



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:45 PM EDT

PDB ID : 6ZLZ / pdb_00006zlz
Title : Crystal Structure of Merkel Cell Polyomavirus Virus-like Particle
Authors : Bayer, N.J.; Stehle, T.; Blaum, B.S.
Deposited on : 2020-07-01
Resolution : 3.52 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

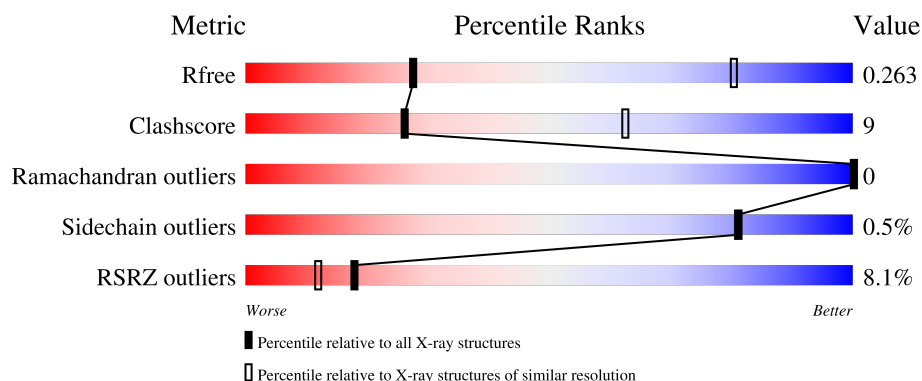
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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

Mol	Chain	Length	Quality of chain
1	A	423	 6% 66% 19% 15%
1	B	423	 8% 67% 20% 12%
1	C	423	 6% 67% 18% 15%
1	D	423	 6% 64% 17% 18%
1	E	423	 7% 66% 19% 14%

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Mol	Chain	Length	Quality of chain
1	F	423	8% 67% 17% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16324 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 Capsid protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2728	1739	446	527	16			
1	B	371	Total	C	N	O	S	0	0	0
			2800	1783	460	542	15			
1	C	360	Total	C	N	O	S	0	0	0
			2728	1742	447	523	16			
1	D	346	Total	C	N	O	S	0	0	0
			2623	1671	431	506	15			
1	E	362	Total	C	N	O	S	0	0	0
			2749	1756	449	531	13			
1	F	358	Total	C	N	O	S	0	0	0
			2690	1714	442	520	14			

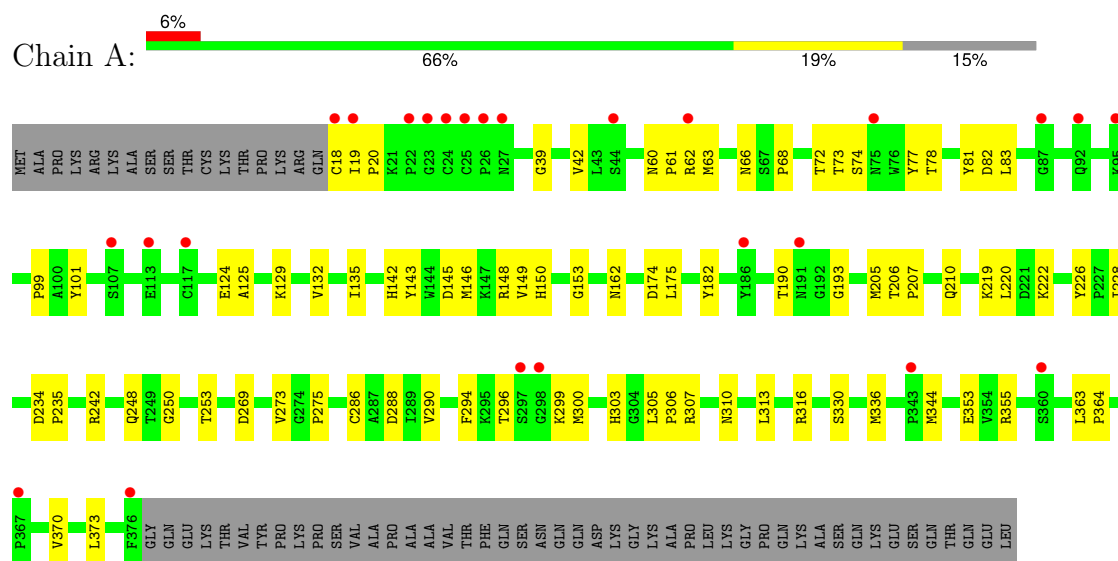
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

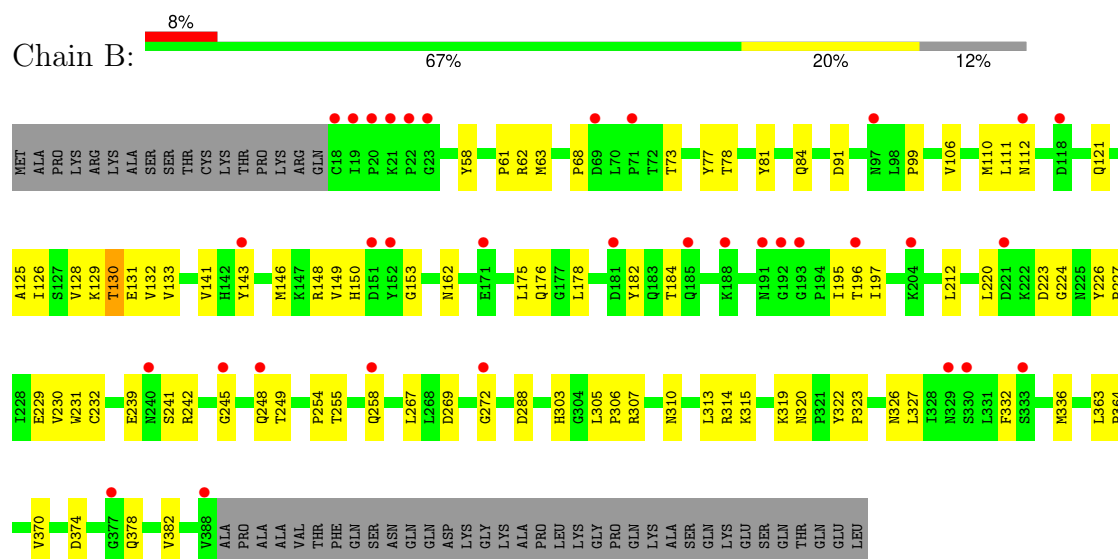
3 Residue-property plots [i](#)

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.

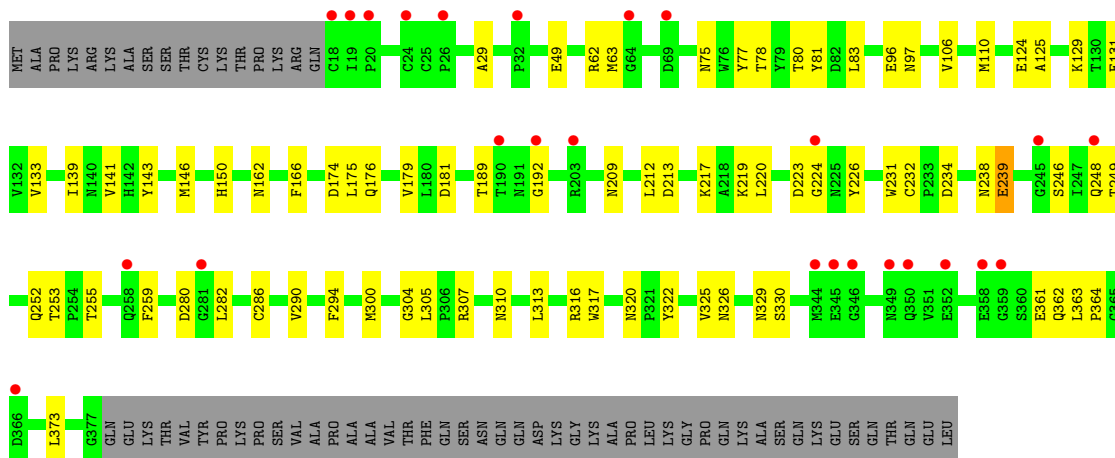
• Molecule 1: Capsid protein VP1



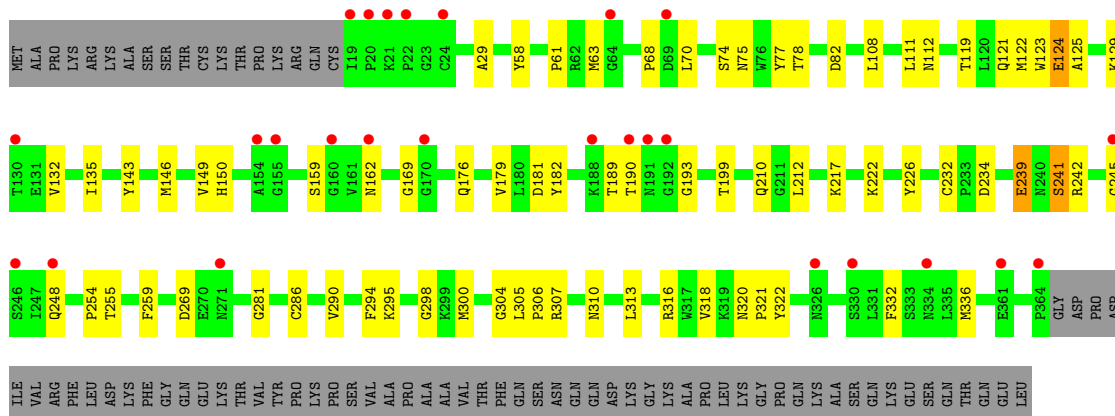
• Molecule 1: Capsid protein VP1



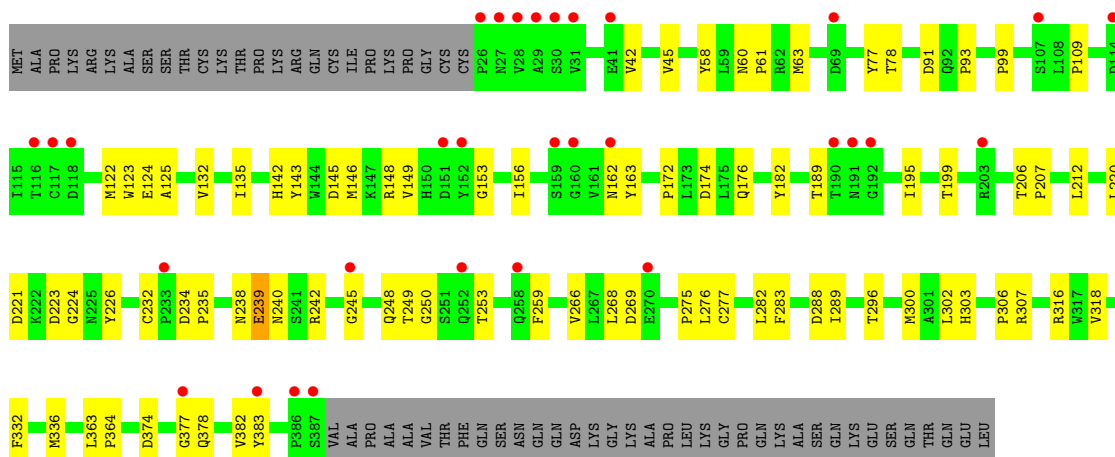
• Molecule 1: Capsid protein VP1



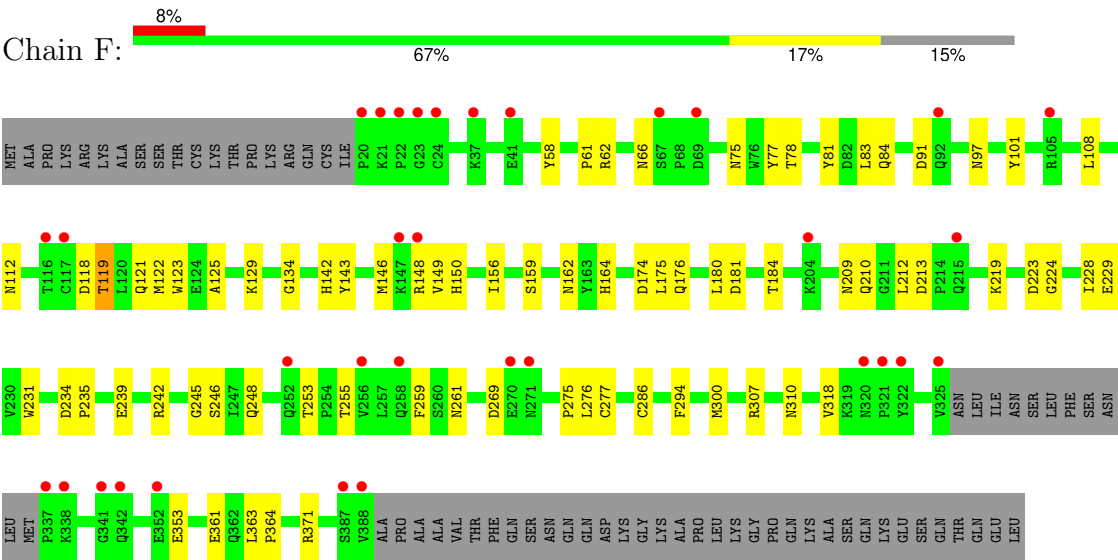
• Molecule 1: Capsid protein VP1



• Molecule 1: Capsid protein VP1



● Molecule 1: Capsid protein VP1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	554.83Å 560.99Å 573.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.52 49.97 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.97-3.52) 100.0 (49.97-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.235 , (Not available) 0.267 , 0.263	Depositor DCC
R_{free} test set	1479 reflections (0.14%)	wwPDB-VP
Wilson B-factor (Å ²)	131.8	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.013 for l,-k,h 0.014 for -k,-h,-l 0.013 for k,-l,-h 0.013 for -l,h,-k	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	16324	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.53	2/2796 (0.1%)	0.50	1/3823 (0.0%)
1	B	0.54	1/2871 (0.0%)	0.56	2/3932 (0.1%)
1	C	0.55	2/2796 (0.1%)	0.55	3/3824 (0.1%)
1	D	0.61	2/2688 (0.1%)	0.60	3/3678 (0.1%)
1	E	0.57	2/2818 (0.1%)	0.57	4/3857 (0.1%)
1	F	0.53	2/2759 (0.1%)	0.56	3/3778 (0.1%)
All	All	0.55	11/16728 (0.1%)	0.56	16/22892 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	ALA	C-N	-8.64	1.21	1.33
1	B	320	ASN	C-N	7.65	1.43	1.34
1	C	29	ALA	C-N	6.70	1.43	1.33
1	E	235	PRO	C-O	-6.45	1.16	1.24
1	F	119	THR	C-N	-6.41	1.24	1.33
1	A	234	ASP	C-O	-6.06	1.17	1.24
1	E	234	ASP	C-O	-5.91	1.16	1.24
1	C	320	ASN	C-N	-5.89	1.26	1.34
1	F	235	PRO	C-O	-5.76	1.17	1.24
1	A	235	PRO	C-O	-5.61	1.17	1.24
1	D	119	THR	C-N	5.10	1.40	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	320	ASN	O-C-N	8.36	128.42	121.31
1	C	29	ALA	CA-C-N	-7.66	110.78	122.81
1	C	29	ALA	C-N-CA	-7.66	110.78	122.81
1	E	199	THR	CA-CB-OG1	-7.54	98.30	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	320	ASN	O-C-N	6.10	126.85	121.18
1	F	108	LEU	CA-C-N	6.09	126.06	120.03
1	F	108	LEU	C-N-CA	6.09	126.06	120.03
1	D	29	ALA	CA-C-N	6.05	131.91	123.07
1	D	29	ALA	C-N-CA	6.05	131.91	123.07
1	E	239	GLU	CB-CA-C	-5.41	100.46	109.55
1	E	239	GLU	CA-C-N	-5.41	114.58	122.86
1	E	239	GLU	C-N-CA	-5.41	114.58	122.86
1	B	130	THR	CB-CA-C	-5.36	99.25	109.66
1	A	353	GLU	CB-CA-C	-5.27	100.52	110.16
1	B	319	LYS	CA-C-O	-5.26	114.65	120.38
1	F	353	GLU	CB-CA-C	-5.11	101.85	110.43

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	2728	0	2632	56	0
1	B	2800	0	2679	65	0
1	C	2728	0	2634	55	0
1	D	2623	0	2536	52	0
1	E	2749	0	2639	64	0
1	F	2690	0	2560	49	0
2	A	2	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
2	E	1	0	0	0	0
All	All	16324	0	15680	301	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 (301) 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:D:169:GLY:HA3	1:D:241:SER:HB3	1.51	0.92
1:F:112:ASN:HD21	1:F:121:GLN:H	1.26	0.83
1:E:242:ARG:HH21	1:E:269:ASP:HB3	1.47	0.80
1:B:242:ARG:HH11	1:B:269:ASP:HB3	1.46	0.79
1:E:174:ASP:H	1:E:238:ASN:HD21	1.32	0.76
1:C:290:VAL:HG21	1:C:305:LEU:HD13	1.68	0.75
1:E:162:ASN:ND2	1:E:289:ILE:O	2.20	0.74
1:A:355:ARG:NH2	1:C:239:GLU:OE1	2.21	0.73
1:D:124:GLU:OE1	1:D:316:ARG:NE	2.23	0.71
1:A:148:ARG:NH1	1:A:153:GLY:O	2.24	0.70
1:B:112:ASN:H	1:B:121:GLN:HE21	1.39	0.70
1:A:143:TYR:HB3	1:A:146:MET:HG3	1.73	0.69
1:F:175:LEU:HA	1:F:234:ASP:H	1.57	0.69
1:B:143:TYR:HB3	1:B:146:MET:HG3	1.74	0.68
1:E:162:ASN:HB3	1:E:248:GLN:HB3	1.76	0.67
1:F:143:TYR:HB3	1:F:146:MET:HB2	1.75	0.67
1:B:128:VAL:HG12	1:B:267:LEU:HD11	1.77	0.67
1:C:133:VAL:HG21	1:D:212:LEU:HD12	1.76	0.67
1:A:162:ASN:OD1	1:A:248:GLN:NE2	2.27	0.66
1:E:143:TYR:HB3	1:E:146:MET:HB2	1.76	0.65
1:B:126:ILE:HD11	1:B:314:ARG:HD3	1.78	0.65
1:A:162:ASN:ND2	1:A:290:VAL:O	2.30	0.65
1:C:223:ASP:OD1	1:C:224:GLY:N	2.30	0.65
1:F:223:ASP:OD1	1:F:224:GLY:N	2.30	0.64
1:B:175:LEU:HD23	1:B:231:TRP:HB3	1.78	0.64
1:C:179:VAL:HG12	1:C:181:ASP:H	1.63	0.64
1:C:175:LEU:HA	1:C:234:ASP:H	1.62	0.64
1:B:148:ARG:NH1	1:B:153:GLY:O	2.31	0.63
1:A:344:MET:HG2	1:B:106:VAL:HG22	1.80	0.63
1:F:129:LYS:HB3	1:F:310:ASN:HB3	1.82	0.62
1:D:143:TYR:HB3	1:D:146:MET:HB2	1.80	0.62
1:B:374:ASP:OD1	1:B:378:GLN:N	2.33	0.61
1:C:162:ASN:HB2	1:C:248:GLN:HB3	1.82	0.61
1:F:175:LEU:HD13	1:F:231:TRP:HB3	1.81	0.61
1:F:286:CYS:HB2	1:F:307:ARG:HD3	1.81	0.61
1:A:286:CYS:HB2	1:A:307:ARG:HD3	1.83	0.60
1:C:175:LEU:HD13	1:C:231:TRP:HB3	1.83	0.60
1:E:374:ASP:OD1	1:E:378:GLN:N	2.33	0.60
1:F:363:LEU:HD12	1:F:364:PRO:HD2	1.84	0.60
1:B:306:PRO:HG2	1:C:212:LEU:HB2	1.83	0.59
1:B:370:VAL:HG13	1:B:382:VAL:HB	1.83	0.59
1:C:325:VAL:HG12	1:C:329:ASN:HD21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:TYR:HB3	1:B:327:LEU:HD11	1.83	0.59
1:D:179:VAL:HG12	1:D:181:ASP:H	1.66	0.59
1:A:294:PHE:HE1	1:A:300:MET:HE3	1.67	0.59
1:C:363:LEU:HD12	1:C:364:PRO:HD2	1.83	0.59
1:A:129:LYS:HB3	1:A:310:ASN:HB3	1.83	0.59
1:E:220:LEU:HA	1:E:226:TYR:HE2	1.68	0.59
1:C:143:TYR:HB3	1:C:146:MET:HG3	1.85	0.58
1:F:361:GLU:OE2	1:F:371:ARG:NH2	2.34	0.58
1:B:242:ARG:NH1	1:B:269:ASP:HB3	2.15	0.58
1:D:290:VAL:HG21	1:D:305:LEU:HG	1.86	0.58
1:B:220:LEU:HA	1:B:226:TYR:HE2	1.69	0.58
1:F:125:ALA:HB3	1:F:275:PRO:HG2	1.85	0.58
1:B:182:TYR:OH	1:F:75:ASN:OD1	2.21	0.58
1:C:209:ASN:ND2	1:C:213:ASP:OD2	2.37	0.57
1:D:242:ARG:NH2	1:D:269:ASP:HB3	2.19	0.57
1:A:373:LEU:HD21	1:C:330:SER:HB3	1.86	0.57
1:B:254:PRO:HB3	1:C:253:THR:HG21	1.87	0.57
1:F:122:MET:HE2	1:F:318:VAL:HG21	1.87	0.56
1:B:220:LEU:HA	1:B:226:TYR:CE2	2.40	0.56
1:E:174:ASP:N	1:E:238:ASN:HD21	2.01	0.56
1:E:363:LEU:HD12	1:E:364:PRO:HD2	1.88	0.56
1:A:18:CYS:SG	1:A:19:ILE:N	2.79	0.56
1:C:49:GLU:OE2	1:C:317:TRP:NE1	2.36	0.56
1:D:70:LEU:O	1:D:74:SER:OG	2.22	0.56
1:A:182:TYR:HA	1:A:205:MET:HE3	1.87	0.55
1:D:294:PHE:HE1	1:D:300:MET:HE3	1.70	0.55
1:A:190:THR:HG23	1:A:193:GLY:H	1.71	0.55
1:B:241:SER:O	1:F:261:ASN:ND2	2.36	0.55
1:A:63:MET:HG3	1:A:99:PRO:HB3	1.88	0.55
1:B:363:LEU:HD12	1:B:364:PRO:HD2	1.89	0.55
1:D:122:MET:HE3	1:D:318:VAL:HG21	1.87	0.55
1:C:174:ASP:OD1	1:C:219:LYS:HG2	2.07	0.55
1:A:174:ASP:OD1	1:A:219:LYS:NZ	2.36	0.54
1:D:63:MET:HE3	1:D:304:GLY:HA3	1.87	0.54
1:A:288:ASP:OD2	1:A:307:ARG:NH1	2.34	0.54
1:D:254:PRO:HB3	1:E:253:THR:HG21	1.90	0.54
1:E:240:ASN:O	1:E:240:ASN:ND2	2.41	0.54
1:C:124:GLU:OE1	1:C:316:ARG:NE	2.37	0.54
1:E:125:ALA:HB3	1:E:275:PRO:HG2	1.90	0.54
1:E:266:VAL:HG12	1:E:268:LEU:H	1.74	0.53
1:C:220:LEU:HA	1:C:226:TYR:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:MET:HE2	1:E:318:VAL:HG21	1.90	0.53
1:E:122:MET:HE3	1:E:276:LEU:HD23	1.90	0.53
1:D:111:LEU:HD11	1:D:123:TRP:NE1	2.24	0.53
1:E:148:ARG:NH1	1:E:153:GLY:O	2.42	0.52
1:C:62:ARG:HG3	1:C:223:ASP:OD1	2.07	0.52
1:D:294:PHE:CE1	1:D:300:MET:HE3	2.44	0.52
1:D:129:LYS:HB3	1:D:310:ASN:HB3	1.92	0.52
1:B:223:ASP:OD1	1:B:224:GLY:N	2.42	0.52
1:B:269:ASP:OD1	1:B:272:GLY:N	2.43	0.52
1:A:294:PHE:CE1	1:A:300:MET:HE3	2.45	0.52
1:C:217:LYS:NZ	1:C:234:ASP:OD2	2.33	0.52
1:D:182:TYR:H	1:D:210:GLN:HE21	1.57	0.52
1:B:143:TYR:HE1	1:C:181:ASP:OD2	1.92	0.51
1:B:162:ASN:ND2	1:B:248:GLN:HE21	2.08	0.51
1:D:162:ASN:HD22	1:D:248:GLN:HE21	1.57	0.51
1:F:81:TYR:O	1:F:83:LEU:HD12	2.11	0.51
1:E:132:VAL:HB	1:E:135:ILE:HD11	1.92	0.51
1:E:223:ASP:OD1	1:E:224:GLY:N	2.43	0.51
1:A:125:ALA:HB3	1:A:275:PRO:HG2	1.93	0.51
1:B:229:GLU:CD	1:F:142:HIS:HE2	2.19	0.51
1:D:162:ASN:ND2	1:D:248:GLN:HE21	2.09	0.51
1:A:330:SER:HB2	1:C:373:LEU:HD23	1.92	0.51
1:A:363:LEU:HD12	1:A:364:PRO:HD2	1.93	0.51
1:C:220:LEU:HA	1:C:226:TYR:CE2	2.45	0.51
1:E:58:TYR:CD2	1:F:212:LEU:HD23	2.46	0.51
1:B:227:PRO:HG2	1:B:230:VAL:HG22	1.92	0.50
1:D:112:ASN:HB2	1:D:121:GLN:NE2	2.26	0.50
1:F:294:PHE:CE1	1:F:300:MET:HE3	2.46	0.50
1:D:61:PRO:HG2	1:D:78:THR:HG22	1.93	0.50
1:F:294:PHE:HE1	1:F:300:MET:HE3	1.76	0.50
1:B:178:LEU:HD13	1:F:134:GLY:HA3	1.94	0.50
1:B:212:LEU:HD23	1:F:58:TYR:CG	2.46	0.50
1:F:176:GLN:HB2	1:F:234:ASP:HB2	1.94	0.50
1:B:230:VAL:HG23	1:B:231:TRP:CD1	2.47	0.50
1:D:149:VAL:HG11	1:E:300:MET:HE1	1.93	0.50
1:E:124:GLU:OE1	1:E:316:ARG:NE	2.41	0.49
1:A:39:GLY:O	1:A:42:VAL:HG22	2.12	0.49
1:B:63:MET:HA	1:B:99:PRO:HA	1.93	0.49
1:D:162:ASN:HD21	1:D:255:THR:HG22	1.76	0.49
1:A:61:PRO:HG2	1:A:78:THR:HG22	1.93	0.49
1:A:242:ARG:NH2	1:A:269:ASP:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:VAL:HB	1:D:135:ILE:HD11	1.94	0.49
1:D:217:LYS:NZ	1:D:234:ASP:OD2	2.34	0.49
1:E:220:LEU:HA	1:E:226:TYR:CE2	2.45	0.49
1:B:61:PRO:HG2	1:B:78:THR:HG22	1.94	0.49
1:B:110:MET:C	1:B:111:LEU:HD12	2.38	0.49
1:D:286:CYS:HB2	1:D:307:ARG:HD3	1.95	0.49
1:A:124:GLU:OE1	1:A:316:ARG:NE	2.43	0.49
1:B:162:ASN:HD22	1:B:248:GLN:HE21	1.61	0.49
1:B:196:THR:HG22	1:B:197:ILE:H	1.78	0.49
1:F:149:VAL:HG23	1:F:150:HIS:ND1	2.28	0.49
1:F:149:VAL:HG12	1:F:156:ILE:HG12	1.93	0.49
1:D:82:ASP:OD1	1:D:295:LYS:NZ	2.36	0.48
1:D:77:TYR:O	1:D:78:THR:OG1	2.26	0.48
1:D:259:PHE:CZ	1:E:245:GLY:HA3	2.48	0.48
1:E:42:VAL:O	1:E:45:VAL:HG12	2.12	0.48
1:A:78:THR:O	1:A:303:HIS:ND1	2.46	0.48
1:B:125:ALA:HA	1:B:313:LEU:HD23	1.95	0.48
1:B:196:THR:HG22	1:B:197:ILE:N	2.28	0.48
1:E:78:THR:O	1:E:303:HIS:ND1	2.43	0.48
1:F:159:SER:OG	1:F:253:THR:O	2.32	0.48
1:B:245:GLY:HA3	1:F:259:PHE:CZ	2.49	0.48
1:C:81:TYR:O	1:C:97:ASN:ND2	2.47	0.48
1:C:174:ASP:O	1:C:238:ASN:ND2	2.29	0.48
1:A:19:ILE:N	1:A:20:PRO:HD3	2.29	0.47
1:B:212:LEU:HD23	1:F:58:TYR:CD2	2.49	0.47
1:E:77:TYR:O	1:E:78:THR:OG1	2.29	0.47
1:B:130:THR:O	1:B:130:THR:HG23	2.14	0.47
1:B:176:GLN:N	1:B:232:CYS:O	2.44	0.47
1:E:145:ASP:O	1:E:296:THR:N	2.48	0.47
1:B:129:LYS:HB3	1:B:310:ASN:HB3	1.96	0.47
1:A:72:THR:HG23	1:A:73:THR:HG22	1.95	0.47
1:B:77:TYR:O	1:B:78:THR:OG1	2.29	0.47
1:B:323:PRO:HG2	1:B:326:ASN:ND2	2.30	0.47
1:C:75:ASN:OD1	1:D:182:TYR:OH	2.21	0.47
1:E:124:GLU:CD	1:E:316:ARG:HE	2.22	0.47
1:D:68:PRO:HA	1:D:74:SER:HB3	1.97	0.47
1:A:222:LYS:H	1:A:226:TYR:HE2	1.63	0.47
1:A:101:TYR:CE1	1:A:228:ILE:HG12	2.50	0.47
1:F:62:ARG:HG3	1:F:223:ASP:OD1	2.14	0.47
1:C:143:TYR:HE1	1:D:181:ASP:OD2	1.97	0.46
1:B:332:PHE:O	1:B:336:MET:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:PHE:HA	1:C:286:CYS:HA	1.97	0.46
1:D:75:ASN:OD1	1:E:182:TYR:OH	2.24	0.46
1:E:125:ALA:O	1:E:275:PRO:HD2	2.14	0.46
1:A:206:THR:HB	1:A:207:PRO:HD2	1.96	0.46
1:E:288:ASP:OD2	1:E:307:ARG:HD2	2.16	0.46
1:A:250:GLY:HA3	1:A:253:THR:OG1	2.16	0.46
1:B:143:TYR:HB3	1:B:146:MET:CG	2.45	0.46
1:E:143:TYR:HE1	1:F:181:ASP:OD2	1.97	0.46
1:C:150:HIS:NE2	1:D:298:GLY:O	2.49	0.46
1:B:112:ASN:N	1:B:121:GLN:HE21	2.12	0.46
1:C:80:THR:HG23	1:C:96:GLU:O	2.16	0.46
1:E:162:ASN:HD22	1:E:163:TYR:N	2.12	0.46
1:B:58:TYR:CE2	1:C:212:LEU:HD22	2.51	0.46
1:B:323:PRO:HG2	1:B:326:ASN:HD22	1.81	0.46
1:C:176:GLN:N	1:C:232:CYS:O	2.35	0.46
1:E:240:ASN:C	1:E:240:ASN:HD22	2.23	0.46
1:A:273:VAL:HG12	1:A:316:ARG:CZ	2.46	0.45
1:D:150:HIS:CE1	1:E:300:MET:HE3	2.51	0.45
1:F:101:TYR:CE1	1:F:228:ILE:HG12	2.51	0.45
1:A:132:VAL:HB	1:A:135:ILE:HD11	1.98	0.45
1:E:172:PRO:HD3	1:E:283:PHE:HE2	1.81	0.45
1:B:62:ARG:HG3	1:B:223:ASP:OD1	2.16	0.45
1:D:176:GLN:N	1:D:232:CYS:O	2.44	0.45
1:E:61:PRO:HG2	1:E:78:THR:HG22	1.99	0.45
1:E:259:PHE:CZ	1:F:245:GLY:HA3	2.52	0.45
1:F:122:MET:HE3	1:F:276:LEU:HD23	1.98	0.45
1:D:108:LEU:HD13	1:D:281:GLY:HA2	1.99	0.45
1:D:159:SER:HA	1:D:255:THR:HG23	1.98	0.45
1:D:332:PHE:O	1:D:336:MET:HG2	2.16	0.45
1:B:73:THR:HG1	1:B:81:TYR:HH	1.54	0.45
1:C:259:PHE:CZ	1:D:245:GLY:HA3	2.52	0.45
1:D:321:PRO:HG2	1:D:322:TYR:CD2	2.52	0.45
1:A:182:TYR:H	1:A:210:GLN:HE21	1.65	0.45
1:E:221:ASP:H	1:E:226:TYR:HE2	1.64	0.45
1:A:143:TYR:HB3	1:A:146:MET:CG	2.44	0.44
1:F:62:ARG:HD2	1:F:66:ASN:HB3	1.99	0.44
1:F:209:ASN:ND2	1:F:213:ASP:OD2	2.50	0.44
1:A:124:GLU:CD	1:A:316:ARG:HE	2.26	0.44
1:A:370:VAL:HG12	1:C:322:TYR:OH	2.17	0.44
1:D:77:TYR:CD2	1:D:78:THR:HG23	2.53	0.44
1:E:242:ARG:NH2	1:E:269:ASP:HB3	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ASN:HA	1:C:329:ASN:HD22	1.82	0.44
1:F:91:ASP:HB3	1:F:184:THR:HG22	2.00	0.44
1:C:129:LYS:HB3	1:C:310:ASN:HB3	1.99	0.44
1:E:143:TYR:HB3	1:E:146:MET:HE3	2.00	0.44
1:F:118:ASP:OD1	1:F:119:THR:N	2.50	0.44
1:F:162:ASN:HB2	1:F:248:GLN:HG2	1.99	0.44
1:B:91:ASP:HB3	1:B:184:THR:HG22	1.99	0.44
1:C:106:VAL:HB	1:C:282:LEU:HB3	1.99	0.44
1:F:77:TYR:CD2	1:F:78:THR:HG23	2.53	0.44
1:A:162:ASN:HB2	1:A:248:GLN:HG2	1.99	0.44
1:C:255:THR:HG21	1:C:290:VAL:HG13	2.00	0.44
1:E:109:PRO:HG2	1:E:123:TRP:HZ2	1.83	0.43
1:A:62:ARG:HD2	1:A:66:ASN:HB3	2.00	0.43
1:A:68:PRO:HA	1:A:74:SER:HB3	2.00	0.43
1:A:175:LEU:HD11	1:A:220:LEU:HD12	1.99	0.43
1:C:110:MET:HG3	1:C:280:ASP:OD2	2.17	0.43
1:D:125:ALA:HA	1:D:313:LEU:HD23	2.00	0.43
1:E:77:TYR:CD2	1:E:78:THR:HG23	2.53	0.43
1:E:91:ASP:OD2	1:E:93:PRO:HD3	2.18	0.43
1:B:258:GLN:HA	1:C:246:SER:HA	2.00	0.43
1:E:162:ASN:HD22	1:E:163:TYR:H	1.64	0.43
1:A:82:ASP:OD2	1:A:299:LYS:HD3	2.17	0.43
1:A:290:VAL:HG21	1:A:305:LEU:HG	2.00	0.43
1:D:70:LEU:H	1:D:70:LEU:HD23	1.83	0.43
1:E:332:PHE:O	1:E:336:MET:HG2	2.19	0.43
1:C:77:TYR:O	1:C:78:THR:OG1	2.29	0.43
1:D:190:THR:O	1:D:193:GLY:N	2.51	0.43
1:D:306:PRO:HG2	1:E:212:LEU:HB2	2.01	0.43
1:F:123:TRP:HB2	1:F:277:CYS:HB2	2.01	0.43
1:D:189:THR:OG1	1:D:199:THR:OG1	2.22	0.43
1:D:222:LYS:H	1:D:226:TYR:HE2	1.66	0.43
1:F:164:HIS:HB2	1:F:246:SER:HB3	2.01	0.43
1:F:242:ARG:HH21	1:F:269:ASP:HB3	1.82	0.43
1:A:99:PRO:HB2	1:A:228:ILE:HD12	1.99	0.43
1:E:148:ARG:HH12	1:F:84:GLN:HG2	1.84	0.43
1:E:277:CYS:SG	1:E:282:LEU:HB3	2.58	0.43
1:B:195:ILE:HB	1:B:226:TYR:CE1	2.54	0.43
1:C:63:MET:HE3	1:C:304:GLY:HA3	2.00	0.43
1:E:374:ASP:OD1	1:E:377:GLY:N	2.52	0.43
1:B:77:TYR:CD2	1:B:78:THR:HG23	2.54	0.42
1:B:111:LEU:HD21	1:B:315:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:HIS:CE1	1:C:300:MET:HE3	2.54	0.42
1:E:149:VAL:HG22	1:E:156:ILE:HG12	2.00	0.42
1:B:78:THR:O	1:B:303:HIS:ND1	2.52	0.42
1:B:255:THR:HG22	1:C:249:THR:OG1	2.19	0.42
1:C:174:ASP:OD1	1:C:219:LYS:NZ	2.36	0.42
1:E:63:MET:HA	1:E:99:PRO:HA	2.01	0.42
1:F:61:PRO:HG2	1:F:78:THR:HG22	2.00	0.42
1:F:180:LEU:O	1:F:210:GLN:NE2	2.50	0.42
1:D:149:VAL:HG13	1:D:150:HIS:ND1	2.34	0.42
1:A:18:CYS:HB3	1:A:20:PRO:HD3	2.01	0.42
1:A:68:PRO:HD3	1:A:77:TYR:CE1	2.54	0.42
1:A:149:VAL:HG13	1:A:150:HIS:ND1	2.34	0.42
1:A:77:TYR:O	1:A:78:THR:OG1	2.31	0.42
1:C:189:THR:O	1:C:192:GLY:N	2.51	0.42
1:C:294:PHE:CE1	1:C:300:MET:HE2	2.55	0.42
1:D:58:TYR:CD2	1:E:212:LEU:HD23	2.55	0.42
1:B:149:VAL:HG11	1:C:300:MET:HE1	2.01	0.42
1:A:60:ASN:HA	1:A:306:PRO:HB3	2.02	0.42
1:F:143:TYR:HB3	1:F:146:MET:HE3	2.02	0.42
1:A:145:ASP:C	1:A:296:THR:HG23	2.45	0.41
1:D:255:THR:OG1	1:E:249:THR:OG1	2.29	0.41
1:E:142:HIS:NE2	1:F:229:GLU:OE2	2.53	0.41
1:A:81:TYR:O	1:A:83:LEU:HD12	2.20	0.41
1:B:84:GLN:HG2	1:F:148:ARG:HH22	1.84	0.41
1:E:195:ILE:HB	1:E:226:TYR:CE1	2.55	0.41
1:F:81:TYR:O	1:F:97:ASN:ND2	2.53	0.41
1:F:174:ASP:OD1	1:F:219:LYS:NZ	2.40	0.41
1:B:288:ASP:OD2	1:B:307:ARG:HD3	2.20	0.41
1:E:288:ASP:OD2	1:E:307:ARG:NH1	2.33	0.41
1:B:249:THR:OG1	1:F:255:THR:HG22	2.20	0.41
1:E:60:ASN:HA	1:E:306:PRO:HB3	2.02	0.41
1:D:135:ILE:HD12	1:D:135:ILE:H	1.85	0.41
1:C:125:ALA:HA	1:C:313:LEU:HD23	2.02	0.41
1:E:206:THR:HB	1:E:207:PRO:HD2	2.02	0.41
1:A:125:ALA:HA	1:A:313:LEU:HD23	2.02	0.41
1:C:252:GLN:HG2	1:C:294:PHE:CE2	2.56	0.41
1:A:330:SER:OG	1:A:336:MET:SD	2.71	0.41
1:B:132:VAL:HG12	1:B:305:LEU:CD1	2.51	0.41
1:B:133:VAL:O	1:B:305:LEU:HD13	2.21	0.41
1:E:189:THR:HG22	1:E:189:THR:O	2.21	0.41
1:E:382:VAL:HG22	1:E:383:TYR:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:ILE:HG21	1:E:302:LEU:HD22	2.02	0.41
1:A:101:TYR:CD1	1:A:228:ILE:HG12	2.56	0.40
1:A:124:GLU:OE2	1:A:273:VAL:HA	2.20	0.40
1:A:142:HIS:O	1:A:142:HIS:ND1	2.54	0.40
1:B:141:VAL:HA	1:B:146:MET:HE1	2.03	0.40
1:C:139:ILE:O	1:C:141:VAL:HG23	2.21	0.40
1:C:361:GLU:HG3	1:C:362:GLN:O	2.21	0.40
1:E:176:GLN:N	1:E:232:CYS:O	2.48	0.40
1:D:239:GLU:H	1:D:239:GLU:HG2	1.47	0.40
1:E:250:GLY:HA3	1:E:253:THR:HG23	2.04	0.40
1:C:81:TYR:O	1:C:83:LEU:HD12	2.22	0.40
1:C:286:CYS:HB2	1:C:307:ARG:HD3	2.04	0.40
1:B:68:PRO:HD3	1:B:77:TYR:CE1	2.56	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	357/423 (84%)	347 (97%)	10 (3%)	0	100	100
1	B	369/423 (87%)	361 (98%)	8 (2%)	0	100	100
1	C	358/423 (85%)	351 (98%)	7 (2%)	0	100	100
1	D	344/423 (81%)	333 (97%)	11 (3%)	0	100	100
1	E	360/423 (85%)	348 (97%)	12 (3%)	0	100	100
1	F	354/423 (84%)	337 (95%)	17 (5%)	0	100	100
All	All	2142/2538 (84%)	2077 (97%)	65 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	299/372 (80%)	299 (100%)	0	100	100
1	B	305/372 (82%)	303 (99%)	2 (1%)	76	78
1	C	297/372 (80%)	295 (99%)	2 (1%)	76	78
1	D	288/372 (77%)	285 (99%)	3 (1%)	68	75
1	E	298/372 (80%)	297 (100%)	1 (0%)	86	83
1	F	289/372 (78%)	288 (100%)	1 (0%)	86	83
All	All	1776/2232 (80%)	1767 (100%)	9 (0%)	81	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	131	GLU
1	B	239	GLU
1	C	131	GLU
1	C	239	GLU
1	D	124	GLU
1	D	239	GLU
1	D	241	SER
1	E	239	GLU
1	F	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	329	ASN
1	B	66	ASN
1	B	75	ASN
1	B	121	GLN
1	B	162	ASN
1	B	210	GLN
1	B	326	ASN

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Mol	Chain	Res	Type
1	B	334	ASN
1	C	66	ASN
1	C	225	ASN
1	C	329	ASN
1	C	334	ASN
1	D	66	ASN
1	D	121	GLN
1	D	162	ASN
1	D	183	GLN
1	D	209	ASN
1	D	210	GLN
1	D	225	ASN
1	E	121	GLN
1	E	162	ASN
1	E	210	GLN
1	E	225	ASN
1	E	238	ASN
1	E	240	ASN
1	E	334	ASN
1	F	162	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	359/423 (84%)	0.69	25 (6%)	22	14	97, 113, 135, 187	2 (0%)
1	B	371/423 (87%)	0.74	34 (9%)	14	9	96, 113, 146, 181	2 (0%)
1	C	360/423 (85%)	0.69	25 (6%)	23	14	92, 106, 134, 169	4 (1%)
1	D	346/423 (81%)	0.61	26 (7%)	20	13	90, 104, 134, 177	3 (0%)
1	E	362/423 (85%)	0.70	31 (8%)	16	11	93, 108, 138, 165	0
1	F	358/423 (84%)	0.79	33 (9%)	14	9	100, 118, 154, 170	2 (0%)
All	All	2156/2538 (84%)	0.70	174 (8%)	18	12	90, 110, 141, 187	13 (0%)

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	CYS	7.9
1	F	20	PRO	7.5
1	F	24	CYS	6.3
1	D	24	CYS	6.1
1	C	18	CYS	6.0
1	C	358	GLU	5.2
1	B	18	CYS	5.2
1	E	117	CYS	5.1
1	F	41	GLU	4.9
1	F	337	PRO	4.7
1	F	325	VAL	4.6
1	D	19	ILE	4.6
1	C	190	THR	4.5
1	A	75	ASN	4.4
1	B	23	GLY	4.4
1	C	359	GLY	4.4
1	E	69	ASP	4.1
1	E	191	ASN	4.1
1	E	190	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	160	GLY	3.9
1	E	28	VAL	3.9
1	A	19	ILE	3.8
1	E	29	ALA	3.8
1	A	298	GLY	3.7
1	D	326	ASN	3.7
1	B	188	LYS	3.6
1	F	37	LYS	3.6
1	E	27	ASN	3.6
1	B	22	PRO	3.5
1	E	387	SER	3.5
1	D	248	GLN	3.5
1	A	95	LYS	3.5
1	B	388	VAL	3.5
1	A	27	ASN	3.5
1	A	22	PRO	3.5
1	A	367	PRO	3.4
1	F	321	PRO	3.4
1	A	25	CYS	3.4
1	A	360	SER	3.4
1	A	24	CYS	3.3
1	A	191	ASN	3.3
1	F	338	LYS	3.3
1	B	20	PRO	3.3
1	F	387	SER	3.3
1	C	346	GLY	3.2
1	C	345	GLU	3.2
1	B	69	ASP	3.2
1	B	21	LYS	3.2
1	D	188	LYS	3.1
1	D	155	GLY	3.1
1	B	185	GLN	3.1
1	D	160	GLY	3.1
1	A	92	GLN	3.1
1	B	248	GLN	3.1
1	E	252	GLN	3.1
1	D	246	SER	3.1
1	A	23	GLY	3.1
1	E	377	GLY	3.1
1	E	31	VAL	3.0
1	B	196	THR	3.0
1	D	192	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	151	ASP	3.0
1	C	248	GLN	2.9
1	D	20	PRO	2.9
1	B	245	GLY	2.9
1	B	330	SER	2.9
1	E	41	GLU	2.9
1	E	270	GLU	2.9
1	C	349	ASN	2.9
1	F	388	VAL	2.8
1	B	192	GLY	2.8
1	E	151	ASP	2.8
1	D	162	ASN	2.8
1	F	147	LYS	2.7
1	D	22	PRO	2.7
1	F	322	TYR	2.7
1	A	376	PHE	2.7
1	D	245	GLY	2.7
1	B	329	ASN	2.7
1	F	105	ARG	2.6
1	D	191	ASN	2.6
1	E	26	PRO	2.6
1	C	24	CYS	2.6
1	D	69	ASP	2.6
1	E	107	SER	2.6
1	C	26	PRO	2.6
1	F	341	GLY	2.6
1	B	221	ASP	2.6
1	F	22	PRO	2.6
1	E	116	THR	2.5
1	E	162	ASN	2.5
1	A	44	SER	2.5
1	E	203	ARG	2.5
1	F	270	GLU	2.5
1	A	26	PRO	2.5
1	F	23	GLY	2.5
1	A	297	SER	2.5
1	F	67	SER	2.5
1	C	352	GLU	2.5
1	B	191	ASN	2.5
1	B	240	ASN	2.5
1	C	281	GLY	2.5
1	E	159	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	203	ARG	2.4
1	F	252	GLN	2.4
1	D	364	PRO	2.4
1	E	192	GLY	2.4
1	C	258	GLN	2.4
1	C	64	GLY	2.4
1	E	30	SER	2.4
1	B	19	ILE	2.4
1	A	87	GLY	2.4
1	F	148	ARG	2.4
1	B	258	GLN	2.4
1	F	215	GLN	2.4
1	B	333	SER	2.3
1	B	112	ASN	2.3
1	B	272	GLY	2.3
1	A	62	ARG	2.3
1	B	181	ASP	2.3
1	C	366	ASP	2.3
1	D	361	GLU	2.3
1	F	69	ASP	2.3
1	F	271	ASN	2.3
1	F	342	GLN	2.3
1	C	192	GLY	2.3
1	F	116	THR	2.3
1	D	330	SER	2.3
1	B	193	GLY	2.3
1	D	170	GLY	2.3
1	E	245	GLY	2.3
1	D	130	THR	2.2
1	D	154	ALA	2.2
1	A	117	CYS	2.2
1	B	97	ASN	2.2
1	B	143	TYR	2.2
1	F	21	LYS	2.2
1	C	344	MET	2.2
1	A	113	GLU	2.2
1	C	32	PRO	2.2
1	D	271	ASN	2.2
1	C	350	GLN	2.2
1	B	377	GLY	2.2
1	C	20	PRO	2.2
1	B	152	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	334	ASN	2.2
1	C	69	ASP	2.1
1	A	186	TYR	2.1
1	E	152	TYR	2.1
1	C	224	GLY	2.1
1	A	107	SER	2.1
1	E	258	GLN	2.1
1	C	19	ILE	2.1
1	B	71	PRO	2.1
1	C	245	GLY	2.1
1	D	64	GLY	2.1
1	B	204	LYS	2.1
1	A	343	PRO	2.1
1	E	386	PRO	2.1
1	F	320	ASN	2.1
1	F	204	LYS	2.1
1	B	118	ASP	2.1
1	E	114	ASP	2.1
1	F	352	GLU	2.1
1	D	21	LYS	2.1
1	E	233	PRO	2.1
1	F	258	GLN	2.1
1	E	383	TYR	2.0
1	F	92	GLN	2.0
1	F	256	VAL	2.0
1	B	171	GLU	2.0
1	E	118	ASP	2.0
1	F	117	CYS	2.0
1	D	190	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

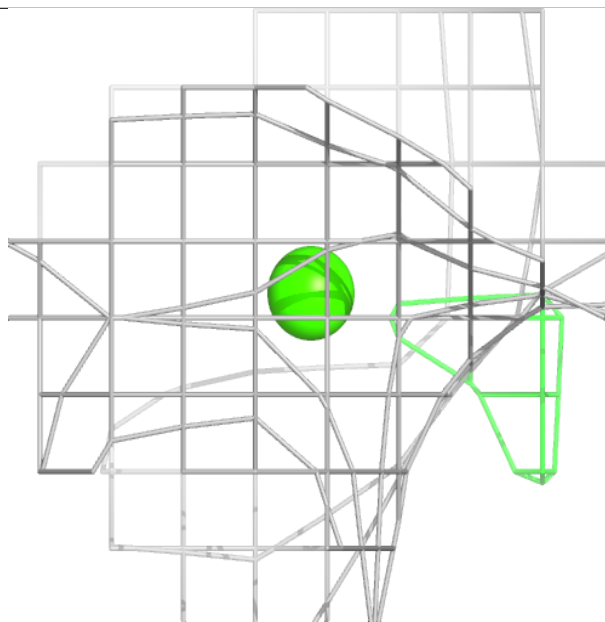
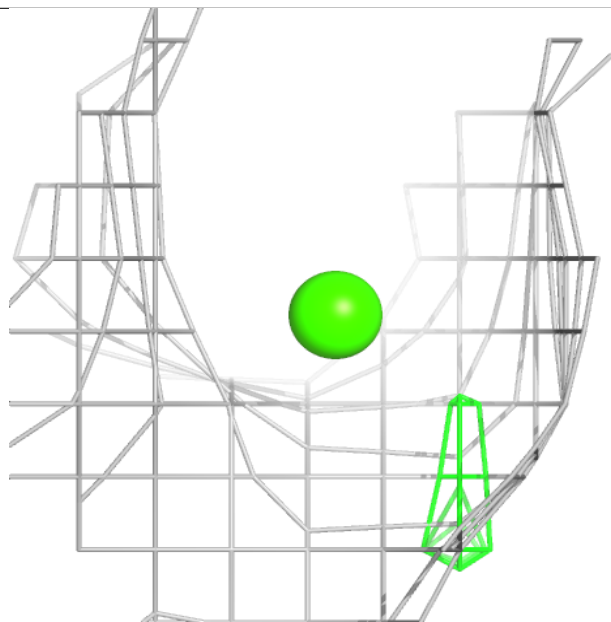
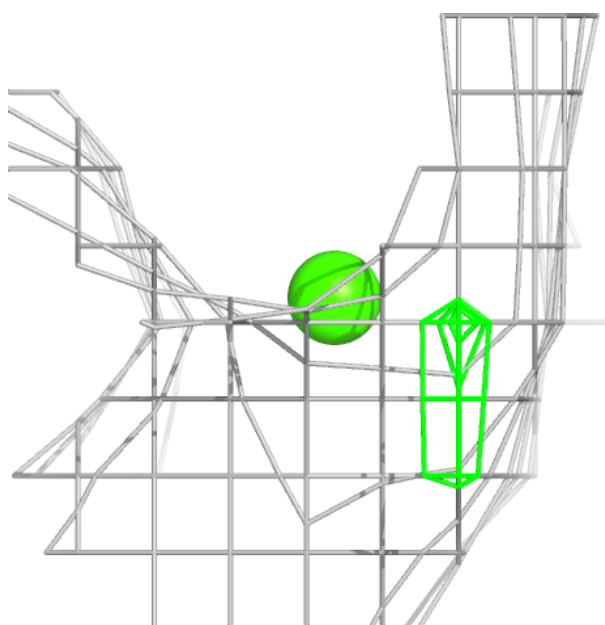
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	501	1/1	0.63	0.32	116,116,116,116	1
2	CA	E	501	1/1	0.73	0.28	116,116,116,116	1
2	CA	C	501	1/1	0.93	0.12	116,116,116,116	0
2	CA	A	502	1/1	0.96	0.07	116,116,116,116	1
2	CA	B	501	1/1	0.96	0.15	116,116,116,116	1
2	CA	D	501	1/1	0.98	0.06	116,116,116,116	0

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

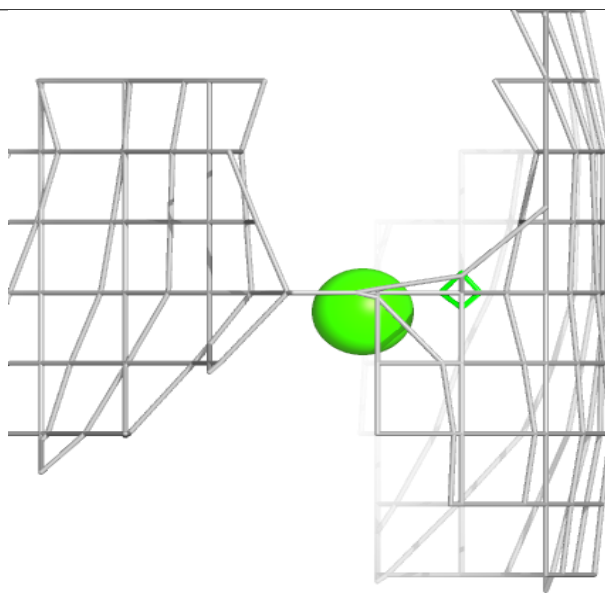
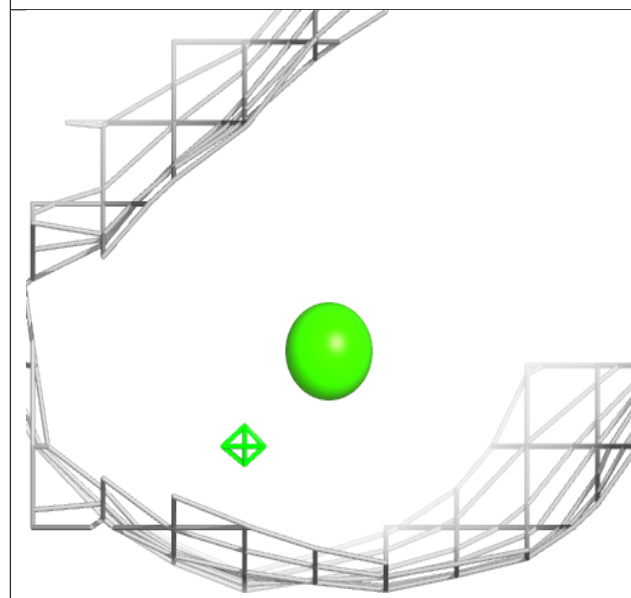
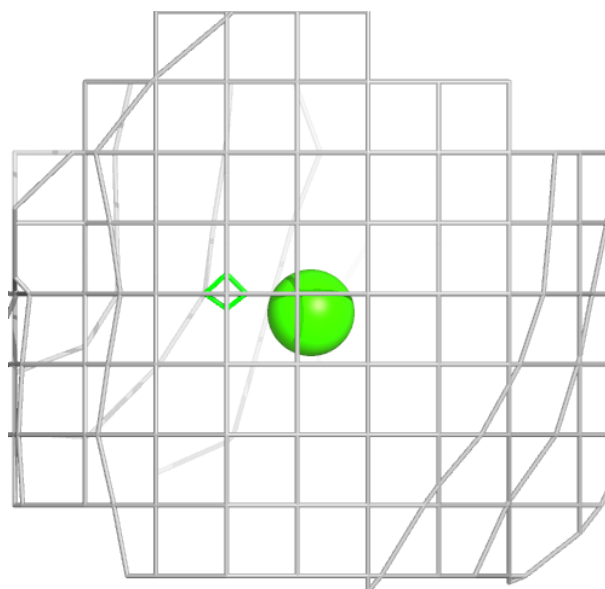
Electron density around CA A 501:

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



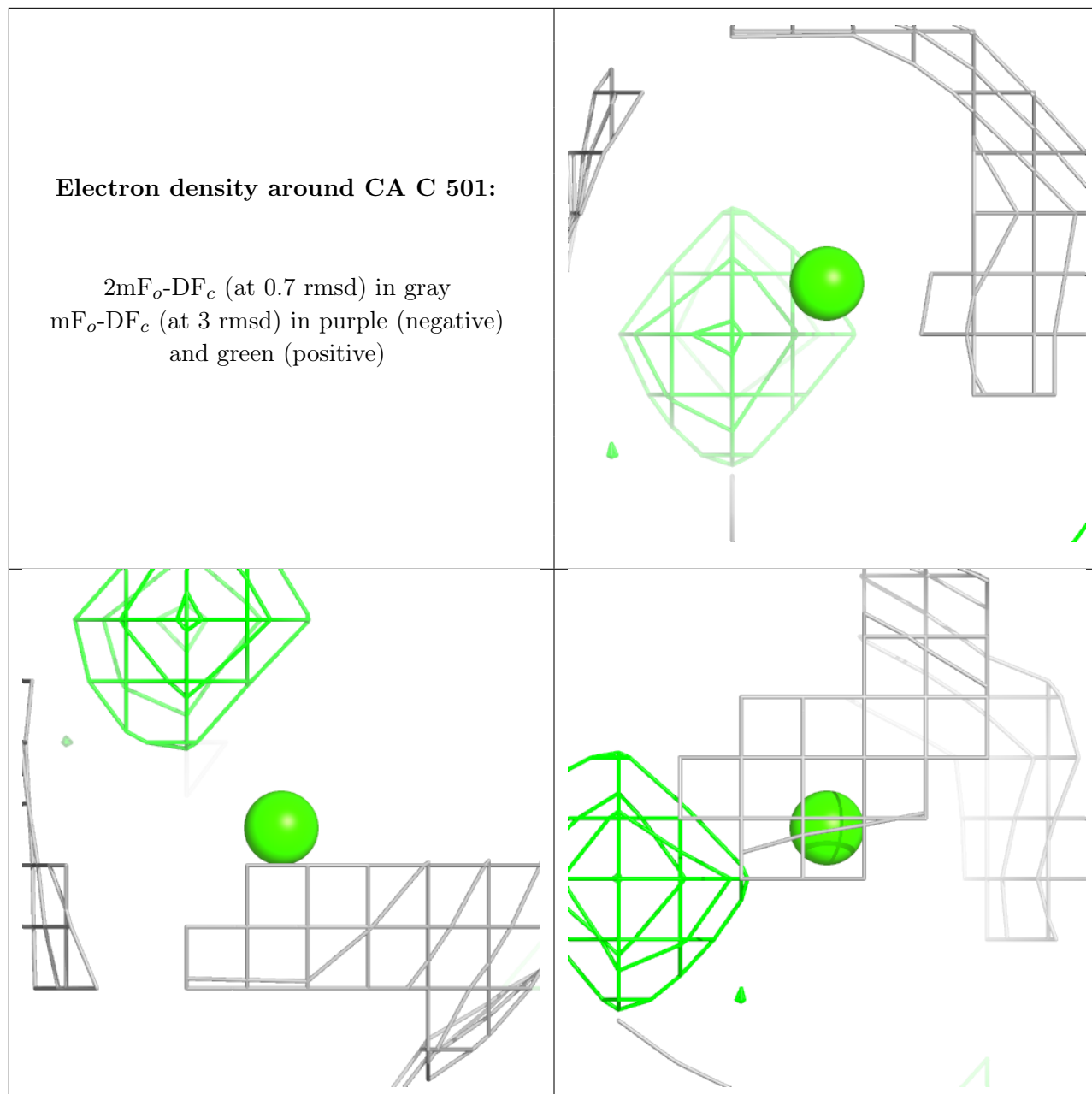
Electron density around CA E 501:

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



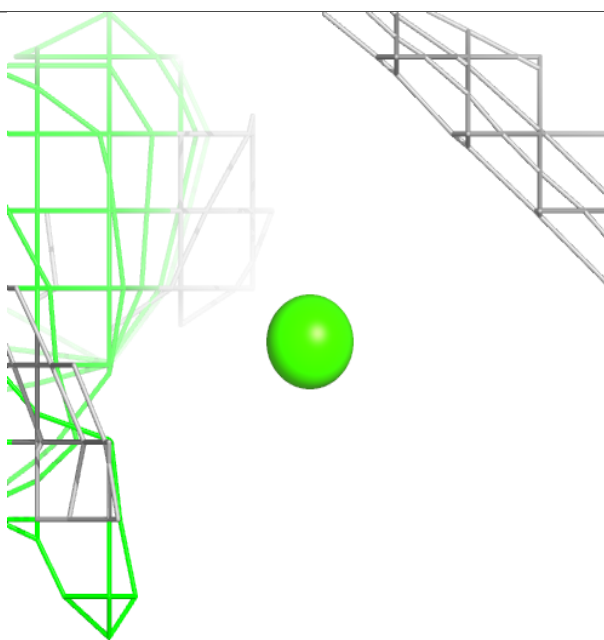
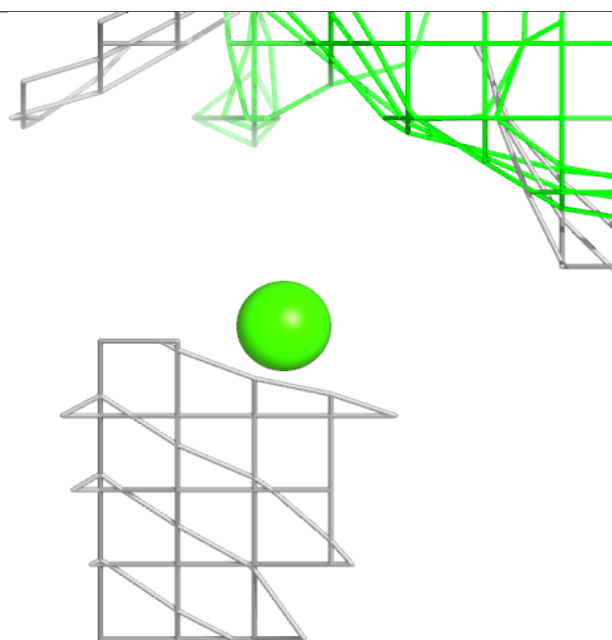
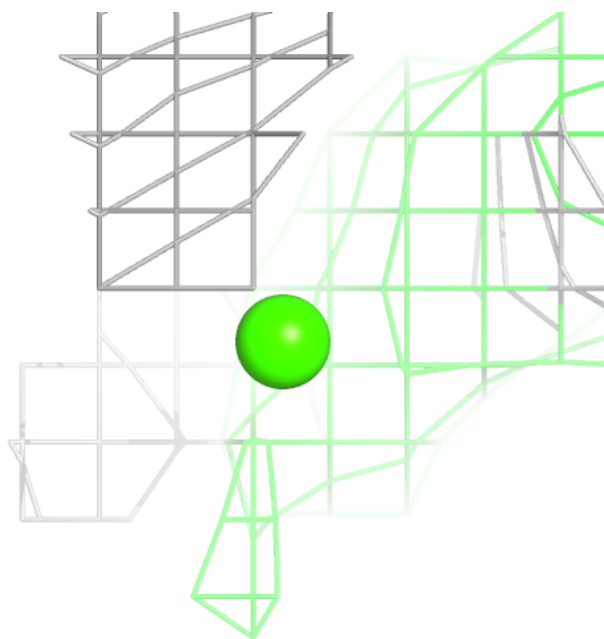
Electron density around CA C 501:

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



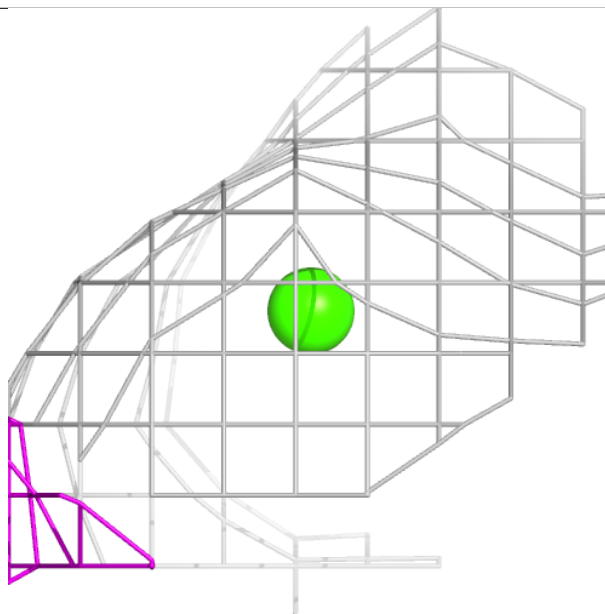
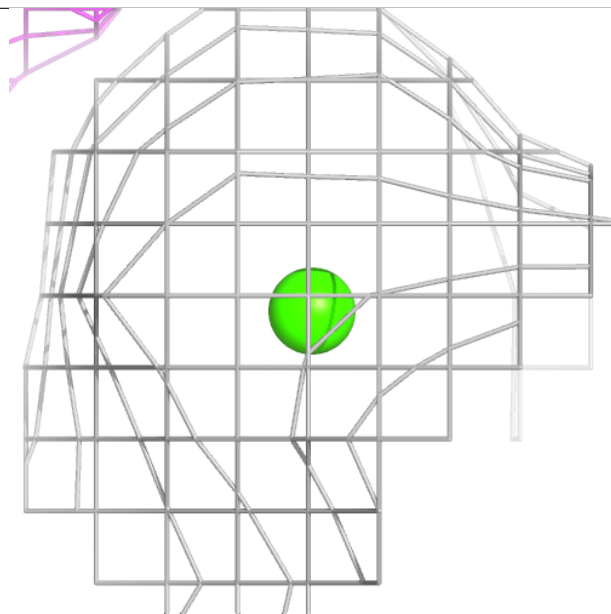
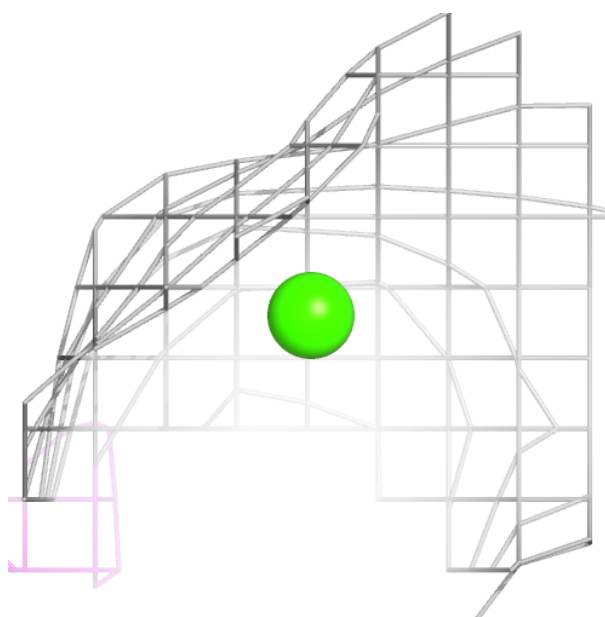
Electron density around CA A 502:

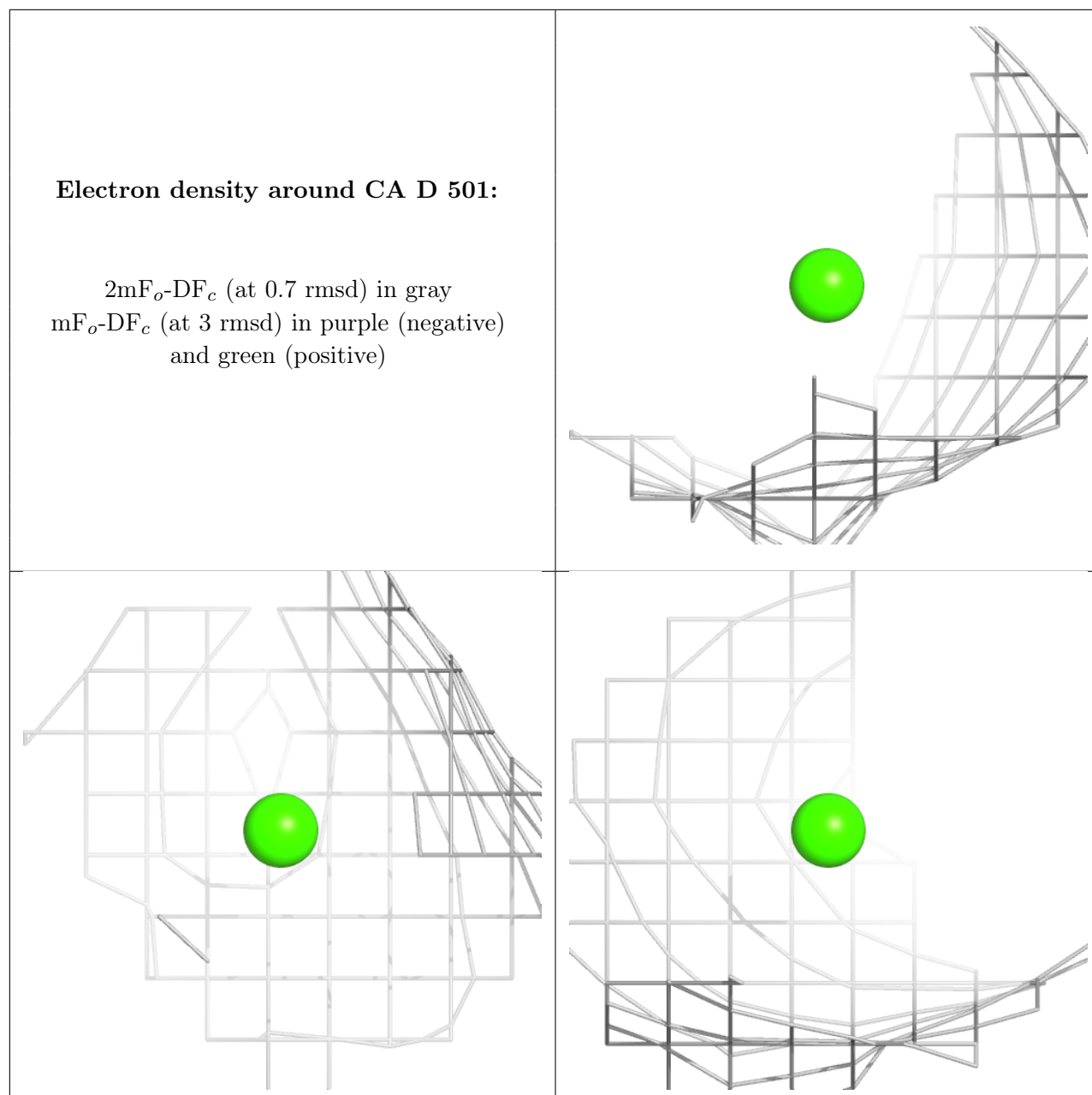
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 501:

$2mF_o-DF_c$ (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.