Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2026 – 06:31 PM JST

PDB ID	:	9UIX / pdb_00009uix
Title	:	Plasmodium vivax cytoplasmic Phenylalanyl-tRNA synthetase in complex with Phenylalanine in space group P212121
Authors	:	Mutharasappan, N.; Manickam, Y.; Sharma, A.
Deposited on	:	2025-04-16
Resolution	:	3.26 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*
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:

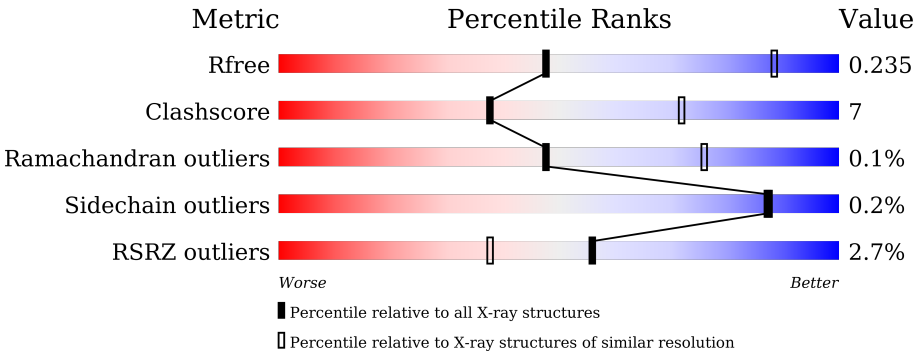
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.26 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	304	83% 16%
1	C	304	79% 20%
2	B	618	84% 15%
3	D	618	5% 83% 17%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14991 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 Phenylalanine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2506	1619	422	454	11			
1	C	304	Total	C	N	O	S	0	0	0
			2519	1627	425	456	11			

- Molecule 2 is a protein called Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	616	Total	C	N	O	S	0	0	0
			4956	3173	805	946	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP A5K464
B	1	GLY	-	expression tag	UNP A5K464

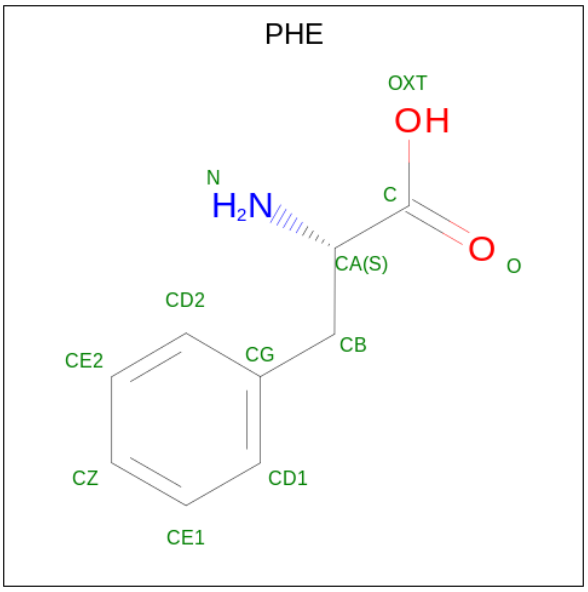
- Molecule 3 is a protein called Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	616	Total	C	N	O	S	0	0	0
			4928	3159	799	938	32			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP A5K464
D	1	GLY	-	expression tag	UNP A5K464

- Molecule 4 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 12 9 1 2	0	0
4	C	1	Total C N O 12 9 1 2	0	0

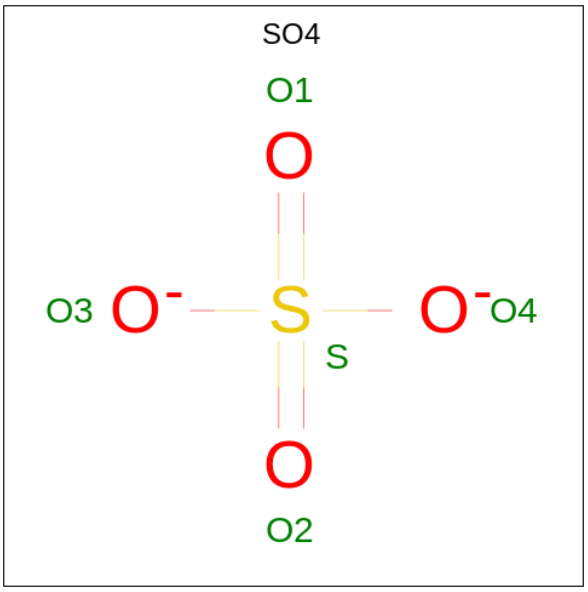
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

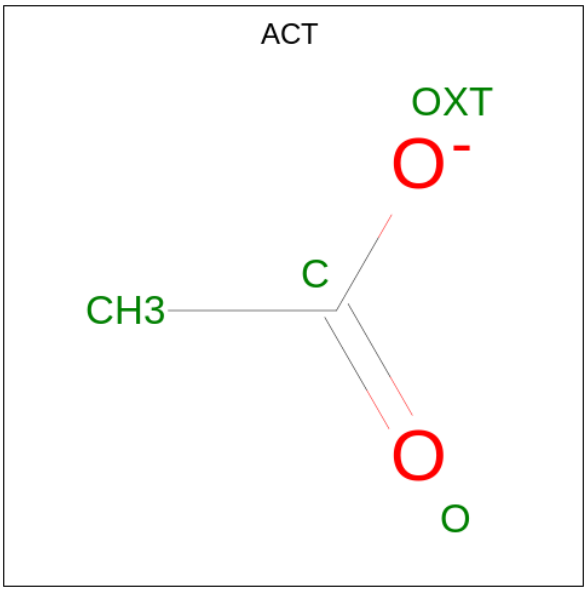
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	0	0
6	D	1	Total Mg 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 2 2	0	0

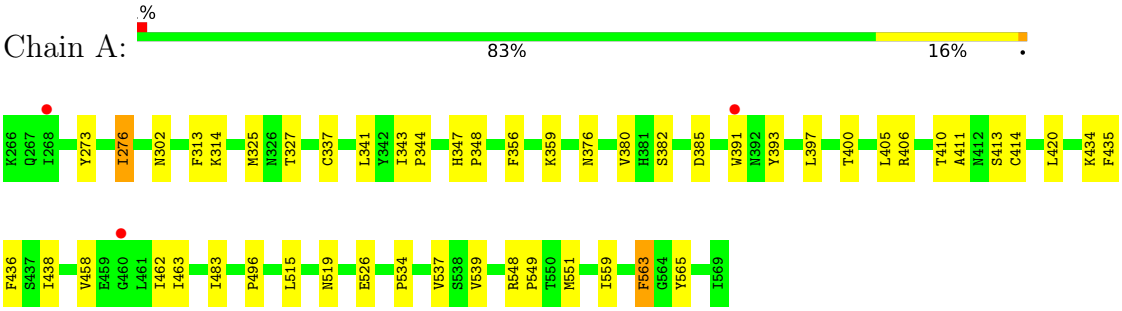
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	8	Total O 9 9	0	1
9	B	8	Total O 8 8	0	0
9	C	9	Total O 10 10	0	1
9	D	10	Total O 13 13	0	3

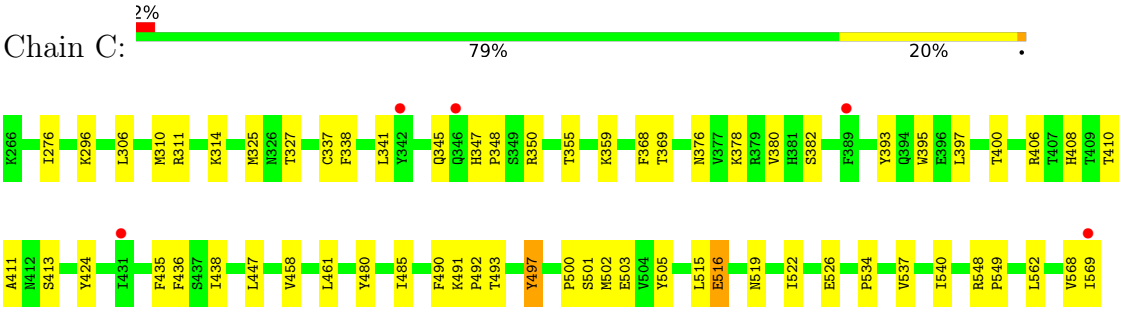
3 Residue-property plots (i)

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.

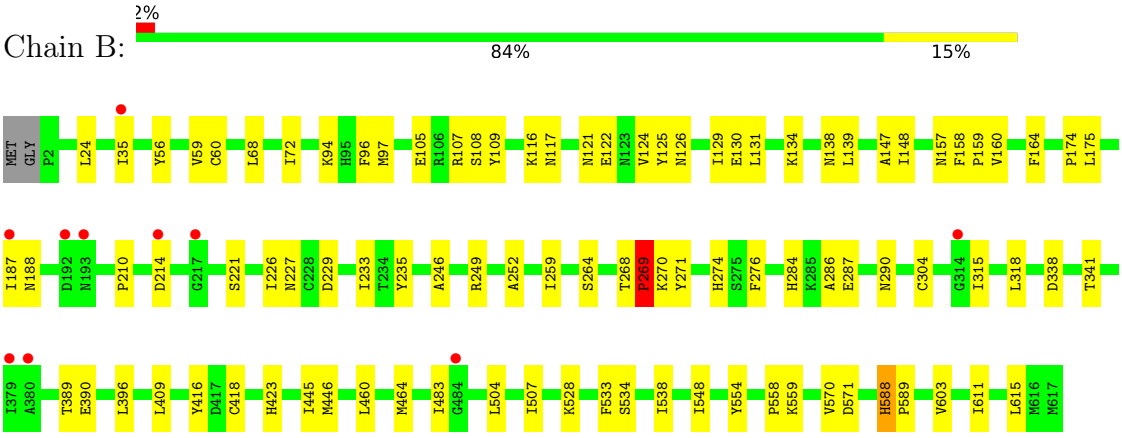
• Molecule 1: Phenylalanine–tRNA ligase alpha subunit



• Molecule 1: Phenylalanine–tRNA ligase alpha subunit

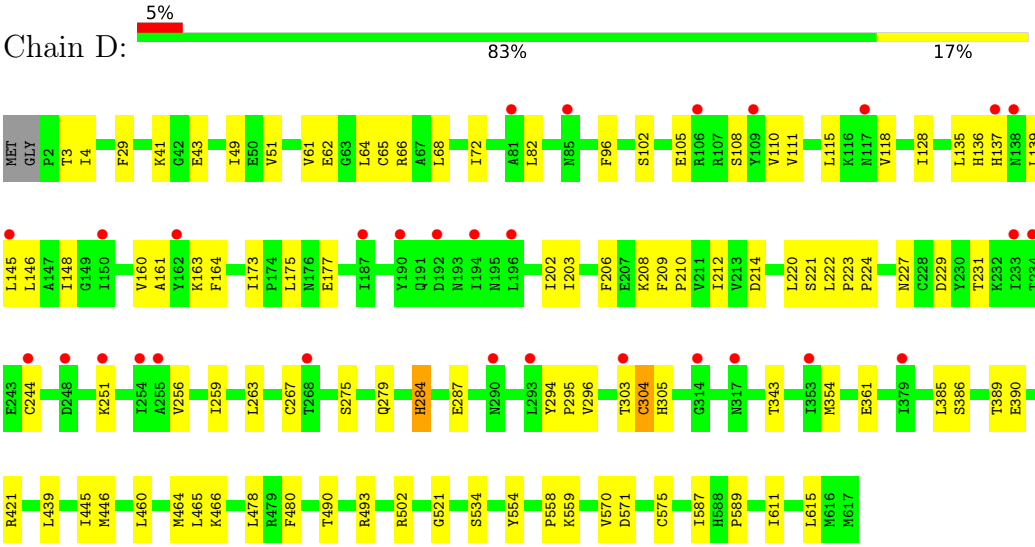


• Molecule 2: Phenylalanine–tRNA ligase beta subunit



• Molecule 3: Phenylalanine–tRNA ligase beta subunit

Chain D:


5%
83%
17%
MET GLY P2 T3 I4 F29 K41 G42 E43 I49 E50 V51 V61 E62 G63 L64 C65 R66 A67 L68 I72 A81 L82 N85 F96 S102 E105 R106 R107 S108 Y109 V110 V111 L115 K116 N117 V118 I128 L135 H136 H137 N138 L139 G140 R143 I144
L145 L146 A147 I148 G149 I150 V160 A161 Y162 K163 F164 I173 P174 L175 N176 E177 I187 Y190 Q191 D192 N193 I194 N195 L196 I202 I203 F206 E207 K208 F209 P210 V211 I212 V213 D214 L220 S221 L222 P223 P224 N227 C228 D229 Y230 T231 K232 I233 T234 T237 I242
E243 C244 D248 K251 I254 A255 V256 I259 L263 C267 T268 S275 Q279 H284 E287 N290 L293 Y294 P295 V296 T303 C304 H305 G314 N317 T343 I353 M354 E361 I379 L385 S386 T389 E390 T402 L409
R421 L439 I445 M446 L460 M464 L465 K466 L478 R479 F480 T490 R493 R502 G521 S534 Y554 P558 K559 V570 D571 C575 I587 H588 P589 I611 L615 M616 M617

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.37Å 157.10Å 190.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.95 – 3.26 110.95 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.0 (110.95-3.26) 99.1 (110.95-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.26Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.221 , 0.246 0.211 , 0.235	Depositor DCC
R_{free} test set	3149 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	103.7	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 94.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14991	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4, ZN, ACT, MG, CME

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	0.25	0/2574	0.37	0/3475
1	C	0.31	0/2587	0.40	1/3491 (0.0%)
2	B	0.27	0/5029	0.37	3/6801 (0.0%)
3	D	0.26	0/5001	0.41	3/6763 (0.0%)
All	All	0.27	0/15191	0.39	7/20530 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	41	LYS	N-CA-C	-7.57	96.18	108.52
3	D	284	HIS	N-CA-C	-6.62	100.09	109.96
2	B	588	HIS	CA-C-N	6.51	126.27	119.05
2	B	588	HIS	C-N-CA	6.51	126.27	119.05
1	C	516	GLU	N-CA-C	-6.39	98.76	108.67
2	B	269	PRO	N-CA-C	-6.19	99.72	112.47
3	D	137	HIS	N-CA-C	5.04	116.47	111.07

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	2506	0	2434	37	0
1	C	2519	0	2458	44	0
2	B	4956	0	4888	65	0
3	D	4928	0	4839	71	0
4	A	12	0	8	1	0
4	C	12	0	8	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	B	4	0	3	0	0
9	A	9	0	0	0	0
9	B	8	0	0	0	0
9	C	10	0	0	1	0
9	D	13	0	0	0	0
All	All	14991	0	14638	206	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 7.

All (206) 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:408:HIS:CE1	1:C:410:THR:HB	2.03	0.93
1:A:276:ILE:HG23	2:B:589:PRO:HB3	1.60	0.84
2:B:389:THR:HG23	2:B:483:ILE:CD1	2.09	0.83
3:D:389:THR:HG21	3:D:502:ARG:HH11	1.43	0.83
3:D:82:LEU:HD22	3:D:295:PRO:HG2	1.60	0.82
3:D:136:HIS:HB3	3:D:143:ARG:HG2	1.61	0.82
3:D:284:HIS:HB3	3:D:287:GLU:O	1.80	0.82
3:D:62:GLU:O	3:D:66:ARG:HG3	1.82	0.79
1:C:408:HIS:ND1	1:C:410:THR:HB	2.01	0.76
3:D:139:LEU:HD12	3:D:139:LEU:O	1.86	0.74
3:D:164:PHE:HB3	3:D:208:LYS:HB2	1.70	0.73
2:B:389:THR:HG23	2:B:483:ILE:HD11	1.72	0.72
2:B:268:THR:CB	2:B:269:PRO:HD3	2.19	0.72
3:D:163:LYS:O	3:D:210:PRO:HA	1.90	0.72
3:D:139:LEU:HG	3:D:146:LEU:HD21	1.73	0.69
3:D:139:LEU:HD11	3:D:251:LYS:HD2	1.74	0.68
3:D:275:SER:HA	3:D:295:PRO:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ASN:HB3	4:C:601:PHE:HB3	1.77	0.67
1:C:276:ILE:HG23	3:D:589:PRO:HB3	1.77	0.66
1:A:519:ASN:HB3	4:A:601:PHE:HB3	1.77	0.66
3:D:82:LEU:CD2	3:D:295:PRO:HG2	2.27	0.65
2:B:446:MET:HE3	1:C:359:LYS:HA	1.79	0.64
2:B:148:ILE:HD13	2:B:259:ILE:HD11	1.79	0.64
1:A:438:ILE:HG12	1:A:458:VAL:HG13	1.80	0.64
1:C:516:GLU:O	1:C:516:GLU:HG3	1.99	0.63
3:D:43:GLU:O	3:D:43:GLU:HG3	1.99	0.62
3:D:202:ILE:HG22	3:D:203:ILE:HG23	1.81	0.62
3:D:296:VAL:HG12	3:D:296:VAL:O	2.00	0.61
3:D:82:LEU:HD22	3:D:295:PRO:CG	2.31	0.61
3:D:139:LEU:HD12	3:D:139:LEU:C	2.25	0.59
1:C:337:CYS:HA	1:C:411:ALA:HB2	1.85	0.59
1:C:500:PRO:HA	3:D:361:GLU:HG3	1.84	0.59
1:A:313:PHE:HE1	1:A:483:ILE:HD13	1.68	0.59
3:D:210:PRO:O	3:D:222:LEU:HD12	2.02	0.59
2:B:389:THR:CG2	2:B:483:ILE:HD13	2.33	0.58
1:C:378:LYS:HG3	1:C:395:TRP:HB3	1.85	0.58
1:A:343:ILE:HG12	1:A:496:PRO:HB2	1.85	0.58
3:D:148:ILE:HD13	3:D:259:ILE:HD11	1.84	0.58
1:A:551:MET:SD	1:A:559:ILE:HG13	2.44	0.58
1:A:548:ARG:HB3	1:A:549:PRO:HD3	1.86	0.57
2:B:558:PRO:HA	2:B:570:VAL:HG12	1.86	0.57
3:D:209:PHE:HB3	3:D:222:LEU:HD11	1.85	0.57
2:B:389:THR:CG2	2:B:483:ILE:CD1	2.81	0.57
2:B:122:GLU:HA	2:B:235:TYR:HE2	1.70	0.57
1:A:420:LEU:HD23	1:A:463:ILE:HD13	1.87	0.57
3:D:304:CME:HZ3	3:D:305:HIS:HE1	1.69	0.56
1:C:408:HIS:ND1	1:C:410:THR:CB	2.68	0.56
1:A:359:LYS:HA	3:D:446:MET:HE3	1.87	0.56
3:D:409:LEU:HD22	3:D:445:ILE:HD11	1.86	0.56
2:B:315:ILE:HG21	2:B:318:LEU:HD13	1.88	0.55
1:A:563:PHE:C	1:A:563:PHE:CD2	2.84	0.55
1:A:325:MET:HG3	1:A:435:PHE:HB3	1.90	0.54
2:B:121:ASN:H	2:B:124:VAL:HB	1.72	0.54
3:D:221:SER:HA	3:D:227:ASN:HA	1.90	0.54
2:B:409:LEU:HD22	2:B:445:ILE:HD11	1.90	0.53
3:D:164:PHE:CE1	3:D:210:PRO:HB3	2.43	0.53
1:C:410:THR:O	1:C:413:SER:HB2	2.08	0.53
2:B:122:GLU:HA	2:B:235:TYR:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:ILE:HD12	1:A:559:ILE:H	1.75	0.52
3:D:68:LEU:O	3:D:72:ILE:HG12	2.08	0.52
3:D:4:ILE:HD11	3:D:64:LEU:HD13	1.91	0.52
1:A:515:LEU:HD12	1:A:548:ARG:HH21	1.74	0.52
2:B:122:GLU:CB	2:B:235:TYR:HE2	2.22	0.52
2:B:389:THR:HG23	2:B:483:ILE:HD13	1.87	0.52
3:D:105:GLU:HA	3:D:108:SER:OG	2.10	0.52
3:D:136:HIS:CB	3:D:143:ARG:HG2	2.38	0.51
2:B:24:LEU:HG	2:B:35:ILE:HD11	1.92	0.51
2:B:483:ILE:HB	2:B:504:LEU:HD13	1.92	0.51
2:B:117:ASN:HB3	2:B:268:THR:CB	2.41	0.51
2:B:105:GLU:HA	2:B:108:SER:OG	2.11	0.51
2:B:270:LYS:HB3	2:B:271:TYR:CD2	2.46	0.50
1:C:325:MET:HG3	1:C:435:PHE:HB3	1.93	0.50
2:B:175:LEU:HB3	2:B:226:ILE:HD11	1.92	0.50
3:D:203:ILE:HB	3:D:206:PHE:HD2	1.76	0.50
1:A:273:TYR:HA	1:A:276:ILE:HD12	1.94	0.50
1:A:434:LYS:HG2	1:A:462:ILE:HG12	1.94	0.50
1:A:534:PRO:HG2	1:A:537:VAL:HG13	1.93	0.50
2:B:160:VAL:HG12	2:B:214:ASP:HA	1.93	0.50
3:D:558:PRO:HA	3:D:570:VAL:HG12	1.94	0.50
1:C:338:PHE:HZ	1:C:355:THR:CG2	2.25	0.50
2:B:390:GLU:OE1	1:C:311:ARG:NE	2.40	0.49
2:B:107:ARG:HH12	2:B:147:ALA:HB3	1.77	0.49
1:C:380:VAL:HG11	1:C:526:GLU:HB3	1.93	0.49
3:D:175:LEU:HA	3:D:229:ASP:HB2	1.93	0.49
1:C:503:GLU:CD	9:C:701:HOH:O	2.54	0.49
1:C:327:THR:HB	1:C:406:ARG:HH12	1.77	0.49
1:A:356:PHE:HB2	1:A:405:LEU:HB2	1.93	0.49
1:C:368:PHE:CD2	1:C:369:THR:HG22	2.48	0.48
3:D:102:SER:HB2	3:D:164:PHE:HB2	1.95	0.48
3:D:421:ARG:HD2	3:D:439:LEU:HD21	1.95	0.48
2:B:164:PHE:CE1	2:B:210:PRO:HB3	2.49	0.48
3:D:111:VAL:HG12	3:D:294:TYR:CE2	2.48	0.48
2:B:611:ILE:O	2:B:615:LEU:HG	2.14	0.48
1:C:306:LEU:HD13	1:C:562:LEU:HD21	1.95	0.48
3:D:460:LEU:O	3:D:464:MET:HG2	2.13	0.48
2:B:59:VAL:HG22	2:B:134:LYS:HB3	1.95	0.47
1:A:376:ASN:O	1:A:380:VAL:HG23	2.14	0.47
2:B:109:TYR:CG	2:B:249:ARG:HB2	2.50	0.47
3:D:465:LEU:HD21	3:D:587:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:LYS:HD2	2:B:274:HIS:NE2	2.29	0.47
1:C:438:ILE:HG12	1:C:458:VAL:HG13	1.97	0.47
1:C:534:PRO:HG2	1:C:537:VAL:HG13	1.96	0.47
2:B:56:TYR:CZ	2:B:139:LEU:HD13	2.49	0.47
1:C:341:LEU:O	1:C:497:TYR:HB3	2.14	0.47
1:C:548:ARG:HB3	1:C:549:PRO:HD3	1.96	0.47
1:A:327:THR:HB	1:A:406:ARG:HH12	1.80	0.47
2:B:264:SER:CB	2:B:271:TYR:HA	2.45	0.47
1:A:565:TYR:CE1	3:D:466:LYS:HB2	2.50	0.46
2:B:157:ASN:O	2:B:214:ASP:HB2	2.14	0.46
2:B:122:GLU:CA	2:B:235:TYR:HE2	2.28	0.46
1:C:338:PHE:CZ	1:C:355:THR:HG21	2.51	0.46
2:B:287:GLU:HB3	2:B:290:ASN:HB2	1.98	0.46
2:B:460:LEU:O	2:B:464:MET:HG2	2.16	0.46
1:A:410:THR:O	1:A:413:SER:HB2	2.15	0.45
3:D:490:THR:HB	3:D:493:ARG:HB2	1.97	0.45
1:A:397:LEU:O	1:A:400:THR:HG22	2.15	0.45
2:B:187:ILE:HG13	2:B:188:ASN:H	1.80	0.45
2:B:126:ASN:HA	2:B:129:ILE:HG22	1.98	0.45
2:B:221:SER:HA	2:B:227:ASN:HA	1.98	0.45
3:D:611:ILE:O	3:D:615:LEU:HG	2.16	0.45
1:A:337:CYS:HA	1:A:411:ALA:HB2	1.98	0.45
2:B:246:ALA:HB3	2:B:252:ALA:HB2	1.99	0.45
2:B:559:LYS:HD2	2:B:571:ASP:CG	2.42	0.45
3:D:118:VAL:HG12	3:D:267:CYS:HA	1.98	0.45
1:A:302:ASN:HB2	3:D:402:THR:HG23	1.98	0.45
1:A:463:ILE:HB	1:A:539:VAL:HG22	1.99	0.45
1:C:480:TYR:CD1	1:C:485:ILE:HD12	2.52	0.45
2:B:528:LYS:HG3	2:B:533:PHE:CE2	2.52	0.44
1:C:568:VAL:HG12	1:C:569:ILE:HG13	1.98	0.44
3:D:223:PRO:HA	3:D:224:PRO:HA	1.74	0.44
3:D:210:PRO:O	3:D:223:PRO:HD2	2.17	0.44
3:D:96:PHE:CZ	3:D:279:GLN:HB3	2.53	0.44
1:A:438:ILE:HG23	1:A:458:VAL:HG22	1.98	0.44
1:C:338:PHE:HZ	1:C:355:THR:HG21	1.82	0.44
1:C:347:HIS:CG	1:C:348:PRO:HD2	2.53	0.44
2:B:68:LEU:O	2:B:72:ILE:HG12	2.17	0.44
1:A:276:ILE:HG22	1:A:276:ILE:O	2.17	0.44
2:B:174:PRO:O	2:B:229:ASP:HB2	2.17	0.44
2:B:588:HIS:CG	2:B:589:PRO:HD2	2.52	0.44
1:C:424:TYR:CE2	1:C:534:PRO:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:PHE:HB2	1:C:461:LEU:HG	1.99	0.44
3:D:111:VAL:HG23	3:D:256:VAL:HG21	1.99	0.44
3:D:115:LEU:HD12	3:D:115:LEU:HA	1.73	0.44
2:B:338:ASP:HB3	2:B:341:THR:H	1.82	0.43
2:B:507:ILE:HG13	2:B:603:VAL:HG22	1.99	0.43
1:C:397:LEU:O	1:C:400:THR:HG22	2.19	0.43
2:B:94:LYS:O	2:B:158:PHE:HB3	2.19	0.43
2:B:268:THR:CB	2:B:269:PRO:CD	2.94	0.43
3:D:386:SER:O	3:D:390:GLU:HG2	2.18	0.43
1:A:314:LYS:HG3	1:A:436:PHE:CZ	2.54	0.43
3:D:385:LEU:O	3:D:389:THR:HG23	2.19	0.43
1:A:348:PRO:HG3	2:B:138:ASN:O	2.18	0.43
2:B:588:HIS:HA	2:B:589:PRO:HD3	1.79	0.43
1:C:376:ASN:O	1:C:380:VAL:HG23	2.19	0.43
3:D:534:SER:HB3	3:D:554:TYR:CZ	2.54	0.43
1:A:341:LEU:HD21	1:A:414:CYS:HB2	2.01	0.42
1:C:447:LEU:HD23	1:C:447:LEU:HA	1.69	0.42
1:A:563:PHE:CD2	1:A:563:PHE:O	2.72	0.42
3:D:559:LYS:HD2	3:D:571:ASP:CG	2.45	0.42
3:D:135:LEU:HD23	3:D:135:LEU:HA	1.67	0.42
3:D:389:THR:HG21	3:D:502:ARG:NH1	2.23	0.42
2:B:284:HIS:HE1	2:B:286:ALA:HB3	1.85	0.42
2:B:396:LEU:HD11	2:B:504:LEU:HD21	2.02	0.42
2:B:60:CYS:HB3	2:B:131:LEU:HD13	2.01	0.42
2:B:416:TYR:CZ	2:B:423:HIS:HB3	2.54	0.42
1:C:310:MET:HG2	1:C:438:ILE:HD12	2.02	0.42
2:B:105:GLU:HA	2:B:108:SER:HG	1.85	0.42
3:D:354:MET:HE3	3:D:354:MET:HB2	1.90	0.42
3:D:209:PHE:HB3	3:D:222:LEU:CD1	2.50	0.42
1:C:493:THR:O	1:C:501:SER:HB2	2.20	0.41
3:D:51:VAL:HG11	3:D:64:LEU:HD12	2.02	0.41
1:A:380:VAL:HG11	1:A:526:GLU:HB3	2.02	0.41
2:B:130:GLU:O	2:B:134:LYS:HG2	2.20	0.41
3:D:160:VAL:HG12	3:D:214:ASP:HA	2.02	0.41
3:D:303:THR:HA	3:D:343:THR:HG22	2.02	0.41
1:A:382:SER:HA	1:A:393:TYR:O	2.20	0.41
2:B:534:SER:HB3	2:B:554:TYR:CZ	2.55	0.41
3:D:3:THR:HA	3:D:49:ILE:O	2.20	0.41
1:C:382:SER:HA	1:C:393:TYR:O	2.20	0.41
1:C:490:PHE:HB3	1:C:502:MET:HE2	2.03	0.41
1:C:505:TYR:HA	1:C:515:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:140:GLY:HA2	3:D:145:LEU:HB2	2.02	0.41
2:B:117:ASN:O	2:B:268:THR:N	2.54	0.41
3:D:173:ILE:HD11	3:D:177:GLU:C	2.46	0.41
1:A:344:PRO:HG3	1:A:391:TRP:CE2	2.56	0.41
2:B:538:ILE:HA	2:B:548:ILE:HD11	2.02	0.41
1:C:491:LYS:HB2	3:D:29:PHE:CE2	2.56	0.41
3:D:110:VAL:HA	3:D:244:CYS:O	2.21	0.41
3:D:478:LEU:HB3	3:D:480:PHE:CE2	2.55	0.41
1:A:380:VAL:HG22	1:A:385:ASP:HB3	2.02	0.41
1:C:491:LYS:HG2	1:C:492:PRO:O	2.21	0.41
2:B:97:MET:HB2	2:B:276:PHE:HE1	1.86	0.41
1:C:296:LYS:O	3:D:521:GLY:HA3	2.20	0.41
1:C:314:LYS:HG3	1:C:436:PHE:CZ	2.56	0.41
1:C:522:ILE:HG13	1:C:540:ILE:HG22	2.03	0.41
1:A:344:PRO:HG2	1:A:347:HIS:CB	2.51	0.40
1:A:420:LEU:HD12	1:A:420:LEU:HA	1.97	0.40
2:B:125:TYR:HE2	2:B:233:ILE:HG13	1.86	0.40
2:B:187:ILE:HG13	2:B:188:ASN:N	2.36	0.40
3:D:128:ILE:HG12	3:D:263:LEU:HD21	2.04	0.40
3:D:161:ALA:O	3:D:212:ILE:HA	2.21	0.40
2:B:611:ILE:HD12	2:B:615:LEU:HD21	2.03	0.40
2:B:96:PHE:HB3	2:B:159:PRO:HB3	2.04	0.40
3:D:61:VAL:O	3:D:65:CYS:HB2	2.22	0.40
3:D:220:LEU:HD22	3:D:231:THR:HG21	2.03	0.40
1:C:345:GLN:HA	1:C:350:ARG:NH1	2.36	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	302/304 (99%)	287 (95%)	15 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	302/304 (99%)	290 (96%)	12 (4%)	0	100 100
2	B	612/618 (99%)	589 (96%)	22 (4%)	1 (0%)	43 70
3	D	612/618 (99%)	586 (96%)	26 (4%)	0	100 100
All	All	1828/1844 (99%)	1752 (96%)	75 (4%)	1 (0%)	48 76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	269	PRO

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	272/279 (98%)	270 (99%)	2 (1%)	76 79
1	C	275/279 (99%)	274 (100%)	1 (0%)	84 84
2	B	551/570 (97%)	551 (100%)	0	100 100
3	D	542/570 (95%)	542 (100%)	0	100 100
All	All	1640/1698 (97%)	1637 (100%)	3 (0%)	87 87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	A	563	PHE
1	C	497	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	77	ASN
2	B	121	ASN

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Mol	Chain	Res	Type
2	B	279	GLN
2	B	299	ASN
1	C	345	GLN
1	C	394	GLN
3	D	121	ASN
3	D	191	GLN

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	$\#\|Z\| > 2$
2	CME	B	418	2	8,9,10	0.49	0	5,9,11	1.92	2 (40%)
3	CME	D	304	3	8,9,10	0.51	0	5,9,11	9.73	2 (40%)
3	CME	D	575	3	8,9,10	0.58	0	5,9,11	1.41	1 (20%)
2	CME	B	304	2	8,9,10	0.47	0	5,9,11	1.69	1 (20%)

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
2	CME	B	418	2	-	2/5/8/10	-
3	CME	D	304	3	-	2/5/8/10	-
3	CME	D	575	3	-	3/5/8/10	-
2	CME	B	304	2	-	1/5/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	304	CME	CB-SG-SD	18.14	150.81	103.82
3	D	304	CME	CE-SD-SG	11.96	158.55	103.45
2	B	304	CME	CE-SD-SG	3.18	118.09	103.45
2	B	418	CME	CB-SG-SD	3.13	111.94	103.82
2	B	418	CME	CE-SD-SG	2.48	114.86	103.45
3	D	575	CME	CB-SG-SD	2.21	109.55	103.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	304	CME	CE-SD-SG-CB
3	D	575	CME	CE-SD-SG-CB
3	D	304	CME	CE-SD-SG-CB
3	D	304	CME	N-CA-CB-SG
2	B	418	CME	CZ-CE-SD-SG
2	B	418	CME	CA-CB-SG-SD
3	D	575	CME	CA-CB-SG-SD
3	D	575	CME	SD-CE-CZ-OH

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	304	CME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	PHE	C	601	-	11,12,12	0.70	1 (9%)	14,15,15	0.95	2 (14%)
7	SO4	B	702	-	4,4,4	0.60	0	6,6,6	0.04	0
8	ACT	B	703	-	3,3,3	1.05	0	3,3,3	1.18	0
4	PHE	A	601	-	11,12,12	0.70	1 (9%)	14,15,15	0.95	2 (14%)
7	SO4	C	603	-	4,4,4	0.60	0	6,6,6	0.06	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	PHE	C	601	-	-	0/8/8/8	0/1/1/1
4	PHE	A	601	-	-	0/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	PHE	OXT-C	-2.15	1.23	1.30
4	A	601	PHE	OXT-C	-2.15	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	PHE	OXT-C-O	-2.69	117.99	124.09
4	A	601	PHE	OXT-C-O	-2.66	118.06	124.09
4	A	601	PHE	OXT-C-CA	2.24	121.03	113.38
4	C	601	PHE	OXT-C-CA	2.24	121.02	113.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	PHE	1	0

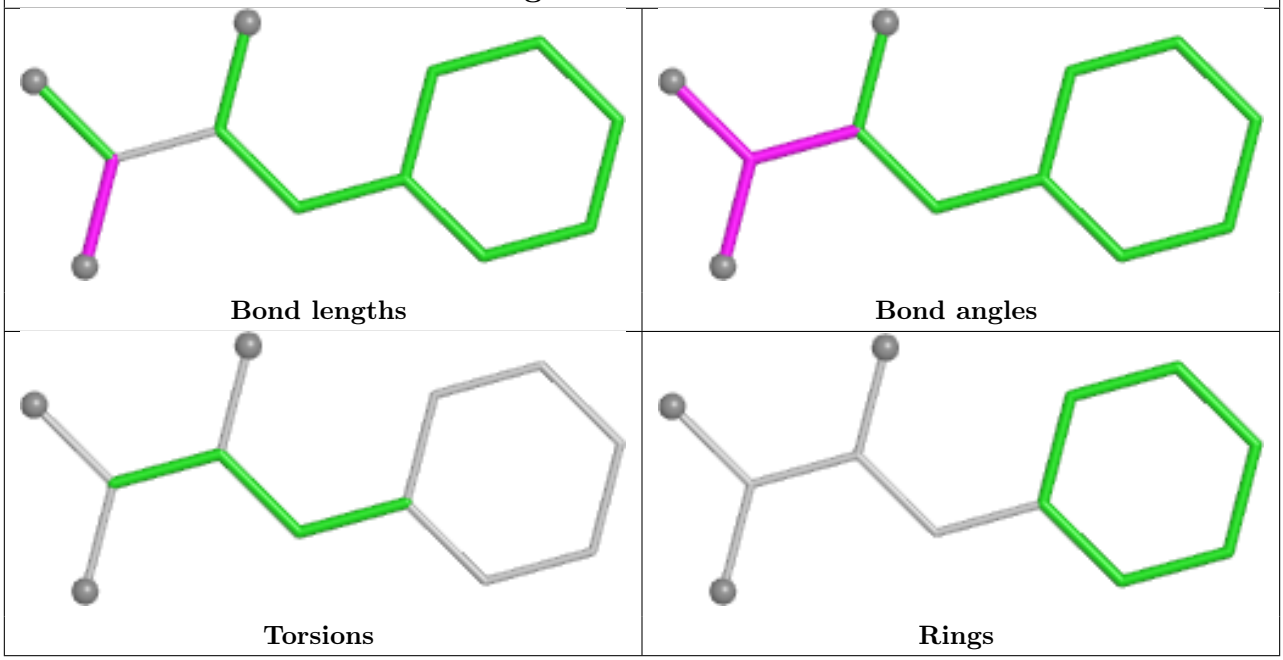
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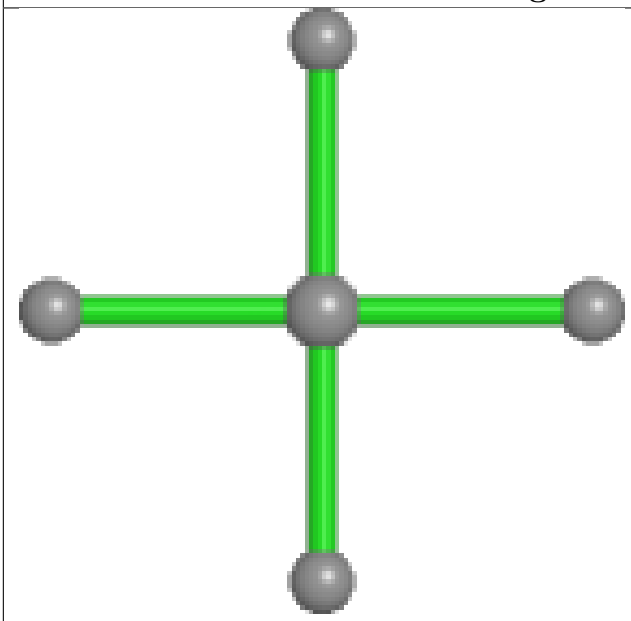
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	PHE	1	0

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.

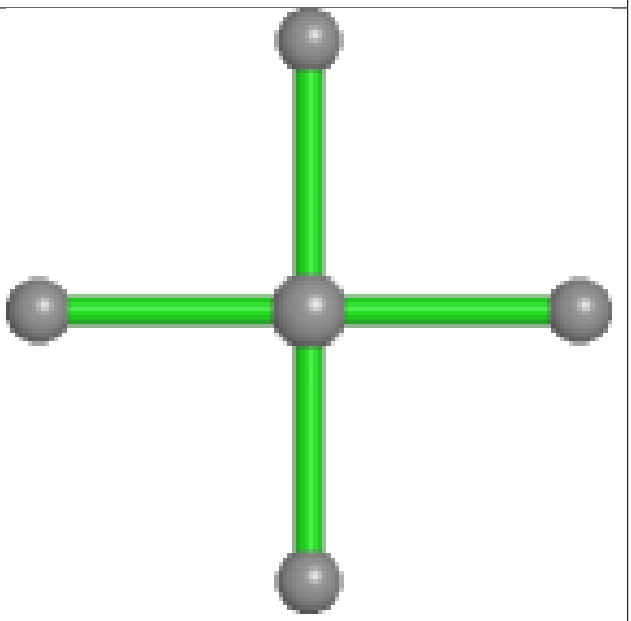
Ligand PHE C 601



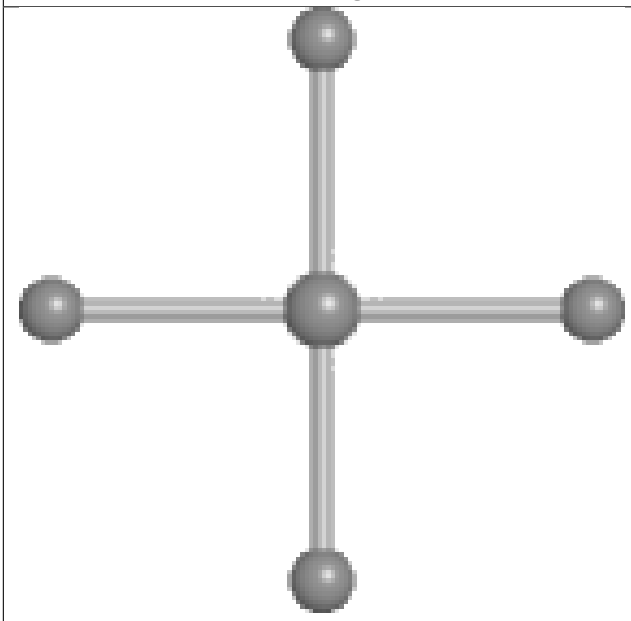
Ligand SO4 B 702



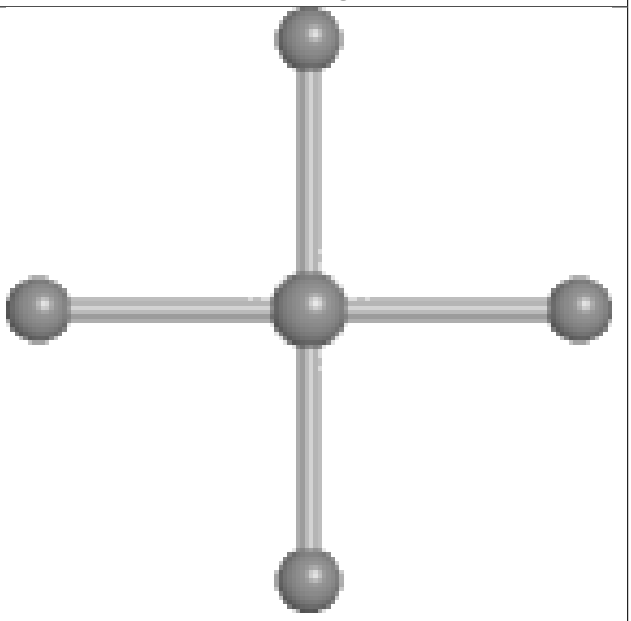
Bond lengths



Bond angles

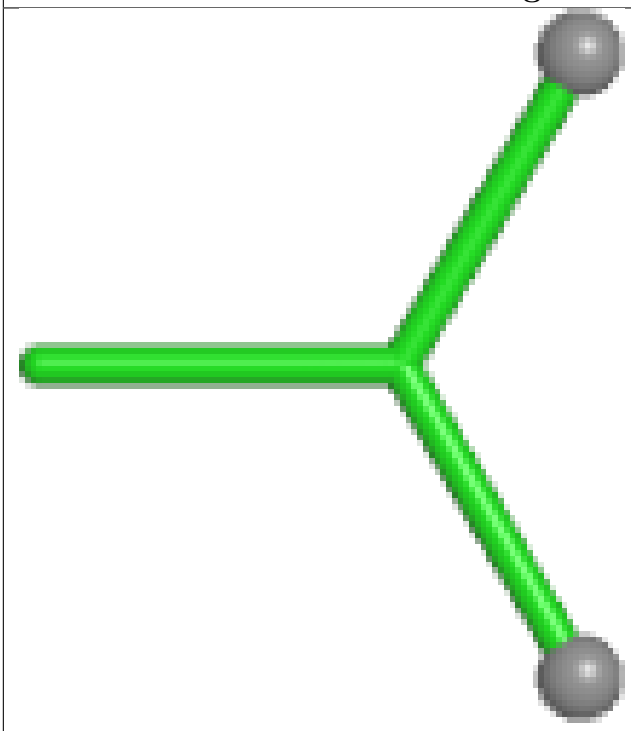


Torsions

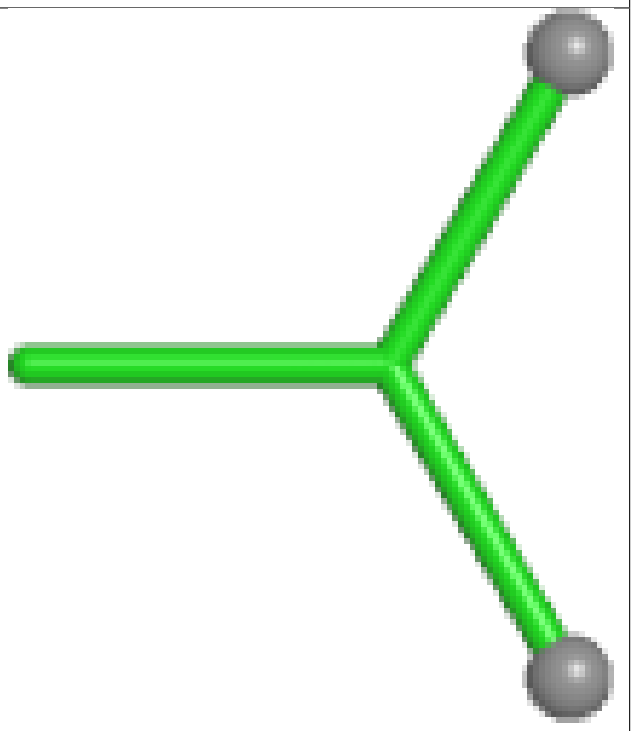


Rings

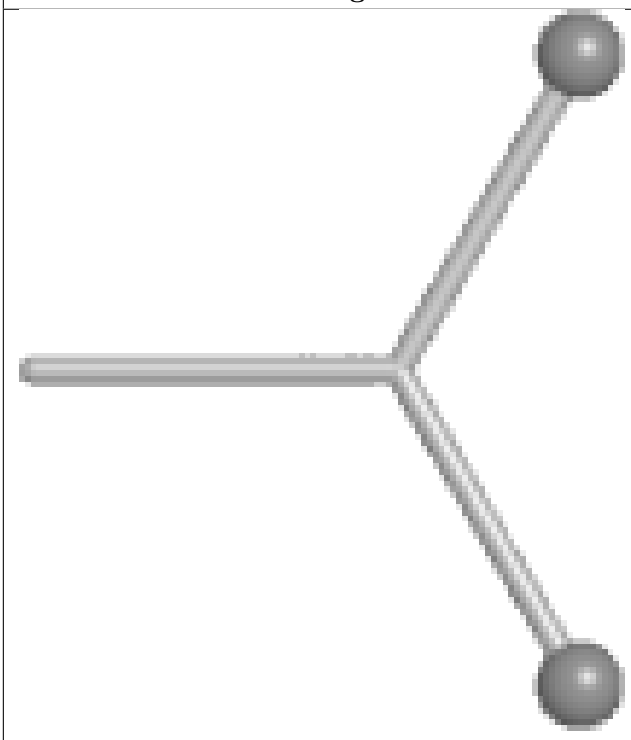
Ligand ACT B 703



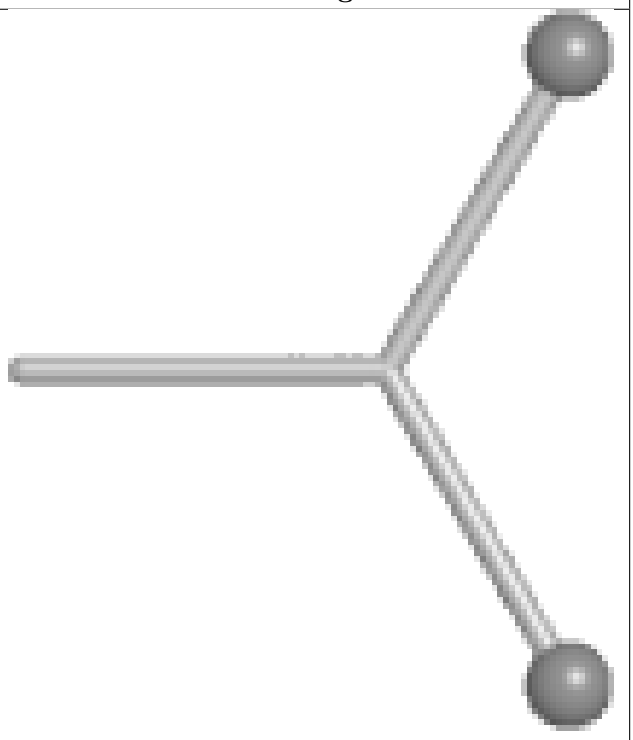
Bond lengths



Bond angles

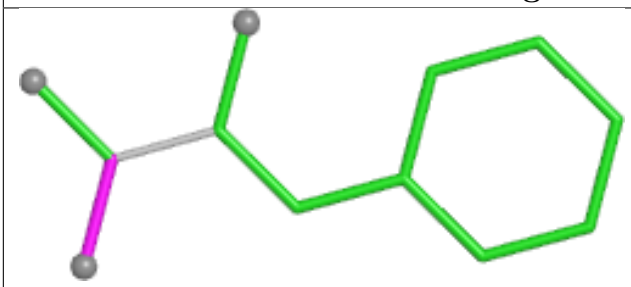


Torsions

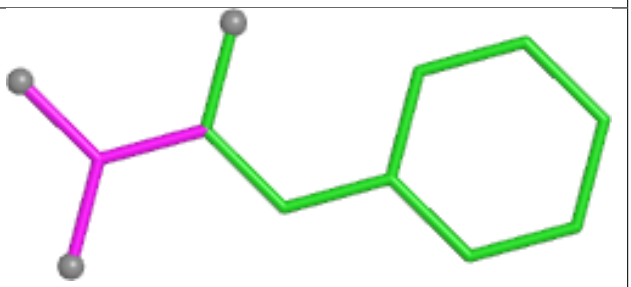


Rings

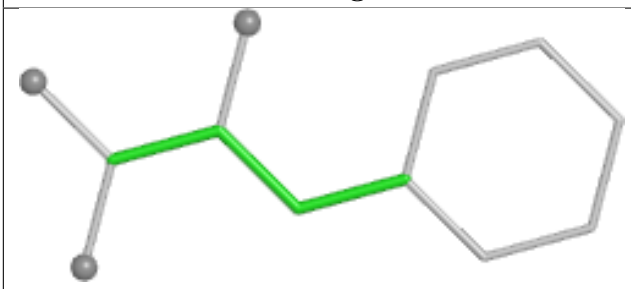
Ligand PHE A 601



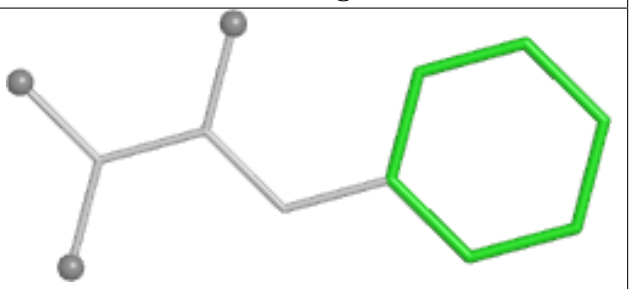
Bond lengths



Bond angles

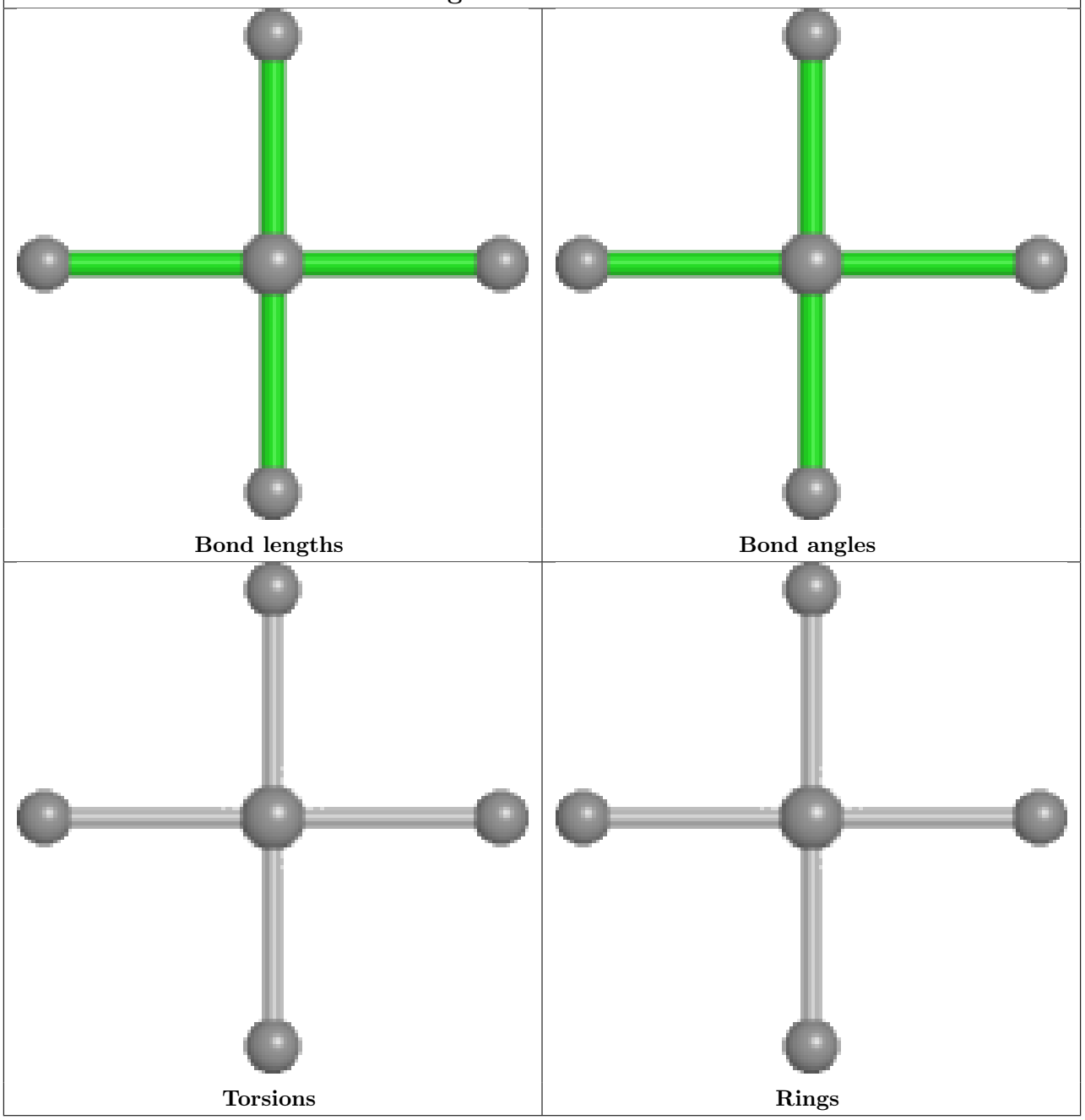


Torsions



Rings

Ligand SO4 C 603



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^{th} 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	304/304 (100%)	-0.06	3 (0%)	79	62	60, 86, 130, 163	0
1	C	304/304 (100%)	-0.02	5 (1%)	70	52	56, 81, 124, 145	0
2	B	614/618 (99%)	0.06	10 (1%)	70	52	62, 90, 124, 182	0
3	D	614/618 (99%)	0.29	32 (5%)	33	22	66, 102, 161, 210	0
All	All	1836/1844 (99%)	0.10	50 (2%)	56	38	56, 91, 141, 210	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	314	GLY	4.4
3	D	254	ILE	4.0
3	D	248	ASP	4.0
3	D	242	ILE	4.0
1	C	389	PHE	3.7
3	D	192	ASP	3.6
3	D	138	ASN	3.6
1	A	268	ILE	3.5
1	C	569	ILE	3.5
3	D	251	LYS	3.4
3	D	190	TYR	3.4
2	B	192	ASP	3.3
1	C	431	ILE	3.2
2	B	214	ASP	3.2
2	B	484	GLY	3.0
3	D	150	ILE	3.0
3	D	290	ASN	2.9
3	D	244	CYS	2.9
2	B	35	ILE	2.8
3	D	237	THR	2.7
2	B	187	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	137	HIS	2.6
2	B	314	GLY	2.6
3	D	303	THR	2.6
3	D	106	ARG	2.6
3	D	234	THR	2.6
3	D	268	THR	2.5
2	B	380	ALA	2.3
3	D	85	ASN	2.3
1	A	460	GLY	2.3
3	D	196	LEU	2.3
3	D	379	ILE	2.3
3	D	81	ALA	2.3
3	D	353	ILE	2.2
3	D	255	ALA	2.2
2	B	193	ASN	2.2
3	D	187	ILE	2.2
3	D	145	LEU	2.2
3	D	293	LEU	2.2
2	B	217	GLY	2.2
3	D	109	TYR	2.1
3	D	317	ASN	2.1
1	C	342	TYR	2.1
3	D	194	ILE	2.1
3	D	117	ASN	2.1
3	D	162	TYR	2.1
1	A	391	TRP	2.0
1	C	346	GLN	2.0
2	B	379	ILE	2.0
3	D	233	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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
3	CME	D	575	10/11	0.82	0.14	97,114,158,161	0
3	CME	D	304	10/11	0.86	0.19	80,95,108,125	4
2	CME	B	304	10/11	0.86	0.15	101,117,124,129	4
2	CME	B	418	10/11	0.95	0.10	79,92,119,140	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

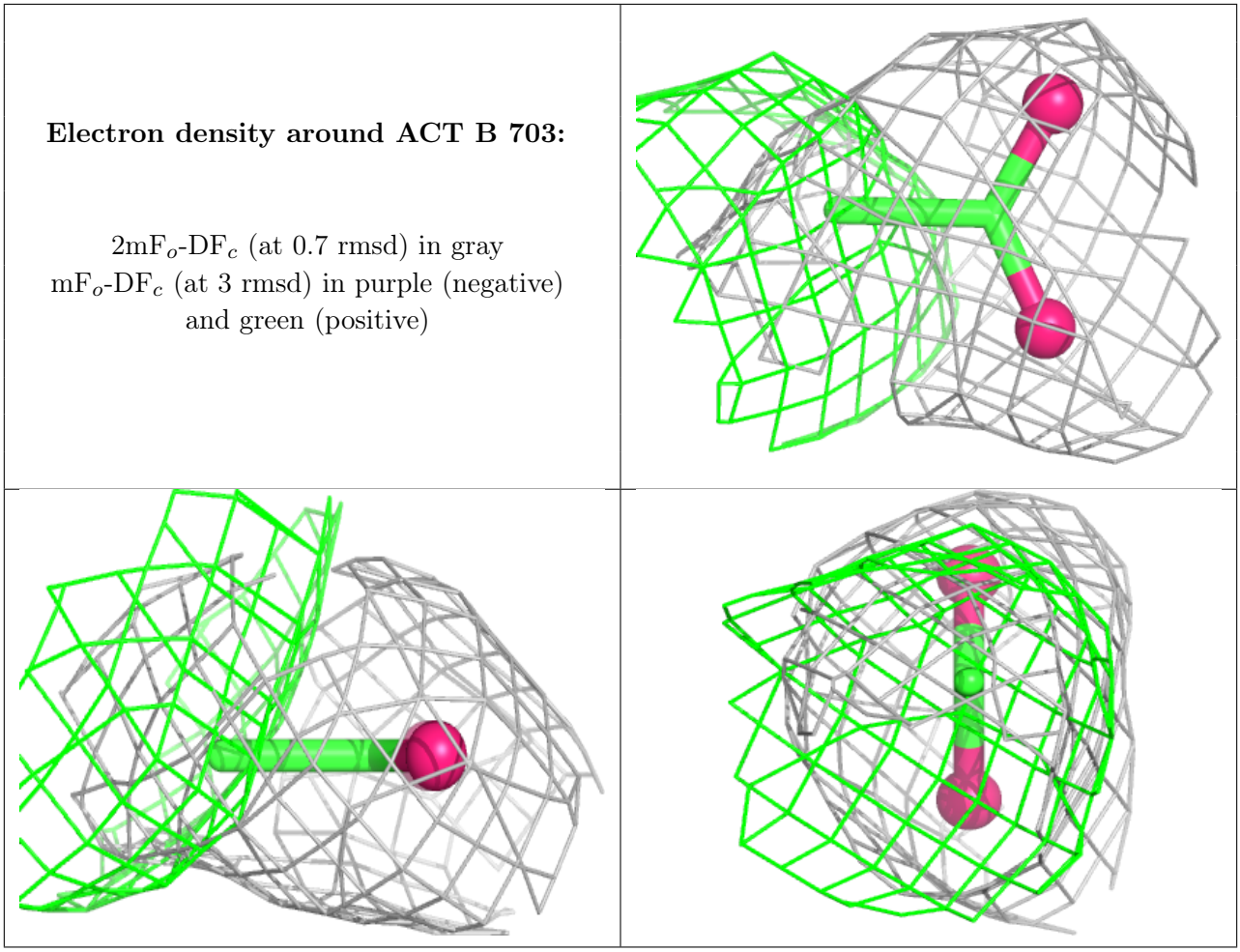
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	ACT	B	703	4/4	0.57	0.24	95,109,109,116	0
7	SO4	C	603	5/5	0.80	0.20	101,102,145,157	0
7	SO4	B	702	5/5	0.86	0.24	75,76,107,119	5
5	ZN	A	602	1/1	0.91	0.14	92,92,92,92	1
6	MG	B	701	1/1	0.92	0.13	53,53,53,53	0
4	PHE	C	601	12/12	0.92	0.14	54,69,75,76	0
4	PHE	A	601	12/12	0.93	0.13	60,83,96,99	0
6	MG	D	701	1/1	0.94	0.10	56,56,56,56	0
5	ZN	C	602	1/1	0.96	0.12	104,104,104,104	1

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

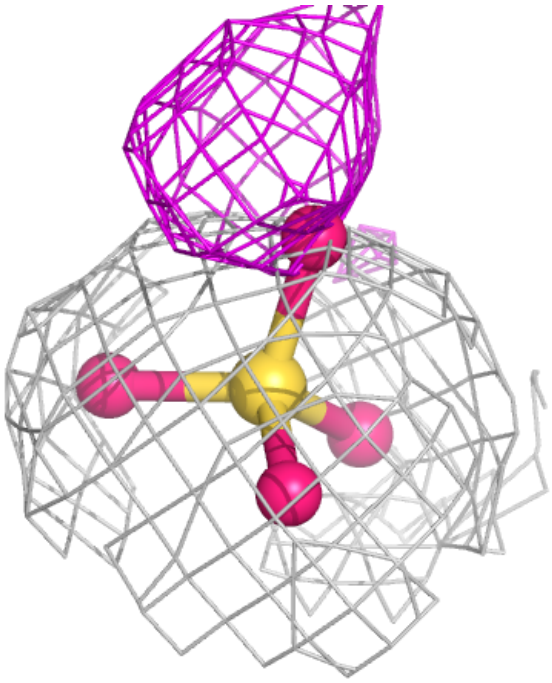
Electron density around ACT B 703:

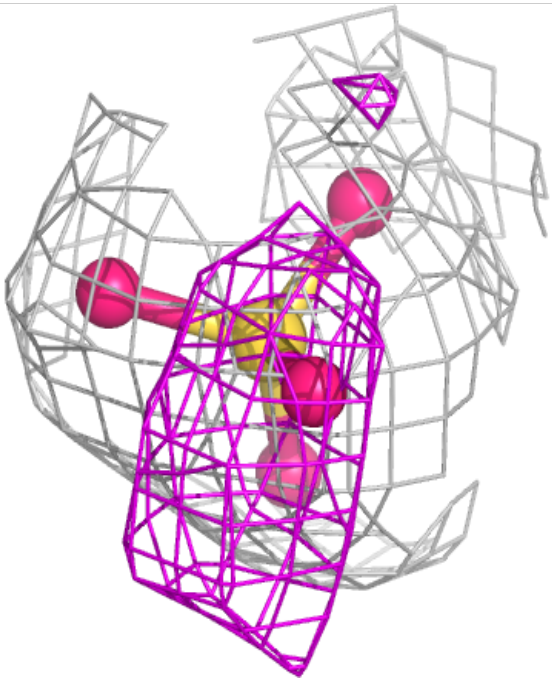
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

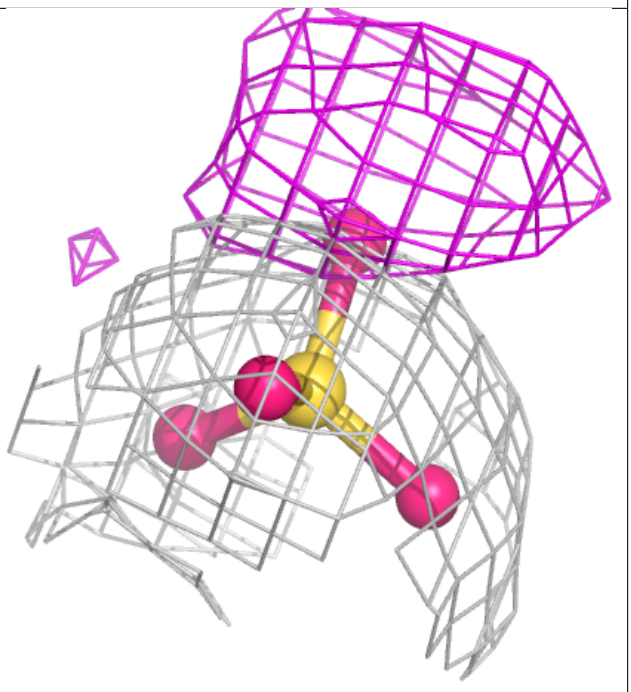


Electron density around SO4 C 603:

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

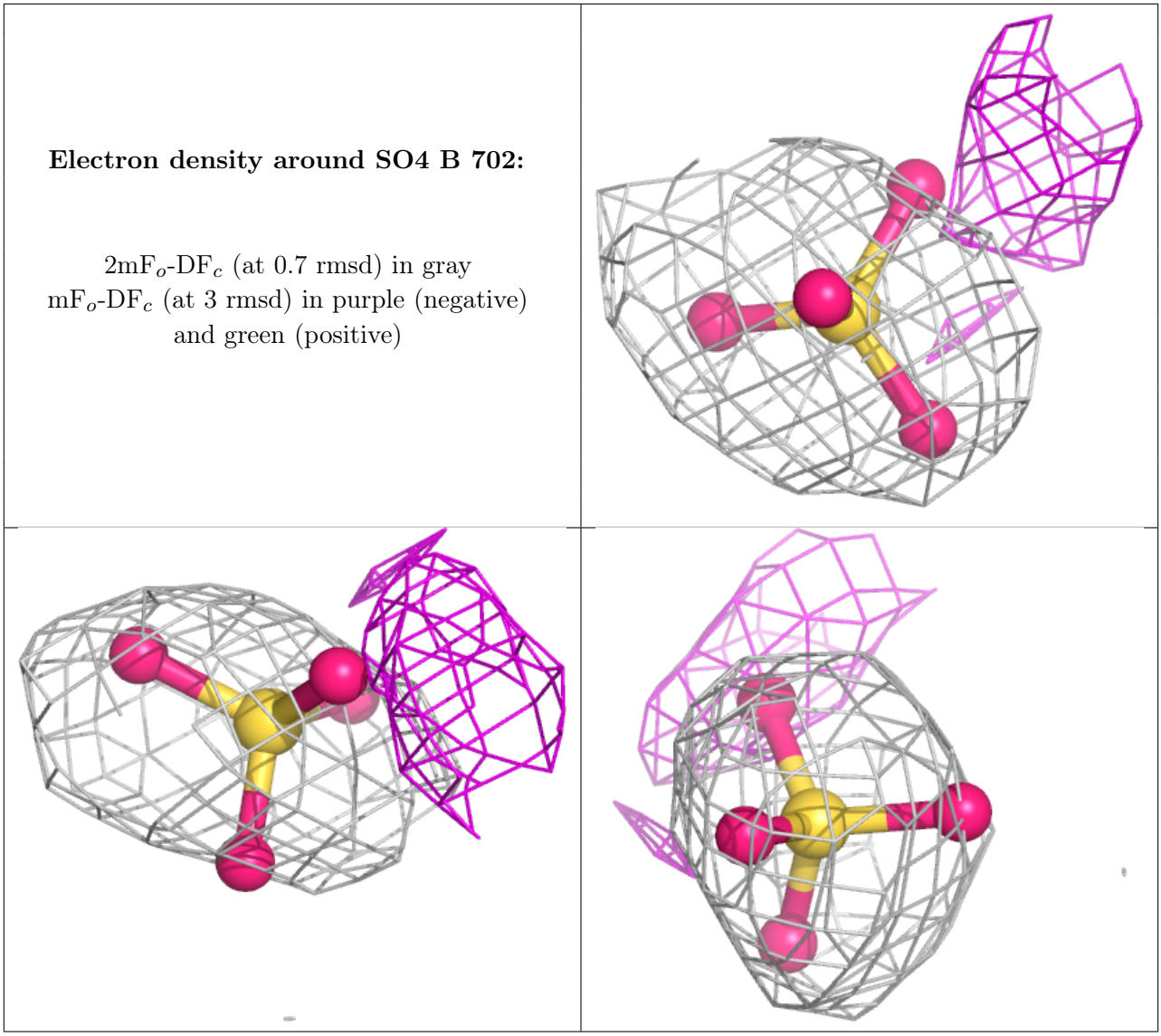






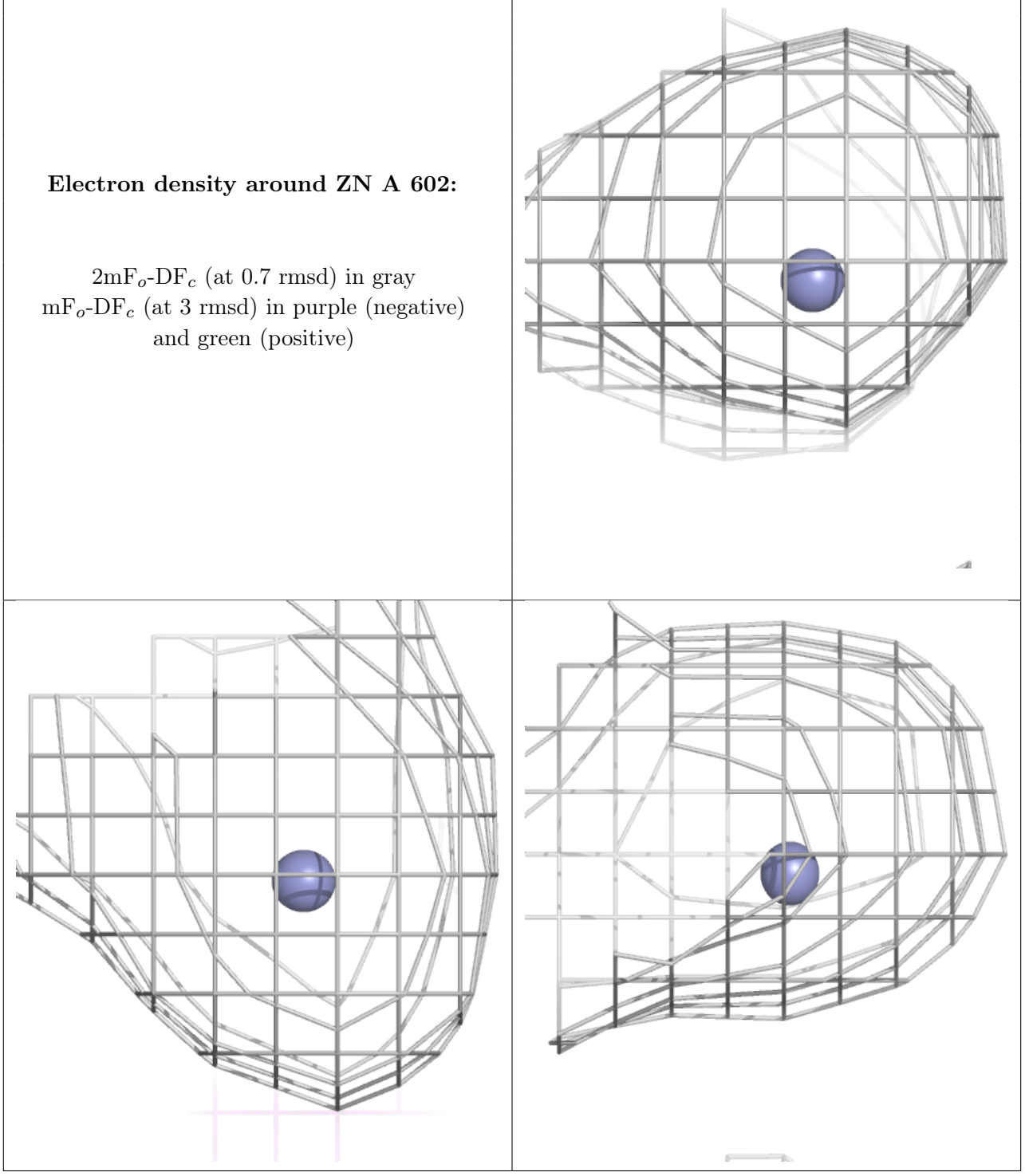
Electron density around SO4 B 702:

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



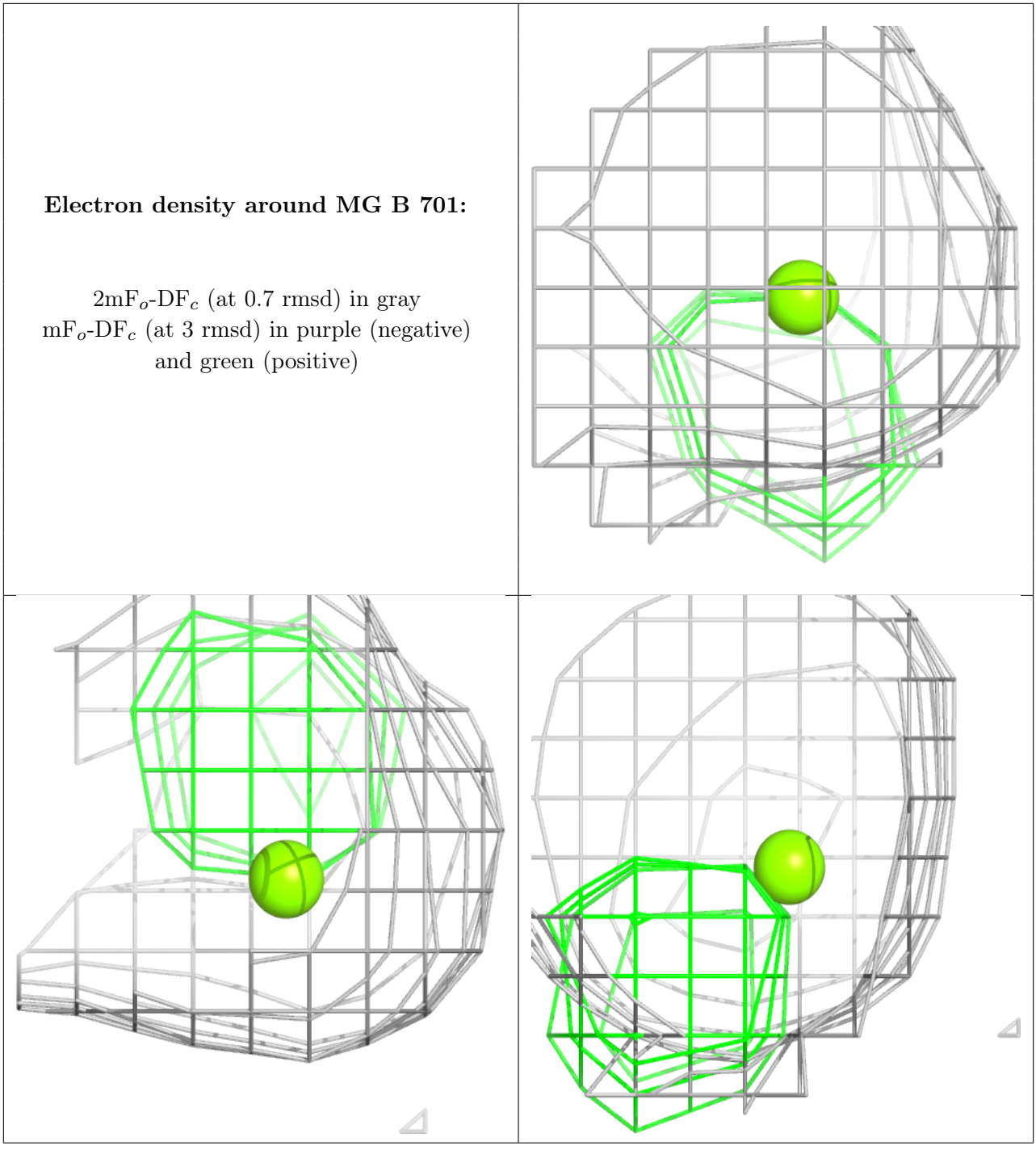
Electron density around ZN A 602:

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



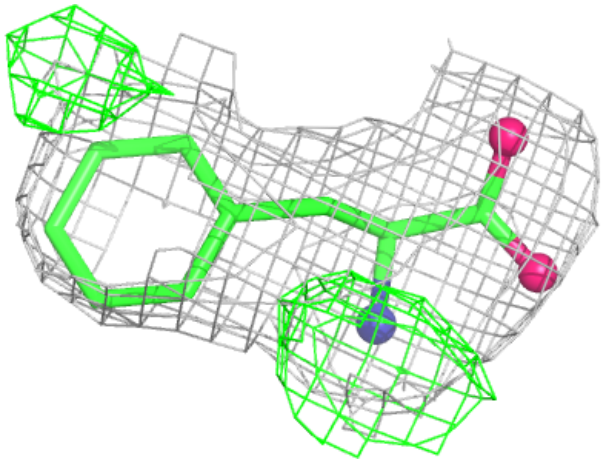
Electron density around MG B 701:

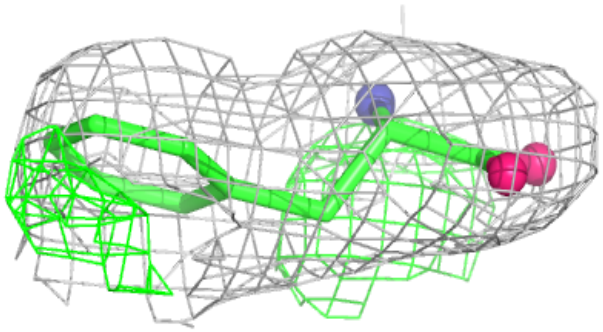
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

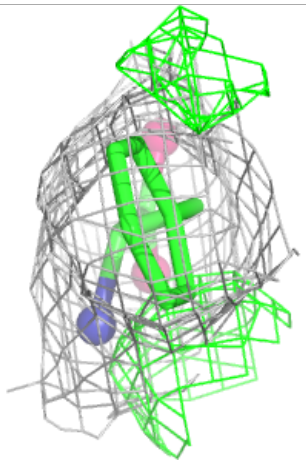


Electron density around PHE C 601:

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

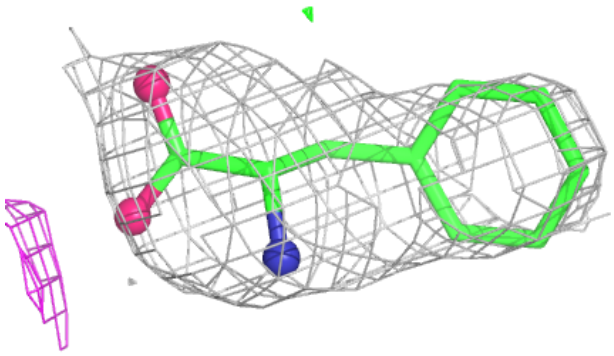


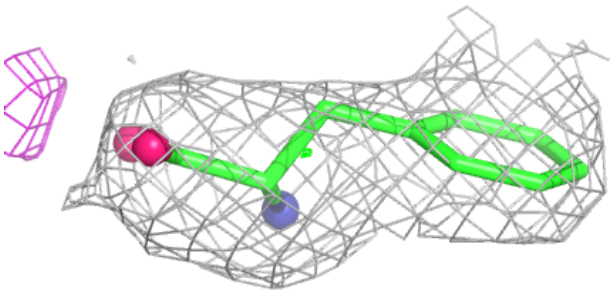


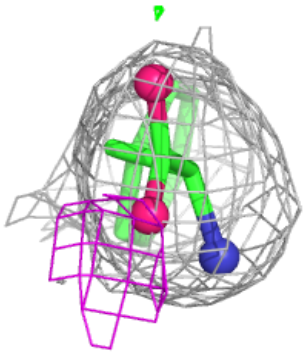


Electron density around PHE A 601:

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

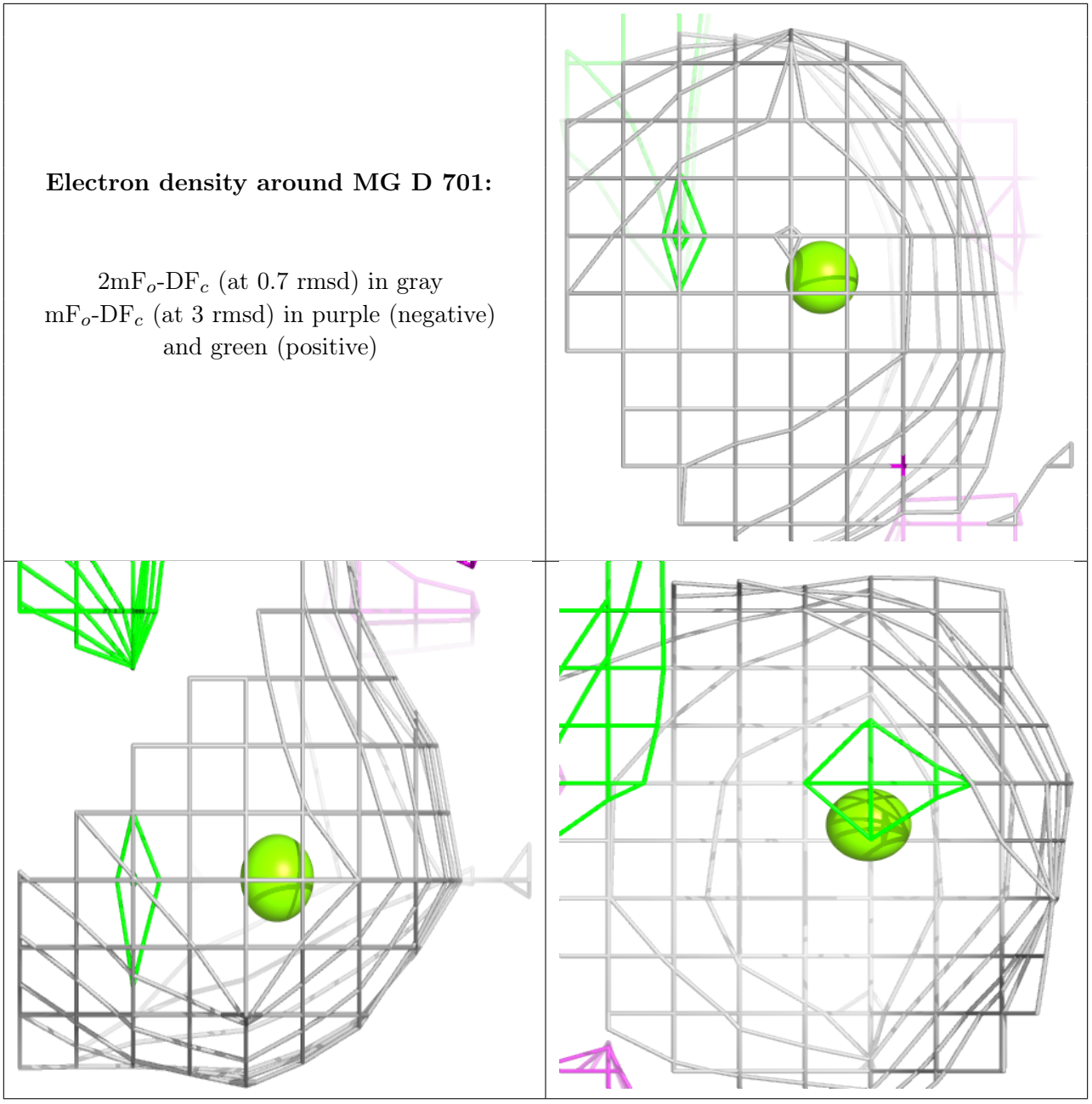






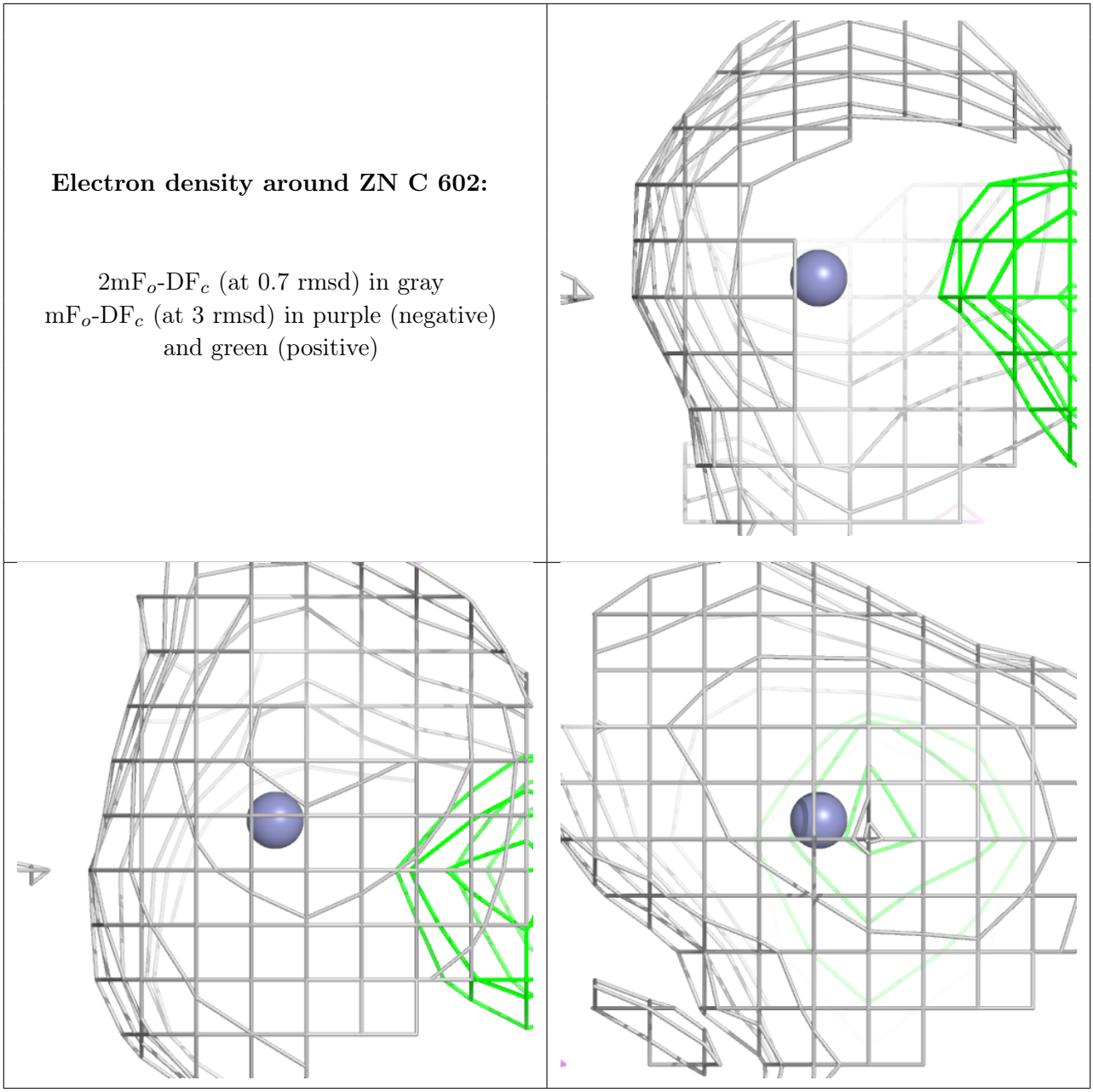
Electron density around MG D 701:

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



Electron density around ZN C 602:

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



6.5 Other polymers

There are no such residues in this entry.