase

Chain K:

• Molecule 1: Hydroxylamine reductase

Chain M:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	67.95Å 67.95Å 469.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.82 48.05 – 2.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.05-2.82) 100.0 (48.05-2.82)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.234 , 0.259 0.232 , 0.258	Depositor DCC
R_{free} test set	2554 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.5	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.159 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15353	wwPDB-VP
Average B, all atoms (Å^2)	69.0	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SF4, FE, FS2, CSS

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	0.30	0/3912	0.56	0/5306
1	B	0.31	0/3910	0.58	0/5306
1	K	0.30	0/3870	0.54	0/5249
1	M	0.31	0/3847	0.55	0/5220
All	All	0.30	0/15539	0.56	0/21081

There are no bond length outliers.

There are no bond angle outliers.

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	3837	0	3800	96	0
1	B	3835	0	3788	84	0
1	K	3796	0	3750	73	0
1	M	3773	0	3722	72	0
2	A	9	0	0	1	0
2	B	9	0	0	1	0
2	K	9	0	0	2	0
2	M	9	0	0	2	0
3	A	8	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	0	0	0
3	K	8	0	0	1	0
3	M	8	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
5	A	2	0	0	0	0
5	B	15	0	0	1	0
5	K	8	0	0	0	0
5	M	15	0	0	1	0
All	All	15353	0	15060	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (303) 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:M:85:CYS:HB2	1:M:136:ASN:HD21	1.34	0.91
1:A:261:CYS:HB2	2:A:601:FS2:S5	2.17	0.83
1:M:19:PRO:HB3	1:M:25:PRO:HD3	1.62	0.80
1:A:362:ARG:HE	1:K:362:ARG:HH12	1.30	0.79
1:A:359:GLU:HG3	1:A:362:ARG:HH22	1.49	0.78
1:B:419:MET:HE3	1:B:424:LEU:HA	1.65	0.77
1:A:73:THR:OG1	3:A:602:SF4:S1	2.44	0.76
1:K:85:CYS:HB2	1:K:136:ASN:HD21	1.53	0.74
1:M:37:LEU:HD22	1:M:44:GLY:HA2	1.71	0.73
1:K:77:ARG:HB2	1:M:60:PRO:HG2	1.70	0.72
1:A:265:PRO:HB3	1:A:273:MET:HE1	1.72	0.71
1:A:180:VAL:HG22	1:A:236:GLN:HB3	1.73	0.70
1:M:97:ASN:HD21	1:M:442:TRP:HE1	1.40	0.70
1:K:102:ILE:HG23	1:K:126:LEU:HD22	1.74	0.69
1:B:59:ARG:HB2	1:B:60:PRO:HD3	1.75	0.69
1:A:50:PRO:O	1:A:52:ARG:N	2.26	0.68
1:B:265:PRO:O	1:B:270:ARG:NH2	2.26	0.68
1:M:252:SER:HA	1:M:272:ARG:HH12	1.58	0.68
1:B:8:CYS:HA	1:B:56:ARG:HH22	1.60	0.67
1:M:330:LYS:HB2	1:M:416:LEU:HD21	1.76	0.67
1:M:23:ILE:HD11	1:M:33:PRO:HD3	1.77	0.67
1:B:330:LYS:HB2	1:B:416:LEU:HD21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASN:ND2	1:B:434:GLU:OE2	2.27	0.66
1:M:255:VAL:HB	1:M:273:MET:HG2	1.77	0.66
1:B:49:GLU:HG2	1:B:52:ARG:HD3	1.78	0.66
1:A:47:GLN:HE22	1:A:82:LYS:HE2	1.61	0.66
1:K:244:GLN:HE22	1:K:263:LEU:H	1.44	0.65
1:A:358:THR:HG22	1:A:379:ARG:HB3	1.77	0.65
1:A:176:ALA:HB2	1:A:228:ARG:HH21	1.62	0.65
1:M:2:LYS:HB3	1:M:11:ILE:HD11	1.78	0.64
1:M:102:ILE:HG23	1:M:126:LEU:HD22	1.78	0.64
1:A:330:LYS:HB2	1:A:416:LEU:HD21	1.80	0.64
1:A:127:GLU:OE1	1:B:113:ARG:NH1	2.33	0.62
1:M:347:CSS:SG	1:M:437:ALA:HB2	2.39	0.62
1:A:332:LEU:HB3	1:A:338:ILE:HG22	1.80	0.62
1:B:347:CSS:HB2	2:B:601:FS2:S6	2.41	0.61
1:A:402:ASP:O	1:A:405:VAL:HG22	2.01	0.60
1:M:97:ASN:HD22	1:M:461:TRP:HE1	1.50	0.60
1:M:347:CSS:HB2	2:M:601:FS2:S6	2.42	0.60
1:A:347:CSS:SG	1:A:437:ALA:HB2	2.42	0.60
1:M:41:CYS:HB2	1:M:84:VAL:HG22	1.84	0.60
1:K:472:ASP:OD1	1:K:473:LYS:N	2.35	0.60
1:B:163:LYS:NZ	1:B:408:GLU:OE1	2.35	0.59
1:K:68:TYR:HA	1:K:73:THR:HG21	1.83	0.59
1:K:464:ASP:HA	1:K:467:ILE:HG22	1.84	0.58
1:B:264:LEU:HD23	1:B:281:LEU:HD22	1.85	0.58
1:K:138:ASN:HD21	1:K:143:GLU:HG2	1.68	0.58
1:B:347:CSS:SG	1:B:437:ALA:HB2	2.44	0.58
1:B:368:THR:HG21	1:B:490:MET:HE1	1.86	0.58
1:B:174:GLU:O	1:B:228:ARG:NH2	2.36	0.57
1:K:70:CYS:O	1:K:73:THR:HG23	2.05	0.57
1:B:468:ASN:HA	1:B:471:VAL:HG22	1.86	0.57
1:M:174:GLU:O	1:M:228:ARG:NH2	2.38	0.57
1:A:193:HIS:CD2	1:A:217:GLU:HG2	2.40	0.57
1:A:333:VAL:HG11	1:A:417:PHE:CE1	2.40	0.57
1:A:166:HIS:ND1	1:A:195:LEU:HD12	2.20	0.57
1:A:414:SER:HA	1:A:424:LEU:HD21	1.87	0.57
1:B:223:GLY:HA2	1:B:228:ARG:HH21	1.71	0.56
1:K:137:VAL:HG22	1:M:260:ASN:HB3	1.87	0.56
1:K:332:LEU:HB3	1:K:338:ILE:HG22	1.87	0.56
1:M:383:MET:HE3	1:M:385:LEU:HD21	1.87	0.56
1:B:332:LEU:HB3	1:B:338:ILE:HG22	1.87	0.56
1:K:30:GLN:HG3	1:K:30:GLN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:SER:OG	1:A:217:GLU:N	2.38	0.56
1:A:137:VAL:HG22	1:B:260:ASN:HB3	1.87	0.55
1:A:166:HIS:HD1	1:A:195:LEU:HD12	1.71	0.55
1:K:453:TYR:HA	1:K:477:THR:O	2.05	0.55
1:K:37:LEU:HD23	1:K:44:GLY:HA2	1.88	0.55
1:K:73:THR:HG22	3:K:602:SF4:S1	2.47	0.55
1:A:85:CYS:HB2	1:A:136:ASN:HD21	1.72	0.54
1:M:108:TYR:CE1	1:M:401:ASN:HB3	2.42	0.54
1:A:359:GLU:HG3	1:A:362:ARG:NH2	2.20	0.54
1:M:184:ASP:OD1	1:M:307:GLU:HB2	2.06	0.54
1:M:361:VAL:HG21	1:M:380:PHE:HB3	1.89	0.54
1:A:440:ILE:O	1:A:444:LEU:HG	2.08	0.54
1:K:166:HIS:ND1	1:K:195:LEU:HD12	2.23	0.54
1:A:192:GLY:O	1:A:217:GLU:HB3	2.07	0.53
1:K:385:LEU:O	1:K:393:ARG:HD3	2.09	0.53
1:A:453:TYR:HA	1:A:477:THR:O	2.08	0.53
1:A:362:ARG:HE	1:K:362:ARG:NH1	2.02	0.53
1:B:131:TYR:O	1:B:137:VAL:HG11	2.08	0.53
1:A:193:HIS:H	1:A:259:SER:HB3	1.73	0.53
1:K:374:ALA:O	1:K:377:LYS:HE3	2.09	0.53
1:K:435:GLN:OE1	1:M:134:LEU:HD13	2.09	0.53
1:M:361:VAL:HG21	1:M:380:PHE:CB	2.38	0.53
1:A:60:PRO:C	1:A:62:ASP:H	2.12	0.53
1:K:458:LEU:HD13	1:K:467:ILE:HD12	1.89	0.53
1:K:468:ASN:HA	1:K:471:VAL:HG22	1.91	0.52
1:B:440:ILE:O	1:B:444:LEU:HG	2.10	0.52
1:K:11:ILE:HD11	1:K:51:LEU:HD22	1.91	0.52
1:M:237:LEU:HD21	1:M:251:TYR:CD2	2.44	0.52
1:K:182:ALA:HB1	1:K:305:LEU:HD13	1.92	0.52
1:M:397:LEU:HD13	1:M:405:VAL:HG22	1.91	0.52
1:M:6:LYS:HB3	1:M:82:LYS:HD3	1.91	0.52
1:A:298:LYS:O	1:A:302:LEU:HD23	2.10	0.52
1:B:244:GLN:HG3	1:B:248:PHE:CE2	2.45	0.52
1:A:186:PRO:HB2	1:A:210:VAL:HG12	1.91	0.51
1:B:266:ARG:NH2	5:B:702:HOH:O	2.41	0.51
1:A:74:VAL:HG12	1:A:75:ARG:HE	1.75	0.51
1:A:397:LEU:HD13	1:A:405:VAL:HG23	1.91	0.51
1:B:3:TYR:O	1:B:11:ILE:HD12	2.10	0.51
1:M:244:GLN:HG3	1:M:248:PHE:CE2	2.45	0.51
1:M:223:GLY:HA2	1:M:228:ARG:HH21	1.74	0.51
1:A:269:TYR:HA	1:A:272:ARG:HE	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:TYR:HA	1:B:477:THR:O	2.11	0.51
1:A:435:GLN:OE1	1:A:435:GLN:N	2.44	0.51
1:B:108:TYR:CE1	1:B:401:ASN:HB3	2.46	0.51
1:K:177:GLU:HG3	1:K:312:THR:OG1	2.11	0.51
1:A:419:MET:HE3	1:A:424:LEU:HA	1.92	0.50
1:K:193:HIS:NE2	2:K:601:FS2:O9	2.44	0.50
1:A:488:LYS:O	1:A:488:LYS:HD3	2.11	0.50
1:B:244:GLN:HE22	1:B:263:LEU:H	1.59	0.50
1:M:261:CYS:HB2	2:M:601:FS2:S5	2.52	0.50
1:K:135:THR:HG23	1:M:435:GLN:HE22	1.77	0.50
1:M:402:ASP:O	1:M:405:VAL:HG13	2.12	0.50
1:K:440:ILE:O	1:K:444:LEU:HG	2.11	0.49
1:A:137:VAL:HG22	1:B:260:ASN:CB	2.42	0.49
1:K:407:VAL:O	1:K:410:VAL:HG22	2.13	0.49
1:M:453:TYR:HA	1:M:477:THR:O	2.12	0.49
1:B:243:ASP:O	1:B:246:GLU:HG2	2.13	0.49
1:K:246:GLU:OE1	1:K:246:GLU:N	2.44	0.49
1:A:138:ASN:HD21	1:A:143:GLU:HG2	1.78	0.49
1:K:347:CSS:HB3	1:K:433:MET:HB3	1.93	0.49
1:A:29:PHE:CZ	1:A:45:LYS:HG3	2.48	0.49
1:K:244:GLN:HG3	1:K:248:PHE:CE2	2.47	0.49
1:B:374:ALA:O	1:B:377:LYS:HE3	2.13	0.49
1:A:265:PRO:HB3	1:A:273:MET:CE	2.43	0.48
1:A:406:ALA:O	1:A:410:VAL:HG13	2.13	0.48
1:K:419:MET:HE3	1:K:424:LEU:HA	1.95	0.48
1:K:166:HIS:CE1	1:K:195:LEU:HD12	2.48	0.48
1:M:132:SER:HA	1:M:137:VAL:HG11	1.96	0.48
1:A:60:PRO:O	1:A:62:ASP:N	2.45	0.48
1:B:155:ASN:ND2	1:B:443:SER:OG	2.40	0.48
1:M:440:ILE:O	1:M:444:LEU:HG	2.13	0.48
1:A:115:LEU:HD21	1:A:196:LYS:HB2	1.95	0.48
1:A:271:ASP:O	1:A:298:LYS:HE2	2.13	0.48
1:B:12:TYR:OH	1:B:32:LEU:HD11	2.13	0.48
1:B:361:VAL:HG21	1:B:380:PHE:CB	2.43	0.48
1:K:7:VAL:HG13	1:K:82:LYS:O	2.14	0.48
1:K:402:ASP:O	1:K:405:VAL:HG13	2.13	0.48
1:A:298:LYS:HE3	1:A:302:LEU:HD21	1.94	0.48
1:M:188:ILE:HA	1:M:254:ALA:O	2.14	0.48
1:B:59:ARG:CB	1:B:60:PRO:HD3	2.43	0.48
1:B:49:GLU:HG3	1:B:50:PRO:HD2	1.96	0.47
1:K:349:SER:OG	1:K:351:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ILE:HD12	1:A:367:ASP:O	2.14	0.47
1:M:90:THR:HB	1:M:463:ASN:HD21	1.79	0.47
1:M:138:ASN:HD21	1:M:143:GLU:HG2	1.79	0.47
1:A:37:LEU:HD12	1:A:42:ASN:O	2.14	0.47
1:K:347:CSS:SG	1:K:437:ALA:HB2	2.55	0.47
1:B:131:TYR:HA	1:B:134:LEU:HD13	1.97	0.47
1:B:466:ILE:O	1:B:469:VAL:HG12	2.15	0.47
1:K:179:ARG:NH1	1:K:310:SER:OG	2.48	0.47
1:M:342:PHE:CD1	1:M:427:SER:HB2	2.49	0.47
1:A:179:ARG:HH11	1:A:183:LEU:HD21	1.80	0.47
1:B:368:THR:CG2	1:B:490:MET:HE1	2.45	0.47
1:B:156:LEU:HD22	1:B:443:SER:HB3	1.98	0.46
1:B:236:GLN:HG3	1:B:237:LEU:N	2.30	0.46
1:B:237:LEU:HD21	1:B:251:TYR:CD2	2.49	0.46
1:M:357:TYR:O	1:M:361:VAL:HG22	2.15	0.46
1:B:72:GLN:HB3	1:B:84:VAL:HG11	1.98	0.46
1:B:357:TYR:O	1:B:361:VAL:HG22	2.15	0.46
1:M:269:TYR:HD1	1:M:273:MET:HG3	1.79	0.46
1:A:75:ARG:HH12	1:B:60:PRO:HA	1.80	0.46
1:B:338:ILE:HD12	1:B:367:ASP:O	2.15	0.46
1:B:403:SER:O	1:B:406:ALA:HB3	2.15	0.46
1:B:371:LEU:HD23	1:B:395:ILE:HB	1.97	0.46
1:K:325:LEU:HD23	1:K:328:LYS:HB3	1.98	0.46
1:M:76:GLY:O	1:M:77:ARG:HD2	2.15	0.46
1:M:485:ASP:O	1:M:489:MET:HG3	2.16	0.46
1:A:106:SER:HB3	1:B:127:GLU:HA	1.98	0.46
1:A:237:LEU:HD21	1:A:251:TYR:CG	2.51	0.46
1:B:338:ILE:HD13	1:B:369:VAL:HG13	1.97	0.46
1:A:330:LYS:HB2	1:A:416:LEU:CD2	2.45	0.46
1:A:403:SER:O	1:A:406:ALA:HB3	2.16	0.46
1:A:407:VAL:O	1:A:410:VAL:HG22	2.16	0.46
1:K:191:THR:HG23	1:K:215:HIS:HD2	1.81	0.46
1:K:397:LEU:HD13	1:K:405:VAL:HG22	1.98	0.45
1:M:374:ALA:O	1:M:377:LYS:HE3	2.15	0.45
1:A:261:CYS:N	1:B:136:ASN:O	2.49	0.45
1:A:359:GLU:CD	1:A:482:PRO:HG3	2.37	0.45
1:A:363:LYS:HD3	1:A:483:GLU:HG2	1.98	0.45
1:B:361:VAL:HG21	1:B:380:PHE:HB3	1.97	0.45
1:K:339:ARG:NH1	1:K:367:ASP:OD2	2.50	0.45
1:M:236:GLN:HG3	1:M:237:LEU:N	2.31	0.45
1:M:260:ASN:ND2	1:M:434:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:GLU:OE2	1:K:290:TYR:OH	2.30	0.45
1:M:12:TYR:OH	1:M:32:LEU:HD11	2.16	0.45
1:M:243:ASP:O	1:M:246:GLU:HG2	2.17	0.45
1:A:7:VAL:HG13	1:A:82:LYS:O	2.16	0.45
1:K:366:GLU:HA	1:K:393:ARG:NH1	2.32	0.45
1:A:59:ARG:HH12	1:B:59:ARG:HA	1.81	0.45
1:B:244:GLN:HG3	1:B:248:PHE:CD2	2.52	0.45
1:B:329:ILE:O	1:B:333:VAL:HG13	2.16	0.45
1:K:242:PHE:CB	1:K:350:PRO:HG3	2.47	0.45
1:K:259:SER:OG	1:K:260:ASN:N	2.50	0.45
1:M:50:PRO:O	1:M:51:LEU:HD22	2.16	0.45
1:B:414:SER:HA	1:B:424:LEU:HD11	1.98	0.44
1:K:340:ARG:HB3	1:K:490:MET:HE2	1.98	0.44
1:K:371:LEU:HD23	1:K:395:ILE:HB	1.99	0.44
1:B:93:ARG:HB3	1:B:461:TRP:O	2.18	0.44
1:A:131:TYR:HA	1:A:134:LEU:HD13	2.00	0.44
1:M:3:TYR:CZ	1:M:50:PRO:HB3	2.52	0.44
1:M:264:LEU:HD23	1:M:281:LEU:HD22	1.98	0.44
1:M:361:VAL:HA	1:M:364:LEU:HD12	1.99	0.44
1:A:241:TRP:CH2	1:A:350:PRO:HD3	2.52	0.44
1:K:320:SER:HA	1:K:323:LEU:HG	2.00	0.44
1:A:412:ALA:O	1:A:416:LEU:N	2.49	0.44
1:A:108:TYR:CE1	1:A:436:LYS:HD3	2.52	0.44
1:B:109:LEU:HD11	1:B:122:VAL:HG12	1.98	0.44
1:B:333:VAL:HG21	1:B:417:PHE:CE1	2.53	0.44
1:A:362:ARG:NE	1:K:362:ARG:HH12	2.07	0.44
1:B:333:VAL:HG12	1:B:338:ILE:HG23	1.98	0.44
1:B:340:ARG:NH1	1:B:427:SER:OG	2.51	0.44
1:M:102:ILE:CG2	1:M:126:LEU:HD22	2.45	0.44
1:A:179:ARG:NH1	1:A:183:LEU:HD21	2.33	0.44
1:A:472:ASP:OD1	1:A:473:LYS:N	2.51	0.44
1:M:248:PHE:CE2	1:M:255:VAL:HG11	2.53	0.43
1:A:237:LEU:HD21	1:A:251:TYR:CD1	2.53	0.43
1:K:64:ASP:O	1:K:93:ARG:NH1	2.51	0.43
1:A:467:ILE:O	1:A:471:VAL:HG23	2.19	0.43
1:B:41:CYS:HB2	1:B:84:VAL:HG22	2.00	0.43
1:B:452:MET:O	1:B:476:LEU:HD12	2.19	0.43
1:B:485:ASP:O	1:B:489:MET:HG3	2.18	0.43
1:K:306:LYS:HE2	1:K:306:LYS:HB3	1.81	0.43
1:M:27:THR:CG2	1:M:31:GLU:HB3	2.49	0.43
1:A:138:ASN:HB3	1:A:144:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:HB1	1:A:227:LEU:HD13	2.01	0.43
1:M:220:PRO:HG2	1:M:399:GLN:HG2	1.99	0.43
1:M:371:LEU:HD23	1:M:395:ILE:HB	2.01	0.43
1:A:100:PHE:O	1:A:435:GLN:HB3	2.17	0.43
1:B:58:VAL:HG21	1:B:63:ILE:HG12	2.00	0.43
1:B:402:ASP:O	1:B:405:VAL:HG13	2.18	0.43
1:B:436:LYS:O	1:B:440:ILE:HG13	2.18	0.43
1:K:329:ILE:CD1	1:K:391:ILE:HG12	2.48	0.43
1:K:330:LYS:HA	1:K:417:PHE:HE1	1.84	0.43
1:A:329:ILE:HD11	1:A:391:ILE:HG21	2.01	0.43
1:K:341:PHE:HD1	1:K:369:VAL:HG22	1.84	0.42
1:M:248:PHE:O	1:M:272:ARG:NH2	2.52	0.42
1:A:130:PHE:CZ	1:B:130:PHE:CE2	3.07	0.42
1:K:347:CSS:SD	2:K:601:FS2:O9	2.77	0.42
1:A:23:ILE:HD13	1:A:23:ILE:HA	1.90	0.42
1:A:77:ARG:HG3	1:B:61:GLU:HB2	2.01	0.42
1:B:347:CSS:SD	1:B:434:GLU:HG2	2.59	0.42
1:A:220:PRO:HG2	1:A:399:GLN:HG2	2.02	0.42
1:B:98:LEU:O	1:B:102:ILE:HG13	2.20	0.42
1:K:108:TYR:CE1	1:K:401:ASN:HB3	2.55	0.42
1:A:217:GLU:OE2	1:A:374:ALA:HA	2.19	0.42
1:B:46:ASP:C	1:B:48:PHE:H	2.22	0.42
1:A:312:THR:O	1:A:313:LEU:HD12	2.20	0.42
1:B:57:ARG:HD3	1:B:57:ARG:HA	1.95	0.42
1:B:72:GLN:O	1:B:84:VAL:HG21	2.19	0.42
1:B:188:ILE:HA	1:B:254:ALA:O	2.20	0.42
1:K:215:HIS:HE1	1:K:243:ASP:OD1	2.03	0.42
1:M:18:ASP:OD2	1:M:21:SER:OG	2.26	0.42
1:A:244:GLN:HG3	1:A:248:PHE:CE2	2.55	0.41
1:A:374:ALA:O	1:A:377:LYS:HG2	2.20	0.41
1:B:317:PHE:CG	1:B:395:ILE:HG23	2.56	0.41
1:K:269:TYR:HA	1:K:272:ARG:HG3	2.01	0.41
1:M:398:GLY:HA3	1:M:402:ASP:OD2	2.20	0.41
1:B:265:PRO:HG2	1:B:270:ARG:NH1	2.35	0.41
1:K:82:LYS:HE3	1:K:88:GLU:HG2	2.02	0.41
1:A:6:LYS:HE3	1:A:49:GLU:HB3	2.02	0.41
1:A:59:ARG:NH1	1:B:59:ARG:HA	2.35	0.41
1:M:163:LYS:NZ	5:M:703:HOH:O	2.53	0.41
1:A:126:LEU:O	1:A:130:PHE:CD2	2.73	0.41
1:B:381:ASN:OD1	1:B:381:ASN:N	2.54	0.41
1:K:333:VAL:HG21	1:K:417:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:128:ARG:HE	1:M:128:ARG:HB2	1.74	0.41
1:M:98:LEU:O	1:M:102:ILE:HG13	2.20	0.41
1:B:4:ARG:HH22	1:B:53:GLY:HA2	1.85	0.41
1:M:84:VAL:HB	3:M:602:SF4:S3	2.60	0.41
1:M:381:ASN:N	1:M:381:ASN:OD1	2.50	0.41
1:M:136:ASN:ND2	1:M:139:PHE:HZ	2.18	0.41
1:A:463:ASN:OD1	1:A:466:ILE:HG13	2.20	0.41
1:K:69:GLN:OE1	1:M:103:LYS:NZ	2.52	0.41
1:A:374:ALA:O	1:A:377:LYS:HE3	2.20	0.41
1:B:338:ILE:CD1	1:B:369:VAL:HG13	2.51	0.41
1:K:348:ASP:OD2	1:K:379:ARG:NE	2.50	0.41
1:K:131:TYR:HA	1:K:134:LEU:HD13	2.02	0.41
1:K:261:CYS:HA	1:M:136:ASN:HB2	2.02	0.41
1:K:293:SER:OG	1:K:294:PRO:HD3	2.21	0.41
1:M:403:SER:OG	1:M:440:ILE:HD13	2.21	0.41
1:A:59:ARG:NH1	1:B:58:VAL:O	2.54	0.40
1:A:70:CYS:HB2	1:B:433:MET:O	2.21	0.40
1:A:244:GLN:HG3	1:A:248:PHE:CD2	2.55	0.40
1:B:68:TYR:HB3	1:B:78:ALA:HA	2.03	0.40
1:A:108:TYR:CE1	1:A:401:ASN:HB3	2.56	0.40
1:A:236:GLN:HG3	1:A:237:LEU:N	2.36	0.40
1:A:466:ILE:O	1:A:470:LEU:HD22	2.21	0.40
1:B:472:ASP:OD1	1:B:473:LYS:N	2.54	0.40
1:K:260:ASN:OD1	1:K:261:CYS:N	2.42	0.40
1:M:68:TYR:HB3	1:M:78:ALA:HA	2.03	0.40
1:A:374:ALA:HB2	1:A:400:CYS:HB3	2.03	0.40
1:K:433:MET:O	1:M:70:CYS:HB2	2.21	0.40
1:M:340:ARG:NH2	1:M:426:LEU:O	2.55	0.40
1:B:9:ASP:OD2	1:B:56:ARG:HG3	2.20	0.40
1:M:95:GLN:HG2	1:M:144:PHE:CZ	2.57	0.40
1:A:172:GLU:OE1	1:A:320:SER:HB2	2.20	0.40
1:A:315:THR:HA	1:A:396:ASP:HB3	2.02	0.40
1:K:236:GLN:HG3	1:K:237:LEU:N	2.37	0.40
1:K:244:GLN:NE2	1:K:263:LEU:H	2.16	0.40
1:K:329:ILE:O	1:K:333:VAL:HG22	2.22	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	488/506 (96%)	454 (93%)	31 (6%)	3 (1%)	25	54
1	B	488/506 (96%)	454 (93%)	28 (6%)	6 (1%)	13	37
1	K	482/506 (95%)	454 (94%)	28 (6%)	0	100	100
1	M	479/506 (95%)	448 (94%)	31 (6%)	0	100	100
All	All	1937/2024 (96%)	1810 (93%)	118 (6%)	9 (0%)	29	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	61	GLU
1	B	56	ARG
1	B	51	LEU
1	B	59	ARG
1	B	61	GLU
1	A	216	SER
1	B	380	PHE
1	B	374	ALA

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	418/430 (97%)	400 (96%)	18 (4%)	29	60
1	B	418/430 (97%)	405 (97%)	13 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	414/430 (96%)	398 (96%)	16 (4%)	32	64
1	M	412/430 (96%)	398 (97%)	14 (3%)	37	69
All	All	1662/1720 (97%)	1601 (96%)	61 (4%)	34	66

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	49	GLU
1	A	68	TYR
1	A	70	CYS
1	A	75	ARG
1	A	131	TYR
1	A	137	VAL
1	A	161	LEU
1	A	178	VAL
1	A	229	LYS
1	A	312	THR
1	A	314	THR
1	A	369	VAL
1	A	375	CYS
1	A	403	SER
1	A	448	ASN
1	A	454	ILE
1	A	475	GLU
1	B	68	TYR
1	B	70	CYS
1	B	81	VAL
1	B	131	TYR
1	B	180	VAL
1	B	276	CYS
1	B	298	LYS
1	B	375	CYS
1	B	397	LEU
1	B	410	VAL
1	B	465	ASP
1	B	469	VAL
1	B	470	LEU
1	K	24	LYS
1	K	68	TYR
1	K	70	CYS

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Mol	Chain	Res	Type
1	K	90	THR
1	K	126	LEU
1	K	131	TYR
1	K	135	THR
1	K	262	VAL
1	K	268	SER
1	K	272	ARG
1	K	281	LEU
1	K	325	LEU
1	K	339	ARG
1	K	369	VAL
1	K	433	MET
1	K	449	LEU
1	M	68	TYR
1	M	70	CYS
1	M	126	LEU
1	M	128	ARG
1	M	131	TYR
1	M	134	LEU
1	M	184	ASP
1	M	272	ARG
1	M	273	MET
1	M	339	ARG
1	M	369	VAL
1	M	375	CYS
1	M	410	VAL
1	M	454	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	136	ASN
1	A	448	ASN
1	B	47	GLN
1	B	155	ASN
1	B	215	HIS
1	B	244	GLN
1	K	136	ASN
1	K	215	HIS
1	K	244	GLN
1	M	69	GLN

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Mol	Chain	Res	Type
1	M	95	GLN
1	M	97	ASN
1	M	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	CSS	M	347	1,2	4,6,7	1.36	1 (25%)	1,6,8	0.70	0
1	CSS	B	347	1,2	4,6,7	1.24	0	1,6,8	0.81	0
1	CSS	A	347	1,2	4,6,7	1.07	0	1,6,8	0.43	0
1	CSS	K	347	1	4,6,7	1.03	0	1,6,8	0.08	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
1	CSS	M	347	1,2	-	1/1/5/7	-
1	CSS	B	347	1,2	-	1/1/5/7	-
1	CSS	A	347	1,2	-	1/1/5/7	-
1	CSS	K	347	1	-	1/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	347	CSS	CB-SG	-2.18	1.74	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	347	CSS	N-CA-CB-SG
1	B	347	CSS	N-CA-CB-SG
1	K	347	CSS	N-CA-CB-SG
1	M	347	CSS	N-CA-CB-SG

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	347	CSS	2	0
1	B	347	CSS	3	0
1	A	347	CSS	1	0
1	K	347	CSS	3	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	SF4	B	602	1	0,12,12	-	-	-		
2	FS2	M	601	1	0,14,14	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	FS2	A	601	1	0,14,14	-	-	-		
2	FS2	K	601	1	0,14,14	-	-	-		
3	SF4	M	602	1	0,12,12	-	-	-		
3	SF4	K	602	1	0,12,12	-	-	-		
3	SF4	A	602	1	0,12,12	-	-	-		
2	FS2	B	601	1	0,14,14	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	K	602	1	-	-	0/6/5/5
3	SF4	B	602	1	-	-	0/6/5/5
3	SF4	A	602	1	-	-	0/6/5/5
3	SF4	M	602	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.
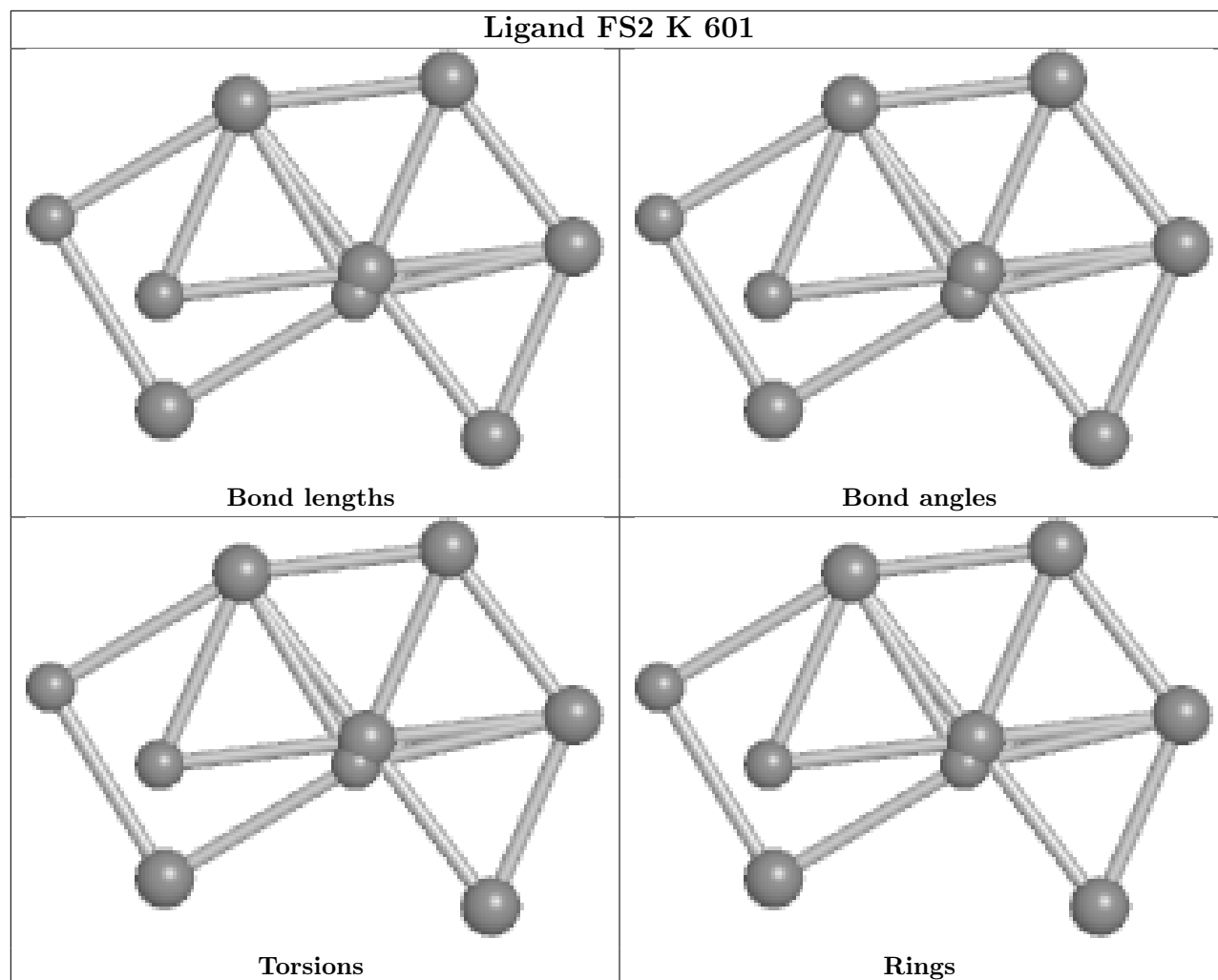
7 monomers are involved in 9 short contacts:

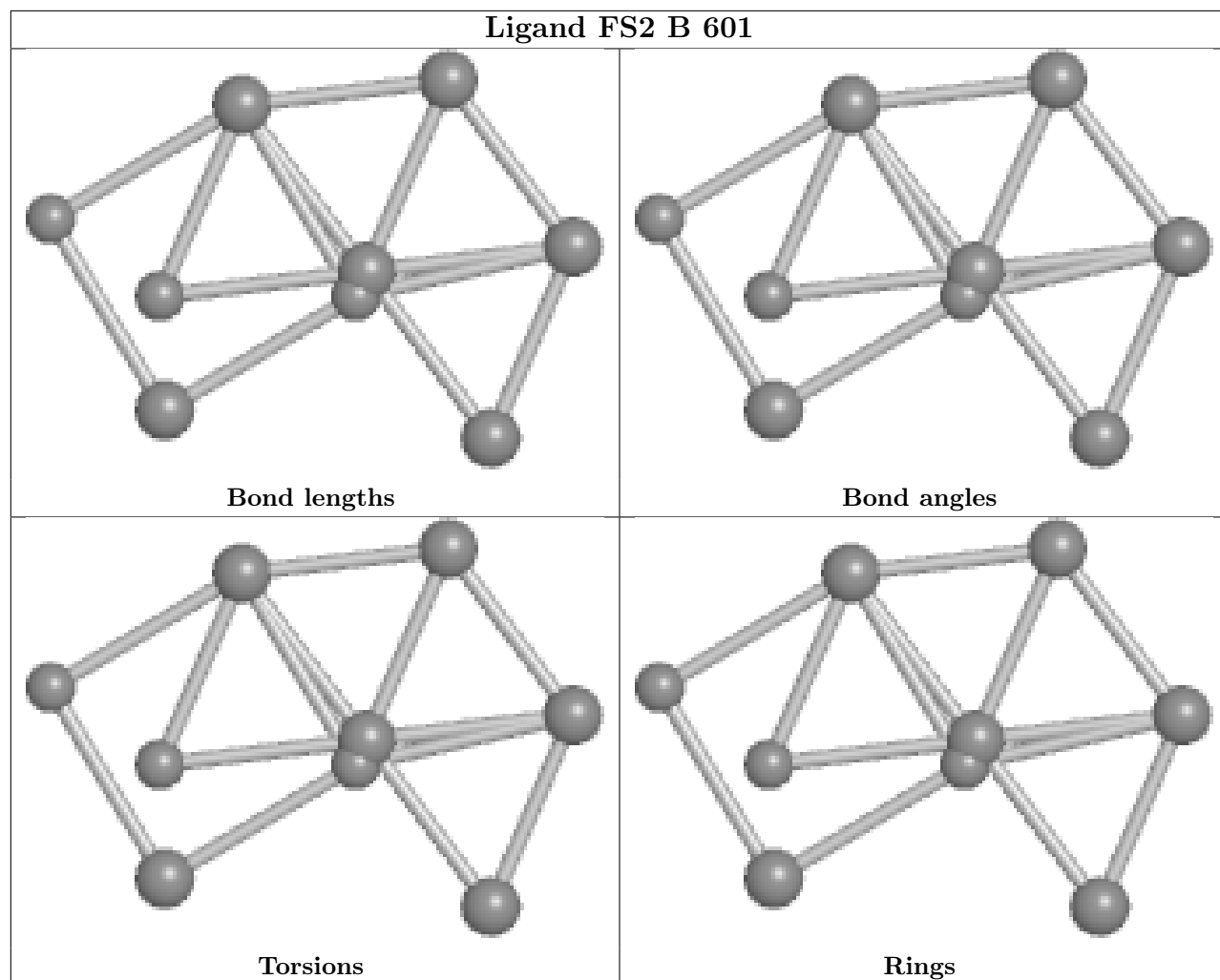| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	601	FS2	2	0
2	A	601	FS2	1	0
2	K	601	FS2	2	0
3	M	602	SF4	1	0
3	K	602	SF4	1	0
3	A	602	SF4	1	0
2	B	601	FS2	1	0

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 then 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 FS2 M 601

Bond lengths

Bond angles

Torsions

Rings

Ligand FS2 A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand FS2 K 601

Bond lengths

Bond angles

Torsions

Rings
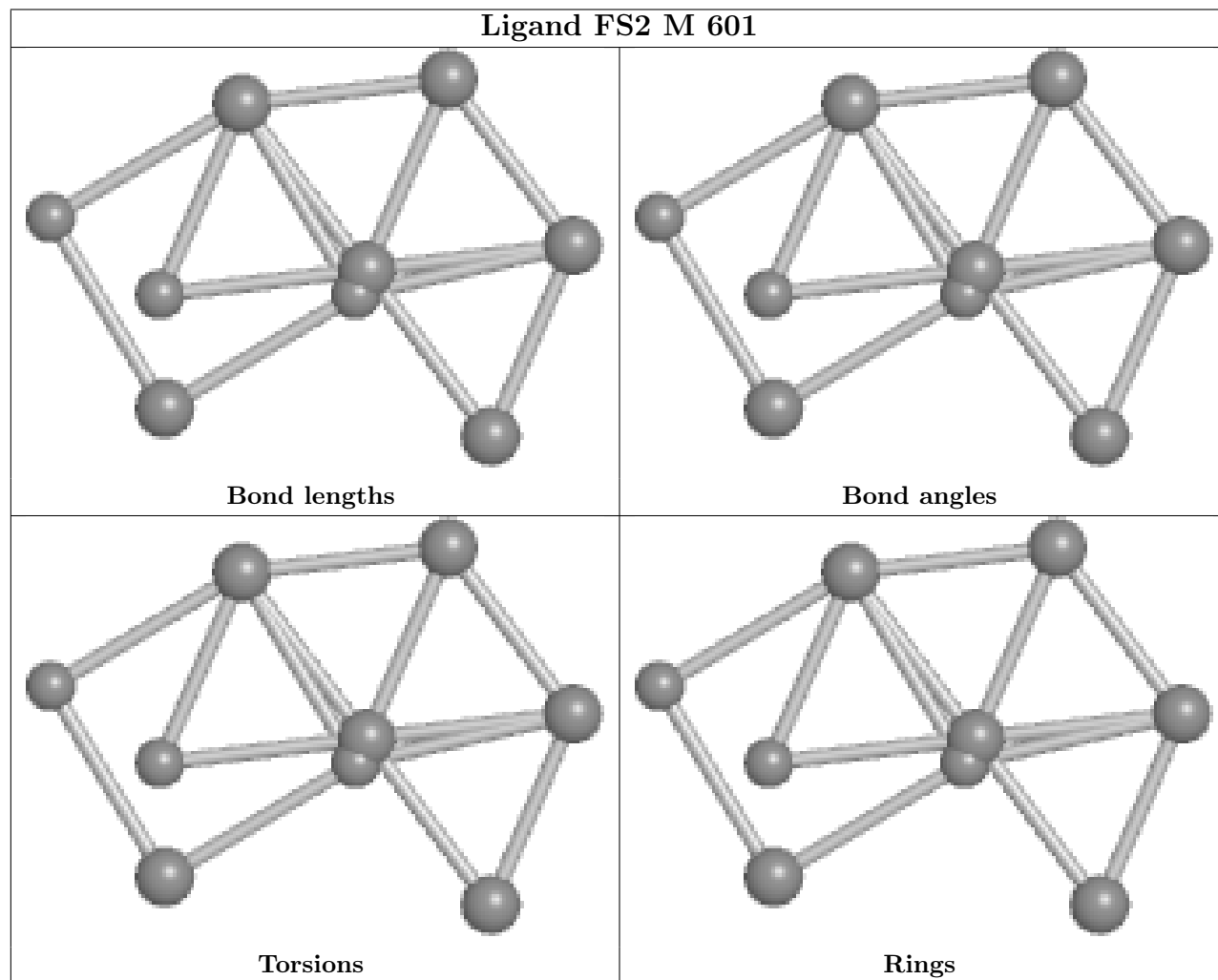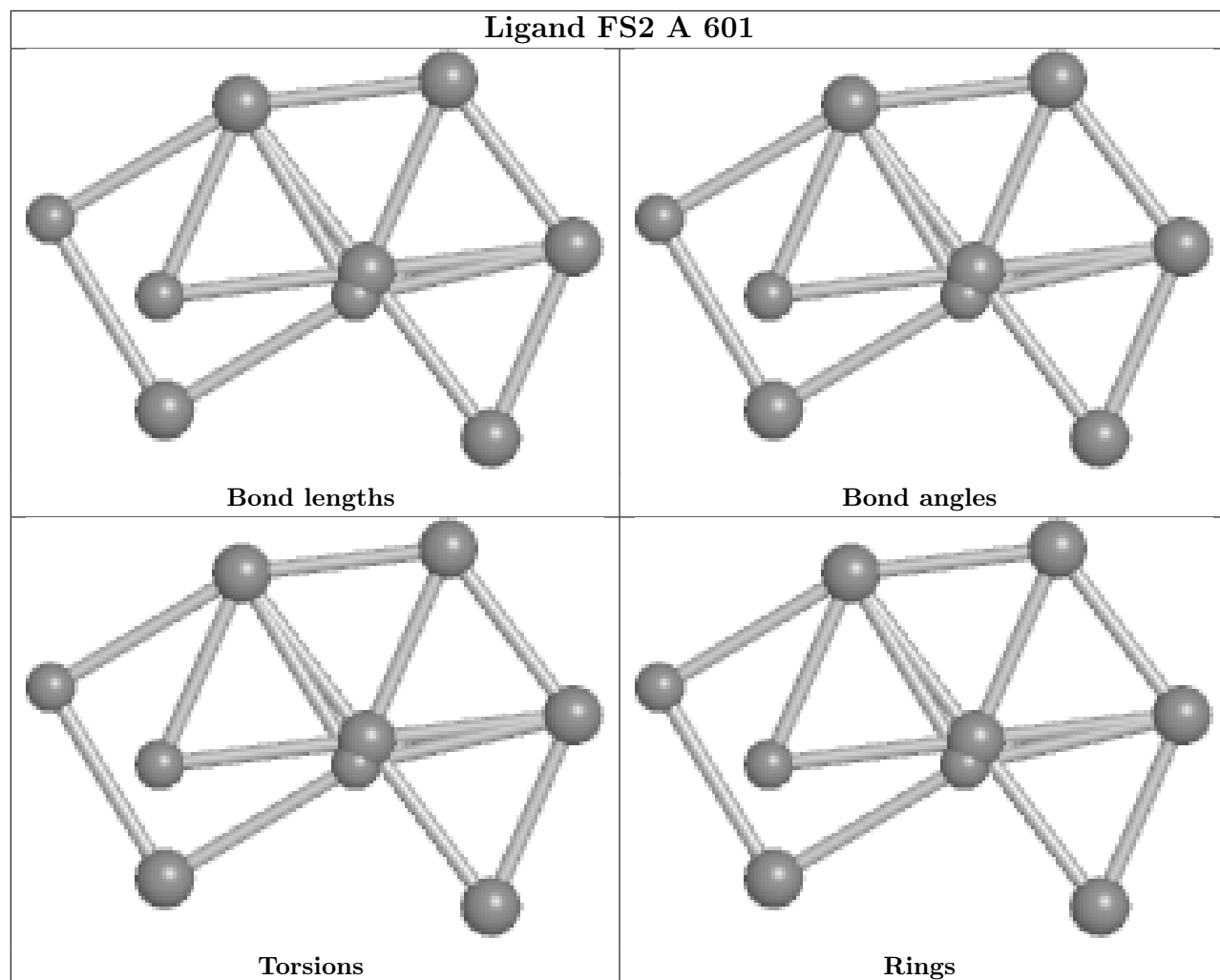
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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(Å²)	Q<0.9
1	A	490/506 (96%)	-0.13	10 (2%)	65	56	44, 73, 102, 142	0
1	B	490/506 (96%)	-0.07	25 (5%)	28	19	38, 51, 189, 240	0
1	K	486/506 (96%)	-0.12	12 (2%)	57	47	43, 74, 102, 119	0
1	M	483/506 (95%)	-0.10	29 (6%)	21	14	37, 51, 177, 245	0
All	All	1949/2024 (96%)	-0.11	76 (3%)	39	29	37, 60, 132, 245	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	PRO	9.4
1	B	26	GLY	9.1
1	B	30	GLN	7.7
1	B	12	TYR	7.5
1	B	14	PRO	7.0
1	M	13	ASP	7.0
1	M	12	TYR	6.4
1	B	3	TYR	6.3
1	B	6	LYS	5.8
1	M	26	GLY	5.7
1	B	19	PRO	5.7
1	B	20	THR	5.5
1	B	29	PHE	5.4
1	B	53	GLY	5.0
1	B	36	TRP	5.0
1	M	35	ASP	5.0
1	M	14	PRO	4.9
1	M	40	VAL	4.9
1	M	28	PRO	4.7
1	M	7	VAL	4.6
1	B	51	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	13	ASP	4.2
1	B	4	ARG	4.2
1	M	19	PRO	4.1
1	A	58	VAL	4.1
1	M	39	PRO	4.0
1	A	394	LEU	4.0
1	M	36	TRP	4.0
1	M	48	PHE	3.9
1	B	24	LYS	3.9
1	B	7	VAL	3.8
1	B	5	CYS	3.7
1	M	24	LYS	3.7
1	K	235	GLY	3.7
1	M	2	LYS	3.6
1	B	23	ILE	3.6
1	M	8	CYS	3.6
1	B	11	ILE	3.6
1	M	37	LEU	3.6
1	M	49	GLU	3.5
1	K	234	ALA	3.5
1	A	26	GLY	3.4
1	M	23	ILE	3.3
1	M	16	VAL	3.2
1	M	47	GLN	3.1
1	K	53	GLY	3.1
1	B	17	GLY	3.1
1	M	29	PHE	3.0
1	K	190	ALA	3.0
1	K	392	PRO	3.0
1	A	392	PRO	2.9
1	A	326	ALA	2.9
1	B	15	GLU	2.7
1	M	20	THR	2.7
1	K	233	LEU	2.7
1	A	395	ILE	2.7
1	M	15	GLU	2.7
1	M	10	TYR	2.6
1	M	34	GLU	2.6
1	B	50	PRO	2.5
1	M	32	LEU	2.4
1	K	388	ILE	2.4
1	M	27	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	28	PRO	2.3
1	B	52	ARG	2.2
1	A	12	TYR	2.1
1	A	388	ILE	2.1
1	K	369	VAL	2.1
1	K	227	LEU	2.1
1	M	11	ILE	2.1
1	A	274	PHE	2.1
1	K	12	TYR	2.1
1	A	57	ARG	2.1
1	K	13	ASP	2.1
1	K	343	LEU	2.0
1	M	3	TYR	2.0

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

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, 95th 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($\mathring{A}^2$)	Q<0.9
1	CSS	B	347	7/8	0.92	0.14	53,54,60,66	0
1	CSS	K	347	7/8	0.93	0.16	68,69,71,82	0
1	CSS	M	347	7/8	0.94	0.12	51,52,58,67	0
1	CSS	A	347	7/8	0.95	0.11	73,74,76,88	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 95th 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($\mathring{A}^2$)	Q<0.9
4	FE	B	603	1/1	0.61	0.14	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\mathring{A}^2$)	Q<0.9
2	FS2	K	601	9/9	0.93	0.11	86,101,124,133	0
4	FE	A	603	1/1	0.94	0.18	157,157,157,157	0
2	FS2	B	601	9/9	0.96	0.07	57,68,83,90	0
2	FS2	A	601	9/9	0.96	0.08	92,96,124,137	0
2	FS2	M	601	9/9	0.97	0.07	62,67,78,98	0
4	FE	K	603	1/1	0.97	0.07	69,69,69,69	0
4	FE	M	603	1/1	0.97	0.10	135,135,135,135	0
3	SF4	K	602	8/8	0.98	0.08	60,69,83,88	0
3	SF4	A	602	8/8	0.99	0.10	47,55,66,66	0
3	SF4	M	602	8/8	0.99	0.09	65,76,86,92	0
3	SF4	B	602	8/8	0.99	0.11	62,67,71,84	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.
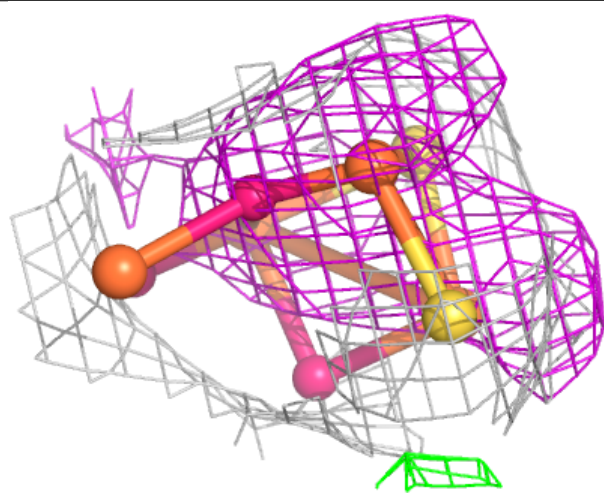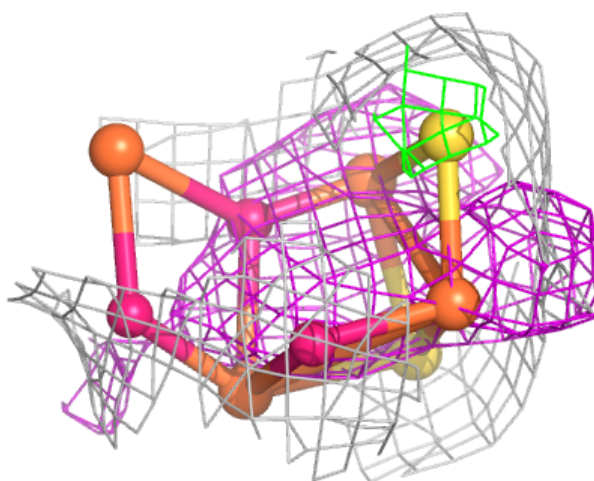
Electron density around FS2 K 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
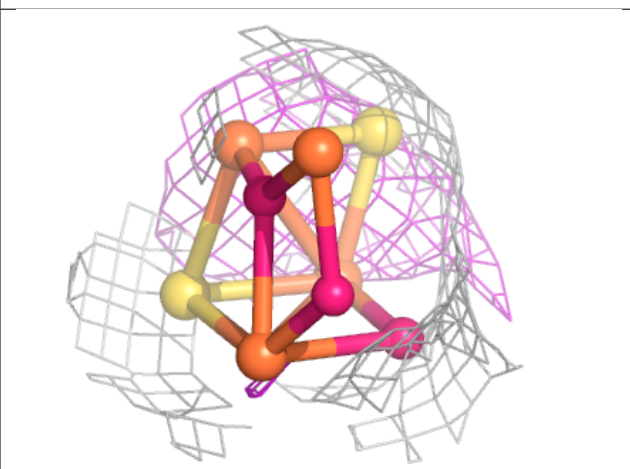$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
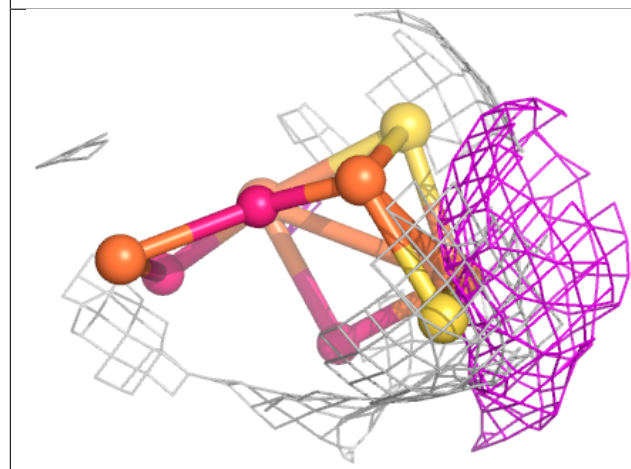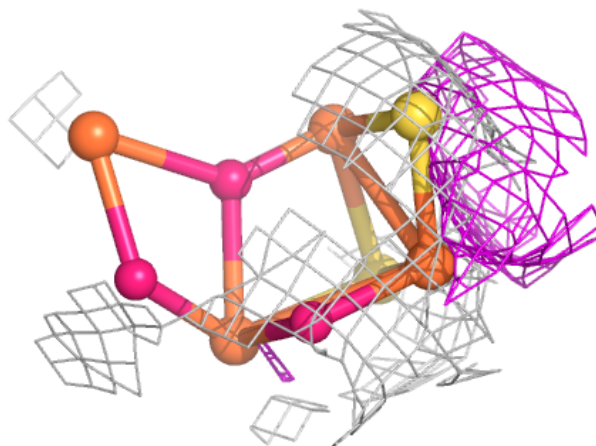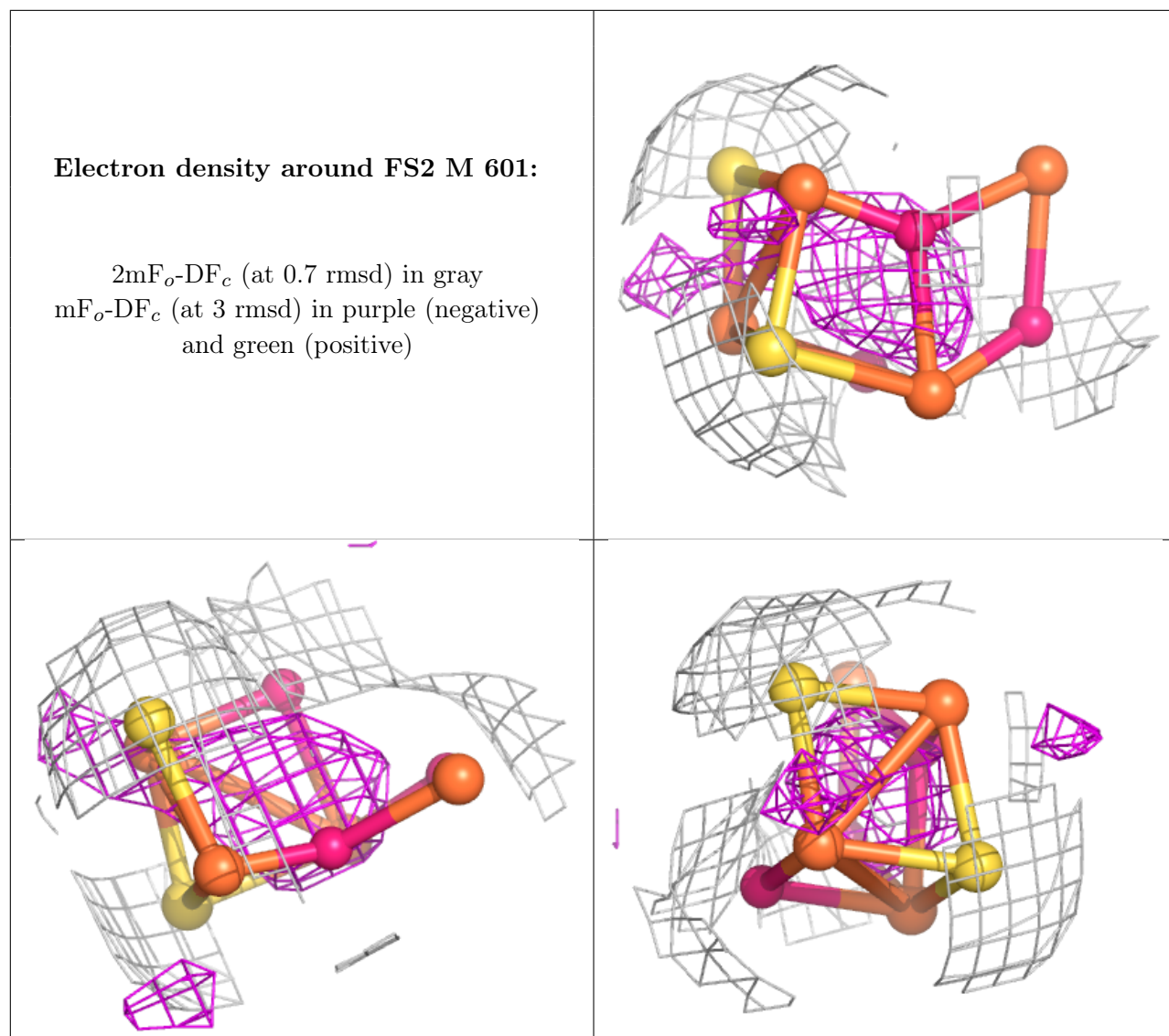and green (positive)
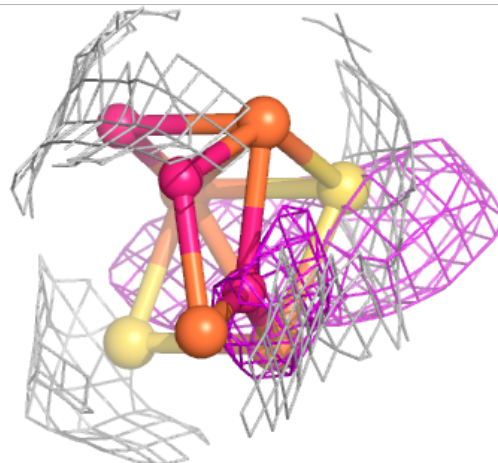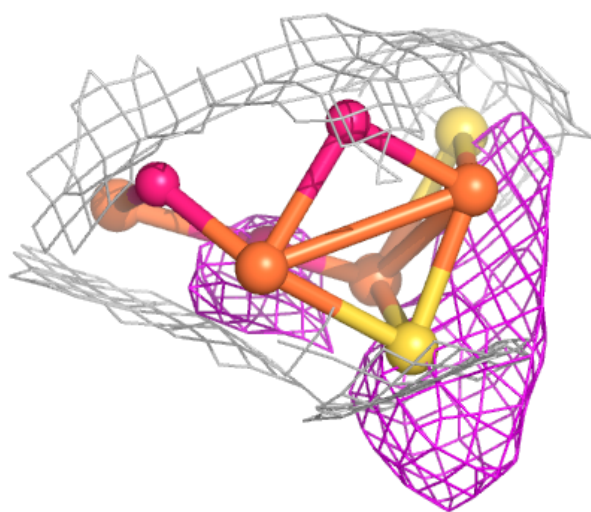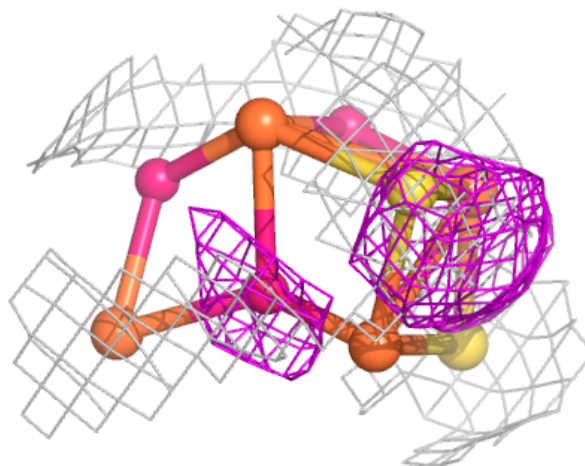
Electron density around FS2 B 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
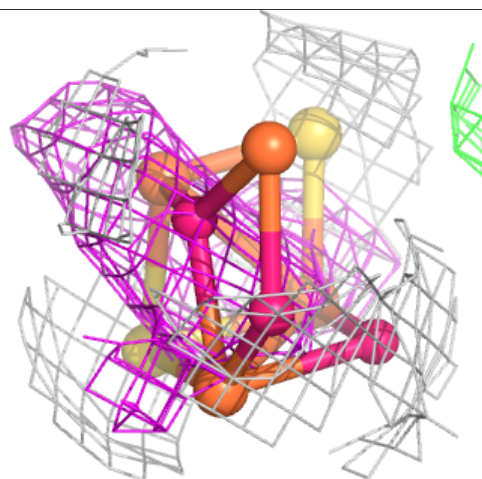
Electron density around FS2 A 601:

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

Electron density around FS2 M 601:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.