Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2024 – 04:20 pm BST

PDB ID	:	9EVV
Title	:	His579Leu variant of L-arabinonate dehydratase co-crystallized with 2-oxobutyrate
Authors	:	Ren, Y.; Rouvinen, J.; Hakulinen, N.
Deposited on	:	2024-04-02
Resolution	:	2.44 Å(reported)

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

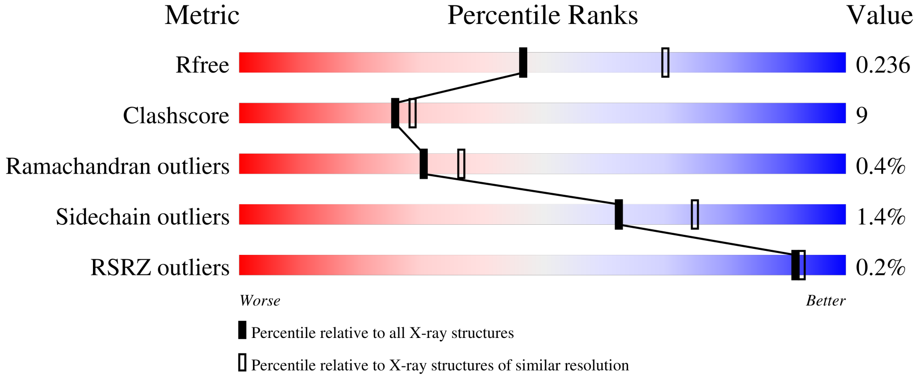
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

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 2.44 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	2124 (2.46-2.42)
Clashscore	180529	2259 (2.46-2.42)
Ramachandran outliers	177936	2244 (2.46-2.42)
Sidechain outliers	177891	2244 (2.46-2.42)
RSRZ outliers	164620	2124 (2.46-2.42)

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	588	
1	B	588	
1	C	588	
1	D	588	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 17865 atoms, of which 5 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 L-arabinonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total 4355	C 2729	N 767	O 825	S 34	0	1	0
1	B	575	Total 4347	C 2724	N 764	O 825	S 34	0	0	0
1	C	575	Total 4353	C 2728	N 765	O 826	S 34	0	1	0
1	D	575	Total 4347	C 2724	N 764	O 825	S 34	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP B5ZZ34
A	-7	ASP	-	expression tag	UNP B5ZZ34
A	-6	TRP	-	expression tag	UNP B5ZZ34
A	-5	SER	-	expression tag	UNP B5ZZ34
A	-4	HIS	-	expression tag	UNP B5ZZ34
A	-3	PRO	-	expression tag	UNP B5ZZ34
A	-2	GLN	-	expression tag	UNP B5ZZ34
A	-1	PHE	-	expression tag	UNP B5ZZ34
A	0	GLU	-	expression tag	UNP B5ZZ34
A	1	LYS	-	expression tag	UNP B5ZZ34
A	579	LEU	HIS	engineered mutation	UNP B5ZZ34
B	-8	MET	-	initiating methionine	UNP B5ZZ34
B	-7	ASP	-	expression tag	UNP B5ZZ34
B	-6	TRP	-	expression tag	UNP B5ZZ34
B	-5	SER	-	expression tag	UNP B5ZZ34
B	-4	HIS	-	expression tag	UNP B5ZZ34
B	-3	PRO	-	expression tag	UNP B5ZZ34
B	-2	GLN	-	expression tag	UNP B5ZZ34
B	-1	PHE	-	expression tag	UNP B5ZZ34
B	0	GLU	-	expression tag	UNP B5ZZ34
B	1	LYS	-	expression tag	UNP B5ZZ34

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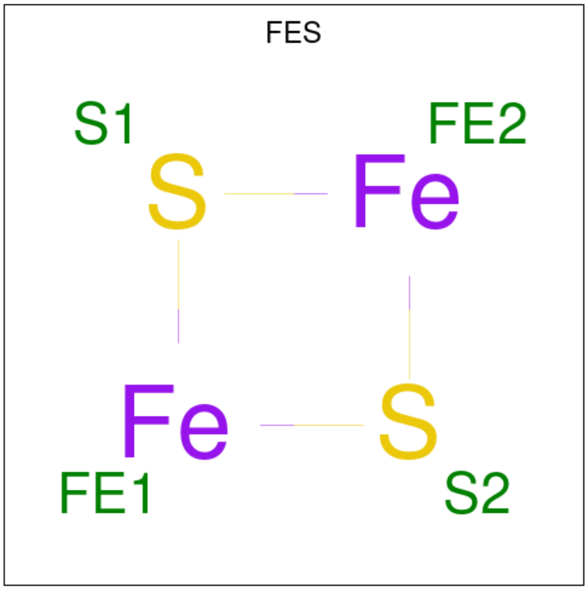
Chain	Residue	Modelled	Actual	Comment	Reference
B	579	LEU	HIS	engineered mutation	UNP B5ZZ34
C	-8	MET	-	initiating methionine	UNP B5ZZ34
C	-7	ASP	-	expression tag	UNP B5ZZ34
C	-6	TRP	-	expression tag	UNP B5ZZ34
C	-5	SER	-	expression tag	UNP B5ZZ34
C	-4	HIS	-	expression tag	UNP B5ZZ34
C	-3	PRO	-	expression tag	UNP B5ZZ34
C	-2	GLN	-	expression tag	UNP B5ZZ34
C	-1	PHE	-	expression tag	UNP B5ZZ34
C	0	GLU	-	expression tag	UNP B5ZZ34
C	1	LYS	-	expression tag	UNP B5ZZ34
C	579	LEU	HIS	engineered mutation	UNP B5ZZ34
D	-8	MET	-	initiating methionine	UNP B5ZZ34
D	-7	ASP	-	expression tag	UNP B5ZZ34
D	-6	TRP	-	expression tag	UNP B5ZZ34
D	-5	SER	-	expression tag	UNP B5ZZ34
D	-4	HIS	-	expression tag	UNP B5ZZ34
D	-3	PRO	-	expression tag	UNP B5ZZ34
D	-2	GLN	-	expression tag	UNP B5ZZ34
D	-1	PHE	-	expression tag	UNP B5ZZ34
D	0	GLU	-	expression tag	UNP B5ZZ34
D	1	LYS	-	expression tag	UNP B5ZZ34
D	579	LEU	HIS	engineered mutation	UNP B5ZZ34

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

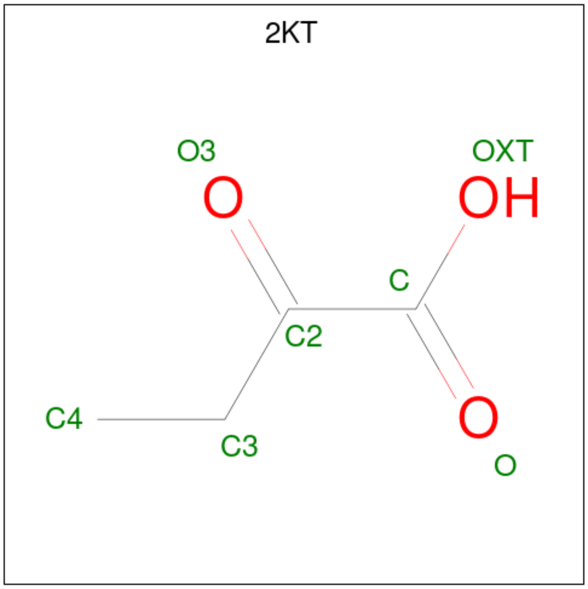
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 2-KETOBUTYRIC ACID (three-letter code: 2KT) (formula: $C_4H_6O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C H O 12 4 5 3	0	0

- Molecule 5 is water.

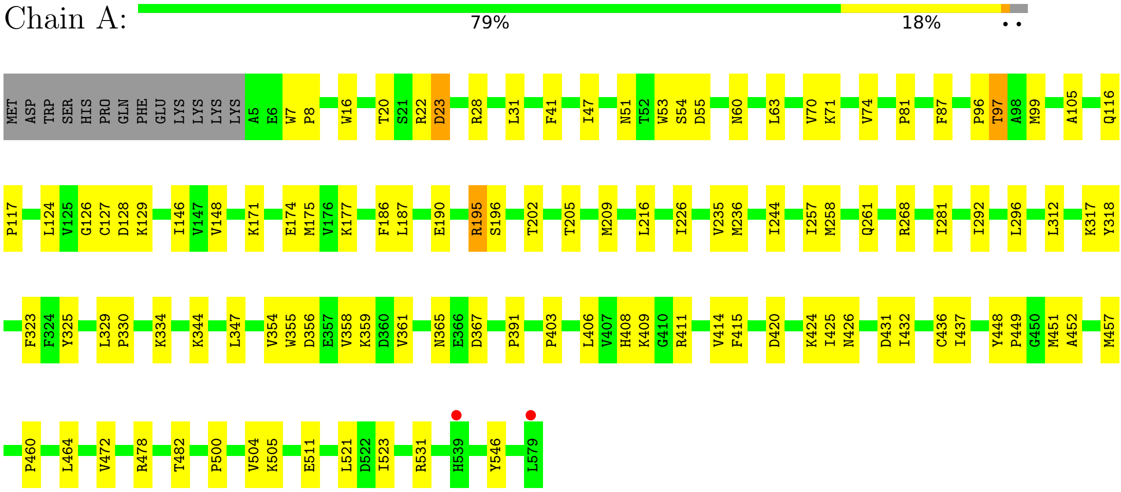
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	87	Total O 87 87	0	0
5	B	103	Total O 103 103	0	0
5	C	122	Total O 122 122	0	0
5	D	119	Total O 119 119	0	0

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.

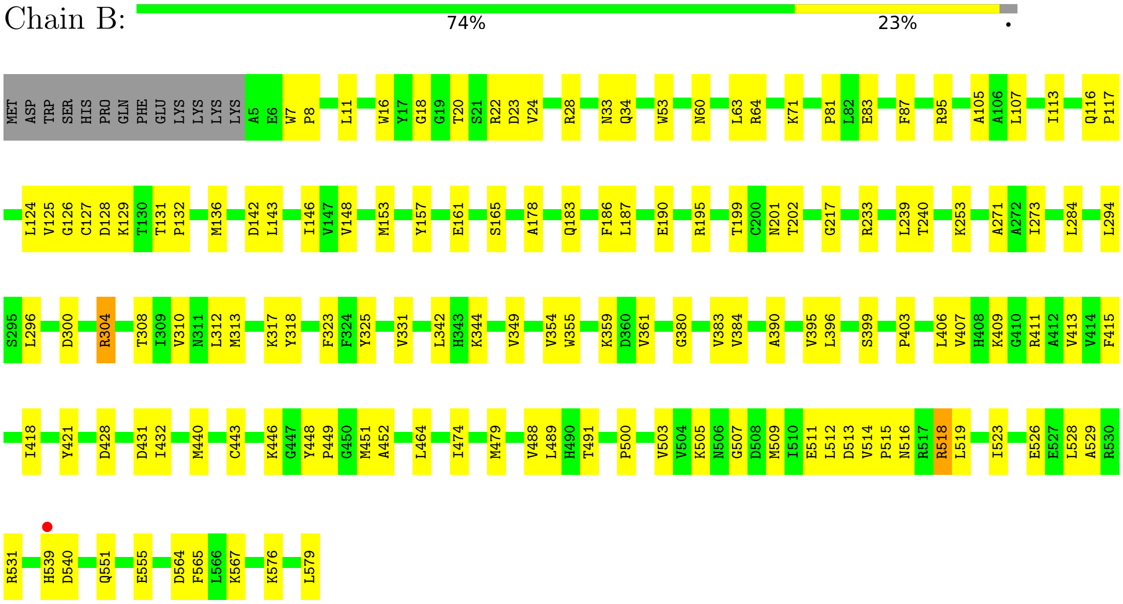
- Molecule 1: L-arabinonate dehydratase

Chain A:



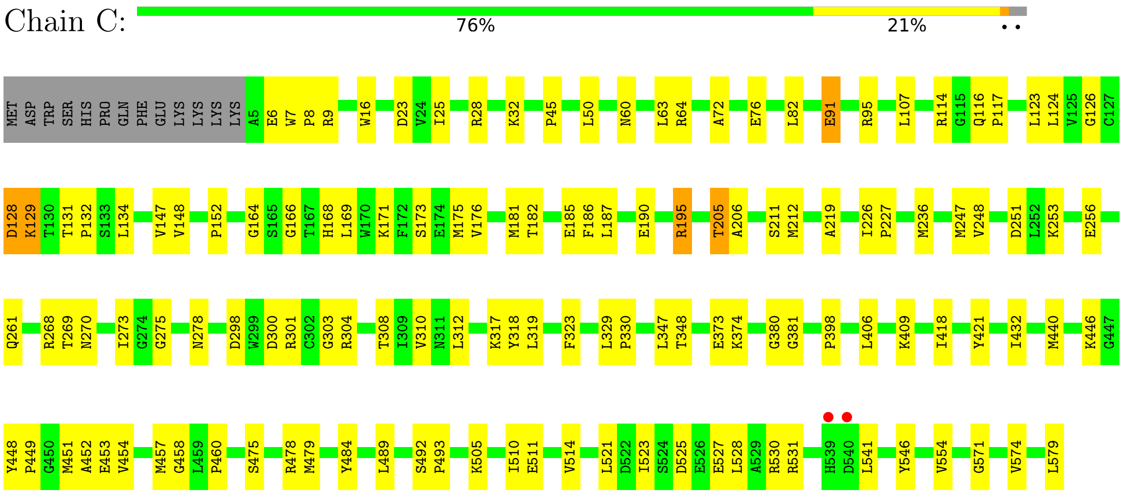
- Molecule 1: L-arabinonate dehydratase

Chain B:



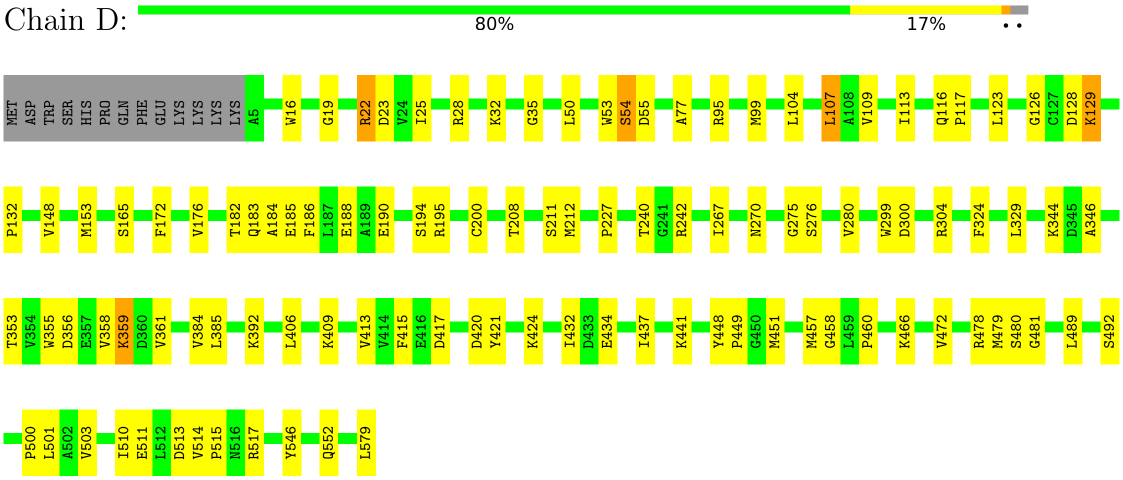
- Molecule 1: L-arabinonate dehydratase

Chain C:



- Molecule 1: L-arabinonate dehydratase

Chain D:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.95Å 148.21Å 165.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.44 48.48 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.48-2.44) 99.7 (48.48-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.185 , 0.237 0.184 , 0.236	Depositor DCC
R_{free} test set	96248 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17865	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: MG, FES, KCX, 2KT

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	0.41	0/4430	0.64	0/5998
1	B	0.43	0/4419	0.64	0/5984
1	C	0.41	0/4428	0.64	0/5996
1	D	0.42	0/4419	0.64	0/5984
All	All	0.42	0/17696	0.64	0/23962

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	4355	0	4337	80	0
1	B	4347	0	4324	94	0
1	C	4353	0	4332	98	0
1	D	4347	0	4324	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
4	D	7	5	5	1	0
5	A	87	0	0	2	0
5	B	103	0	0	1	0
5	C	122	0	0	3	0
5	D	119	0	0	1	0
All	All	17860	5	17322	326	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 9.

All (326) 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:C:523:ILE:HD11	1:C:528:LEU:HB2	1.55	0.88
1:C:187:LEU:HD22	1:D:25:ILE:HD11	1.57	0.86
1:A:409:LYS:HG3	1:A:511:GLU:HG2	1.61	0.83
1:C:212:MET:HE1	1:C:270:ASN:HB2	1.62	0.80
1:D:270:ASN:OD1	1:D:275:GLY:HA3	1.82	0.79
1:A:60:ASN:HB3	1:A:63:LEU:HD22	1.67	0.77
1:C:28:ARG:HD2	1:D:190:GLU:OE2	1.84	0.77
1:A:171:LYS:O	1:A:175:MET:HG3	1.85	0.77
1:A:546:TYR:HB2	1:B:107:LEU:HD11	1.66	0.76
1:D:358:VAL:O	1:D:361:VAL:HG22	1.85	0.76
1:C:269:THR:O	1:C:273:ILE:HG12	1.86	0.75
1:C:432:ILE:HD13	1:C:460:PRO:HG2	1.67	0.74
1:C:546:TYR:HB2	1:D:107:LEU:HD21	1.70	0.74
1:B:509:MET:HB2	5:B:708:HOH:O	1.87	0.73
1:A:356:ASP:HA	1:A:359:LYS:HE2	1.72	0.71
1:B:146:ILE:HD13	1:B:240:THR:HG23	1.72	0.71
1:A:174:GLU:OE1	1:A:177:LYS:HE2	1.90	0.71
1:A:505:LYS:HB2	1:A:531:ARG:NH1	2.06	0.71
1:B:523:ILE:HG21	1:B:531:ARG:NH2	2.04	0.71
1:B:16:TRP:CD2	1:B:117:PRO:HB3	2.26	0.70
1:A:420:ASP:OD1	1:A:424:LYS:HE3	1.91	0.70
1:B:271:ALA:O	1:B:308:THR:HG22	1.92	0.70
1:C:60:ASN:HB3	1:C:63:LEU:HD22	1.72	0.70
1:C:212:MET:HE1	1:C:270:ASN:CB	2.23	0.69
1:C:451:MET:HG2	1:C:478:ARG:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:ASP:OD1	1:D:515:PRO:HD2	1.93	0.69
1:C:182:THR:HG23	1:C:185:GLU:OE2	1.93	0.69
1:B:124:LEU:HD23	1:B:148:VAL:HB	1.75	0.69
1:A:325:TYR:OH	1:C:195:ARG:NH2	2.25	0.68
1:B:142:ASP:OD2	1:B:253:LYS:HE3	1.93	0.67
1:C:527:GLU:HA	1:C:530:ARG:HG2	1.75	0.67
1:B:523:ILE:HD11	1:B:528:LEU:HB2	1.78	0.66
1:C:64:ARG:HB2	5:C:760:HOH:O	1.95	0.65
1:C:205:THR:HG23	1:C:278:ASN:HB2	1.78	0.65
1:B:308:THR:CG2	1:B:380:GLY:HA3	2.26	0.65
1:A:20:THR:HB	1:B:187:LEU:HD11	1.79	0.65
1:D:172:PHE:O	1:D:176:VAL:HG23	1.97	0.65
1:D:16:TRP:CD2	1:D:117:PRO:HB3	2.31	0.64
1:D:182:THR:OG1	1:D:185:GLU:HG3	1.97	0.64
1:C:152:PRO:HD2	1:C:227:PRO:HA	1.80	0.64
1:C:479:MET:HG2	1:C:489:LEU:HD11	1.80	0.64
1:B:308:THR:HG23	1:B:380:GLY:HA3	1.78	0.63
1:C:91:GLU:HG3	1:C:128:ASP:HB2	1.80	0.63
1:A:216:LEU:HD13	1:A:258:MET:HE3	1.79	0.63
1:A:70:VAL:O	1:A:74:VAL:HG23	1.99	0.62
1:D:500:PRO:O	1:D:503:VAL:HG22	1.99	0.62
1:A:403:PRO:HA	1:A:406:LEU:CD1	2.29	0.62
1:C:190:GLU:OE2	1:D:28:ARG:HD2	2.00	0.62
1:D:300:ASP:O	1:D:304:ARG:HG3	1.99	0.61
1:A:505:LYS:HB2	1:A:531:ARG:HH12	1.64	0.61
1:D:28:ARG:HD3	1:D:32:LYS:HE3	1.83	0.61
1:A:505:LYS:HE3	1:A:531:ARG:CZ	2.31	0.61
1:D:50:LEU:HD22	1:D:123:LEU:HD23	1.83	0.61
1:A:235:VAL:CG2	1:D:35:GLY:HA2	2.31	0.61
1:D:392:LYS:HB2	1:D:492:SER:HB3	1.83	0.60
1:A:408:HIS:HD2	1:A:437:ILE:HD11	1.66	0.59
1:C:312:LEU:HD11	1:C:323:PHE:HB2	1.85	0.59
1:D:409:LYS:NZ	1:D:511:GLU:OE2	2.35	0.59
1:B:390:ALA:HB2	1:B:491:THR:HG23	1.84	0.59
1:C:432:ILE:HD13	1:C:460:PRO:CG	2.33	0.59
1:A:281:ILE:HD11	1:A:451:MET:HE1	1.85	0.59
1:D:50:LEU:HD22	1:D:123:LEU:CD2	2.33	0.59
1:D:195:ARG:HD2	1:D:195:ARG:O	2.02	0.59
1:B:124:LEU:CD2	1:B:148:VAL:HB	2.32	0.58
1:A:415:PHE:CD2	1:A:457:MET:HE1	2.39	0.58
1:A:7:TRP:CD2	1:A:8:PRO:HA	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:TRP:CD2	1:C:117:PRO:HB3	2.39	0.58
1:D:356:ASP:OD1	1:D:359:LYS:HE3	2.04	0.58
1:D:276:SER:HB2	1:D:481:GLY:HA3	1.86	0.58
1:C:479:MET:HG2	1:C:489:LEU:CD1	2.33	0.58
1:C:164:GLY:H	1:C:168:HIS:CD2	2.22	0.58
1:D:346:ALA:O	1:D:353:THR:HA	2.04	0.57
1:A:16:TRP:CD2	1:A:117:PRO:HB3	2.40	0.57
1:A:28:ARG:HD2	1:B:190:GLU:OE2	2.04	0.57
1:A:190:GLU:OE2	1:B:28:ARG:HD2	2.04	0.57
1:C:300:ASP:OD2	1:C:304:ARG:NH2	2.38	0.57
1:D:448:TYR:HB3	1:D:449:PRO:C	2.24	0.57
1:B:22:ARG:HG3	1:B:23:ASP:N	2.20	0.57
1:B:284:LEU:HD23	1:B:294:LEU:HD23	1.85	0.57
1:C:317:LYS:HD3	1:C:318:TYR:CZ	2.40	0.56
1:D:413:VAL:HG21	1:D:432:ILE:HG13	1.88	0.56
1:C:45:PRO:HB3	1:C:248:VAL:HG11	1.86	0.56
1:C:406:LEU:HG	1:C:514:VAL:HG21	1.87	0.56
1:A:268:ARG:HD2	5:A:704:HOH:O	2.06	0.56
1:A:312:LEU:HD21	1:A:323:PHE:HB2	1.86	0.56
1:A:408:HIS:CD2	1:A:437:ILE:HD11	2.41	0.56
1:A:202:THR:OG1	1:A:482:THR:HG22	2.06	0.55
1:C:510:ILE:HG13	1:C:521:LEU:HD12	1.88	0.55
1:A:235:VAL:HG23	1:D:35:GLY:HA2	1.89	0.55
1:A:403:PRO:HA	1:A:406:LEU:HD12	1.89	0.55
1:C:7:TRP:CD2	1:C:8:PRO:HA	2.42	0.54
1:C:129:KCX:C	1:C:132:PRO:HD2	2.37	0.54
1:B:409:LYS:HE3	1:B:511:GLU:HG2	1.89	0.54
1:D:421:TYR:OH	1:D:458:GLY:N	2.40	0.54
1:C:124:LEU:CD2	1:C:148:VAL:HB	2.38	0.54
1:C:131:THR:HB	1:C:132:PRO:HD3	1.89	0.54
1:C:6:GLU:O	1:C:9:ARG:HD3	2.08	0.54
1:D:441:LYS:HE2	1:D:501:LEU:O	2.07	0.53
1:D:437:ILE:HG23	1:D:472:VAL:HG12	1.90	0.53
1:B:153:MET:HG3	1:B:199:THR:O	2.08	0.53
1:C:453:GLU:HA	1:C:478:ARG:O	2.08	0.53
1:D:22:ARG:HG3	1:D:23:ASP:N	2.23	0.53
1:B:317:LYS:HD3	1:B:318:TYR:CZ	2.44	0.53
1:D:104:LEU:HD12	1:D:104:LEU:O	2.09	0.53
1:D:466:LYS:HE3	5:D:706:HOH:O	2.09	0.52
1:B:300:ASP:OD2	1:B:304:ARG:NH2	2.41	0.52
1:B:539:HIS:O	1:B:540:ASP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:THR:HG22	1:B:313:MET:HB2	1.92	0.52
1:D:420:ASP:OD1	1:D:424:LYS:HE3	2.10	0.52
1:B:421:TYR:CB	1:B:440:MET:CE	2.88	0.52
1:C:310:VAL:HG12	1:C:312:LEU:HG	1.91	0.52
1:B:116:GLN:HB3	1:B:117:PRO:HD2	1.92	0.52
1:C:123:LEU:HD22	1:C:134:LEU:HD23	1.91	0.52
1:C:171:LYS:O	1:C:175:MET:HG3	2.09	0.52
1:D:148:VAL:HG23	1:D:240:THR:HG21	1.90	0.52
1:C:187:LEU:CD2	1:D:25:ILE:HD11	2.36	0.52
1:D:421:TYR:CD1	1:D:457:MET:CE	2.93	0.52
1:B:7:TRP:CD2	1:B:8:PRO:HA	2.44	0.51
1:C:347:LEU:HG	1:C:348:THR:N	2.25	0.51
1:C:421:TYR:CE1	1:C:457:MET:HB3	2.45	0.51
1:D:409:LYS:HD2	1:D:511:GLU:HG2	1.90	0.51
1:C:418:ILE:HD13	1:C:454:VAL:HG21	1.91	0.51
1:C:298:ASP:OD1	1:C:301:ARG:NH2	2.42	0.51
1:A:365:ASN:OD1	1:A:367:ASP:HB2	2.11	0.51
1:B:312:LEU:HD11	1:B:323:PHE:HB2	1.92	0.51
1:B:421:TYR:HB3	1:B:440:MET:CE	2.40	0.51
1:B:308:THR:HG21	1:B:399:SER:HB3	1.92	0.51
1:C:28:ARG:HD3	1:C:32:LYS:NZ	2.26	0.50
1:B:355:TRP:O	1:B:359:LYS:HB3	2.12	0.50
1:C:329:LEU:N	1:C:330:PRO:CD	2.74	0.50
1:A:195:ARG:HD2	1:A:195:ARG:C	2.32	0.50
1:B:411:ARG:HG2	1:B:507:GLY:HA2	1.93	0.50
1:B:411:ARG:NH1	1:B:431:ASP:OD2	2.44	0.50
1:B:195:ARG:HD2	1:B:195:ARG:O	2.11	0.50
1:A:448:TYR:N	1:A:449:PRO:HA	2.27	0.50
1:D:109:VAL:O	1:D:113:ILE:HG13	2.12	0.50
1:C:268:ARG:HD2	5:C:737:HOH:O	2.12	0.50
1:C:116:GLN:HB3	1:C:117:PRO:HD2	1.93	0.50
1:C:270:ASN:OD1	1:C:275:GLY:HA3	2.12	0.50
1:A:344:LYS:HG2	1:A:355:TRP:HB2	1.94	0.49
1:B:403:PRO:HA	1:B:406:LEU:HG	1.94	0.49
1:C:206:ALA:HB2	3:C:602:FES:S2	2.52	0.49
1:B:60:ASN:HB3	1:B:63:LEU:HD13	1.93	0.49
1:B:178:ALA:HB2	1:B:464:LEU:HB3	1.94	0.49
1:B:418:ILE:HA	1:B:440:MET:HE2	1.93	0.49
1:B:446:LYS:HE2	1:B:551:GLN:O	2.12	0.49
1:C:398:PRO:HD2	5:C:740:HOH:O	2.11	0.49
1:D:300:ASP:OD1	1:D:304:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ILE:HD12	1:A:472:VAL:HB	1.95	0.49
1:D:53:TRP:CG	1:D:54:SER:N	2.80	0.49
1:B:7:TRP:HZ3	1:B:11:LEU:HD21	1.78	0.49
1:A:187:LEU:HD11	1:B:20:THR:HB	1.95	0.49
1:B:63:LEU:HD23	1:B:124:LEU:HB3	1.95	0.49
1:C:107:LEU:HD21	1:D:546:TYR:HB2	1.94	0.49
1:D:448:TYR:N	1:D:449:PRO:HA	2.28	0.48
1:B:71:LYS:HG2	1:B:81:PRO:HB2	1.95	0.48
1:D:184:ALA:O	1:D:188:GLU:HG3	2.14	0.48
1:D:280:VAL:HG22	1:D:299:TRP:CD2	2.47	0.48
1:C:176:VAL:HA	1:C:181:MET:O	2.14	0.48
1:D:50:LEU:N	1:D:50:LEU:CD1	2.76	0.48
1:B:354:VAL:HG13	1:B:355:TRP:N	2.28	0.48
1:D:421:TYR:CD1	1:D:457:MET:HE3	2.48	0.48
1:C:448:TYR:HB3	1:C:449:PRO:C	2.34	0.48
1:C:273:ILE:HG22	1:C:310:VAL:HG21	1.95	0.48
1:B:500:PRO:O	1:B:503:VAL:HG22	2.14	0.48
1:C:95:ARG:HD3	1:D:16:TRP:CZ2	2.49	0.48
1:B:407:VAL:HA	1:B:512:LEU:O	2.14	0.47
1:B:474:ILE:HD13	1:B:519:LEU:HD11	1.96	0.47
1:D:432:ILE:HD13	1:D:460:PRO:CG	2.44	0.47
1:B:183:GLN:OE1	1:B:183:GLN:HA	2.13	0.47
1:C:190:GLU:HG3	1:D:25:ILE:HG23	1.96	0.47
1:D:300:ASP:HB2	1:D:384:VAL:HG23	1.97	0.47
1:A:358:VAL:O	1:A:361:VAL:HG22	2.15	0.47
1:A:505:LYS:HE3	1:A:531:ARG:NH1	2.29	0.47
1:B:157:TYR:HA	1:B:161:GLU:O	2.13	0.47
1:C:211:SER:HB3	1:C:329:LEU:HD13	1.96	0.47
1:B:555:GLU:OE2	1:B:567:LYS:NZ	2.40	0.47
1:C:91:GLU:HG3	1:C:128:ASP:CB	2.44	0.47
1:C:253:LYS:N	1:C:256:GLU:OE1	2.33	0.47
1:C:579:LEU:C	1:C:579:LEU:HD12	2.34	0.47
1:D:267:ILE:HD13	1:D:299:TRP:HA	1.95	0.47
1:A:420:ASP:CG	1:A:424:LYS:HE3	2.35	0.47
1:B:125:VAL:HG11	1:B:131:THR:HA	1.97	0.47
1:B:513:ASP:HB3	1:B:518:ARG:HG2	1.97	0.47
1:D:434:GLU:CD	1:D:434:GLU:H	2.18	0.47
1:B:443:CYS:O	1:B:451:MET:HA	2.14	0.47
1:B:448:TYR:N	1:B:449:PRO:HA	2.30	0.47
1:A:432:ILE:HD13	1:A:460:PRO:HG3	1.96	0.47
1:C:523:ILE:CD1	1:C:528:LEU:HB2	2.38	0.47

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:A:124:LEU:CD2	1:A:148:VAL:HB	2.45	0.46
1:B:16:TRP:CE3	1:B:117:PRO:HB3	2.50	0.46
1:D:344:LYS:HB3	1:D:355:TRP:HB2	1.98	0.46
1:A:99:MET:HB2	1:A:478:ARG:NH2	2.30	0.46
1:A:448:TYR:CE2	1:A:452:ALA:HB2	2.51	0.46
1:B:421:TYR:HB2	1:B:440:MET:HE3	1.96	0.46
1:A:96:PRO:O	1:A:97:THR:HB	2.14	0.46
1:D:451:MET:HG2	1:D:478:ARG:HG3	1.97	0.46
1:D:153:MET:SD	1:D:194:SER:HB3	2.56	0.46
1:B:448:TYR:CE2	1:B:452:ALA:HB2	2.50	0.46
1:B:505:LYS:NZ	1:B:531:ARG:CZ	2.79	0.46
1:C:25:ILE:HG23	1:D:190:GLU:HG3	1.98	0.46
1:A:146:ILE:HG22	1:A:244:ILE:HD13	1.98	0.45
1:C:523:ILE:HD11	1:C:528:LEU:CB	2.37	0.45
1:C:418:ILE:HD12	1:C:440:MET:CE	2.46	0.45
1:C:505:LYS:HD2	1:C:531:ARG:HD3	1.97	0.45
1:C:114:ARG:HD3	1:C:571:GLY:O	2.17	0.45
1:C:152:PRO:HD2	1:C:226:ILE:O	2.17	0.45
1:D:479:MET:HG2	1:D:489:LEU:HD11	1.97	0.45
1:D:183:GLN:OE1	1:D:183:GLN:HA	2.17	0.45
1:B:505:LYS:HE3	1:B:531:ARG:NE	2.32	0.45
1:C:23:ASP:OD1	1:C:579:LEU:HD11	2.17	0.45
1:D:276:SER:HB2	1:D:481:GLY:CA	2.46	0.45
1:B:132:PRO:O	1:B:136:MET:HG3	2.17	0.44
1:C:318:TYR:O	1:C:319:LEU:HD23	2.17	0.44
1:B:474:ILE:HG12	1:B:488:VAL:HB	1.99	0.44
1:C:440:MET:HB3	1:C:475:SER:HB3	1.99	0.44
1:D:480:SER:OG	4:D:603:2KT:H31	2.17	0.44
1:B:233:ARG:HA	1:B:233:ARG:HD3	1.75	0.44
1:C:317:LYS:HD3	1:C:318:TYR:CE1	2.51	0.44
1:C:107:LEU:C	1:C:107:LEU:HD23	2.38	0.44
1:D:129:KCX:C	1:D:132:PRO:HD2	2.47	0.44
1:B:415:PHE:CD1	1:B:421:TYR:HA	2.53	0.44
1:D:552:GLN:O	1:D:552:GLN:HG3	2.17	0.44
1:D:385:LEU:HD23	1:D:517:ARG:HA	2.00	0.44
1:A:124:LEU:HD22	1:A:148:VAL:HB	1.99	0.44
1:A:391:PRO:CD	1:A:500:PRO:HG2	2.47	0.44
1:B:113:ILE:CG2	1:B:143:LEU:HD12	2.48	0.44
1:C:409:LYS:HG3	1:C:511:GLU:HG2	1.98	0.43
1:A:521:LEU:HG	1:A:523:ILE:HG12	2.01	0.43
1:B:564:ASP:OD1	1:B:565:PHE:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:TRP:CE2	1:D:95:ARG:HD3	2.53	0.43
1:C:28:ARG:NH1	1:D:190:GLU:OE1	2.47	0.43
1:D:406:LEU:HD22	1:D:514:VAL:HG21	1.99	0.43
1:A:55:ASP:HB2	1:B:83:GLU:O	2.18	0.43
1:B:523:ILE:HG21	1:B:531:ARG:HH22	1.78	0.43
1:A:205:THR:O	1:A:209:MET:HG2	2.17	0.43
1:C:187:LEU:HD22	1:D:25:ILE:CD1	2.38	0.43
1:A:71:LYS:HG2	1:A:81:PRO:HB2	1.99	0.43
1:D:50:LEU:N	1:D:50:LEU:HD12	2.33	0.43
1:B:165:SER:HB2	1:B:201:ASN:H	1.84	0.43
1:A:414:VAL:HG21	1:A:504:VAL:HG12	2.00	0.43
1:D:479:MET:HG2	1:D:489:LEU:CD1	2.48	0.43
1:A:436:CYS:O	1:A:437:ILE:HD13	2.18	0.43
1:C:147:VAL:HB	1:C:219:ALA:HB2	2.00	0.43
1:D:19:GLY:O	1:D:28:ARG:NH2	2.48	0.43
1:A:99:MET:HG2	1:A:478:ARG:NE	2.33	0.42
1:B:33:ASN:OD1	1:B:34:GLN:HG2	2.19	0.42
1:B:217:GLY:O	1:B:349:VAL:HG22	2.19	0.42
1:D:208:THR:O	1:D:212:MET:HG2	2.19	0.42
1:A:425:ILE:HG23	1:A:426:ASN:N	2.33	0.42
1:C:492:SER:HA	1:C:493:PRO:C	2.39	0.42
1:A:261:GLN:CD	1:A:261:GLN:H	2.21	0.42
1:A:432:ILE:HD13	1:A:460:PRO:CG	2.50	0.42
1:A:16:TRP:CE2	1:B:95:ARG:HD3	2.55	0.42
1:B:448:TYR:HB3	1:B:449:PRO:C	2.39	0.42
1:C:448:TYR:CE2	1:C:452:ALA:HB2	2.54	0.42
1:A:23:ASP:OD2	1:A:23:ASP:N	2.52	0.42
1:D:415:PHE:CD2	1:D:457:MET:HE1	2.55	0.42
1:A:451:MET:CE	1:A:478:ARG:HG3	2.50	0.42
1:B:383:VAL:HG22	1:B:396:LEU:O	2.20	0.42
1:B:474:ILE:CD1	1:B:519:LEU:HD11	2.50	0.42
1:B:513:ASP:CG	1:B:516:ASN:HB2	2.40	0.42
1:A:53:TRP:HB2	1:A:63:LEU:HB2	2.01	0.42
1:A:87:PHE:CD1	1:A:105:ALA:HB2	2.55	0.42
1:A:226:ILE:HD11	1:A:236:MET:CE	2.49	0.42
1:A:354:VAL:O	1:A:358:VAL:HG22	2.19	0.42
1:B:18:GLY:O	1:B:24:VAL:HG21	2.19	0.42
1:B:87:PHE:CD1	1:B:105:ALA:HB2	2.55	0.42
1:B:523:ILE:CD1	1:B:528:LEU:HB2	2.49	0.42
1:D:77:ALA:HB2	1:D:242:ARG:HA	2.02	0.42
1:C:247:MET:O	1:C:251:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG21	1:A:244:ILE:HG21	2.01	0.42
1:B:296:LEU:O	1:B:384:VAL:HG21	2.20	0.42
1:D:116:GLN:HB3	1:D:117:PRO:HD2	2.01	0.42
1:C:82:LEU:CD2	1:D:55:ASP:HB3	2.50	0.41
1:C:308:THR:OG1	1:C:380:GLY:HA3	2.20	0.41
1:D:437:ILE:HD12	1:D:510:ILE:HB	2.02	0.41
1:D:165:SER:HB2	1:D:200:CYS:HB3	2.02	0.41
1:D:211:SER:HA	1:D:329:LEU:HD22	2.01	0.41
1:A:31:LEU:HD23	1:A:41:PHE:HE2	1.86	0.41
1:B:331:VAL:HG22	1:B:361:VAL:HG23	2.01	0.41
1:C:303:GLY:O	1:C:381:GLY:HA3	2.21	0.41
1:A:116:GLN:HB3	1:A:117:PRO:HD2	2.03	0.41
1:B:239:LEU:HD23	1:B:239:LEU:HA	1.88	0.41
1:A:257:ILE:HG23	1:A:347:LEU:O	2.20	0.41
1:B:325:TYR:OH	1:D:195:ARG:NH2	2.50	0.41
1:C:16:TRP:CH2	1:C:574:VAL:HG13	2.56	0.41
1:C:176:VAL:HG22	1:C:181:MET:O	2.20	0.41
1:C:446:LYS:HE2	1:C:554:VAL:HG12	2.03	0.41
1:C:530:ARG:HG3	1:C:531:ARG:N	2.36	0.41
1:A:16:TRP:CE3	1:A:117:PRO:HB3	2.55	0.41
1:B:421:TYR:HB3	1:B:440:MET:HE1	2.02	0.41
1:D:227:PRO:HD3	1:D:324:PHE:CD2	2.56	0.41
1:A:296:LEU:HD23	1:A:296:LEU:HA	1.70	0.41
1:A:317:LYS:HD3	1:A:318:TYR:CZ	2.55	0.41
1:B:479:MET:HG2	1:B:489:LEU:HD11	2.03	0.41
1:C:421:TYR:OH	1:C:458:GLY:N	2.54	0.41
1:B:342:LEU:HD23	1:B:344:LYS:HG2	2.02	0.41
1:C:541:LEU:HD23	1:C:541:LEU:HA	1.88	0.41
1:A:190:GLU:OE1	1:B:28:ARG:NH1	2.54	0.41
1:A:448:TYR:O	1:B:576:LYS:HE3	2.20	0.41
1:B:146:ILE:CD1	1:B:240:THR:HG23	2.46	0.41
1:B:273:ILE:HA	1:B:310:VAL:HB	2.02	0.41
1:B:383:VAL:O	1:B:395:VAL:HA	2.21	0.41
1:B:514:VAL:HB	1:B:515:PRO:HD3	2.02	0.41
1:C:72:ALA:O	1:C:76:GLU:HG3	2.21	0.41
1:C:312:LEU:HD22	1:C:319:LEU:N	2.36	0.41
1:C:169:LEU:O	1:C:173:SER:OG	2.36	0.41
1:C:579:LEU:HD12	1:C:579:LEU:O	2.20	0.41
1:A:51:ASN:OD1	1:A:63:LEU:HB3	2.20	0.40
1:A:190:GLU:HB3	5:A:708:HOH:O	2.20	0.40
1:A:292:ILE:HD13	1:A:292:ILE:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:N	1:A:330:PRO:CD	2.85	0.40
1:B:53:TRP:CZ2	1:B:64:ARG:CZ	3.04	0.40
1:B:526:GLU:O	1:B:529:ALA:HB3	2.21	0.40
1:C:373:GLU:HG2	1:C:374:LYS:HG2	2.03	0.40
1:C:484:TYR:CD1	1:C:484:TYR:N	2.89	0.40
1:A:334:LYS:NZ	1:A:361:VAL:O	2.51	0.40
1:B:413:VAL:HG21	1:B:432:ILE:HD12	2.03	0.40
1:C:166:GLY:O	1:C:169:LEU:HB2	2.21	0.40
1:C:50:LEU:HD12	1:C:123:LEU:CD2	2.51	0.40
1:A:177:LYS:HE3	1:A:464:LEU:CD1	2.50	0.40
1:A:403:PRO:HA	1:A:406:LEU:HD11	2.04	0.40
1:A:411:ARG:NH1	1:A:431:ASP:O	2.55	0.40
1:D:432:ILE:HD13	1:D:460:PRO:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	573/588 (97%)	553 (96%)	17 (3%)	3 (0%)	25	30
1	B	572/588 (97%)	546 (96%)	24 (4%)	2 (0%)	37	44
1	C	573/588 (97%)	553 (96%)	18 (3%)	2 (0%)	37	44
1	D	572/588 (97%)	550 (96%)	19 (3%)	3 (0%)	25	30
All	All	2290/2352 (97%)	2202 (96%)	78 (3%)	10 (0%)	30	36

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	128	ASP
1	D	128	ASP

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Mol	Chain	Res	Type
1	A	128	ASP
1	B	128	ASP
1	D	54	SER
1	A	97	THR
1	D	126	GLY
1	A	126	GLY
1	C	126	GLY
1	B	126	GLY

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	461/473 (98%)	454 (98%)	7 (2%)	60	73
1	B	460/473 (97%)	454 (99%)	6 (1%)	65	77
1	C	461/473 (98%)	455 (99%)	6 (1%)	65	77
1	D	460/473 (97%)	453 (98%)	7 (2%)	60	73
All	All	1842/1892 (97%)	1816 (99%)	26 (1%)	62	75

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	23	ASP
1	A	54	SER
1	A	127	CYS
1	A	186	PHE
1	A	195	ARG
1	A	196	SER
1	B	127	CYS
1	B	186	PHE
1	B	304	ARG
1	B	428	ASP
1	B	518	ARG
1	B	579	LEU

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Mol	Chain	Res	Type
1	C	91	GLU
1	C	186	PHE
1	C	195	ARG
1	C	205	THR
1	C	236	MET
1	C	525	ASP
1	D	22	ARG
1	D	99	MET
1	D	107	LEU
1	D	186	PHE
1	D	359	LYS
1	D	417	ASP
1	D	579	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	490	HIS
1	C	516	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	KCX	A	129	2,1	9,11,12	0.79	0	5,12,14	2.87	2 (40%)
1	KCX	B	129	2,1	9,11,12	0.85	1 (11%)	5,12,14	1.61	1 (20%)
1	KCX	C	129	2,1	9,11,12	0.90	0	5,12,14	1.80	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	KCX	D	129	2,1	9,11,12	1.10	1 (11%)	5,12,14	2.12	2 (40%)

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	KCX	A	129	2,1	-	3/9/10/12	-
1	KCX	B	129	2,1	-	5/9/10/12	-
1	KCX	C	129	2,1	-	1/9/10/12	-
1	KCX	D	129	2,1	-	5/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	KCX	OQ1-CX	2.14	1.25	1.21
1	B	129	KCX	OQ1-CX	2.01	1.25	1.21

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	KCX	OQ1-CX-NZ	-4.44	118.07	124.96
1	A	129	KCX	CD-CE-NZ	-4.32	99.86	112.21
1	D	129	KCX	OQ1-CX-NZ	-3.95	118.84	124.96
1	C	129	KCX	OQ1-CX-NZ	-3.30	119.84	124.96
1	B	129	KCX	CD-CE-NZ	-2.87	104.00	112.21
1	D	129	KCX	CD-CE-NZ	-2.40	105.36	112.21
1	C	129	KCX	CE-NZ-CX	-2.26	118.25	121.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	129	KCX	C-CA-CB-CG
1	B	129	KCX	C-CA-CB-CG
1	D	129	KCX	C-CA-CB-CG
1	D	129	KCX	CG-CD-CE-NZ
1	B	129	KCX	CG-CD-CE-NZ
1	B	129	KCX	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
1	D	129	KCX	CA-CB-CG-CD
1	A	129	KCX	CA-CB-CG-CD
1	A	129	KCX	CG-CD-CE-NZ
1	B	129	KCX	CE-CD-CG-CB
1	B	129	KCX	N-CA-CB-CG
1	D	129	KCX	CE-CD-CG-CB
1	C	129	KCX	CA-CB-CG-CD
1	D	129	KCX	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	129	KCX	1	0
1	D	129	KCX	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	FES	C	602	5,1	0,4,4	-	-	-		
3	FES	D	602	1	0,4,4	-	-	-		
3	FES	A	602	5,1	0,4,4	-	-	-		
3	FES	B	602	5,1	0,4,4	-	-	-		
4	2KT	D	603	2	6,6,6	1.90	3 (50%)	7,7,7	1.53	2 (28%)

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	FES	C	602	5,1	-	-	0/1/1/1
3	FES	D	602	1	-	-	0/1/1/1
3	FES	A	602	5,1	-	-	0/1/1/1
3	FES	B	602	5,1	-	-	0/1/1/1
4	2KT	D	603	2	-	1/6/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	603	2KT	C2-C	2.91	1.57	1.53
4	D	603	2KT	O-C	2.58	1.29	1.22
4	D	603	2KT	C3-C2	2.27	1.55	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	603	2KT	C3-C2-C	2.67	121.32	116.25
4	D	603	2KT	OXT-C-O	-2.22	118.54	123.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	603	2KT	OXT-C-C2-C3

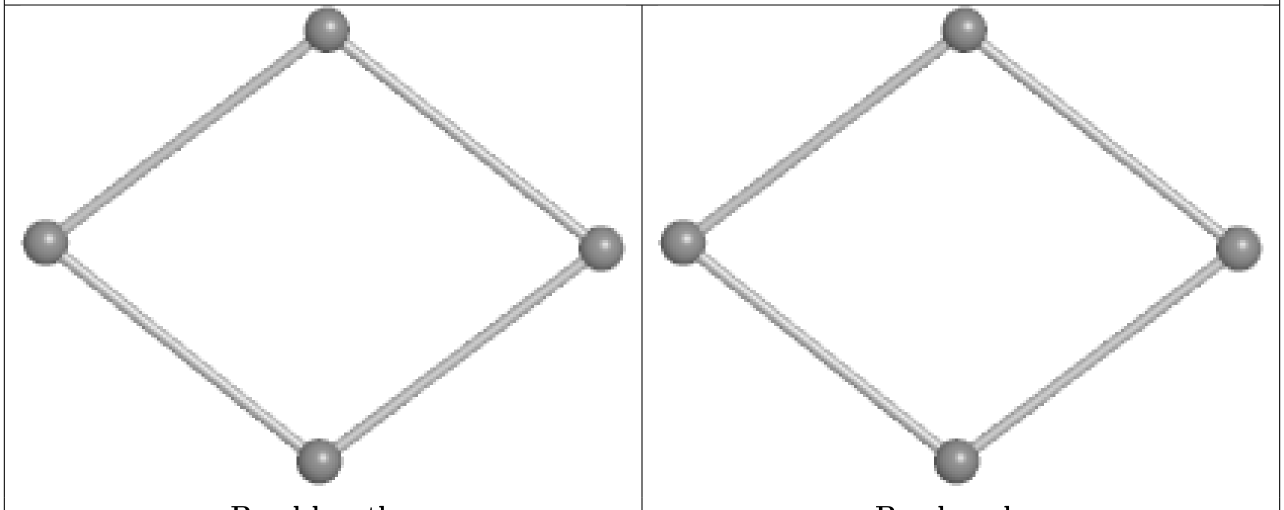
There are no ring outliers.

2 monomers are involved in 2 short contacts:

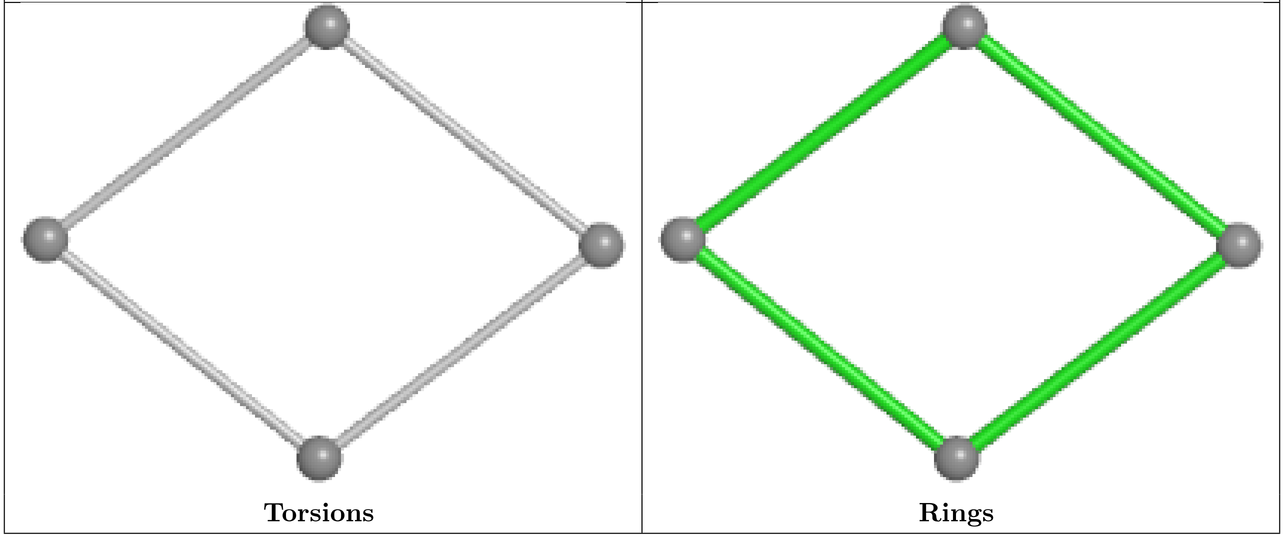
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	FES	1	0
4	D	603	2KT	1	0

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 FES C 602

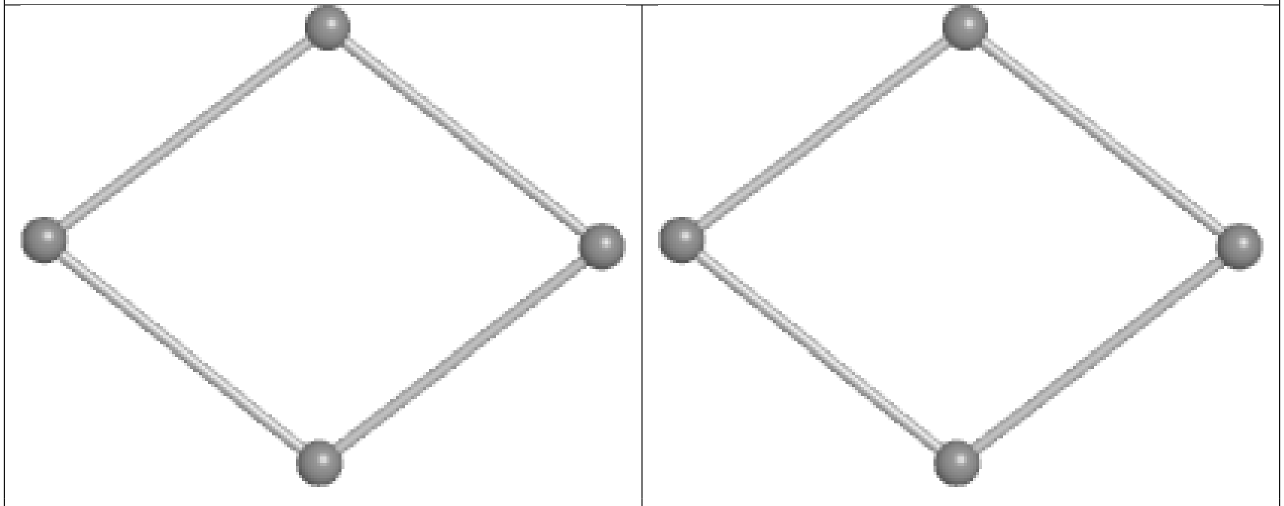


Bond lengths **Bond angles**



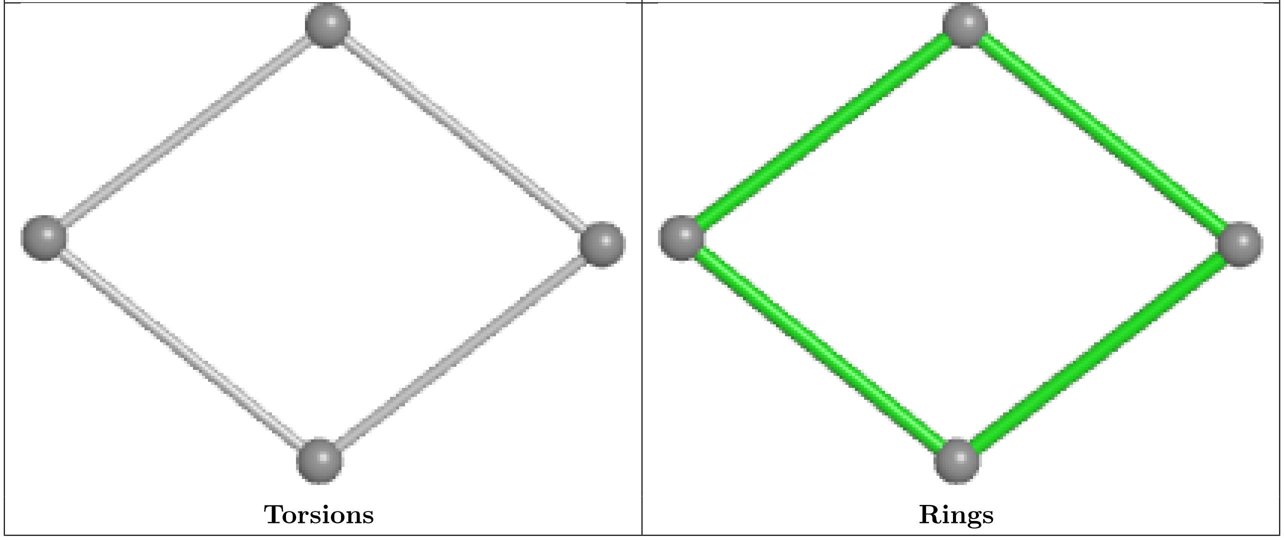
Torsions **Rings**

Ligand FES D 602



Bond lengths

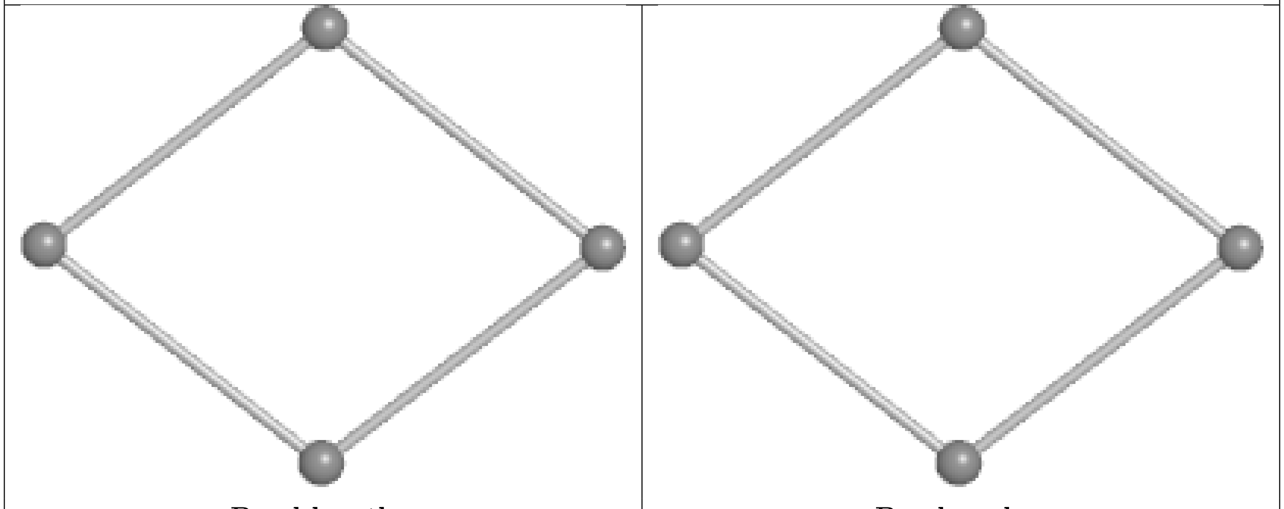
Bond angles



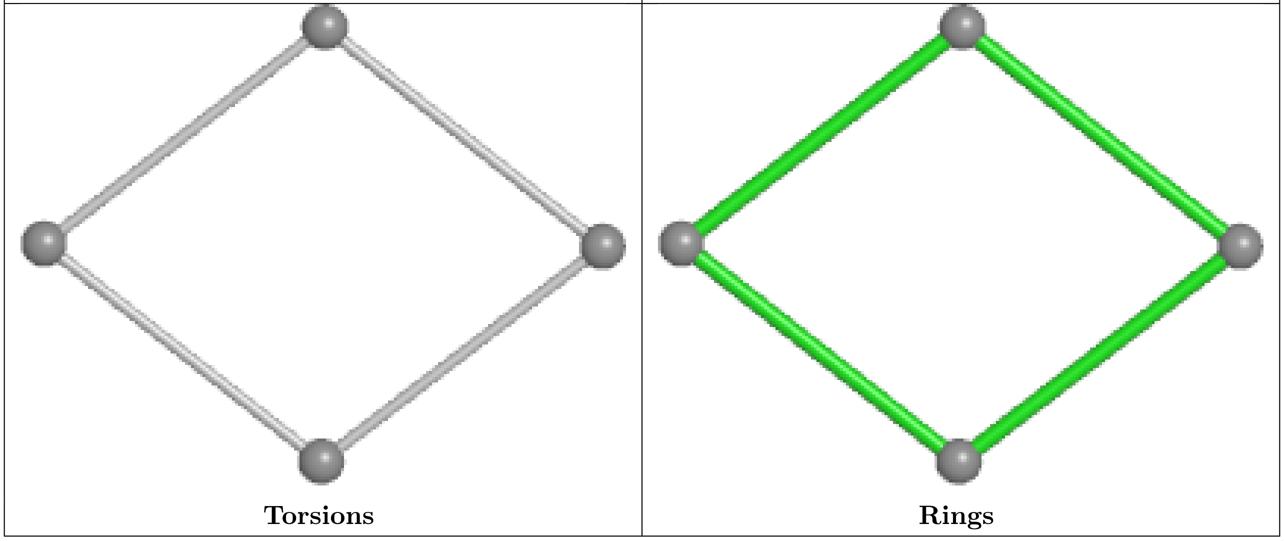
Torsions

Rings

Ligand FES A 602

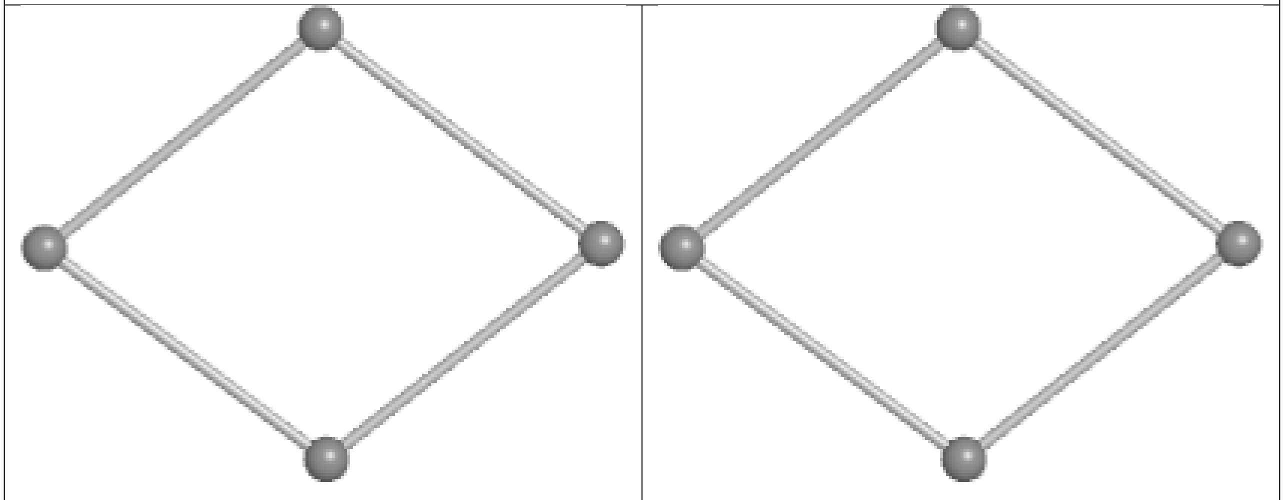


Bond lengths **Bond angles**



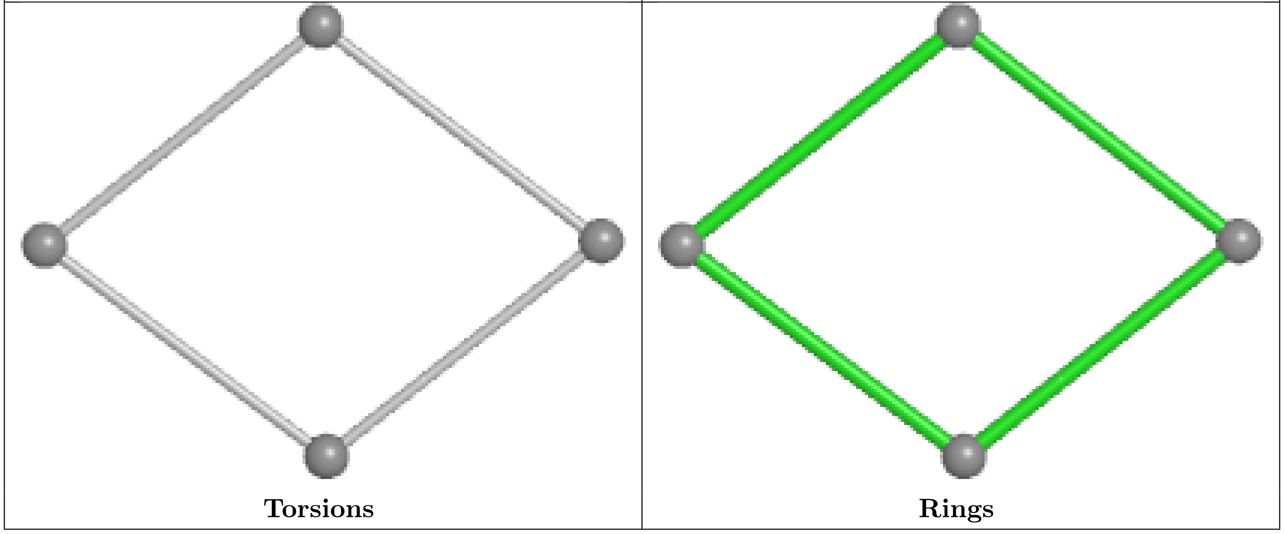
Torsions **Rings**

Ligand FES B 602



Bond lengths

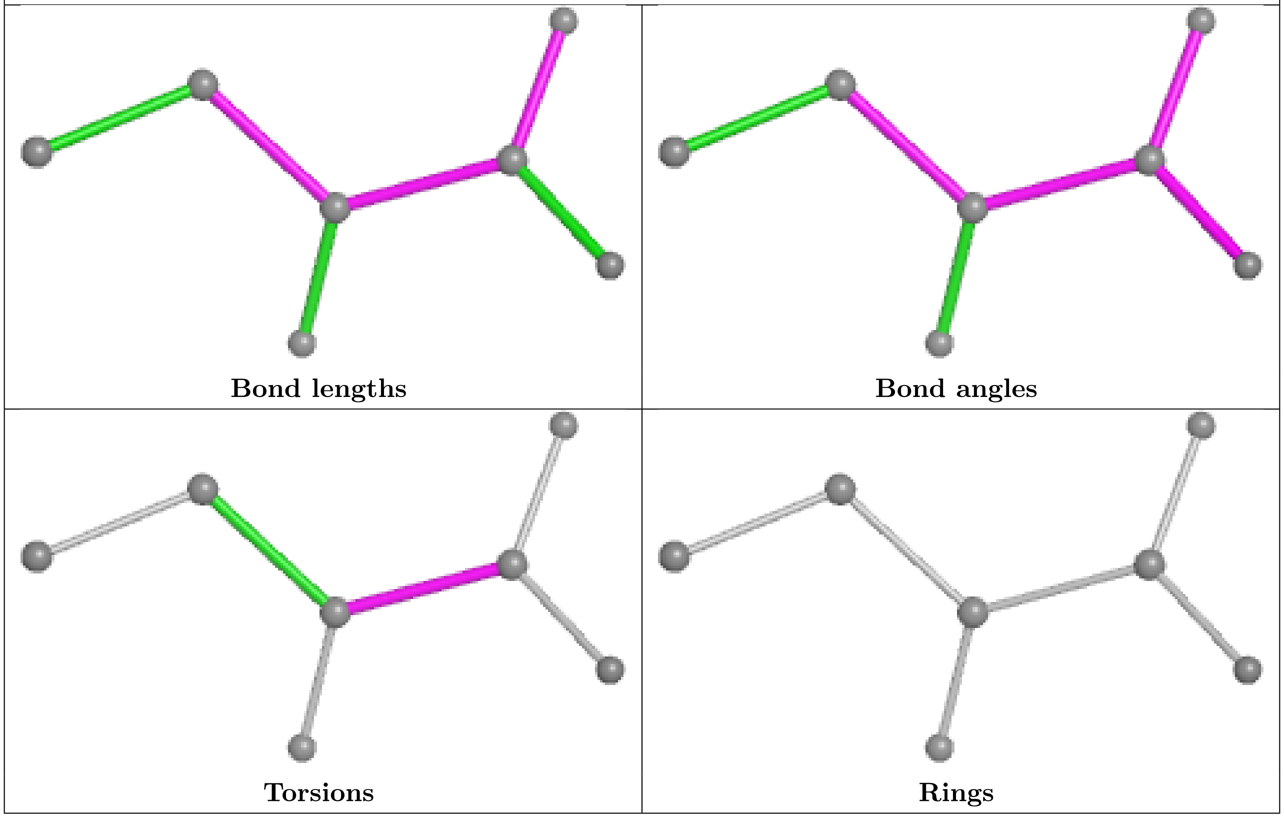
Bond angles



Torsions

Rings

Ligand 2KT D 603



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(Å^2)	Q<0.9
1	A	574/588 (97%)	-0.28	2 (0%)	90	91	31, 41, 55, 90	1 (0%)
1	B	574/588 (97%)	-0.24	1 (0%)	92	93	28, 40, 62, 97	0
1	C	574/588 (97%)	-0.18	2 (0%)	90	91	23, 40, 64, 98	1 (0%)
1	D	574/588 (97%)	-0.34	0	100	100	29, 39, 51, 65	0
All	All	2296/2352 (97%)	-0.26	5 (0%)	92	93	23, 40, 60, 98	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	540	ASP	3.1
1	B	539	HIS	2.7
1	A	579	LEU	2.4
1	C	539	HIS	2.1
1	A	539	HIS	2.1

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(Å^2)	Q<0.9
1	KCX	A	129	12/13	0.92	0.09	27,37,44,45	0
1	KCX	B	129	12/13	0.92	0.08	31,36,42,46	0
1	KCX	D	129	12/13	0.92	0.09	31,38,42,42	0
1	KCX	C	129	12/13	0.94	0.07	31,38,42,42	0

6.3 Carbohydrates ⓘ

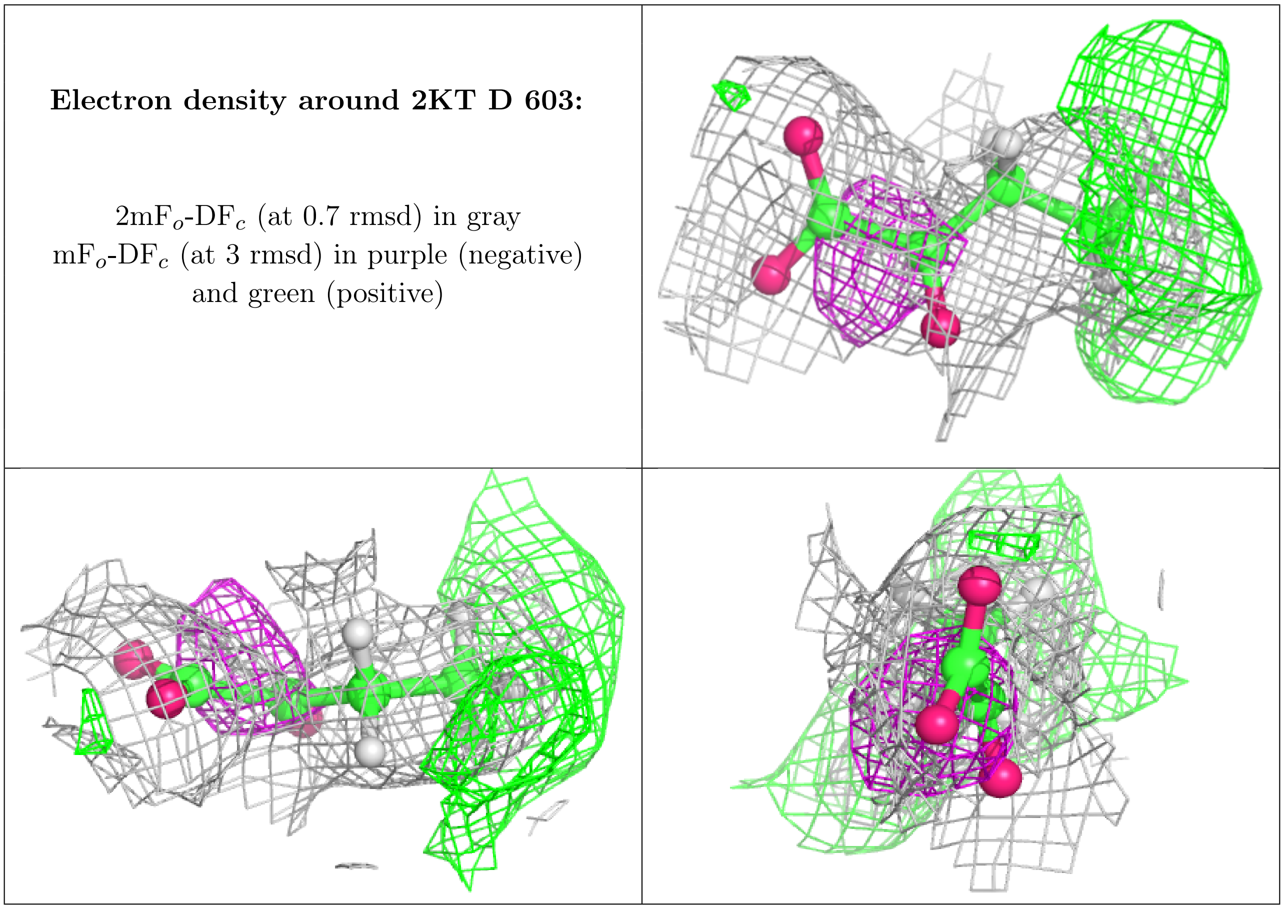
There are no monosaccharides in this entry.

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, 95^{th} 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^2)	Q<0.9
4	2KT	D	603	7/7	0.68	0.17	32,48,58,58	0
2	MG	B	601	1/1	0.90	0.06	40,40,40,40	0
3	FES	D	602	4/4	0.96	0.06	34,38,39,42	0
3	FES	B	602	4/4	0.97	0.05	38,40,44,45	4
3	FES	C	602	4/4	0.97	0.05	39,42,43,44	4
2	MG	A	601	1/1	0.97	0.04	40,40,40,40	0
2	MG	C	601	1/1	0.97	0.04	41,41,41,41	0
2	MG	D	601	1/1	0.98	0.03	33,33,33,33	0
3	FES	A	602	4/4	0.98	0.04	36,37,40,42	4

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.

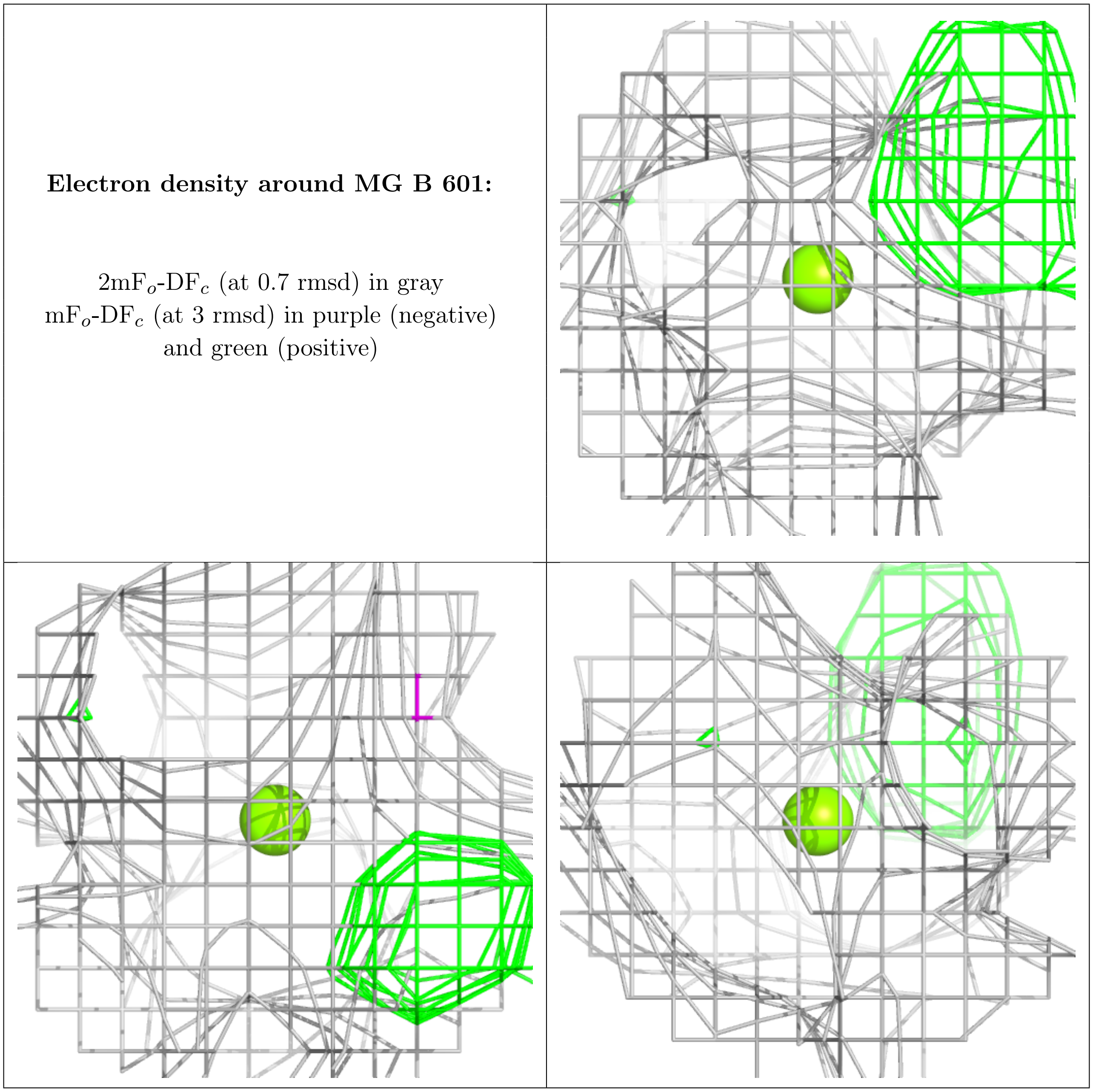


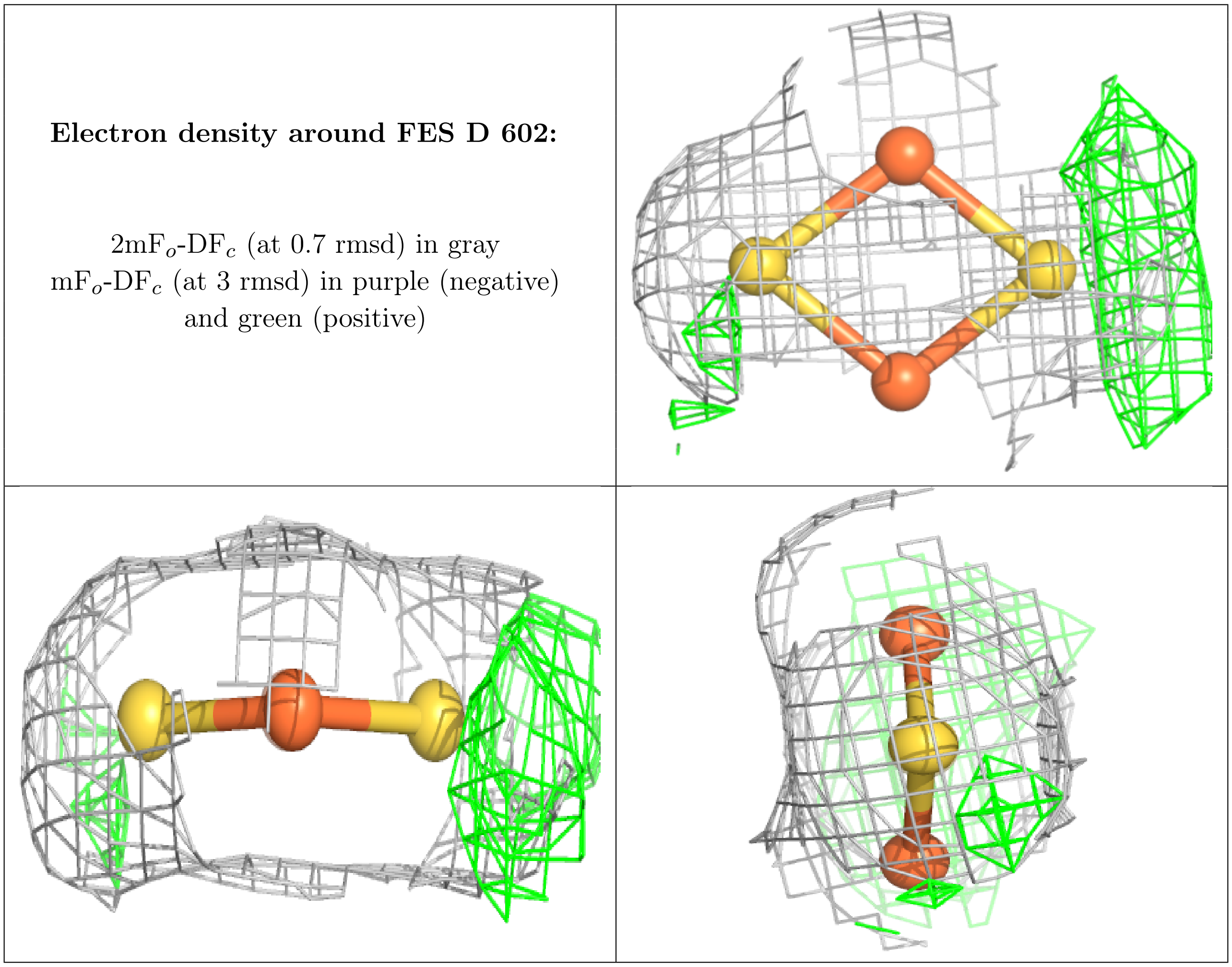
Electron density around 2KT D 603:

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

Electron density around MG 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)



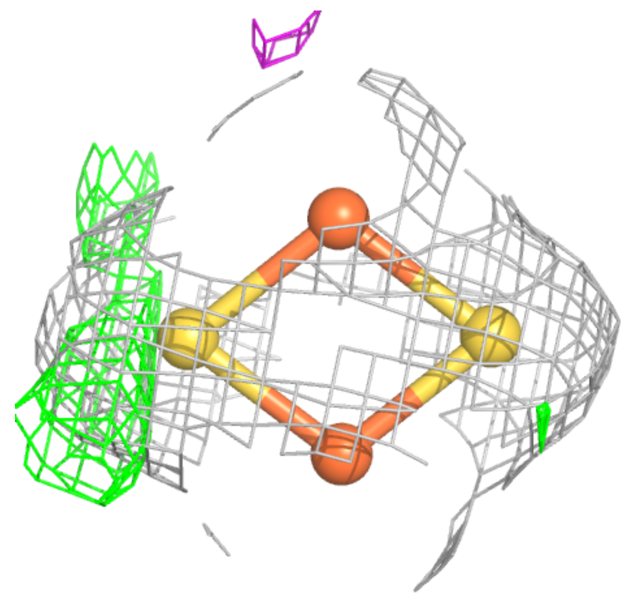


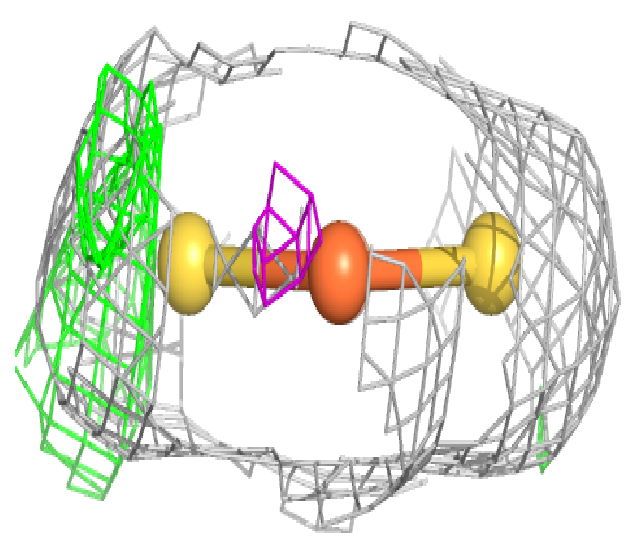
Electron density around FES D 602:

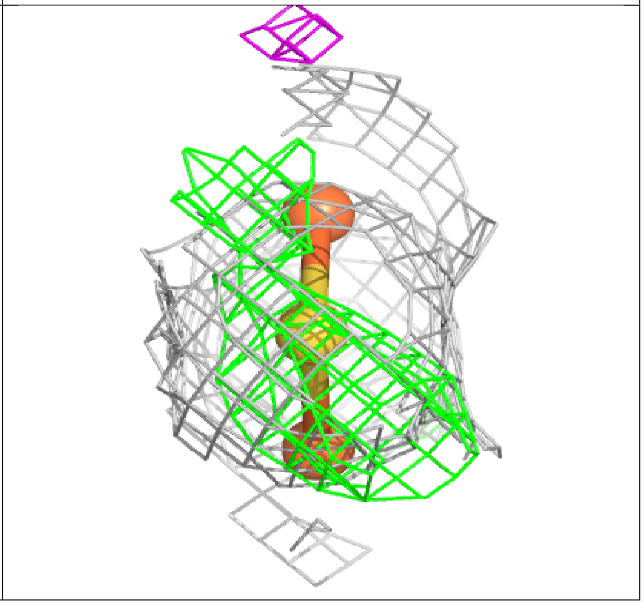
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FES B 602:

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







Electron density around FES C 602:

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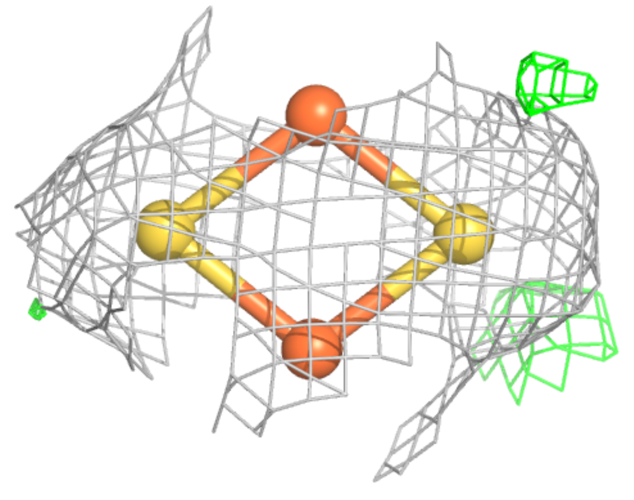
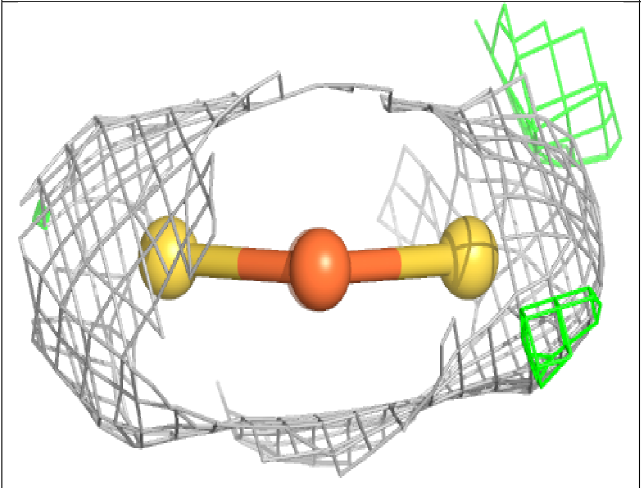
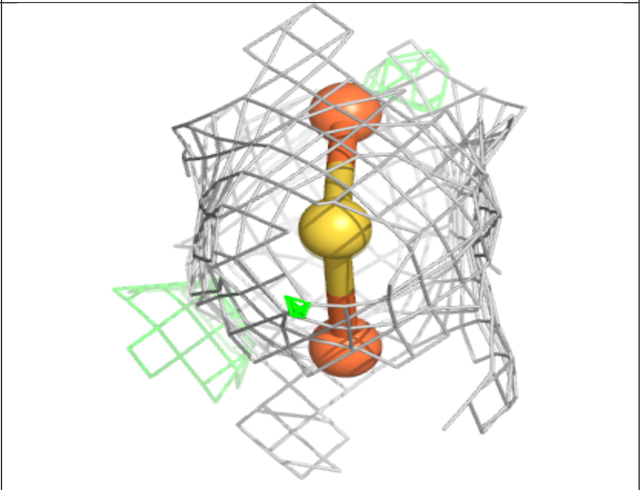
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around MG A 601:

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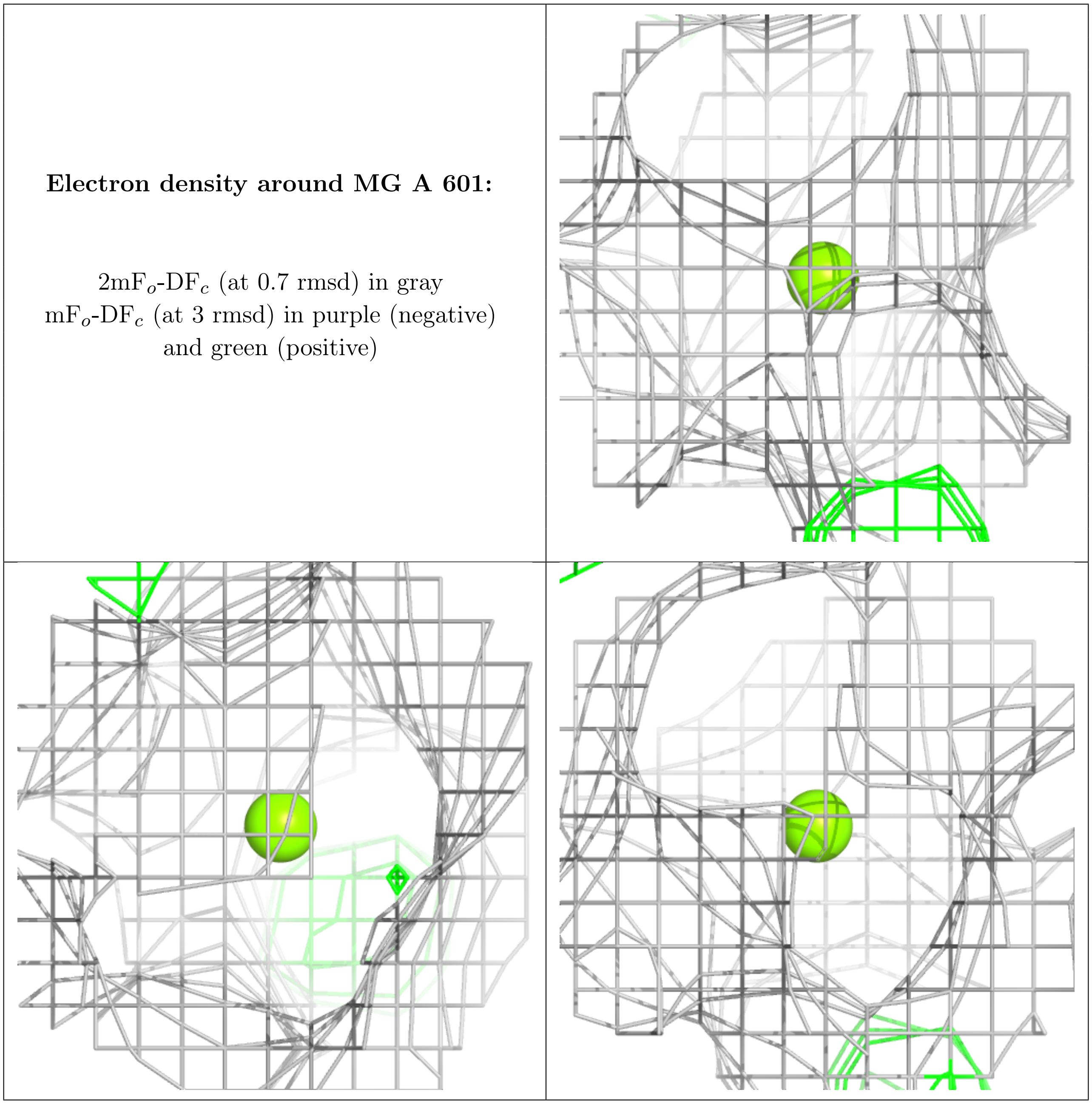
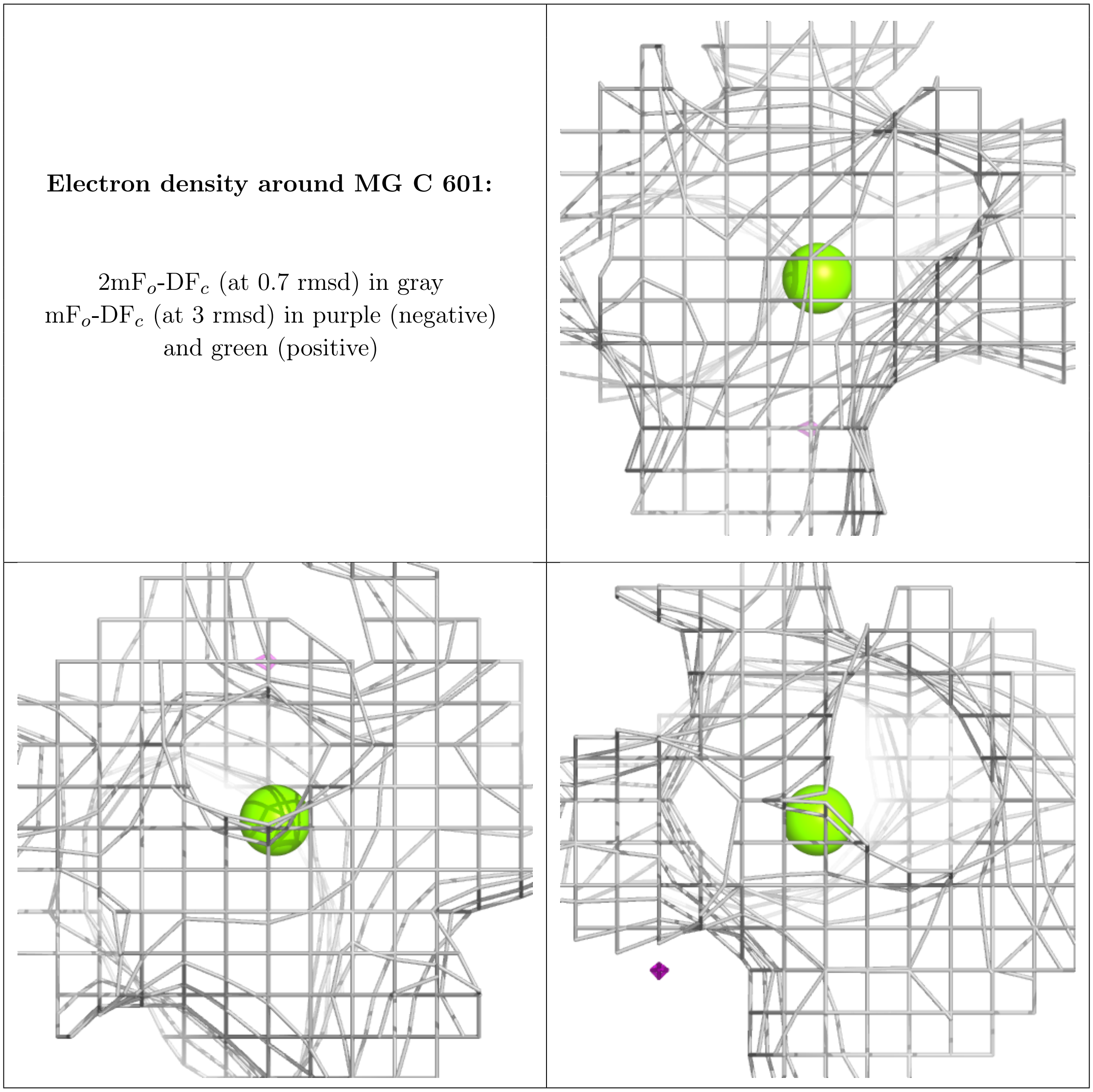
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around MG C 601:

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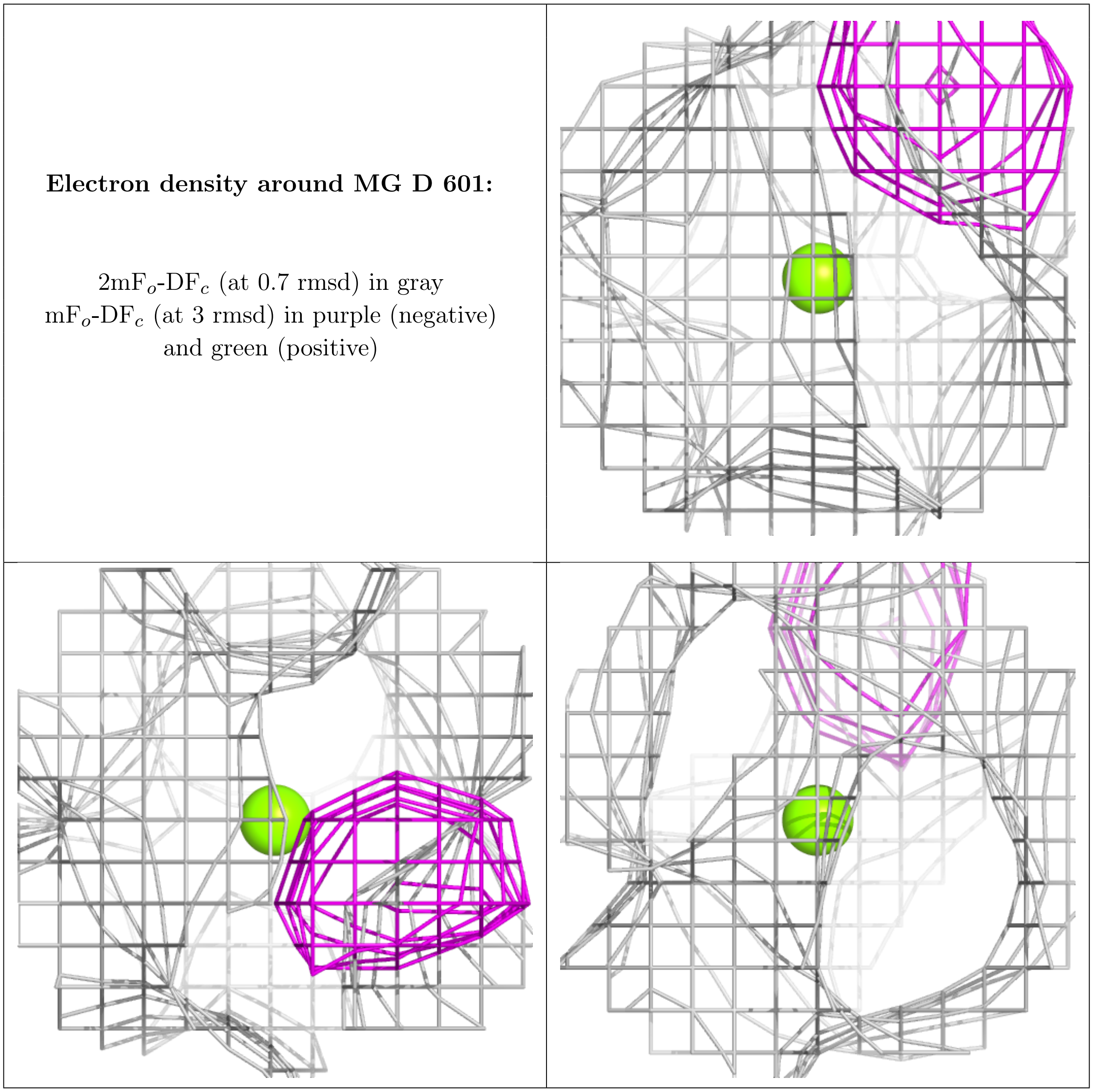
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG D 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 FES A 602:

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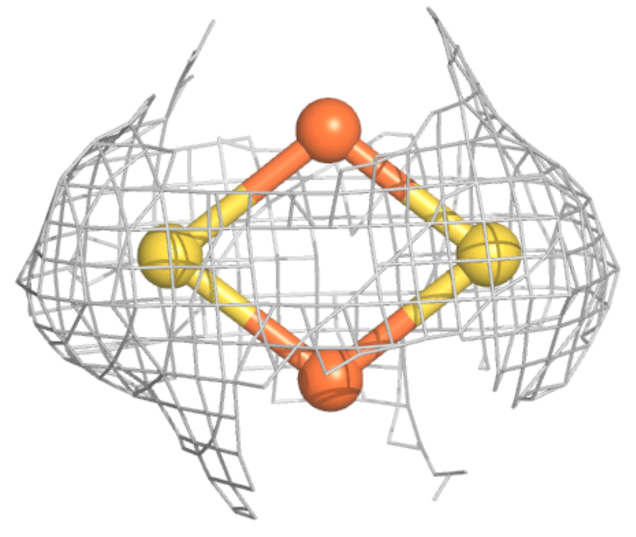
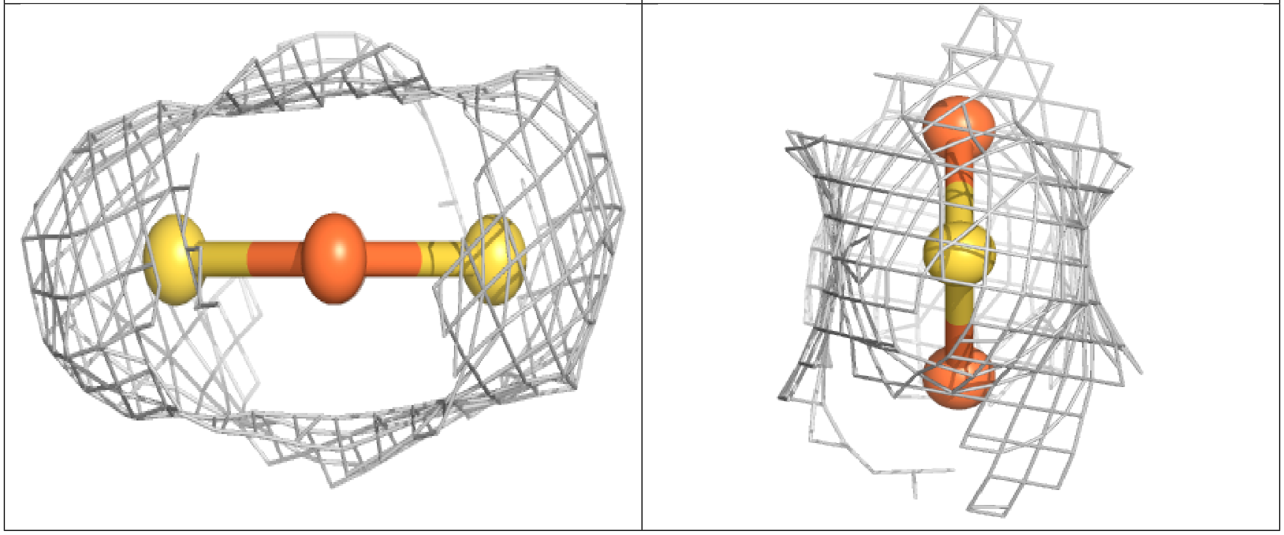
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.