



Full wwPDB X-ray Structure Validation Report i

Oct 12, 2020 – 08:06 PM EDT

PDB ID : 6UT3
Title : X-ray structure of Thermococcus gammatolerans McrB AAA+ domain hexamer in P21 symmetry
Authors : Niu, Y.; Hosford, C.J.; Chappie, J.S.
Deposited on : 2019-10-29
Resolution : 2.95 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 i symbol.

The following versions of software and data (see [references](#) i) 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	:	2.14.6
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)	:	2.14.6

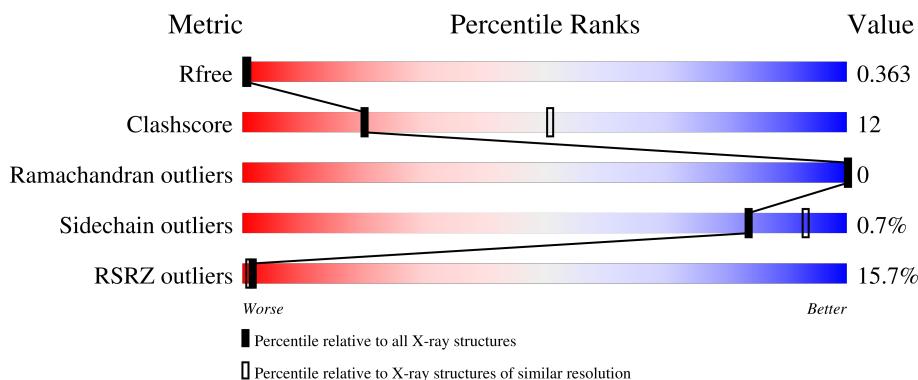
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



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Mol	Chain	Length	Quality of chain			
1	F	428	5%	42%	13%	45%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GSP	C	701	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15959 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.

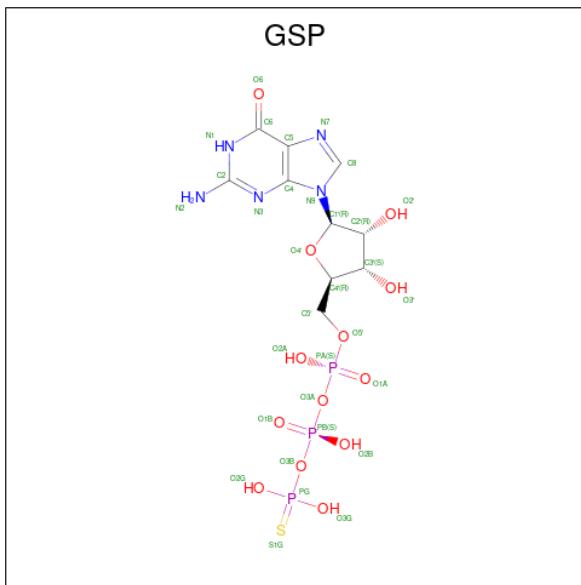
- Molecule 1 is a protein called GTPase subunit of restriction endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C 2453	N 1575	O 425	S 451	2	0	0
1	B	365	Total	C 2667	N 1722	O 455	S 487	3	0	0
1	C	375	Total	C 2981	N 1938	O 507	S 533	3	0	0
1	D	381	Total	C 3016	N 1959	O 516	S 538	3	0	0
1	E	384	Total	C 2952	N 1919	O 495	S 535	3	0	0
1	F	235	Total	C 1758	N 1139	O 294	S 323	2	0	0

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

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

- Molecule 3 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S) (labeled as "Ligand of Interest" by author).

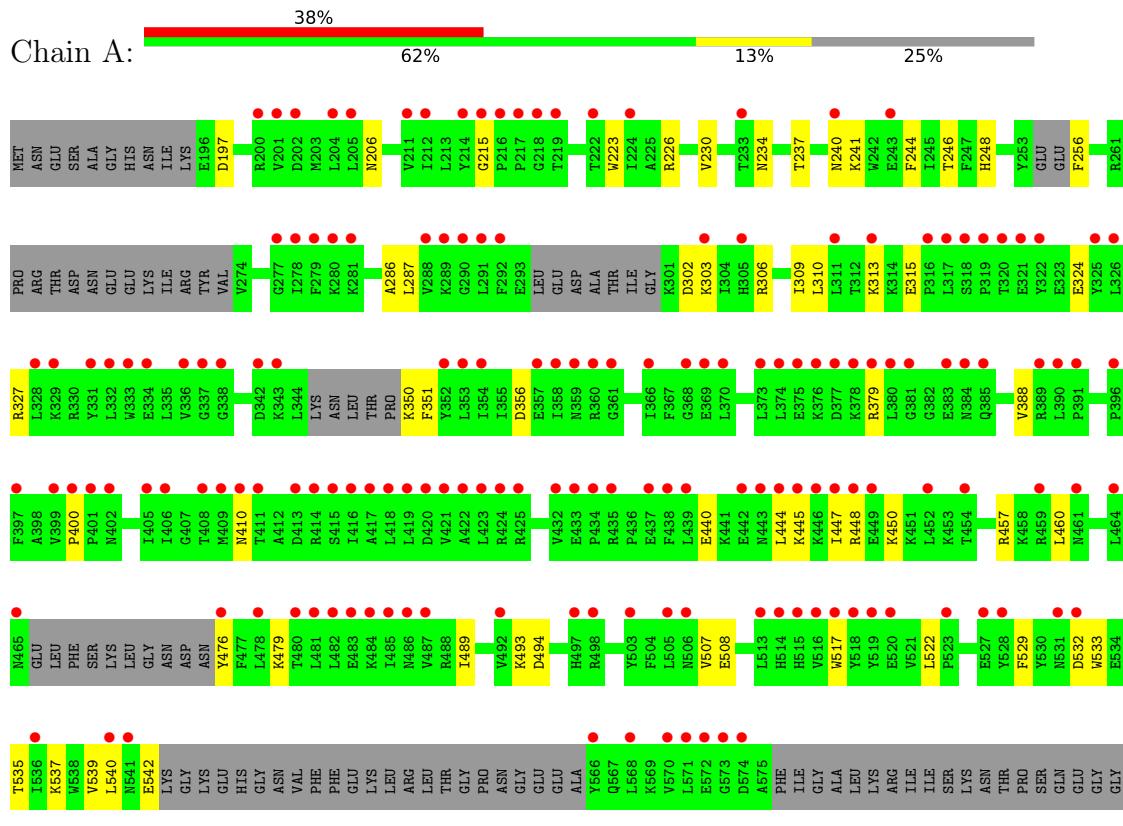


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total		C	N	O	P	S	
			32		10	5	13	3	1	0
3	C	1	Total		C	N	O	P	S	
			32		10	5	13	3	1	0
3	D	1	Total		C	N	O	P	S	
			32		10	5	13	3	1	0
3	E	1	Total		C	N	O	P	S	
			32		10	5	13	3	1	0

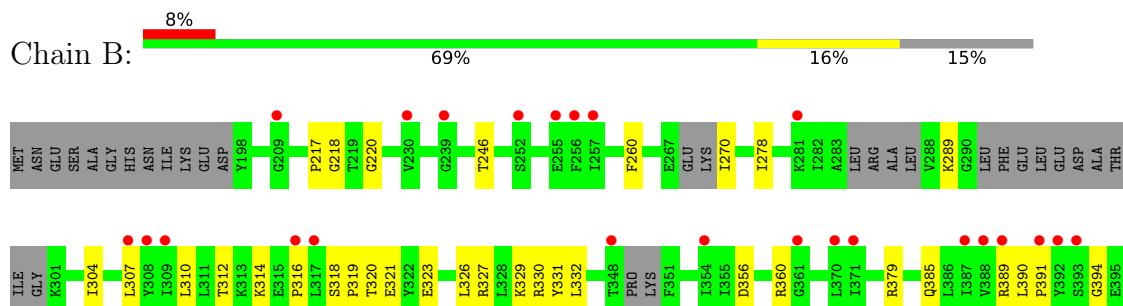
3 Residue-property plots [\(i\)](#)

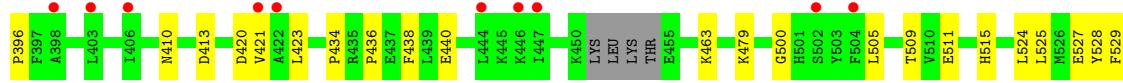
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GTPase subunit of restriction endonuclease

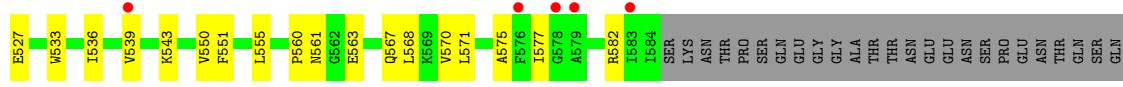


- Molecule 1: GTPase subunit of restriction endonuclease

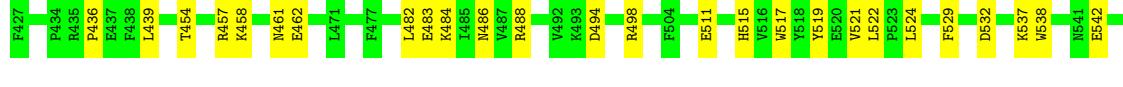


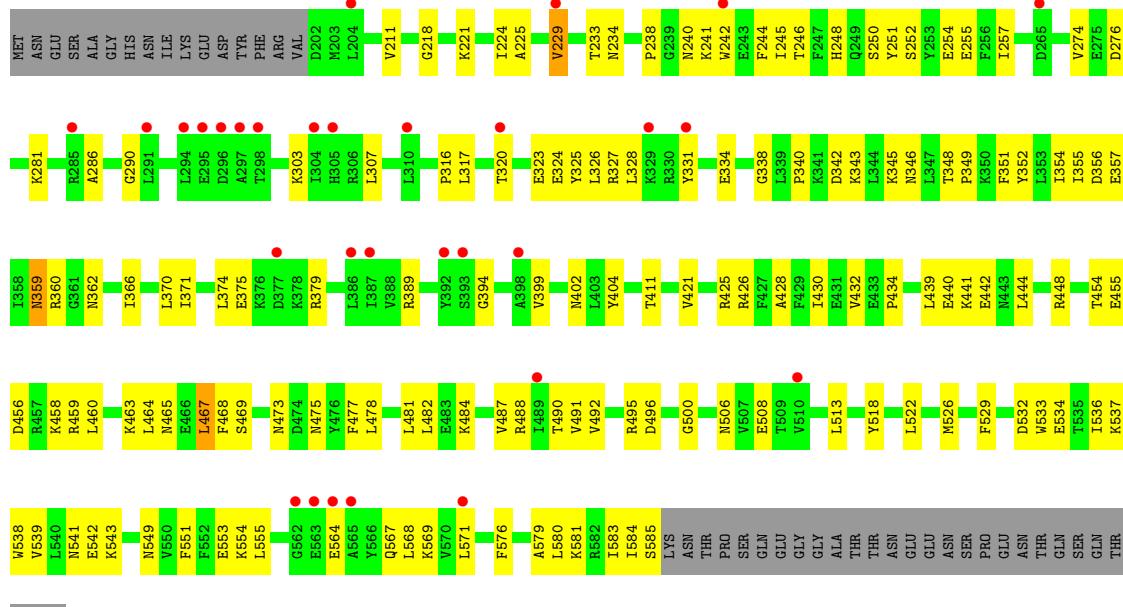


- Molecule 1: GTPase subunit of restriction endonuclease

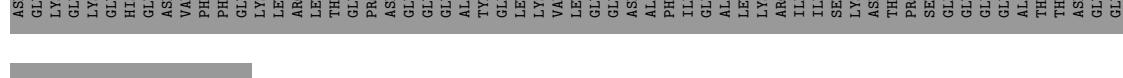
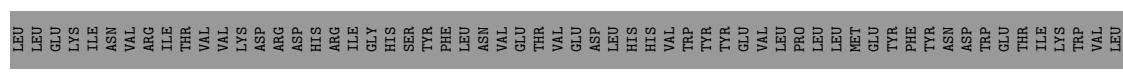
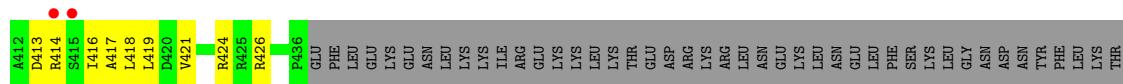


- Molecule 1: GTPase subunit of restriction endonuclease





- Molecule 1: GTPase subunit of restriction endonuclease



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.47 Å 109.62 Å 120.78 Å 90.00° 108.33° 90.00°	Depositor
Resolution (Å)	114.65 – 2.95 114.65 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (114.65-2.95) 96.9 (114.65-2.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.23 (at 2.86 Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R , R_{free}	0.345 , 0.363 0.345 , 0.363	Depositor DCC
R_{free} test set	2000 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 106.0	EDS
L-test for twinning ²	$< L > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15959	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [\(i\)](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GSP, MG

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	0.35	0/2492	0.62	0/3369
1	B	0.37	0/2714	0.60	0/3688
1	C	0.36	0/3045	0.58	0/4125
1	D	0.35	0/3081	0.57	0/4173
1	E	0.47	0/3015	0.71	0/4096
1	F	0.41	0/1792	0.60	0/2439
All	All	0.39	0/16139	0.62	0/21890

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 [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2453	0	2337	48	0
1	B	2667	0	2432	62	0
1	C	2981	0	2910	72	0
1	D	3016	0	2938	66	0
1	E	2952	0	2808	117	0
1	F	1758	0	1679	45	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	C	64	0	24	16	0
3	D	32	0	12	1	0
3	E	32	0	12	1	0
All	All	15959	0	15152	388	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 12.

All (388) 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:E:240:ASN:O	1:E:241:LYS:HG2	1.29	1.29
1:E:342:ASP:HA	1:E:345:LYS:HD2	1.38	1.04
1:A:529:PHE:CB	1:A:532:ASP:HB3	1.90	1.00
1:B:390:LEU:HD12	1:B:391:PRO:HD2	1.41	0.98
1:E:240:ASN:O	1:E:241:LYS:CG	2.15	0.94
3:C:701:GSP:C8	3:C:701:GSP:C5'	2.53	0.91
1:E:229:VAL:HG21	1:E:354:ILE:HD11	1.54	0.90
1:E:529:PHE:HB3	1:E:532:ASP:HB3	1.55	0.88
1:D:288:VAL:HG21	1:D:307:LEU:HD22	1.57	0.87
1:B:390:LEU:HD12	1:B:391:PRO:CD	2.08	0.84
1:B:389:ARG:HA	1:B:396:PRO:HA	1.59	0.84
3:C:701:GSP:C8	3:C:701:GSP:H5'2	2.15	0.82
1:C:560:PRO:HB3	1:D:538:TRP:CD1	2.15	0.82
1:B:323:GLU:N	1:B:323:GLU:OE2	2.14	0.81
1:B:389:ARG:HA	1:B:396:PRO:CA	2.10	0.81
1:E:490:THR:HG22	1:E:495:ARG:HA	1.61	0.81
1:A:241:LYS:O	1:A:241:LYS:HG2	1.82	0.80
1:A:522:LEU:HA	1:A:539:VAL:CB	2.11	0.80
1:E:440:GLU:HG3	1:E:442:GLU:HG2	1.64	0.80
1:E:456:ASP:HB3	1:E:459:ARG:HE	1.47	0.79
1:F:315:GLU:N	1:F:316:PRO:HD2	1.99	0.78
1:A:241:LYS:HB2	1:A:351:PHE:CD1	2.19	0.78
1:B:390:LEU:HD23	1:B:394:GLY:HA3	1.65	0.77
1:C:577:ILE:HD12	1:C:577:ILE:N	1.99	0.77
3:C:701:GSP:H5'1	3:C:701:GSP:C8	2.19	0.77
1:B:289:LYS:HE3	1:B:304:ILE:CB	2.16	0.76
1:B:379:ARG:O	1:B:385:GLN:HG3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:ASN:O	1:E:346:ASN:OD1	2.04	0.75
1:B:440:GLU:N	1:B:440:GLU:OE1	2.20	0.75
1:C:560:PRO:HB3	1:D:538:TRP:CG	2.22	0.74
1:C:550:VAL:HA	1:C:582:ARG:HH22	1.52	0.74
1:C:555:LEU:HD21	1:C:567:GLN:HB2	1.68	0.74
1:B:505:LEU:HD12	3:C:701:GSP:H1'	1.69	0.74
1:C:570:VAL:O	1:C:570:VAL:HG23	1.88	0.74
1:A:241:LYS:HB2	1:A:351:PHE:HD1	1.54	0.72
1:E:254:GLU:OE1	1:E:254:GLU:N	2.23	0.71
1:F:287:LEU:HB2	1:F:400:PRO:HG3	1.71	0.71
1:A:246:THR:HA	1:A:356:ASP:HB2	1.74	0.69
1:F:418:LEU:HD23	1:F:418:LEU:C	2.13	0.68
1:A:315:GLU:HB3	1:B:389:ARG:HG3	1.74	0.68
1:B:548:GLY:O	1:B:569:LYS:NZ	2.26	0.68
1:C:367:PHE:HE2	1:C:427:PHE:HZ	1.40	0.68
1:E:441:LYS:HZ2	1:E:468:PHE:HD2	1.41	0.68
1:A:529:PHE:CB	1:A:535:THR:HB	2.24	0.68
1:E:454:THR:O	1:E:454:THR:HG22	1.94	0.67
1:C:563:GLU:N	1:C:563:GLU:OE1	2.21	0.67
1:E:459:ARG:O	1:E:463:LYS:HG3	1.95	0.66
1:E:478:LEU:HD21	1:E:513:LEU:HD11	1.77	0.66
1:C:436:PRO:HG2	1:C:483:GLU:HG2	1.76	0.66
3:C:702:GSP:S1G	1:D:426:ARG:NH1	2.69	0.66
1:E:542:GLU:HG3	1:E:542:GLU:O	1.96	0.66
1:F:416:ILE:O	1:F:416:ILE:HG22	1.94	0.66
1:A:537:LYS:HG3	1:A:537:LYS:O	1.96	0.66
1:E:456:ASP:O	1:E:459:ARG:HG3	1.95	0.66
1:C:413:ASP:HB3	1:C:416:ILE:HG12	1.77	0.65
1:E:334:GLU:O	1:E:338:GLY:N	2.30	0.65
1:C:577:ILE:HD12	1:C:577:ILE:H	1.58	0.64
1:B:278:ILE:HD11	1:B:310:LEU:O	1.97	0.64
1:C:442:GLU:N	1:C:442:GLU:OE1	2.29	0.64
1:D:458:LYS:HA	1:D:461:ASN:ND2	2.12	0.64
1:E:323:GLU:HA	1:E:326:LEU:HD12	1.79	0.63
1:E:229:VAL:CG2	1:E:354:ILE:HD11	2.27	0.63
1:B:524:LEU:HD13	1:C:424:ARG:HD2	1.78	0.63
1:D:305:HIS:O	1:D:309:ILE:HG12	1.98	0.63
1:E:238:PRO:HA	1:E:242:TRP:CE3	2.33	0.63
1:B:220:GLY:HA2	3:C:701:GSP:PA	2.39	0.63
1:E:534:GLU:HB3	1:E:543:LYS:HE2	1.81	0.63
1:E:488:ARG:O	1:E:491:VAL:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ARG:CA	1:B:396:PRO:HA	2.29	0.62
1:F:289:LYS:O	1:F:292:PHE:HB2	1.99	0.62
1:B:314:LYS:HD3	1:C:330:ARG:HD2	1.80	0.62
1:B:537:LYS:HD2	1:B:542:GLU:CB	2.29	0.62
3:C:701:GSP:H5'2	3:C:701:GSP:H8	1.64	0.62
1:E:362:ASN:O	1:E:366:ILE:HG12	2.00	0.62
1:E:455:GLU:HA	1:E:458:LYS:CE	2.30	0.62
1:F:306:ARG:O	1:F:309:ILE:HG12	1.99	0.62
1:D:281:LYS:HZ3	1:D:311:LEU:HA	1.64	0.61
1:E:477:PHE:HE1	1:E:581:LYS:HG2	1.65	0.61
1:B:555:LEU:HD21	1:B:567:GLN:HB2	1.81	0.61
1:B:217:PRO:HG2	1:C:421:VAL:HG22	1.82	0.61
1:D:308:TYR:CE2	1:D:312:THR:HG21	2.36	0.61
1:E:439:LEU:HD11	1:E:482:LEU:HD22	1.82	0.60
1:B:390:LEU:CD1	1:B:391:PRO:HD2	2.26	0.60
1:E:491:VAL:HG23	1:E:492:VAL:HG13	1.83	0.60
1:E:440:GLU:CG	1:E:442:GLU:HG2	2.32	0.59
1:F:302:ASP:O	1:F:306:ARG:HG2	2.02	0.59
1:E:238:PRO:HA	1:E:242:TRP:HE3	1.68	0.59
1:B:217:PRO:HG2	1:C:421:VAL:CG2	2.33	0.59
1:C:560:PRO:HD3	1:D:538:TRP:CD2	2.38	0.59
1:E:342:ASP:O	1:E:345:LYS:HB2	2.02	0.59
1:D:380:LEU:HB2	1:D:400:PRO:HA	1.84	0.59
3:C:702:GSP:O1A	1:D:378:LYS:NZ	2.34	0.58
1:D:292:PHE:CZ	1:D:305:HIS:HA	2.38	0.58
1:F:287:LEU:HD13	1:F:287:LEU:C	2.23	0.58
1:A:533:TRP:O	1:A:537:LYS:N	2.26	0.58
1:A:246:THR:CA	1:A:356:ASP:HB2	2.32	0.58
1:F:224:ILE:HA	1:F:227:LYS:HB2	1.85	0.58
1:F:306:ARG:O	1:F:310:LEU:HG	2.04	0.58
1:B:312:THR:CB	1:B:316:PRO:HB3	2.34	0.58
1:E:327:ARG:NE	1:E:331:TYR:OH	2.37	0.57
1:A:444:LEU:HG	1:A:445:LYS:HG3	1.86	0.57
1:B:260:PHE:O	1:B:270:ILE:N	2.37	0.57
1:B:390:LEU:HG	1:B:391:PRO:O	2.04	0.57
1:B:511:GLU:O	1:B:515:HIS:ND1	2.36	0.57
1:D:379:ARG:NH2	1:D:403:LEU:O	2.37	0.57
1:C:511:GLU:O	1:C:515:HIS:ND1	2.37	0.57
1:E:458:LYS:H	1:E:458:LYS:HE2	1.68	0.57
1:B:389:ARG:HA	1:B:396:PRO:CB	2.34	0.57
1:F:306:ARG:HB2	1:F:328:LEU:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LYS:HG2	1:A:448:ARG:CB	2.35	0.57
1:D:289:LYS:HG3	1:D:349:PRO:HG3	1.86	0.57
1:F:287:LEU:HD23	1:F:400:PRO:HB3	1.86	0.56
1:C:577:ILE:N	1:C:577:ILE:CD1	2.68	0.56
1:D:537:LYS:NZ	1:D:542:GLU:OE2	2.37	0.56
1:D:289:LYS:CG	1:D:349:PRO:HG3	2.36	0.56
1:E:338:GLY:C	1:E:340:PRO:HD3	2.25	0.56
1:E:441:LYS:NZ	1:E:465:ASN:HA	2.21	0.56
1:E:568:LEU:C	1:E:568:LEU:HD23	2.26	0.56
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.70	0.56
1:A:447:ILE:O	1:A:450:LYS:HE3	2.06	0.56
1:C:577:ILE:H	1:C:577:ILE:CD1	2.19	0.56
1:B:318:SER:O	1:B:319:PRO:C	2.43	0.55
1:B:326:LEU:O	1:B:329:LYS:HB2	2.05	0.55
1:E:352:TYR:CD1	1:E:404:TYR:HB2	2.41	0.55
1:A:445:LYS:NZ	1:A:507:VAL:O	2.40	0.55
1:B:536:ILE:O	1:B:539:VAL:HG22	2.06	0.55
1:B:314:LYS:HD3	1:C:330:ARG:CD	2.36	0.55
1:E:233:THR:O	1:E:234:ASN:HB2	2.07	0.55
1:C:527:GLU:OE2	1:D:414:ARG:NH2	2.39	0.55
1:D:457:ARG:HG2	1:D:458:LYS:N	2.21	0.55
1:F:315:GLU:N	1:F:316:PRO:CD	2.68	0.55
1:E:455:GLU:HG2	1:E:455:GLU:O	2.06	0.55
1:B:307:LEU:HD12	1:B:307:LEU:O	2.07	0.55
1:C:377:ASP:OD2	3:C:701:GSP:O3'	2.24	0.55
1:F:210:GLN:NE2	1:F:374:LEU:O	2.38	0.55
1:E:477:PHE:CE1	1:E:581:LYS:HG2	2.41	0.54
1:E:290:GLY:HA2	1:E:349:PRO:HD2	1.89	0.54
1:E:357:GLU:HB3	1:E:360:ARG:HG3	1.90	0.54
1:A:215:GLY:O	1:A:410:ASN:ND2	2.40	0.54
1:C:570:VAL:O	1:C:570:VAL:CG2	2.56	0.54
1:E:320:THR:O	1:E:324:GLU:N	2.40	0.54
1:B:360:ARG:NH2	1:C:420:ASP:OD2	2.41	0.54
1:D:321:GLU:HA	1:D:324:GLU:CB	2.38	0.54
1:C:379:ARG:HG2	1:C:399:VAL:HG13	1.89	0.54
1:D:202:ASP:O	1:D:206:ASN:ND2	2.40	0.53
1:E:371:ILE:O	1:E:426:ARG:NE	2.39	0.53
1:F:291:LEU:HD21	1:F:336:VAL:HG12	1.89	0.53
1:A:230:VAL:O	1:A:234:ASN:ND2	2.41	0.53
1:A:517:TRP:CD1	1:A:542:GLU:HG2	2.42	0.53
1:D:511:GLU:O	1:D:515:HIS:ND1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:389:ARG:NH1	1:E:394:GLY:O	2.39	0.53
1:E:568:LEU:HD23	1:E:569:LYS:N	2.24	0.53
1:D:255:GLU:OE2	1:D:261:ARG:NH2	2.42	0.53
1:D:347:LEU:HD12	1:D:402:ASN:HB2	1.89	0.53
1:F:324:GLU:O	1:F:328:LEU:HG	2.07	0.53
1:A:460:LEU:HD21	1:A:508:GLU:HG2	1.91	0.53
1:E:448:ARG:NH1	1:E:506:ASN:HA	2.23	0.53
1:A:197:ASP:N	1:A:197:ASP:OD1	2.42	0.53
1:E:481:LEU:HD12	1:E:583:ILE:HD11	1.91	0.53
1:B:218:GLY:HA3	1:B:500:GLY:HA3	1.90	0.53
1:C:458:LYS:HA	1:C:461:ASN:HD22	1.73	0.53
1:C:258:GLU:OE1	1:C:280:LYS:NZ	2.41	0.52
1:B:560:PRO:HB3	1:C:543:LYS:HE3	1.92	0.52
1:E:488:ARG:HD3	1:E:539:VAL:HA	1.91	0.52
1:D:281:LYS:NZ	1:D:311:LEU:HA	2.23	0.52
1:E:221:LYS:O	1:E:224:ILE:HG22	2.09	0.52
1:D:517:TRP:HA	1:D:521:VAL:HG22	1.92	0.52
1:E:541:ASN:ND2	1:E:585:SER:O	2.42	0.52
1:D:389:ARG:NH1	1:D:394:GLY:O	2.43	0.52
1:A:248:HIS:CD2	1:B:421:VAL:HG21	2.45	0.52
1:C:426:ARG:NH1	3:C:701:GSP:S1G	2.78	0.52
1:D:529:PHE:HB3	1:D:532:ASP:HB3	1.92	0.52
1:F:307:LEU:O	1:F:310:LEU:HB2	2.10	0.52
1:F:421:VAL:HA	1:F:424:ARG:HD3	1.91	0.52
1:B:220:GLY:HA2	3:C:701:GSP:O3A	2.10	0.52
1:D:389:ARG:HA	1:D:396:PRO:HA	1.91	0.52
1:F:413:ASP:O	1:F:417:ALA:HB2	2.09	0.52
1:F:417:ALA:O	1:F:419:LEU:HG	2.10	0.52
1:C:204:LEU:HD12	1:C:430:ILE:HD11	1.91	0.52
1:B:327:ARG:HA	1:B:330:ARG:CG	2.40	0.51
1:C:560:PRO:HD3	1:D:538:TRP:CE3	2.45	0.51
1:E:316:PRO:HA	1:F:330:ARG:HD2	1.92	0.51
1:E:464:LEU:HA	1:E:467:LEU:HB2	1.91	0.51
1:D:555:LEU:HD13	1:E:487:VAL:HG23	1.91	0.51
1:C:494:ASP:N	1:C:494:ASP:OD1	2.44	0.51
1:D:257:ILE:HG22	1:D:258:GLU:HG2	1.91	0.51
1:A:457:ARG:HB3	1:A:457:ARG:CZ	2.39	0.51
1:C:551:PHE:O	1:C:568:LEU:HD12	2.11	0.51
1:F:202:ASP:O	1:F:206:ASN:ND2	2.41	0.51
1:F:326:LEU:HB3	1:F:330:ARG:HH21	1.76	0.51
1:D:313:LYS:NZ	1:D:317:LEU:HA	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ASP:N	1:C:202:ASP:OD1	2.42	0.51
1:C:380:LEU:HB2	1:C:400:PRO:HA	1.93	0.51
1:B:540:LEU:HD12	1:B:552:PHE:CE2	2.46	0.51
1:C:442:GLU:CD	1:C:442:GLU:H	2.09	0.51
1:E:379:ARG:HG2	1:E:399:VAL:HG23	1.93	0.51
1:E:464:LEU:HD21	1:E:508:GLU:HA	1.93	0.51
1:E:241:LYS:HA	1:E:351:PHE:CD2	2.47	0.50
1:D:307:LEU:HA	1:D:310:LEU:HD12	1.93	0.50
1:B:434:PRO:HB3	1:B:500:GLY:HA2	1.93	0.50
1:C:218:GLY:HA3	1:C:500:GLY:HA3	1.93	0.50
1:D:524:LEU:HD11	1:E:421:VAL:HG23	1.93	0.50
1:F:378:LYS:HD3	1:F:386:LEU:HD12	1.92	0.50
1:B:220:GLY:HA2	3:C:701:GSP:O5'	2.11	0.50
1:E:274:VAL:HG13	1:E:274:VAL:O	2.11	0.50
1:C:286:ALA:O	1:C:402:ASN:ND2	2.42	0.50
1:D:216:PRO:O	1:D:221:LYS:NZ	2.44	0.50
1:E:303:LYS:HA	1:E:307:LEU:HG	1.94	0.50
1:B:436:PRO:HB2	1:B:479:LYS:HG2	1.94	0.50
1:E:454:THR:O	1:E:455:GLU:HB3	2.11	0.50
1:F:416:ILE:O	1:F:416:ILE:CG2	2.59	0.50
1:B:565:ALA:HB2	1:C:491:VAL:HA	1.94	0.49
1:D:454:THR:O	1:D:457:ARG:NH2	2.38	0.49
1:F:293:GLU:OE1	1:F:293:GLU:N	2.44	0.49
1:D:436:PRO:HB3	1:D:482:LEU:HB3	1.93	0.49
1:E:554:LYS:NZ	1:E:555:LEU:O	2.44	0.49
1:A:479:LYS:NZ	1:A:479:LYS:O	2.45	0.49
1:C:202:ASP:O	1:C:206:ASN:ND2	2.45	0.49
1:E:240:ASN:C	1:E:241:LYS:HG2	2.24	0.49
1:E:533:TRP:O	1:E:537:LYS:HG3	2.11	0.49
1:D:560:PRO:HD3	1:E:538:TRP:CZ3	2.47	0.49
1:A:310:LEU:HD12	1:A:313:LYS:HD2	1.95	0.49
1:E:218:GLY:HA3	1:E:500:GLY:HA3	1.94	0.49
1:E:225:ALA:O	1:E:229:VAL:HG22	2.12	0.49
1:E:533:TRP:O	1:E:536:ILE:HG22	2.13	0.49
1:B:389:ARG:HA	1:B:396:PRO:CG	2.43	0.48
1:B:524:LEU:HB2	1:C:424:ARG:HD3	1.94	0.48
1:A:306:ARG:HD2	1:A:309:ILE:CG2	2.43	0.48
1:C:571:LEU:HD22	1:C:575:ALA:HB1	1.95	0.48
1:E:469:SER:HA	1:E:473:ASN:CG	2.33	0.48
1:E:286:ALA:HB1	1:E:402:ASN:CG	2.33	0.48
1:A:517:TRP:HZ2	1:A:540:LEU:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:439:LEU:HD23	1:E:439:LEU:N	2.28	0.48
1:A:256:PHE:HE2	1:A:388:VAL:HG21	1.79	0.47
1:B:318:SER:CB	1:B:321:GLU:CB	2.92	0.47
1:D:349:PRO:HG2	1:D:402:ASN:HD21	1.79	0.47
1:F:418:LEU:HD23	1:F:419:LEU:N	2.29	0.47
1:E:490:THR:HG22	1:E:495:ARG:CA	2.37	0.47
1:A:287:LEU:HB2	1:A:400:PRO:HB3	1.96	0.47
1:D:284:LEU:O	1:D:288:VAL:HG23	2.14	0.47
1:D:307:LEU:HD23	1:D:307:LEU:C	2.35	0.47
1:D:313:LYS:HZ3	1:D:317:LEU:HA	1.78	0.47
1:E:325:TYR:HA	1:E:328:LEU:HD12	1.97	0.47
1:E:536:ILE:O	1:E:539:VAL:HG22	2.15	0.47
1:E:359:ASN:N	1:E:359:ASN:OD1	2.45	0.47
1:E:211:VAL:HG22	1:E:428:ALA:HB3	1.96	0.47
1:A:537:LYS:CG	1:A:537:LYS:O	2.61	0.47
1:D:292:PHE:HD1	1:D:304:ILE:HD12	1.80	0.47
1:D:560:PRO:HD3	1:E:538:TRP:CE3	2.50	0.47
1:E:484:LYS:HE2	1:E:584:ILE:HG23	1.97	0.47
1:A:241:LYS:HE2	1:A:350:LYS:HG3	1.97	0.47
1:A:256:PHE:CE2	1:A:388:VAL:HG21	2.50	0.47
1:C:495:ARG:O	1:C:498:ARG:NE	2.47	0.47
1:C:462:GLU:HA	1:C:465:ASN:HB2	1.97	0.47
1:D:422:ALA:O	1:D:426:ARG:NH1	2.46	0.47
1:E:370:LEU:HB3	1:E:374:LEU:HG	1.97	0.47
1:A:522:LEU:CA	1:A:539:VAL:CB	2.89	0.46
1:E:441:LYS:HZ3	1:E:465:ASN:HA	1.79	0.46
1:B:527:GLU:HG2	1:C:424:ARG:NH2	2.30	0.46
1:C:213:LEU:HA	1:C:430:ILE:O	2.15	0.46
1:B:525:LEU:HD23	1:B:528:TYR:HD2	1.80	0.46
1:C:443:ASN:OD1	1:C:443:ASN:N	2.48	0.46
3:C:701:GSP:N9	3:C:701:GSP:C5'	2.79	0.46
1:E:375:GLU:OE2	1:E:425:ARG:NH1	2.47	0.46
1:C:418:LEU:O	1:C:424:ARG:NH2	2.48	0.46
1:F:314:LYS:C	1:F:316:PRO:HD2	2.36	0.46
1:A:440:GLU:O	1:A:444:LEU:N	2.49	0.46
1:C:219:THR:OG1	1:C:221:LYS:NZ	2.45	0.46
1:A:517:TRP:CZ2	1:A:540:LEU:HB3	2.51	0.45
1:F:411:THR:O	1:F:414:ARG:HG3	2.16	0.45
1:E:468:PHE:CD1	1:E:475:ASN:HA	2.52	0.45
1:E:411:THR:HG23	1:E:496:ASP:HB3	1.98	0.45
1:D:261:ARG:HD3	1:D:261:ARG:HA	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HH12	1:A:244:PHE:N	2.14	0.45
1:C:384:ASN:ND2	3:C:701:GSP:O3'	2.48	0.45
1:D:202:ASP:OD1	1:D:202:ASP:N	2.49	0.45
1:D:288:VAL:HG21	1:D:307:LEU:CD2	2.39	0.45
1:D:436:PRO:HG2	1:D:483:GLU:HG2	1.97	0.45
1:B:389:ARG:HA	1:B:396:PRO:HG3	1.99	0.45
1:F:287:LEU:HD11	1:F:291:LEU:HD22	1.99	0.45
1:C:425:ARG:NH1	3:C:701:GSP:O2A	2.50	0.45
1:F:375:GLU:HB2	1:F:378:LYS:HG2	1.99	0.45
1:D:287:LEU:O	1:D:291:LEU:HG	2.17	0.44
1:B:463:LYS:HD2	1:B:509:THR:HG22	2.00	0.44
1:C:320:THR:OG1	1:C:321:GLU:OE1	2.34	0.44
1:F:286:ALA:HA	1:F:351:PHE:CE1	2.52	0.44
1:E:580:LEU:O	1:E:583:ILE:HG12	2.17	0.44
1:A:517:TRP:CZ2	1:A:540:LEU:HD22	2.53	0.44
1:D:320:THR:HB	1:D:321:GLU:OE1	2.17	0.44
1:E:456:ASP:HA	1:E:459:ARG:HG3	2.00	0.44
1:F:276:ASP:OD2	1:F:329:LYS:NZ	2.50	0.44
1:F:291:LEU:HD21	1:F:336:VAL:CG1	2.47	0.44
1:D:519:TYR:HE1	1:E:430:ILE:HG23	1.82	0.44
1:E:455:GLU:HA	1:E:458:LYS:NZ	2.33	0.44
1:F:380:LEU:HB2	1:F:400:PRO:HA	1.99	0.44
1:A:241:LYS:HB2	1:A:351:PHE:CE1	2.53	0.43
1:B:320:THR:O	1:B:323:GLU:HB2	2.18	0.43
1:C:436:PRO:HB3	1:C:482:LEU:HB3	2.00	0.43
1:E:281:LYS:NZ	1:E:327:ARG:HH22	2.15	0.43
1:E:551:PHE:O	1:E:568:LEU:HA	2.18	0.43
1:D:486:ASN:HB3	1:D:498:ARG:HD2	2.00	0.43
1:E:348:THR:CB	1:E:349:PRO:HD2	2.48	0.43
1:B:246:THR:HG22	1:B:356:ASP:HB3	2.00	0.43
1:B:356:ASP:OD2	1:C:372:THR:OG1	2.34	0.43
1:E:276:ASP:N	1:E:276:ASP:OD1	2.50	0.43
1:B:531:ASN:HD21	1:C:494:ASP:HA	1.83	0.43
1:A:457:ARG:CG	1:A:457:ARG:HH11	2.31	0.43
1:B:331:TYR:O	1:B:332:LEU:C	2.57	0.43
1:D:461:ASN:OD1	1:D:462:GLU:N	2.51	0.43
1:E:248:HIS:CE1	1:E:250:SER:HB2	2.54	0.43
1:F:306:ARG:HB2	1:F:328:LEU:HD11	2.00	0.43
1:C:261:ARG:HA	1:C:261:ARG:HD3	1.75	0.43
1:D:420:ASP:HB3	1:D:423:LEU:HB3	2.00	0.43
1:E:343:LYS:HB2	1:E:343:LYS:HE3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448:ARG:HD3	1:E:460:LEU:HD21	2.00	0.43
1:A:324:GLU:HG3	1:A:327:ARG:HE	1.84	0.43
1:E:491:VAL:HG21	1:E:538:TRP:CZ3	2.53	0.43
1:A:302:ASP:OD1	1:A:303:LYS:N	2.51	0.43
1:B:436:PRO:C	1:B:438:PHE:N	2.70	0.43
1:E:221:LYS:HG2	1:E:432:VAL:HG21	2.01	0.43
1:E:245:ILE:CG2	1:E:355:ILE:HG12	2.49	0.43
1:E:581:LYS:HA	1:E:584:ILE:HD12	2.00	0.43
1:E:434:PRO:HB3	1:E:500:GLY:HA2	2.01	0.43
1:F:305:HIS:O	1:F:309:ILE:HG23	2.19	0.43
1:D:388:VAL:O	1:D:397:PHE:N	2.52	0.42
1:E:522:LEU:HG	1:E:526:MET:HE2	2.01	0.42
1:C:560:PRO:HD3	1:D:538:TRP:CE2	2.55	0.42
1:A:440:GLU:OE2	1:A:476:TYR:N	2.52	0.42
1:D:379:ARG:HG2	1:D:399:VAL:HG23	2.01	0.42
1:D:211:VAL:HG12	1:D:406:ILE:HG12	2.02	0.42
1:E:554:LYS:HE2	1:E:564:GLU:CB	2.49	0.42
1:B:525:LEU:HB3	1:B:536:ILE:CD1	2.48	0.42
1:C:276:ASP:OD2	1:C:325:TYR:OH	2.35	0.42
1:D:288:VAL:HG12	1:D:292:PHE:CE1	2.54	0.42
1:E:334:GLU:O	1:E:338:GLY:CA	2.67	0.42
1:E:491:VAL:CG2	1:E:538:TRP:HZ3	2.32	0.42
1:A:286:ALA:HA	1:A:351:PHE:HD2	1.84	0.42
1:E:252:SER:HB3	1:E:255:GLU:HG3	2.01	0.42
1:B:385:GLN:CD	1:B:385:GLN:C	2.78	0.42
1:E:323:GLU:O	1:E:326:LEU:HB2	2.19	0.42
1:A:206:ASN:OD1	1:A:379:ARG:NH1	2.53	0.42
1:B:410:ASN:ND2	1:B:413:ASP:OD2	2.53	0.42
1:C:257:ILE:HG22	1:C:258:GLU:HG2	2.02	0.42
1:F:257:ILE:HD11	1:F:370:LEU:HD13	2.02	0.42
1:E:244:PHE:HD2	1:F:388:VAL:HG23	1.85	0.42
1:A:489:ILE:HD12	1:A:493:LYS:HG2	2.02	0.42
1:D:439:LEU:HA	1:D:439:LEU:HD23	1.91	0.42
1:E:454:THR:O	1:E:454:THR:CG2	2.63	0.42
1:E:518:TYR:OH	1:E:571:LEU:N	2.53	0.42
1:C:488:ARG:HD3	1:C:539:VAL:HA	2.02	0.41
1:A:223:TRP:CZ3	1:A:450:LYS:HE2	2.55	0.41
1:E:549:ASN:OD1	1:E:579:ALA:HB2	2.19	0.41
1:C:410:ASN:HD21	1:C:412:ALA:HB3	1.86	0.41
1:D:222:THR:OG1	3:D:700:GSP:O1B	2.38	0.41
1:D:494:ASP:N	1:D:494:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:571:LEU:C	1:E:576:PHE:HB2	2.40	0.41
1:E:448:ARG:O	1:E:448:ARG:HG2	2.20	0.41
1:C:274:VAL:HG11	1:C:393:SER:HB3	2.02	0.41
1:E:456:ASP:HB3	1:E:459:ARG:NE	2.25	0.41
1:B:327:ARG:O	1:B:330:ARG:HG3	2.20	0.41
3:C:701:GSP:N9	3:C:701:GSP:H5'1	2.35	0.41
1:C:347:LEU:HD12	1:C:402:ASN:HB2	2.02	0.41
1:C:560:PRO:HG2	1:C:561:ASN:H	1.86	0.41
1:F:243:GLU:HB2	1:F:282:ILE:HD12	2.03	0.41
1:E:317:LEU:HD12	1:E:317:LEU:HA	1.95	0.41
1:E:478:LEU:CD2	1:E:513:LEU:HD11	2.49	0.41
1:E:553:GLU:O	1:E:567:GLN:N	2.53	0.41
1:A:237:THR:HG23	1:A:240:ASN:OD1	2.20	0.41
1:C:310:LEU:HD13	1:C:325:TYR:HB2	2.01	0.41
1:A:494:ASP:OD1	1:A:494:ASP:N	2.53	0.41
1:D:522:LEU:HA	1:D:522:LEU:HD23	1.89	0.41
1:B:327:ARG:O	1:B:330:ARG:N	2.54	0.40
1:C:437:GLU:CD	1:C:437:GLU:H	2.24	0.40
1:C:454:THR:HG22	1:C:455:GLU:H	1.86	0.40
1:D:289:LYS:HE2	1:D:308:TYR:CE1	2.56	0.40
1:D:484:LYS:HZ3	1:D:488:ARG:HH12	1.69	0.40
1:C:533:TRP:HA	1:C:536:ILE:HG22	2.02	0.40
1:E:440:GLU:O	1:E:444:LEU:N	2.48	0.40
1:B:420:ASP:OD2	1:B:423:LEU:N	2.54	0.40
1:C:456:ASP:OD1	1:C:456:ASP:N	2.48	0.40
1:F:292:PHE:CE1	1:F:304:ILE:HG22	2.56	0.40
1:F:350:LYS:HA	1:F:402:ASN:HB2	2.03	0.40
1:C:470:LYS:HA	1:C:470:LYS:HD3	1.89	0.40
1:F:295:GLU:O	1:F:299:ILE:N	2.55	0.40
1:C:433:GLU:OE2	1:C:495:ARG:NH2	2.54	0.40
1:E:246:THR:HB	1:F:369:GLU:HG3	2.03	0.40
1:E:323:GLU:HA	1:E:326:LEU:HB2	2.04	0.40
3:E:700:GSP:PG	1:F:426:ARG:HH12	2.44	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	307/428 (72%)	275 (90%)	32 (10%)	0	100 100
1	B	353/428 (82%)	338 (96%)	15 (4%)	0	100 100
1	C	369/428 (86%)	353 (96%)	16 (4%)	0	100 100
1	D	377/428 (88%)	358 (95%)	19 (5%)	0	100 100
1	E	382/428 (89%)	360 (94%)	22 (6%)	0	100 100
1	F	233/428 (54%)	224 (96%)	9 (4%)	0	100 100
All	All	2021/2568 (79%)	1908 (94%)	113 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	237/385 (62%)	237 (100%)	0	100 100
1	B	237/385 (62%)	235 (99%)	2 (1%)	81 92
1	C	302/385 (78%)	299 (99%)	3 (1%)	76 90
1	D	302/385 (78%)	302 (100%)	0	100 100
1	E	285/385 (74%)	279 (98%)	6 (2%)	53 80
1	F	168/385 (44%)	168 (100%)	0	100 100
All	All	1531/2310 (66%)	1520 (99%)	11 (1%)	84 93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	529	PHE
1	B	552	PHE
1	C	437	GLU
1	C	442	GLU
1	C	443	ASN
1	E	229	VAL
1	E	251	TYR
1	E	257	ILE
1	E	356	ASP
1	E	359	ASN
1	E	467	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	C	248	HIS
1	C	384	ASN
1	C	461	ASN
1	C	501	HIS
1	E	443	ASN

5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	GSP	C	701	2	26,34,34	1.11	1 (3%)	28,54,54	2.34	5 (17%)
3	GSP	C	702	2	26,34,34	1.12	1 (3%)	28,54,54	2.42	5 (17%)
3	GSP	D	700	2	26,34,34	1.12	1 (3%)	28,54,54	2.30	5 (17%)
3	GSP	E	700	2	26,34,34	1.11	1 (3%)	28,54,54	2.34	6 (21%)

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	GSP	C	701	2	-	5/17/38/38	0/3/3/3
3	GSP	C	702	2	-	1/17/38/38	0/3/3/3
3	GSP	D	700	2	-	0/17/38/38	0/3/3/3
3	GSP	E	700	2	-	0/17/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	700	GSP	C6-N1	3.95	1.39	1.33
3	C	702	GSP	C6-N1	3.94	1.39	1.33
3	E	700	GSP	C6-N1	3.92	1.39	1.33
3	C	701	GSP	C6-N1	3.85	1.39	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	GSP	C5-C6-N1	-8.81	111.38	123.43
3	D	700	GSP	C5-C6-N1	-8.78	111.42	123.43
3	C	702	GSP	C5-C6-N1	-8.76	111.45	123.43
3	E	700	GSP	C5-C6-N1	-8.73	111.49	123.43
3	D	700	GSP	C6-N1-C2	5.83	125.19	115.93
3	C	701	GSP	C6-N1-C2	5.82	125.18	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	700	GSP	C6-N1-C2	5.80	125.15	115.93
3	C	702	GSP	C6-N1-C2	5.77	125.11	115.93
3	C	702	GSP	PA-O3A-PB	-4.59	117.07	132.83
3	C	701	GSP	C2-N3-C4	-2.93	112.02	115.36
3	D	700	GSP	C2-N3-C4	-2.92	112.02	115.36
3	E	700	GSP	C2-N3-C4	-2.84	112.11	115.36
3	C	702	GSP	C2-N3-C4	-2.77	112.19	115.36
3	D	700	GSP	N3-C2-N1	-2.70	123.62	127.22
3	C	702	GSP	N3-C2-N1	-2.67	123.66	127.22
3	E	700	GSP	N3-C2-N1	-2.67	123.67	127.22
3	C	701	GSP	N3-C2-N1	-2.61	123.74	127.22
3	D	700	GSP	PA-O3A-PB	-2.59	123.94	132.83
3	C	701	GSP	O4'-C1'-C2'	-2.56	103.18	106.93
3	E	700	GSP	PA-O3A-PB	-2.55	124.06	132.83
3	E	700	GSP	O4'-C1'-C2'	-2.35	103.48	106.93

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	701	GSP	C5'-O5'-PA-O3A
3	C	701	GSP	O4'-C4'-C5'-O5'
3	C	701	GSP	C3'-C4'-C5'-O5'
3	C	701	GSP	C4'-C5'-O5'-PA
3	C	701	GSP	C5'-O5'-PA-O1A
3	C	702	GSP	PB-O3B-PG-O2G

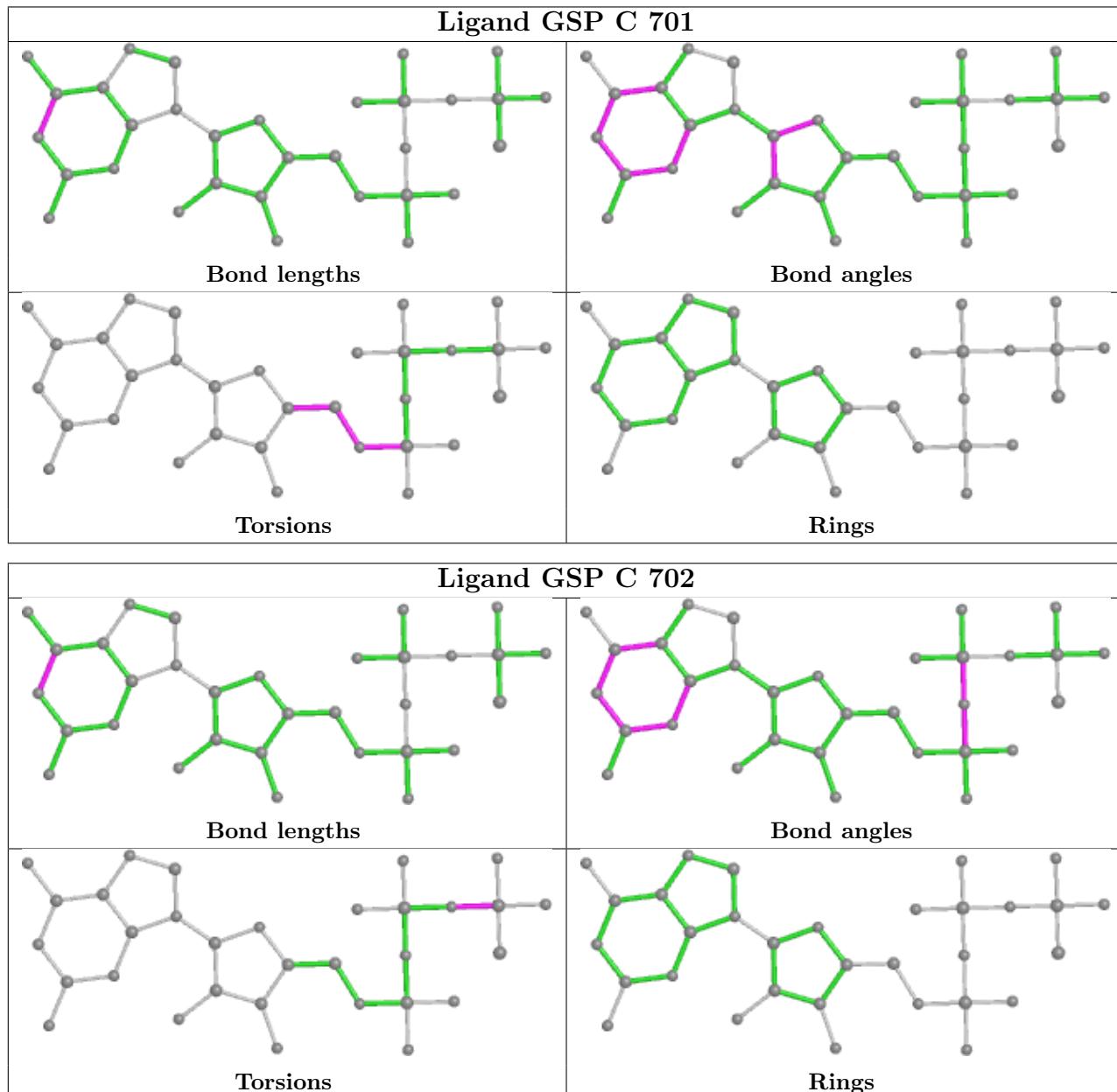
There are no ring outliers.

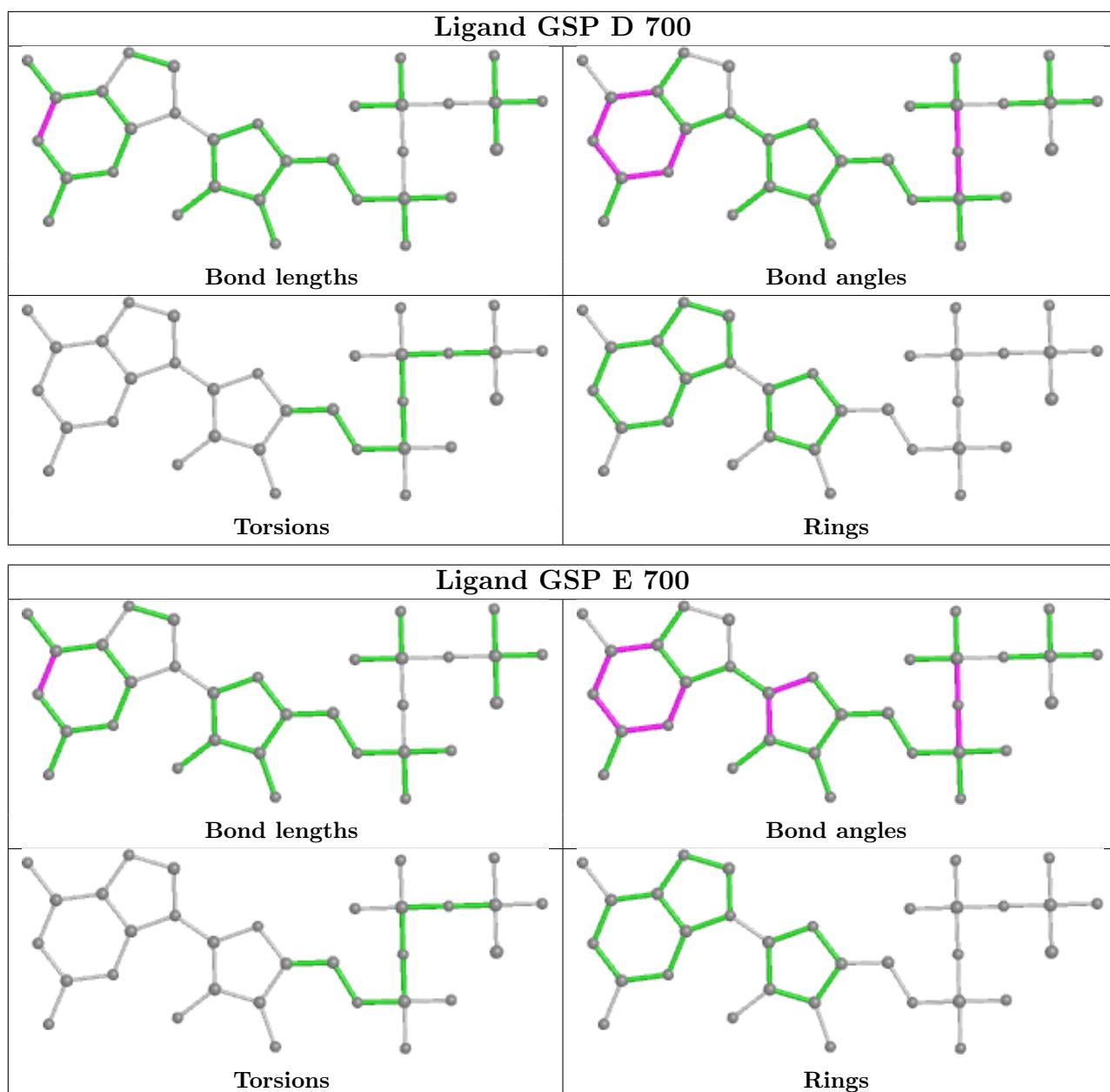
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	701	GSP	14	0
3	C	702	GSP	2	0
3	D	700	GSP	1	0
3	E	700	GSP	1	0

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

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





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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	321/428 (75%)	3.48	164 (51%) 0 0	70, 211, 232, 246	0
1	B	365/428 (85%)	0.51	35 (9%) 8 4	30, 119, 167, 186	0
1	C	375/428 (87%)	0.58	37 (9%) 7 4	46, 103, 140, 175	0
1	D	381/428 (89%)	0.61	36 (9%) 8 5	77, 108, 140, 155	0
1	E	384/428 (89%)	0.35	30 (7%) 13 7	30, 114, 151, 187	0
1	F	235/428 (54%)	0.48	22 (9%) 8 5	30, 119, 156, 170	0
All	All	2061/2568 (80%)	0.97	324 (15%) 2 1	30, 118, 219, 246	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	SER	22.6
1	A	399	VAL	21.1
1	A	317	LEU	19.1
1	A	406	ILE	17.2
1	A	519	TYR	16.9
1	A	280	LYS	16.0
1	A	358	ILE	15.8
1	A	381	GLY	14.8
1	A	216	PRO	14.7
1	A	572	GLU	14.2
1	A	476	TYR	13.7
1	A	424	ARG	13.6
1	A	359	ASN	13.3
1	A	333	TRP	13.2
1	C	271	ARG	12.9
1	A	281	LYS	12.7
1	A	322	TYR	12.4
1	A	419	LEU	11.8
1	A	400	PRO	11.5

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Mol	Chain	Res	Type	RSRZ
1	A	360	ARG	11.3
1	A	420	ASP	11.1
1	A	217	PRO	11.0
1	A	417	ALA	10.7
1	A	211	VAL	10.6
1	A	277	GLY	10.6
1	A	418	LEU	10.5
1	A	390	LEU	10.2
1	A	278	ILE	10.1
1	A	421	VAL	10.0
1	A	409	MET	9.3
1	A	205	LEU	9.1
1	A	215	GLY	9.0
1	A	391	PRO	8.9
1	B	387	ILE	8.8
1	A	352	TYR	8.8
1	A	370	LEU	8.6
1	A	316	PRO	8.5
1	A	288	VAL	8.4
1	A	434	PRO	8.2
1	A	573	GLY	8.2
1	A	212	ILE	8.2
1	A	432	VAL	8.0
1	A	279	PHE	7.5
1	A	528	TYR	7.5
1	A	515	HIS	7.4
1	A	516	VAL	7.3
1	A	385	GLN	7.3
1	A	334	GLU	7.2
1	A	541	ASN	7.2
1	B	388	VAL	7.1
1	D	270	ILE	7.0
1	A	354	ILE	6.8
1	A	465	ASN	6.8
1	A	425	ARG	6.7
1	A	410	ASN	6.7
1	A	374	LEU	6.6
1	A	366	ILE	6.6
1	A	369	GLU	6.6
1	A	292	PHE	6.5
1	A	439	LEU	6.5
1	A	405	ILE	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	6.4
1	A	377	ASP	6.3
1	A	384	ASN	6.3
1	A	204	LEU	6.2
1	A	319	PRO	6.2
1	A	291	LEU	6.1
1	A	214	TYR	6.1
1	B	239	GLY	6.1
1	A	571	LEU	5.9
1	A	331	TYR	5.8
1	A	570	VAL	5.8
1	A	332	LEU	5.8
1	A	396	PRO	5.7
1	A	368	GLY	5.6
1	D	240	ASN	5.6
1	A	513	LEU	5.6
1	A	240	ASN	5.5
1	A	389	ARG	5.5
1	F	270	ILE	5.5
1	A	449	GLU	5.4
1	A	503	TYR	5.3
1	E	304	ILE	5.3
1	A	353	LEU	5.2
1	A	401	PRO	5.1
1	A	422	ALA	5.1
1	E	296	ASP	5.1
1	F	246	THR	5.0
1	B	257	ILE	5.0
1	A	336	VAL	5.0
1	A	444	LEU	4.9
1	E	562	GLY	4.9
1	A	527	GLU	4.9
1	A	447	ILE	4.9
1	A	414	ARG	4.9
1	F	220	GLY	4.9
1	A	487	VAL	4.8
1	E	392	TYR	4.8
1	A	482	LEU	4.7
1	C	270	ILE	4.7
1	D	243	GLU	4.7
1	A	338	GLY	4.7
1	F	405	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	376	LYS	4.6
1	A	222	THR	4.6
1	A	438	PHE	4.6
1	C	579	ALA	4.6
1	A	402	ASN	4.5
1	A	375	GLU	4.5
1	B	361	GLY	4.4
1	B	403	LEU	4.4
1	A	483	GLU	4.3
1	E	305	HIS	4.3
1	A	485	ILE	4.3
1	A	218	GLY	4.3
1	B	348	THR	4.3
1	B	447	ILE	4.2
1	A	497	HIS	4.2
1	A	443	ASN	4.1
1	C	576	PHE	4.1
1	A	320	THR	4.1
1	A	224	ILE	4.1
1	A	243	GLU	4.1
1	A	219	THR	4.0
1	B	421	VAL	4.0
1	E	298	THR	4.0
1	C	510	VAL	4.0
1	E	565	ALA	4.0
1	C	464	LEU	4.0
1	C	471	LEU	3.9
1	A	531	ASN	3.9
1	D	239	GLY	3.9
1	C	231	GLU	3.9
1	A	452	LEU	3.9
1	A	484	LYS	3.9
1	B	252	SER	3.9
1	A	517	TRP	3.9
1	C	325	TYR	3.8
1	C	507	VAL	3.8
1	A	329	LYS	3.8
1	B	444	LEU	3.8
1	B	406	ILE	3.8
1	A	492	VAL	3.8
1	B	354	ILE	3.7
1	B	371	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	492	VAL	3.7
1	E	571	LEU	3.7
1	F	414	ARG	3.7
1	A	397	PHE	3.7
1	A	481	LEU	3.7
1	D	238	PRO	3.6
1	F	245	ILE	3.6
1	A	433	GLU	3.6
1	D	271	ARG	3.6
1	A	506	ASN	3.6
1	A	435	ARG	3.6
1	A	303	LYS	3.5
1	C	450	LYS	3.5
1	F	269	LYS	3.5
1	D	308	TYR	3.5
1	A	202	ASP	3.5
1	A	305	HIS	3.5
1	A	343	LYS	3.5
1	E	297	ALA	3.4
1	A	378	LYS	3.4
1	B	422	ALA	3.4
1	A	337	GLY	3.3
1	A	461	ASN	3.3
1	A	361	GLY	3.3
1	C	513	LEU	3.3
1	F	251	TYR	3.2
1	A	290	GLY	3.2
1	A	233	THR	3.2
1	D	427	PHE	3.2
1	E	563	GLU	3.2
1	A	448	ARG	3.2
1	A	379	ARG	3.2
1	B	316	PRO	3.2
1	E	510	VAL	3.1
1	A	536	ILE	3.1
1	A	325	TYR	3.1
1	E	285	ARG	3.1
1	F	263	ARG	3.0
1	A	342	ASP	3.0
1	C	392	TYR	3.0
1	A	498	ARG	3.0
1	C	348	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	393	SER	3.0
1	A	459	ARG	3.0
1	E	265	ASP	3.0
1	F	400	PRO	3.0
1	C	263	ARG	3.0
1	A	416	ILE	2.9
1	B	392	TYR	2.9
1	E	204	LEU	2.9
1	A	478	LEU	2.9
1	D	568	LEU	2.9
1	A	514	HIS	2.8
1	D	223	TRP	2.8
1	E	294	LEU	2.8
1	A	328	LEU	2.8
1	A	415	SER	2.8
1	D	387	ILE	2.8
1	E	387	ILE	2.8
1	D	386	LEU	2.8
1	C	444	LEU	2.8
1	A	357	GLU	2.7
1	B	502	SER	2.7
1	E	310	LEU	2.7
1	D	477	PHE	2.7
1	A	445	LYS	2.7
1	B	209	GLY	2.7
1	C	264	THR	2.7
1	A	201	VAL	2.7
1	A	373	LEU	2.7
1	B	230	VAL	2.7
1	E	564	GLU	2.7
1	E	229	VAL	2.7
1	A	442	GLU	2.6
1	D	471	LEU	2.6
1	A	454	THR	2.6
1	A	505	LEU	2.6
1	F	240	ASN	2.6
1	B	398	ALA	2.6
1	E	398	ALA	2.6
1	E	329	LYS	2.6
1	A	486	ASN	2.6
1	A	408	THR	2.6
1	C	452	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	200	ARG	2.6
1	C	578	GLY	2.5
1	D	504	PHE	2.5
1	C	224	ILE	2.5
1	C	497	HIS	2.5
1	A	289	LYS	2.5
1	C	327	ARG	2.5
1	A	321	GLU	2.5
1	A	464	LEU	2.5
1	E	242	TRP	2.5
1	F	356	ASP	2.5
1	C	508	GLU	2.5
1	C	509	THR	2.5
1	D	547	HIS	2.5
1	D	291	LEU	2.5
1	C	482	LEU	2.4
1	E	386	LEU	2.4
1	C	525	LEU	2.4
1	E	331	TYR	2.4
1	E	291	LEU	2.4
1	C	463	LYS	2.4
1	B	307	LEU	2.4
1	B	317	LEU	2.4
1	A	566	TYR	2.4
1	D	566	TYR	2.4
1	F	406	ILE	2.4
1	E	320	THR	2.4
1	C	451	LYS	2.4
1	D	550	VAL	2.3
1	B	309	ILE	2.3
1	F	213	LEU	2.3
1	D	438	PHE	2.3
1	A	574	ASP	2.3
1	A	380	LEU	2.3
1	A	540	LEU	2.3
1	A	568	LEU	2.3
1	B	391	PRO	2.3
1	D	493	LYS	2.3
1	C	467	LEU	2.3
1	F	411	THR	2.3
1	B	308	TYR	2.3
1	F	326	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	299	ILE	2.3
1	F	415	SER	2.3
1	D	352	TYR	2.3
1	D	292	PHE	2.3
1	A	313	LYS	2.2
1	F	386	LEU	2.2
1	C	539	VAL	2.2
1	D	403	LEU	2.2
1	C	230	VAL	2.2
1	A	413	ASP	2.2
1	D	212	ILE	2.2
1	F	216	PRO	2.2
1	C	322	TYR	2.2
1	A	446	LYS	2.2
1	B	281	LYS	2.2
1	A	411	THR	2.2
1	E	489	ILE	2.2
1	B	446	LYS	2.2
1	A	311	LEU	2.2
1	B	370	LEU	2.2
1	E	377	ASP	2.2
1	C	449	GLU	2.2
1	F	354	ILE	2.1
1	B	255	GLU	2.1
1	C	393	SER	2.1
1	A	480	THR	2.1
1	A	532	ASP	2.1
1	D	213	LEU	2.1
1	D	439	LEU	2.1
1	A	383	GLU	2.1
1	D	371	ILE	2.1
1	F	234	ASN	2.1
1	B	256	PHE	2.1
1	C	439	LEU	2.1
1	C	583	ILE	2.1
1	A	326	LEU	2.1
1	E	295	GLU	2.1
1	E	393	SER	2.1
1	A	437	GLU	2.1
1	A	523	PRO	2.1
1	D	434	PRO	2.1
1	C	519	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	549	ASN	2.1
1	A	520	GLU	2.1
1	B	504	PHE	2.1
1	D	358	ILE	2.0
1	D	529	PHE	2.0
1	A	518	TYR	2.0
1	B	389	ARG	2.0
1	B	576	PHE	2.0
1	D	541	ASN	2.0
1	D	221	LYS	2.0
1	D	311	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

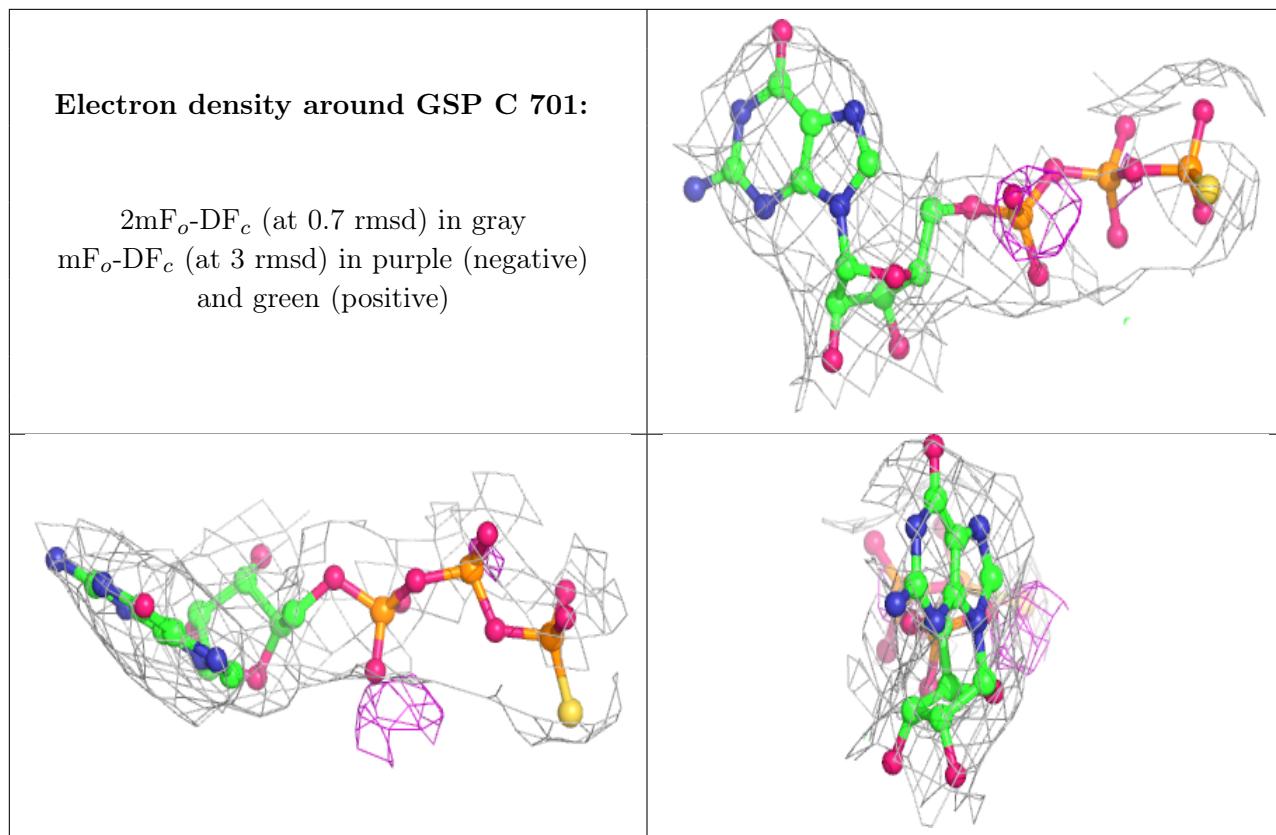
There are no monosaccharides in this entry.

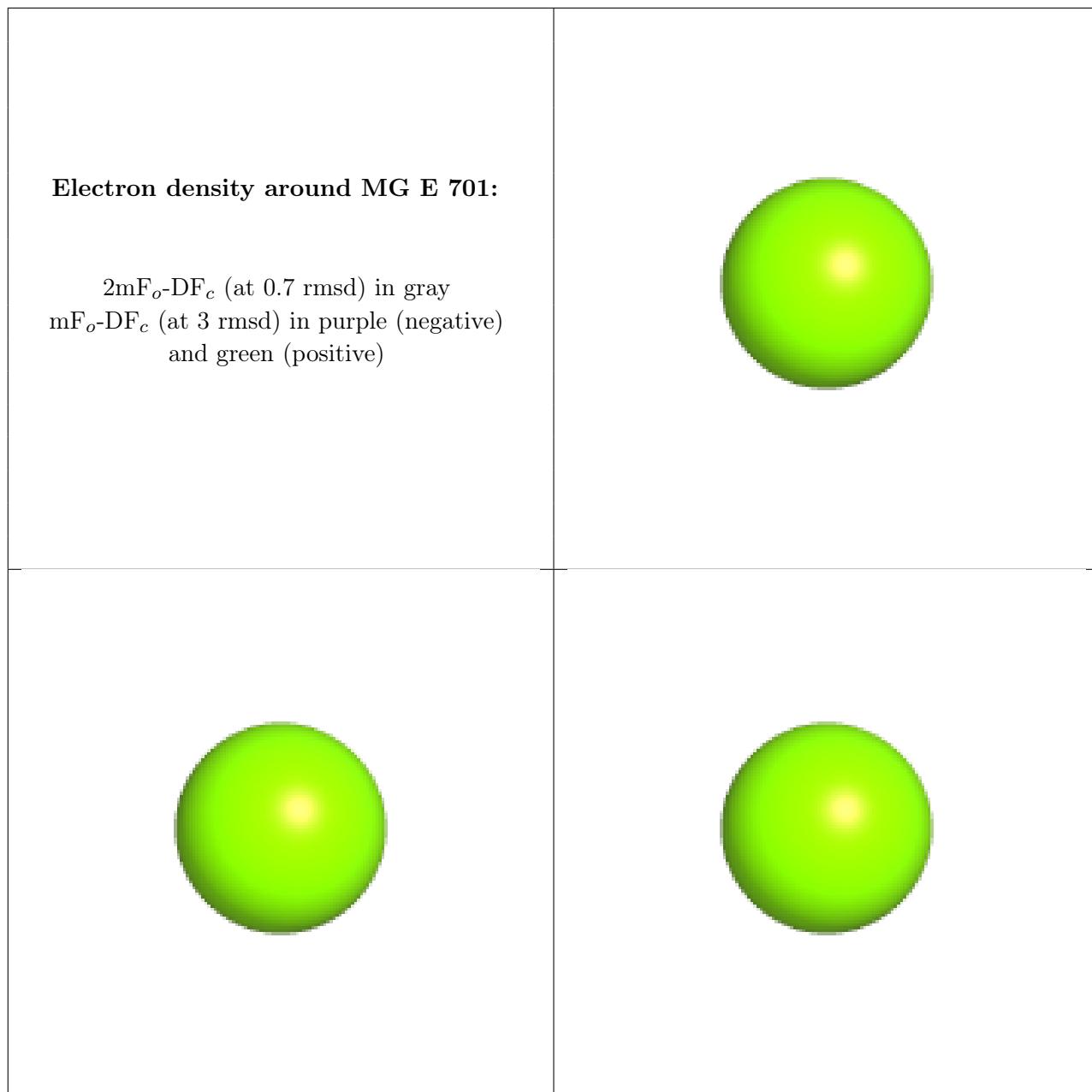
6.4 Ligands [\(i\)](#)

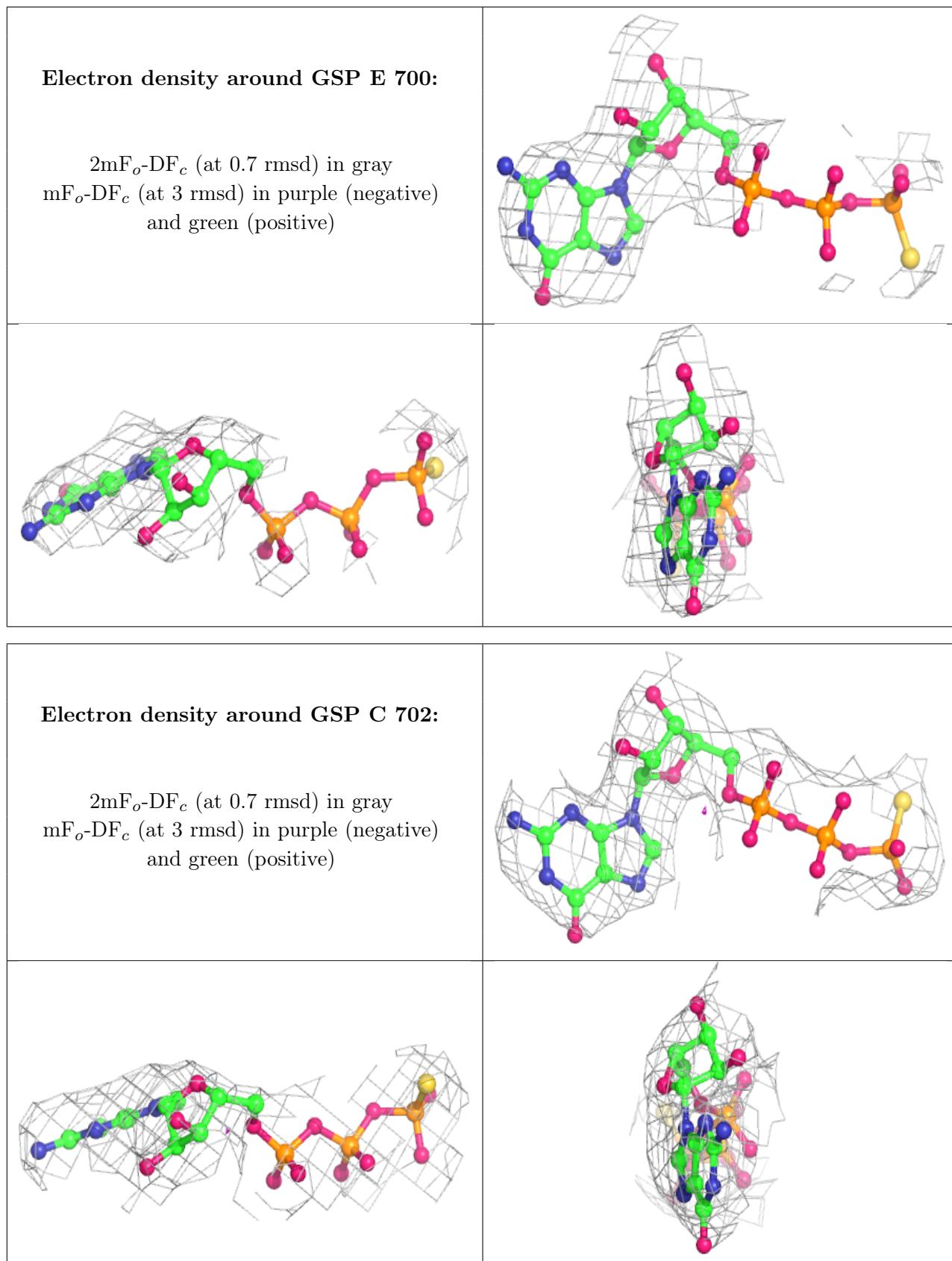
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

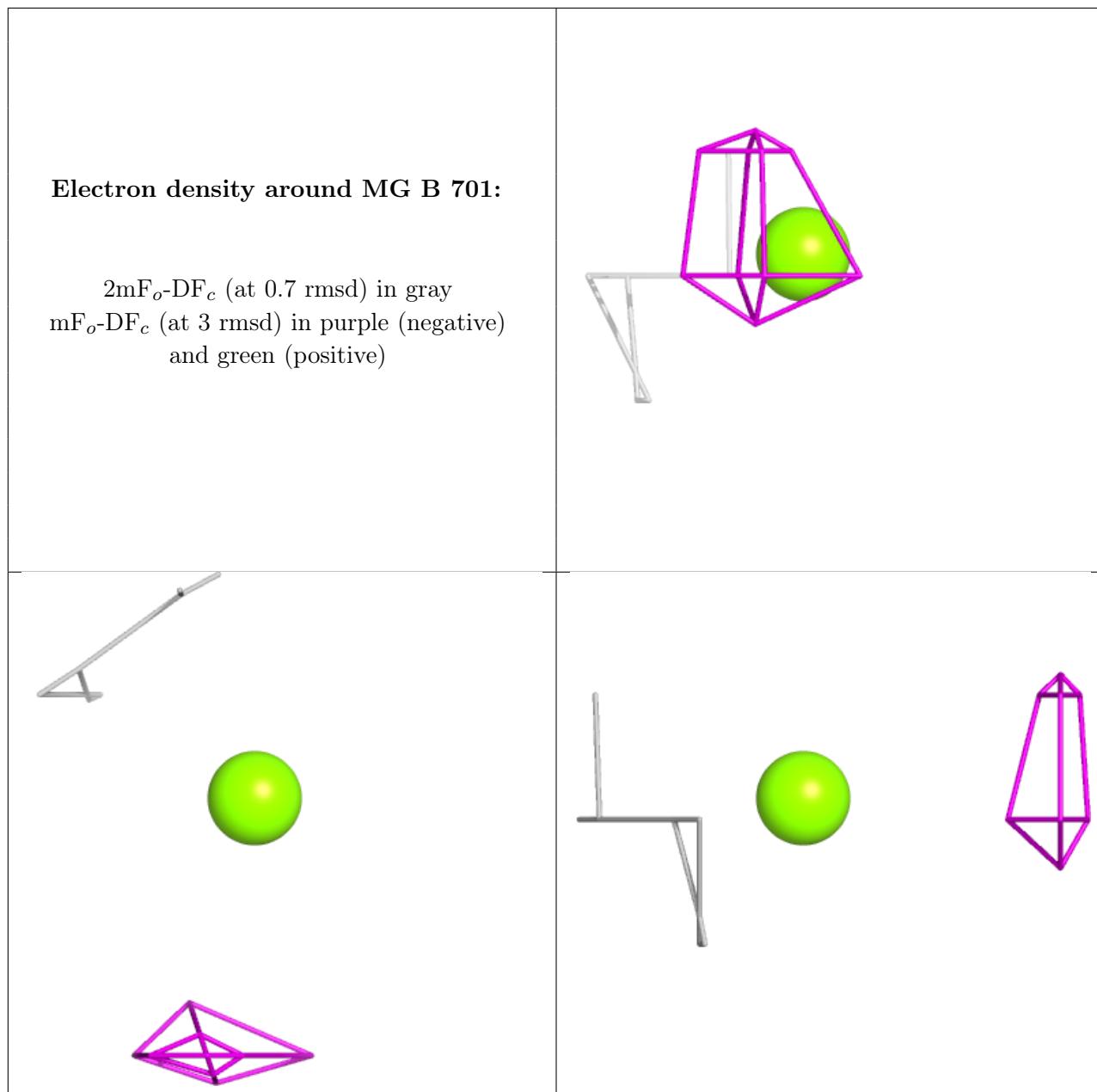
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GSP	C	701	32/32	0.88	0.19	120,120,120,120	0
2	MG	E	701	1/1	0.90	0.18	100,100,100,100	0
3	GSP	E	700	32/32	0.93	0.17	113,113,113,113	0
3	GSP	C	702	32/32	0.93	0.18	101,101,101,101	0
2	MG	B	701	1/1	0.93	0.06	115,115,115,115	0
2	MG	D	701	1/1	0.94	0.15	84,84,84,84	0
3	GSP	D	700	32/32	0.96	0.19	107,107,107,107	0
2	MG	C	703	1/1	0.98	0.13	80,80,80,80	0

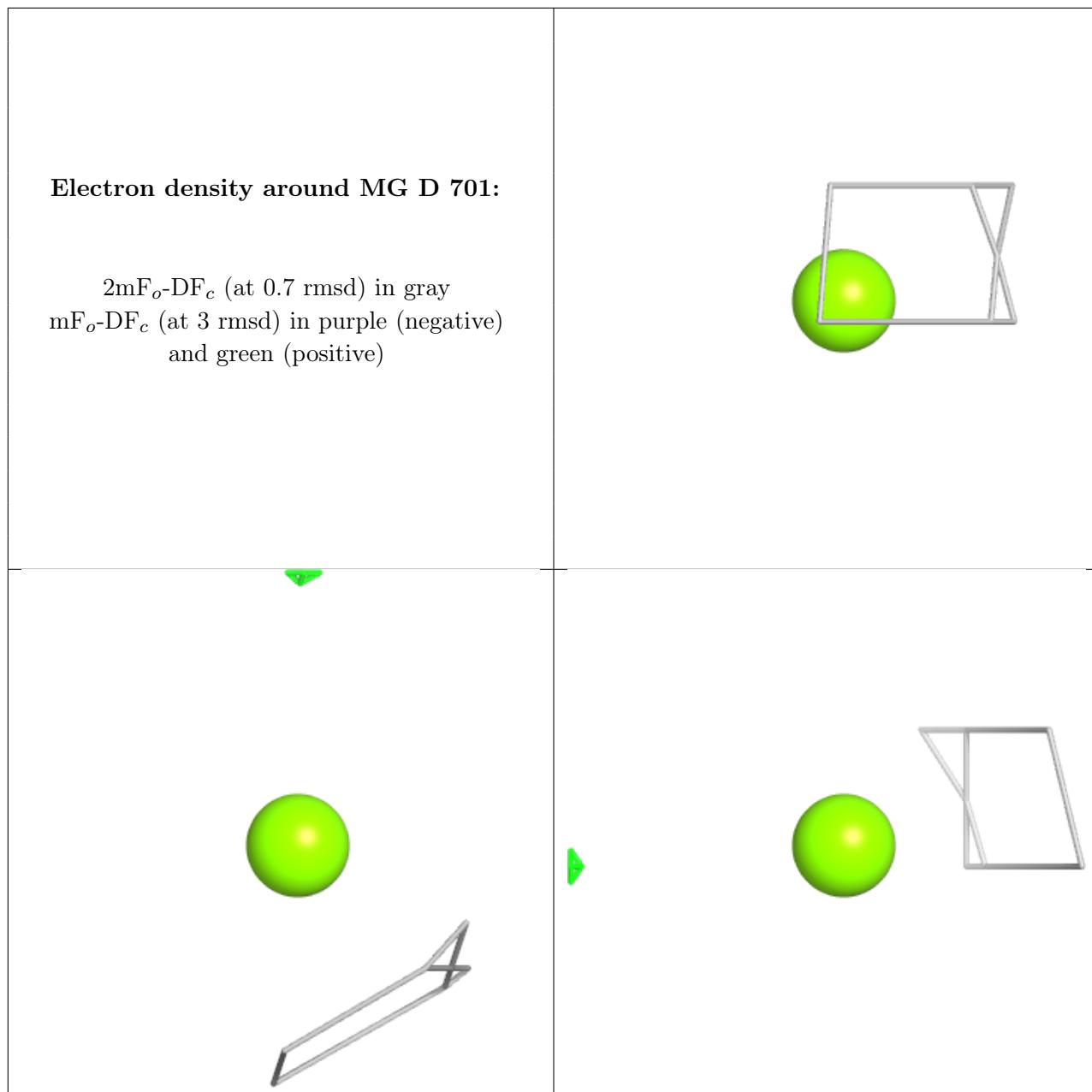
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

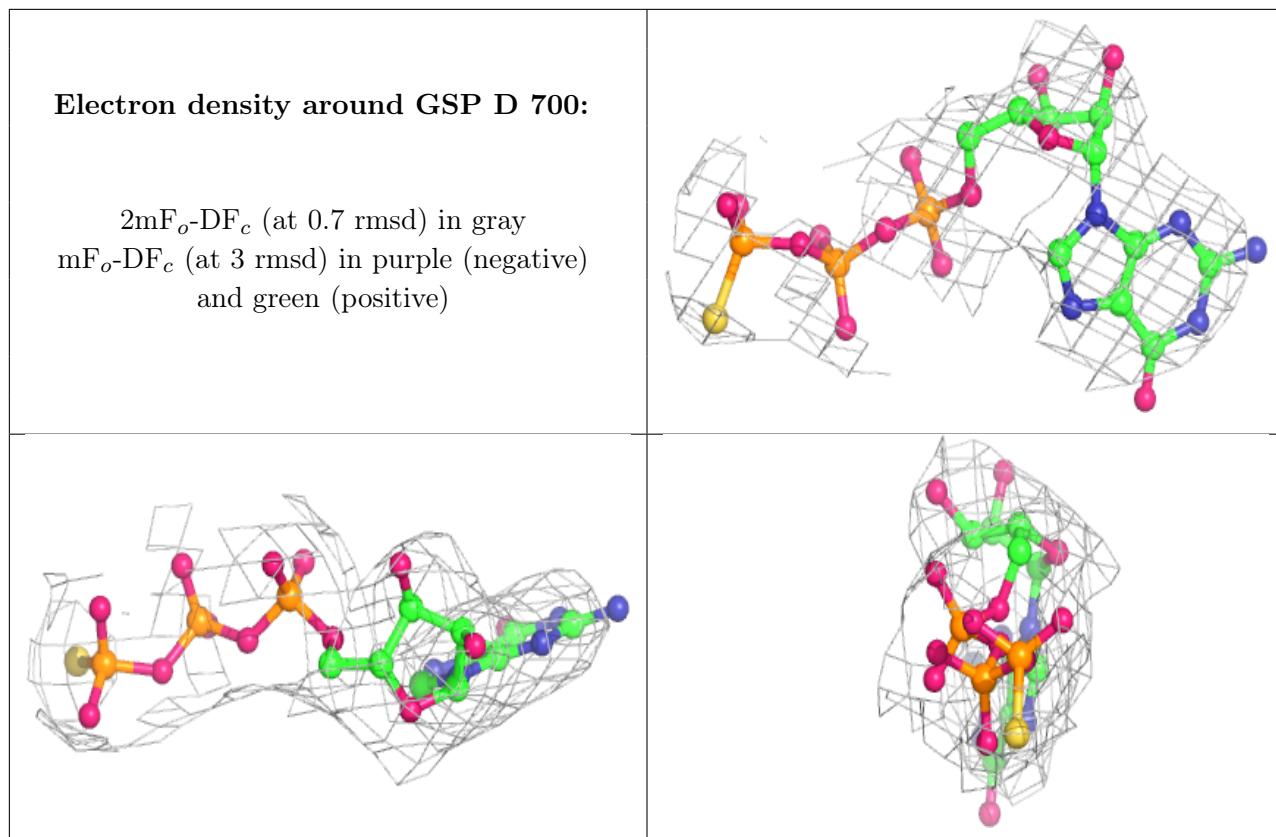


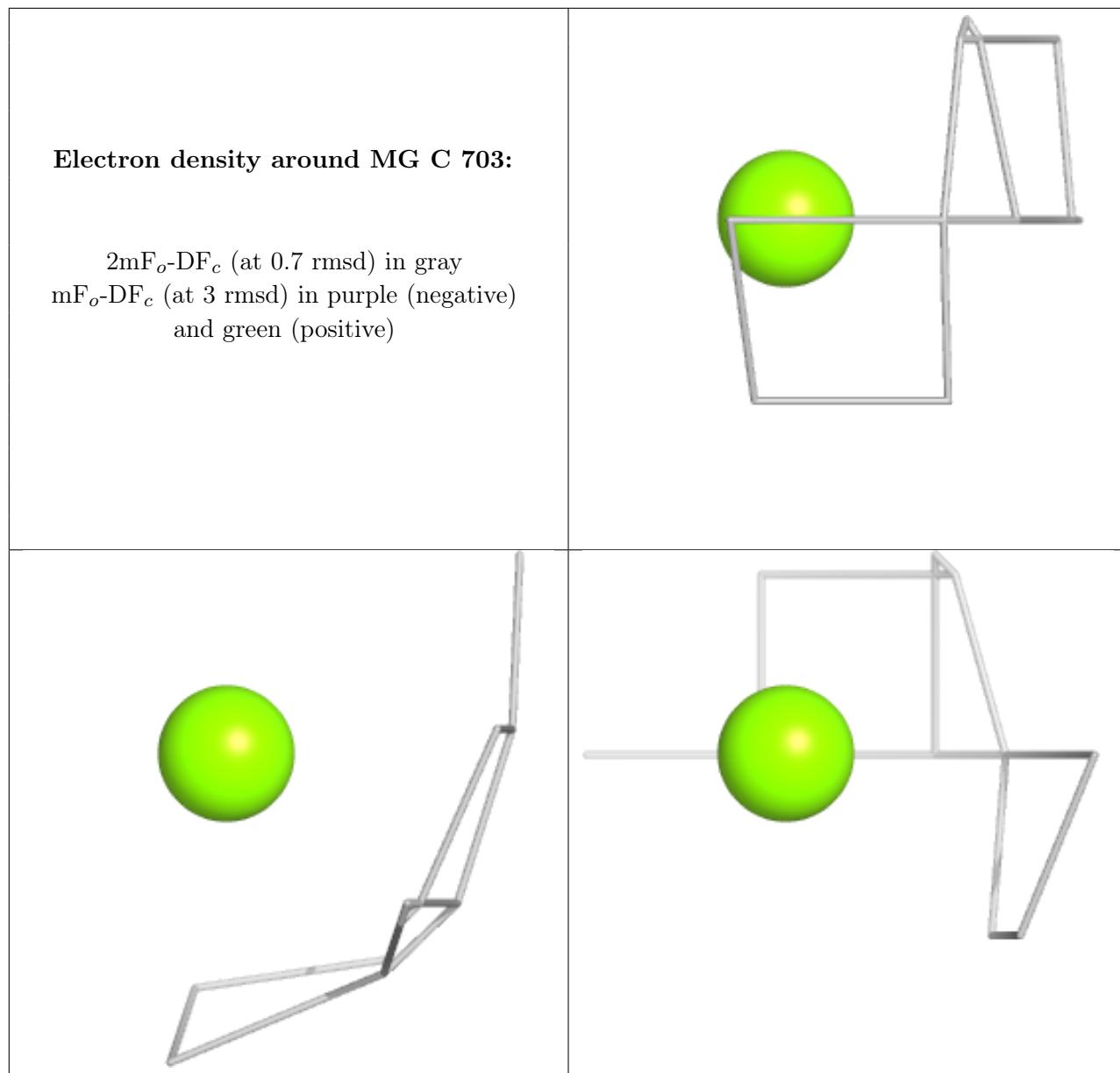












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.